

Enantioselective C–H annulations enabled by either nickel- or cobalt-electrocatalysed C–H activation for catalyst-controlled chemodivergence

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Supplementary Methods

General Information

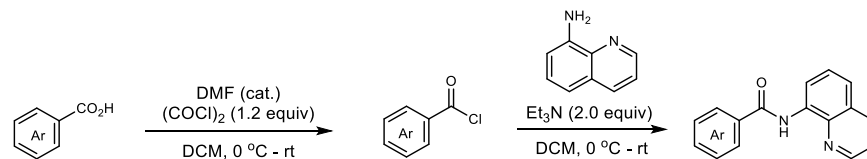
NMR spectra were recorded on the Bruker Avance Neo 300, 400, 500 and 600 MHz spectrometers. Chemical shifts are stated as δ -values in parts per million (ppm) referenced to the residual proton peak of the deuterated solvent (^1H ; CDCl_3 : 7.26 ppm, CD_2Cl_2 : 5.32 ppm) or the carbon peak of the solvent (^{13}C : CDCl_3 : 77.16 ppm, CD_2Cl_2 : 54.00 ppm). Data are reported as follows: chemical shift (δ) and coupling constants J are reported in Hertz (Hz). The evaluation of the NMR spectra was carried out with the software MNova NMR v 10.0.2 from Mestrelab Research. Yields refer to isolated compounds, estimated to be >95% pure as determined by ^1H NMR spectroscopy, unless otherwise noted.

Electrospray-ionization mass spectra (ESI-MS) were recorded on Bruker Daltonik micrOTOF and maXis. High resolution mass spectrometry (HR-ESI-MS) was recorded on Exactive Plus, 2.9 Build 290492 by Thermo Fisher Scientific. IR spectra were recorded on a Bruker FT-IR Alpha-P device and were recorded in the range from 4000 to 400 cm^{-1} . HPLC chromatograms were recorded on an Agilent 1290 Infinity or Jasco AS-4150 using CHIRALPAK® IA-3, IB-3, IC-3, ID-3, IE-3, IF-3, IG-3, IH-3, AD-3, OD-3, OG-3, and OJ-3 columns. Optical rotations were measured with Anton Paar MCP 150 at 20 °C under a Na/Hg lamp, $\lambda = 589 \text{ nm}$ (c in g/100 mL). Values were denoted as specific rotations: $[\alpha]_D^{20}$. Headspace analysis was performed on an Agilent 7890B GC System using a Thermal Conductivity Detector and a 5Å MS column.

Electrocatalytic reactions were performed with Platinum (Pt) electrodes (10 mm $\times$ 15 mm $\times$ 0.25 mm, 99.9%; obtained from ChemPur®, Germany), Nickel foam (Ni) electrodes (10 mm $\times$ 15 mm $\times$ 1.4 mm, RCM-Ni5763; obtained from Recemat BV, Germany), and graphite felt (GF) electrodes (10 mm $\times$ 15 mm $\times$ 6 mm, SIGRACELL® GFA 6 EA, obtained from SGL Carbon, Germany) connected using stainless steel adapters. Electrocatalytic reactions were conducted using an AUTOLAB multichannel line from METROHM or Rohde & Schwarz Galvanostat (HMP4040). Spectroelectrochemical analyses (SEC) were measured using an AUTOLAB potentiostat with the TSC Spectro cell from rhd instruments (Pt mesh working electrode; Glassy carbon counter electrode; Ag-wire pseudo reference electrodes). Temperature control was ensured with the AUTOLAB Microcell HC. Avantes AvaLight-DH-S-BAL was used as the light source and an Avantes AvaSpec-ULS2048x64-EVO was used for absorption measurement. The evaluation of the data was carried out with the software AvaSoft 8 from Avantes and Nova 2.1. Cyclic voltammograms (CV) were measured using the Metrohm Autolab PGSTAT204 potentiostat (Glassy carbon electrode; Pt wire counter electrode; SCE reference) or AUTOLAB potentiostat with the TSC Spectro cell from rhd instruments (Pt mesh working electrode; Glassy carbon counter electrode; Ag-wire pseudo reference electrodes).

Synthesis of Substrates and Ligands

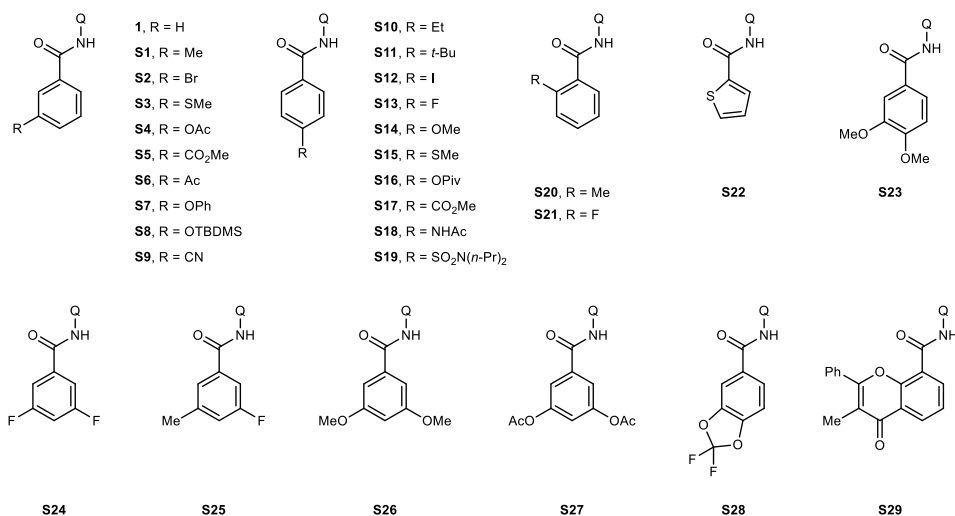
General procedure for amide synthesis



Preparation of acyl chloride: To an oven dried Schlenk flask, carboxylic acid derivative (1.0 equiv), DMF (2-3 drops), and anhydrous DCM (0.5 M) were added under a nitrogen atmosphere. Oxalyl chloride (1.2 equiv) was added dropwise at 0 °C. The mixture was stirred at room temperature for 6 h. Volatiles were then removed under reduced pressure to afford the crude acyl chloride, which was used immediately without further purification.

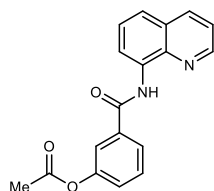
Preparation of amide: The acid chloride was dissolved in DCM (0.5 mL/mmol) followed by dropwise addition of a solution of 8-aminoquinoline (1.3 equiv) and Et₃N (2.0 equiv) in DCM (1.5 mL/mmol) at 0 °C. The resulting reaction mixture was then warmed to room temperature and stirred overnight. The reaction was then quenched with aq. NaHCO₃ solution, and the organic layer was separated. The aqueous layer was extracted with DCM (3 times). The combined organic layer was washed with brine and dried over Na₂SO₄. Purification by column chromatography on silica gel furnished the amide.

The amides **1**, **S1-S29** were synthesized according to the general procedure for amide synthesis starting from the carboxylic acid derivative or directly from the corresponding acid chloride. The characterization data were consistent with those reported in the literature¹⁻⁸.



Characterization data for amides not described in the literature:

3-(Quinolin-8-ylcarbamoyl)phenyl acetate (**S4**)



Prepared according to general procedure for amide synthesis, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **S4** as a white solid.

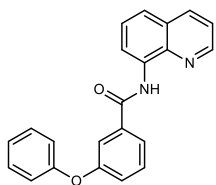
¹H NMR (400 MHz, CDCl₃) δ 10.72 (s, 1H), 8.92 (d, *J* = 7.2 Hz, 1H), 8.89 – 8.84 (m, 1H), 8.20 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.81 (s, 1H), 7.64 – 7.54 (m, 3H), 7.53 – 7.46 (m, 1H), 7.33 (d, *J* = 6.9 Hz, 1H), 2.37 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 169.4 (C_q), 164.5 (C_q), 151.2 (C_q), 148.5 (CH), 138.9 (C_q), 137.0 (C_q), 136.6 (CH), 134.6 (C_q), 130.0 (CH), 128.2 (C_q), 127.6 (CH), 125.4 (CH), 124.6 (CH), 122.0 (CH), 121.9 (CH), 121.1 (CH), 116.8 (CH), 21.3 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3351, 1768, 1673, 1526, 1480, 1425, 1328, 1268, 1207, 826 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₅N₂O₃: 307.1077; found: 307.1071.

3-Phenoxy-*N*-(quinolin-8-yl)benzamide (**S7**)



Prepared according to general procedure for amide synthesis, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **S7** as a white solid.

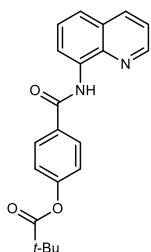
¹H NMR (400 MHz, CDCl₃) δ 10.72 (s, 1H), 8.91 (d, *J* = 7.3 Hz, 1H), 8.84 (d, *J* = 4.3 Hz, 1H), 8.19 (d, *J* = 8.2 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 1H), 7.73 (s, 1H), 7.64 – 7.45 (m, 4H), 7.43 – 7.34 (m, 2H), 7.22 (d, *J* = 8.1 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 8.2 Hz, 2H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 164.9 (C_q), 158.2 (C_q), 156.7 (C_q), 148.5 (CH), 138.9 (C_q), 137.2 (C_q), 136.5 (CH), 134.6 (C_q), 130.3 (CH), 130.1 (CH), 128.1 (C_q), 127.6 (CH), 124.0 (CH), 122.0 (CH), 121.9 (CH), 121.9 (CH), 121.8 (CH), 119.5 (CH), 117.7 (CH), 116.7 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 1670, 1530, 1476, 1328, 1272, 1223, 826, 798, 762, 742 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₂H₁₇N₂O₂: 341.1285; found: 341.1275.

4-(Quinolin-8-ylcarbamoyl)phenyl pivalate (**S16**)



Prepared according to general procedure for amide synthesis, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **S16** as a brown solid.

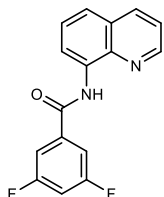
¹H NMR (300 MHz, CDCl₃) δ 10.72 (s, 1H), 8.92 (dd, *J* = 7.3, 1.8 Hz, 1H), 8.85 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.19 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.11 (d, *J* = 8.8 Hz, 2H), 7.63 – 7.53 (m, 2H), 7.49 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.28 – 7.23 (m, 2H), 1.40 (s, 9H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 176.9 (C_q), 164.9 (C_q), 154.1 (C_q), 148.5 (CH), 138.9 (C_q), 136.6 (CH), 134.7 (C_q), 132.7 (C_q), 128.9 (CH), 128.1 (C_q), 127.6 (CH), 122.1 (CH), 121.9 (CH), 121.9 (CH), 116.7 (CH), 39.4 (C_q), 27.3 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2974, 1745, 1671, 1598, 1525, 1503, 1424, 1204, 1164, 1102 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₁H₂₁N₂O₃: 349.1552; found: 349.1551.

3,5-Difluoro-*N*-(quinolin-8-yl)benzamide (**S24**)



Prepared according to general procedure for amide synthesis, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **S24** as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 10.70 (s, 1H), 9.00 – 8.68 (m, 2H), 8.21 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.65 – 7.56 (m, 4H), 7.51 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.15 – 6.84 (m, 1H) ppm.

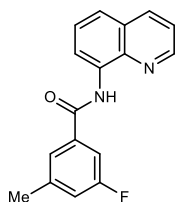
¹³C NMR (101 MHz, CDCl₃) δ 163.3 (dd, *J*_{CF} = 250.7, 12.0 Hz, C_q), 162.9 (t, *J*_{CF} = 2.9 Hz, C_q), 148.6 (CH), 138.8 (C_q), 138.7 (t, *J*_{CF} = 8.3 Hz, C_q), 136.6 (CH), 134.1 (C_q), 128.1 (C_q), 127.5 (CH), 122.4 (CH), 122.0 (CH), 116.9 (CH), 110.7 (dd, *J*_{CF} = 19.1, 7.5 Hz, CH), 107.4 (t, *J*_{CF} = 25.4 Hz, CH) ppm.

¹⁹F NMR (377 MHz, CDCl₃) δ -107.8 ppm.

IR (ATR): $\tilde{\nu}$ = 3351, 3054, 1668, 1527, 1480, 1420, 1304, 822, 754, 607 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₆H₁₁F₂N₂O₁: 285.0834; found: 285.0831.

3-Fluoro-5-methyl-N-(quinolin-8-yl)benzamide (S25)



Prepared according to general procedure for amide synthesis, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **S25** as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 10.68 (s, 1H), 8.91 (dd, *J* = 7.3, 1.7 Hz, 1H), 8.88 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.20 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.68 – 7.65 (m, 1H), 7.64 – 7.54 (m, 3H), 7.50 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.12 – 7.07 (m, 1H), 2.49 (s, 3H) ppm.

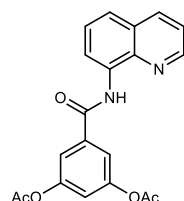
¹³C NMR (101 MHz, CDCl₃) δ 164.5 (d, *J*_{CF} = 2.8 Hz, C_q), 163.0 (d, *J*_{CF} = 247.0 Hz, C_q), 148.5 (CH), 141.3 (d, *J*_{CF} = 7.9 Hz, C_q), 138.9 (C_q), 137.3 (d, *J*_{CF} = 7.4 Hz, C_q), 136.6 (CH), 134.5 (C_q), 128.1 (C_q), 127.6 (CH), 123.8 (d, *J*_{CF} = 2.7 Hz, CH), 122.1 (CH), 121.9 (CH), 119.6 (d, *J*_{CF} = 21.2 Hz, CH), 116.8 (CH), 111.7 (d, *J*_{CF} = 23.1 Hz, CH), 21.6 (d, *J*_{CF} = 1.8 Hz, CH₃) ppm.

¹⁹F NMR (377 MHz, CDCl₃) δ -122.8 ppm.

IR (ATR): $\tilde{\nu}$ = 3360, 1665, 1526, 1465, 1421, 1295, 962, 823, 786, 671 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₄F₁N₂O₁: 281.1085; found: 281.1079.

5-(Quinolin-8-ylcarbamoyl)-1,3-phenylene diacetate (S27)



Prepared according to general procedure for amide synthesis, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **S27** as a white solid.

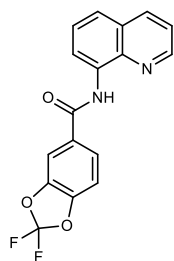
¹H NMR (400 MHz, CDCl₃) δ 10.65 (s, 1H), 8.92 – 8.82 (m, 2H), 8.18 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.71 – 7.64 (m, 2H), 7.61 – 7.53 (m, 2H), 7.47 (dd, *J* = 8.2, 4.3 Hz, 1H), 7.19 (t, *J* = 2.1 Hz, 1H), 2.35 (s, 6H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 168.9 (C_q), 163.5 (C_q), 151.4 (C_q), 148.5 (CH), 138.8 (C_q), 137.5 (C_q), 136.5 (CH), 134.3 (C_q), 128.1 (C_q), 127.5 (CH), 122.2 (CH), 121.9 (CH), 119.2 (CH), 118.1 (CH), 116.9 (CH), 21.2 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3341, 1761, 1658, 1530, 1294, 1187, 1128, 1023, 895, 827 cm⁻¹;

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₀H₁₇N₂O₅: 365.1132; found: 365.1125.

2,2-Difluoro-*N*-(quinolin-8-yl)benzo[*d*][1,3]dioxole-5-carboxamide (28)



Prepared according to general procedure for amide synthesis, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **S28** as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 10.69 (s, 1H), 8.88 (dd, *J* = 7.2, 1.8 Hz, 1H), 8.86 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.21 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.87 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.82 (d, *J* = 1.8 Hz, 1H), 7.66 – 7.54 (m, 2H), 7.50 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.22 (d, *J* = 8.3 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 163.8 (C_q), 148.5 (CH), 146.3 (C_q), 144.3 (C_q), 138.8 (C_q), 136.6 (CH), 134.4 (C_q), 131.9 (t, *J*_{CF} = 256.8 Hz, C_q), 131.8 (C_q), 128.2 (C_q), 127.6 (CH), 123.6 (CH), 122.1 (CH), 122.0 (CH), 116.8 (CH), 109.6 (CH), 109.3 (CH) ppm.

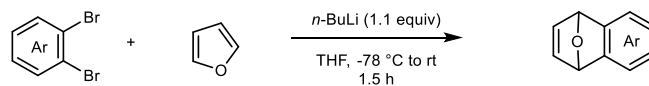
¹⁹F NMR (377 MHz, CDCl₃) δ -49.7 ppm.

IR (ATR): $\tilde{\nu}$ = 3363, 3072, 1667, 1532, 1478, 1233, 1203, 1132, 786, 600 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₁F₂N₂O₃: 329.0732; found: 329.0729.

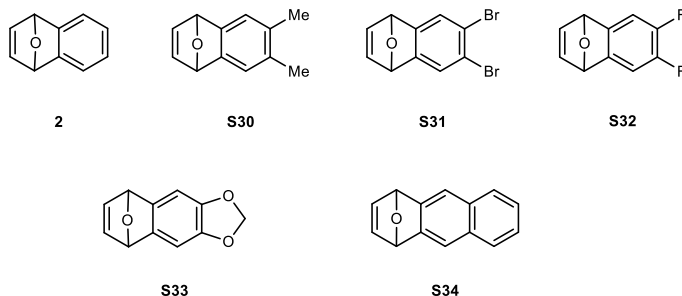
Procedures for alkene synthesis

General procedure for 7-oxabenzonorbornadiene synthesis



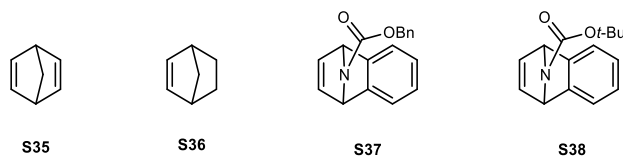
To a stirred solution of 1,2-dibromobenzene derivative (1.0 equiv) and freshly distilled furan (2 mL/equiv) in anhydrous THF (0.5 M) was added *n*-BuLi (1.1 equiv, 2.5 M in hexane) dropwise at -78 °C under nitrogen atmosphere. The solution was stirred for 1.5 h at -78 °C. Water was then slowly added and the reaction mixture was allowed to warm to room temperature. Diethyl ether was then added to the reaction mixture and the organic phase was separated. The aqueous solution was extracted with diethyl ether (3 times), and the combined organic solution was dried over Na₂SO₄. The solvent was then removed in vacuo and the resulting mixture was purified by column chromatography on silica to give the alkene.

Alkenes **2**, **S30-S34** were synthesized according to general procedure starting from the corresponding 1,2-dibromobenzene derivative. The characterization data were consistent with those reported in the literature^{6,8,9}.

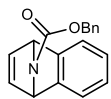


Synthesis of other alkenes

S35 and **S36** were purchased from commercial sources. Alkenes **S37** and **S38** were synthesized according to a literature procedure¹⁰.



Benzyl 1,4-dihydro-1,4-epiminonaphthalene-9-carboxylate (S37)



Prepared according to a literature procedure¹⁰, isolation by column chromatography (dichloromethane) yielded **S37** as a brown sticky solid.

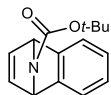
¹H NMR (400 MHz, CDCl₃) δ 7.46 – 7.17 (m, 7H), 7.12 – 6.87 (m, 4H), 5.60 (s, 2H), 5.07 (s, 2H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 155.4 (C_q), 148.2 (C_q), 146.5 – 139.7 (broad, CH), 136.4 (C_q), 128.6 (CH), 128.2 (CH), 127.9 (CH), 125.3 (CH), 122.9 – 119.5 (broad, CH), 67.3 (CH₂), 66.4 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 1692, 1391, 1321, 1245, 1081, 861, 809, 746, 698, 569 cm⁻¹.

HRMS (ESI): m/z [M+H]⁺ calcd for C₁₈H₁₆N₁O₂: 278.1176; found: 278.1173.

tert-Butyl 1,4-dihydro-1,4-epiminonaphthalene-9-carboxylate (S38)



Prepared according to a literature procedure¹⁰, isolation by column chromatography (dichloromethane) yielded **S38** as a brown sticky solid.

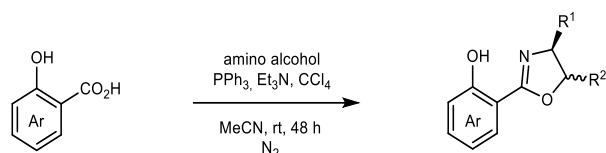
¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.16 (m, 2H), 7.04 – 6.90 (m, 4H), 5.65 – 5.37 (m, 2H), 1.38 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 155.3 (C_q), 148.4 (C_q), 145.2 – 140.4 (broad, CH), 125.1 (CH), 122.2 – 119.8 (broad, CH), 80.7 (C_q), 68.7 – 63.6 (broad, CH), 28.3 (CH₃) ppm.

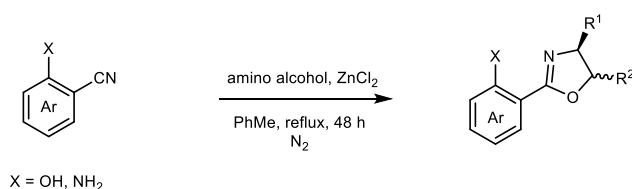
IR (ATR): $\tilde{\nu}$ = 2980, 1689, 1356, 1329, 1248, 1156, 1075, 855, 787, 745 cm⁻¹.

HRMS (ESI): m/z [M+Na]⁺ calcd for C₁₅H₁₇N₁Na₁O₂: 266.1152; found: 266.1149.

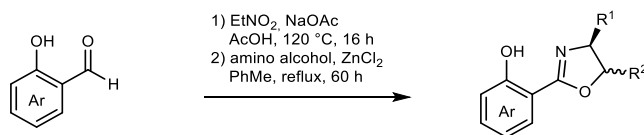
Procedures for ligand synthesis



Procedure A: To an oven dried Schlenk flask were added salicylic acid derivative (1.0 equiv), amino alcohol (1.0 equiv), triphenylphosphine (3.0 equiv), and acetonitrile (5 mL/mmol) under nitrogen atmosphere. Triethylamine (4.0 equiv) was added, and a clear colorless solution was obtained. Then, CCl_4 (10.0 equiv) was added dropwise to the reaction mixture over 30 minutes. During the addition of CCl_4 , a precipitate formed, and the reaction mixture turned dark red. The reaction was stirred for 48 h at room temperature, resulting in a dark red suspension. Subsequently, diethyl ether was added to the solution and the formed suspension was filtered. The solvent was removed under reduced pressure and the concentrated residue was purified by column chromatography (*n*-hexane/ethyl acetate) on silica gel to afford the chiral ligand.



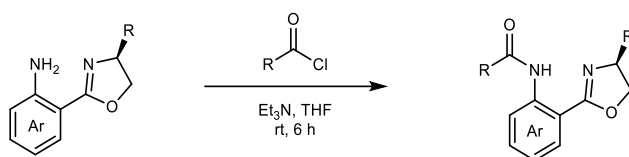
Procedure B: Zinc chloride (1.5 equiv) was melted under vacuum in a Schlenk-flask using a heat gun. After cooling and refilling with nitrogen, toluene (17 mL/mmol) and amino alcohol (1.5 equiv) were added, followed by the addition of the corresponding benzonitrile derivative (1.0 equiv). Next, the reaction mixture was heated to reflux and maintained at this temperature for 48 h. The solvent was then removed under reduced pressure and the crude residue was purified by column chromatography (*n*-hexane/ethyl acetate) on silica gel to afford the chiral ligand.



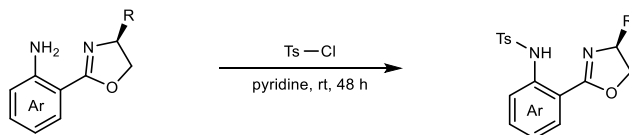
Procedure C: A pressure tube was charged with nitroethane (2.0 equiv), sodium acetate (2.0 equiv), hydroxybenzaldehyde derivative (1.0 equiv), and acetic acid (0.2 mL/mmol). The reaction mixture was heated to 120 °C for 16 h followed by the addition to ice-cooled water after cooling to room temperature. Then, the aqueous phase was extracted with ethyl acetate (3 times), and the combined organic phases were washed with saturated NaHCO_3 solution (2 times). The

solvent was removed under reduced pressure, yielding the corresponding hydroxybenzonitrile derivative as a pale-yellow solid, which was used immediately without further purification.

Zinc chloride (1.0 equiv) was melted in a Schlenk-flask using a heat gun. After cooling and flushing with nitrogen, hydroxybenzonitrile derivative (1.0 equiv) obtained from the first step and amino alcohol derivative (1.0 equiv) were added and dissolved in anhydrous toluene (8.8 mL/mmol). Then, the mixture was heated to reflux for 60 h. Next, the solvent was removed under reduced pressure and the resulting residue was purified by column chromatography (*n*-hexane/ethyl acetate), to afford the chiral ligand.



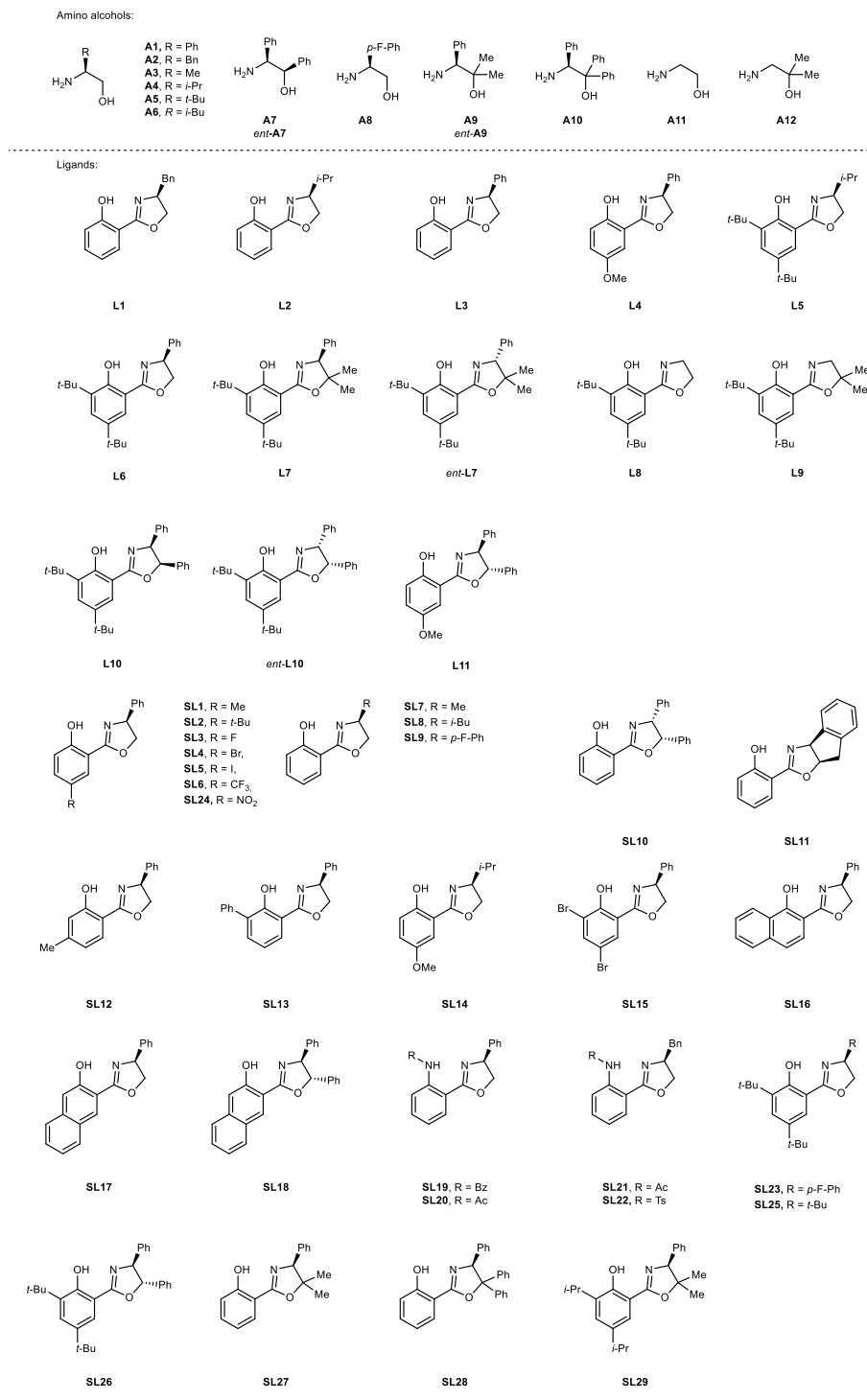
Procedure D: To an oven dried Schlenk flask were added aniline derivative (1.0 equiv), acid chloride (1.0 equiv), and THF (2 mL/mmol) under nitrogen atmosphere. Then, the mixture was stirred and Et₃N (1.5 equiv) was added dropwise. After stirring for 6 h at room temperature the reaction was quenched with saturated aq. NaHCO₃ and extracted with ethyl acetate (3 times). The organic layer was dried over Na₂SO₄ and concentrated under reduced pressure and the resulting residue was purified by column chromatography (*n*-hexane/ethyl acetate), to afford the chiral ligand.



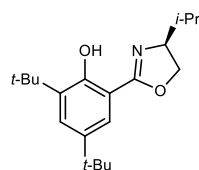
Procedure E: To an oven dried Schlenk flask were added aniline derivative (1.0 equiv), and dry pyridine (5 mL/mmol) under nitrogen atmosphere. *p*-Tosyl chloride (1.2 equiv) was added dropwise at 0 °C. Then, the mixture was stirred at room temperature for 48 h. After reaction completion the reaction mixture was transferred to a separation funnel with ethyl acetate and washed with water (3 times). The combined organic phases were dried over Na₂SO₄. Afterwards, the solvent was removed under reduced pressure and the resulting residue was purified by column chromatography (*n*-hexane/ethyl acetate), to afford the chiral ligand.

The chiral ligands **L1-9**, **L11**, **SL1-9**, **SL11-18**, **SL23-26**, and **SL28-29** were synthesized according to procedure **A**. The chiral ligand **L10** was synthesized according to procedure **C**. The chiral ligands

SL10 and **SL27** were synthesized according to procedure **B**. The chiral ligands **SL19-21** were synthesized according to procedure **B** and **D**. The chiral ligand **SL22** was prepared according to procedure **B** and **E**. The characterization data were consistent with those reported in the literature¹¹⁻¹⁵. The amino alcohols **A1-7**, *ent*-**A7**, **A11-12** were purchased from commercial sources. **A8**¹³, **A9**¹⁶, *ent*-**A9**¹⁶, and **A10**¹⁶ were synthesized according to literature procedures.



(S)-2,4-Di-*tert*-butyl-6-(4-isopropyl-4,5-dihydrooxazol-2-yl)phenol (L5)



Prepared according to general procedure **A**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **L5** as a white solid.

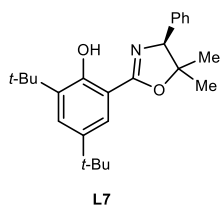
¹H NMR (400 MHz, CDCl₃) δ 12.71 (s, 1H), 7.53 (s, 1H), 7.44 (s, 1H), 4.49 – 4.32 (m, 1H), 4.26 – 3.96 (m, 2H), 1.89 – 1.74 (m, 1H), 1.45 (s, 9H), 1.31 (s, 9H), 1.04 (d, *J* = 6.6 Hz, 3H), 0.96 (d, *J* = 6.6 Hz, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.1 (C_q), 157.1 (C_q), 140.0 (C_q), 136.5 (C_q), 128.0 (CH), 122.2 (CH), 109.9 (C_q), 71.8 (CH), 69.8 (CH₂), 35.3 (C_q), 34.4 (C_q), 33.2 (CH), 31.7 (CH₃), 29.6 (CH₃), 19.0 (CH₃), 18.8 (CH₃) ppm.

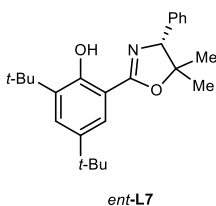
IR (ATR): $\tilde{\nu}$ = 2958, 2907, 2872, 1636, 1467, 1439, 1219, 1102, 978, 786 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₀H₃₂NO₂: 318.2428; found: 318.2431.

(S)-2,4-Di-*tert*-butyl-6-(5,5-dimethyl-4-phenyl-4,5-dihydrooxazol-2-yl)phenol (L7) and (R)-2,4-Di-*tert*-butyl-6-(5,5-dimethyl-4-phenyl-4,5-dihydrooxazol-2-yl)phenol (*ent*-L7)



L7



***ent*-L7**

Prepared according to procedure **A** using amino alcohol **A9**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **L7** as a white solid. *ent*-**L7** was prepared following the procedure **A** using amino alcohol *ent*-**A9**.

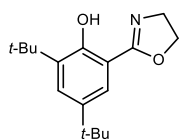
¹H NMR (400 MHz, CDCl₃) δ 12.87 (s, 1H), 7.60 – 7.55 (m, 1H), 7.50 – 7.46 (m, 1H), 7.39 – 7.29 (m, 3H), 7.28 – 7.27 (m, 1H), 7.26 – 7.24 (m, 1H), 5.10 (s, 1H), 1.68 (s, 3H), 1.46 (s, 9H), 1.34 (s, 9H), 0.95 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.6 (C_q), 157.6 (C_q), 140.0 (C_q), 138.6 (C_q), 136.7 (C_q), 128.5 (CH), 128.3 (CH), 127.8 (CH), 127.2 (CH), 122.4 (CH), 110.2 (C_q), 87.0 (C_q), 77.3 (CH), 35.3 (C_q), 34.5 (C_q), 31.7 (CH₃), 29.6 (CH₃), 29.0 (CH₃), 23.9 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2963, 2908, 1631, 1439, 1370, 1254, 1222, 1101, 759, 700 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₅H₃₄NO₂: 380.2584; found: 380.2574.

2,4-Di-*tert*-butyl-6-(4,5-dihydrooxazol-2-yl)phenol (**L8**)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **L8** as a white solid.

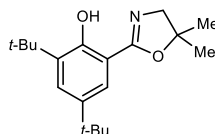
¹H NMR (400 MHz, CDCl₃) δ 12.55 (s, 1H), 7.54 (d, *J* = 2.5 Hz, 1H), 7.43 (d, *J* = 2.5 Hz, 1H), 4.41 (t, *J* = 9.5 Hz, 2H), 4.10 (t, *J* = 9.3 Hz, 2H), 1.44 (s, 9H), 1.31 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 167.3 (C_q), 156.9 (C_q), 140.1 (C_q), 136.6 (C_q), 128.1 (CH), 122.3 (CH), 110.0 (C_q), 66.7 (CH₂), 53.6 (CH₂), 35.3 (C_q), 34.4 (C_q), 31.7 (CH₃), 29.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2958, 1635, 1446, 1365, 1249, 1191, 1098, 1016, 959, 800 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₂₆N₁O₂: 276.1958; found: 276.1956.

2,4-Di-*tert*-butyl-6-(5,5-dimethyl-4,5-dihydrooxazol-2-yl)phenol (**L9**)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **L9** as a white solid.

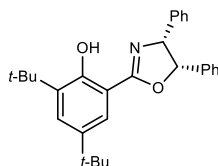
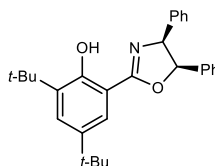
¹H NMR (400 MHz, CDCl₃) δ 12.80 (s, 1H), 7.51 (d, *J* = 2.5 Hz, 1H), 7.42 (d, *J* = 2.5 Hz, 1H), 3.79 (s, 2H), 1.50 (s, 6H), 1.44 (s, 9H), 1.31 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.2 (C_q), 157.1 (C_q), 139.9 (C_q), 136.5 (C_q), 127.8 (CH), 122.2 (CH), 110.4 (C_q), 83.6 (C_q), 65.4 (CH₂), 35.3 (C_q), 34.4 (C_q), 31.7 (CH₃), 29.6 (CH₃), 27.5 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2961, 2870, 1629, 1438, 1372, 1251, 1100, 1032, 820, 799 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₃₀N₁O₂: 304.2271; found: 304.2267.

2,4-Di-*tert*-butyl-6-((4*S*,5*R*)-4,5-diphenyl-4,5-dihydrooxazol-2-yl)phenol (**L10**) and 2,4-Di-*tert*-butyl-6-((4*R*,5*S*)-4,5-diphenyl-4,5-dihydrooxazol-2-yl)phenol (*ent*-**L10**)



Prepared according to procedure **C** using amino alcohol **A7**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **L10** as a white solid. *ent*-**L10** was prepared following procedure **C** using amino alcohol *ent*-**A7**.

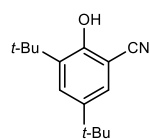
¹H NMR (400 MHz, CDCl₃) δ 12.63 (s, 1H), 7.80 – 7.68 (m, 1H), 7.59 – 7.49 (m, 1H), 7.19 – 6.87 (m, 10H), 5.98 (d, *J* = 10.0 Hz, 1H), 5.81 (d, *J* = 10.1 Hz, 1H), 1.49 (s, 9H), 1.34 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 167.7 (C_q), 157.6 (C_q), 140.4 (C_q), 137.4 (C_q), 136.9 (C_q), 136.1 (C_q), 128.7 (CH), 127.9 (CH), 127.9 (CH), 127.9 (CH), 127.8 (CH), 127.3 (CH), 126.7 (CH), 122.6 (CH), 109.6 (C_q), 84.5 (CH), 73.4 (CH), 35.4 (C_q), 34.5 (C_q), 31.7 (CH₃), 29.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3032, 2963, 1634, 1454, 1439, 1362, 1252, 1188, 1103, 695 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₉H₃₄NO₂: 428.2584; found: 428.2576.

Characterization data of the intermediate product 3,5-di-*tert*-butyl-2-hydroxybenzonitrile (**L10'**)



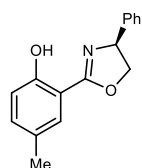
¹H NMR (400 MHz, CDCl₃) δ 7.54 – 7.50 (m, 1H), 7.32 – 7.29 (m, 1H), 5.77 (s, 1H), 1.41 (s, 9H), 1.29 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 154.9 (C_q), 143.8 (C_q), 137.2 (C_q), 129.9 (CH), 126.1 (CH), 117.4 (C_q), 99.7 (C_q), 35.3 (C_q), 34.6 (C_q), 31.4 (CH₃), 29.5 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3032, 2963, 1634, 1454, 1439, 1362, 1252, 1188, 1103, 695 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₅H₂₂NO: 232.1696; found: 232.1690.

(**S**)-4-Methyl-2-(4-phenyl-4,5-dihydrooxazol-2-yl)phenol (**SL1**)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/dichloromethane) yielded **SL1** as a white solid.

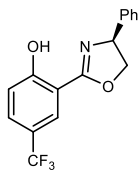
¹H NMR (400 MHz, CDCl₃) δ 11.91 (s, 1H), 7.52 (s, 1H), 7.42 – 7.34 (m, 2H), 7.33 – 7.27 (m, 3H), 7.22 (d, *J* = 8.4 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 1H), 5.70 – 5.33 (m, 1H), 4.94 – 4.64 (m, 1H), 4.35 – 4.09 (m, 1H), 2.31 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.5 (C_q), 158.1 (C_q), 141.8 (C_q), 134.7 (CH), 129.0 (CH), 128.2 (CH), 128.0 (CH), 128.0 (C_q), 126.6 (CH), 116.8 (CH), 110.2 (C_q), 74.1 (CH₂), 69.0 (CH), 20.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 1638, 1614, 1253, 1203, 1068, 1021, 772, 752, 726, 696 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₆H₁₆NO₂: 254.1176; found: 254.1165.

(S)-4-Methyl-2-(4-phenyl-4,5-dihydrooxazol-2-yl)phenol (SL6)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/dichloromethane) yielded **SL6** as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 12.37 (s, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.45 – 7.27 (m, 6H), 7.14 (d, *J* = 8.1 Hz, 1H), 5.57 – 5.42 (m, 1H), 4.93 – 4.69 (m, 1H), 4.37 – 4.20 (m, 1H) ppm.

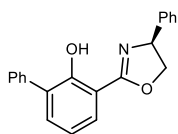
¹³C NMR (101 MHz, CDCl₃) δ 165.6 (C_q), 160.3 (C_q), 141.2 (C_q), 135.2 (q, *J*_{CF} = 32.6 Hz, C_q), 129.1 (CH), 129.1 (CH), 128.2 (CH), 126.6 (CH), 123.6 (q, *J*_{CF} = 272.7 Hz, C_q), 115.3 (q, *J*_{CF} = 3.6 Hz, CH), 114.3 (q, *J*_{CF} = 3.6 Hz, CH), 113.4 (C_q), 74.4 (CH₂), 69.1 (CH) ppm.

¹⁹F NMR (377 MHz, CDCl₃) δ –63.4 ppm.

IR (ATR): $\tilde{\nu}$ = 1621, 1332, 1230, 1154, 1114, 1076, 923, 740, 697, 686 cm^{–1}.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₆H₁₃F₃NO₂: 308.0893; found: 308.0893.

(S)-3-(4-Phenyl-4,5-dihydrooxazol-2-yl)-[1,1'-biphenyl]-2-ol (SL13)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/dichloromethane) yielded **SL13** as a white solid.

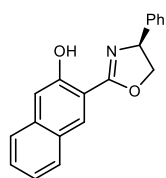
¹H NMR (400 MHz, CDCl₃) δ 12.73 (s, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.47 – 7.40 (m, 2H), 7.39 – 7.27 (m, 6H), 7.07 – 6.89 (m, 1H), 5.72 – 5.31 (m, 1H), 5.04 – 4.65 (m, 1H), 4.37 – 4.23 (m, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.7 (C_q), 157.5 (C_q), 141.6 (C_q), 137.9 (C_q), 134.7 (CH), 129.9 (C_q), 129.5 (CH), 129.0 (CH), 128.2 (CH), 128.0 (CH), 127.7 (CH), 127.3 (CH), 126.6 (CH), 118.8 (CH), 110.9 (C_q), 74.2 (CH₂), 68.9 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 1629, 1429, 1363, 1250, 1141, 955, 800, 754, 695, 647 cm^{–1}.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₁H₁₈NO₂: 316.1293; found: 316.1332.

(S)-3-(4-Phenyl-4,5-dihydrooxazol-2-yl)naphthalen-2-ol (SL17)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL17** as a white solid.

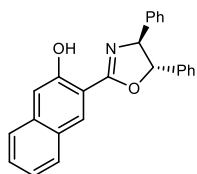
¹H NMR (400 MHz, CDCl₃) δ 11.87 (s, 1H), 8.34 (s, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.53 – 7.45 (m, 1H), 7.42 – 7.29 (m, 7H), 5.60 – 5.49 (m, 1H), 4.87 (t, *J* = 9.2 Hz, 1H), 4.38 – 4.27 (m, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.1 (C_q), 155.6 (C_q), 141.5 (C_q), 137.0 (C_q), 130.1 (CH), 129.1 (CH), 128.9 (CH), 128.5 (CH), 128.1 (CH), 127.2 (C_q), 126.7 (CH), 126.5 (CH), 123.8 (CH), 112.8 (C_q), 111.1 (CH), 74.2 (CH₂), 69.3 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 1650, 1606, 1522, 1467, 1360, 1311, 1054, 948, 755, 475 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₆NO₂: 290.1176; found: 290.1178.

3-((4S,5S)-4,5-Diphenyl-4,5-dihydrooxazol-2-yl)naphthalen-2-ol (SL18)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL18** as a white solid.

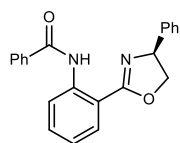
¹H NMR (400 MHz, CDCl₃) δ 11.85 (s, 1H), 8.43 (s, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.54 – 7.29 (m, 13H), 5.45 (d, *J* = 7.8 Hz, 1H), 5.38 (d, *J* = 7.8 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 165.5 (C_q), 155.8 (C_q), 141.1 (C_q), 139.5 (C_q), 137.1 (C_q), 130.3 (CH), 129.3 (CH), 129.1 (CH), 129.1 (CH), 128.9 (CH), 128.6 (CH), 128.3 (CH), 127.2 (C_q), 126.7 (CH), 126.5 (CH), 126.1 (CH), 123.8 (CH), 112.7 (C_q), 111.2 (CH), 88.6 (CH), 77.9 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3030, 1650, 1521, 1455, 1284, 1224, 959, 755, 697, 476 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₅H₂₀NO₂: 366.1489; found: 366.1489.

(S)-N-(2-(4-Phenyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (SL19)



Prepared according to procedures **B** and **D**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL19** as a white solid.

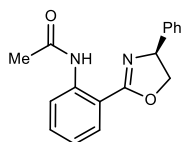
¹H NMR (400 MHz, CDCl₃) δ 13.09 (s, 1H), 9.01 (d, *J* = 8.5 Hz, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.92 (d, *J* = 7.9 Hz, 2H), 7.62 – 7.54 (m, 1H), 7.47 – 7.31 (m, 6H), 7.25 – 7.19 (m, 2H), 7.18 – 7.10 (m, 1H), 5.62 – 5.47 (m, 1H), 4.88 – 4.74 (m, 1H), 4.38 – 4.27 (m, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.2 (C_q), 165.1 (C_q), 141.6 (C_q), 140.7 (C_q), 135.2 (C_q), 133.2 (CH), 131.7 (CH), 129.6 (CH), 129.1 (CH), 128.5 (CH), 128.1 (CH), 127.9 (CH), 126.9 (CH), 122.6 (CH), 120.1 (CH), 113.4 (C_q), 73.5 (CH₂), 70.3 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 1679, 1633, 1616, 1541, 1449, 1277, 1063, 975, 800, 701 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₂H₁₉N₂O₂: 343.1441; found: 343.1439.

(S)-N-(2-(4-Phenyl-4,5-dihydrooxazol-2-yl)phenyl)acetamide (SL20)



Prepared according to procedures **B** and **D**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL20** as a white solid.

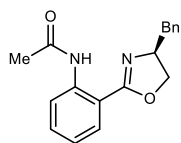
¹H NMR (400 MHz, CDCl₃) δ 12.24 (s, 1H), 8.74 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 7.9 Hz, 1H), 7.55 – 7.46 (m, 1H), 7.44 – 7.37 (m, 2H), 7.36 – 7.29 (m, 3H), 7.15 – 7.06 (m, 1H), 5.72 – 5.27 (m, 1H), 4.82 – 4.66 (m, 1H), 4.27 – 4.13 (m, 1H), 2.14 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 169.4 (C_q), 165.0 (C_q), 142.0 (C_q), 140.4 (C_q), 133.0 (CH), 129.5 (CH), 129.0 (CH), 128.0 (CH), 126.5 (CH), 122.4 (CH), 119.9 (CH), 112.9 (C_q), 73.5 (CH₂), 70.0 (CH), 25.5 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3060, 1698, 1633, 1613, 1536, 1448, 1299, 1045, 951, 755 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₇N₂O₂: 281.1285; found: 281.1281.

(S)-N-(2-(4-Benzyl-4,5-dihydrooxazol-2-yl)phenyl)acetamide (SL21)



Prepared according to procedure **B** and **D**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL21** as a white solid.

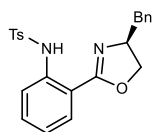
¹H NMR (400 MHz, CDCl₃) δ 12.15 (s, 1H), 8.72 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.51 – 7.41 (m, 1H), 7.38 – 7.22 (m, 5H), 7.12 – 6.97 (m, 1H), 4.77 – 4.61 (m, 1H), 4.50 – 4.37 (m, 1H), 4.17 – 3.99 (m, 1H), 3.08 – 2.85 (m, 2H), 2.02 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 169.5 (C_q), 164.1 (C_q), 140.3 (C_q), 138.2 (C_q), 132.8 (CH), 129.3 (CH), 129.3 (CH), 128.7 (CH), 126.8 (CH), 122.3 (CH), 119.7 (CH), 112.8 (C_q), 71.0 (CH₂), 68.0 (CH), 42.4 (CH₂), 25.4 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 1685, 1636, 1447, 1361, 1361, 1065, 775, 749, 682 cm⁻¹.

HRMS (ESI): m/z [M+H]⁺ calcd for C₁₈H₁₉N₂O₂: 295.1441; found: 295.1432.

(S)-N-(2-(4-Benzyl-4,5-dihydrooxazol-2-yl)phenyl)-4-methylbenzenesulfonamide (SL22)



Prepared according to procedure **B** and **E**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL22** as a white solid.

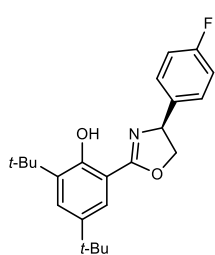
¹H NMR (400 MHz, CDCl₃) δ 12.32 (s, 1H), 7.79 – 7.63 (m, 4H), 7.38 – 7.32 (m, 3H), 7.30 – 7.25 (m, 3H), 7.20 (d, *J* = 7.9 Hz, 2H), 7.05 – 6.91 (m, 1H), 4.78 – 4.56 (m, 1H), 4.40 – 4.25 (m, 1H), 4.14 – 4.00 (m, 1H), 3.20 (dd, *J* = 13.7, 5.8 Hz, 1H), 2.76 (dd, *J* = 13.7, 8.0 Hz, 1H), 2.36 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 164.0 (C_q), 143.6 (C_q), 139.4 (C_q), 137.6 (C_q), 137.2 (C_q), 132.6 (CH), 129.7 (CH), 129.5 (CH), 129.4 (CH), 128.9 (CH), 127.3 (CH), 126.9 (CH), 122.4 (CH), 117.9 (CH), 113.5 (C_q), 70.8 (CH₂), 67.7 (CH), 41.8 (CH₂), 21.7 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 1633, 1498, 1340, 1152, 1060, 937, 751, 698, 564, 503 cm⁻¹.

HRMS (ESI): m/z [M+H]⁺ calcd for C₂₃H₂₃N₂O₃S: 407.1424; found: 407.1428.

(S)-2,4-Di-*tert*-butyl-6-(4-(4-fluorophenyl)-4,5-dihydrooxazol-2-yl)phenol (SL23)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/dichloromethane) yielded **SL23** as a white solid.

¹H NMR (400 MHz, CDCl₃) δ 12.45 (s, 1H), 7.61 (s, 1H), 7.48 (s, 1H), 7.32 – 7.25 (m, 2H), 7.14 – 7.00 (m, 2H), 5.51 – 5.38 (m, 1H), 4.91 – 4.68 (m, 1H), 4.26 – 4.12 (m, 1H), 1.45 (s, 9H), 1.33 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 167.4 (C_q), 162.5 (d, *J*_{CF} = 246.3 Hz, C_q), 157.3 (C_q), 140.4 (C_q), 137.7 (d, *J*_{CF} = 3.2 Hz, C_q), 136.8 (C_q), 128.6 (CH), 128.4 (d, *J*_{CF} = 8.1 Hz, CH), 122.5 (CH), 115.8

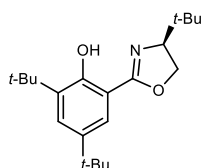
(d, $J_{\text{CF}} = 21.5$ Hz, CH), 109.6 (C_q), 73.9 (CH₂), 68.5 (CH), 35.4 (C_q), 34.4 (C_q), 31.7 (CH₃), 29.6 (CH₃) ppm.

¹⁹F NMR (377 MHz, CDCl₃) δ -114.63 ppm.

IR (ATR): $\tilde{\nu} = 1629, 1509, 1438, 1232, 1101, 978, 826, 812, 573, 529$ cm⁻¹.

HRMS (ESI): m/z [M+H]⁺ calcd for C₂₃H₂₉FNO₂: 370.2177; found: 370.2179.

(S)-2,4-Di-*tert*-butyl-6-(4-(*tert*-butyl)-4,5-dihydrooxazol-2-yl)phenol (SL25)



Prepared according to procedure A, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL25** as a white solid.

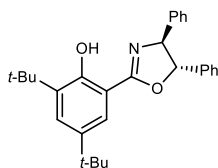
¹H NMR (400 MHz, CDCl₃) δ 12.72 (s, 1H), 7.52 (s, 1H), 7.44 (s, 1H), 4.42 – 4.27 (m, 1H), 4.24 – 4.16 (m, 1H), 4.16 – 4.09 (m, 1H), 1.45 (s, 9H), 1.31 (s, 9H), 0.96 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.1 (C_q), 157.2 (C_q), 140.0 (C_q), 136.5 (C_q), 128.0 (CH), 122.2 (CH), 109.9 (C_q), 75.2 (CH), 67.9 (CH₂), 35.3 (C_q), 34.4 (C_q), 33.9 (C_q), 31.7 (CH₃), 29.6 (CH₃), 26.0 (CH₃) ppm.

IR (ATR): $\tilde{\nu} = 2957, 2908, 2869, 1635, 1440, 1364, 1254, 1219, 1105, 978$ cm⁻¹.

HRMS (ESI): m/z [M+H]⁺ calcd for C₂₁H₃₄NO₂: 332.2584; found: 332.2585.

2,4-Di-*tert*-butyl-6-((4*S*,5*S*)-4,5-diphenyl-4,5-dihydrooxazol-2-yl)phenol (SL26)



Prepared according to general procedure C, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL26** as a white solid.

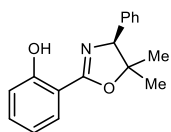
¹H NMR (400 MHz, CDCl₃) δ 12.56 (s, 1H), 7.69 (s, 1H), 7.52 (s, 1H), 7.46 – 7.26 (m, 10H), 5.36 (d, $J = 7.6$ Hz, 1H), 5.29 (d, $J = 7.7$ Hz, 1H), 1.47 (s, 9H), 1.33 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.8 (C_q), 157.5 (C_q), 141.5 (C_q), 140.4 (C_q), 139.9 (C_q), 136.9 (C_q), 129.1 (CH), 129.0 (CH), 128.9 (CH), 128.7 (CH), 128.1 (CH), 126.7 (CH), 126.2 (CH), 122.6 (CH), 109.6 (C_q), 88.2 (CH), 77.8 (CH), 35.4 (C_q), 34.5 (C_q), 31.7 (CH₃), 29.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu} = 2956, 2910, 2869, 1633, 1439, 1252, 1102, 972, 909, 697$ cm⁻¹.

HRMS (ESI): m/z [M+H]⁺ calcd for C₂₉H₃₄NO₂: 428.2584; found: 428.2572.

(S)-2-(5,5-Dimethyl-4-phenyl-4,5-dihydrooxazol-2-yl)phenol (SL27)



Prepared according to procedure **B**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL27** as a white solid.

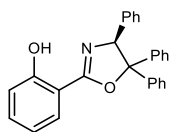
¹H NMR (300 MHz, CDCl₃) δ 12.14 (s, 1H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.18 (m, 6H), 7.08 (d, *J* = 8.2 Hz, 1H), 6.96 – 6.83 (m, 1H), 5.11 (s, 1H), 1.68 (s, 3H), 0.96 (s, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 165.4 (C_q), 160.2 (C_q), 138.0 (C_q), 133.4 (CH), 128.3 (CH), 128.1 (CH), 127.7 (CH), 126.9 (CH), 118.5 (CH), 116.8 (CH), 110.8 (C_q), 87.2 (C_q), 76.9 (CH), 28.7 (CH₃), 23.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2978, 1639, 1616, 1492, 1460, 1358, 1261, 1237, 1070, 756 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₈NO₂: 268.1338; found: 268.1332.

(S)-2-(4,5,5-Triphenyl-4,5-dihydrooxazol-2-yl)phenol (SL28)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL28** as a yellow oil.

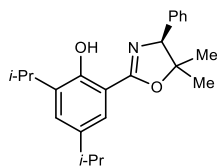
¹H NMR (300 MHz, CDCl₃) δ 12.14 (s, 1H), 8.08 (d, *J* = 6.5 Hz, 1H), 7.79 (d, *J* = 7.2 Hz, 2H), 7.53 – 7.47 (m, 3H), 7.43 – 7.39 (m, 1H), 7.17 – 7.11 (m, 4H), 7.09 – 7.02 (m, 8H), 6.26 (s, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ 165.0 (C_q), 160.5 (C_q), 143.8 (C_q), 139.7 (C_q), 138.2 (C_q), 134.0 (CH), 128.7 (CH), 128.5 (CH), 128.3 (CH), 127.9 (CH), 127.6 (CH), 127.5 (CH), 127.1 (CH), 126.9 (CH), 126.7 (CH), 119.0 (CH), 117.2 (CH), 110.6 (C_q), 93.9 (C_q), 78.5 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3061, 3030, 1641, 1490, 1354, 1258, 1156, 757, 731, 700 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₂₂NO₂: 392.1651; found: 392.1649.

(S)-2-(5,5-Dimethyl-4-phenyl-4,5-dihydrooxazol-2-yl)-4,6-diisopropylphenol (SL29)



Prepared according to procedure **A**, isolation by column chromatography (*n*-hexane/ethyl acetate) yielded **SL29** as a white solid.

¹H NMR (300 MHz, CDCl₃) δ 12.56 (s, 1H), 7.42 – 7.17 (m, 7H), 5.10 (s, 1H), 3.42 (hept, *J* = 6.6 Hz, 1H), 2.88 (hept, *J* = 6.9 Hz, 1H), 1.69 (s, 3H), 1.34 – 1.22 (m, 12H), 0.95 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.2 (C_q), 156.1 (C_q), 138.6 (C_q), 138.5 (C_q), 136.1 (C_q), 128.7 (CH), 128.4 (CH), 127.8 (CH), 127.2 (CH), 122.8 (CH), 110.0 (C_q), 87.2 (C_q), 77.2 (CH), 33.7 (CH), 29.0 (CH), 27.1 (CH₃), 24.4 (CH₃), 24.4 (CH₃), 23.9 (CH₃), 22.8 (CH₃), 22.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2929, 2930, 1633, 1468, 1386, 1371, 1236, 1175, 741, 700 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₃H₃₀NO₂: 352.2271; found: 352.2255.

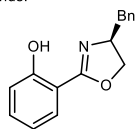
Development of Nickel Catalysis

Supplementary Table 1. Ligand screening.

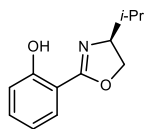
entry	ligand	yield	e.r.	entry	ligand	yield	e.r.
1	L1	<5%	-	20	SL11	26%	50:50
2	L2	11%	59.5:40.5	21	SL12	14%	85.5:14.5
3	L3	25%	79.5:20.5	22	SL13	12%	79.5:20.5
4	L4	16%	75.5:24.5	23	SL14	8%	57.5:42.5
5	L5	13%	58.5:41.5	24	SL15	13%	63:37
6	L6	43%	86:14	25	SL16	12%	73:27
7	L7	29%	93:7	26	SL17	15%	79.5:20.5
8	L10	16%	91:9	27	SL18	15%	88.5:11.5
9	L11	19%	82.5:17.5	28	SL19	38%	50:50
10	SL1	37%	75:25	29	SL20	43%	50:50
11	SL2	20%	76.5:23.5	30	SL21	40%	50:50
12	SL3	30%	76:24	31	SL22	20%	50:50
13	SL4	20%	84:16	32	SL23	20%	90:10
14	SL5	23%	83:17	33	SL24	13%	59:41
15	SL6	6%	88.5:11.5	34	SL25	15%	50:50
16	SL7	<5%	-	35	SL26	37%	87.5:12.5
17	SL8	<5%	-	36	SL27	27%	88:12
18	SL9	7%	89.5:10.5	37	SL28	24%	73:27
19	SL10	18%	21:79	38	SL29	30%	89:11

Reaction conditions: amide (0.2 mmol), alkene (0.3 mmol), Ni(OAc)₂·4H₂O (0.04 mmol), ligand (0.06 mmol), BmimPF₆ (0.05 M), 1,4-dioxane/DMA (4:1, v/v, 5 mL), undivided cell, graphite felt anode (GF), platinum plate cathode (Pt), 600 rpm stirring rate, constant current electrolysis (CCE) at 2.0 mA, 100 °C, 18 h reaction time. Yields determined by ¹H NMR with 1,3,5-trimethoxybenzene as standard. Enantiomeric ratios (e.r.) determined by chiral HPLC using a chiral stationary phase. Bmim = 1-butyl-3-methylimidazolium, DMA = *N,N*-dimethylacetamide.

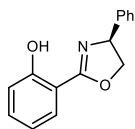
Ligands:



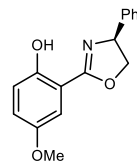
L1



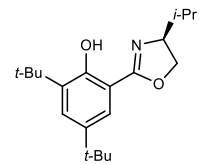
L2



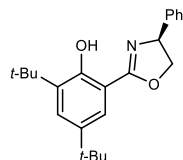
L3



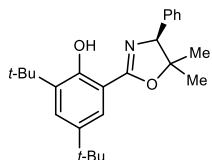
L4



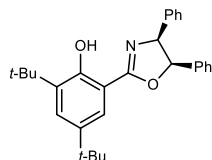
L5



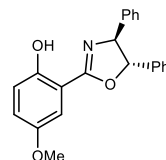
L6



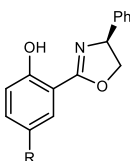
L7



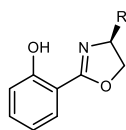
L10



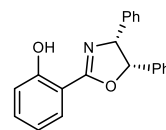
L11



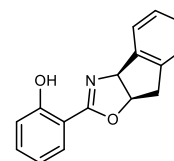
SL1, R = Me
SL2, R = *t*-Bu
SL3, R = F
SL4, R = Br
SL5, R = I
SL6, R = CF₃
SL24, R = NO₂



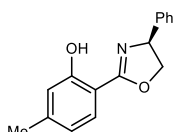
SL7, R = Me
SL8, R = *i*-Bu
SL9, R = *p*-F-Ph



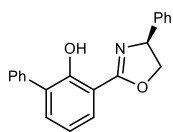
SL10



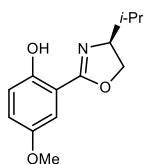
SL11



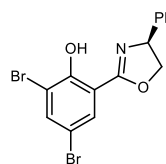
SL12



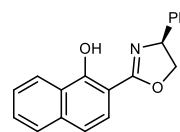
SL13



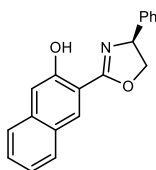
SL14



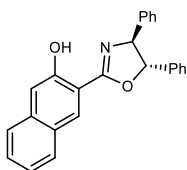
SL15



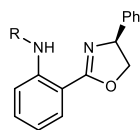
SL16



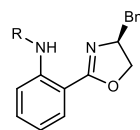
SL17



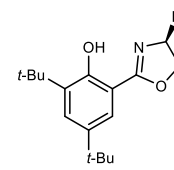
SL18



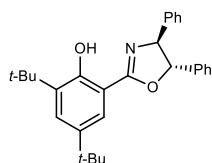
SL19, R = Bz
SL20, R = Ac



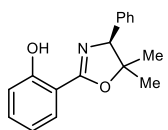
SL21, R = Ac
SL22, R = Ts



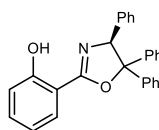
SL23, R = *p*-F-Ph
SL25, R = *t*-Bu



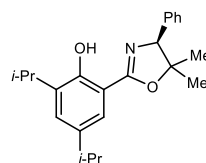
SL26



SL27



SL28



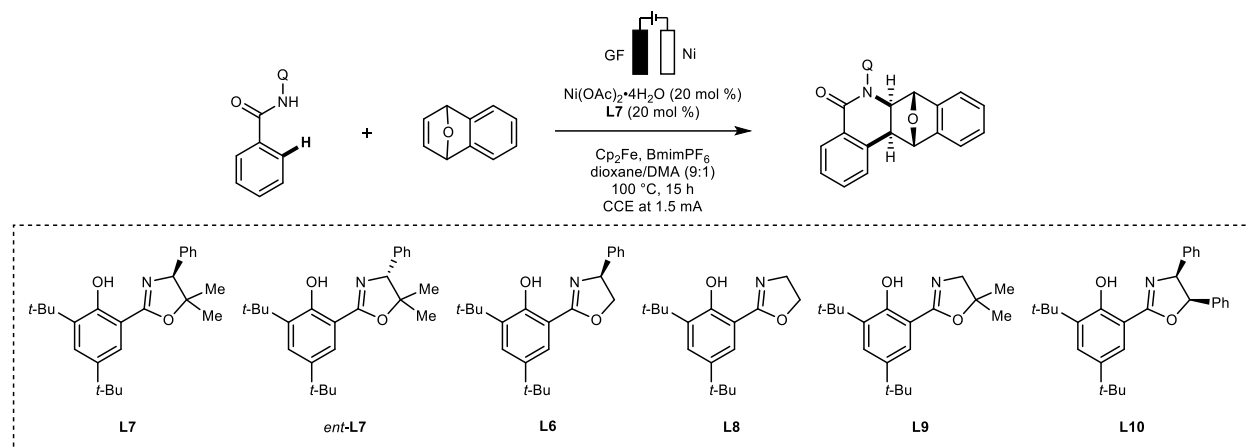
SL29

Supplementary Table 2. Screening of nickel salts.

entry	nickel salt [Ni]	yield	e.r.
1	Ni(OAc) ₂ •4H ₂ O	70%	95:5
2	Ni(OPiv) ₂ •4H ₂ O	50%	80:20
3	Ni(O ₂ CAd) ₂ •4H ₂ O	52%	85:15
4	Ni(O ₂ CMes) ₂ •4H ₂ O	18%	88:12
5	Ni(TFA) ₂ •4H ₂ O	<5%	-
6	NiCl ₂ •6H ₂ O	<5%	-
7	Ni(PF ₆) ₂	<5%	-
8	Ni(BF ₄) ₂ •4H ₂ O	<5%	-
9	Ni(OPh) ₂	<5%	-

Reaction conditions: amide (0.2 mmol), alkene (0.3 mmol), [Ni] (0.04 mmol), ligand **L7** (0.04 mmol), Cp₂Fe (0.06 mmol), BmimPF₆ (0.05 M), 1,4-dioxane/DMA (9:1, v/v, 5 mL). Undivided cell. Graphite felt anode (GF). Nickel foam cathode (Ni). 600 rpm stirring rate. Constant current electrolysis (CCE) at 1.5 mA. 15 h reaction time, 100 °C. Yields determined by ¹H NMR with 1,3,5-trimethoxybenzene as standard. Enantiomeric ratios (e.r.) determined by chiral HPLC using a chiral stationary phase. Bmim = 1-butyl-3-methylimidazolium, DMA = *N,N*-dimethylacetamide Ad = 1-adamantyl. TFA = trifluoro acetate.

Supplementary Table 3. Screening of electrode material and control experiments.



entry	deviation from standard conditions	yield	e.r.
1	-	70%	95:5
2	GF (+) Pt plate (-)	55%	95:5
3	BDD (+) Ni foam (-)	38%	95:5
4	Ni foam (+) Ni foam (-)	63%	94.5:5.5
5	RVC (+) Ni foam (-)	25%	95:5
6	Pt (+) Ni foam (-)	48%	95:5
7	1,4-dioxane/DMA (4:1), 2.0 mA, GF (+) Pt plate (-)	48%	94:6
8	$\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (15 mol %), L7 (15 mol %)	40%	95.5:4.5
9	No Cp_2Fe	25%	93:7
10	<i>ent</i> - L7 instead of L7	70%	5:95
11	L6 instead of L7	48%	90:10
12	L8 instead of L7	45%	50:50
13	L9 instead of L7	46%	50:50
14	L10 instead of L7	42%	81:19
15	No ligand	57%	50:50
16	Under nitrogen atmosphere, no electricity	n.d.	-
17	Under oxygen atmosphere, no electricity	14%	87:13
18	$\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ instead of $\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$	<5%	-

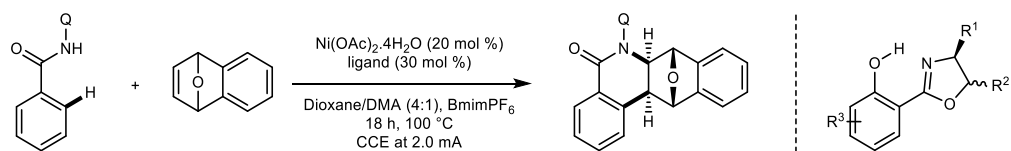
Reaction conditions: amide (0.2 mmol), alkene (0.3 mmol), $\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (0.04 mmol), ligand **L7** (0.04 mmol), Cp_2Fe (0.06 mmol), BmimPF_6 (0.05 M), 1,4-dioxane/DMA (9:1, v/v, 5 mL). Undivided cell. Graphite felt anode (GF). Nickel foam cathode (Ni). 600 rpm stirring rate. Constant current electrolysis (CCE) at 1.5 mA. 15 h reaction time, 100 °C. Yields determined by ^1H NMR with 1,3,5-trimethoxybenzene as standard. Enantiomeric ratios (e.r.) determined by chiral HPLC using a chiral stationary phase. Bmim = 1-butyl-3-methylimidazolium, DMA = *N,N*-dimethylacetamide RVC = reticulated vitreous carbon, BDD = boron doped diamond.

Dataset from Experimental Ligand Screening

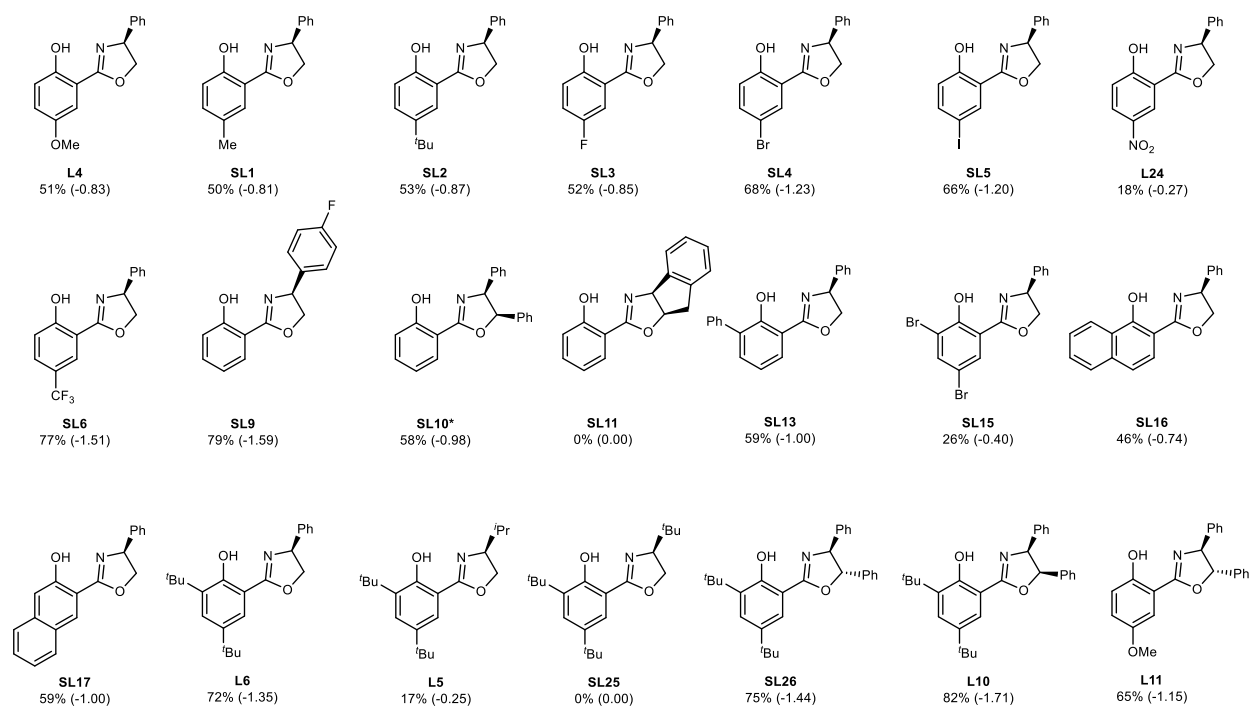
Successfully observed experimental enantioselectivity (ee_{exp}) data of 26 salicyloxazoline ligands was used for statistical analysis and model development (Supplementary Figure 1). The ee_{exp} was converted into Gibbs free energy ($\Delta\Delta G_{\text{exp}}$) using the Supplementary Equation 1:

$$\Delta\Delta G^\ddagger = -RT|\textit{e.r.}| \quad (1)$$

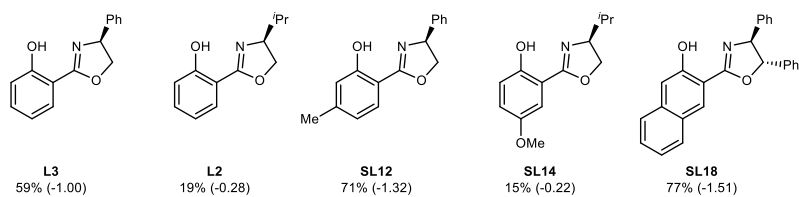
Where, R represents the gas constant ($R = 1.987 \text{ cal K}^{-1} \text{ mol}^{-1}$), T is the temperature considered from the reaction condition ($T = 373.15 \text{ K}$), and $\textit{e.r.}$ represents the enantiomeric ratio ($\textit{e.r.} = \text{major/minor}$). The $\Delta\Delta G_{\text{exp}}$ was taken into consideration given that, with more physical meaning as well as more consistent target variable for statistical analysis and predictive machine learning (ML) model development.



Training (21):



Validation (5):



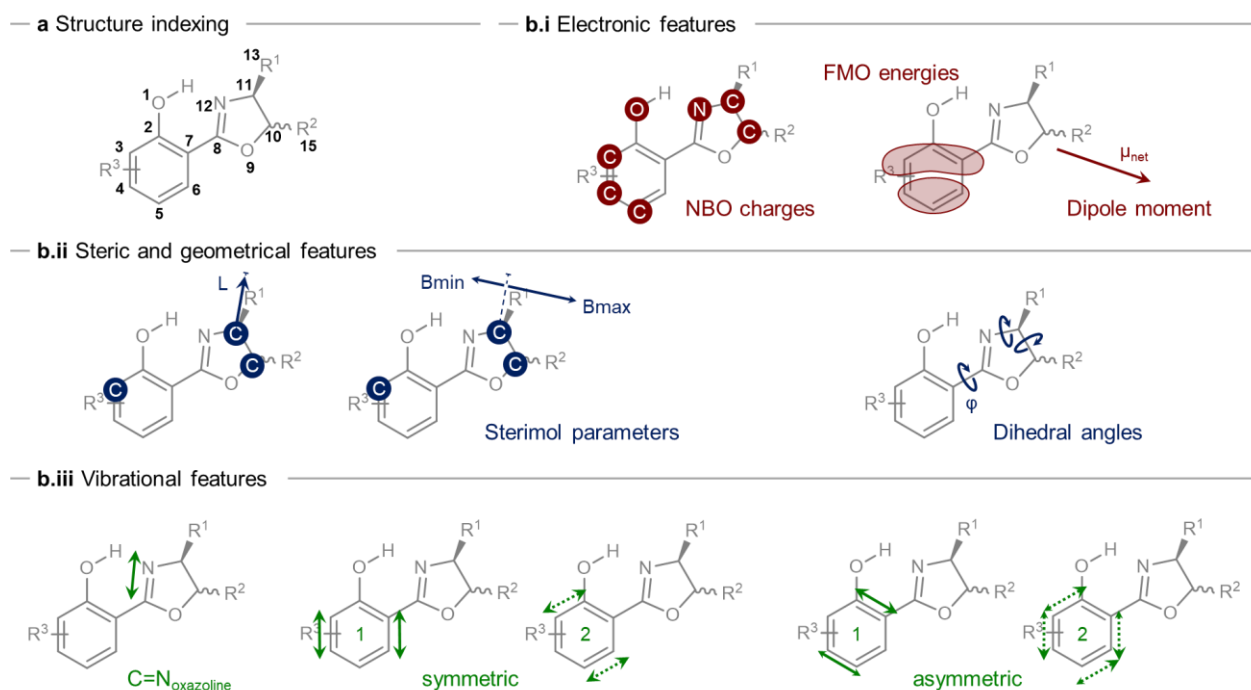
Supplementary Figure 1. Training and validation set of ligands used for ML studies with their respective ee_{exp} ($\Delta\Delta G_{exp}$ in kcal mol⁻¹). * S enantiomer of the SL10 was considered with opposite ee_{exp} value for data analysis and model development.

Descriptor Extraction for Ligand Featurization

The descriptors discussed below (Supplementary Table 4 and Supplementary Figure 2) were calculated with the help of the RDKit¹⁷ library and Gaussian 16, Revision A.03 package¹⁸. Initially the MMFF94¹⁹⁻²⁴ Force Field based 3D structures were generated from SMILES using the ETKDG²⁵ method, integrated in the RDKit library. The structures were then further subjected to conformational search using Grimme's CREST²⁶ conformational search software program, at the GFN2-xTB²⁷ level of theory to get the suitable conformed structures. Afterwards, the selected structures were optimized at a higher level of theory by DFT at TPSS-D3(BJ)/def2-SVP²⁸⁻³¹ level of theory in gas phase.

Supplementary Table 4. List of ligand features used in the ML studies for the ligand-based model.

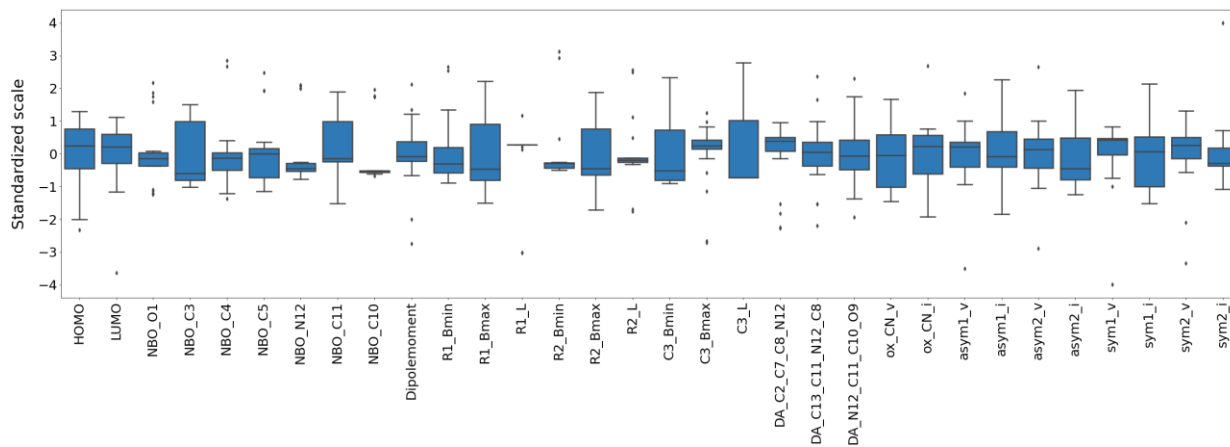
Features	Unit	Description
HOMO, LUMO	a.u.	Frontier molecular orbital energies of the ligand
NBO_O1, NBO_C3, NBO_C4, NBO_C5, NBO_C10, NBO_N12, NBO_C11	e	NBO charges of indexed atoms from the ligand
Dipolemoment	D	Net dipole moment of the ligand
R1_Bmin, R1_Bmax, R1_L	Å	Sterimol features for R ¹ substituent in the oxazoline fragment of the ligand
R2_Bmin, R2_Bmax, R2_L	Å	Sterimol features for R ² substituent in the oxazoline fragment of the ligand
C3_Bmin, C3_Bmax, C3_L	Å	Sterimol features for C3 substituent in the phenol fragment of the ligand
DA_C2_C7_C8_N12, DA_C13_C11_N12_C8, DA_N12_C11_C10_O9	°	Dihedral angles between index atoms from the ligand structure
Ox_CN_v, asym1_v, asym2_v, sym1_v, sym2_v	cm ⁻¹	Vibrational stretching frequency of C=N in the oxazoline fragment, asymmetric and symmetric in the phenol fragment of the ligand
Ox_CN_i, asym1_i, asym2_i, sym1_i, sym2_i	-	IR intensity of vibrations for C=N in the oxazoline fragment, asymmetric and symmetric in the phenol fragment of the ligand



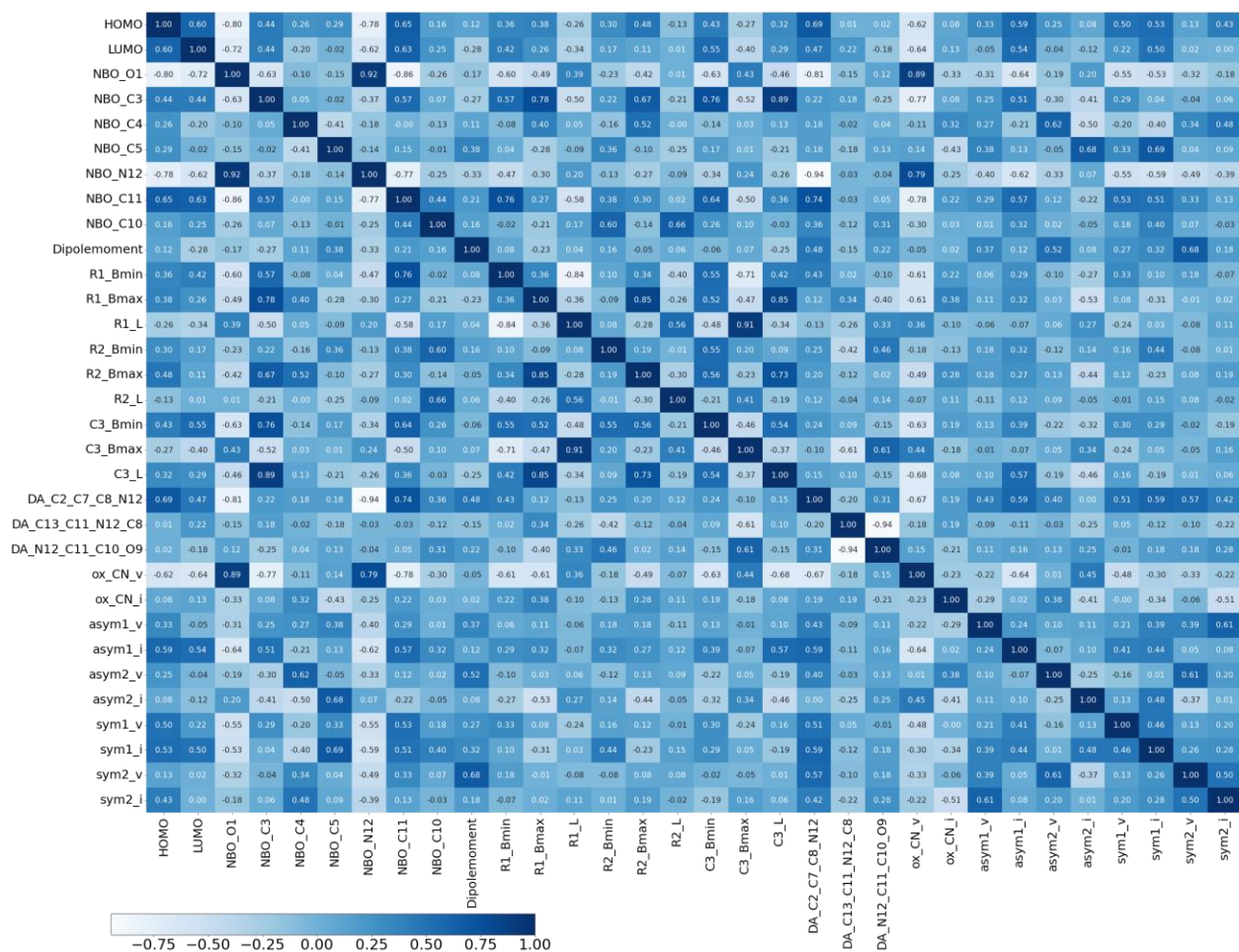
Supplementary Figure 2. Ligand descriptors: a. General atom indexing, b. Calculated ligand parameters for features analysis and model development.

Initially 32 descriptors were abstracted for feature analysis and the ML model development: Frontier molecular orbital (HOMO and LUMO) energies and net dipole moment values were obtained from the single point calculations at the PW6B95-D3(BJ)/def2-TZVPP+SMD(1,4-Dioxane) level of theory on the optimized free ligand structures. The natural bond orbitals (NBO) atomic charges were obtained using Gaussian NBO version 3.1³² from the single point calculations using PW6B95-D3(BJ)/def2-TZVPP on optimized neutral ligand structures. The vibrational stretching frequency of the C=N in the oxazoline fragment, asymmetric and symmetric modes in the phenol fragment of the ligand were obtained from the geometry optimization calculations. The dihedral angles between specific atoms were obtained from the optimized ligand structures. Sterimol parameters (Bmin, Bmax, and L) from several bonds were calculated using DFT-based Steric Parameters (DBSTEP)³³ python package on different bonds in the optimized ligand structure.

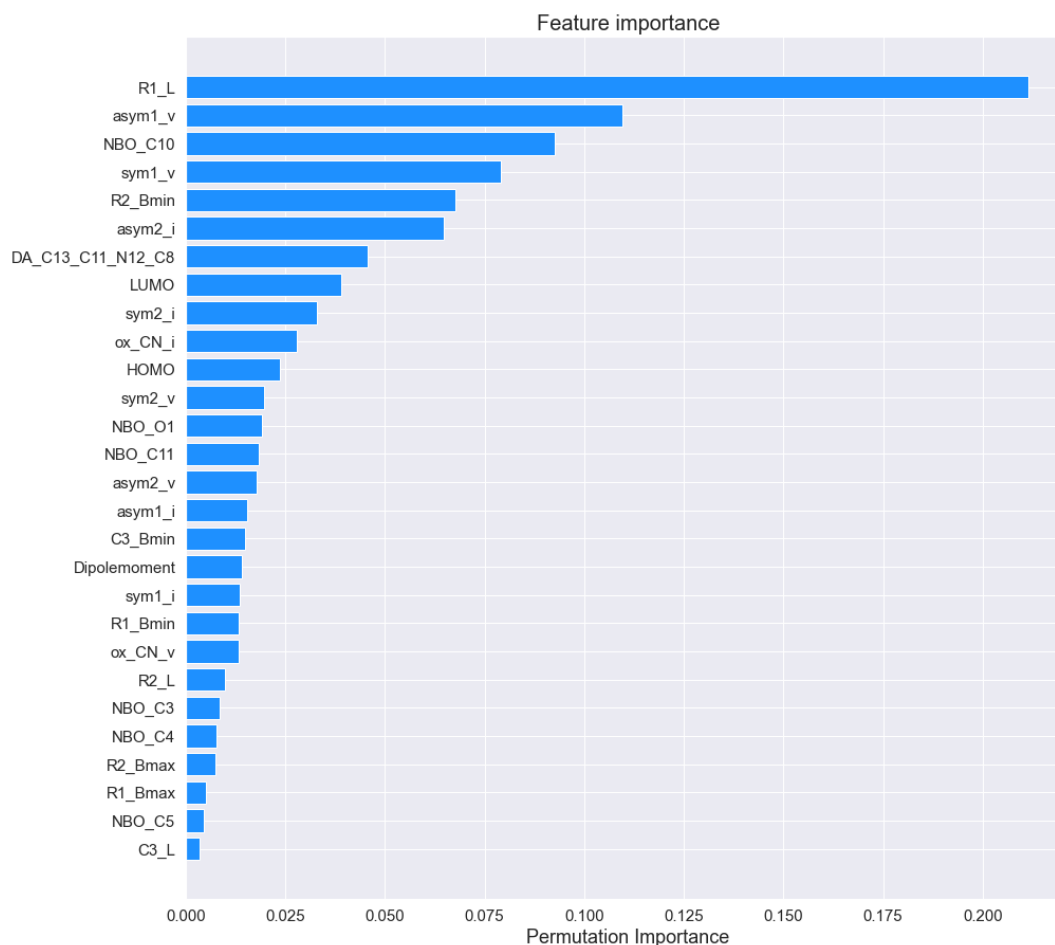
Feature Analysis



Supplementary Figure 3. Box plot of standardized features in the training dataset for each feature. Each box includes a line indicating the median, with the box representing the interquartile range (IQR). The whiskers denote the remaining data distribution within ± 1.5 times the IQR, and outliers beyond this range are indicated as individual points.



Supplementary Figure 4. Pearson correlation heatmap of the training dataset. The color scale bar represents the magnitude and direction of the correlations between the features, with values ranging from -1 (white: strong negative correlation) to +1 (dark blue: strong positive correlation). Each cell displays the correlation coefficient for the respective feature pair.



Supplementary Figure 5. Feature importance with tree-based (random forest regressor) permutation importance method for the training dataset.

With the help of Pearson correlation analysis on the training set, the features with an intercorrelation of $|\text{coefficient}| \geq 0.9$ were removed for further feature selection part. Afterwards, a random forest regressor model was used to assess the permutation importance. Based on the Recursive Feature Elimination (RFE), the top 7 important features were taken for further ML model screening and optimization and training.

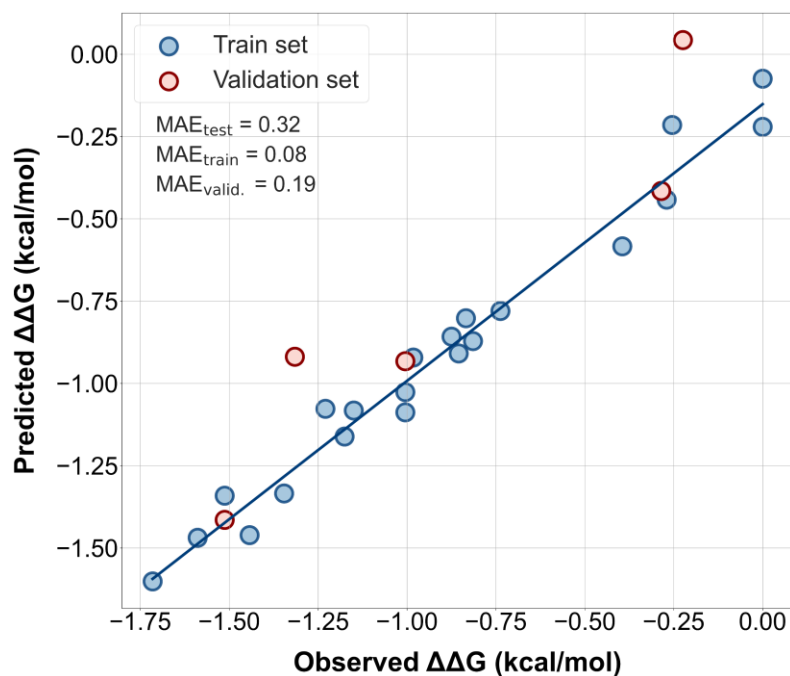
Algorithm Optimization

A group of extensively used ML algorithms like Kernel Ridge Regression (KRR)³⁴, Support Vector Regression (SVR)³⁵, Lasso regression (Lasso)³⁶, eXtreme Gradient Boosting Regression (XGBR)³⁷, Random Forest (RF) regression³⁸, Gaussian Process Regression (GPR)³⁹, Gradient Boosting Regression (GBR)⁴⁰, and Ridge regression⁴¹ were considered during model screening. The final optimizations of all the models were done with Bayesian search hyperparameter

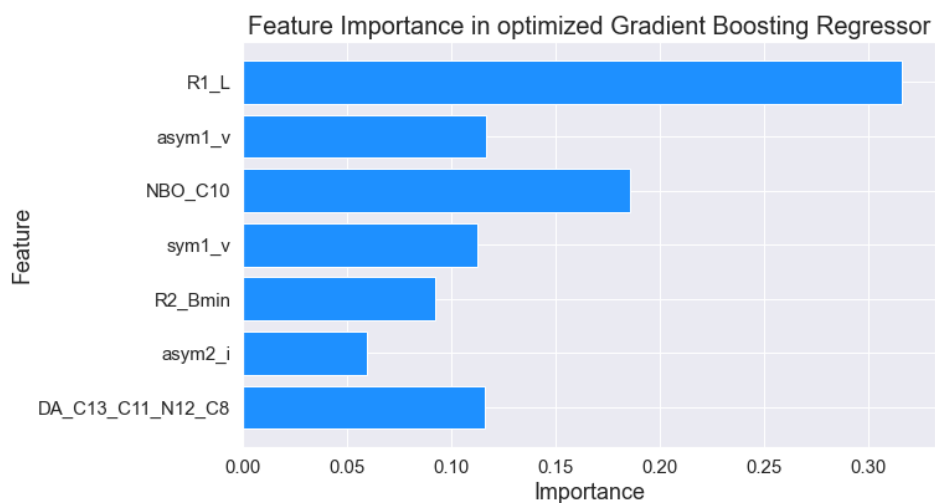
optimization using K-fold (K=3) cross validation within the training set, followed by external validation with the validation set (Supplementary Table 5). All the models have been provided the optimized parameters of the best individual versions.

Supplementary Table 5. Hyperparameters of optimized ML models with test and validation mean absolute error (MAE) in kcal mol⁻¹ unit.

Model	Test MAE	Validation MAE	Optimized parameters
GPR	0.43	0.50	[('kernel__k1__length_scale', 816.6335656907636), ('kernel__k2__noise_level', 0.06434158289435152)]
KRR	0.43	0.49	[('alpha', 0.97440637367698), ('gamma', 1e-06)]
SVR	0.41	0.42	[('C', 0.00026787646509051147), ('gamma', 8.443448902726717e-05), ('kernel', 'linear')]
Lasso	0.42	0.48	[('alpha', 884.7439478702872)]
XGBR	0.35	0.19	[('colsample_bytree', 1.0), ('learning_rate', 1.0), ('max_depth', 2), ('n_estimators', 50), ('reg_alpha', 1e-09), ('reg_lambda', 100.0), ('subsample', 0.7412279484481307)]
RF	0.40	0.31	[('bootstrap', True), ('max_depth', 1), ('max_features', 'log2'), ('min_samples_leaf', 0.014336011077006772), ('min_samples_split', 0.046087724297956614), ('n_estimators', 10)]
GBR	0.32	0.19	[('learning_rate', 0.07042768237611077), ('max_depth', 14), ('min_samples_split', 7), ('n_estimators', 50), ('subsample', 0.612185834327143)]
Ridge	0.40	0.22	[('alpha', 0.4669180289234465)]



Supplementary Figure 6. The selected GBR model used for final predictions.



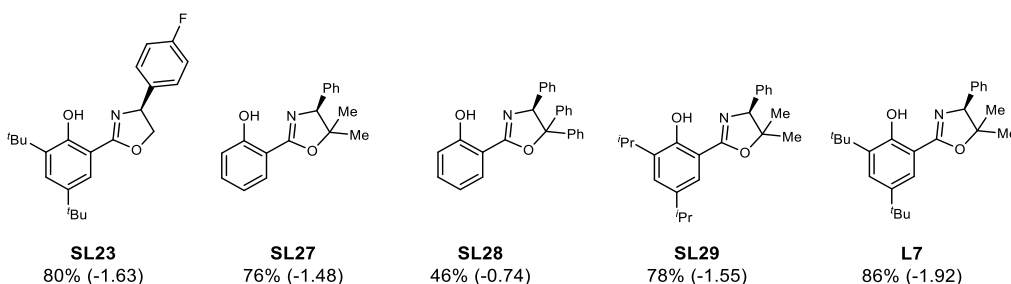
Supplementary Figure 7. Permutation importance from the selected GBR model with the training set.

Prediction Evaluation

Supplementary Table 6. Individual predicted $\Delta\Delta G$ ($\Delta\Delta G_{\text{pred_gbr}}$) against experimentally observed $\Delta\Delta G$ ($\Delta\Delta G_{\text{exp}}$) for the validation dataset. Values in kcal mol⁻¹ unit.

Ligand	$\Delta\Delta G_{\text{exp}}$	$\Delta\Delta G_{\text{pred_gbr}}$
L3	-1.00	-0.93
L2	-0.28	-0.41
SL12	-1.31	-0.92
SL14	-0.22	0.04
SL18	-1.51	-1.41

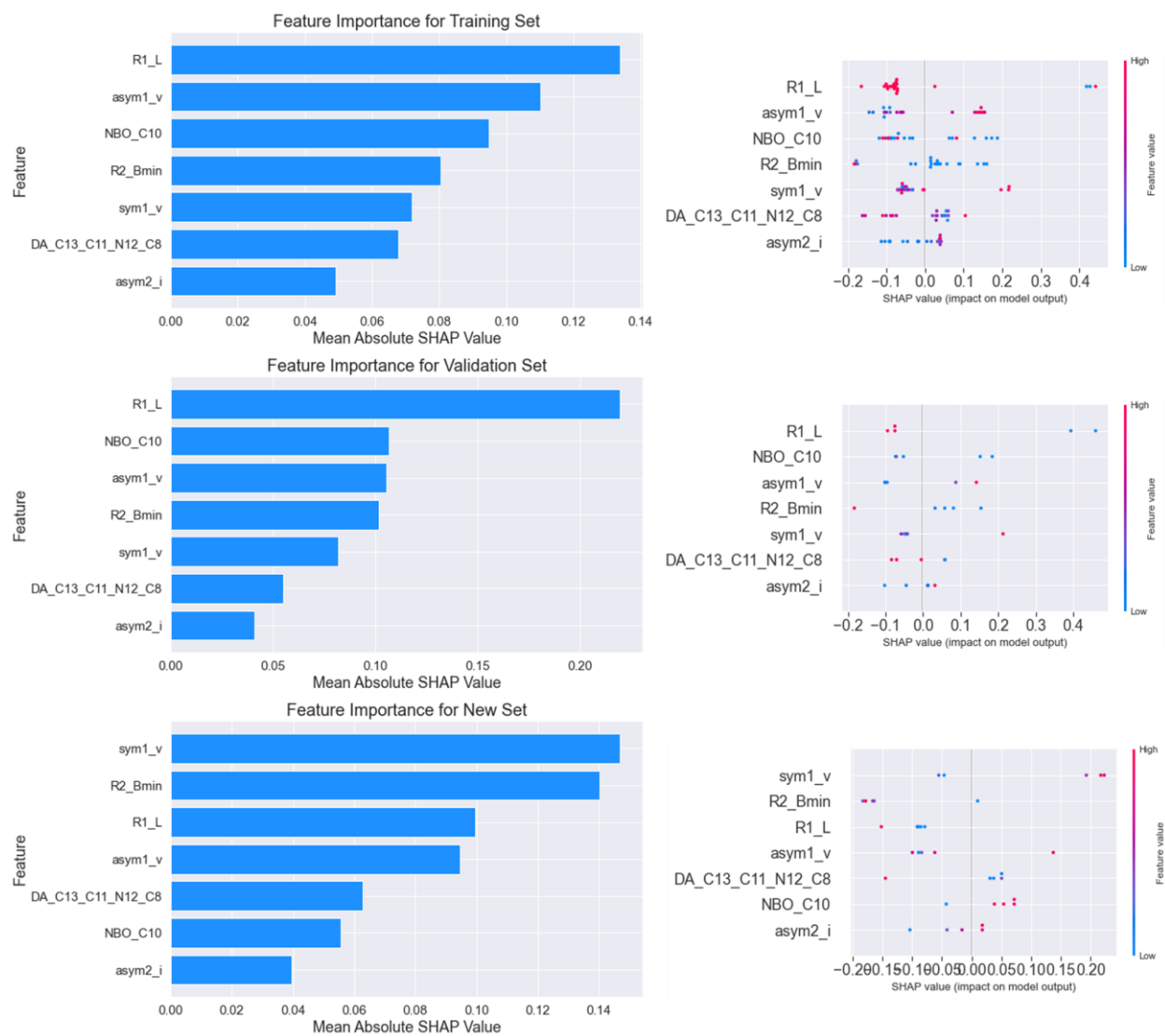
Designed New Ligands



Supplementary Figure 8. Set of new ligands designed further used with their respective ee_{exp} ($\Delta\Delta G_{\text{exp}}$ in kcal mol⁻¹).

Supplementary Table 7. Individual predicted $\Delta\Delta G$ ($\Delta\Delta G_{\text{pred_gbr}}$) against experimentally observed $\Delta\Delta G$ ($\Delta\Delta G_{\text{exp}}$) for set of new ligands. Values in kcal mol⁻¹ unit.

Ligand	$\Delta\Delta G_{\text{pred_gbr}}$	$\Delta\Delta G_{\text{exp}}$
SL23	-1.11	-1.63
SL27	-1.00	-1.48
SL28	-1.13	-0.74
SL29	-0.70	-1.55
L7	-1.16	-1.92

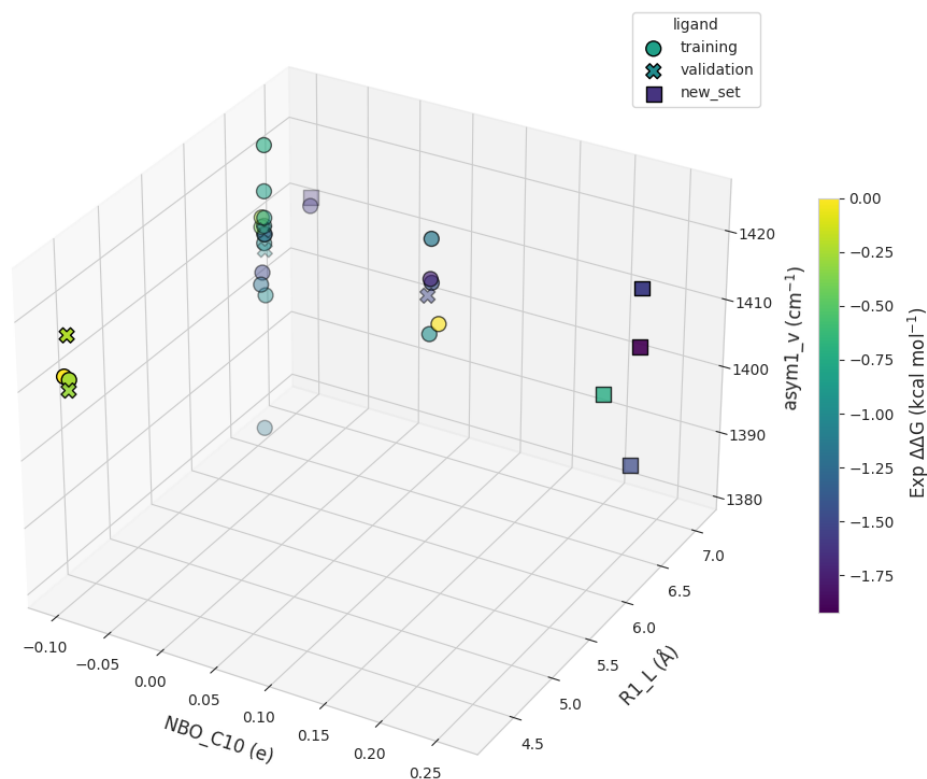


Supplementary Figure 9. Feature wise SHapley Additive exPlanations (SHAP)⁴² impact on the selected GBR model with the training, validation, and the new ligand set.

From the above plot, one can observe that training and validation dataset have similar trend in feature importance towards the model with R1_L, asym1_v, and NBO_C10 having the highest impact among other features. However, this trend changes in the new ligand dataset, indicating the diverseness from the training and validation datasets.

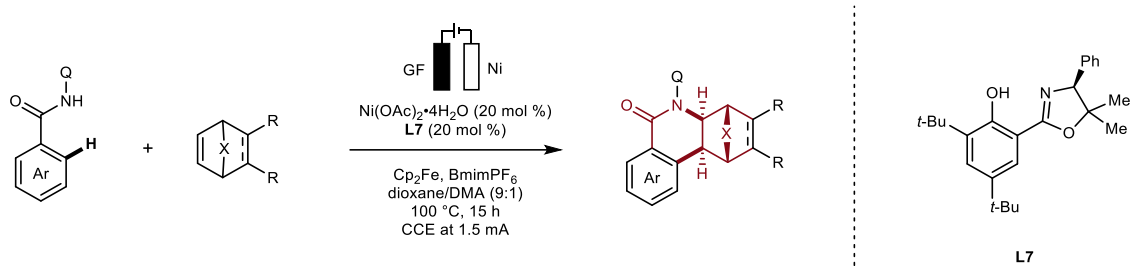
Supplementary Table 8. Measured values of the top three ranking parameters (NBO_C10, R1_L, and asym1_v) for the designed 5 ligands.

Ligand	NBO_C10 (e)	R1_L (Å)	asym1_v (cm ⁻¹)
SL23	-0.09071	7.1	1411.2188
SL27	0.25515	6.5	1391.9974
SL28	0.22833	6.5	1401.3834
SL29	0.25966	6.5	1418.2294
L7	0.25982	6.5	1409.7318



Supplementary Figure 10. Parameter space for the top three ranking parameters (NBO_C10, R1_L, and asym1_v) space for all the studied ligands.

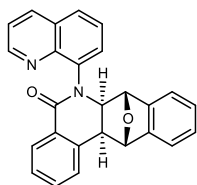
General Procedure for Nickel Catalysis



The electrolysis was carried out in an undivided cell setup. A GF anode (20 mm × 10 mm × 4 mm) and a nickel foam cathode (10 mm × 15 mm × 1.4 mm) with electrode holders made of stainless steel were used. The cell was charged with the amide (0.20 mmol, 1.0 equiv), alkene (0.30 mmol, 1.5 equiv), $\text{Ni(OAc)}_2 \cdot 4\text{H}_2\text{O}$ (10 mg, 0.04 mmol), ligand **L7** (15.2 mg, 0.04 mmol), Cp_2Fe (11.2 mg, 0.06 mmol), BmimPF_6 (73.9 mg, 0.05 M) and a teflon-coated magnetic stirring bar (15 × 6 mm). Then 1,4-dioxane (4.5 mL) and DMA (0.5 mL) were added. The reaction mixture was stirred at 100 °C for 10 min to obtain a homogeneous solution. Subsequently, the electrolysis was performed at 100 °C with a constant current of 1.5 mA maintained for 15 h with a stirring rate of 600 rpm. After completion of the reaction, the reaction mixture was diluted with 2 mL ethyl acetate and transferred to a round bottom flask. The electrodes (nickel foam and graphite felt) were washed in the reaction flask with ethyl acetate (3 × 5 mL) in an ultrasonic cleaner (3 × 3 min) and the washes were combined in the round bottom flask. The solvent was then removed under vacuum and the residue was purified by column chromatography to afford the title compound.

Characterization Data of the Products of Nickel Catalysis

(6aR,7S,12S,12aS)-6-(Quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[b]phenanthridin-5(6H)-one (3)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 4:1) afforded the title compound **3** as a sticky solid (55 mg, 0.14 mmol, 70%), with an enantiomeric ratio of 95:5.

¹H NMR (400 MHz, CDCl₃) δ 9.06 – 8.47 (m, 1H), 8.32 – 8.18 (m, 2H), 8.10 – 7.78 (m, 2H), 7.76 – 7.67 (m, 1H), 7.64 – 7.56 (m, 1H), 7.52 (d, *J* = 7.7 Hz, 1H), 7.45 – 7.34 (m, 3H), 7.24 – 7.17 (m, 1H), 7.13 – 7.03 (m, 1H), 6.95 (d, *J* = 7.3 Hz, 1H), 5.55 – 5.42 (m, 2H), 4.72 (bs, 1H), 3.69 (d, *J* = 8.5 Hz, 1H) ppm.

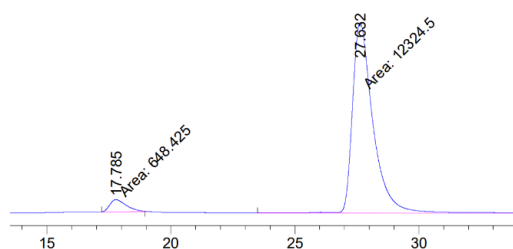
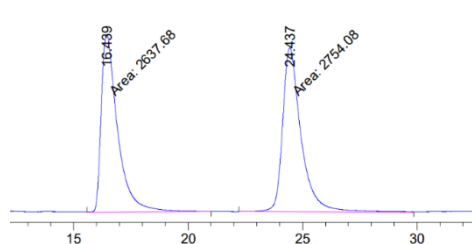
¹³C NMR (101 MHz, CDCl₃) δ 163.0 (C_q), 150.8 (CH), 145.8 (C_q), 144.0 (C_q or CH), 142.5 (C_q), 138.3 (C_q or CH), 137.7 (C_q), 136.7 (CH), 132.6 (CH), 130.1 (C_q), 129.0 (CH), 128.6 (CH), 128.1 (CH), 127.7 (CH), 127.2 (CH), 127.2 (CH), 127.2 (C_q), 126.6 (CH), 121.7 (CH), 120.5 (CH), 119.3 (CH), 88.9 (CH), 84.7 (CH), 63.6 (CH), 43.1 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3003, 1644, 1461, 1421, 1299, 987, 858, 825, 794, 753 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₆H₁₉N₂O₂: 391.1441; found: 391.1440.

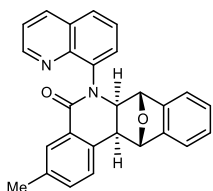
[α]_D²⁰ = +55.80 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 27.6 min, tr(minor) = 17.8 min, 95:5 e.r.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.439	MM	0.8283	2637.67505	53.07174	48.9205	1	17.785	MM	0.7783	648.42511	13.88588	4.9983
2	24.437	MM	0.9382	2754.07983	48.92476	51.0795	2	27.632	MM	0.9582	1.23245e4	214.37813	95.0017

(6aR,7S,12S,12aS)-3-Methyl-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (5)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compound **5** as a sticky solid (45 mg, 0.112 mmol, 56%), with an enantiomeric ratio of 92:8.

¹H NMR (400 MHz, CDCl₃) δ 8.81 (s, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 8.07 (s, 1H), 7.98 – 7.88 (m, 2H), 7.76 – 7.68 (m, 1H), 7.44 – 7.38 (m, 4H), 7.23 – 7.13 (m, 1H), 7.13 – 7.01 (m, 1H), 6.93 (d, *J* = 7.3 Hz, 1H), 5.48 (s, 1H), 5.42 (s, 1H), 4.68 (s, 1H), 3.65 (d, *J* = 8.5 Hz, 1H), 2.40 (s, 3H) ppm.

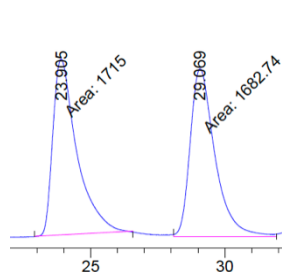
¹³C NMR (101 MHz, CDCl₃) δ 163.3 (C_q), 150.8 (CH), 145.9 (C_q), 142.6 (C_q), 137.0 (C_q), 136.6 (CH), 134.8 (C_q), 133.5 (CH), 132.5 (CH), 130.1 (C_q), 129.2 (CH), 128.6 (CH), 128.1 (CH), 127.7 (CH), 127.2 (CH), 126.9 (C_q), 126.6 (CH), 121.7 (CH), 120.5 (CH), 119.3 (CH), 88.9 (CH), 84.7 (CH), 63.7 (CH), 42.8 (CH), 21.3 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2925, 1653, 1612, 1501, 1459, 1302, 859, 791, 764, 649 cm⁻¹.

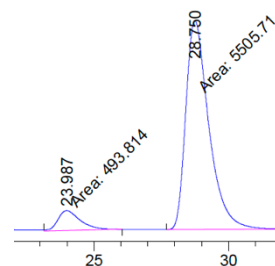
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₂₁N₂O₂: 405.1603; found: 405.1598.

[α]_D²⁰ = +10.2 (c = 0.78, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 28.8 min, tr(minor) = 24.0 min, 92:8 e.r.

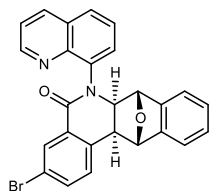


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.905	MM	1.0346	1715.00110	27.62834	50.4747
2	29.069	MM	1.0650	1682.74329	26.33316	49.5253



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.987	MM	0.9437	493.81406	8.72083	8.2309
2	28.750	MM	0.9913	5505.71191	92.56638	91.7691

(6aR,7S,12S,12aS)-3-Bromo-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[b]phenanthridin-5(6H)-one (6)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compound **6** as a sticky solid (49 mg, 0.104 mmol, 52%), with an enantiomeric ratio of 92.5:7.5.

¹H NMR (400 MHz, CDCl₃) δ 8.82 (s, 1H), 8.39 (s, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 8.06 – 7.82 (m, 2H), 7.78 – 7.67 (m, 2H), 7.44 – 7.38 (m, 3H), 7.24 – 7.13 (m, 1H), 7.14 – 7.01 (m, 1H), 6.94 (d, *J* = 7.3 Hz, 1H), 5.49 (s, 1H), 5.40 (s, 1H), 4.68 (s, 1H), 3.63 (d, *J* = 8.5 Hz, 1H) ppm.

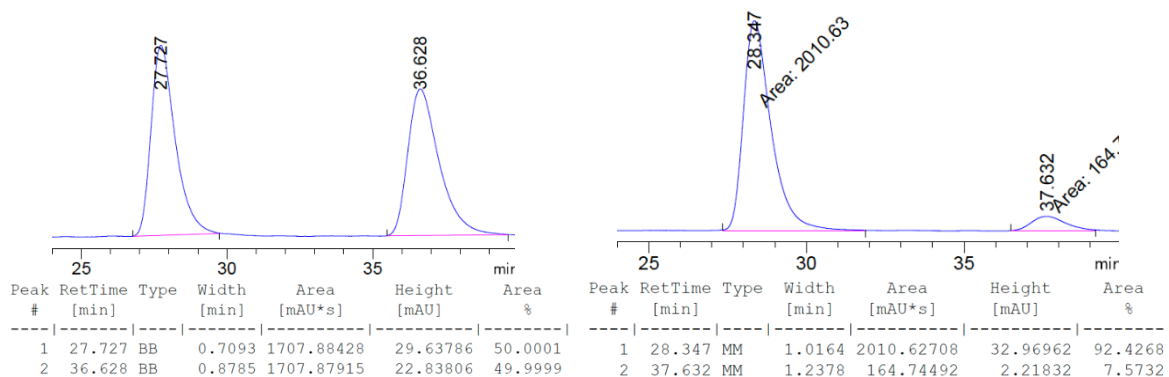
¹³C NMR (101 MHz, CDCl₃) δ 161.7 (C_q), 150.9 (CH), 145.5 (C_q), 142.4 (C_q), 136.7 (CH), 136.7 (C_q), 135.5 (CH), 131.9 (CH), 130.1 (C_q), 130.0 (CH), 129.0 (C_q), 128.9 (CH), 127.8 (CH), 127.4 (CH), 126.7 (CH), 121.8 (CH), 121.3 (C_q), 120.5 (CH), 119.3 (CH), 88.7 (CH), 84.7 (CH), 63.8 (CH), 42.9 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3009, 1652, 1594, 1498, 1446, 1301, 988, 859, 794, 762, 660, 622 cm⁻¹.

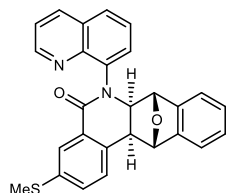
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₆H₁₈BrN₂O₂: 469.0552; found: 469.0546.

[α]_D²⁰ = +19.9 (c = 0.70, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 28.3 min, tr(minor) = 37.6 min, 92.5:7.5 e.r.



(6a*R*,7*S*,12*S*,12a*S*)-3-(Methylthio)-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (7)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:3) afforded the title compound **7** as a sticky solid (52 mg, 0.12 mmol, 60%), with an enantiomeric ratio of 91.5:8.5.

¹H NMR (400 MHz, CDCl₃) δ 9.27 – 8.57 (m, 1H), 8.23 (d, *J* = 8.2 Hz, 1H), 8.14 (s, 1H), 8.04 – 7.64 (m, 3H), 7.58 – 7.34 (m, 4H), 7.27 – 7.16 (m, 1H), 7.13 – 7.03 (m, 1H), 6.98 – 6.87 (m, 1H), 5.57 – 5.47 (m, 1H), 5.46 – 5.35 (m, 1H), 4.69 (s, 1H), 3.65 (d, *J* = 8.6 Hz, 1H), 2.51 (s, 3H) ppm.

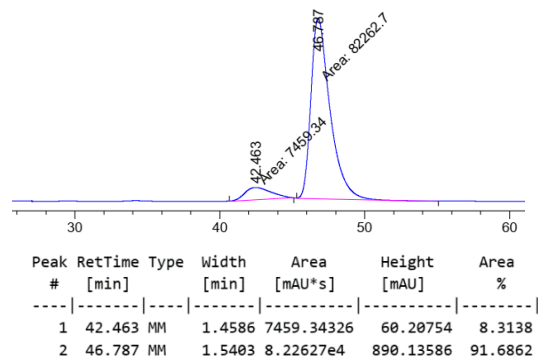
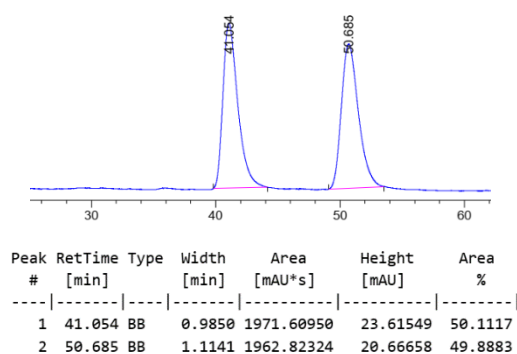
¹³C NMR (101 MHz, CDCl₃) δ 162.7 (C_q), 150.9 (CH), 145.7 (C_q), 142.5 (C_q), 137.9 (C_q), 136.6 (CH), 134.4 (C_q), 132.3 (C_q), 131.2 (CH), 130.0 (C_q), 128.7 (CH), 128.6 (CH), 127.7 (CH), 127.7 (C_q), 127.2 (CH), 126.6 (CH), 125.8 (CH), 121.7 (CH), 120.4 (CH), 119.3 (CH), 88.8 (CH), 84.6 (CH), 63.6 (CH), 42.8, (CH) 15.9 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2923, 1652, 1595, 1446, 1302, 1215, 795, 761, 628 cm⁻¹.

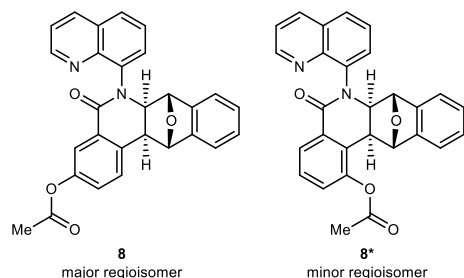
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₂₁N₂O₂S: 437.1325; found: 437.1318.

[α]_D²⁰ = +17.5 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 46.8 min, tr(minor) = 42.5 min, 91.5:8.5 e.r.



(6aR,7S,12S,12aS)-5-Oxo-6-(quinolin-8-yl)-5,6,6a,7,12,12a-hexahydro-7,12-epoxybenzo[*b*]phenanthridin-3-yl acetate (8**) and (6aR,7S,12S,12aS)-5-oxo-6-(quinolin-8-yl)-5,6,6a,7,12,12a-hexahydro-7,12-epoxybenzo[*b*]phenanthridin-1-yl acetate (**8***)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 4:1) afforded the title compounds as a sticky solid (52 mg, 0.116 mmol, 58%), with an enantiomeric ratio of 96:4 (major regioisomer, **8**) and 94:6 (minor regioisomer, **8***) in a regioisomeric ratio of 5:1.

¹H NMR (600 MHz, CDCl₃, major regioisomer, **8**) δ 8.98 – 8.65 (m, 1H), 8.23 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.98 – 7.90 (m, 3H), 7.76 – 7.67 (m, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.44 – 7.38 (m, 2H), 7.36 (dd, *J* = 8.4, 2.6 Hz, 1H), 7.24 – 7.18 (m, 1H), 7.10 – 7.02 (m, 1H), 6.94 (d, *J* = 7.3 Hz, 1H), 5.54 – 5.38 (m, 2H), 4.72 (s, 1H), 3.67 (d, *J* = 8.5 Hz, 1H), 2.32 (s, 3H) ppm.

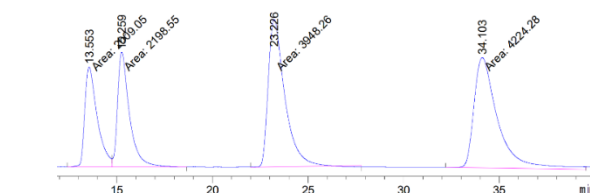
¹³C NMR (126 MHz, CDCl₃, major regioisomer, **8**) δ 169.5 (C_q), 162.2 (C_q), 150.8 (CH), 149.8 (C_q), 145.7 (C_q), 143.8 (C_q), 142.4 (C_q), 138.0 (C_q), 136.6 (CH), 135.2 (C_q), 132.4 (CH), 130.1 (C_q), 129.4 (CH), 128.7 (CH), 128.7 (C_q), 127.7 (CH), 127.3 (CH), 126.6 (CH), 126.3 (CH), 121.8 (CH), 121.6 (CH), 120.5 (CH), 119.3 (CH), 88.7 (CH), 84.6 (CH), 63.6 (CH), 42.8 (CH), 21.2 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3070, 1758, 1655, 1592, 1497, 1473, 1451, 1369, 1302, 1200 cm⁻¹.

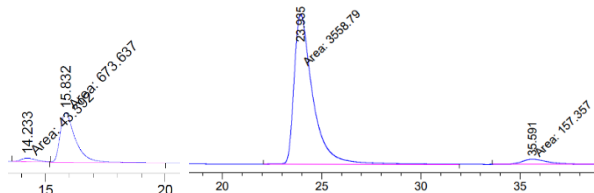
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₁N₂O₄: 449.1496; found: 449.1486.

[α]_D²⁰ = +28.60 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): Major regioisomer: tr(major) = 23.9 min, tr(minor) = 35.6 min, 96:4 e.r., minor regioisomer: tr(major) = 15.8 min, tr(minor) = 14.2 min, 94:6 e.r.



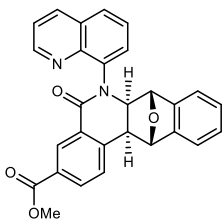
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.553	MF	0.7576	2009.05115	44.19521	16.2280
2	15.259	FM	0.7229	2198.55420	50.68851	17.7587
3	23.226	MM	1.0079	3948.26221	65.28972	31.8919
4	34.103	MM	1.4433	4224.28320	48.78126	34.1214



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.935	MM	1.0988	3558.79248	53.98165	95.7656
2	35.591	MM	1.4462	157.35674	1.81351	4.2344

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.233	MM	0.7116	43.39195	1.01624	6.0516
2	15.832	MM	0.7658	673.63654	14.66112	93.9484

Methyl-(6aR,7S,12S,12aS)-5-oxo-6-(quinolin-8-yl)-5,6,6a,7,12,12a-hexahydro-7,12-epoxybenzo[*b*]phenanthridine-3-carboxylate (9)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 4:1) afforded the title compound **9** as a sticky solid (34 mg, 0.075 mmol, 38%), with an enantiomeric ratio of 94.5:5.5. Crystallization from a saturated solution of chloroform/*i*-propanol yielded crystals suitable for X-ray diffraction analysis.

¹H NMR (400 MHz, CDCl₃) δ 8.91 (s, 1H), 8.82 (s, 1H), 8.30 – 8.22 (m, 2H), 8.02 – 7.85 (m, 2H), 7.79 – 7.69 (m, 1H), 7.62 (d, *J* = 8.1 Hz, 1H), 7.46 – 7.37 (m, 2H), 7.25 – 7.18 (m, 1H), 7.15 – 7.02 (m, 1H), 6.96 (d, *J* = 7.3 Hz, 1H), 5.51 (s, 1H), 5.45 (s, 1H), 4.72 (bs, 1H), 3.93 (s, 3H), 3.72 (d, *J* = 8.6 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 166.6 (C_q), 162.1 (C_q), 150.9 (CH), 145.6 (C_q), 142.6 (C_q), 142.4 (C_q), 136.7 (CH), 133.2 (CH), 130.6 (CH), 130.1 (C_q), 129.5 (C_q), 128.8 (CH), 128.6 (CH), 127.8 (CH), 127.6 (C_q), 127.4 (CH), 126.6 (CH), 121.8 (CH), 120.6 (CH), 119.3 (CH), 88.8 (CH), 84.7 (CH), 63.7 (CH), 52.4 (CH₃), 43.4 (CH) ppm.

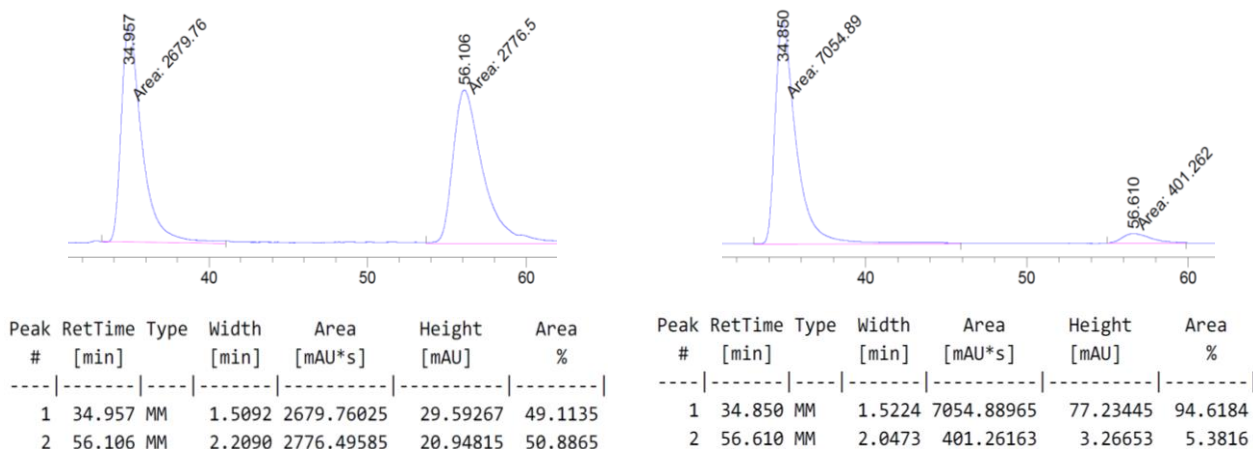
IR (ATR): $\tilde{\nu}$ = 3002, 1720, 1651, 1473, 1434, 1286, 1237, 1119, 975, 758 cm⁻¹.

MP: 225-228 °C.

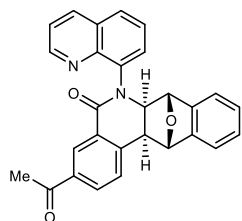
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₁N₂O₄: 449.1496; found: 449.1494.

[α]_D²⁰ = +28.8 (*c* = 0.4, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 34.9 min, tr(minor) = 56.6 min, 94.5:5.5 e.r.



(6aR,7S,12S,12aS)-3-Acetyl-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (10)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:3) afforded the title compound **10** as a sticky solid (36 mg, 0.084 mmol, 42%), with an enantiomeric ratio of 94:6.

¹H NMR (400 MHz, CDCl₃) δ 8.92 – 8.76 (m, 2H), 8.31 – 8.21 (m, 2H), 8.03 – 7.85 (m, 2H), 7.80 – 7.70 (m, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.49 – 7.36 (m, 2H), 7.25 – 7.17 (m, 1H), 7.13 – 7.04 (m, 1H), 6.97 (d, *J* = 7.3 Hz, 1H), 5.59 – 5.51 (m, 1H), 5.48 – 5.42 (m, 1H), 4.71 (bs, 1H), 3.73 (d, *J* = 8.5 Hz, 1H), 2.64 (s, 3H) ppm.

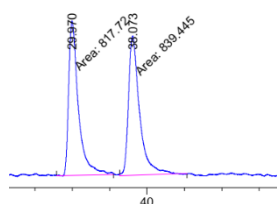
¹³C NMR (101 MHz, CDCl₃) δ 197.7 (C_q), 162.3 (C_q), 151.0 (CH), 145.5 (C_q), 142.8 (C_q), 142.4 (C_q), 136.7 (CH), 136.2 (C_q), 131.4 (CH), 130.1 (C_q), 129.9 (CH), 128.9 (CH), 128.9 (CH), 127.9 (CH), 127.5 (CH), 127.4 (C_q), 126.6 (CH), 122.1 (CH), 121.9 (CH), 120.6 (CH), 119.4 (CH), 88.7 (CH), 84.7 (CH), 63.7 (CH), 43.5 (CH), 26.9 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2926, 1683, 1654, 1606, 1456, 1283, 1237, 844, 762, 667 cm⁻¹.

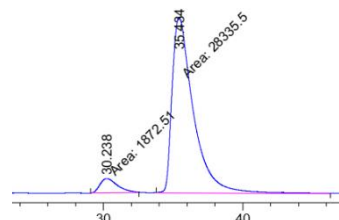
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₁N₂O₃: 433.1541; found: 433.1547.

[α]_D²⁰ = +23.2 (*c* = 0.5, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 35.4 min, tr(minor) = 30.2 min, 94:6 e.r.

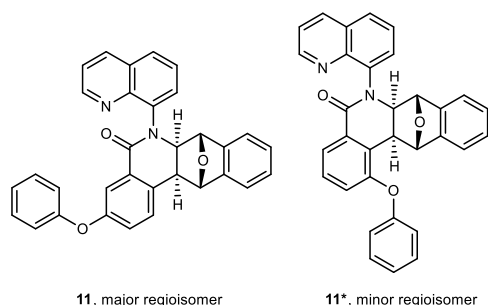


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	29.970	MM	1.5110	817.71991	9.01987	49.3445
2	38.073	MM	1.7201	839.44476	8.13378	50.6555



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.238	MM	1.4503	1872.50806	21.51837	6.1987
2	35.434	MM	1.7747	2.83355e4	266.11151	93.8013

(6aR,7S,12S,12aS)-3-Phenoxy-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (11) and (6aR,7S,12S,12aS)-1-phenoxy-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (11*)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate) afforded the title compounds **11** (43 mg, 0.09 mmol, 45%) and **11*** (18 mg, 0.038 mmol, 19%) as sticky solids. Enantiomeric ratios of 84.5:15.5 (**11**) and $\geq 99.5:0.5$ (**11***) were obtained. Crystallization from a saturated solution of chloroform/*i*-propanol yielded crystals of **11** suitable for X-ray diffraction analysis.

Regioisomer 11

¹H NMR (400 MHz, CDCl₃) δ 9.17 – 8.65 (m, 1H), 8.23 (d, *J* = 8.2 Hz, 1H), 7.96 – 7.90 (m, 2H), 7.88 (s, 1H), 7.77 – 7.66 (m, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.44 – 7.28 (m, 5H), 7.25 – 7.18 (m, 1H), 7.15 – 7.02 (m, 4H), 6.95 (d, *J* = 7.3 Hz, 1H), 5.63 – 5.32 (m, 2H), 4.74 (bs, 1H), 3.68 (d, *J* = 8.6 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 162.5 (C_q), 156.8 (C_q), 156.7 (C_q), 150.8 (CH), 145.7 (C_q), 143.8 (C_q), 142.5 (C_q), 138.1 (C_q), 136.6 (CH), 132.3 (C_q), 129.9 (CH), 129.8 (CH), 128.7 (CH), 128.6 (C_q), 127.7 (CH), 127.2 (CH), 126.5 (CH), 123.7 (CH), 123.6 (CH), 121.7 (CH), 120.4 (CH), 119.3 (CH), 118.1 (CH), 88.9 (CH), 84.6 (CH), 63.6 (CH), 42.6 (CH) ppm.

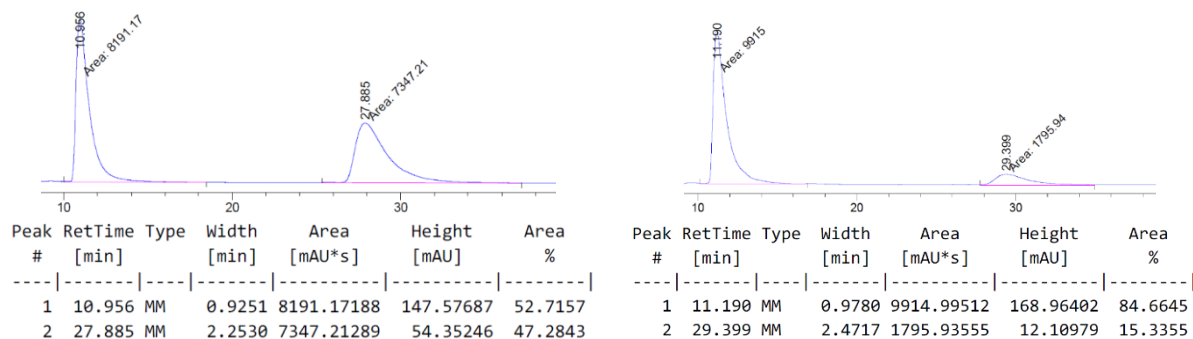
IR (ATR): $\tilde{\nu}$ = 3009, 1644, 1608, 1589, 1487, 1451, 1304, 1260, 1225, 765 cm⁻¹.

MP: 225–227 °C.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₂H₂₃N₂O₃: 483.1703; found: 483.1699.

[α]_D²⁰ = +18.40 (*c* = 1.0, CHCl₃).

R_t (IB column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 11.2 min, tr(minor) = 29.4 min, 84.5:15.5 e.r.



Regioisomer **11***

¹H NMR (400 MHz, CDCl₃) δ 9.00 – 8.67 (m, 1H), 8.25 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 8.02 – 7.84 (m, 2H), 7.79 – 7.69 (m, 1H), 7.47 – 7.40 (m, 3H), 7.40 – 7.29 (m, 2H), 7.21 – 7.12 (m, 5H), 7.06 – 7.01 (m, 1H), 6.93 (d, *J* = 7.3 Hz, 1H), 5.60 (s, 1H), 5.48 (s, 1H), 4.76 (bs, 1H), 3.74 (d, *J* = 8.6 Hz, 1H) ppm.

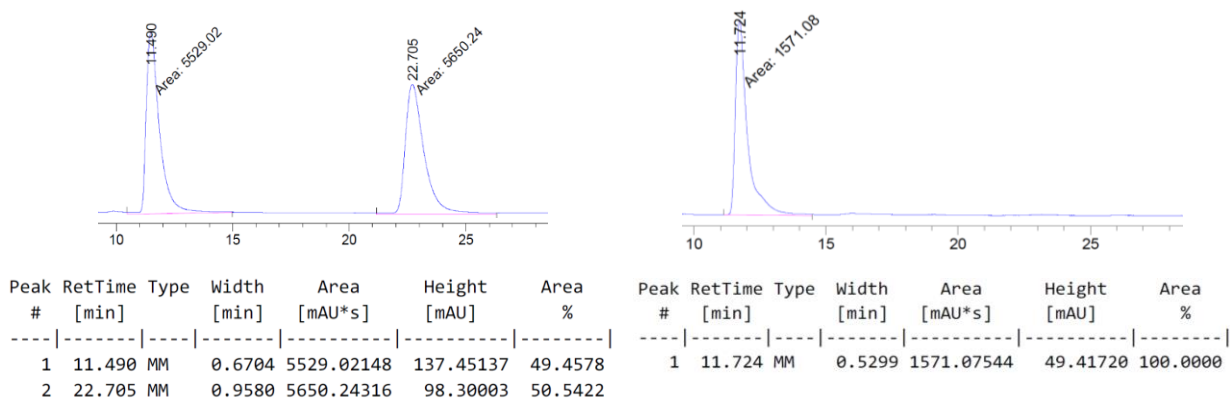
¹³C NMR (101 MHz, CDCl₃) δ 162.7 (C_q), 156.7 (C_q), 153.8 (C_q), 150.8 (CH), 146.4 (C_q), 142.1 (C_q), 136.7 (CH), 132.7 (C_q), 130.3 (CH), 130.0 (CH), 129.0 (C_q), 128.8 (C_q), 128.7 (CH), 127.9 (CH), 127.7 (CH), 127.0 (CH), 126.6 (CH), 124.1 (CH), 123.9 (CH), 121.7 (CH), 120.5 (CH), 119.3 (CH), 118.4 (CH), 87.0 (CH), 84.4 (CH), 63.3 (CH), 39.1 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3007, 1656, 1583, 1489, 1469, 1421, 1318, 1292, 1238, 754 cm⁻¹.

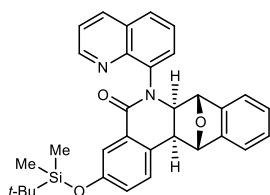
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₂H₂₃N₂O₃: 483.1703; found: 483.1698.

[α]_D²⁰ = +54.60 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 11.7 min, ≥99.5:0.5 e.r.



(6aR,7S,12S,12aS)-3-((*tert*-Butyldimethylsilyl)oxy)-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (12)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:3) afforded the title compound **12** as a sticky solid (71 mg, 0.136 mmol, 68%), with an enantiomeric ratio of 94:6.

¹H NMR (400 MHz, CDCl₃) δ 9.21 – 8.56 (m, 1H), 8.23 (d, *J* = 8.3 Hz, 1H), 8.06 – 7.83 (m, 2H), 7.80 – 7.62 (m, 2H), 7.49 – 7.34 (m, 3H), 7.25 – 7.17 (m, 1H), 7.14 – 7.01 (m, 2H), 6.94 (d, *J* = 7.3 Hz, 1H), 5.48 (s, 1H), 5.42 (s, 1H), 4.74 (s, 1H), 3.63 (d, *J* = 8.6 Hz, 1H), 1.00 (s, 9H), 0.23 (s, 6H) ppm.

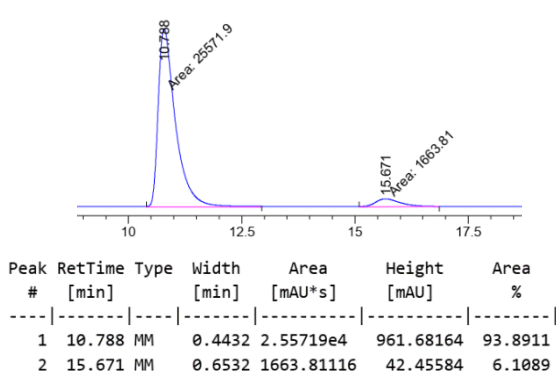
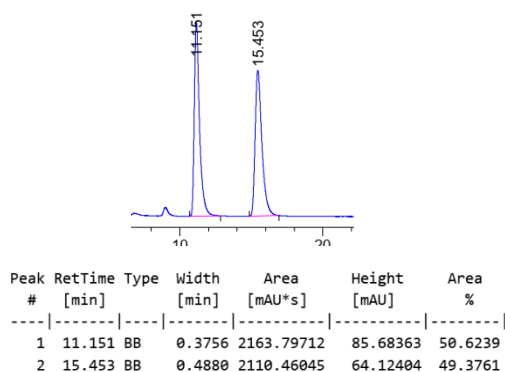
¹³C NMR (101 MHz, CDCl₃) δ 163.0 (C_q), 154.9 (C_q), 150.8 (CH), 145.9 (C_q), 142.5 (C_q), 136.6 (CH), 132.5 (CH), 130.4 (C_q), 130.0 (C_q), 129.4 (CH), 128.6 (CH), 128.1 (C_q), 127.6 (CH), 127.2 (CH), 126.6 (CH), 125.2 (CH), 121.7 (CH), 120.4 (CH), 119.3 (CH), 119.1 (CH), 88.9 (CH), 84.5 (CH), 63.5 (CH), 42.6 (CH), 25.8 (CH₃), 18.3 (C_q), -4.3 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2931, 1653, 1607, 1499, 1449, 1306, 1278, 962, 880, 838, 762 cm⁻¹.

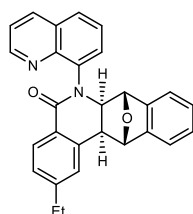
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₂H₃₃N₂O₃Si: 521.2252; found: 521.2255.

[α]_D²⁰ = +38.0 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 10.8 min, tr(minor) = 15.7 min, 94:6 e.r.



(6aR,7S,12S,12aS)-2-Ethyl-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (13)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:2) afforded the title compound **13** as a sticky solid (54 mg, 0.13 mmol, 65%), with an enantiomeric ratio of 95:5.

¹H NMR (300 MHz, CDCl₃) δ 8.82 (s, 1H), 8.31 – 8.11 (m, 2H), 8.03 – 7.82 (m, 2H), 7.81 – 7.62 (m, 1H), 7.50 – 7.36 (m, 2H), 7.32 (s, 1H), 7.26 – 7.17 (m, 2H), 7.11 – 7.03 (m, 1H), 6.94 (d, *J* = 7.2 Hz, 1H), 5.63 – 5.29 (m, 2H), 4.70 (s, 1H), 3.66 (d, *J* = 8.6 Hz, 1H), 2.78 (q, *J* = 7.6 Hz, 2H), 1.34 (t, *J* = 7.6 Hz, 3H) ppm.

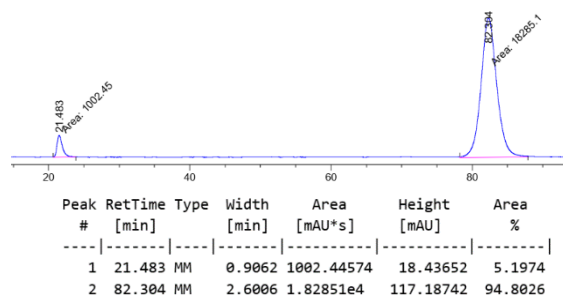
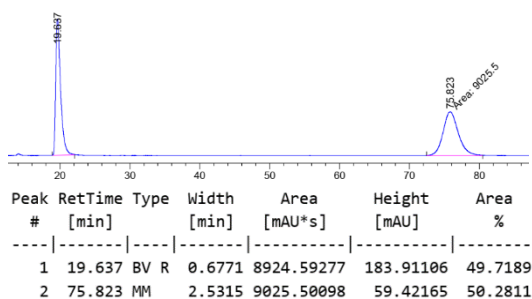
¹³C NMR (101 MHz, CDCl₃) δ 163.2 (C_q), 150.8 (CH), 149.3 (C_q), 145.9 (C_q), 142.6 (C_q), 137.7 (C_q), 136.6 (CH), 132.6 (C_q), 130.1 (C_q), 129.2 (CH), 128.6 (CH), 127.6 (CH), 127.4 (CH), 127.2 (CH), 127.1 (CH), 126.6 (CH), 124.9 (C_q), 121.7 (CH), 120.5 (CH), 119.3 (CH), 88.9 (CH), 84.7 (CH), 63.5 (CH), 43.1 (CH), 29.2 (CH₂), 15.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2968, 1770, 1651, 1611, 1498, 1443, 1299, 987, 758 cm⁻¹.

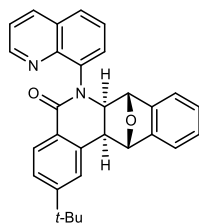
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₃N₂O₂: 419.1751; found: 419.1754.

[α]_D²⁰ = +68.6 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 82.3 min, tr(minor) = 21.5 min, 95:5 e.r.



(6aR,7S,12S,12aS)-2-(tert-Butyl)-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (14)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:1) afforded the title compound **14** as a sticky solid (51 mg, 0.114 mmol, 57%), with an enantiomeric ratio of 96.5:3.5.

¹H NMR (400 MHz, CDCl₃) δ 9.16 – 8.66 (m, 1H), 8.37 – 8.15 (m, 2H), 8.16 – 7.88 (m, 2H), 7.84 – 7.67 (m, 1H), 7.57 – 7.40 (m, 4H), 7.33 – 7.22 (m, 1H), 7.20 – 7.07 (m, 1H), 6.99 (d, *J* = 7.3 Hz, 1H), 5.58 – 5.45 (m, 2H), 4.76 (s, 1H), 3.73 (d, *J* = 8.5 Hz, 1H), 1.48 (s, 9H) ppm.

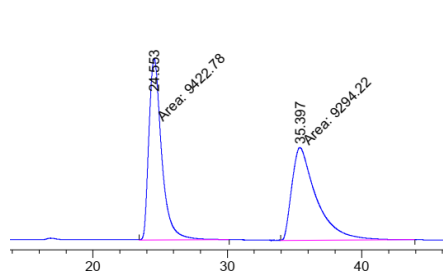
¹³C NMR (101 MHz, CDCl₃) δ 163.1 (C_q), 156.1 (C_q), 150.8 (CH), 145.8 (C_q), 142.7 (C_q), 137.3 (C_q), 136.6 (CH), 132.6 (CH), 130.1 (C_q), 128.9 (CH), 128.5 (CH), 127.6 (CH), 127.2 (CH), 126.6 (CH), 124.7 (C_q), 124.7 (CH), 124.7 (CH), 121.7 (CH), 120.4 (CH), 119.4 (CH), 88.9 (CH), 84.7 (CH), 63.6 (CH), 43.3 (CH), 35.2 (C_q), 31.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2963, 1723, 1692, 1652, 1609, 1436, 1298, 987, 765, 748 cm⁻¹.

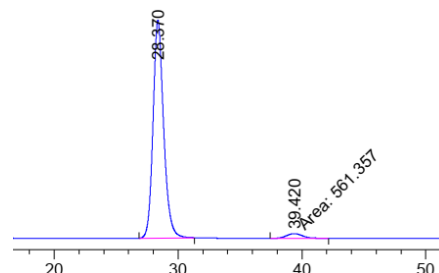
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₀H₂₇N₂O₂: 447.2061; found: 447.2067.

[α]_D²⁰ = +62.9 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 28.4 min, tr(minor) = 39.4 min, 96.5:3.5 e.r.

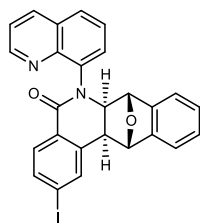


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.553	MM	1.1009	9422.77734	142.65631	50.3434
2	35.397	MM	2.1183	9294.21875	73.12592	49.6566



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.370	BB	0.8635	1.46339e4	246.20056	96.3057
2	39.420	MM	1.6787	561.35730	5.57324	3.6943

(6aR,7S,12S,12aS)-2-Iodo-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (15)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:1) afforded the title compound **15** as a sticky solid (57 mg, 0.11 mmol, 55%), with an enantiomeric ratio of 91:9.

¹H NMR (400 MHz, CDCl₃) δ 9.09 – 8.64 (m, 1H), 8.23 (d, *J* = 8.3 Hz, 1H), 8.04 – 7.82 (m, 4H), 7.80 – 7.61 (m, 2H), 7.51 – 7.35 (m, 2H), 7.26 – 7.17 (m, 1H), 7.16 – 7.04 (m, 1H), 6.95 (d, *J* = 7.4 Hz, 1H), 5.53 – 5.38 (m, 2H), 4.69 (s, 1H), 3.62 (d, *J* = 8.5 Hz, 1H) ppm.

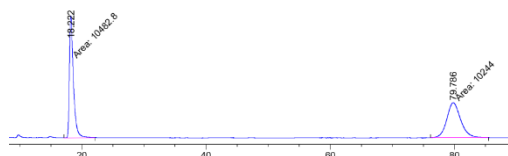
¹³C NMR (101 MHz, CDCl₃) δ 162.6 (C_q), 151.4 (CH), 145.5 (C_q), 143.8 (C_q), 142.4 (C_q), 139.7 (CH), 137.0 (CH), 136.6 (CH), 132.4 (C_q), 130.7 (CH), 130.1 (C_q), 128.7 (CH), 127.8 (CH), 127.4 (CH), 126.8 (C_q), 126.6 (CH), 121.8 (CH), 120.5 (CH), 119.4 (CH), 99.8 (C_q), 88.7 (CH), 84.7 (CH), 63.7 (CH), 42.7 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3004, 2173, 1962, 1652, 1585, 1438, 1296, 986, 760 cm⁻¹.

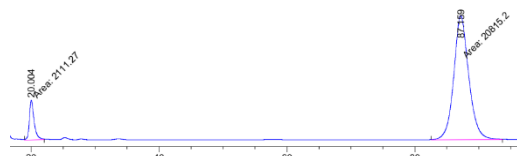
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₆H₁₈N₂O₂I: 517.0407; found: 517.0407.

[α]_D²⁰ = +58.6 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 87.2 min, tr(minor) = 20.0 min, 91:9 e.r.

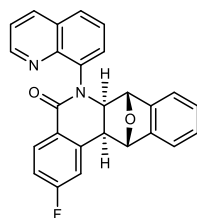


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.222	MM	0.7508	1.04828e4	232.69073	50.5761
2	79.786	MM	2.5602	1.02440e4	66.68620	49.4239



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.004	MM	0.8601	2111.27100	40.90979	9.2089
2	87.159	MM	2.7205	2.08152e4	127.52212	90.7911

(6aR,7S,12S,12aS)-2-Fluoro-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[b]phenanthridin-5(6H)-one (16)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate) afforded the title compound **16** as a sticky solid (39 mg, 0.095 mmol, 48%), with an enantiomeric ratio of 93.5:6.5.

¹H NMR (400 MHz, CDCl₃) δ 9.00 – 8.64 (m, 1H), 8.33 – 8.20 (m, 2H), 7.98 – 7.81 (m, 2H), 7.77 – 7.66 (m, 1H), 7.45 – 7.38 (m, 2H), 7.25 – 7.18 (m, 2H), 7.13 – 7.03 (m, 2H), 6.95 (d, *J* = 7.3 Hz, 1H), 5.58 – 5.36 (m, 2H), 4.71 (bs, 1H), 3.66 (d, *J* = 8.5 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 165.5 (d, *J*_{CF} = 253 Hz, C_q), 162.2 (C_q), 150.9 (CH), 149.6 (C_q), 145.5 (C_q), 144.0 (C_q), 142.4 (C_q), 140.5 (d, *J*_{CF} = 9 Hz, C_q), 136.6 (CH), 132.3 (CH), 132.1 (d, *J*_{CF} = 9 Hz, CH), 130.1 (C_q), 128.7 (CH), 127.8 (CH), 127.4 (CH), 126.6 (CH), 123.7 (d, *J*_{CF} = 3 Hz, C_q), 121.8 (CH), 120.5 (CH), 119.3 (CH), 114.9 (d, *J*_{CF} = 22 Hz, CH), 114.4 (d, *J*_{CF} = 22 Hz, CH), 88.7 (CH), 84.7 (CH), 63.6 (CH), 43.3 (CH) ppm.

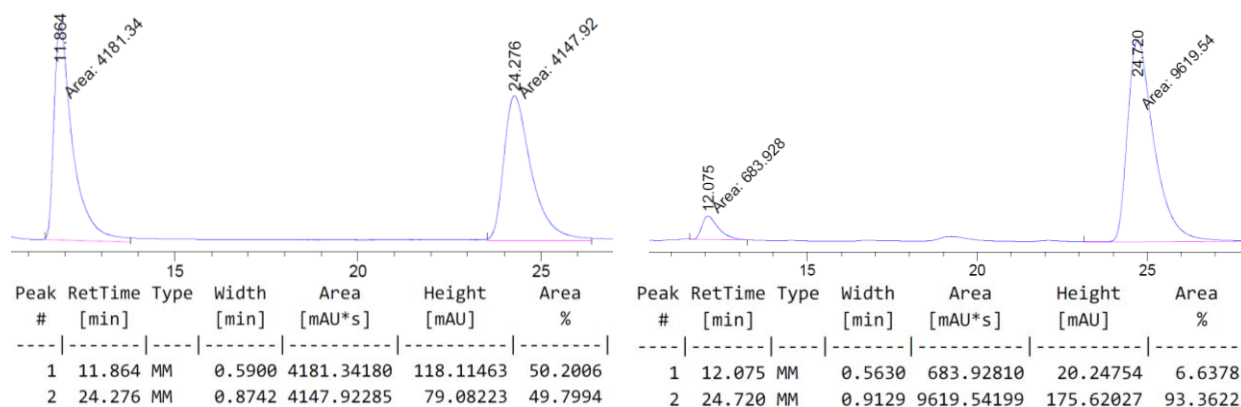
¹⁹F NMR (282 MHz, CDCl₃) δ –107.3 ppm.

IR (ATR): $\tilde{\nu}$ = 3001, 1656, 1610, 1594, 1501, 1447, 1303, 1241, 987, 763 cm⁻¹.

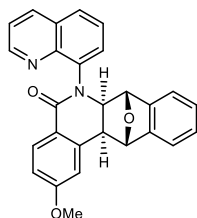
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₆H₁₈FN₂O₂: 409.1347; found: 409.1337.

[α]_D²⁰ = +43.50 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 24.7 min, tr(minor) = 12.1 min, 93.5:6.5 e.r.



(6aR,7S,12S,12aS)-2-Methoxy-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (17)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1 → 4:1) afforded the title compound **17** as a sticky solid (35 mg, 0.084 mmol, 42%), with an enantiomeric ratio of 94.5:5.5.

¹H NMR (400 MHz, CDCl₃) δ 9.08 – 8.72 (m, 1H), 8.51 – 8.22 (m, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 8.03 – 7.97 (m, 1H), 7.92 – 7.32 (m, 4H), 7.24 – 7.19 (m, 1H), 7.11 – 7.05 (m, 1H), 7.01 – 6.85 (m, 3H), 5.65 – 5.22 (m, 2H), 4.66 (s, 1H), 3.94 (s, 3H), 3.71 (s, 1H) ppm.

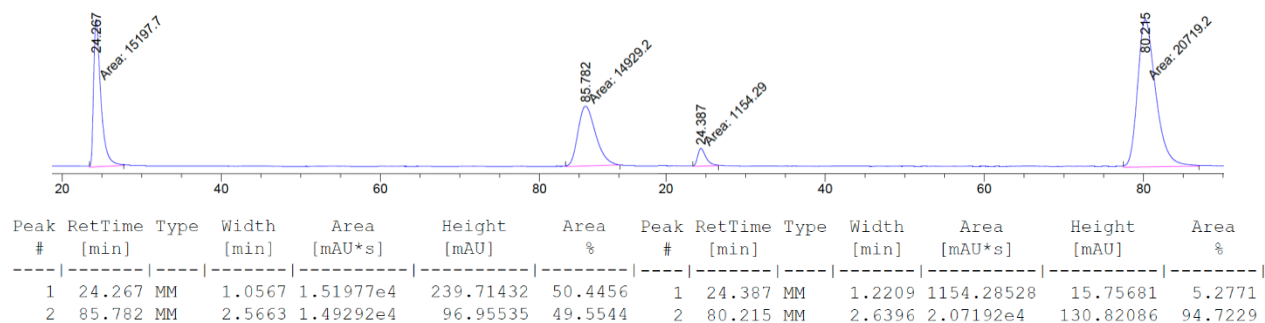
¹³C NMR (101 MHz, CDCl₃) δ 163.2 (C_q), 145.8 (C_q), 142.4 (C_q), 140.0 (C_q), 131.2 (CH), 130.2 (C_q), 128.9 (CH), 127.7 (CH), 127.3 (CH), 121.9 (CH), 120.7 (CH), 120.2 (C_q), 119.4 (CH), 113.0 (CH), 113.0 (CH), 88.9 (CH), 84.8 (CH), 63.9 (CH), 55.8 (CH₃), 43.6 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 2926, 1764, 1649, 1605, 1443, 1302, 1247, 1031, 987, 764 cm⁻¹.

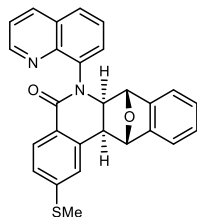
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₂₁N₂O₃: 421.1552; found: 421.1547.

[α]_D²⁰ = +40.47 (*c* = 0.47, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 80.2 min, tr(minor) = 24.4 min, 94.5:5.5 e.r.



(6aR,7S,12S,12aS)-2-(Methylthio)-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (18)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1 → 4:1) afforded the title compound **18** as a sticky solid (69 mg, 0.158 mmol, 79%), with an enantiomeric ratio of 96:4.

¹H NMR (400 MHz, CDCl₃) δ 9.00 – 8.59 (m, 1H), 8.24 (s, 1H), 8.17 (d, *J* = 8.2 Hz, 1H), 8.00 – 7.65 (m, 3H), 7.48 – 7.37 (m, 2H), 7.34 (s, 1H), 7.25 – 7.18 (m, 2H), 7.12 – 7.04 (m, 1H), 6.99 – 6.87 (m, 1H), 5.60 – 5.22 (m, 2H), 4.69 (s, 1H), 3.62 (d, *J* = 8.4 Hz, 1H), 2.59 (s, 3H) ppm.

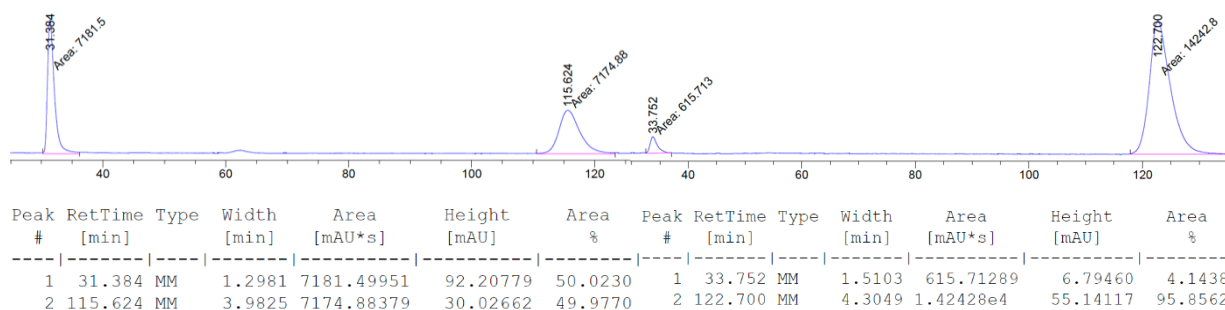
¹³C NMR (101 MHz, CDCl₃) δ 162.9 (C_q), 150.8 (CH), 145.7 (C_q), 144.5 (C_q), 144.1 (C_q), 142.5 (C_q), 138.2 (C_q), 136.7 (CH), 132.5 (CH), 130.1 (C_q), 129.5 (CH), 128.7 (CH), 127.7 (CH), 127.3 (CH), 126.6 (CH), 125.0 (CH), 124.2 (CH), 124.0 (C_q), 121.7 (CH), 120.5 (CH), 119.3 (CH), 88.7 (CH), 84.7 (CH), 63.7 (CH), 43.1 (CH), 15.3 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3004, 1644, 1594, 1472, 1432, 1295, 987, 829, 761, 663 cm⁻¹.

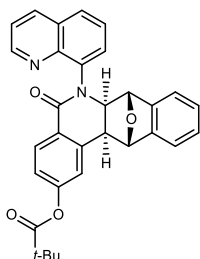
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₂₁N₂O₂S: 437.1324; found: 437.1318.

[α]_D²⁰ = +141.3 (*c* = 0.85, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 122.7 min, tr(minor) = 33.8 min, 96:4 e.r.



(6aR,7S,12S,12aS)-5-Oxo-6-(quinolin-8-yl)-5,6,6a,7,12,12a-hexahydro-7,12-epoxybenzo[*b*]phenanthridin-2-yl pivalate (19**)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 4:1) afforded the title compound **19** as a brown, sticky solid (70 mg, 0.158 mmol, 71%), with an enantiomeric ratio of 92:8.

¹H NMR (300 MHz, CDCl₃) δ 8.82 (s, 1H), 8.28 (d, *J* = 8.6 Hz, 1H), 8.24 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.98 – 7.87 (m, 2H), 7.76 – 7.67 (m, 1H), 7.47 – 7.34 (m, 2H), 7.27 (s, 1H), 7.23 – 7.18 (m, 1H), 7.10 – 7.05 (m, 2H), 6.95 (d, *J* = 7.3 Hz, 1H), 5.51 – 5.46 (m, 2H), 4.71 (s, 1H), 3.66 (d, *J* = 8.7 Hz, 1H), 1.43 (s, 9H) ppm.

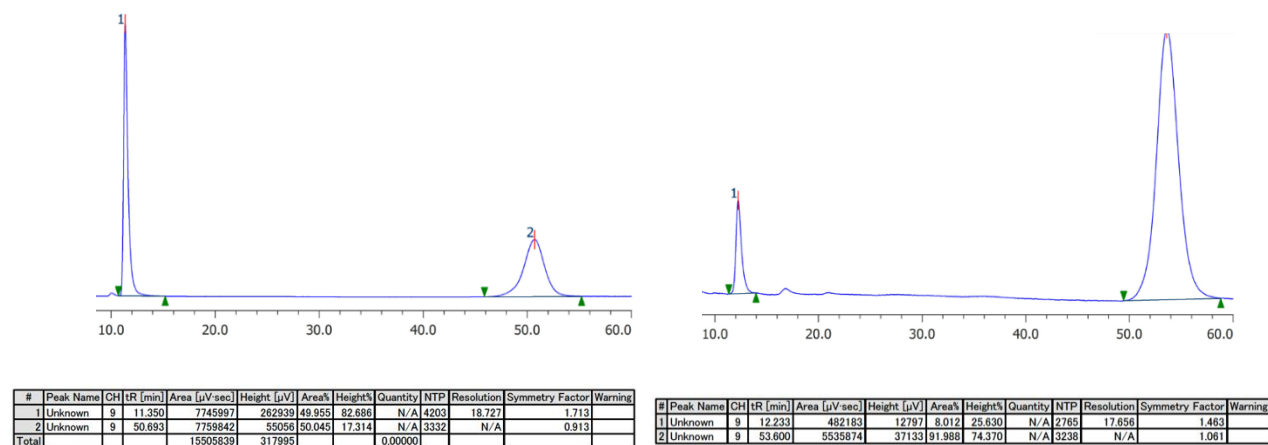
¹³C NMR (101 MHz, CDCl₃) δ 176.8 (C_q), 162.4 (C_q), 154.5 (C_q), 150.8 (CH), 145.6 (C_q), 142.5 (C_q), 139.4 (C_q), 136.6 (CH), 132.4 (CH), 130.9 (CH), 130.0 (C_q), 128.7 (CH), 127.7 (CH), 127.3 (CH), 126.6 (CH), 124.8 (C_q), 121.7 (CH), 120.8 (CH), 120.6 (CH), 120.5 (CH), 119.4 (CH), 88.6 (CH), 84.7 (CH), 63.8 (CH), 43.2 (CH), 39.4 (C_q), 27.3 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3002, 1746, 1650, 1606, 1444, 1300, 1150, 1110, 1092, 722 cm⁻¹.

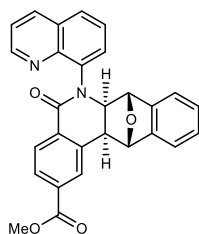
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₁H₂₇N₂O₄: 491.1971; found: 491.1972.

[α]_D²⁰ = + 103.7 (c = 0.72, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 53.6 min, tr(minor) = 12.2 min, 92:8 e.r.



Methyl (6a*R*,7*S*,12*S*,12*aS*)-5-oxo-6-(quinolin-8-yl)-5,6,6a,7,12,12a-hexahydro-7,12-epoxybenzo[*b*]phenanthridine-2-carboxylate (20**)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:3) afforded the title compound **20** as a sticky solid (45 mg, 0.10 mmol, 51%), with an enantiomeric ratio of 92:8.

¹H NMR (300 MHz, CDCl₃) δ 8.82 (bs, 1H), 8.33 (d, *J* = 8.2 Hz, 1H), 8.28 – 8.21 (m, 2H), 8.06 – 7.83 (m, 3H), 7.79 – 7.66 (m, 1H), 7.50 – 7.38 (m, 2H), 7.29 – 7.18 (m, 1H), 7.14 – 7.04 (m, 1H), 6.95 (d, *J* = 7.3 Hz, 1H), 5.54 – 5.45 (m, 2H), 4.72 (bs, 1H), 4.01 (s, 3H), 3.74 (d, *J* = 8.6 Hz, 1H) ppm.

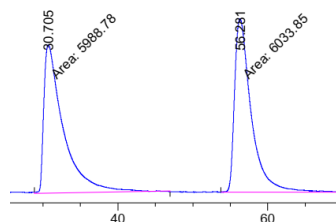
¹³C NMR (75 MHz, CDCl₃) δ 166.6 (C_q), 151.0 (CH), 145.5 (C_q), 142.4 (C_q), 138.0 (C_q), 136.7 (CH), 133.6 (C_q), 130.8 (C_q), 130.1 (C_q), 129.8 (CH), 129.3 (CH), 128.9 (CH), 128.0 (CH), 127.9 (CH), 127.4 (CH), 126.7 (CH), 121.8 (CH), 120.5 (CH), 119.5 (CH), 88.9 (CH), 84.6 (CH), 63.8 (CH), 52.7 (CH₃), 43.0 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3009, 1721, 1652, 1497, 1439, 1278, 1202, 1113. 985, 752 cm⁻¹.

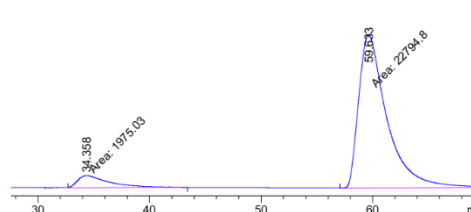
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₁N₂O₄: 449.1501; found: 449.1493.

[α]_D²⁰ = +64.2 (*c* = 0.5, CHCl₃).

R_t (IF column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 59.6 min, tr(minor) = 34.4 min, 92:8 e.r.

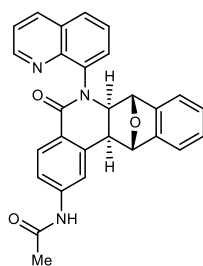


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.705	MM	3.0017	5988.78271	33.25217	49.8126
2	56.281	MM	2.5835	6033.85107	38.92550	50.1874



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	34.358	MM	3.2479	1975.02979	10.13496	7.9735
2	59.633	MM	2.9360	2.27948e4	129.39732	92.0265

***N*-((6*a**R*,7*S*,12*S*,12*a**S*)-5-Oxo-6-(quinolin-8-yl)-5,6,6*a*,7,12,12*a*-hexahydro-7,12-epoxybenzo[*b*]phenanthridin-2-yl)acetamide (**21**)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:9) afforded the title compound **21** as a sticky solid (42 mg, 0.094 mmol, 47%), with an enantiomeric ratio of 89.5:10.5.

¹H NMR (400 MHz, CDCl₃) δ 8.92 – 8.64 (m, 1H), 8.55 (s, 1H), 8.21 (d, *J* = 8.2 Hz, 1H), 8.12 – 7.81 (m, 4H), 7.78 – 7.60 (m, 1H), 7.45 – 7.28 (m, 2H), 7.22 – 7.13 (m, 1H), 7.11 – 7.01 (m, 1H), 6.97 – 6.86 (m, 2H), 5.57 – 5.35 (m, 2H), 4.62 (bs, 1H), 3.60 (d, *J* = 8.6 Hz, 1H), 1.92 (s, 3H) ppm.

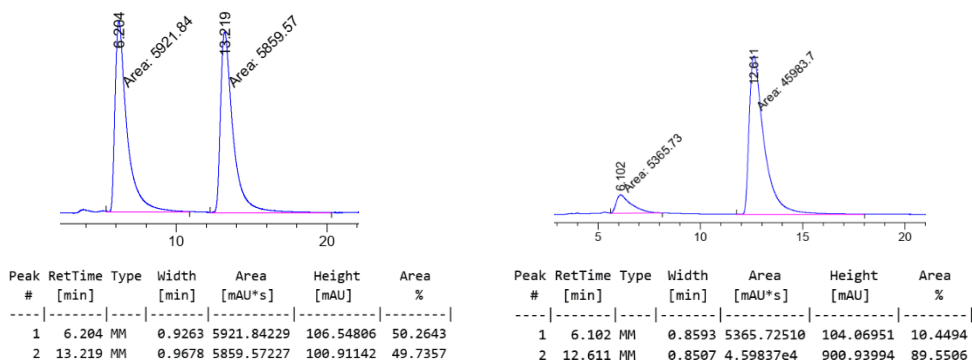
¹³C NMR (101 MHz, CDCl₃) δ 169.4 (C_q), 163.4 (C_q), 150.9 (CH), 145.6 (C_q), 143.9 (C_q), 142.5 (C_q), 139.1 (C_q), 138.3 (C_q), 136.7 (CH), 132.3 (C_q), 130.1 (C_q), 129.6 (CH), 128.9 (CH), 127.8 (CH), 127.2 (CH), 126.6 (CH), 122.3 (C_q), 121.9 (CH), 120.3 (CH), 119.6 (CH), 118.2 (CH), 118.1 (CH), 88.8 (CH), 84.8 (CH), 63.9 (CH), 43.3 (CH), 24.5 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2926, 2192, 1772, 1690, 1649, 1542, 1413, 1310, 1258, 760 cm⁻¹.

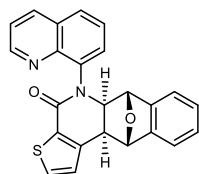
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₂N₃O₃: 448.1638; found: 448.1656.

[α]_D²⁰ = +85.8 (*c* = 0.5, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 12.6 min, tr(minor) = 6.1 min, 89.5:10.5 e.r.



(5aR,6S,11S,11aS)-5-(Quinolin-8-yl)-5a,6,11,11a-tetrahydro-6,11-epoxybenzo[*g*]thieno[2,3-*c*]quinolin-4(5*H*)-one (22)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate) afforded the title compound **22** as a sticky solid (53 mg, 0.133 mmol, 67%), with an enantiomeric ratio of 93:7.

¹H NMR (400 MHz, CDCl₃) δ 8.84 (s, 1H), 8.23 (d, *J* = 8.2 Hz, 1H), 7.97 – 7.88 (m, 2H), 7.77 – 7.66 (m, 1H), 7.59 (d, *J* = 5.0 Hz, 1H), 7.45 – 7.34 (m, 2H), 7.22 – 7.15 (m, 2H), 7.11 – 7.02 (m, 1H), 6.91 (d, *J* = 7.3 Hz, 1H), 5.49 (s, 1H), 5.44 (s, 1H), 4.80 (s, 1H), 3.69 (d, *J* = 8.6 Hz, 1H) ppm.

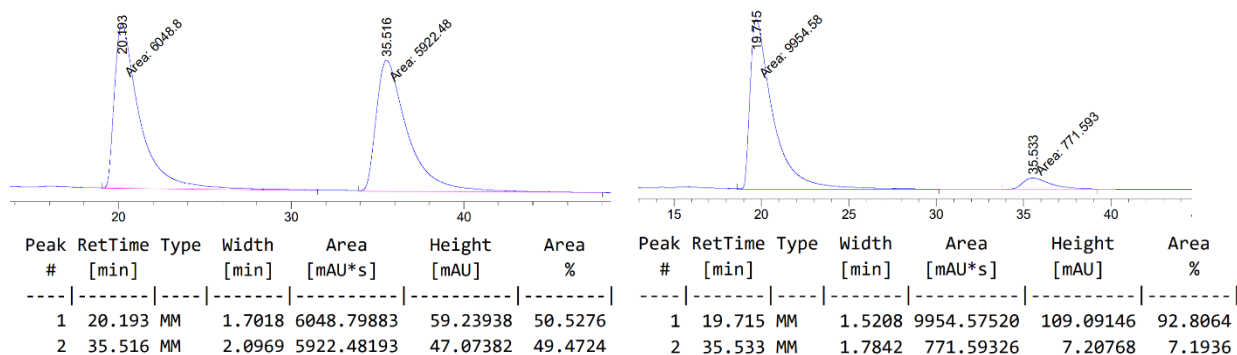
¹³C NMR (101 MHz, CDCl₃) δ 159.9 (C_q), 150.8 (CH), 145.4 (CH), 144.1 (C_q), 142.7 (C_q), 142.0 (C_q), 137.5 (C_q), 136.7 (CH), 132.6 (C_q), 132.2 (CH), 131.8 (C_q), 130.1 (C_q), 128.7 (CH), 127.7 (CH), 127.3 (CH), 126.7 (CH), 126.6 (CH), 121.7 (CH), 120.3 (CH), 119.5 (CH), 86.6 (CH), 84.8 (CH), 66.1 (CH), 42.1 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3007, 1640, 1594, 1443, 1319, 1304, 1159, 1123, 983, 756 cm⁻¹.

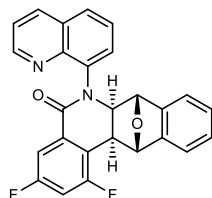
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₄H₁₇N₂O₂S: 397.1005; found: 397.1001.

[α]_D²⁰ = +28.00 (*c* = 1.0, CHCl₃).

R_t (IB column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 19.7 min, tr(minor) = 35.5 min, 93:7 e.r.



(6aR,7S,12S,12aS)-1,3-Difluoro-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[b]phenanthridin-5(6H)-one (23)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compound **23** as a sticky solid (68 mg, 0.16 mmol, 80%), with an enantiomeric ratio of 83:17.

¹H NMR (400 MHz, CDCl₃) δ 9.47 – 8.62 (m, 1H), 8.25 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.03 – 7.91 (m, 2H), 7.83 – 7.75 (m, 1H), 7.76 – 7.69 (m, 1H), 7.46 – 7.40 (m, 2H), 7.25 – 7.19 (m, 1H), 7.15 – 7.03 (m, 2H), 6.96 (d, *J* = 7.3 Hz, 1H), 5.62 – 5.38 (m, 2H), 4.85 – 4.62 (m, 1H), 3.69 (d, *J* = 8.7 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 161.9 (dd, *J*_{CF} = 248.4, 12.3 Hz, C_q), 161.1 (C_q), 160.2 (dd, *J*_{CF} = 248.8, 11.1 Hz, C_q), 151.0 (CH), 145.6 (C_q), 143.7 (C_q), 142.0 (C_q), 137.7 (C_q), 136.7 (CH), 132.3 (CH), 130.2 (dd, *J*_{CF} = 8.9, 4.7 Hz, C_q), 129.0 (CH), 127.9 (CH), 127.4 (CH), 126.6 (CH), 121.9 (CH), 121.4 (dd, *J*_{CF} = 15.6, 3.4 Hz, C_q), 120.5 (CH), 119.5 (CH), 111.5 (dd, *J*_{CF} = 23.3, 3.6 Hz, CH), 107.6 (dd, *J*_{CF} = 26.2, 24.8 Hz, CH), 86.8 (CH), 84.5 (CH), 63.6 (CH), 37.8 (CH) ppm.

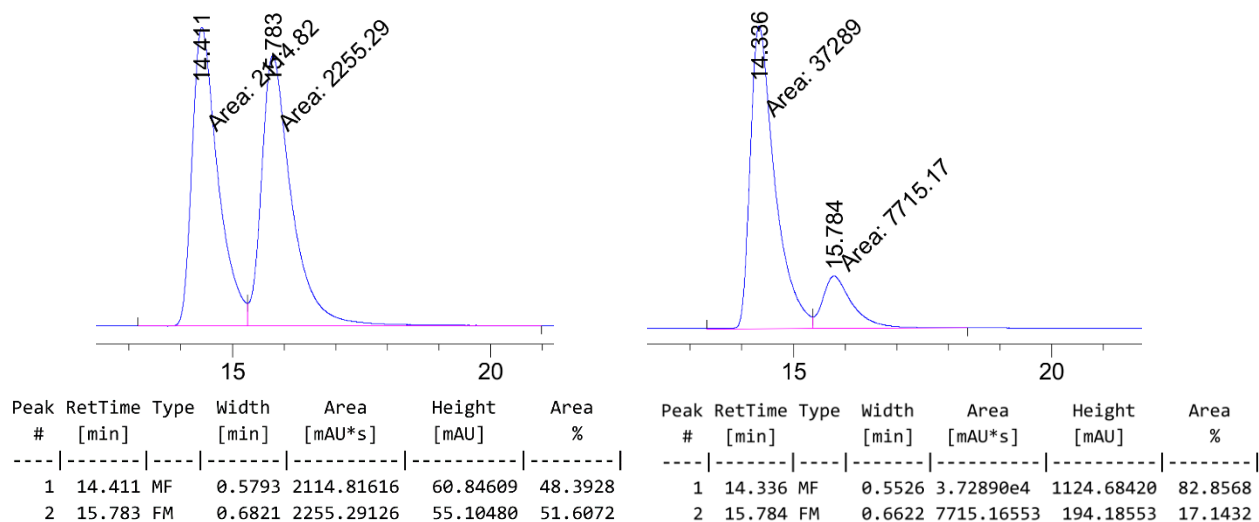
¹⁹F NMR (377 MHz, CDCl₃) δ -110.33, -114.17 ppm.

IR (ATR): $\tilde{\nu}$ = 3010, 1658, 1599, 1463, 1322, 1108, 998, 858, 756, 648 cm⁻¹.

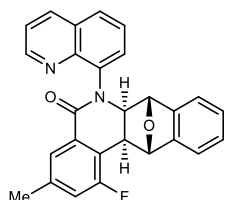
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₆H₁₇F₂N₂O₂: 427.1253; found: 427.1252.

[α]_D²⁰ = +45.3 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 60/40, 1.0 mL/min, 273.4 nm): tr(major) = 14.3 min, tr(minor) = 15.8 min, 83:17 e.r.



(6aR,7S,12S,12aS)-1-Fluoro-3-methyl-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (24)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compound **24** as a sticky solid (67 mg, 0.16 mmol, 79%), with an enantiomeric ratio of 82.5:17.5.

¹H NMR (400 MHz, CDCl₃) δ 8.98 – 8.66 (m, 1H), 8.24 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.01 – 7.80 (m, 3H), 7.81 – 7.67 (m, 1H), 7.51 – 7.35 (m, 2H), 7.24 – 7.19 (m, 1H), 7.17 (dd, *J* = 10.5, 1.4 Hz, 1H), 7.11 – 7.04 (m, 1H), 6.94 (d, *J* = 7.2 Hz, 1H), 5.68 – 5.22 (m, 2H), 4.71 (s, 1H), 3.69 (dd, *J* = 8.7, 2.1 Hz, 1H), 2.41 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 162.3 (C_q), 159.8 (d, *J*_{CF} = 245.3 Hz, C_q), 150.8 (CH), 145.8 (C_q), 143.7 (C_q), 142.1 (C_q), 138.8 (d, *J*_{CF} = 8.0 Hz, C_q), 138.1 (C_q), 136.5 (CH), 132.3 (CH), 130.0 (C_q), 128.6 (CH), 128.4 (d, *J*_{CF} = 3.9 Hz, C_q), 127.7 (CH), 127.1 (CH), 126.5 (CH), 125.0 (d, *J*_{CF} = 2.6 Hz, CH), 122.1 (d, *J*_{CF} = 15.7 Hz, C_q), 121.7 (CH), 120.3 (CH), 119.4 (CH), 119.4 (d, *J*_{CF} = 20.5 Hz, CH), 86.8 (d, *J*_{CF} = 2.8 Hz, CH), 84.4 (CH), 63.4 (CH), 37.8 (CH), 21.3 (d, *J*_{CF} = 1.8 Hz, CH₃). ppm.

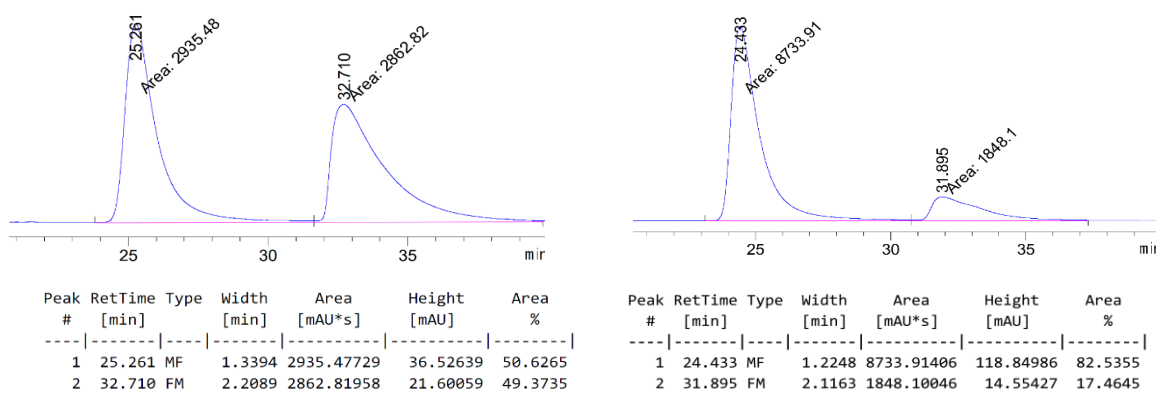
¹⁹F NMR (377 MHz, CDCl₃) δ -119.58 ppm.

IR (ATR): $\tilde{\nu}$ = 3009, 1658, 1584, 1496, 1464, 1316, 1272, 986, 861, 757 cm⁻¹.

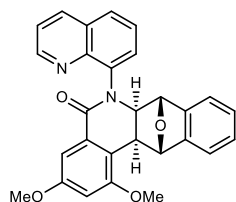
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₂₀F₁N₂O₂: 423.1503; found: 423.1501.

[α]_D²⁰ = +33.4 (*c* = 1.0, CHCl₃).

R_t (IF column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 24.4 min, tr(minor) = 31.9 min, 82.5:17.5 e.r.



(6aR,7S,12S,12aS)-1,3-Dimethoxy-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (25)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:3) afforded the title compound **25** as a sticky solid (58 mg, 0.13 mmol, 64%), with an enantiomeric ratio of 94:6.

¹H NMR (400 MHz, CDCl₃) δ 9.29 – 8.60 (m, 1H), 8.23 (dd, *J* = 8.2, 1.7 Hz, 1H), 8.09 – 7.77 (m, 2H), 7.77 – 7.66 (m, 1H), 7.46 – 7.34 (m, 3H), 7.20 (td, *J* = 7.4, 1.1 Hz, 1H), 7.06 (td, *J* = 7.5, 1.1 Hz, 1H), 6.94 (d, *J* = 7.3 Hz, 1H), 6.72 (d, *J* = 2.5 Hz, 1H), 5.45 (s, 1H), 5.41 (s, 1H), 4.67 (bs, 1H), 4.00 (s, 3H), 3.85 (s, 3H), 3.59 (d, *J* = 8.8 Hz, 1H) ppm.

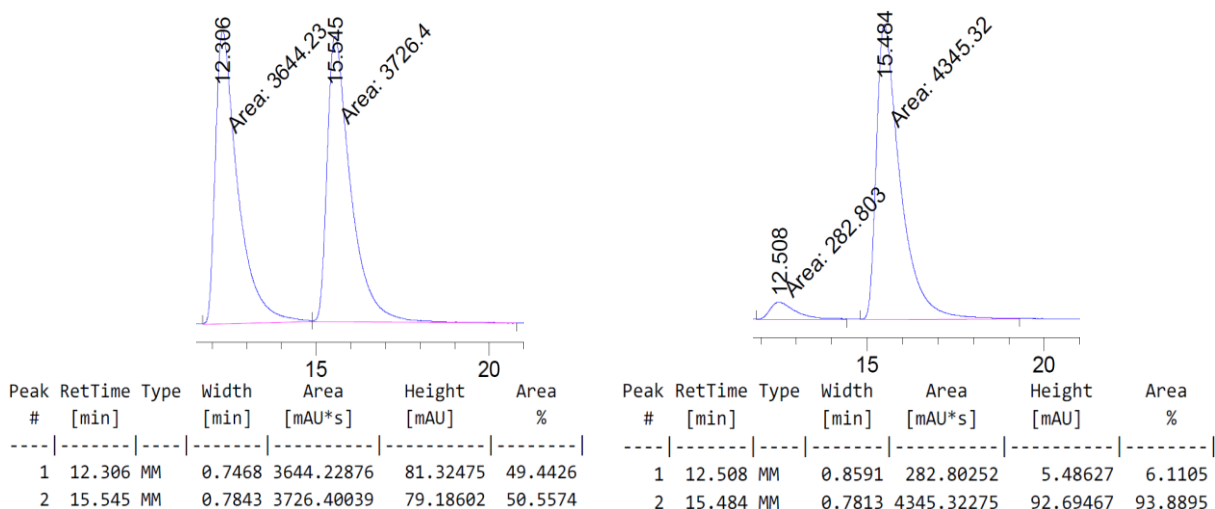
¹³C NMR (101 MHz, CDCl₃) δ 163.0 (C_q), 159.7 (C_q), 157.4 (C_q), 150.8 (CH), 146.7 (C_q), 143.9 (C_q), 142.3 (C_q), 138.3 (C_q), 136.5 (CH), 132.5 (CH), 130.0 (C_q), 128.6 (CH), 128.4 (C_q), 127.6 (CH), 126.9 (CH), 126.6 (CH), 121.7 (CH), 120.5 (CH), 119.5 (C_q), 119.2 (CH), 103.1 (CH), 102.7 (CH), 86.7 (CH), 84.4 (CH), 63.2 (CH), 56.1 (CH₃), 55.7 (CH₃), 38.7 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 1651, 1608, 1471, 1363, 1306, 1211, 1155, 1084, 743, 651 cm⁻¹.

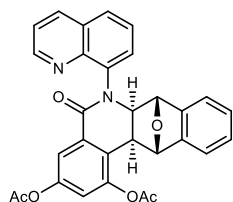
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₃N₂O₄: 451.1652; found: 451.1651.

[α]_D²⁰ = +30.30 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 15.5 min, tr(minor) = 12.5 min, 94:6 e.r.



(6aR,7S,12S,12aS)-5-Oxo-6-(quinolin-8-yl)-5,6,6a,7,12,12a-hexahydro-7,12-epoxybenzo[b]phenanthridine-1,3-diyl diacetate (26)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:3) afforded the title compound **26** as a sticky solid (33 mg, 0.07 mmol, 33%), with an enantiomeric ratio of 90:10.

¹H NMR (400 MHz, CDCl₃) δ 9.05 – 8.59 (m, 1H), 8.24 (dd, *J* = 8.4, 1.8 Hz, 1H), 8.03 – 7.79 (m, 3H), 7.77 – 7.69 (m, 1H), 7.42 (dd, *J* = 8.4, 4.1 Hz, 1H), 7.33 – 7.28 (m, 2H), 7.21 (td, *J* = 7.4, 1.0 Hz, 1H), 7.09 (td, *J* = 7.5, 1.1 Hz, 1H), 6.97 (dd, *J* = 7.4, 1.0 Hz, 1H), 5.52 – 5.41 (m, 2H), 4.74 (bs, 1H), 3.52 (d, *J* = 8.5 Hz, 1H), 2.47 (s, 3H), 2.31 (s, 3H) ppm.

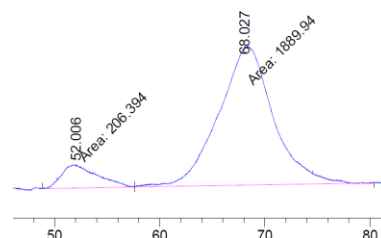
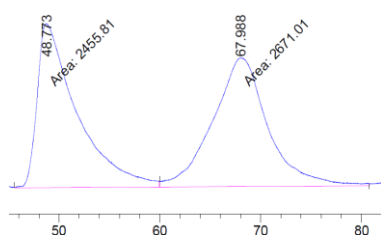
¹³C NMR (101 MHz, CDCl₃) δ 169.0 (C_q), 168.3 (C_q), 161.6 (C_q), 150.9 (CH), 149.8 (C_q), 148.3 (C_q), 146.3 (C_q), 142.1 (C_q), 136.6 (CH), 132.5 (CH), 130.1 (C_q), 129.4 (C_q), 128.9 (CH), 127.9 (CH), 127.4 (CH), 127.3 (C_q), 126.6 (CH), 121.8 (CH), 121.0 (CH), 120.2 (CH), 119.5 (CH), 118.5 (CH), 86.9 (CH), 84.4 (CH), 63.2 (CH), 39.3 (CH), 21.4 (CH₃), 21.2 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3021, 1769, 1657, 1457, 1312, 1202, 1186, 1027, 764, 646 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₀H₂₃N₂O₆: 507.1551; found: 507.1548.

[α]_D²⁰ = +27.40 (*c* = 0.5, CHCl₃).

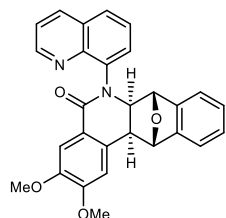
R_t (IF column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 68.0 min, tr(minor) = 52.0 min, 90:10 e.r.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	48.773	MF	4.5571	2455.80566	8.98153	47.9012
2	67.988	FM	6.3159	2671.01343	7.04834	52.0988

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	52.006	MF	3.9317	206.39441	8.74908e-1	9.8455
2	68.027	FM	5.9778	1889.93665	5.26934	90.1545

(6aR,7S,12S,12aS)-2,3-Dimethoxy-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (27)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate) afforded the title compound **27** as a sticky solid (65 mg, 0.144 mmol, 72%), with an enantiomeric ratio of 92:8.

¹H NMR (400 MHz, CDCl₃) δ 8.81 (s, 1H), 8.22 (d, *J* = 8.3 Hz, 1H), 7.95 – 7.89 (m, 2H), 7.75 (s, 1H), 7.74 – 7.66 (m, 1H), 7.47 – 7.36 (m, 2H), 7.23 – 7.16 (m, 1H), 7.12 – 7.03 (m, 1H), 6.94 (d, *J* = 7.2 Hz, 1H), 6.88 (s, 1H), 5.49 (s, 1H), 5.44 (s, 1H), 4.69 (s, 1H), 4.03 (s, 3H), 3.91 (s, 3H), 3.60 (d, *J* = 8.6 Hz, 1H) ppm.

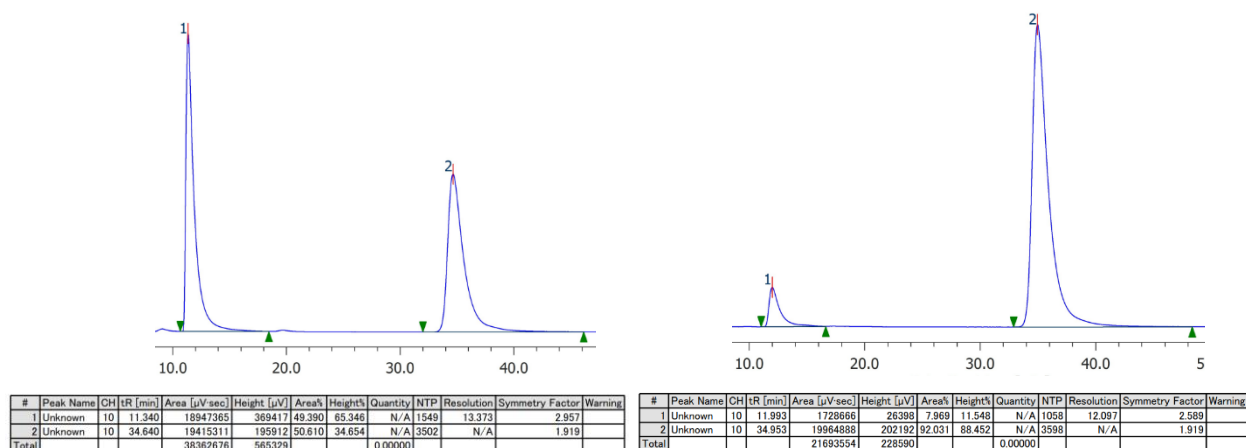
¹³C NMR (101 MHz, CDCl₃) δ 163.0 (C_q), 152.9 (C_q), 150.8 (CH), 148.4 (C_q), 145.7 (C_q), 144.1 (C_q), 142.6 (C_q), 138.4 (C_q), 136.6 (CH), 132.5 (CH), 131.1 (C_q), 130.0 (C_q), 128.5 (CH), 127.6 (CH), 127.2 (CH), 126.5 (CH), 121.6 (CH), 120.4 (CH), 120.3 (C_q), 119.3 (CH), 110.7 (CH), 109.7 (CH), 88.4 (CH), 84.8 (CH), 63.7 (CH), 56.4 (CH₃), 56.1 (CH₃), 43.0 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3003, 1644, 1602, 1516, 1455, 1434, 1297, 1271, 1220, 761 cm⁻¹.

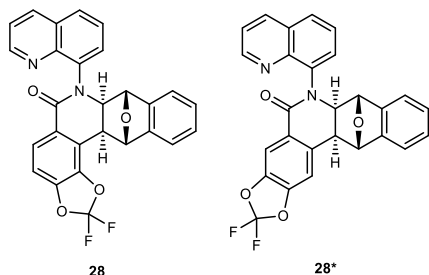
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₃N₂O₄: 451.1652; found: 451.1647.

[α]_D²⁰ = +50.0 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 275.0 nm): tr(major) = 35.0 min, tr(minor) = 12.0 min, 92:8 e.r.



(7aR,8S,13S,13aS)-2,2-Difluoro-7-(quinolin-8-yl)-7a,8,13,13a-tetrahydro-8,13-epoxybenzo[b][1,3]dioxolo[4,5-k]phenanthridin-6(7H)-one (**28**) and (6aR,7S,12S,12aS)-2,2-difluoro-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[b][1,3]dioxolo[4,5-j]phenanthridin-5(6H)-one (**28***)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compounds **28** (72 mg, 0.15 mmol, 76%), with an enantiomeric ratio of 88:12, and **28*** (8 mg, 0.017 mmol, 9%), with an enantiomeric ratio of 78.5:21.5, as sticky solids.

Characterization Data for **28**:

¹H NMR (400 MHz, CDCl₃) δ 9.20 – 8.61 (m, 1H), 8.25 (d, *J* = 7.4 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 8.00 – 7.92 (m, 2H), 7.83 – 7.66 (m, 1H), 7.51 – 7.38 (m, 2H), 7.26 – 7.20 (m, 1H), 7.15 – 7.06 (m, 2H), 6.96 (d, *J* = 7.3 Hz, 1H), 5.63 – 5.47 (m, 2H), 4.77 – 4.56 (m, 1H), 3.72 (d, *J* = 8.5 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 161.8 (C_q), 150.9 (CH), 146.4 (C_q), 145.1 (C_q), 143.7 (C_q), 142.1 (C_q), 140.5 (C_q), 137.9 (C_q), 136.7 (CH), 132.3 (CH), 132.2 (t, *J*_{CF} = 257.6 Hz, C_q), 130.1 (C_q), 128.9 (CH), 128.0 (CH), 127.5 (CH), 126.6 (CH), 125.9 (CH), 123.3 (C_q), 121.8 (CH), 120.9 (C_q), 120.4 (CH), 119.8 (CH), 108.6 (CH), 85.8 (CH), 84.8 (CH), 63.8 (CH), 38.0 (CH) ppm.

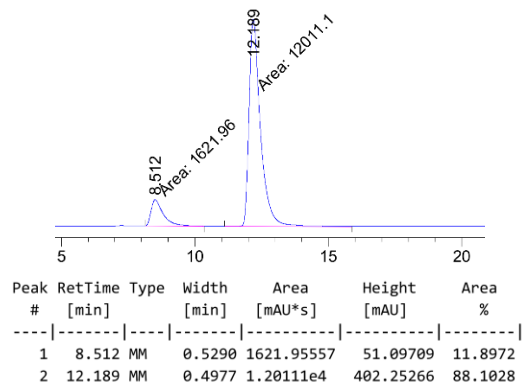
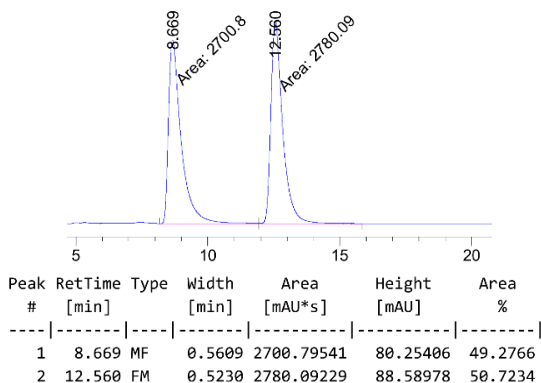
¹⁹F NMR (377 MHz, CDCl₃) δ -48.82 ppm.

IR (ATR): $\tilde{\nu}$ = 3009, 1667, 1636, 1469, 1429, 1240, 1159, 1100, 755, 647 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₁₇F₂N₂O₄: 471.1151; found: 471.1152.

[α]_D²⁰ = +56.6 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 12.2 min, tr(minor) = 8.5 min, 88:12 e.r.



Characterization Data for **28***:

¹H NMR (400 MHz, CDCl₃) δ 8.92 – 8.73 (m, 1H), 8.25 (d, *J* = 7.4 Hz, 1H), 7.99 – 7.91 (m, 3H), 7.79 – 7.68 (m, 1H), 7.49 – 7.35 (m, 2H), 7.25 – 7.17 (m, 2H), 7.12 – 7.05 (m, 1H), 6.96 (d, *J* = 7.3 Hz, 1H), 5.50 (s, 1H), 5.40 (s, 1H), 4.68 (s, 1H), 3.67 (d, *J* = 8.6 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 161.7 (C_q), 151.0 (CH), 147.0 (C_q), 145.4 (C_q), 143.4 (C_q), 142.3 (C_q), 137.9 (C_q), 136.7 (CH), 134.9 (C_q), 132.4 (CH), 131.8 (t, *J*_{CF} = 256.9 Hz, C_q), 130.1 (C_q), 128.9 (CH), 127.9 (CH), 127.5 (CH), 126.6 (CH), 123.9 (C_q), 121.9 (CH), 120.6 (CH), 119.4 (CH), 111.4 (C_q), 110.0 (CH), 108.5 (CH), 88.8 (CH), 84.8 (CH), 63.5 (CH), 43.6 (CH) ppm.

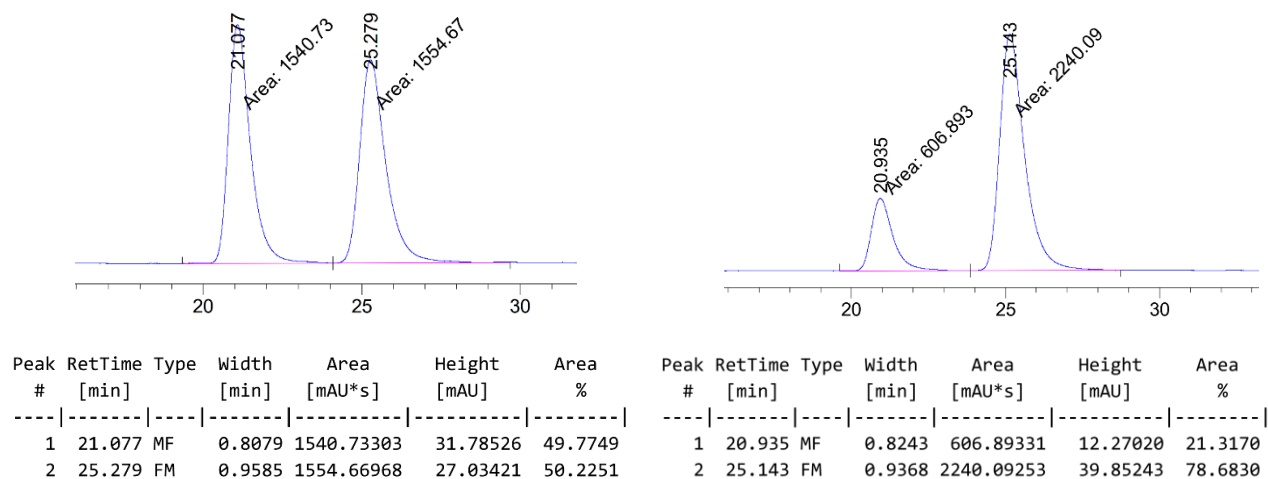
¹⁹F NMR (377 MHz, CDCl₃) δ -50.32 ppm.

IR (ATR): $\tilde{\nu}$ = 3008, 1657, 1627, 1467, 1308, 1246, 1157, 914, 759, 661 cm⁻¹.

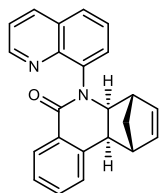
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₁₇F₂N₂O₄: 471.1151; found: 471.1152.

[α]_D²⁰ = +34.3 (c = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 25.1 min, tr(minor) = 20.9 min, 78.5:21.5 e.r.



(1*R*,4*S*,4*aS*,10*bS*)-5-(Quinolin-8-yl)-1,4*a*,5,10*b*-tetrahydro-1,4-methanophenanthridin-6(4*H*)-one (29)



Prepared according to general procedure on a 0.2 mmol scale using 4 mmol of the alkene, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compound **29** as a sticky solid (23 mg, 0.068 mmol, 34%), with an enantiomeric ratio of 83.5:16.5.

¹H NMR (400 MHz, CDCl₃) δ 9.18 – 8.77 (m, 1H), 8.32 – 8.17 (m, 2H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.77 – 7.59 (m, 2H), 7.57 – 7.47 (m, 1H), 7.46 – 7.37 (m, 2H), 7.36 – 7.30 (m, 1H), 6.40 (dd, *J* = 5.7, 2.9 Hz, 1H), 5.87 (dd, *J* = 5.8, 3.1 Hz, 1H), 4.52 – 3.94 (m, 1H), 3.50 – 3.29 (m, 1H), 3.14 – 2.60 (m, 2H), 2.34 – 1.77 (m, 1H), 1.57 – 1.40 (m, 1H) ppm.

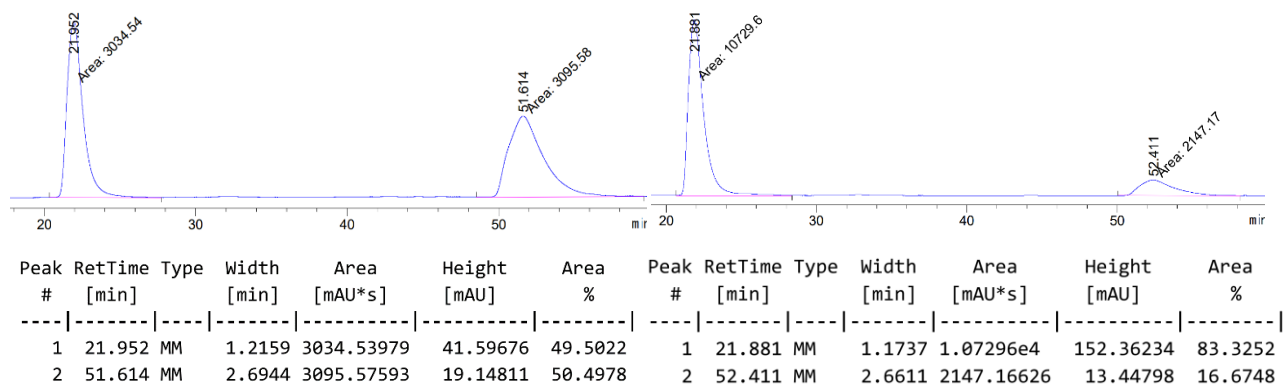
¹³C NMR (101 MHz, CDCl₃) δ 163.9 (C_q), 150.7 (CH), 144.1 (C_q), 140.1 (C_q), 139.6 (CH), 138.8 (C_q), 136.6 (CH), 135.3 (CH), 132.3 (CH), 132.1 (CH), 130.1 (C_q), 128.8 (CH), 128.3 (CH), 128.3 (CH), 126.8 (C_q), 126.5 (CH), 126.3 (CH), 121.5 (CH), 61.7 (CH), 53.5 (CH), 49.2 (CH), 43.2 (CH₂), 40.1 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 2979, 2930, 1647, 1603, 1465, 1425, 1298, 794, 753, 696 cm⁻¹.

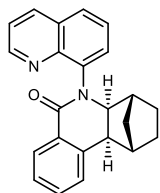
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₃H₁₉N₂O₁: 339.1492; found: 339.1488.

[α]_D²⁰ = +10.8 (*c* = 0.5, CHCl₃).

R_t (IE column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 21.9 min, tr(minor) = 52.4 min, 83.5:16.5 e.r.



(1*S*,4*R*,4*aS*,10*bS*)-5-(Quinolin-8-yl)-1,3,4,4*a*,5,10*b*-hexahydro-1,4-methanophenanthridin-6(2*H*)-one (30)



Prepared according to general procedure on a 0.2 mmol scale using 4 mmol of the alkene, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compound **30** as a sticky solid (25 mg, 0.073 mmol, 37%), with an enantiomeric ratio of 89:11.

¹H NMR (400 MHz, CDCl₃) δ 9.09 – 8.72 (m, 1H), 8.31 – 8.09 (m, 2H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.74 – 7.59 (m, 2H), 7.53 – 7.46 (m, 1H), 7.40 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.34 – 7.27 (m, 2H), 4.64 – 4.06 (m, 1H), 3.57 – 3.29 (m, 1H), 2.49 (s, 1H), 2.42 – 2.23 (m, 1H), 2.08 – 1.86 (m, 1H), 1.73 – 0.93 (m, 5H) ppm.

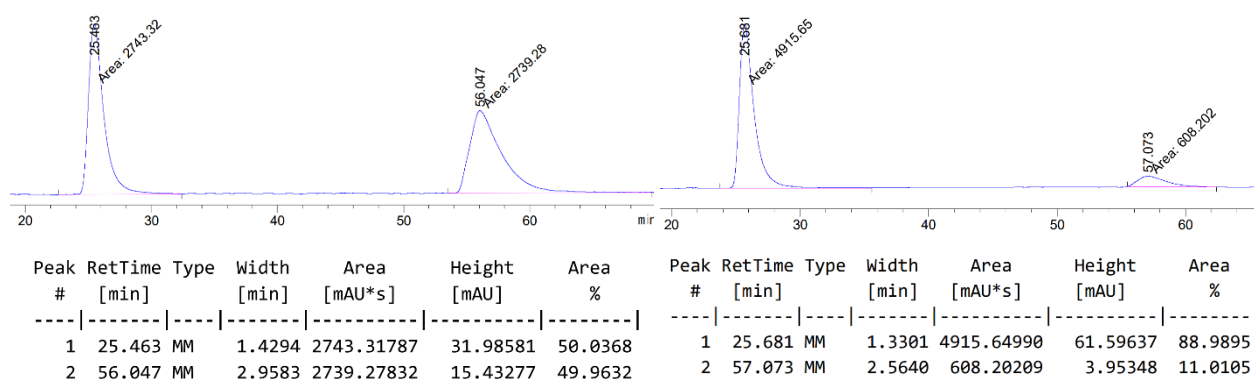
¹³C NMR (101 MHz, CDCl₃) δ 163.5 (C_q), 150.6 (CH), 144.1 (C_q), 140.3 (C_q), 138.7 (C_q), 136.6 (CH), 132.2 (CH), 132.2 (CH), 130.1 (C_q), 128.4 (CH), 128.4 (CH), 128.1 (CH), 126.6 (C_q), 126.4 (CH), 126.2 (CH), 121.5 (CH), 65.6 (CH), 48.6 (CH), 45.1 (CH), 43.1 (CH), 32.9 (CH₂), 30.1 (CH₂), 26.1 (CH₂) ppm.

IR (ATR): $\tilde{\nu}$ = 2956, 2872, 1647, 1466, 1425, 1320, 1287, 795, 752, 694 cm⁻¹.

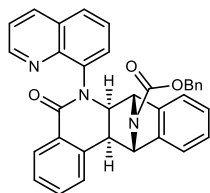
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₃H₂₁N₂O₁: 341.1648; found: 341.1647.

[α]_D²⁰ = +42.2 (*c* = 0.5, CHCl₃).

R_t (IE column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 25.7 min, tr(minor) = 57.1 min, 89:11 e.r.



Benzyl (6a*R*,7*S*,12*S*,12a*R*)-5-oxo-6-(quinolin-8-yl)-5,6,6a,7,12,12a-hexahydro-7,12-epiminobenzo[*b*]phenanthridine-13-carboxylate (31)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compound **31** as a sticky solid (52 mg, 0.10 mmol, 50%), with an enantiomeric ratio of 96:4.

¹H NMR (500 MHz, CDCl₃, 60 °C) δ 8.77 – 8.74 (m, 1H), 8.25 (dd, *J* = 7.8, 1.4 Hz, 1H), 8.21 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.91 (d, *J* = 7.4 Hz, 1H), 7.71 – 7.64 (m, 1H), 7.61 – 7.56 (m, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.42 – 7.34 (m, 3H), 7.33 – 7.01 (m, 8H), 6.93 (d, *J* = 7.3 Hz, 1H), 5.43 (s, 1H), 5.37 (s, 1H), 5.05 – 4.93 (m, 1H), 4.87 – 4.80 (m, 1H), 4.71 (d, *J* = 8.3 Hz, 1H), 3.67 (d, *J* = 8.6 Hz, 1H) ppm.

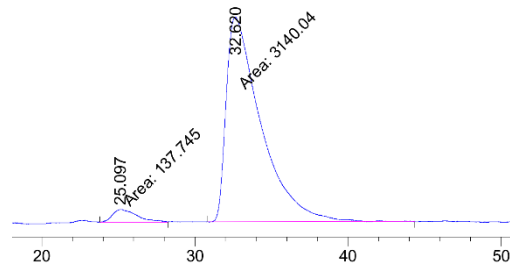
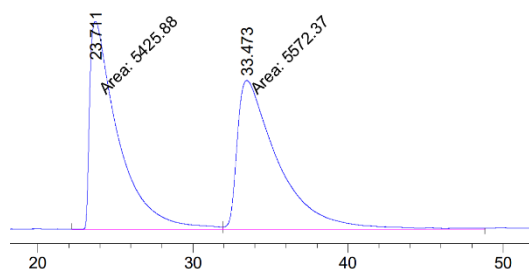
¹³C NMR (126 MHz, CDCl₃, 60 °C) δ 162.9 (C_q), 155.0 (C_q), 150.6 (CH), 145.8 (C_q), 144.3 (C_q), 142.1 (C_q), 138.4 (C_q), 137.2 (C_q), 136.6 (CH), 136.4 (C_q), 132.9 (CH), 132.6 (CH), 130.2 (C_q), 129.1 (CH), 128.6 (CH), 128.5 (CH), 128.5 (CH), 128.1 (CH), 127.9 (CH), 127.7 (CH), 127.5 (CH), 127.2 (CH), 127.2 (C_q), 126.8 (CH), 121.5 (CH), 121.3 (CH), 119.9 (CH), 71.0 (CH), 67.4 (CH₂), 66.9 (CH), 63.9 (CH), 44.0 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3011, 1705, 1652, 1464, 1419, 1292, 1217, 1090, 751, 694 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₄H₂₆N₃O₃: 524.1969; found: 524.1979.

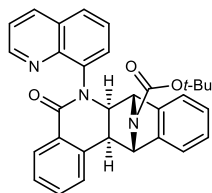
[α]_D²⁰ = +92.4 (*c* = 1.0, CHCl₃).

R_t (IF column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 32.6 min, tr(minor) = 25.1 min, 96:4 e.r.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.711	MF	2.1260	5425.87988	42.53541	49.3340	1	25.097	MM	1.8717	137.74529	1.22659	4.2024
2	33.473	FM	3.0525	5572.36572	30.42483	50.6660	2	32.620	MM	2.6293	3140.03516	19.90442	95.7976

tert-Butyl (6a*R*,7*S*,12*S*,12a*R*)-5-oxo-6-(quinolin-8-yl)-5,6,6a,7,12,12a-hexahydro-7,12-epiminobenzo[*b*]phenanthridine-13-carboxylate (32)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compound **32** as a sticky solid (44 mg, 0.090 mmol, 45%), with an enantiomeric ratio of 96:4.

¹H NMR (500 MHz, CDCl₃, 60 °C) δ 8.80 – 8.70 (m, 1H), 8.32 – 8.15 (m, 3H), 7.93 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.80 – 7.71 (m, 1H), 7.65 – 7.58 (m, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.46 – 7.34 (m, 3H), 7.24 – 7.15 (m, 1H), 7.09 – 7.01 (m, 1H), 6.92 (d, *J* = 7.3 Hz, 1H), 5.39 (s, 1H), 5.28 (s, 1H), 4.69 (s, 1H), 3.65 (d, *J* = 8.5 Hz, 1H), 1.22 (s, 9H) ppm.

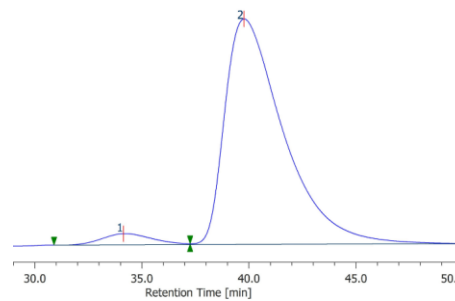
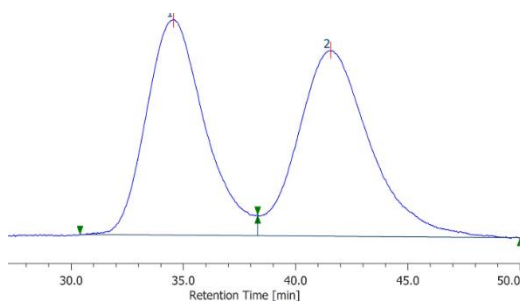
¹³C NMR (126 MHz, CDCl₃, 60 °C) δ 162.8 (C_q), 154.0 (C_q), 150.6 (CH), 146.0 (C_q), 144.3 (C_q), 142.3 (C_q), 138.5 (C_q), 137.5 (C_q), 136.6 (CH), 133.1 (CH), 132.5 (CH), 130.2 (C_q), 129.1 (CH), 128.5 (CH), 128.4 (CH), 127.5 (CH), 127.3 (C_q), 127.3 (CH), 127.0 (CH), 126.8 (CH), 121.5 (CH), 121.1 (CH), 119.7 (CH), 80.5 (C_q), 70.8 (CH), 66.1 (CH), 64.1 (CH), 44.1 (CH), 28.2 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2978, 2930, 1694, 1652, 1466, 1389, 1295, 1158, 1093, 754 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₁H₂₈N₃O₃: 490.2125; found: 490.2123.

[α]_D²⁰ = +74.2 (*c* = 1.0, CHCl₃).

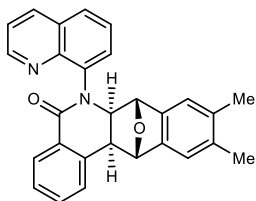
R_t (OD column, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min, 210.0 nm): tr(major) = 39.8 min, tr(minor) = 34.1 min, 96:4 e.r.



#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	11	34.563	4422219	24525	48.535	53.730	N/A	885	1.370		N/A
2	Unknown	11	41.557	4689122	21120	51.465	46.270	N/A	884	N/A		N/A

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	11	34.140	3325936	20624	4.044	4.732	N/A	1000	1.237		N/A
2	Unknown	11	39.767	78910868	415219	95.956	95.268	N/A	1096	N/A		1.943

(6aR,7S,12S,12aS)-9,10-Dimethyl-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[b]phenanthridin-5(6H)-one (33)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 2:1) afforded the title compound **33** as a sticky solid (63 mg, 0.151 mmol, 76%), with an enantiomeric ratio of 94.5:5.5.

¹H NMR (400 MHz, CDCl₃) δ 9.12 – 8.64 (m, 1H), 8.35 – 8.19 (m, 2H), 8.08 – 7.84 (m, 2H), 7.77 – 7.67 (m, 1H), 7.63 – 7.56 (m, 1H), 7.50 (d, *J* = 7.9 Hz, 1H), 7.47 – 7.34 (m, 2H), 7.20 (s, 1H), 6.74 (s, 1H), 5.57 – 5.31 (m, 2H), 4.70 (bs, 1H), 3.66 (d, *J* = 8.6 Hz, 1H), 2.25 (s, 3H), 2.13 (s, 3H) ppm.

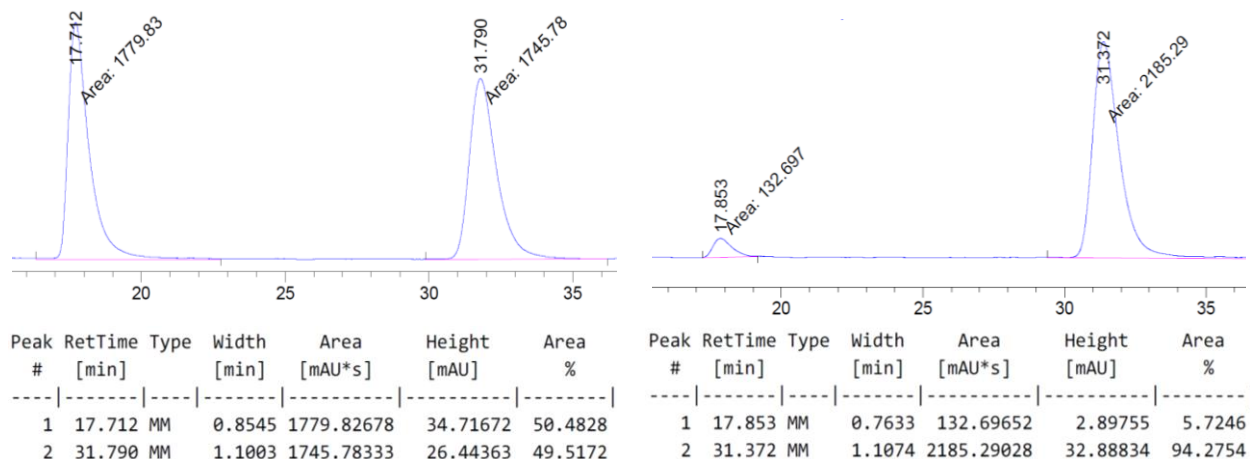
¹³C NMR (101 MHz, CDCl₃) δ 163.1 (C_q), 150.7 (CH), 144.0 (C_q), 143.7 (C_q), 140.3 (C_q), 138.3 (C_q), 138.0 (C_q), 136.6 (CH), 135.8 (C_q), 135.4 (C_q), 132.5 (CH), 130.0 (C_q), 128.9 (CH), 128.5 (CH), 128.1 (CH), 127.2 (C_q), 127.1 (CH), 126.6 (CH), 121.7 (CH), 120.6 (CH), 88.9 (CH), 84.5 (CH), 63.8 (CH), 43.5 (CH), 20.1 (CH₃), 19.9 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3006, 1649, 1603, 1461, 1422, 1297, 983, 860, 793, 750 cm⁻¹.

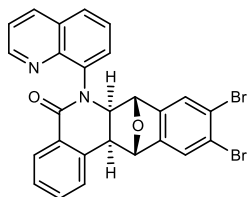
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₈H₂₃N₂O₂: 419.1754; found: 419.1749.

[α]_D²⁰ = +62.10 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 31.4 min, tr(minor) = 17.9 min, 94.5:5.5 e.r.



(6a*R*,7*S*,12*S*,12a*S*)-9,10-Dibromo-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[*b*]phenanthridin-5(6*H*)-one (34)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 3:1) afforded the title compound **34** as a sticky solid (57 mg, 0.104 mmol, 52%), with an enantiomeric ratio of 95:5.

¹H NMR (400 MHz, CDCl₃) δ 9.02 – 8.65 (m, 1H), 8.28 – 8.21 (m, 2H), 8.01 – 7.83 (m, 2H), 7.74 – 7.66 (m, 2H), 7.76 – 7.65 (m, 1H), 7.49 – 7.38 (m, 3H), 7.21 (s, 1H), 5.46 (s, 1H), 5.39 (s, 1H), 4.73 (bs, 1H), 3.68 (d, *J* = 8.6 Hz, 1H) ppm.

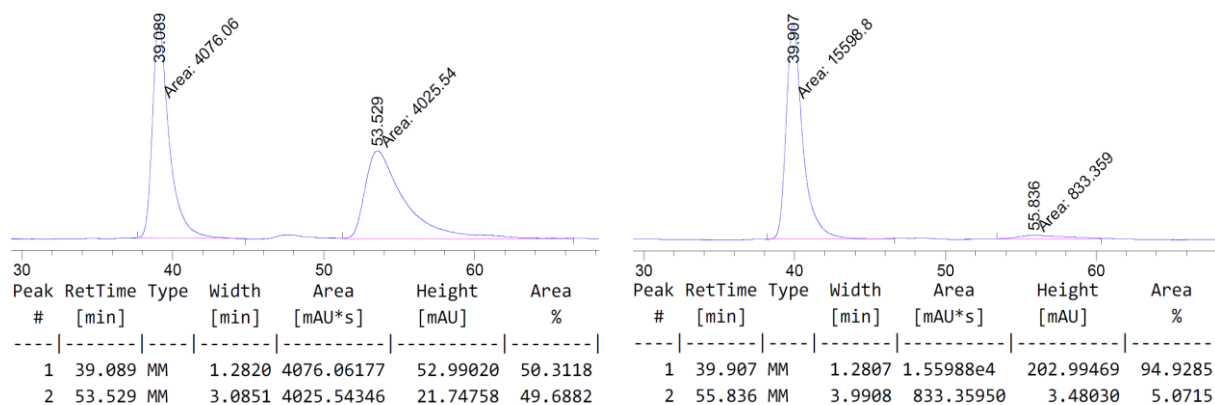
¹³C NMR (101 MHz, CDCl₃) δ 162.8 (C_q), 151.0 (CH), 146.7 (C_q), 143.6 (C_q), 136.9 (C_q), 136.7 (CH), 132.8 (CH), 130.1 (C_q), 129.0 (C_q), 128.9 (CH), 128.0 (CH), 127.5 (CH), 127.1 (C_q), 126.6 (CH), 125.8 (CH), 124.8 (CH), 123.8 (C_q), 123.3 (C_q), 121.8 (CH), 88.2 (CH), 84.1 (CH), 63.2 (CH), 42.8 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3008, 1649, 1601, 1461, 1422, 1295, 1216, 988, 859, 742 cm⁻¹.

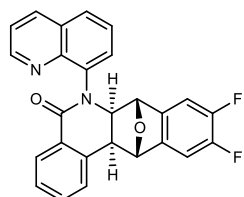
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₆H₁₇Br₂N₂O₂: 546.9651; found: 546.9642.

[α]_D²⁰ = +59.2 (*c* = 0.5, CHCl₃).

R_t (IF column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 39.9 min, tr(minor) = 55.8 min, 95:5 e.r.



(6aR,7S,12S,12aS)-9,10-Difluoro-6-(quinolin-8-yl)-6a,7,12,12a-tetrahydro-7,12-epoxybenzo[b]phenanthridin-5(6H)-one (35)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 3:1) afforded the title compound **35** as a sticky solid (44 mg, 0.10 mmol, 52%), with an enantiomeric ratio of 96.5:3.5.

¹H NMR (600 MHz, CDCl₃) δ 8.82 (s, 1H), 8.28 – 8.20 (m, 2H), 8.02 – 7.85 (m, 2H), 7.75 – 7.67 (m, 1H), 7.63 – 7.57 (m, 1H), 7.48 (d, *J* = 7.7 Hz, 1H), 7.45 – 7.36 (m, 2H), 7.24 (dd, *J* = 8.6, 6.8 Hz, 1H), 6.83 – 6.75 (m, 1H), 5.47 (s, 1H), 5.41 (s, 1H), 4.73 (s, 1H), 3.66 (d, *J* = 8.5 Hz, 1H) ppm.

¹³C NMR (151 MHz, CDCl₃) δ 162.9 (C_q), 150.9 (CH), 149.7 (dd, *J*_{CF} = 248.7, 47.9 Hz, C_q), 149.7 (dd, *J*_{CF} = 248.8, 47.9 Hz, C_q), 143.9 (CH), 141.7 (dd, *J*_{CF} = 6.1, 3.0 Hz, C_q), 138.5 (bs, C_q), 138.0 (C_q), 137.1 (C_q), 136.7 (CH), 132.7 (CH), 132.5 (C_q), 130.1 (C_q), 129.1 (CH), 128.8 (CH), 128.0 (CH), 127.5 (CH), 127.1 (C_q), 126.6 (CH), 121.8 (CH), 110.6 (d, *J*_{CF} = 19.9 Hz, CH), 109.5 (d, *J*_{CF} = 19.7 Hz, CH), 88.5 (CH), 84.4 (CH), 63.3 (CH), 43.0 (CH) ppm.

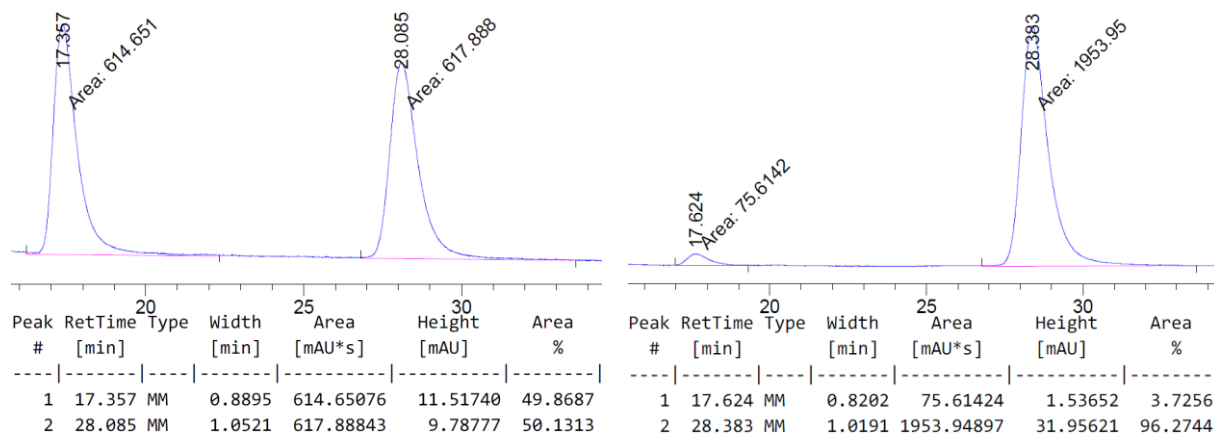
¹⁹F NMR (282 MHz, CDCl₃) δ -137.86 (d, *J*_{FF} = 18.7 Hz), -138.49 (d, *J*_{FF} = 18.7 Hz) ppm.

IR (ATR): $\tilde{\nu}$ = 3007, 1650, 1480, 1426, 1359, 1318, 1066, 862, 755, 607 cm⁻¹.

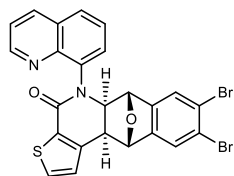
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₆H₁₇F₂N₂O₂: 427.1253; found: 427.1221.

[α]_D²⁰ = +33.4 (c = 2.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 273.4 nm): tr(major) = 28.4 min, tr(minor) = 17.6 min, 96.5:3.5 e.r.



(5aR,6S,11S,11aS)-8,9-Dibromo-5-(quinolin-8-yl)-5a,6,11,11a-tetrahydro-6,11-epoxybenzo[*g*]thieno[2,3-*c*]quinolin-4(5H)-one (36)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate) afforded the title compound **36** as a sticky solid (55 mg, 0.10 mmol, 50%), with an enantiomeric ratio of 95:5.

¹H NMR (400 MHz, CDCl₃) δ 8.87 (s, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.87 (s, 1H), 7.74 – 7.64 (m, 2H), 7.61 (d, *J* = 4.8 Hz, 1H), 7.44 (dd, *J* = 7.9, 3.9 Hz, 1H), 7.20 – 7.10 (m, 2H), 5.45 (s, 1H), 5.39 (s, 1H), 4.99 – 4.65 (m, 1H), 3.70 (d, *J* = 8.6 Hz, 1H) ppm.

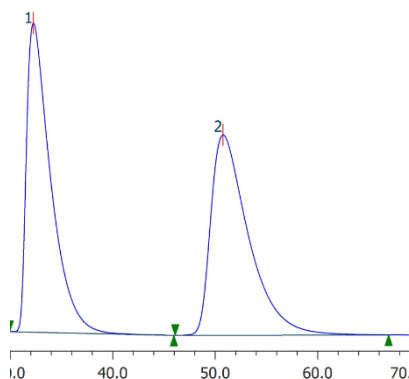
¹³C NMR (101 MHz, CDCl₃) δ 159.7 (C_q), 151.0 (CH), 146.3 (C_q), 144.3 (C_q), 143.7 (C_q), 141.2 (C_q), 136.7 (CH), 132.6 (CH), 131.9 (C_q), 130.1 (C_q), 129.0 (CH), 126.6 (CH), 126.5 (CH), 125.7 (CH), 125.0 (CH), 123.8 (C_q), 123.4 (C_q), 121.9 (CH), 86.0 (CH), 84.3 (CH), 65.9 (CH), 41.9 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3009, 1640, 1441, 1317, 1302, 1211, 983, 860, 799, 749 cm⁻¹.

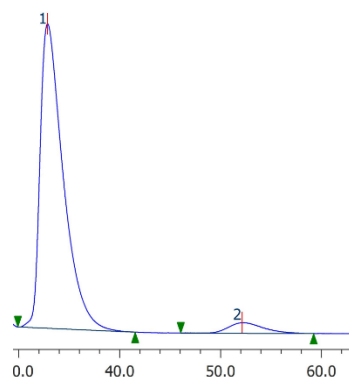
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₄H₁₅Br₂N₂O₂S: 552.9216; found: 552.9213.

[α]_D²⁰ = +28.8 (*c* = 1.0, CHCl₃).

R_t (OD column, *n*-hexane/*i*-PrOH 60/40, 1.0 mL/min, 273.0 nm): tr(major) = 32.8 min, tr(minor) = 52.1 min, 95:5 e.r.

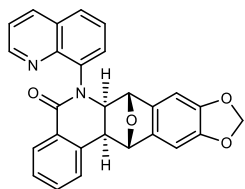


#	Peak Name	CH	TR [min]	Area [μV.sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	10	32.247	21852686	133366	49.607	60.644	N/A	971	3.503		2.350
2	Unknown	10	50.750	22199020	86549	50.393	39.356	N/A	989	N/A		1.943
Total				44051706	219915			0.00000				



#	Peak Name	CH	TR [min]	Area [μV.sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	10	32.833	11516953	72483	95.073	96.657	N/A	1067	3.783		1.923
2	Unknown	10	52.113	596901	2507	4.927	3.343	N/A	1130	N/A		1.392
Total				12113854	74990			0.00000				

(6aR,7S,13S,13aS)-6-(Quinolin-8-yl)-6a,7,13,13a-tetrahydro-7,13-epoxy[1,3]dioxolo[4',5':4,5]benzo[1,2-b]phenanthridin-5(6H)-one (37)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 3:1) afforded the title compound **37** as a sticky solid (59 mg, 0.135 mmol, 68%), with an enantiomeric ratio of 94.5:5.5.

¹H NMR (400 MHz, CDCl₃) δ 9.06 – 8.60 (m, 1H), 8.34 – 8.17 (m, 2H), 8.05 – 7.81 (m, 2H), 7.75 – 7.66 (m, 1H), 7.64 – 7.55 (m, 1H), 7.52 – 7.34 (m, 3H), 6.90 (s, 1H), 6.43 (s, 1H), 6.04 – 5.77 (m, 2H), 5.53 – 5.21 (m, 2H), 4.66 (bs, 1H), 3.62 (d, *J* = 8.6 Hz, 1H) ppm.

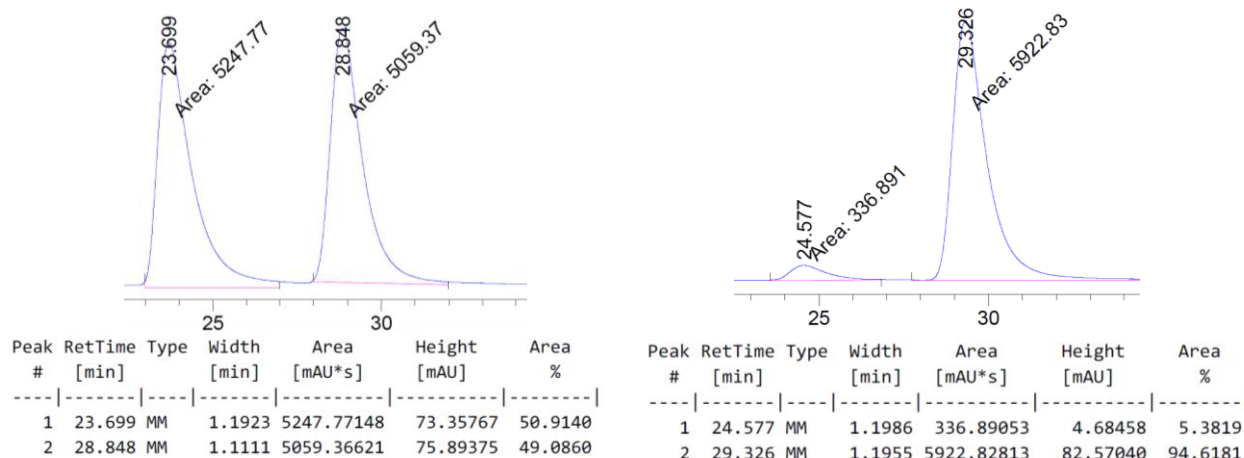
¹³C NMR (101 MHz, CDCl₃) δ 163.0 (C_q), 150.8 (CH), 147.2 (C_q), 146.8 (C_q), 144.0 (C_q), 139.5 (C_q), 137.7 (C_q), 136.6 (CH), 136.1 (C_q), 132.5 (CH), 130.0 (C_q), 129.0 (CH), 128.6 (CH), 128.1 (CH), 127.2 (CH), 127.1 (C_q), 126.6 (CH), 121.7 (CH), 102.5 (CH), 101.5 (CH), 101.4 (CH₂), 88.9 (CH), 84.6 (CH), 63.6 (CH), 43.3 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3007, 1650, 1462, 1430, 1315, 1291, 1037, 853, 793, 760 cm⁻¹.

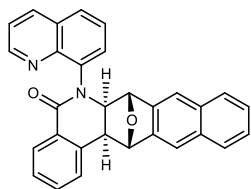
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₁₉N₂O₄: 435.1339; found: 435.1330.

[α]_D²⁰ = +31.5 (c = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 29.3 min, tr(minor) = 24.6 min, 94.5:5.5 e.r.



(6aR,7S,14S,14aS)-6-(Quinolin-8-yl)-6a,7,14,14a-tetrahydro-7,14-epoxynaphtho[2,3-b]phenanthridin-5(6H)-one (38)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 3:1) afforded the title compound **38** as a sticky solid (57 mg, 0.13 mmol, 65%), with an enantiomeric ratio of 91:9.

¹H NMR (400 MHz, CDCl₃) δ 8.81 (s, 1H), 8.32 – 8.24 (m, 2H), 8.13 – 7.93 (m, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.81 – 7.71 (m, 2H), 7.67 – 7.60 (m, 2H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.45 – 7.39 (m, 3H), 7.36 (s, 1H), 5.62 (s, 1H), 5.57 (s, 1H), 4.85 (s, 1H), 3.81 (d, *J* = 8.6 Hz, 1H) ppm.

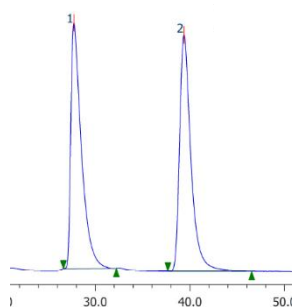
¹³C NMR (101 MHz, CDCl₃) δ 163.1 (C_q), 150.8 (CH), 143.3 (C_q), 140.1 (C_q), 137.6 (C_q), 136.9 (CH), 133.2 (C_q), 133.0 (CH), 132.9 (C_q), 132.7 (CH), 130.2 (C_q), 129.0 (CH), 128.8 (CH), 128.4 (CH), 128.2 (CH), 128.2 (CH), 127.3 (CH), 127.2 (C_q), 126.7 (CH), 126.4 (CH), 126.3 (CH), 121.8 (CH), 119.2 (CH), 117.7 (CH), 88.9 (CH), 84.6 (CH), 64.3 (CH), 44.3 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 1648, 1462, 1275, 1216, 984, 858, 746, 655, 598, 480 cm⁻¹.

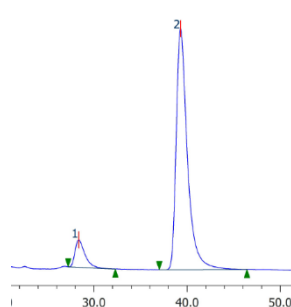
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₃₀H₂₁N₂O₂: 441.1598; found: 441.1597.

[α]_D²⁰ = +86.2 (*c* = 0.5, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 275 nm): tr(major) = 39.3 min, tr(minor) = 28.4 min, 91:9 e.r.



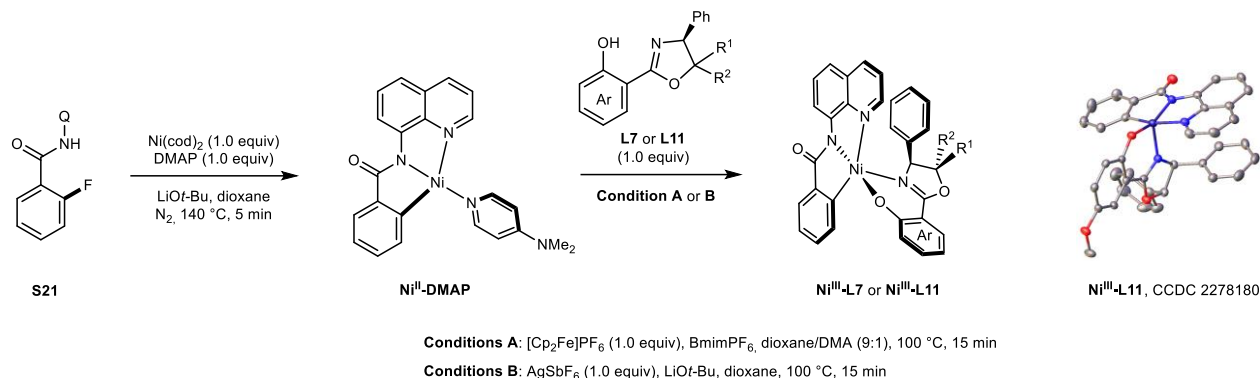
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor
1	Unknown	10	27.733	10113770	130701	49.158	51.007	N/A	3334	5.877	2.260
2	Unknown	10	39.363	10460315	125542	50.842	48.993	N/A	5916	N/A	1.586



#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor
1	Unknown	10	28.380	523737	7182	9.099	10.261	N/A	3798	5.656	1.608
2	Unknown	10	39.280	5232324	62815	90.901	89.739	N/A	5986	N/A	1.602

Synthesis of the Cyclometalated Nickel Complexes

Synthesis using a chemical oxidant



General procedure:

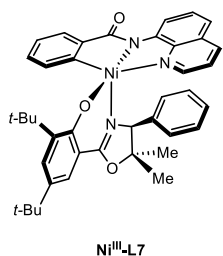
Step 1:

A pressure tube containing 2-fluoro-N-(quinolin-8-yl)benzamide **S21** (506 mg, 1.90 mmol, 1.0 equiv), Ni(cod)_2 (523 mg, 1.90 mmol, 1.0 equiv), LiOt-Bu (304 mg, 3.80 mmol, 2.0 equiv), 4-dimethylaminopyridine (DMAP) (232 mg, 1.90 mmol, 1.0 equiv), and dry 1,4-dioxane (8 mL) was prepared in the glove box. The reaction mixture was heated at 140 °C for 5 minutes, generating an orange suspension. Then, after the reaction mixture has cooled down to room temperature, ether (5 mL) was added. The suspension was next filtered, yielding an orange solid. For further purification, the solid was filtered through a plug of silica gel with acetone as eluent. Then, the solvent was removed under reduced pressure, yielding the desired complex **Ni^{II}-DMAP** as an orange powder. **Ni^{II}-DMAP** was used directly after preparation for the analytical measurements and the subsequent reaction.

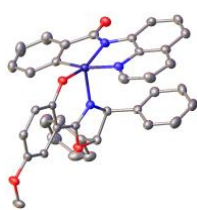
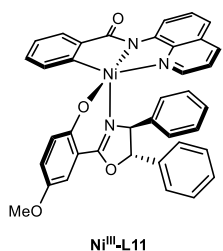
Step 2:

Condition A: A pressure tube was charged with complex **Ni^{II}-DMAP** (1.0 equiv), ligand (1.0 equiv), BmimPF₆ (0.05 M), $[\text{Cp}_2\text{Fe}]\text{PF}_6$ (1.0 equiv), and 1,4-dioxane/DMA (9:1, v/v, 0.023 M). Then, the reaction mixture was stirred for 15 minutes at 100 °C. Next, the solvent was removed under reduced pressure and the residue was purified by column chromatography, affording the desired complex.

Condition B: A pressure tube was charged with complex **Ni^{II}-DMAP** (1.0 equiv), ligand (1.0 equiv), LiOt-Bu (1.0 equiv), AgSbF₆ (1.0 equiv), and 1,4-dioxane (0.1 M). Then, the reaction mixture was stirred for 15 minutes at 100 °C. Next, the solvent was removed under reduced pressure and the residue was purified by column chromatography, affording the desired complex.

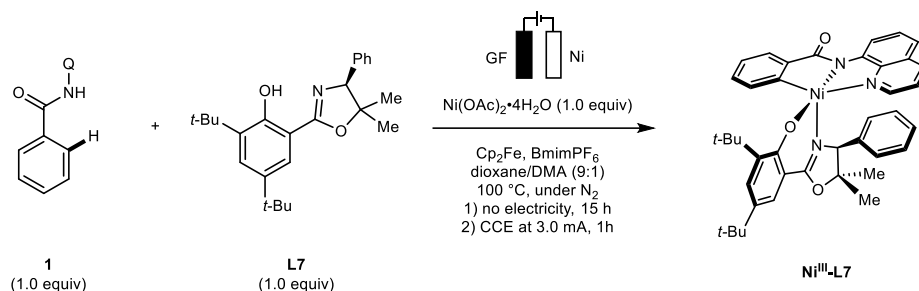


Complex Ni^{III}-L7: Prepared according to general procedure with **Condition A** on a 0.12 mmol scale, column chromatography (*n*-hexane/acetone = 3:1) afforded the title compound **Ni^{III}-L7** as a dark red solid (45 mg, 0.066 mmol, 56%). Furthermore, Cp₂Fe (0.070 mmol, 58%) could be reisolated from the reaction mixture.



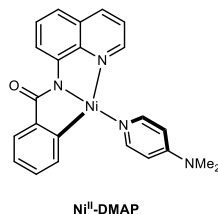
Complex Ni^{III}-L11: Prepared according to general procedure with **Condition B** on a 0.47 mmol scale, column chromatography (*n*-hexane/acetone = 3:1) afforded the title compound **Ni^{III}-L11** as a dark red solid (63 mg, 0.098 mmol, 21%).

Electrochemical Synthesis

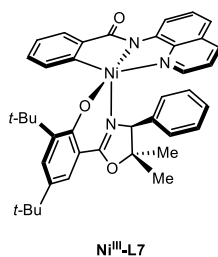


The electrolysis was carried out in an undivided cell setup under an atmosphere of N₂. A GF anode (20 mm × 10 mm × 4 mm) and a nickel foam cathode (10 mm × 15 mm × 1.4 mm) with electrode holders made of stainless steel were used. The cell was charged with the amide **1** (25 mg, 0.10 mmol, 1.0 equiv), ligand **L7** (38 mg, 0.10 mmol, 1.0 equiv), Ni(OAc)₂·4H₂O (25 mg, 0.10 mmol, 1.0 equiv), BmimPF₆ (85 mg, 3.0 equiv), Cp₂Fe (56 mg, 3.0 equiv), and a teflon-coated magnetic stirring bar (15 × 6 mm). Then, dioxane/DMA (9:1, v/v, 5 mL) was added, and mixture was stirred at 100 °C for 15 h without electricity with a stirring rate of 600 rpm. Then, the electrolysis was performed with a constant current of 3.0 mA maintained for 1 h. After completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by column chromatography (*n*-hexane/acetone = 3:1), yielding the title compound **Ni^{III}-L7** as a dark red solid (6 mg, 9 μmol, 8% yield).

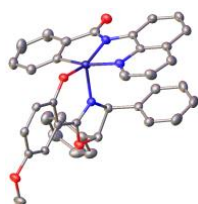
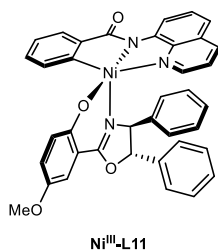
Characterization data for nickel complexes



Complex **Ni^{II}-DMAP**: **¹H NMR** (300 MHz, CD₂Cl₂) δ 8.81 (d, J = 7.7 Hz, 1H), 8.71 (d, J = 7.3 Hz, 2H), 8.14 (dd, J = 8.2 Hz, J = 1.7 Hz, 1H), 7.53 – 7.40 (m, 1H), 7.28 (d, J = 6.8 Hz, 1H), 7.22 – 7.11 (m, 3H), 7.02 – 6.93 (m, 1H), 6.88 – 6.80 (m, 1H), 6.63 (d, J = 7.1 Hz, 2H), 5.95 (d, J = 7.3 Hz, 1H), 3.10 (s, 6H) ppm. **¹³C NMR** (101 MHz, CD₂Cl₂) δ 151.2 (CH), 145.9 (CH), 138.1 (CH), 134.3 (CH), 130.0 (CH), 129.4 (CH), 125.3 (CH), 124.7 (CH), 121.6 (CH), 118.6 (CH), 116.6 (CH), 108.6 (CH), 39.7 (CH₃) ppm. **IR** (ATR): $\tilde{\nu}$ = 1620, 1497, 1463, 1439, 1394, 1385, 1346, 784, 762, 733 cm⁻¹. **HRMS** (ESI): m/z [M+H]⁺ calcd for C₂₃H₂₁N₄ONi: 427.1063; found: 427.1086.



Complex **Ni^{III}-L7**: **Elemental Analysis**: Anal. Calcd for C₄₁H₄₂N₃NiO₃: C, 72.05; H, 6.19; N, 6.15. Found: C, 71.96; H, 6.31; N, 5.99. **IR** (ATR): $\tilde{\nu}$ = 3057, 2958, 1644, 1618, 1500, 1464, 1429, 1382, 1332, 1249 cm⁻¹. **HRMS** (ESI): m/z [M+H]⁺ calcd for C₄₁H₄₃N₃NiO₃: 683.2652; found: 683.2623.

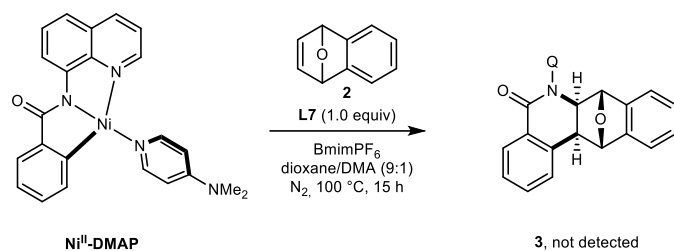


Ni^{III}-L11, CCDC 2278180

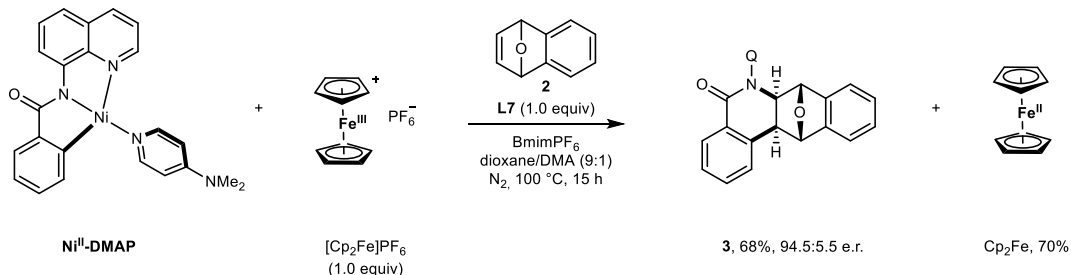
Complex **Ni^{III}-L11**: Crystallization by vapor diffusion (THF/*n*-pentane) yielded crystals suitable for X-ray diffraction analysis. **IR** (ATR): $\tilde{\nu}$ = 2931, 1738, 1650, 1629, 1599, 1499, 1461, 1382, 1330, 1210 cm⁻¹. **HRMS** (ESI): m/z [M+H]⁺ calcd for C₃₈H₂₉N₃O₄Ni: 649.1506; found: 649.1483.

Reactions with Cyclometalated Nickel Complexes

Stoichiometric Reactions Using Nickel(II) Complex

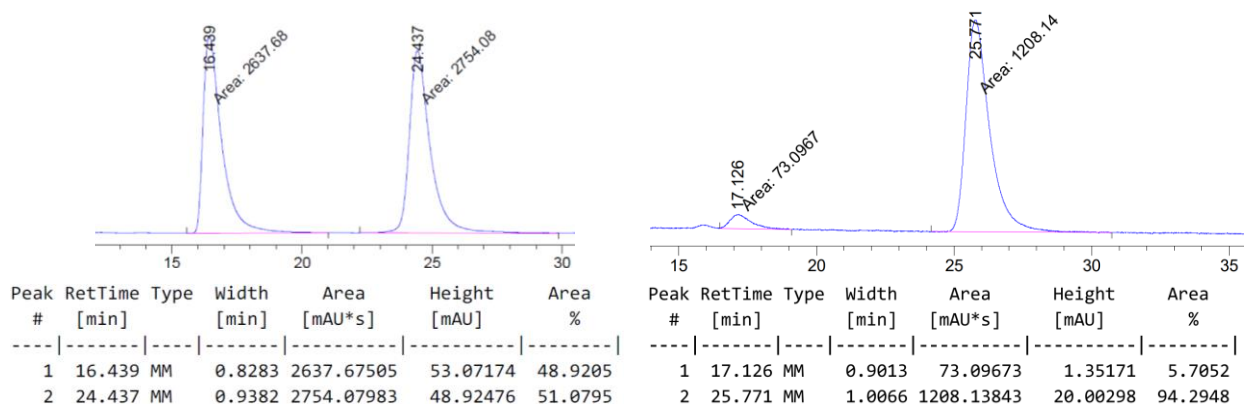


Ni^{II}-DMAP (17 mg, 0.04 mmol, 1.0 equiv), alkene **2** (43 mg, 0.30 mmol), ligand **L7** (15 mg, 0.04 mmol, 1.0 equiv), and **BmimPF₆** (15 mg, 0.052 mmol, 1.3 equiv) were dissolved in a mixture of degassed 1,4-dioxane and DMA (9:1, v/v, 5 mL). The reaction mixture was heated for 15 h at 100 °C under an atmosphere of N₂. After filtration through a pad of silica, the solvent was removed under reduced pressure and the yield was examined with ¹H NMR spectroscopy, utilizing 1,3,5-trimethoxybenzene as the internal standard. Here, no product formation was detected.

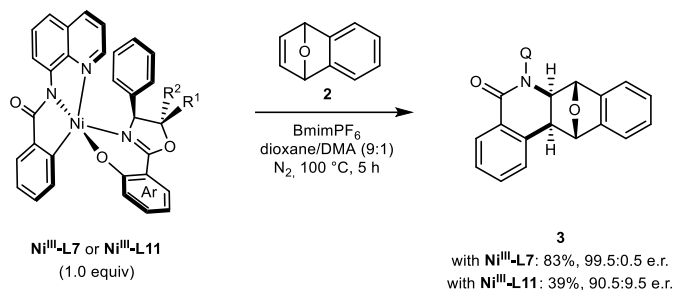


Ni^{II}-DMAP (17 mg, 0.04 mmol, 1.0 equiv), alkene **2** (43 mg, 0.30 mmol), ligand **L7** (15 mg, 0.04 mmol, 1.0 equiv), **[Cp₂Fe]PF₆** (13 mg, 0.04 mmol, 1.0 equiv), and **BmimPF₆** (15 mg, 0.052 mmol, 1.3 equiv) were dissolved in a mixture of degassed 1,4-dioxane and DMA (9:1, v/v, 5 mL). The reaction mixture was heated for 15 h at 100 °C under an atmosphere of N₂. After filtration through a pad of silica, the solvent was removed under reduced pressure and the yield was examined with ¹H NMR spectroscopy, utilizing 1,3,5-trimethoxybenzene as the internal standard. Product **3** was obtained in 68% yield with an enantiomeric ratio of 94.5:5.5.

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 25.8 min, tr(minor) = 17.1 min, 94.5:5.5.



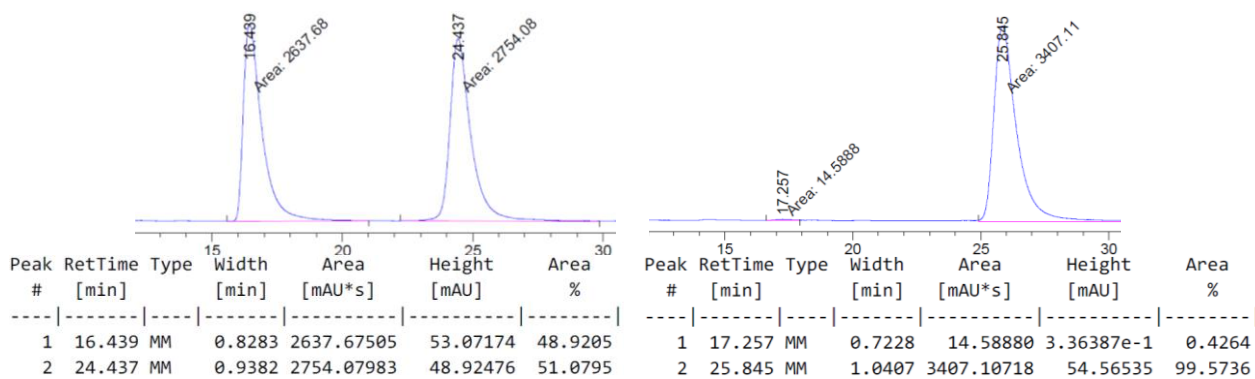
Stoichiometric Reactions Using the Nickel(III) Complexes



General Procedure: The complex $\text{Ni}^{\text{III}}\text{-L7}$ or $\text{Ni}^{\text{III}}\text{-L11}$ (1.0 equiv), alkene **2** (7.5 equiv), and BmimPF_6 (0.05 M) were dissolved in a mixture of degassed 1,4-dioxane and DMA (9:1, v/v, 40 mM). The reaction mixture was heated for 5 h at 100 °C under an atmosphere of N_2 . After filtration through a pad of silica, the solvent was removed under reduced pressure and the yield was examined with ^1H NMR spectroscopy, utilizing 1,3,5-trimethoxybenzene as the internal standard.

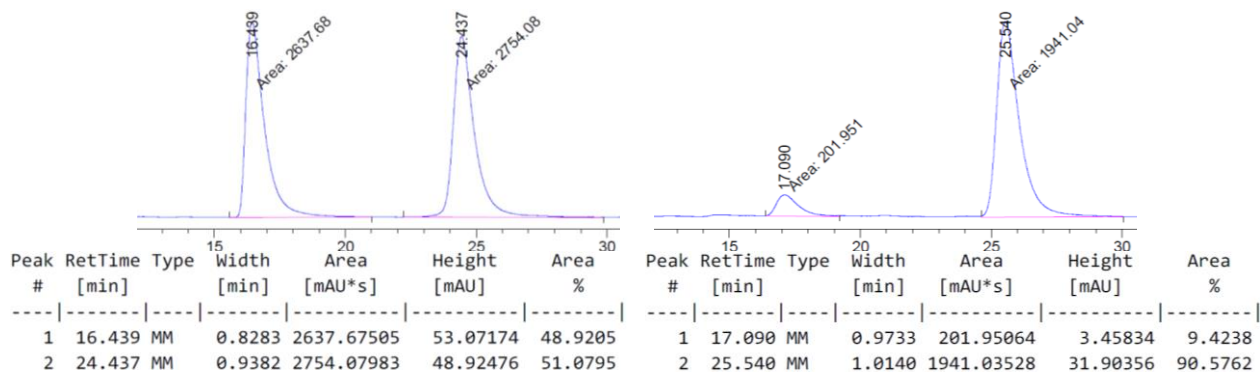
With $\text{Ni}^{\text{III}}\text{-L7}$: The stoichiometric reaction was performed on a 0.04 mmol scale. Product **3** was obtained in 83% yield with an enantiomeric ratio of 99.5:0.5.

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): $t_r(\text{major}) = 25.8$ min, $t_r(\text{minor}) = 17.3$ min, 99.5:0.5.

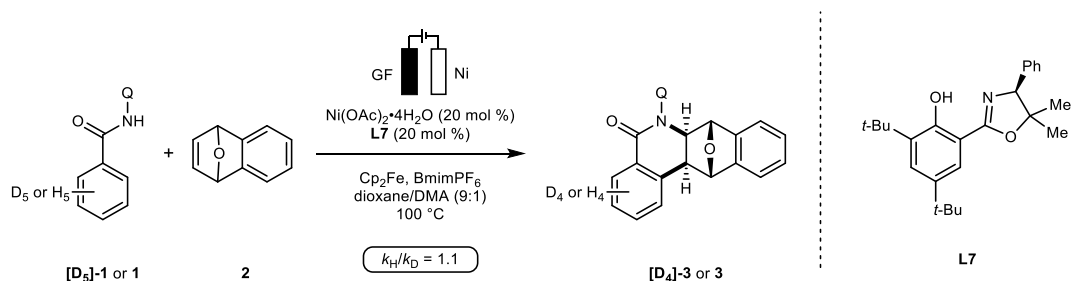


With Ni^{III}-L11: The stoichiometric reaction was performed on a 0.04 mmol scale. Product **3** was obtained in 39% yield with an enantiomeric ratio of 90.5:9.5.

R_t (IA column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 25.5 min, tr(minor) = 17.1 min, 90.5:9.5 e.r.



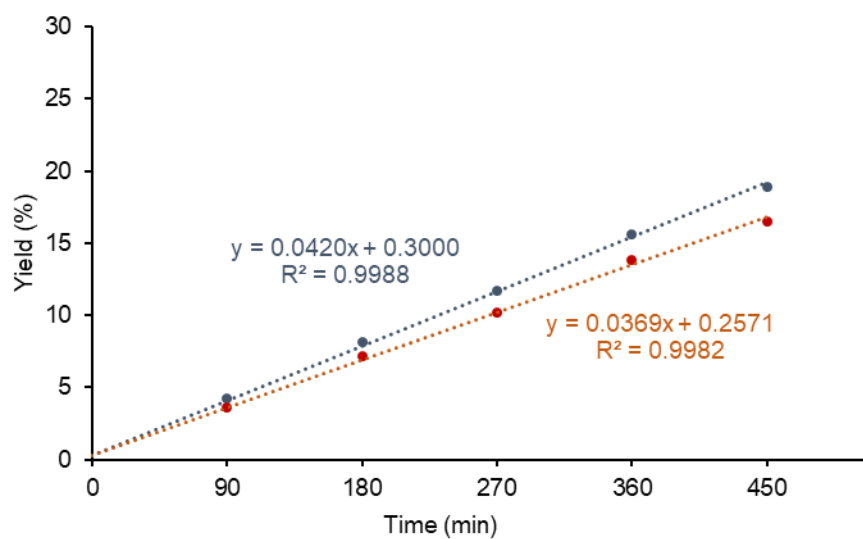
KIE Study for Nickel Catalysis



The KIE was determined in independent reactions, utilizing the deuterated and the non-deuterated amide on a 0.4 mmol scale. The electrolysis was carried out in an undivided cell setup. A GF anode (20 mm $\times$ 10 mm $\times$ 4 mm) and a nickel foam cathode (10 mm $\times$ 15 mm $\times$ 1.4 mm) with electrode holders made of stainless steel were used. The cell was charged with the amide (0.40 mmol, 1.0 equiv), alkene (0.60 mmol, 1.5 equiv), $Ni(OAc)_2 \cdot 4H_2O$ (20 mg, 0.08 mmol), ligand **L7** (30.4 mg, 0.08 mmol), Cp_2Fe (22.4 mg, 0.12 mmol), $BmimPF_6$ (0.05 M) and a teflon-coated magnetic stirring bar (15 $\times$ 6 mm). Then 1,4-dioxane (5.4 mL) and DMA (0.6 mL) were added. The reaction mixture was stirred at $100\text{ }^\circ\text{C}$ for 10 min to obtain a homogeneous solution. Subsequently, the electrolysis was performed at $100\text{ }^\circ\text{C}$ with a constant current of 1.5 mA and a stirring rate of 600 rpm. For 1H NMR spectroscopic quantification of the product formation, 4,4'-dimethylbenzophenone (42.1 mg, 0.20 mmol) was used. At defined reaction times, aliquots (200 μL) of the reaction mixture were taken with a syringe. The samples were directly quenched with triethylamine (0.5 mL), filtered through a silica plug (3.5 cm), and eluted with ethyl acetate (6 mL). After evaporation of the solvent 1H NMR spectra (in $CDCl_3$) were recorded.

Supplementary Table 9. Measured product formation of product 3 and [D₄]-3.

Time (min)	Yield 3	Yield [D ₄]-3
90	4.2%	3.6%
180	8.1%	7.2%
270	11.7%	10.2%
360	15.6%	13.8%
450	18.9%	16.5%



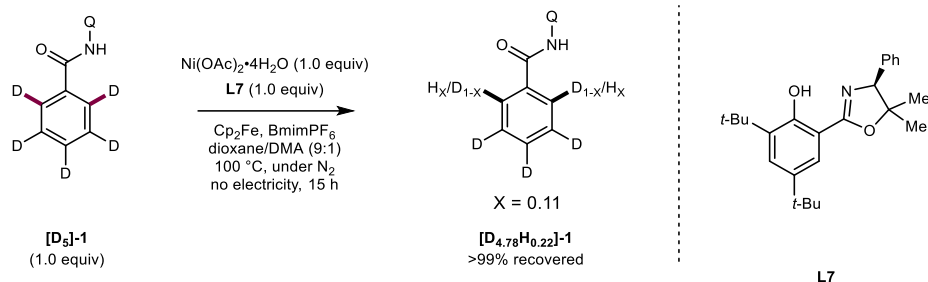
Supplementary Figure 11. Time course of yields in parallel reactions using 1 (blue) or [D₅]-1 (red).

Calculation of the KIE from the determined slopes:

$$\frac{k_{\text{H}}}{k_{\text{D}}} \approx \frac{0.0420\% \cdot \text{min}^{-1}}{0.0369\% \cdot \text{min}^{-1}} = 1.1$$

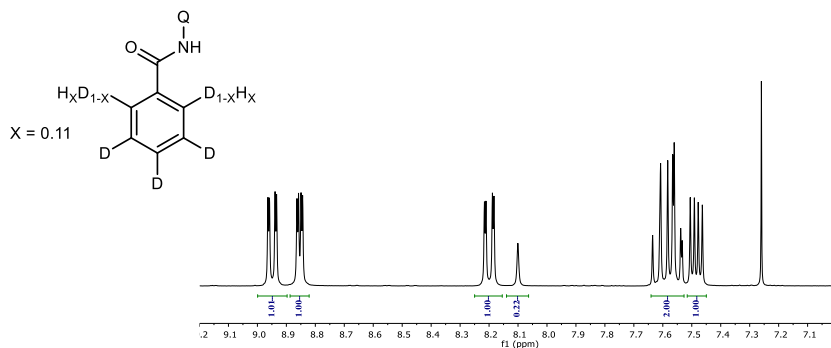
H/D Exchange Studies for Nickel Catalysis

H/D Exchange Experiment for Nickel Catalysis without Electricity

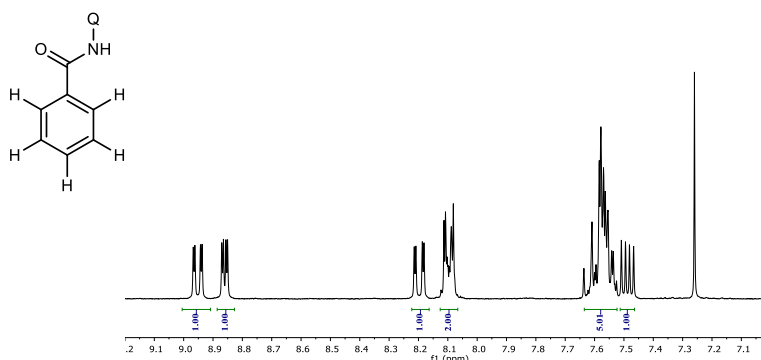


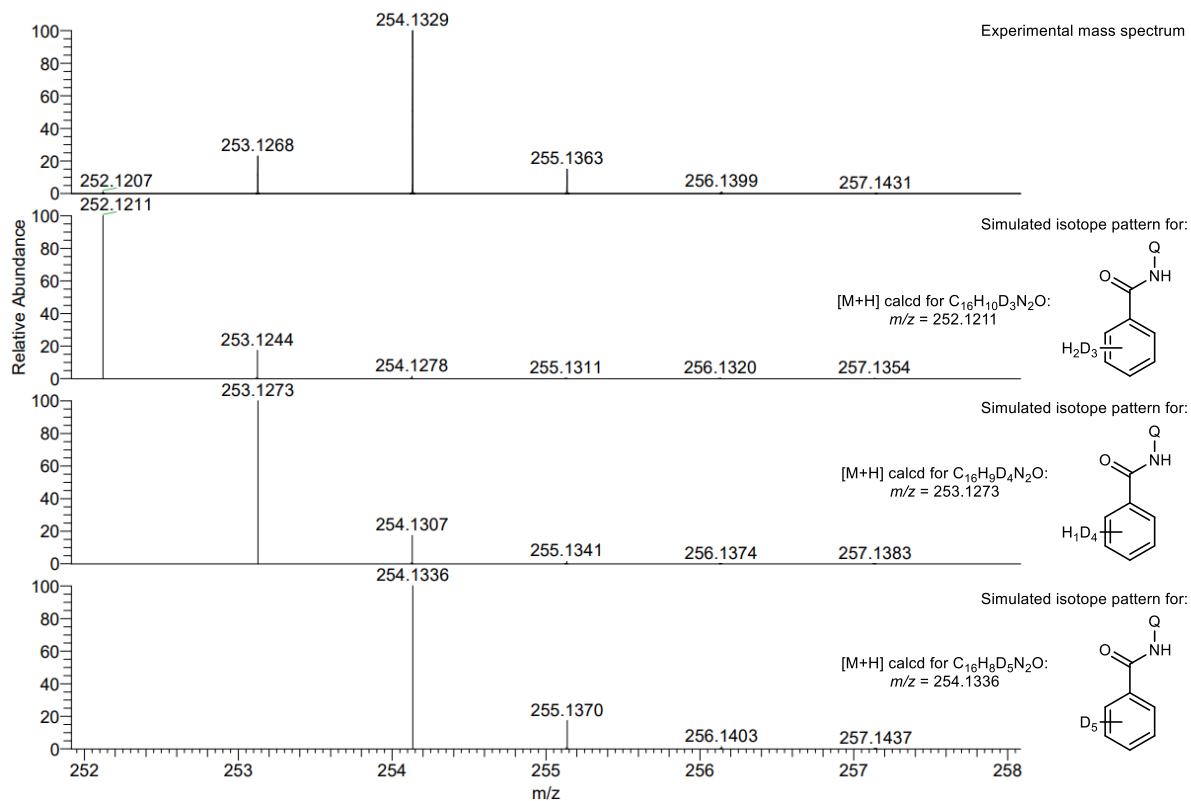
[D₅]-1 (25 mg, 0.1 mmol, 1.0 equiv), ligand **L7** (38 mg, 0.1 mmol, 1.0 equiv), and BmimPF_6 (37 mg, 0.05 M), Cp_2Fe (5.6 mg, 0.03 mmol, 0.3 equiv), and $\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (25 mg, 0.1 mmol, 1.0 equiv) were dissolved in a mixture of degassed 1,4-dioxane and DMA (9:1, v/v, 2.5 mL). The reaction mixture was heated for 15 h at 100 °C under an atmosphere of N_2 . Then, the solvent was removed under reduced pressure and the residue was purified by column chromatography (*n*-hexane/EtOAc = 3:1). The recovered benzamide was analyzed by means of ^1H NMR spectroscopy (in CDCl_3).

^1H NMR spectrum obtained for recovered benzamide:

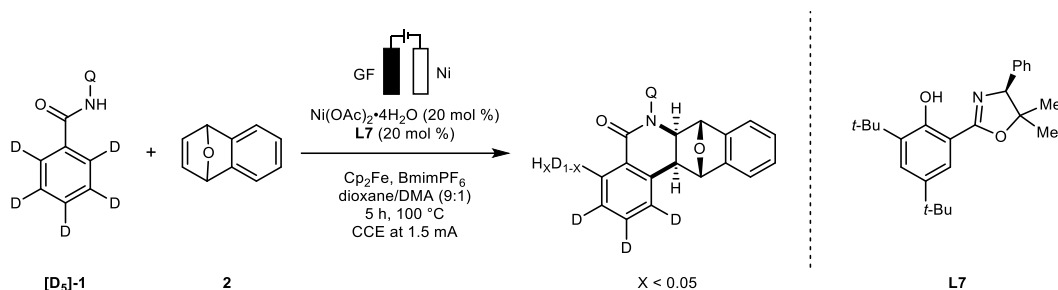


^1H NMR spectrum for H₅-benzamide **1**:



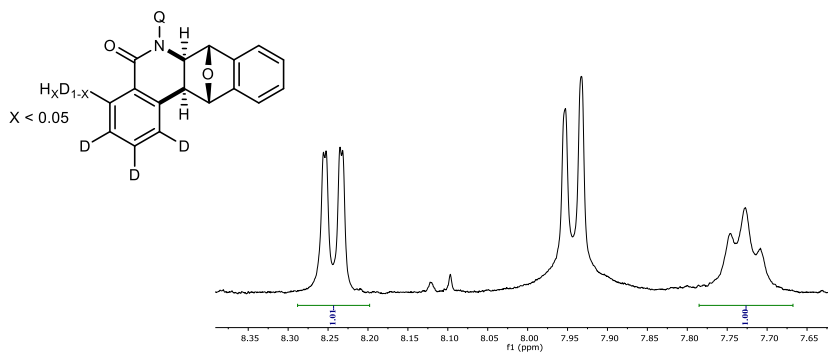


H/D Exchange Experiment for Nickel Catalysis under Conditions of Catalysis

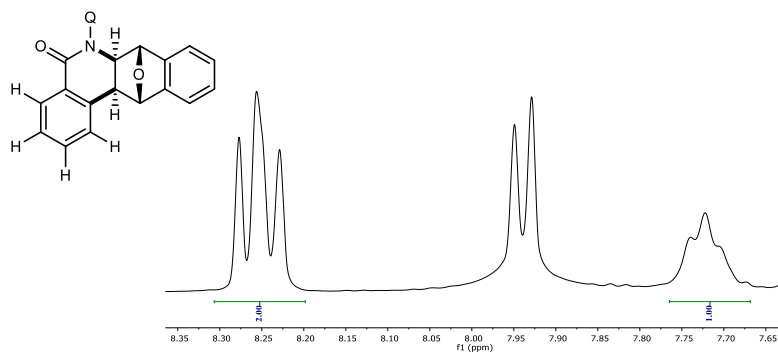


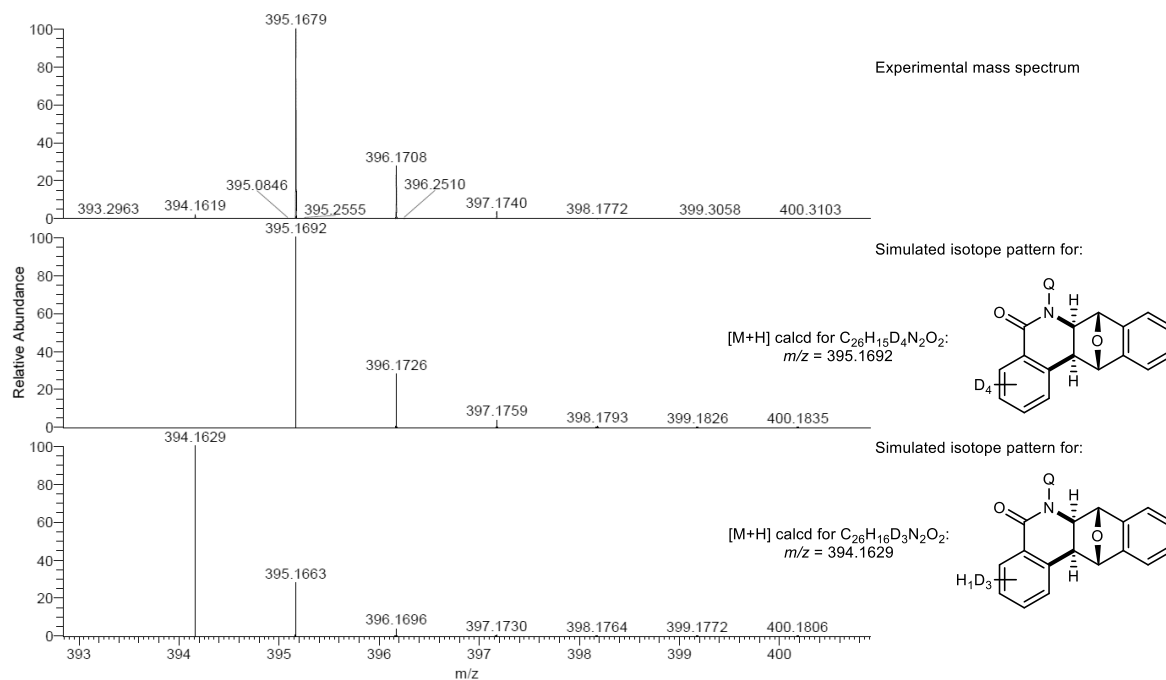
The catalytic reaction was conducted according to the general procedure on a 0.2 mmol scale with the deuterated benzamide **[D₅]-1** and an altered reaction time of 5 h. Then, the solvent was removed under reduced pressure and the residue was purified by column chromatography (*n*-hexane/EtOAc = 3:1). The product was analyzed by means of ^1H NMR spectroscopy (in CDCl_3), showing a fully deuterated benzamide motif. Hence, under the catalytic conditions no relevant H/D exchange occurs.

^1H NMR spectrum obtained from D_5 -benzamide **[D₅]-1**:

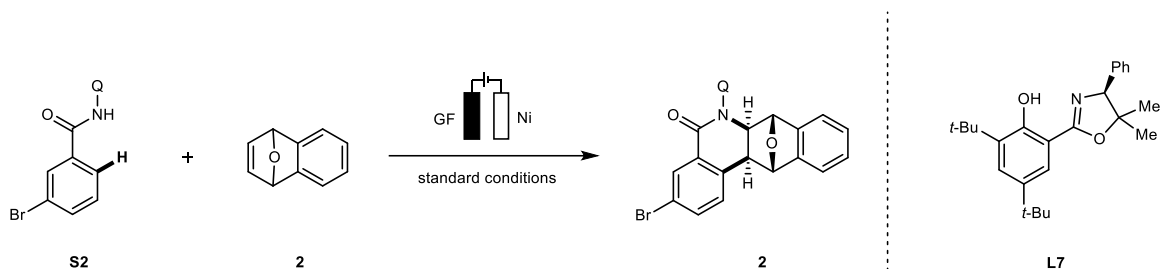


^1H NMR spectrum obtained from H_5 -benzamide **1**:

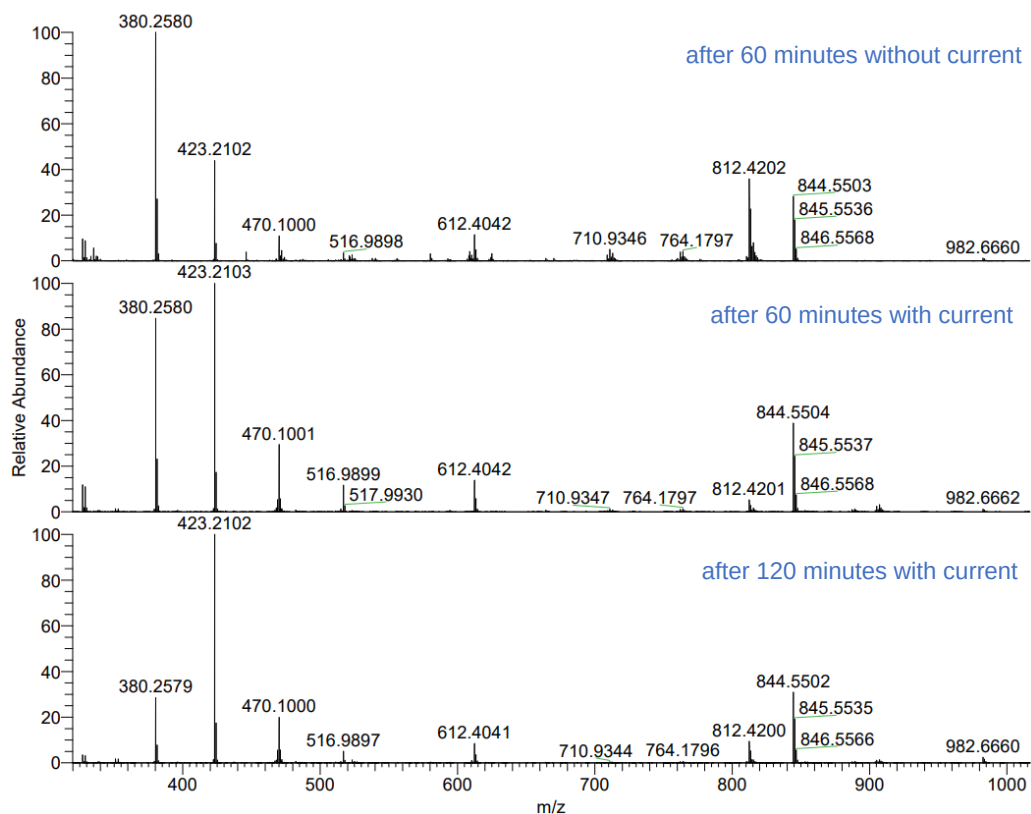




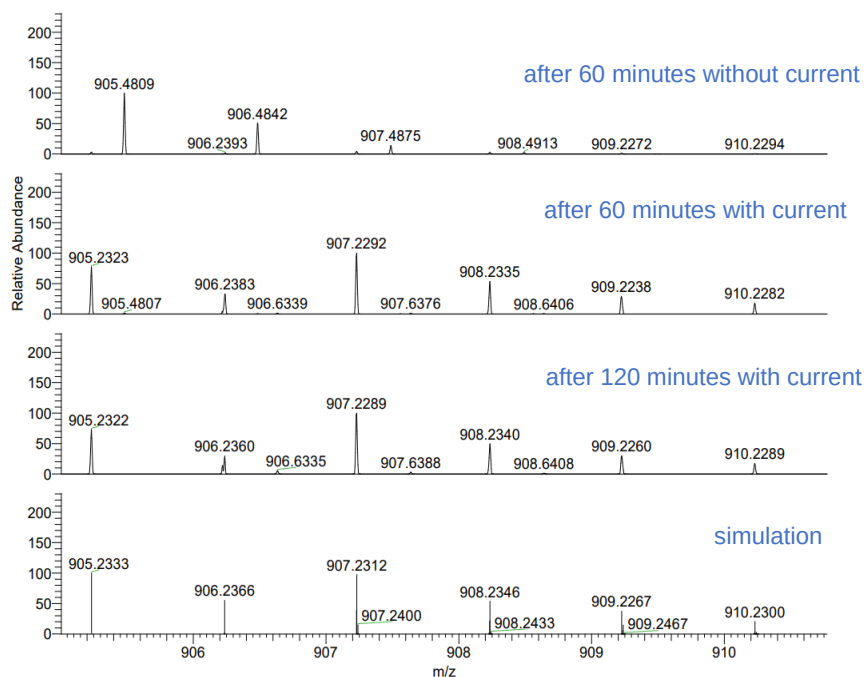
Monitoring the Nickel Catalysis by Mass Spectrometry



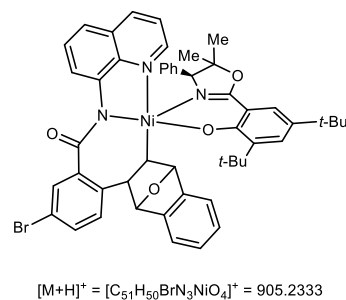
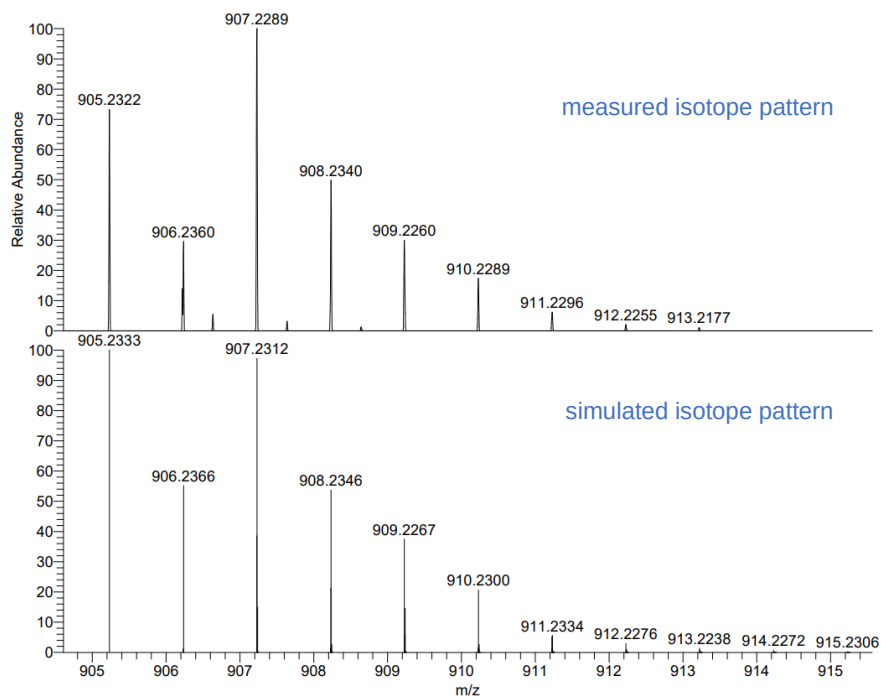
Electrocatalysis was performed according to the general procedure using benzamide **S2**. The first aliquot (50 μL) was taken after stirring the reactions mixture at 100 $^{\circ}\text{C}$ for 60 minutes without current. The aliquot was diluted with THF (500 μL), filtered through an HPLC filter, and directly analyzed via HR ESI MS. In an identical manner, aliquots were analyzed after 60 minutes and 120 minutes applying current.



Supplementary Figure 12. HR-ESI-mass spectrometric monitoring of the enantioselective electrochemical nickel-catalyzed C–H activation with total m/z range.



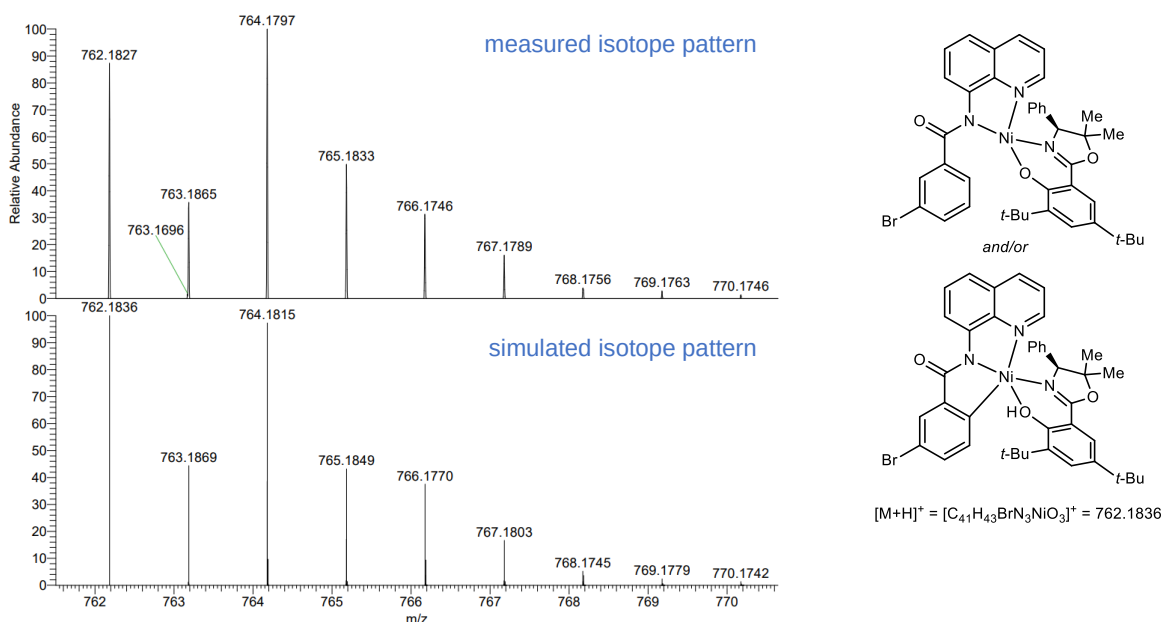
Supplementary Figure 13. HR-ESI-mass spectrometric monitoring of the enantioselective electrochemical nickel-catalyzed C–H activation. m/z calculated for $[\text{C}_{51}\text{H}_{50}\text{BrN}_3\text{NiO}_4]^+ = 905.2333$.



Supplementary Figure 14. Comparison of measured and simulated isotope pattern. m/z calculated for $[\text{C}_{51}\text{H}_{50}\text{BrN}_3\text{NiO}_4]^+ = 905.2333$.

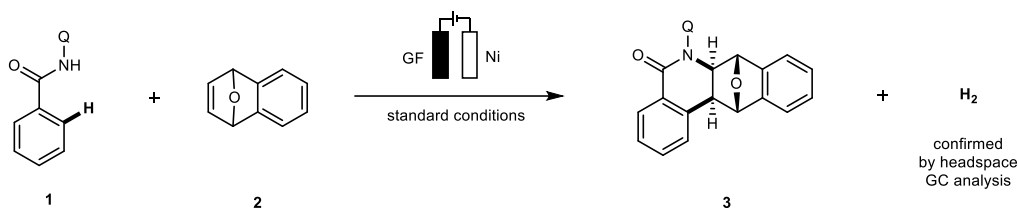


Supplementary Figure 15. HR-ESI-mass spectrometric monitoring of the enantioselective electrochemical nickel-catalyzed C–H activation. m/z calculated for $[\text{C}_{41}\text{H}_{43}\text{BrN}_3\text{NiO}_3]^+ = 762.1836$.

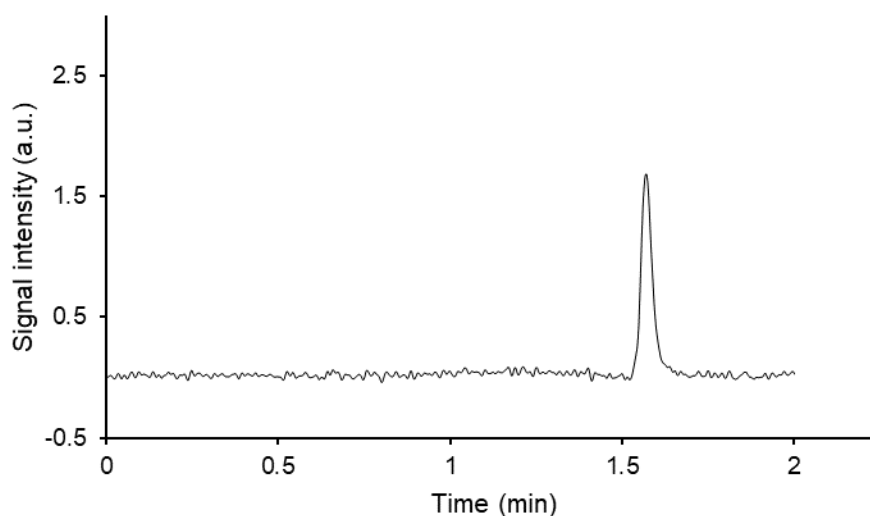


Supplementary Figure 16. Comparison of measured and simulated isotope pattern. m/z calculated for $[\text{C}_{41}\text{H}_{43}\text{BrN}_3\text{NiO}_3]^+ = 762.1836$.

Detection of Hydrogen Gas for Nickel Catalysis

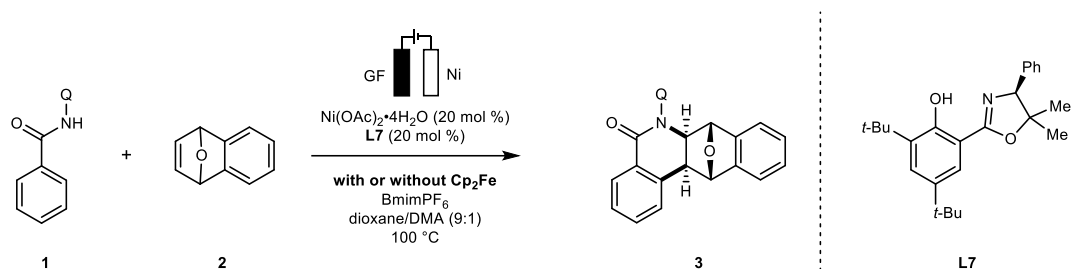


Electrocatalysis was performed according to the general procedure. A septum was used instead of a teflon cap. After completion of the reaction, 1 mL gas volume of the headspace was carefully collected using a gas syringe and directly analyzed. The peak at 1.56 min assigned to hydrogen gas is clearly visible.



Supplementary Figure 17. Chromatogram detected via headspace GC analysis for enantioselective electrochemical nickel-catalyzed C–H activation.

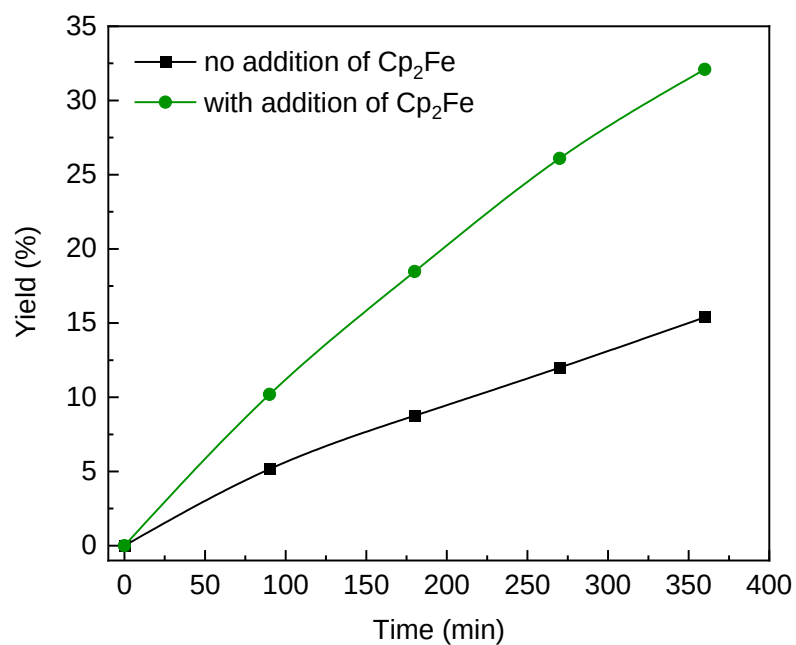
Kinetic Study for Nickel Catalysis



Reaction monitoring was performed with and without the addition of Cp_2Fe (30 mol %) on a 0.2 mmol scale. The electrolysis was carried out in an undivided cell setup. A GF anode (20 mm × 10 mm × 4 mm) and a nickel foam cathode (10 mm × 15 mm × 1.4 mm) with electrode holders made of stainless steel were used. The cell was charged with the amide (0.20 mmol, 1.0 equiv), alkene (0.30 mmol, 1.5 equiv), $\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (10 mg, 0.04 mmol), ligand **L7** (15.2 mg, 0.04 mmol), Cp_2Fe (11.2 mg, 0.06 mmol or no addition), BmimPF_6 (0.05 M) and a teflon-coated magnetic stirring bar (15 × 6 mm). Then 1,4-dioxane (4.5 mL) and DMA (0.5 mL) were added. The reaction mixture was stirred at 100 °C for 10 min to obtain a homogeneous solution. Subsequently, the electrolysis was performed at 100 °C with a constant current of 1.5 mA and a stirring rate of 600 rpm. For ^1H NMR spectroscopic quantification of the product formation, 4,4'-dimethylbenzophenone (21 mg, 0.10 mmol) was used. At defined reaction times, aliquots (200 μL) of the reaction mixture were taken with a syringe. The samples were directly quenched with triethylamine (0.5 mL), filtered through a silica plug (3.5 cm), and eluted with ethyl acetate (6 mL). After evaporation of the solvent ^1H NMR spectra (in CDCl_3) were recorded.

Supplementary Table 10. Measured product formation of product 3.

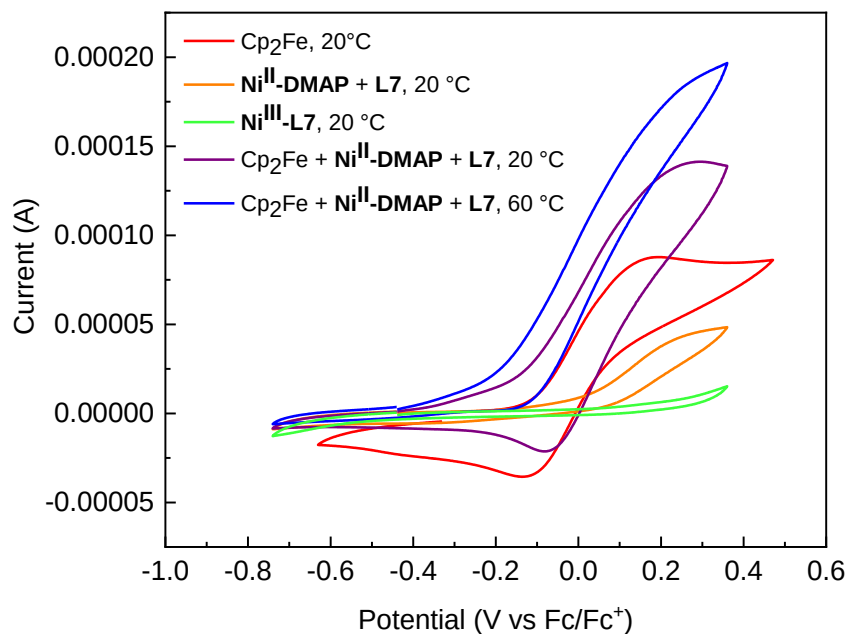
Time (min)	Without addition of Cp ₂ Fe	With addition of Cp ₂ Fe
90	5.2%	10.2%
180	8.8%	18.5%
270	12.0%	26.1%
360	15.4%	32.1%



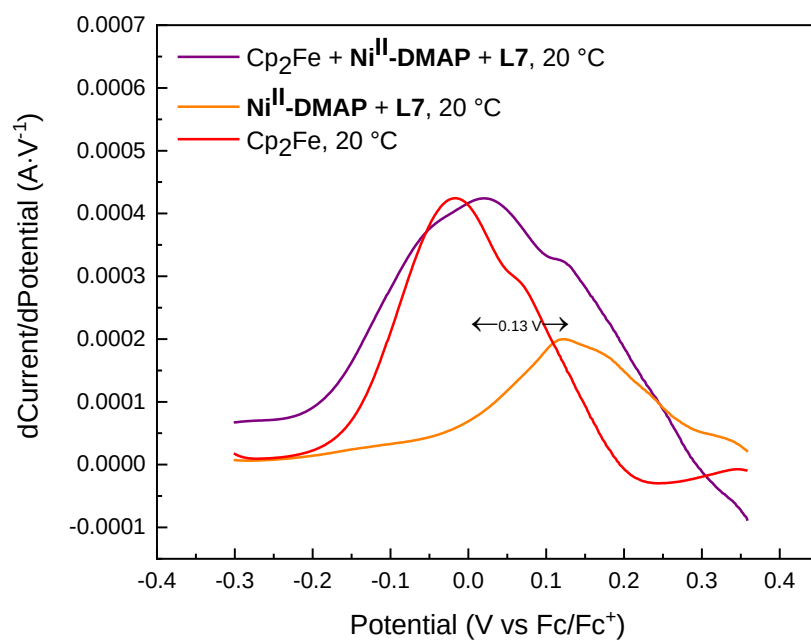
Supplementary Figure 18. Time course of yields in parallel reactions with (green) and without (black) the addition of Cp₂Fe (30 mol %).

Electroanalytical Investigations for Nickel Catalysis

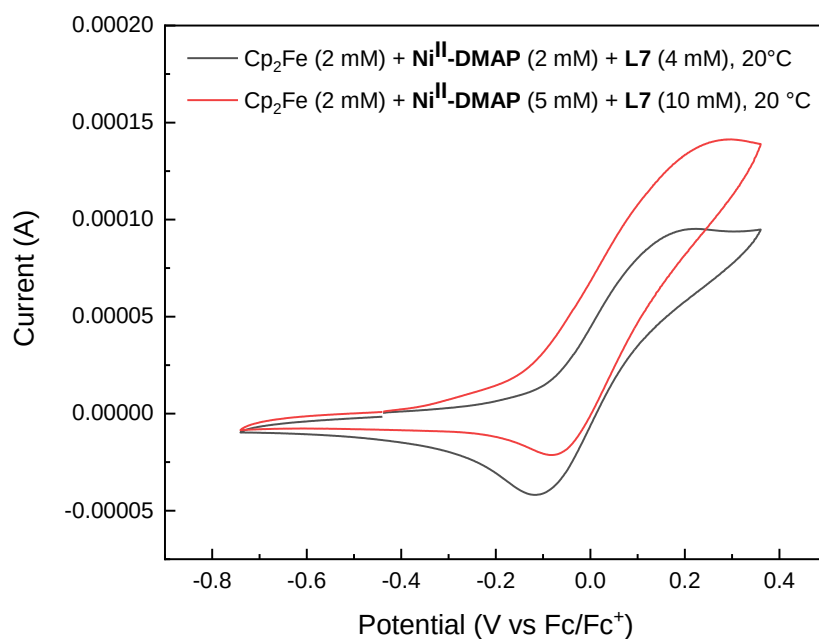
Cyclic Voltammetry (CV)



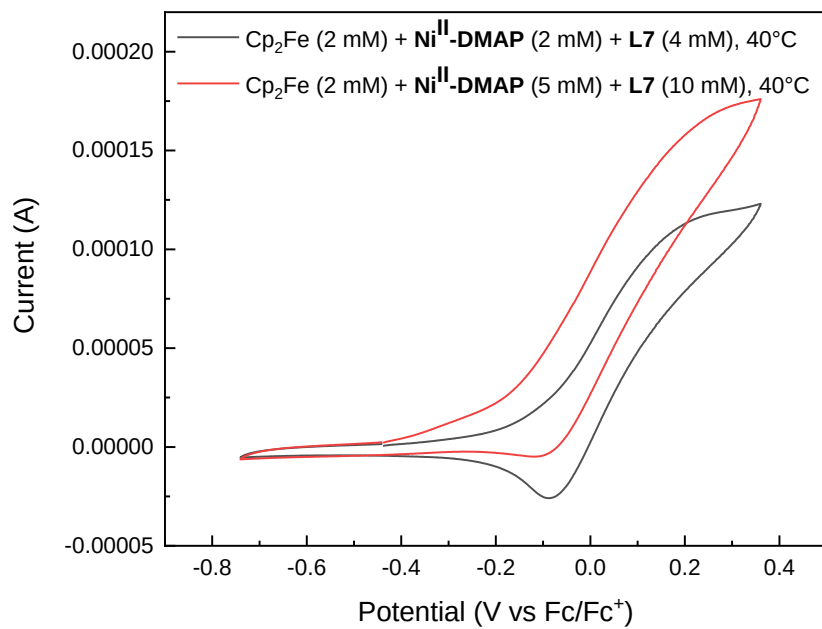
Supplementary Figure 19. Cyclic voltammograms at 50 mVs⁻¹ using dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte. Measurement temperature used as indicated. (red) Cp₂Fe (2 mM); (orange) Ni^{II}-DMAP (5 mM) and L7 (10 mM); (green) Ni^{III}-L7 (5 mM); (purple and blue) Cp₂Fe (2 mM) and Ni^{II}-DMAP (5 mM) and L7 (10 mM).



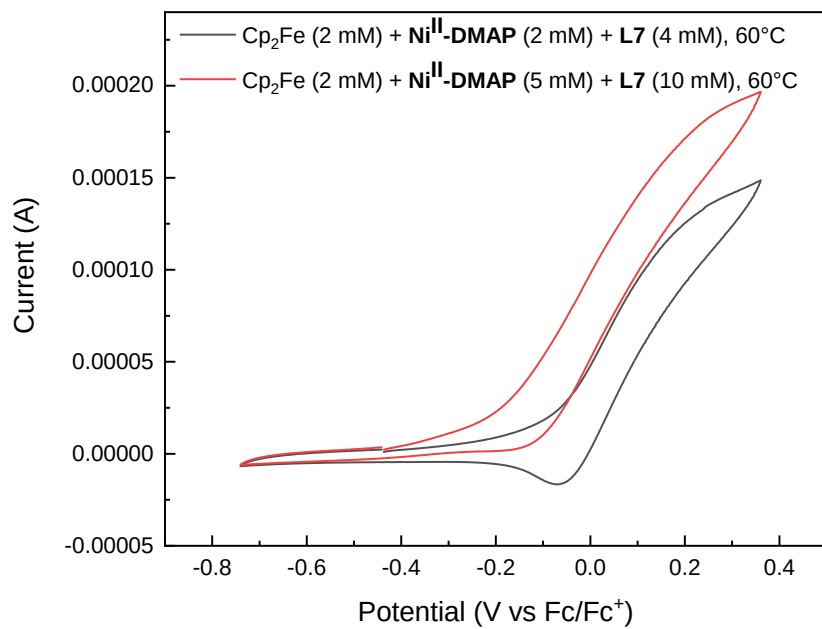
Supplementary Figure 20. First derivative of the oxidation waves. Cyclic voltammograms at 50 mVs^{-1} using dioxane/DMA (4:1) and $n\text{-Bu}_4\text{NPF}_6$ (0.1 M) as the electrolyte. Measurement temperature used as indicated. (red) Cp_2Fe (2 mM); (orange) $\text{Ni}^{\text{II}}\text{-DMAP}$ (5 mM) and **L7** (10 mM); (purple) Cp_2Fe (2 mM) and $\text{Ni}^{\text{II}}\text{-DMAP}$ (5 mM) and **L7** (10 mM).



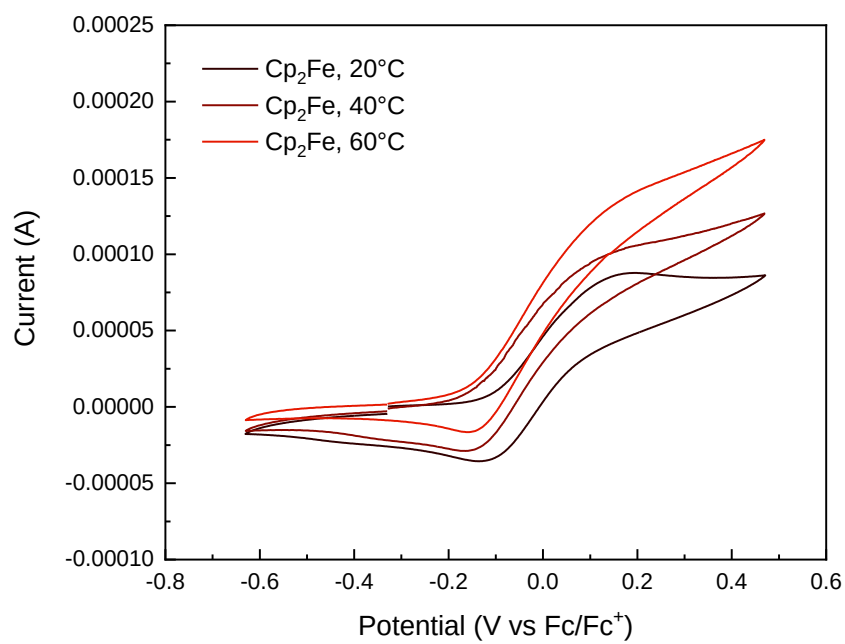
Supplementary Figure 21. Cyclic voltammograms at 50 mVs⁻¹ using dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte at 20 °C. (grey) Cp₂Fe (2 mM) and Ni^{II}-DMAP (2 mM) and L7 (4 mM); (red) Cp₂Fe (2 mM) and Ni^{II}-DMAP (5 mM) and L7 (10 mM).



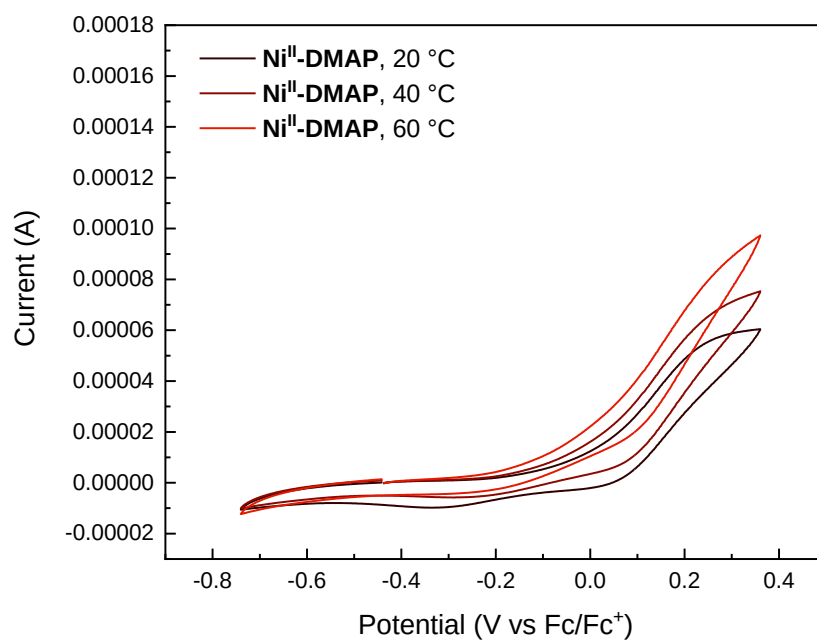
Supplementary Figure 22. Cyclic voltammograms at 50 mVs⁻¹ using dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte at 40 °C. (grey) Cp₂Fe (2 mM) and Ni^{II}-DMAP (2 mM) and L7 (4 mM); (red) Cp₂Fe (2 mM) and Ni^{II}-DMAP (5 mM) and L7 (10 mM).



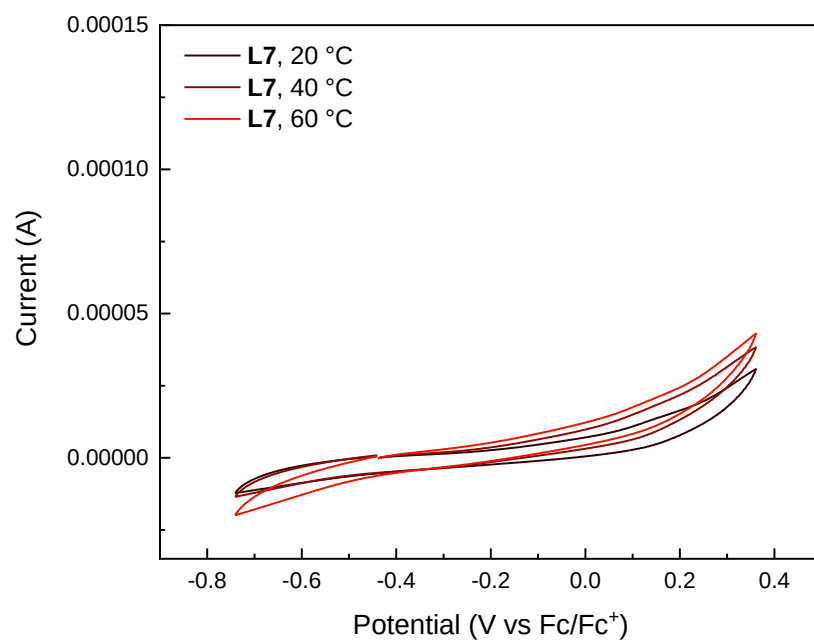
Supplementary Figure 23. Cyclic voltammograms at 50 mVs^{-1} using dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte at 60 °C. (grey) Cp₂Fe (2 mM) and Ni^{II}-DMAP (2 mM) and L7 (4 mM); (red) Cp₂Fe (2 mM) and Ni^{II}-DMAP (5 mM) and L7 (10 mM).



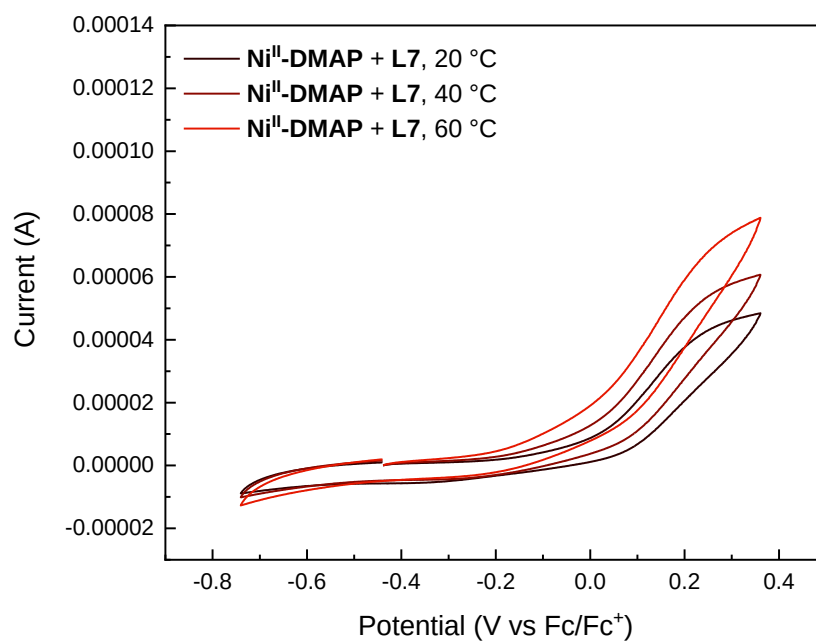
Supplementary Figure 24. Cyclic voltammograms at 50 mVs⁻¹ using dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte. Measurement temperature used as indicated. Cp₂Fe (2 mM).



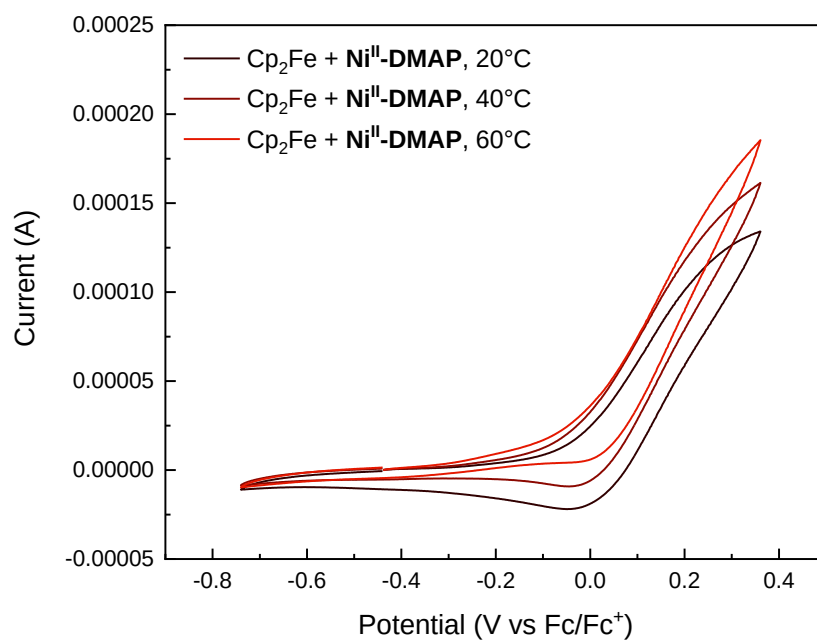
Supplementary Figure 25. Cyclic voltammograms at 50 mVs⁻¹ using dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte. Measurement temperature used as indicated. **Ni^{II}-DMAP** (5 mM).



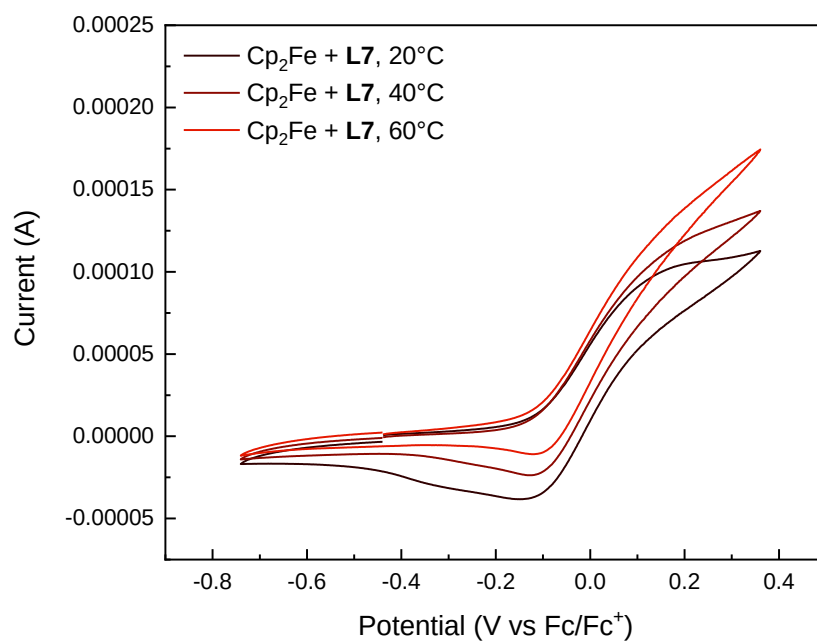
Supplementary Figure 26. Cyclic voltammograms at 50 mVs⁻¹ using dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte. Measurement temperature used as indicated. **L7** (10 mM).



Supplementary Figure 27. Cyclic voltammograms at 50 mVs^{-1} using dioxane/DMA (4:1) and $n\text{-Bu}_4\text{NPF}_6$ (0.1 M) as the electrolyte. Measurement temperature used as indicated. Ni^{II} -DMAP (5 mM) and L7 (10 mM).

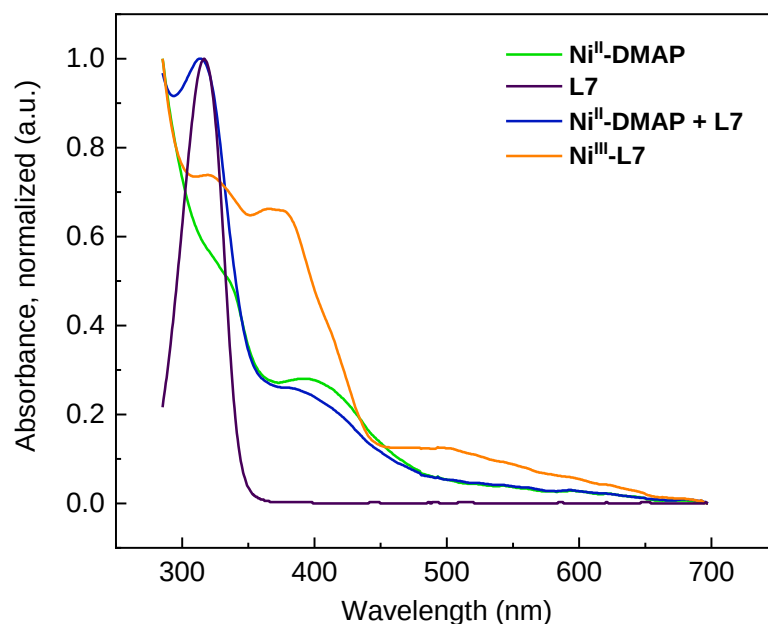


Supplementary Figure 28. Cyclic voltammograms at 50 mVs^{-1} using dioxane/DMA (4:1) and $n\text{-Bu}_4\text{NPF}_6$ (0.1 M) as the electrolyte. Measurement temperature used as indicated. Cp_2Fe (2 mM) and $\text{Ni}^{\text{II}}\text{-DMAP}$ (5 mM).

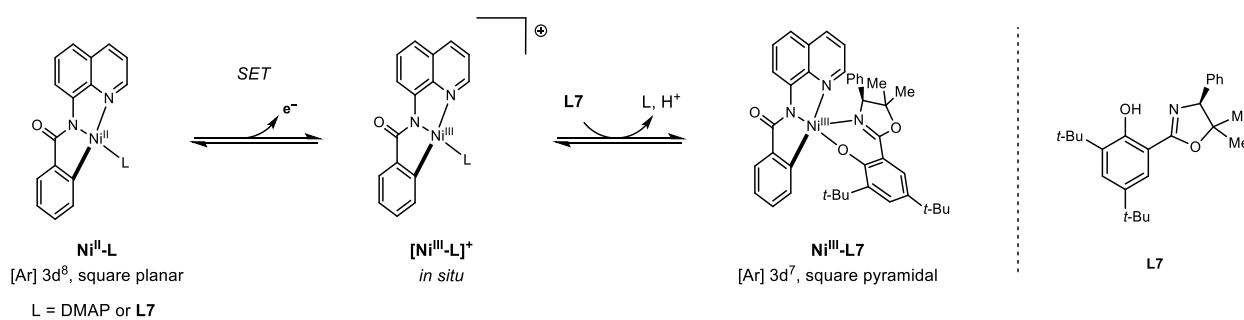


Supplementary Figure 29. Cyclic voltammograms at 50 mVs⁻¹ using dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte. Measurement temperature used as indicated. Cp₂Fe (2 mM) and **L7** (10 mM).

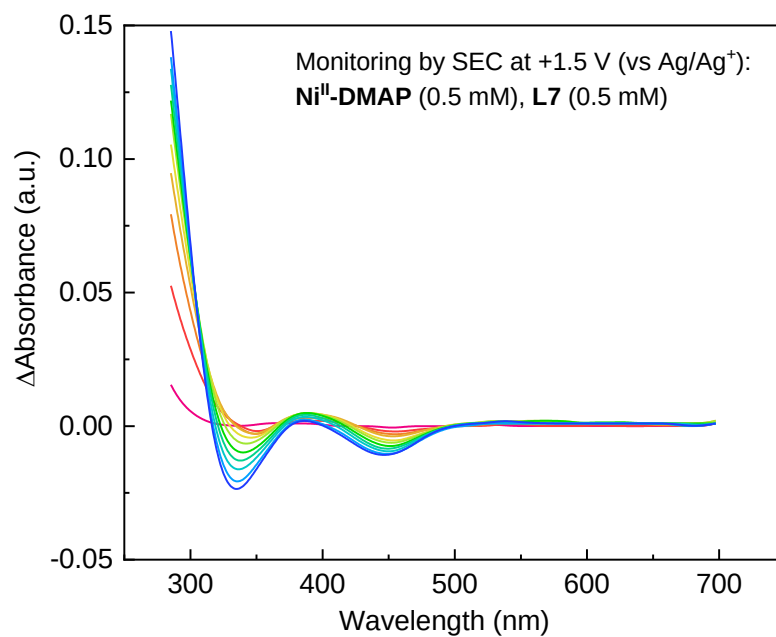
Spectroelectrochemistry (SEC)



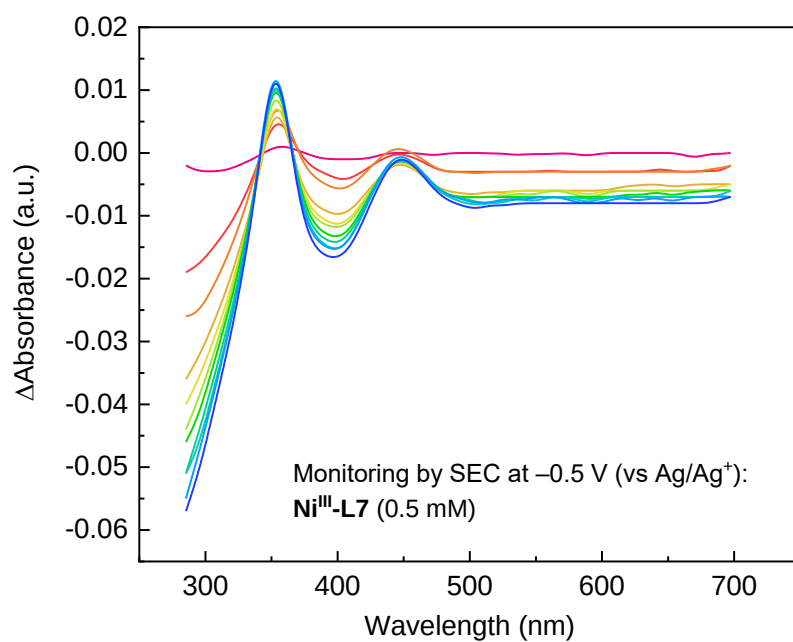
Supplementary Figure 30. UV-vis spectra in dioxane/DMA (4:1) at 20 °C. (green) **Ni^{II}-DMAP** (0.5 mM); (purple) **L7** (0.5 mM); (blue) **Ni^{II}-DMAP** (0.5 mM) and **L7** (0.5 mM); (orange) **Ni^{III}-L7** (0.5 mM).



Supplementary Figure 31. Scheme of the redox process to be investigated by SEC.



Supplementary Figure 32. Monitoring by SEC with dioxane/DMA (4:1) and *n*-Bu₄NPF₆ (0.1 M) as the electrolyte at 20 °C. **Ni^{II}-DMAP** (0.5 mM) and **L7** (0.5 mM). A potential of +1.5 V (vs Ag/Ag⁺) was applied over 300 s.

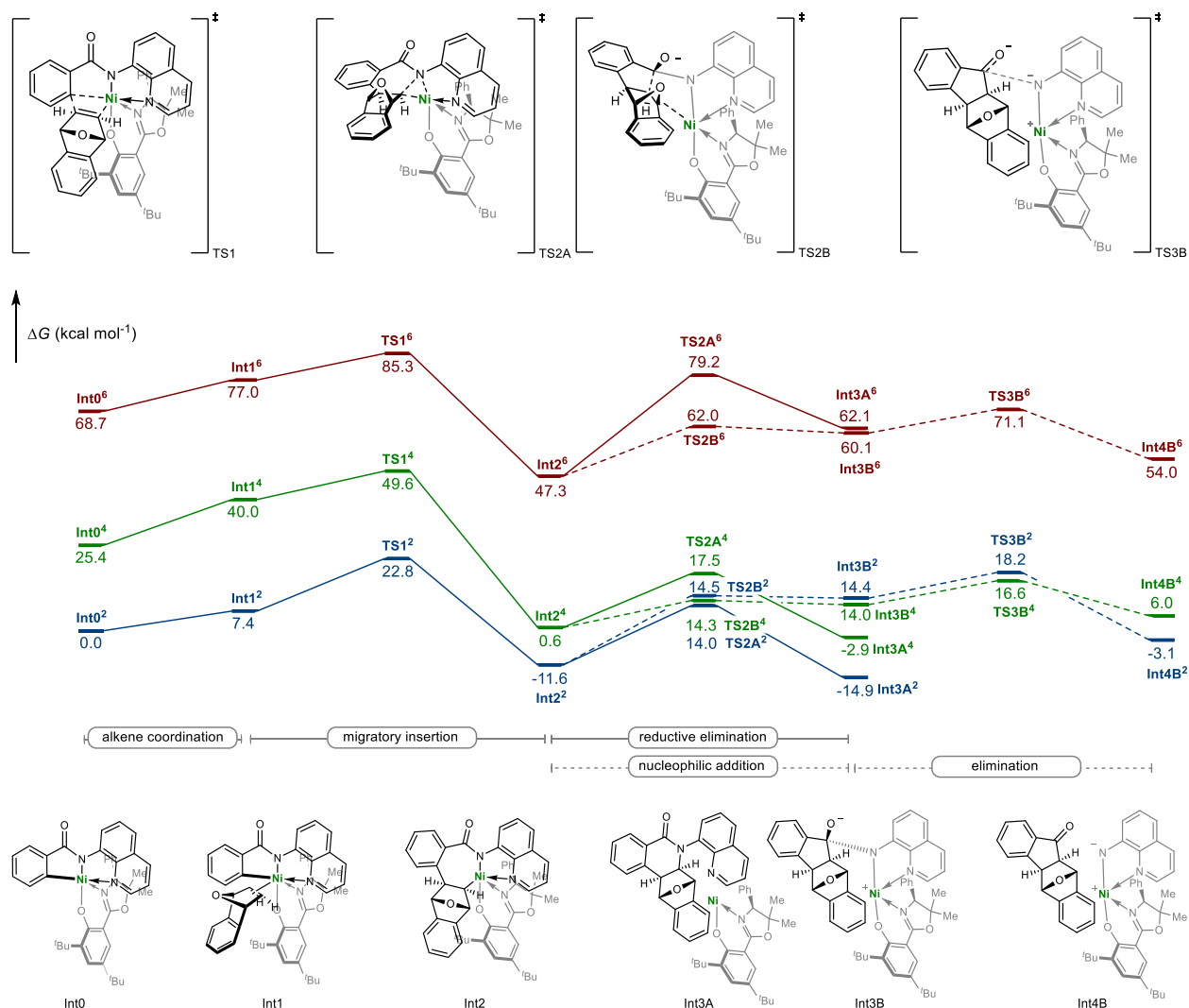


Supplementary Figure 33. Monitoring by SEC with dioxane/DMA (4:1) and $n\text{-Bu}_4\text{NPF}_6$ (0.1 M) as the electrolyte at 20 °C. $\text{Ni}^{\text{III}}\text{-L7}$ (0.5 mM). A potential of -0.5 V (vs Ag/Ag^+) was applied over 300 s.

Computational Methods

All DFT calculations were performed using Gaussian 16, Revision A.03 package¹⁸. Geometry optimizations were performed at the TPSS⁴³ level of theory in combination with Grimme's D3 dispersion corrections with a Becke-Johnson damping scheme (D3BJ)^{44,45} in the gas phase. All atoms were described with a def2-SVP basis set²⁸⁻³¹. Analytical frequencies were carried out at the same level of theory to identify each stationary point as either an intermediate (no imaginary frequencies) or a transition state (single imaginary frequency). These also provided thermal and non-thermal corrections to the Gibbs free energy (G) at 373.15 K and 1 atm. Moreover, Intrinsic reaction coordinate (IRC)⁴⁶ calculations were performed to validate the connectivity between the stationary points. The electronic energy was then refined through single-point calculations at the PW6B95⁴⁷ level of theory on the optimized geometries with a def2-TZVP basis set²⁸⁻³¹ in combination with a standalone version of Grimme's dispersion correction D4. Solvent effects were included implicitly through the use of the SMD model⁴⁸ with a dielectric constant of $\epsilon = 2.2099$, which corresponds to 1,4-dioxane (for the nickel-catalyzed reaction energy profile), and with a dielectric constant of $\epsilon = 6.2528$, which corresponds to acetic acid (for the cobalt-catalyzed reaction energy profile). Energies reported in the energy profiles are based on gas-phase Gibbs free energies with a def2-SVP basis set for which the electronic energies were corrected to PW6B95-D4 with a def2-TZVPP basis set including respective solvent effects. Additionally, different functionals were considered to compute the chemodivergent step for geometry optimization (PBE0-D4)⁴⁹ and energy refinement (B3LYP-D4).⁵⁰

Computational Studies for Nickel Catalysis



Supplementary Figure 34. Computed Gibbs free energy ($\Delta G_{373.15}$) profile for the nickel-catalyzed carboamination (— A) and carboacylation (--- B) pathways in kcal mol⁻¹ at the PW6B95-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory. The superscripted numbers (2/4/6) in each stationary point labels represent the respective spin multiplicity.

Supplementary Table 11. Calculated electronic and Gibbs free energies ($\Delta G_{373.15}$) at the PW6B95-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory, for all structures involved in the nickel catalysis reaction energy profile (all in Hartree).[#]

Structure	Electronic Energy	Total Gibbs Free Energy
alkene ¹	-461.821868	-461.723558
Int0 ²	-3490.222298	-3489.641971
Int0 ⁴	-3490.176103	-3489.601540
Int0 ⁶	-3490.103365	-3489.532543
Int1 ²	-3952.058160	-3951.353658
Int1 ⁴	-3952.005914	-3951.306631
Int1 ⁶	-3951.938128	-3951.242776
TS1 ²	-3952.038191	-3951.329258
TS1 ⁴	-3951.990364	-3951.286512
TS1 ⁶	-3951.926815	-3951.229531
Int2 ²	-3952.095341	-3951.383968
Int2 ⁴	-3952.069701	-3951.364564
Int2 ⁶	-3951.987743	-3951.290092
TS2A ²	-3952.051257	-3951.343275
TS2A ⁴	-3952.044255	-3951.337587
TS2A ⁶	-3951.938692	-3951.239271
TS2B ²	-3952.047839	-3951.342486
TS2B ⁴	-3952.047430	-3951.342769
TS2B ⁶	-3951.967690	-3951.266633
Int3A ²	-3952.101299	-3951.389333
Int3A ⁴	-3952.079710	-3951.370229
Int3A ⁶	-3951.970368	-3951.266512
Int3B ²	-3952.050404	-3951.342592
Int3B ⁴	-3952.049771	-3951.343255
Int3B ⁶	-3951.972521	-3951.269822
TS3B ²	-3952.041798	-3951.336443
TS3B ⁴	-3952.044124	-3951.339111
TS3B ⁶	-3951.952393	-3951.252244
Int4B ²	-3952.077437	-3951.370528
Int4B ⁴	-3952.059227	-3951.355952
Int4B ⁶	-3951.977765	-3951.279456

[#]Superscripted 1, 2, 4, and 6 corresponds to the spin multiplicity as singlet, doublet, quartet and sextet, respectively.

Supplementary Table 12. Relative Gibbs free energy ($\Delta G_{373.15}$) for chemodivergent step in the nickel catalysis between carboamination (— A) and carboacylation (--- B) pathways, computed at different level of theory (all in kcal mol⁻¹).

Functional	Spin multiplicity	Int2	TS2A	TS2B	Int3A	Int3B	$\Delta\Delta G^{\ddagger}_{(B-A)}$
PW6B95-D4ⁱ	Doublet	0.0	25.5	26.0	-3.4	26.0	0.3
	Quartet	12.2	29.1	25.9	8.6	25.5	
B3LYP-D4ⁱ	Doublet	0.0	25.7	27.2	-2.4	27.6	1.5
	Quartet	13.0	28.6	27.3	9.6	27.2	
PBE0-D4ⁱⁱ	Doublet	0.0	23.2	24.4	10.4	56.7	1.2
	Quartet	11.6	27.6	24.4	5.4	22.9	
	Sextet	69.4	84.2	69.0	79.9	65.0	

[#]Level of theory: i) Functional/ def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP; ii) Functional/ def2-TZVPP+SMD(1,4-Dioxane)//PBE0-D3(BJ)/def2-SVP.

Supplementary Table 13. Calculated electronic and Gibbs free energies ($\Delta G_{373.15}$) at the B3LYP-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory, for structures involved in the chemodivergent step in the nickel catalysis reaction energy profile (all in Hartree).[#]

Structure	Electronic Energy	Total Gibbs Free Energy
Int2²	-3948.394491	-3947.630236
Int2⁴	-3948.367207	-3947.609444
TS2A²	-3948.348923	-3947.589349
TS2A⁴	-3948.343645	-3947.584631
TS2B²	-3948.344416	-3947.586822
TS2B⁴	-3948.343738	-3947.586711
Int3A²	-3948.399362	-3947.634104
Int3A⁴	-3948.377577	-3947.614928
Int3B²	-3948.346913	-3947.586290
Int3B⁴	-3948.346209	-3947.586819

[#]Superscripted 2, and 4 corresponds to the spin multiplicity as doublet, and quartet, respectively.

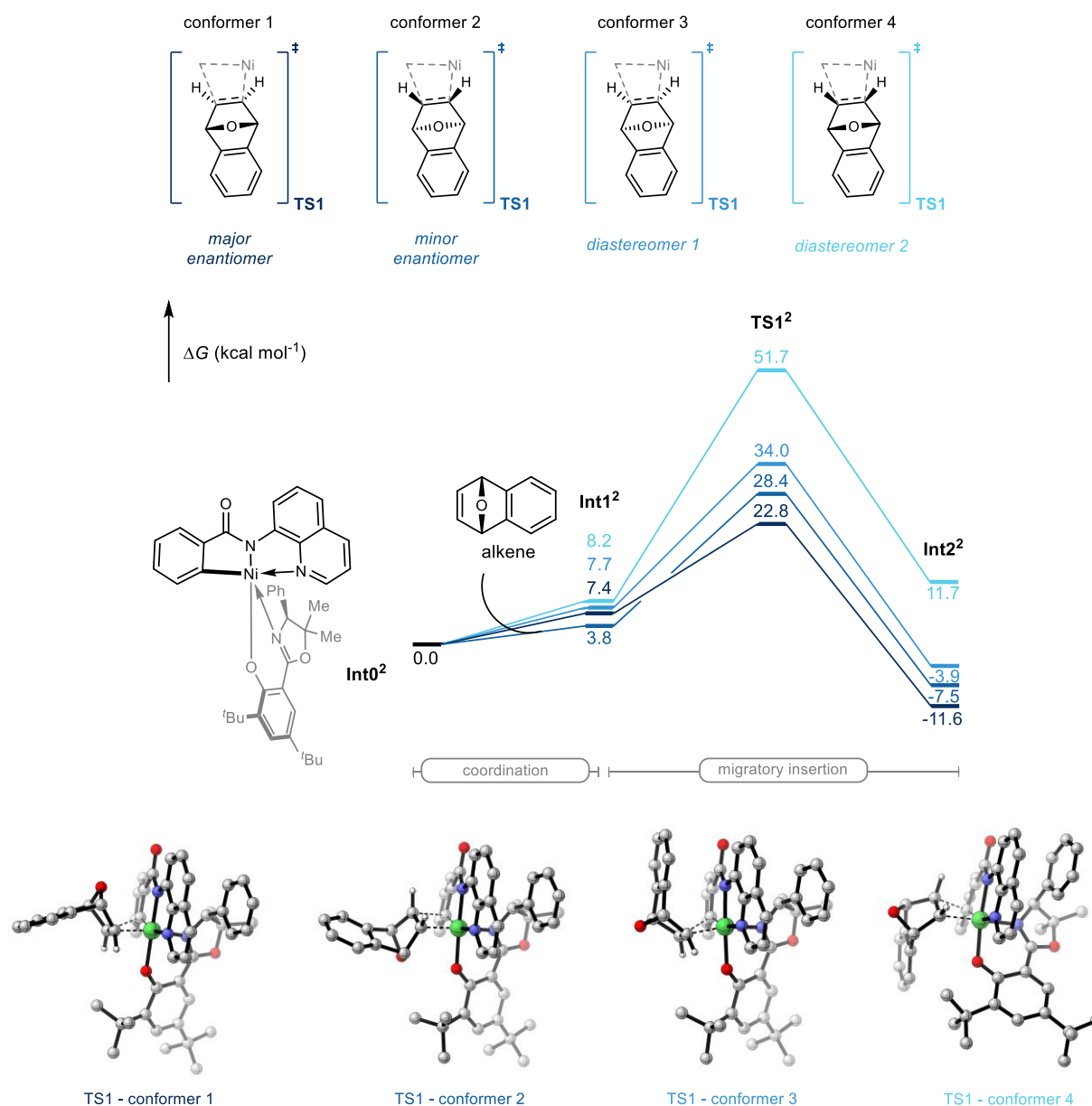
Supplementary Table 14. Calculated electronic and Gibbs free energies ($\Delta G_{373.15}$) at the PBE0-D4/def2-TZVPP+SMD(1,4-Dioxane)//PBE0-D3(BJ)/def2-SVP level of theory, for structures involved in the chemodivergent step in the nickel catalysis reaction energy profile (all in Hartree).[#]

Structure	Electronic Energy	Total Gibbs Free Energy
Int2²	-3945.131235	-3944.353522
Int2⁴	-3945.105774	-3944.335021
Int2⁶	-3945.029431	-3944.242984
TS2A²	-3945.088699	-3944.316616
TS2A⁴	-3945.080981	-3944.309573
TS2A⁶	-3944.984345	-3944.219409
TS2B²	-3945.086339	-3944.314567
TS2B⁴	-3945.085832	-3944.314669
TS2B⁶	-3945.009592	-3944.243624
Int3A²	-3945.136836	-3944.336917
Int3A⁴	-3945.121542	-3944.344932
Int3A⁶	-3945.020949	-3944.226567
Int3B²	-3945.058351	-3944.263104
Int3B⁴	-3945.089078	-3944.317101
Int3B⁶	-3945.018147	-3944.249991

[#]Superscripted 2, 4, and 6 corresponds to the spin multiplicity as doublet, quartet and sextet, respectively.

Conformational analysis of the stereo-determining step

Since the migratory insertion has been revealed to be the enantio-determining step, four possible coordination conformations of alkene were considered, between the coordination and migratory insertion elementary steps. (Supplementary Figure 35). Here the **conformer 1** corresponds to major enantiomer, whereas **conformer 2** to minor enantiomer. The **conformer 3** and **conformer 4** are diastereomers.



Supplementary Figure 35. Relative Gibbs free energies ($\Delta G_{373.15}$) for all the major coordinating conformations of the 7-oxabenzonorbornadiene substrate for the enantio-determining step in the nickel catalysis in doublet spin state, which corresponds to the ground state. Non-relevant hydrogens in the transition state structures were omitted for clarity.

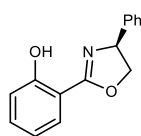
Supplementary Table 15. Calculated electronic and Gibbs free energies ($\Delta G_{373.15}$) at the PW6B95-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory, for all structures involved in the conformational analysis in the nickel catalysis (all in Hartree).[#]

Structure	Electronic Energy	Total Gibbs Free Energy
alkene¹	-461.821868	-461.723558
Int0²	-3490.222298	-3489.641971
Int1 - conformer 1²	-3952.058160	-3951.353658
Int1 - conformer 2²	-3952.065383	-3951.359406
Int1 - conformer 3²	-3952.060263	-3951.353269
Int1 - conformer 4²	-3952.058102	-3951.352518
TS1 - conformer 1²	-3952.038191	-3951.329258
TS1 - conformer 2²	-3952.028466	-3951.320242
TS1 - conformer 3²	-3952.022438	-3951.311335
TS1 - conformer 4²	-3951.993762	-3951.283073
Int2 - conformer 1²	-3952.095341	-3951.383968
Int2 - conformer 2²	-3952.091626	-3951.377485
Int2 - conformer 3²	-3952.085789	-3951.371693
Int2 - conformer 4²	-3952.061923	-3951.346918

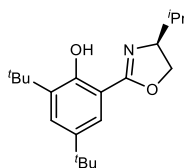
[#]Superscripted 1, 2, 4, and 6 corresponds to the spin multiplicity as singlet, doublet, quartet and sextet, respectively.

Efficacy analysis of ligand in the stereo-determining step

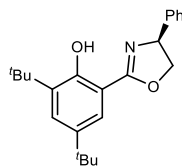
To investigate the effect each substituent of **L7** ligand, three other ligands were considered bearing different substituent pattern such as: the phenyl and di-methyl substituent (**L5** and **L6**) at oxazoline and tertiary-butyl group at the phenyl part of the ligand (**L3**). The effect of the substituents was assessed for the enantio-determining step (Supplementary Figure 36). Due to different alkene coordinating conformation intermediates, the cyclometalated complex was taken as the reference for the reaction profile.



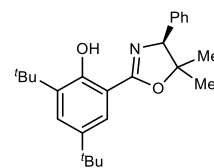
L3



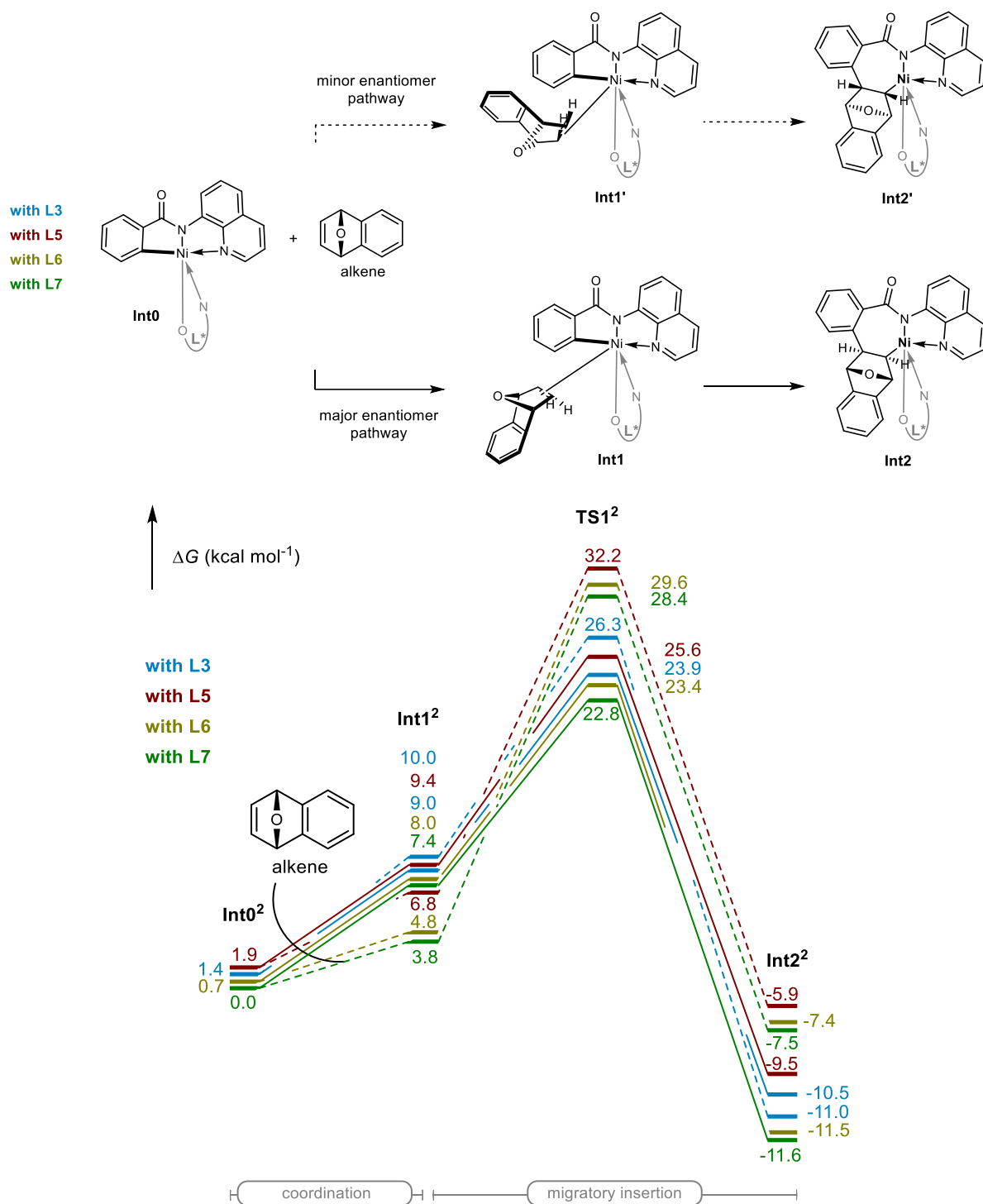
L5



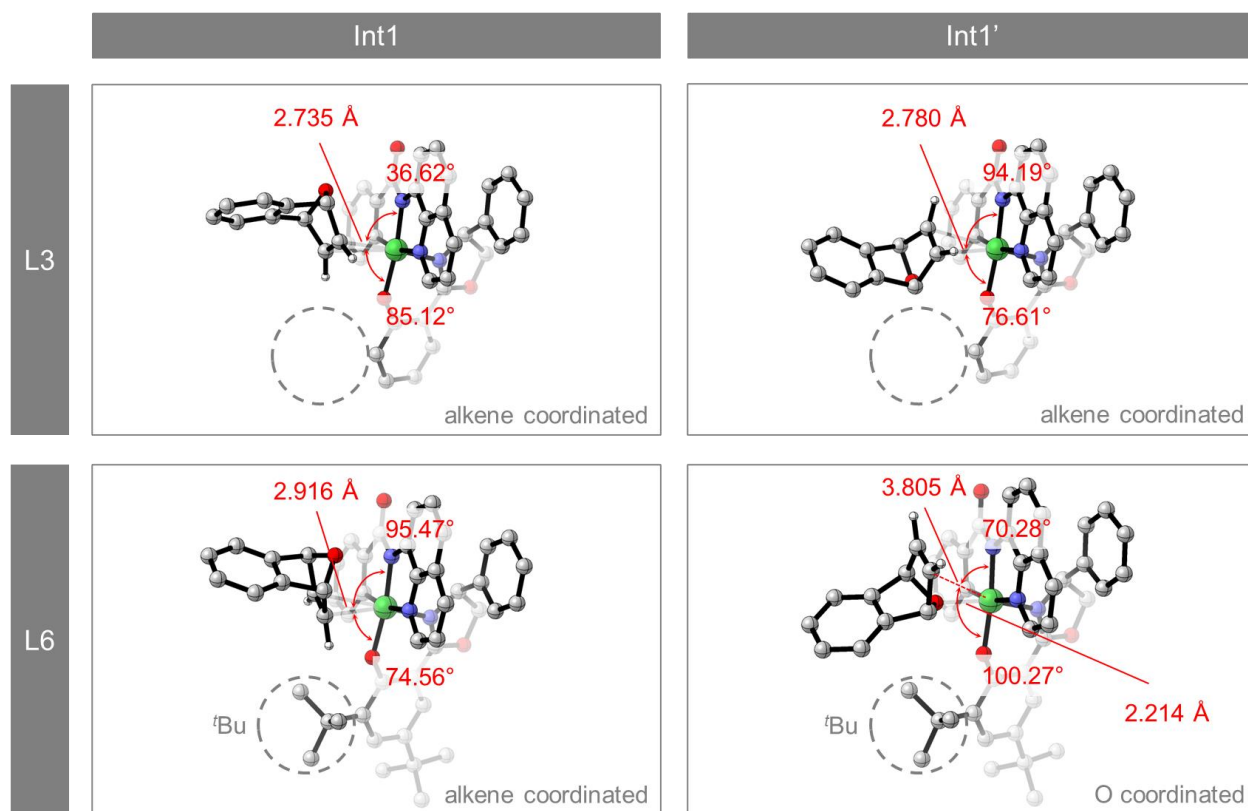
L6



L7

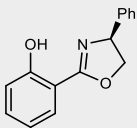
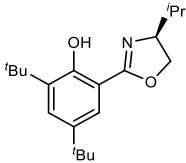
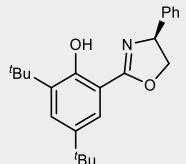
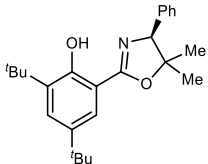


Supplementary Figure 36. Relative Gibbs free energies ($\Delta G_{373.15}$) for the major (—) and minor (---) enantiomer pathways with the four considered ligands for the enantio-determining step in the nickel catalysis. All the computed pathways are for the doublet spin state as the ground state.

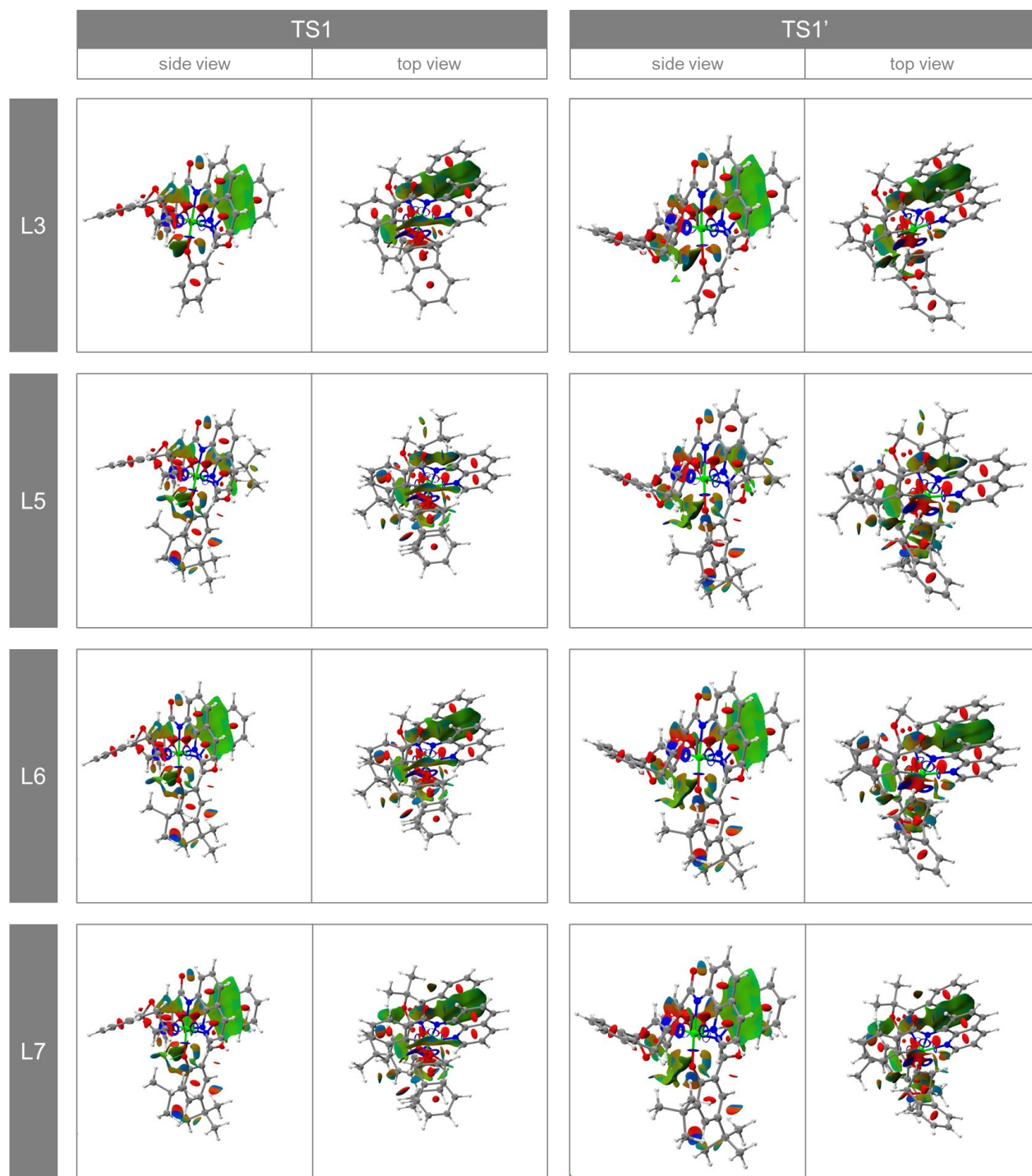


Supplementary Figure 37. 3D structures for the major (**Int1**²) and minor (**Int1'**²) enantiomer with **L3** and **L6** ligand. Non-relevant hydrogens in the transition state structures were omitted for clarity.

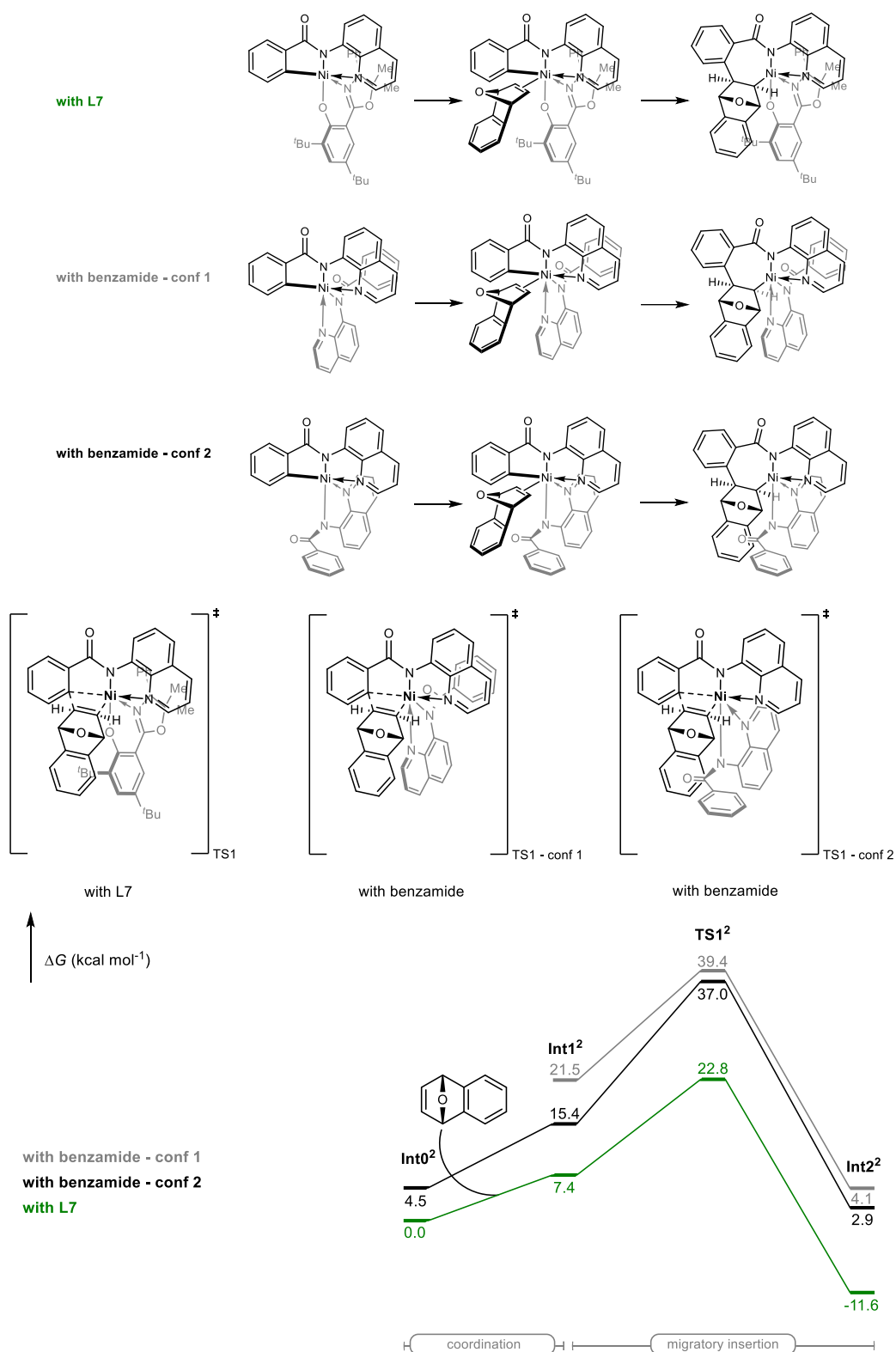
Supplementary Table 16. Calculated electronic and Gibbs free energies ($\Delta G_{373.15}$) at the PW6B95-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory, for the mentioned structures involved in the ligand efficacy analysis in the nickel catalysis (all in Hartree).[#]

Ligand (L*)	Structure	Electronic Energy	Total Gibbs Free Energy
 L3	L3 ¹	-785.952845	-785.781686
	Int0 ²	-3096.411774	-3096.073357
	Int1 ²	-3558.246749	-3557.784821
	Int1' ²	-3558.244864	-3557.783255
	TS1 ²	-3558.227049	-3557.761169
	TS1' ²	-3558.222794	-3557.757301
	Int2 ²	-3558.285037	-3557.815999
	Int2' ²	-3558.286735	-3557.816674
 L5	L5 ¹	-987.681113	-987.308519
	Int0 ²	-3298.136195	-3297.599525
	Int1 ²	-3759.971607	-3759.311121
	Int1' ²	-3759.978166	-3759.315167
	TS1 ²	-3759.950072	-3759.285213
	TS1' ²	-3759.939532	-3759.274800
	Int2 ²	-3760.009955	-3759.341165
	Int2' ²	-3760.004920	-3759.335480
 L6	L6 ¹	-1100.989910	-1100.626073
	Int0 ²	-3411.450844	-3410.918953
	Int1 ²	-3873.286231	-3872.630895
	Int1' ²	-3873.293185	-3872.635943
	TS1 ²	-3873.265365	-3872.606382
	TS1' ²	-3873.255828	-3872.596405
	Int2 ²	-3873.324430	-3872.661899
	Int2' ²	-3873.320544	-3872.655429
 L7	L7 ¹	-1179.760690	-1179.348003
	Int0 ²	-3490.222298	-3489.641971
	Int1 ²	-3952.058160	-3951.353658
	Int1' ²	-3952.065383	-3951.359406
	TS1 ²	-3952.038191	-3951.329258
	TS1' ²	-3952.028466	-3951.320242
	Int2 ²	-3952.095341	-3951.383968
	Int2' ²	-3952.091626	-3951.377485

[#]Superscripted 1, and 2 corresponds to the spin multiplicity as singlet, and doublet respectively.



Supplementary Figure 38. Non-Covalent Interaction (NCI) plot for major (TS1) and minor (TS1') enantiomer pathways with all the four ligands (L3, L5, L6, and L7) made using the NCIPLOT⁵¹ program. Red represents strong repulsive interactions, whereas green and blue represent weak and strong attractive interactions in the plotted surfaces, respectively.



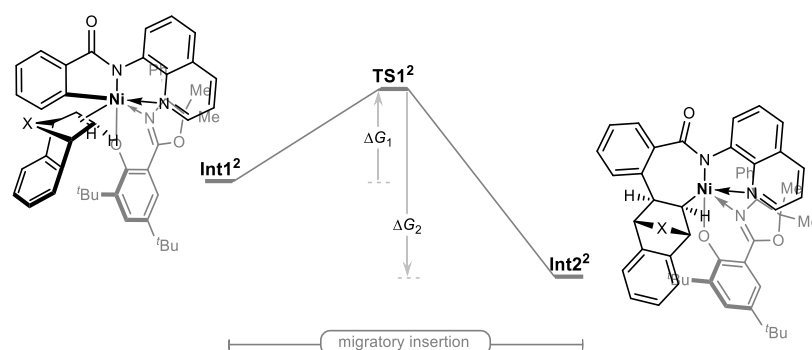
Supplementary Figure 39. Relative Gibbs free energies ($\Delta G_{373.15}$) for the enantio-determining step with a coordinated benzamide as a ligand complex in two conformations (conf 1 and conf 2).

Supplementary Table 17. Calculated electronic and Gibbs free energies ($\Delta G_{373.15}$) at the PW6B95-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory, for all structures involved in the benzamide coordinated complex performing the migratory insertion step in the nickel catalysis (all in Hartree).[#]

Structure	Electronic Energy	Total Gibbs Free Energy
Int0 - conf 2²	-3113.502469	-3113.171220
Int1 - conf 1²	-3575.322600	-3574.867611
Int1 - conf 2²	-3575.334064	-3574.877326
TS1 - conf 1²	-3575.298595	-3574.839122
TS1 - conf 1⁴	-3575.256451	-3574.801601
TS1 - conf 2²	-3575.302777	-3574.842858
TS1 - conf 2⁴	-3575.252350	-3574.797512
TS1 - conf 2⁶	-3575.181448	-3574.731294
Int2 - conf 1²	-3575.359675	-3574.895266
Int2 - conf 2²	-3575.361136	-3574.897312

[#]Superscripted 2, 4, and 6 corresponds to the spin multiplicity as doublet, quartet and sextet, respectively.

Effect of the Oxa-Bridge of the Alkene on the Insertion Step

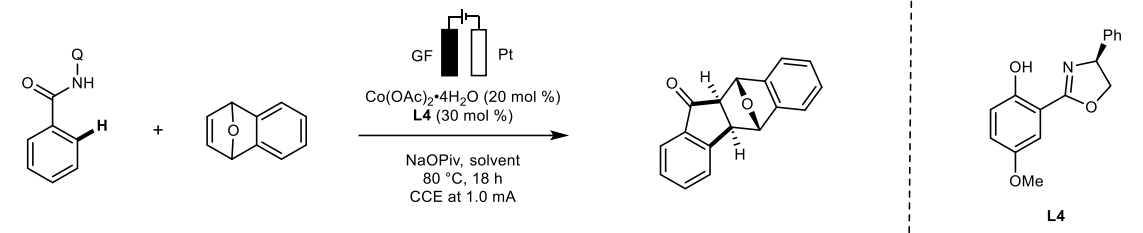


Supplementary Table 18. Computed energy barrier ($\Delta G_{373.15}$) in kcal mol⁻¹ for the migratory insertion of the alkene with bridged atoms as well as in absence of the bridged atom in doublet spin state. Calculations were performed at the PW6B95-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory.

X	ΔG_1 (kcal mol ⁻¹)	ΔG_2 (kcal mol ⁻¹)
O	15.3111	-19.0196
CH₂	18.2712	-12.9604
no bridge	23.2956	-3.5292

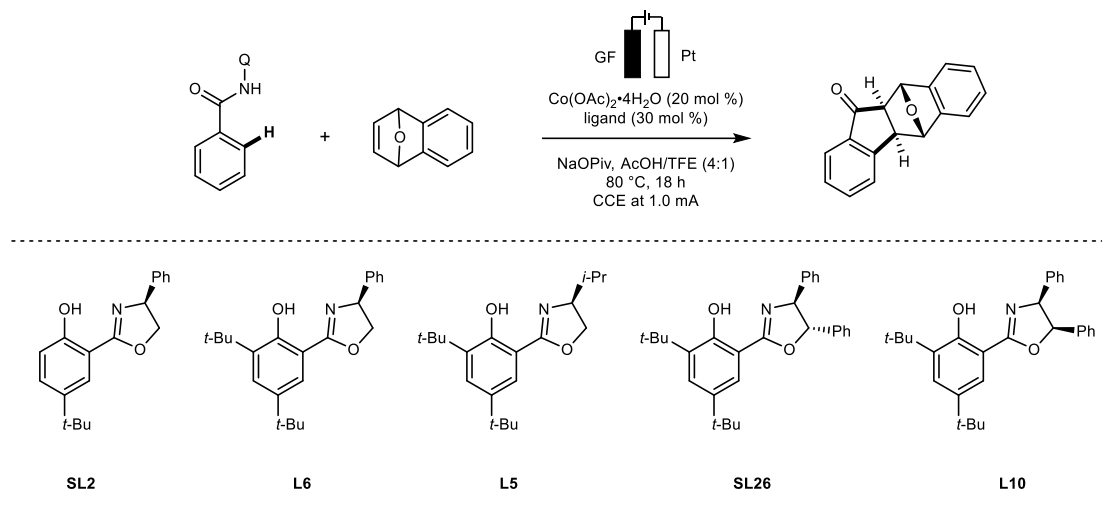
Development of Cobalt Catalysis

Supplementary Table 19. Solvent effect.

			
entry	solvent	yield	e.r.
1	TFE	31%	86.5:13.5
2 ^a	DCE/TFE (4:1)	19%	64.5:35.5
3 ^a	<i>t</i> -AmOH/TFE (4:1)	17%	56.5:43.5
4 ^a	MeCN/TFE (4:1)	12%	67:33
5	AcOH/TFE (4:1)	30%	94:6
6	AcOH/TFE (1:1)	31%	92.5:7.5
7 ^a	DCE/AcOH (1:1)	28%	90:10
8 ^a	AcOH	51%	92.5:7.5

Reaction conditions: amide (0.2 mmol), alkene (0.3 mmol), Co(OAc)₂·4H₂O (0.04 mmol), ligand **L4** (0.06 mmol), NaOPiv (0.6 mmol), solvent (5 mL), undivided cell, graphite felt anode (GF), platinum plate cathode (Pt), 600 rpm stirring rate, constant current electrolysis (CCE) at 1.0 mA, 80 °C, 18 h reaction time. Yields determined by ¹H NMR with 1,3,5-trimethoxybenzene as standard. Enantiomeric ratios (e.r.) determined by chiral HPLC using a chiral stationary phase. [a] *n*-Bu₄NPF₆ (0.02 M). TFE = 2,2,2-trifluoroethanol. DCE = 1,2-dichloroethane.

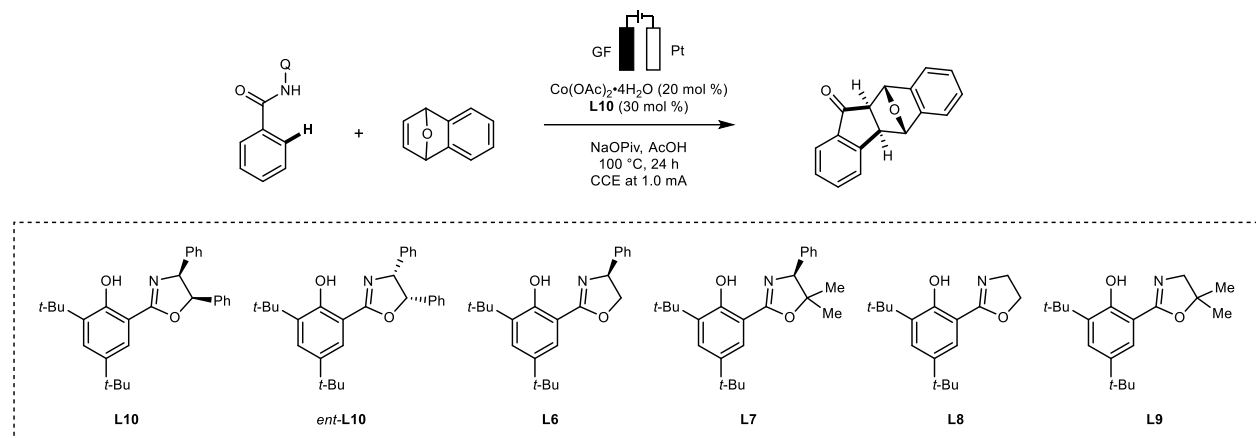
Supplementary Table 20. Optimization – ligand screening.



entry	ligand	yield	e.r.
1	SL2	44%	86.5:13.5
2	L6	40%	94:6
3	L5	24%	88:12
4	SL26	35%	83:17
5	L10	37%	96:4

Reaction conditions: amide (0.2 mmol), alkene (0.3 mmol), $\text{Co(OAc)}_2 \cdot 4\text{H}_2\text{O}$ (0.04 mmol), ligand (0.06 mmol), NaOPiv (0.6 mmol), AcOH/TFE (4:1, v/v, 5 mL), undivided cell, graphite felt anode (GF), platinum plate cathode (Pt), 600 rpm stirring rate, constant current electrolysis (CCE) at 1.0 mA, 80 °C, 18 h reaction time. Yields determined by ^1H NMR with 1,3,5-trimethoxybenzene as standard. Enantiomeric ratios (e.r.) determined by chiral HPLC using a chiral stationary phase. TFE = 2,2,2-trifluoroethanol.

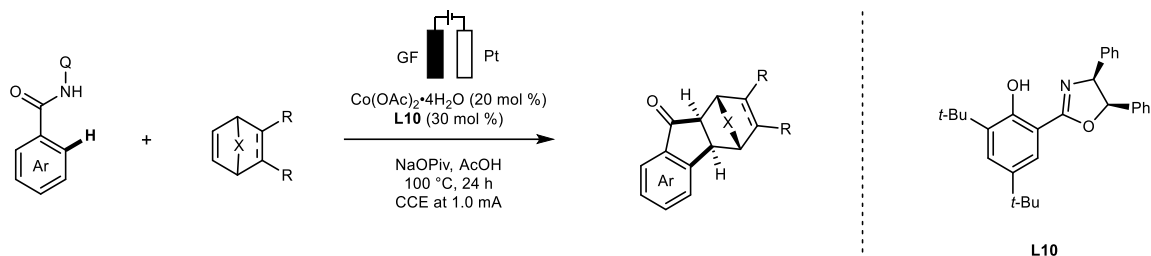
Supplementary Table 21. Optimization – screening of reaction parameters and control experiments.



entry	deviation from standard conditions	yield	e.r.
1	-	75%	95:5
2	addition of <i>n</i> -Bu ₄ NPF ₆ (0.02 M)	66%	95:5
3	addition of <i>n</i> -Bu ₄ NClO ₄ (0.02 M)	39%	94:6
4	$\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (10 mol %), L10 (15 mol %)	47%	93.5:6.5
5	ent-L10 instead of L10	73%	5.5:94.5
6	L6 instead of L10	75%	93.5:6.5
7	L7 instead of L10	50%	91:9
8	L8 instead of L10	53%	50:50
9	L9 instead of L10	78%	50:50
10	No ligand	15%	50:50
11	GF (+) Stainless steel (-)	55%	95:5
12	GF (+) Ni foam (-)	20%	95.5:4.5
13	addition of Cp ₂ Fe (30 mol %)	17%	93:7
14	under nitrogen atmosphere	61%	94:6
15	Ni(OAc) ₂ •4H ₂ O instead of $\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$	n.d.	-
16	no electricity	n.d.	-

Reaction conditions: amide (0.2 mmol), alkene (0.3 mmol), $\text{Co}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (0.04 mmol), ligand **L10** (0.06 mmol), NaOPiv (0.6 mmol), AcOH (5 mL), undivided cell, graphite felt anode (GF), platinum plate cathode (Pt), 600 rpm stirring rate, constant current electrolysis (CCE) at 1.0 mA, 100 °C, 24 h reaction time. Yields determined by ¹H NMR with 1,3,5-trimethoxybenzene as standard. Enantiomeric ratios (e.r.) determined by chiral HPLC using a chiral stationary phase.

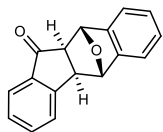
General Procedure for Cobalt Catalysis



The electrolysis was carried out in an undivided cell setup. A GF anode (20 mm × 10 mm × 4 mm) and a platinum plate cathode (20 mm × 10 mm × 0.125 mm) with electrode holders made of stainless steel were used. The cell was charged with the benzamide (0.20 mmol, 1.0 equiv), alkene (0.30 mmol, 1.5 equiv), $\text{Co(OAc)}_2 \cdot 4\text{H}_2\text{O}$ (10 mg, 0.04 mmol), ligand **L10** (25.7 mg, 0.06 mmol), NaOPiv (0.6 mmol), and a teflon-coated magnetic stirring bar (15 × 6 mm). Then AcOH (5.0 mL) was added. The reaction mixture was stirred at 100 °C for 10 min to obtain a homogeneous solution. Subsequently, the electrolysis was performed at 100 °C with a constant current of 1.0 mA maintained for 24 h with a stirring rate of 600 rpm. After completion of the reaction, the reaction mixture was diluted with 2 mL ethyl acetate and transferred to a round bottom flask. The electrodes (platinum plate and graphite felt) were washed in the reaction flask with ethyl acetate (3 × 5 mL) in an ultrasonic cleaner (3 × 3 min) and the washes were combined in the round bottom flask. The solvent was then removed under vacuum and the residue was purified by column chromatography to afford the title compound.

Characterization Data of the Products of Cobalt Catalysis

(4*bR*,5*S*,10*R*,10*aR*)-4*b*,5,10,10*a*-Tetrahydro-11*H*-5,10-epoxybenzo[*b*]fluoren-11-one (**4**)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 4:1) afforded the title compound **4** as a sticky solid (37 mg, 0.15 mmol, 75%), with an enantiomeric ratio of 95:5. Minor amount of the carboamination product was obtained (0.03 mmol). Crystallization of **4** from a saturated solution of chloroform/*i*-propanol yielded crystals suitable for X-ray diffraction analysis.

¹H NMR (400 MHz, CDCl₃) δ 7.77 (d, *J* = 7.6 Hz, 1H), 7.72 – 7.63 (m, 2H), 7.49 – 7.34 (m, 3H), 7.28 – 7.20 (m, 2H), 5.63 (s, 1H), 5.34 (s, 1H), 3.55 (d, *J* = 5.8 Hz, 1H), 2.89 (d, *J* = 5.8 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 204.5 (C_q), 154.4 (C_q), 145.5 (C_q), 144.7 (C_q), 140.0 (C_q), 135.5 (CH), 128.5 (CH), 127.4 (CH), 127.3 (CH), 126.1 (CH), 124.1 (CH), 119.9 (CH), 119.8 (CH), 83.2 (CH), 82.3 (CH), 55.4 (CH), 48.6 (CH) ppm.

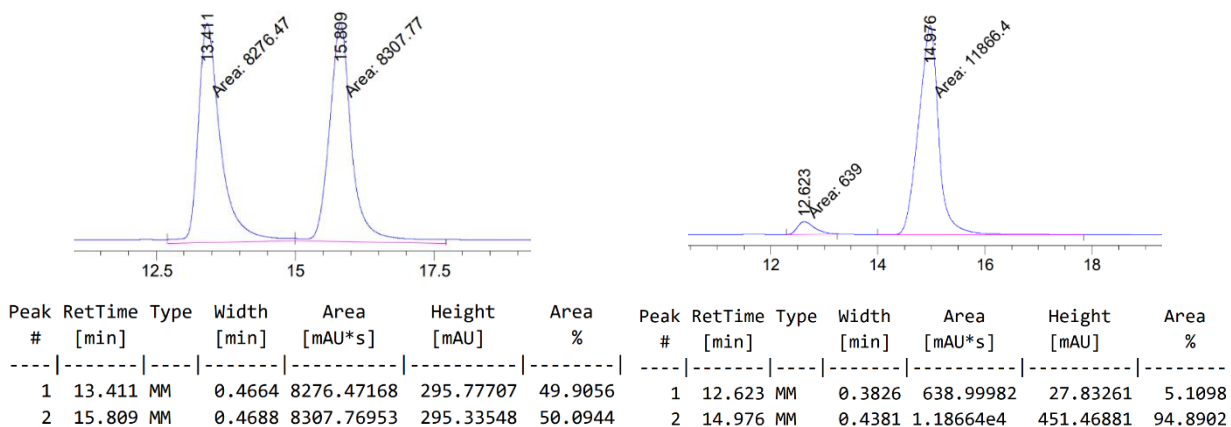
IR (ATR): $\tilde{\nu}$ = 3023, 1702, 1603, 1463, 1282, 1143, 1041, 976, 858, 767 cm⁻¹.

MP: 180-185 °C.

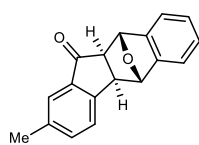
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₃O₂: 249.0910; found: 249.0904.

[α]_D²⁰ = +97.5 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 15.0 min, tr(minor) = 12.6 min, 95:5 e.r.



(5*S*,10*R*)-2-Methyl-4*b*,5,10,10*a*-tetrahydro-11*H*-5,10-epoxybenzo[*b*]fluoren-11-one (39)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane → *n*-hexane/ethyl acetate = 4:1) afforded the title compound **39** as a sticky solid (35 mg, 0.13 mmol, 67%), with an enantiomeric ratio of 94:6. Minor amount of the carboamination product was obtained (0.06 mmol).

¹H NMR (400 MHz, CDCl₃) δ 7.60 – 7.48 (m, 3H), 7.43 – 7.34 (m, 2H), 7.29 – 7.20 (m, 2H), 5.61 (s, 1H), 5.30 (s, 1H), 3.50 (d, *J* = 5.6 Hz, 1H), 2.88 (d, *J* = 5.6 Hz, 1H), 2.42 (s, 3H) ppm.

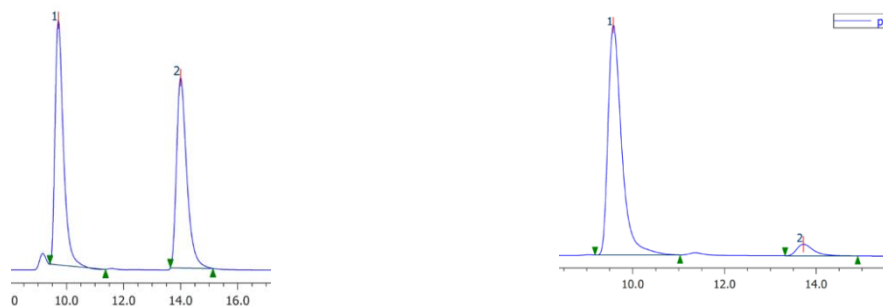
¹³C NMR (101 MHz, CDCl₃) δ 204.7 (C_q), 151.9 (C_q), 145.5 (C_q), 144.7 (C_q), 140.2 (C_q), 138.6 (C_q), 136.7 (CH), 127.4 (CH), 127.2 (CH), 125.8 (CH), 124.1 (CH), 119.9 (CH), 119.8 (CH), 83.2 (CH), 82.2 (CH), 55.8 (CH), 48.2 (CH), 21.3 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2924, 2177, 1709, 1617, 1491, 1285, 859, 813, 748 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₄NaO₂: 285.0891; found: 285.0896.

[α]_D²⁰ = +74.1 (*c* = 0.23, CHCl₃).

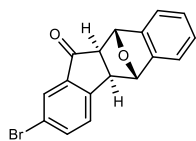
R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 9.6 min, tr(minor) = 13.7 min, 94:6 e.r.



#	Peak Name	CH	tr [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	2	9.710	5191981	253992	51.196	56.203	N/A	5713	7.481	1.565	
2	Unknown	2	13.993	4949434	197925	48.804	43.797	N/A	7788	N/A	1.504	

#	Peak Name	CH	tr [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	9.580	3810966	184074	34.251	95.247	N/A	5601	7.205	1.581	
2	Unknown	9	13.720	232462	9185	5.749	4.753	N/A	7347	N/A	1.525	
Total				4043428	193259		0.00000					

(5*S*,10*R*)-2-Bromo-4b,5,10,10a-tetrahydro-11*H*-5,10-epoxybenzo[*b*]fluoren-11-one (40)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane → *n*-hexane/ethyl acetate = 4:1) afforded the title compound **40** as a sticky solid (45 mg, 0.14 mmol, 69%), with an enantiomeric ratio of 95.5:4.5. Minor amount of the carboamination product was obtained (0.028 mmol).

¹H NMR (400 MHz, CDCl₃) δ 7.88 (s, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.42 – 7.35 (m, 2H), 7.25 – 7.22 (m, 2H), 5.62 (s, 1H), 5.31 (s, 1H), 3.50 (d, *J* = 5.8 Hz, 1H), 2.91 (d, *J* = 5.8 Hz, 1H) ppm.

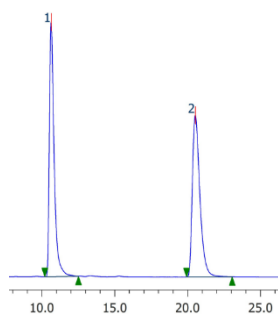
¹³C NMR (101 MHz, CDCl₃) δ 203.1 (C_q), 152.9 (C_q), 145.2 (C_q), 144.4 (C_q), 141.7 (C_q), 138.2 (CH), 127.6 (CH), 127.6 (CH), 127.4 (CH), 127.1 (CH), 122.8 (C_q), 119.9 (CH), 119.8 (CH), 83.0 (CH), 82.4 (CH), 55.9 (CH), 48.3 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 1711, 1596, 1464, 1417, 1185, 980, 858, 747, 629 cm⁻¹.

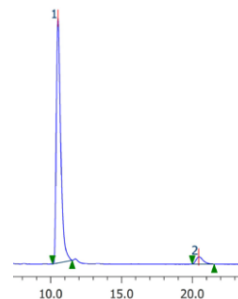
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₁BrNaO₂: 348.9840; found: 348.9836.

[α]_D²⁰ = +16.1 (*c* = 2.7, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 10.5 min, tr(minor) = 20.4 min, 95.5:4.5 e.r.

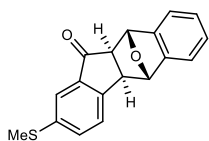


#	Peak Name	CH	tr [min]	Area [μVsec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	2	10.637	7535084	330326	49.938	61.153	N/A	5797	13.429	1.717	
2	Unknown	2	20.527	7553901	209835	50.062	38.847	N/A	7998	N/A	1.511	



#	Peak Name	CH	tr [min]	Area [μVsec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	10.517	4852305	221768	95.506	97.147	N/A	5800	13.530	1.645	
2	Unknown	9	20.443	228341	6512	4.494	2.853	N/A	7920	N/A	1.464	
Total				5080646	228280			0.00000				

(4bR,5S,10R,10aR)-2-(Methylthio)-4b,5,10,10a-tetrahydro-11H-5,10-epoxybenzo[b]fluoren-11-one (41)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 5:1) afforded the title compound **41** as a sticky solid (29 mg, 0.10 mmol, 48%), with an enantiomeric ratio of 91.5:8.5. Minor amount of the carboamination product was obtained (0.06 mmol).

¹H NMR (400 MHz, CDCl₃) δ 7.60 – 7.54 (m, 3H), 7.44 – 7.38 (m, 1H), 7.38 – 7.33 (m, 1H), 7.25 – 7.18 (m, 2H), 5.61 (s, 1H), 5.30 (s, 1H), 3.49 (d, *J* = 5.7 Hz, 1H), 2.89 (d, *J* = 5.7 Hz, 1H), 2.52 (s, 3H) ppm.

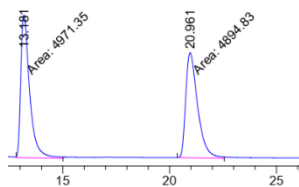
¹³C NMR (101 MHz, CDCl₃) δ 204.1 (C_q), 151.3 (C_q), 145.4 (C_q), 144.5 (C_q), 140.6 (C_q), 140.2 (C_q), 134.1 (CH), 127.5 (CH), 127.3 (CH), 126.1 (CH), 120.2 (CH), 119.9 (CH), 119.8 (CH), 83.1 (CH), 82.2 (CH), 55.8 (CH), 48.2 (CH), 15.8 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2923, 1706, 1472, 1194, 1146, 980, 857, 748, 636 cm⁻¹.

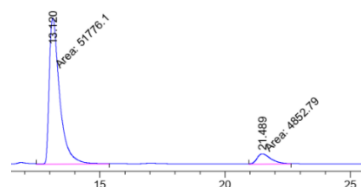
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₅O₂S: 295.0793; found: 295.0781.

[α]_D²⁰ = +84.6 (*c* = 0.5, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 13.1 min, tr(minor) = 21.5 min, 91.5:8.5 e.r.

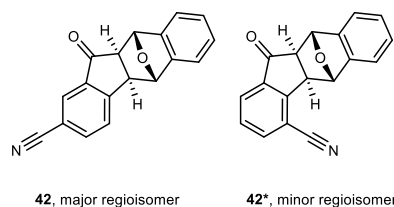


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.181	MM	0.4828	4971.34912	171.61287	50.3878
2	20.961	MM	0.6452	4894.82617	126.45004	49.6122



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.120	MM	0.4816	5.17761e4	1791.67029	91.4305
2	21.489	MM	0.6421	4852.78711	125.97066	8.5695

(4*b*R,5*S*,10*R*,10*a*R)-11-Oxo-4*b*,10,10*a*,11-tetrahydro-5*H*-5,10-epoxybenzo[*b*]fluorene-2-carbonitrile (42) and **(4*b*R,5*S*,10*R*,10*a*R)-11-oxo-4*b*,10,10*a*,11-tetrahydro-5*H*-5,10-epoxybenzo[*b*]fluorene-4-carbonitrile (42*)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 1:3) afforded the title compounds **42** (26 mg, 0.094 mmol, 47%) with an enantiomeric ratio of 94.5:5.5 and **42*** (7.7 mg, 0.028 mmol, 14%) with an enantiomeric ratio of 96.5:3.5 as sticky solids.

Regioisomer 42

¹H NMR (400 MHz, CDCl₃) δ 8.03 (s, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.52 – 7.35 (m, 2H), 7.33 – 7.22 (m, 2H), 5.65 (s, 1H), 5.36 (s, 1H), 3.62 (d, *J* = 6.0 Hz, 1H), 2.96 (d, *J* = 6.0 Hz, 1H) ppm.

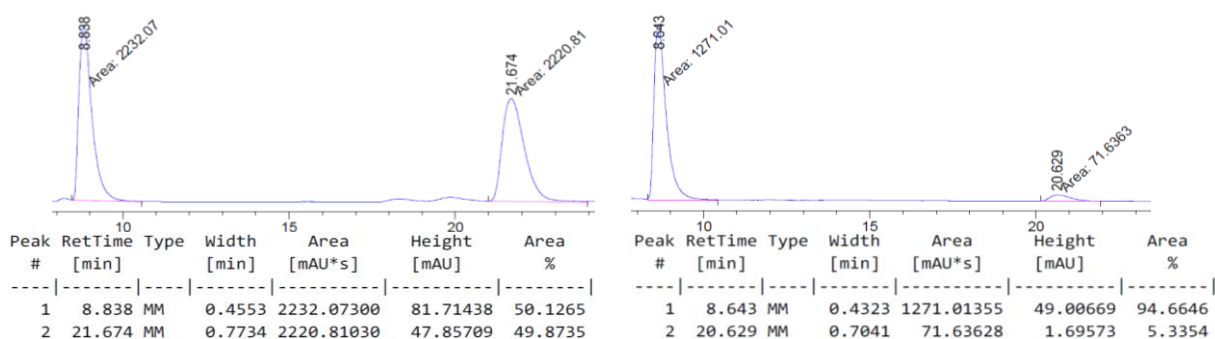
¹³C NMR (101 MHz, CDCl₃) δ 202.4 (C_q), 158.2 (C_q), 144.9 (C_q), 144.2 (C_q), 140.5 (C_q), 138.0 (CH), 128.2 (CH), 127.8 (CH), 127.6 (CH), 127.3 (CH), 120.0 (CH), 119.9 (CH), 117.9 (C_q), 112.9 (C_q), 83.1 (CH), 82.6 (CH), 55.6 (CH), 49.1 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3057, 2229, 1718, 1614, 1482, 1288, 1155, 982, 861, 749 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₂NO₂: 274.0863; found: 274.0854.

[α]_D²⁰ = +52.0 (*c* = 0.5, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 60/40, 1.0 mL/min, 250.4 nm): tr(major) = 8.6 min, tr(minor) = 20.6 min, 94.5:5.5 e.r.



Regioisomer 42*

¹H NMR (400 MHz, CDCl₃) δ 8.08 – 7.85 (m, 2H), 7.62 – 7.56 (m, 1H), 7.55 – 7.45 (m, 1H), 7.44 – 7.34 (m, 1H), 7.33 – 7.19 (m, 2H), 5.67 (s, 1H), 5.59 (s, 1H), 3.75 (d, *J* = 5.9 Hz, 1H), 2.99 (d, *J* = 5.9 Hz, 1H) ppm.

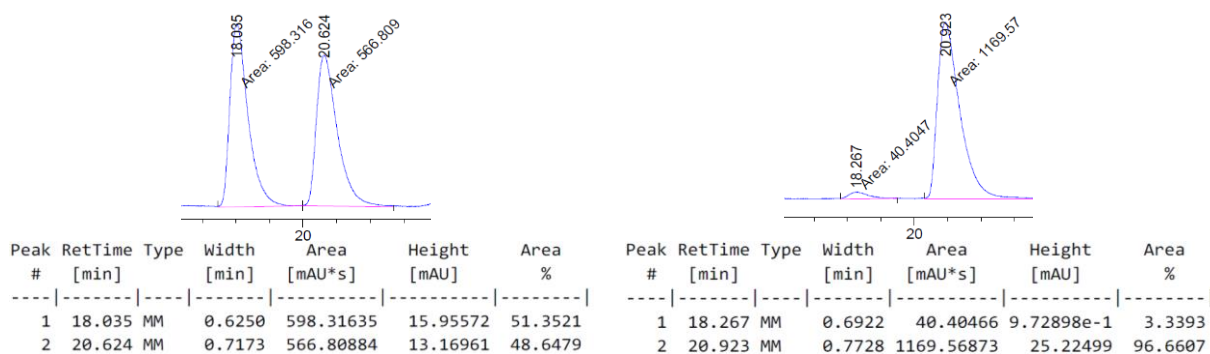
¹³C NMR (101 MHz, CDCl₃) δ 202.5 (C_q), 156.8 (C_q), 144.9 (C_q), 144.0 (C_q), 141.0 (C_q), 138.3 (CH), 129.4 (CH), 128.4 (CH), 127.8 (CH), 127.7 (CH), 120.3 (CH), 119.9 (CH), 116.3 (C_q), 111.0 (C_q), 82.6 (CH), 82.0 (CH), 55.7 (CH), 48.4 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 2929, 2359, 1720, 1583, 1471, 1459, 1328, 1272, 1145, 981 cm⁻¹.

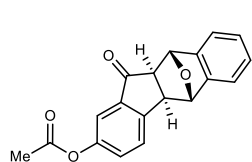
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₂NO₂: 274.0863; found: 274.0859.

[α]_D²⁰ = +9.29 (c = 0.14, CHCl₃).

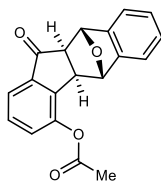
R_t (IA column, *n*-hexane/*i*-PrOH 90/10, 1.0 mL/min, 250.4 nm): tr(major) = 20.9 min, tr(minor) = 18.3 min, 96.5:3.5 e.r.



(4bR,5S,10R,10aR)-11-Oxo-4b,10,10a,11-tetrahydro-5H-5,10-epoxybenzo[b]fluoren-2-yl acetate (43) and **(4bR,5S,10R,10aR)-11-oxo-4b,10,10a,11-tetrahydro-5H-5,10-epoxybenzo[b]fluoren-4-yl acetate (43*)**



43, major regioisomer



43*, minor regioisomer

Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 4:1) afforded the title compounds **43** (31 mg, 0.10 mmol, 51%) with an enantiomeric ratio of 93:7 and **43*** (11 mg, 0.036 mmol, 18%) with an enantiomeric ratio of 91.5:8.5.

Minor amount of the carboamination product was obtained (0.04 mmol). Crystallization of **43** from a saturated solution of chloroform/*i*-propanol yielded crystals suitable for X-ray diffraction analysis.

Regioisomer **43**

¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, *J* = 8.2 Hz, 1H), 7.46 (s, 1H), 7.43 – 7.39 (m, 2H), 7.38 – 7.33 (m, 1H), 7.25 – 7.21 (m, 2H), 5.62 (s, 1H), 5.32 (s, 1H), 3.53 (d, *J* = 5.8 Hz, 1H), 2.93 (d, *J* = 5.8 Hz, 1H), 2.33 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 203.6 (C_q), 169.3 (C_q), 151.6 (C_q), 150.9 (C_q), 145.3 (C_q), 144.5 (C_q), 141.3 (C_q), 129.2 (CH), 127.5 (CH), 127.3 (CH), 126.9 (CH), 119.9 (CH), 119.8 (CH), 116.7 (CH), 83.1 (CH), 82.3 (CH), 56.2 (CH), 48.2 (CH), 21.2 (CH₃) ppm.

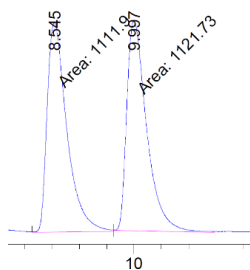
IR (ATR): $\tilde{\nu}$ = 3012, 1765, 1711, 1483, 1370, 1266, 1203, 1183, 1012, 638 cm⁻¹.

MP: 156-158 °C.

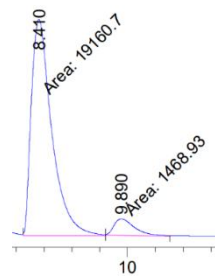
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₅O₄: 307.0965; found: 307.0962.

[α]_D²⁰ = +86.1 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 60/40, 1.0 mL/min, 250.4 nm): tr(major) = 8.4 min, tr(minor) = 9.9 min, 93:7 e.r.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.545	MM	0.4173	1111.90491	44.41251	49.7800
2	9.997	MM	0.4194	1121.73083	44.58188	50.2200



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.410	MM	0.4274	1.91607e4	747.14648	92.8795
2	9.890	MM	0.4300	1468.93066	56.93113	7.1205

Regioisomer **43***

¹H NMR (400 MHz, CDCl₃) δ 7.66 (d, *J* = 7.1 Hz, 1H), 7.51 – 7.42 (m, 2H), 7.39 – 7.32 (m, 2H), 7.31 – 7.20 (m, 2H), 5.63 (s, 1H), 5.36 (s, 1H), 3.47 (d, *J* = 5.7 Hz, 1H), 2.90 (d, *J* = 5.8 Hz, 1H), 2.47 (s, 3H) ppm.

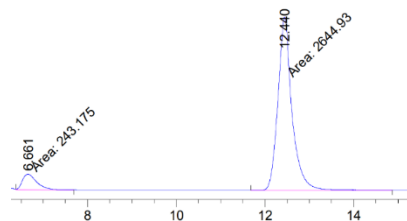
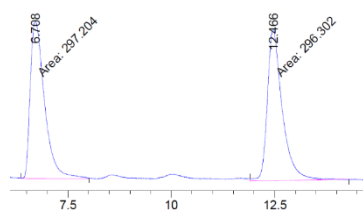
¹³C NMR (101 MHz, CDCl₃) δ 203.6 (C_q), 168.7 (C_q), 148.3 (C_q), 145.4 (C_q), 145.4 (C_q), 144.4 (C_q), 141.9 (C_q), 130.0 (CH), 128.4 (CH), 127.6 (CH), 127.4 (CH), 121.8 (CH), 120.0 (CH), 119.5 (CH), 82.2 (CH), 81.5 (CH), 55.5 (CH), 46.1 (CH), 21.1 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 1964, 1769, 1715, 1371, 1270, 1202, 1180, 882, 762, 636 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₅O₄: 307.0965; found: 307.0968.

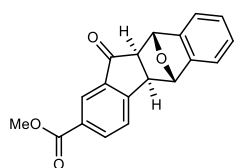
[α]_D²⁰ = +9.20 (c = 0.25, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 60/40, 1.0 mL/min, 250.4 nm): tr(major) = 12.4 min, tr(minor) = 6.7 min, 91.5:8.5 e.r.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.708	MM	0.3997	297.20432	12.39254	50.0760	1	6.661	MM	0.3806	243.17505	10.64953	8.4199
2	12.466	MM	0.4142	296.30209	11.92272	49.9240	2	12.440	MM	0.3703	2644.93164	119.03104	91.5801

Methyl-(4b*R*,5*S*,10*R*,10a*R*)-11-oxo-4*b*,10,10a,11-tetrahydro-5*H*-5,10-epoxybenzo[*b*]fluorene-2-carboxylate (44**)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 4:1) afforded the title compound **44** as a sticky solid (41 mg, 0.13 mmol, 67%), with an enantiomeric ratio of 96.5:3.5.

¹H NMR (400 MHz, CDCl₃) δ 8.42 (s, 1H), 8.36 (d, *J* = 7.9 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.46 – 7.35 (m, 2H), 7.28 – 7.21 (m, 2H), 5.65 (s, 1H), 5.37 (s, 1H), 3.95 (s, 3H), 3.59 (d, *J* = 5.9 Hz, 1H), 2.95 (d, *J* = 5.9 Hz, 1H) ppm.

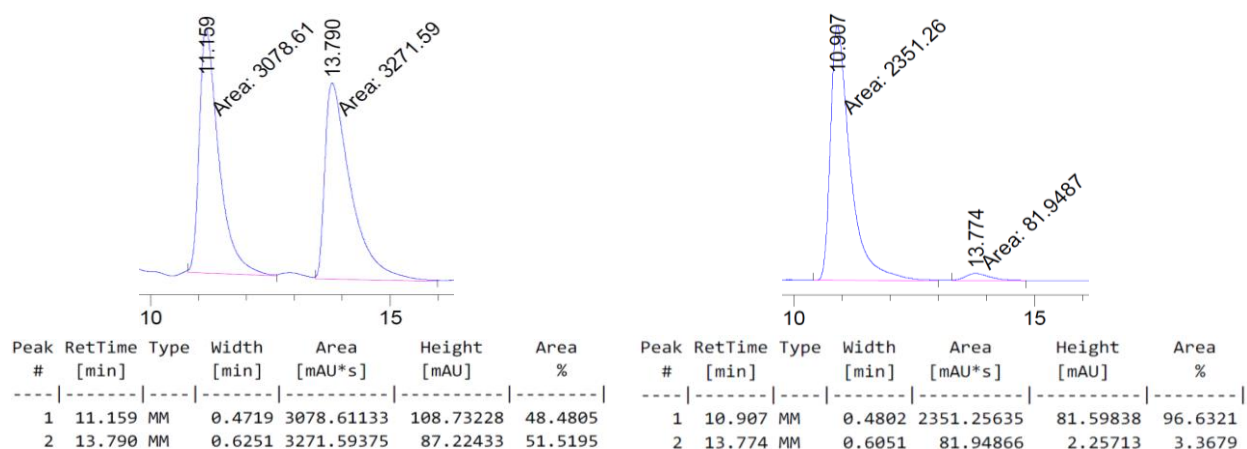
¹³C NMR (101 MHz, CDCl₃) δ 203.6 (C_q), 166.2 (C_q), 158.5 (C_q), 145.2 (C_q), 144.5 (C_q), 140.2 (C_q), 136.2 (CH), 130.9 (C_q), 127.6 (CH), 127.4 (CH), 126.3 (CH), 125.6 (CH), 119.9 (CH), 119.8 (CH), 83.2 (CH), 82.5 (CH), 55.8 (CH), 52.6 (CH₃), 48.8 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 2952, 1711, 1616, 1427, 1304, 1243, 1208, 1112, 975, 748 cm⁻¹.

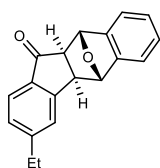
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₅O₄: 307.0965; found: 307.0959.

[α]_D²⁰ = +88.0 (*c* = 0.5, CHCl₃).

R_t (IB column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 10.9 min, tr(minor) = 13.8 min, 96.5:3.5 e.r.



(4bR,5S,10R,10aR)-3-Ethyl-4b,5,10,10a-tetrahydro-11H-5,10-epoxybenzo[b]fluoren-11-one
(45)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 5:1) afforded the title compound **45** as a sticky solid (30 mg, 0.11 mmol, 55%), with an enantiomeric ratio of 92.5:7.5. Minor amount of the carboamination product was obtained (0.06 mmol).

¹H NMR (400 MHz, CDCl₃) δ 7.74 (d, *J* = 7.7 Hz, 1H), 7.56 (s, 1H), 7.50 – 7.40 (m, 2H), 7.39 – 7.26 (m, 3H), 5.67 (s, 1H), 5.40 (s, 1H), 3.56 (d, *J* = 6.0 Hz, 1H), 2.93 (d, *J* = 6.0 Hz, 1H), 2.85 (q, *J* = 7.6 Hz, 2H), 1.38 (t, *J* = 7.6 Hz, 3H) ppm.

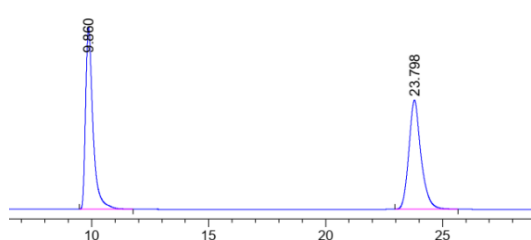
¹³C NMR (101 MHz, CDCl₃) δ 204.0 (C_q), 155.0 (C_q), 153.0 (C_q), 145.6 (C_q), 144.8 (C_q), 138.0 (C_q), 128.7 (CH), 127.4 (CH), 127.2 (CH), 125.2 (CH), 124.1 (CH), 119.8 (CH), 119.7 (CH), 83.2 (CH), 82.2 (CH), 55.7 (CH), 48.4 (CH), 29.6 (CH₂), 15.4 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2965, 1705, 1607, 1458, 1288, 1146, 979, 845, 761, 646 cm⁻¹.

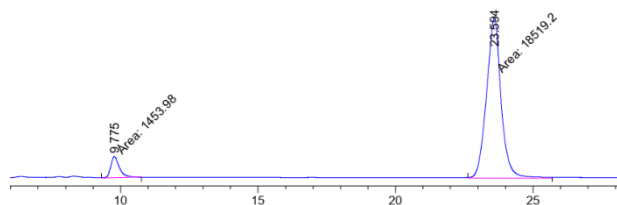
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₇O₂: 277.1229; found: 277.1220.

[α]_D²⁰ = +103.4 (*c* = 0.5, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 23.6 min, tr(minor) = 9.8 min, 92.5:7.5 e.r.

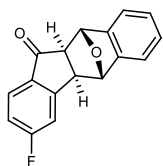


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.860	BB	0.3318	9004.50000	409.11438	50.4561
2	23.798	BB	0.5234	8841.70605	245.35020	49.5439



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.775	MM	0.3663	1453.98157	66.15005	7.2797
2	23.594	MM	0.6103	1.85192e4	505.75339	92.7203

(4bR,5S,10R,10aR)-3-Fluoro-4b,5,10,10a-tetrahydro-11H-5,10-epoxybenzo[b]fluoren-11-one
(46)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 4:1) afforded the title compound **46** as a sticky solid (44 mg, 0.16 mmol, 82%), with an enantiomeric ratio of 96:4. Minor amount of the carboamination product was obtained (0.02 mmol). Crystallization of **46** from a saturated solution of chloroform/*i*-propanol yielded crystals suitable for X-ray diffraction analysis.

¹H NMR (400 MHz, CDCl₃) δ 7.79 (dd, *J* = 8.2, 5.5 Hz, 1H), 7.45 – 7.33 (m, 3H), 7.29 – 7.24 (m, 2H), 7.20 – 7.10 (m, 1H), 5.64 (s, 1H), 5.35 (s, 1H), 3.54 (d, *J* = 5.8 Hz, 1H), 2.94 (d, *J* = 5.8 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 202.6 (C_q), 167.7 (d, *J*_{CF} = 257.4 Hz, C_q), 157.2 (d, *J*_{CF} = 9.7 Hz, C_q), 145.1 (C_q), 144.5 (C_q), 136.4 (C_q), 127.6 (CH), 127.4 (CH), 126.5 (d, *J*_{CF} = 10.5 Hz, CH), 119.9 (CH), 119.8 (CH), 116.8 (d, *J*_{CF} = 23.8 Hz, CH), 112.9 (d, *J*_{CF} = 22.3 Hz, CH), 83.0 (CH), 82.3 (CH), 55.8 (CH), 48.4 (CH) ppm.

¹⁹F NMR (377 MHz, CDCl₃) δ –101.6 ppm.

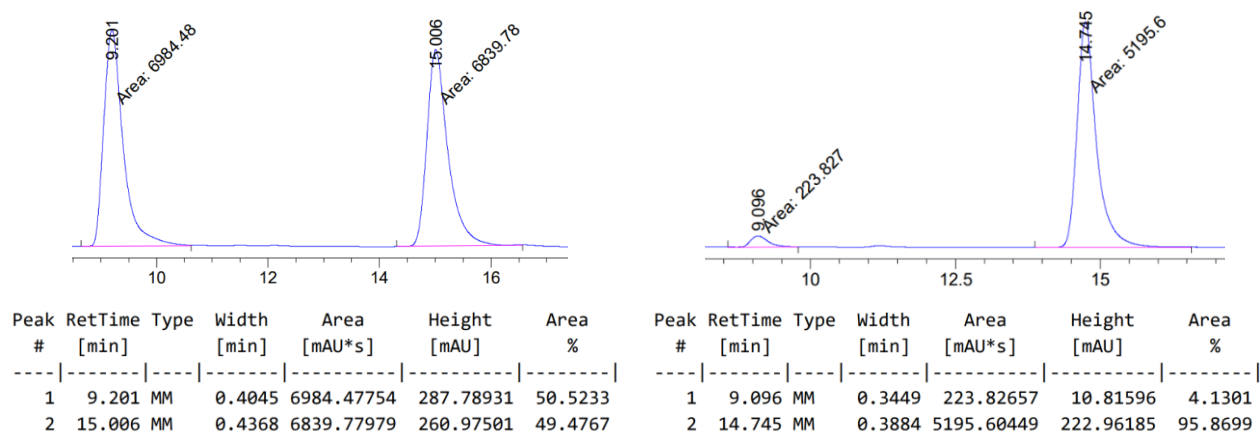
IR (ATR): $\tilde{\nu}$ = 3004, 1709, 1615, 1592, 1483, 1460, 1248, 1137, 1088, 747 cm^{–1}.

MP: 224–229 °C.

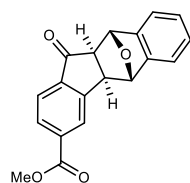
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₂FO₂: 267.0816; found: 267.0847.

[α]_D²⁰ = +103.2 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 14.7 min, tr(minor) = 9.1 min, 96:4 e.r.



Methyl (4b*R*,5*S*,10*R*,10a*R*)-11-oxo-4b,10,10a,11-tetrahydro-5*H*-5,10-epoxybenzo[*b*]fluorene-3-carboxylate (47)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 4:1) afforded the title compound **47** as a sticky solid (43 mg, 0.14 mmol, 70%), with an enantiomeric ratio of 96:4. Minor amount of the carboamination product was obtained (0.014 mmol).

¹H NMR (400 MHz, CDCl₃) δ 8.36 (s, 1H), 8.10 (d, *J* = 8.1 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.48 – 7.34 (m, 2H), 7.29 – 7.21 (m, 2H), 5.64 (s, 1H), 5.38 (s, 1H), 3.99 (s, 3H), 3.60 (d, *J* = 5.9 Hz, 1H), 2.94 (d, *J* = 5.7 Hz, 1H) ppm.

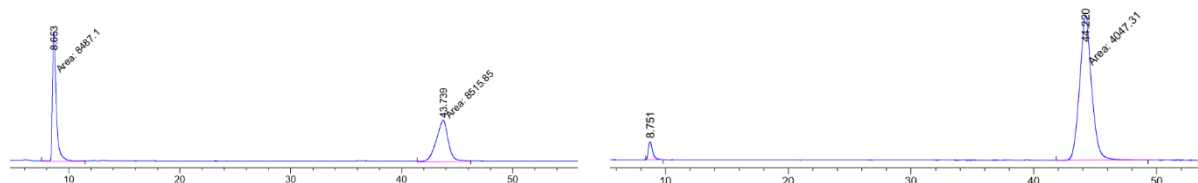
¹³C NMR (101 MHz, CDCl₃) δ 204.0 (C_q), 166.3 (C_q), 154.2 (C_q), 145.3 (C_q), 144.5 (C_q), 143.1 (C_q), 136.2 (C_q), 129.7 (CH), 127.6 (CH), 127.5 (CH), 127.5 (CH), 124.0 (CH), 119.9 (CH), 119.9 (CH), 83.2 (CH), 82.5 (CH), 55.9 (CH), 52.8 (CH₃), 48.6 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 2952, 1713, 1438, 1305, 1274, 1217, 1142, 979, 850, 758 cm⁻¹.

HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₉H₁₅O₄: 307.0970; found: 307.0956.

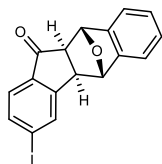
[α]_D²⁰ = +98.8 (*c* = 0.33, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 44.2 min, tr(minor) = 8.8 min, 96:4 e.r.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %	Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.653	MM	0.4126	8487.09668	342.82516	49.9154	1	8.751	BB	0.3296	177.28110	7.45116	4.1964
2	43.739	MM	1.2849	8515.85254	110.46417	50.0846	2	44.220	MM	1.1332	4047.30615	59.52468	95.8036

(4bR,5S,10R,10aR)-3-Iodo-4b,5,10,10a-tetrahydro-11H-5,10-epoxybenzo[*b*]fluoren-11-one
(48)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 5:1) afforded the title compound **48** as a sticky solid (37 mg, 0.10 mmol, 49%), with an enantiomeric ratio of 95.5:4.5. Minor amount of the carboamination product was obtained (0.04 mmol).

¹H NMR (400 MHz, CDCl₃) δ 8.11 (s, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.44 – 7.31 (m, 2H), 7.28 – 7.20 (m, 2H), 5.61 (s, 1H), 5.34 (s, 1H), 3.51 (d, *J* = 5.8 Hz, 1H), 2.86 (d, *J* = 5.8 Hz, 1H) ppm.

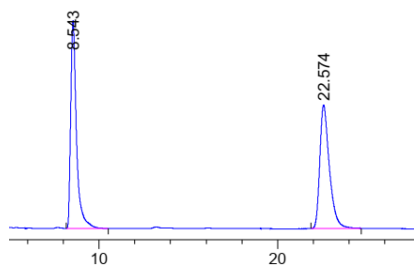
¹³C NMR (101 MHz, CDCl₃) δ 203.6 (C_q), 155.8 (C_q), 145.2 (C_q), 144.5 (C_q), 139.3 (C_q), 137.9 (CH), 135.6 (CH), 127.6 (CH), 127.4 (CH), 125.2 (CH), 119.9 (CH), 119.8 (CH), 104.0 (C_q), 83.1 (CH), 82.3 (CH), 55.4 (CH), 48.1 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3006, 1705, 1588, 1569, 1270, 1216, 976, 839, 754, 639 cm⁻¹.

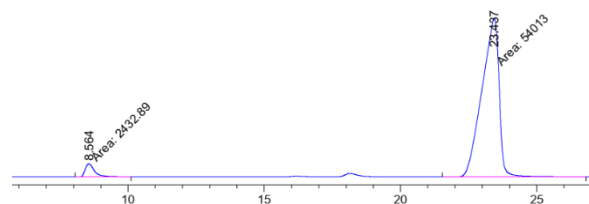
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₂IO₂: 374.9882; found: 374.9864.

[α]_D²⁰ = +98.0 (c = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 273.4 nm): tr(major) = 23.4 min, tr(minor) = 8.6 min, 95.5:4.5 e.r.

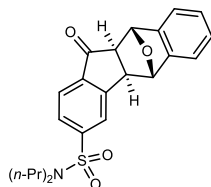


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.543	BB	0.3388	3116.53955	137.82825	50.5700
2	22.574	BB	0.5375	3046.28125	81.79549	49.4300



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.564	MM	0.4016	2432.88940	100.96854	4.3101
2	23.437	MM	0.7314	5.40130e4	1230.87830	95.6899

(4bR,5S,10R,10aR)-11-Oxo-*N,N*-dipropyl-4b,10,10a,11-tetrahydro-5*H*-5,10-epoxybenzo[*b*]fluorene-3-sulfonamide (49)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 3:1) afforded the title compound **49** as a sticky solid (45 mg, 0.11 mmol, 55%), with an enantiomeric ratio of 96:4. Minor amount of the carboamination product was obtained (0.03 mmol).

¹H NMR (400 MHz, CDCl₃) δ 8.16 – 8.13 (m, 1H), 7.86 – 7.80 (m, 2H), 7.46 – 7.42 (m, 1H), 7.39 – 7.35 (m, 1H), 7.28 – 7.22 (m, 2H), 5.64 (s, 1H), 5.36 (s, 1H), 3.61 (d, *J* = 5.9 Hz, 1H), 3.18 – 3.11 (m, 4H), 2.96 (d, *J* = 5.9 Hz, 1H), 1.59 (sextett, *J* = 7.4 Hz, 4H), 0.90 (t, *J* = 7.4 Hz, 1H) ppm.

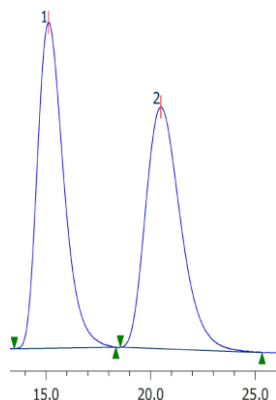
¹³C NMR (101 MHz, CDCl₃) δ 203.4 (C_q), 154.8 (C_q), 146.6 (C_q), 145.0 (C_q), 144.2 (C_q), 142.4 (C_q), 127.7 (CH), 127.5 (CH), 126.9 (CH), 125.0 (CH), 124.8 (CH), 119.9 (CH), 83.2 (CH), 82.5 (CH), 55.8 (CH), 50.2 (CH₂), 48.7 (CH), 22.2 (CH₂), 11.3 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2968, 1718, 1601, 1342, 1188, 1151, 1000, 844, 746, 619 cm⁻¹.

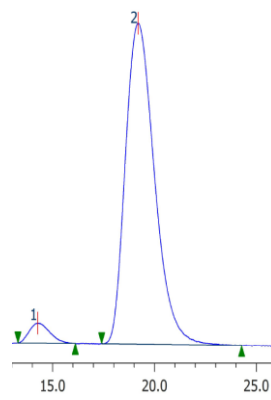
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₃H₂₆O₄SN: 412.1577; found: 412.1582.

[α]_D²⁰ = +103.90 (*c* = 1.0, CHCl₃).

R_t (AS column, *n*-hexane/*i*-PrOH 70/30, 1.0 mL/min, 273.0 nm): tr(major) = 19.2 min, tr(minor) = 14.3 min, 96:4 e.r.

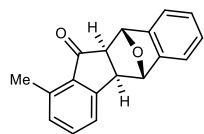


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	10	15.117	2646968	30244	50.247	57.389	N/A	703	2.011	1.377	
2	Unknown	10	20.480	2620946	22456	49.753	42.611	N/A	713	N/A	1.323	



#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	14.273	203081	2898	4.246	5.897	N/A	919	2.198	1.289	
2	Unknown	9	19.193	4580326	46249	95.754	94.103	N/A	869	N/A	1.311	

(4*bR*,5*S*,10*R*,10*aR*)-1-Methyl-4*b*,5,10,10*a*-tetrahydro-11*H*-5,10-epoxybenzo[*b*]fluoren-11-one (50)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 4:1) afforded the title compound **50** as a sticky solid (42 mg, 0.16 mmol, 80%), with an enantiomeric ratio of 93:7.

Minor amount of the carboamination product was obtained (0.02 mmol).

¹H NMR (400 MHz, CDCl₃) δ 7.58 – 7.50 (m, 1H), 7.47 (d, *J* = 7.5 Hz, 1H), 7.44 – 7.36 (m, 2H), 7.25 – 7.21 (m, 2H), 7.17 (d, *J* = 7.2 Hz, 1H), 5.62 (s, 1H), 5.31 (s, 1H), 3.47 (d, *J* = 5.9 Hz, 1H), 2.84 (d, *J* = 6.0 Hz, 1H), 2.66 (s, 3H) ppm.

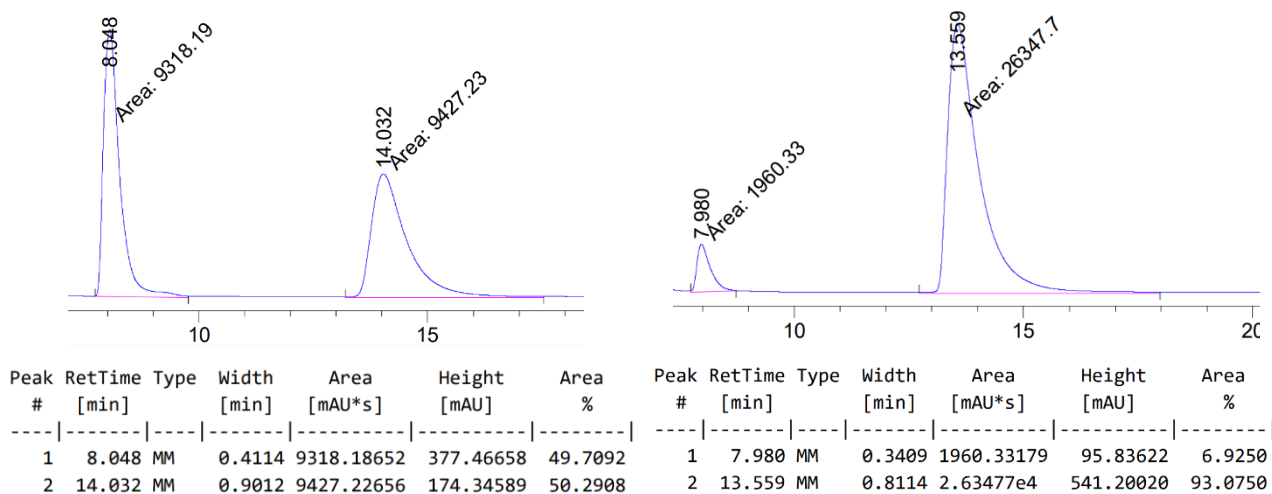
¹³C NMR (101 MHz, CDCl₃) δ 205.3 (C_q), 155.1 (C_q), 145.6 (C_q), 144.7 (C_q), 139.4 (C_q), 137.4 (C_q), 134.8 (CH), 130.3 (CH), 127.3 (CH), 127.2 (CH), 123.4 (CH), 119.9 (CH), 119.7 (CH), 83.4 (CH), 82.4 (CH), 55.5 (CH), 47.8 (CH), 18.6 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3012, 1700, 1594, 1476, 1196, 1141, 979, 853, 757, 637 cm⁻¹.

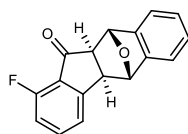
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₅O₂: 263.1067; found: 263.1077.

[α]_D²⁰ = +82.8 (*c* = 1.0, CHCl₃).

R_t (IF column, *n*-hexane/*i*-PrOH 50/50, 1.0 mL/min, 250.4 nm): tr(major) = 13.6 min, tr(minor) = 8.0 min, 93:7 e.r.



(4bR,5S,10R,10aR)-1-Fluoro-4b,5,10,10a-tetrahydro-11H-5,10-epoxybenzo[*b*]fluoren-11-one
(51)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 3:1) afforded the title compound **51** as a sticky solid (30 mg, 0.11 mmol, 56%), with an enantiomeric ratio of 97:3.

¹H NMR (400 MHz, CDCl₃) δ 7.66 (td, *J* = 7.9, 5.0 Hz, 1H), 7.47 – 7.40 (m, 2H), 7.39 – 7.34 (m, 1H), 7.26 – 7.20 (m, 2H), 7.05 (t, *J* = 8.7 Hz, 1H), 5.66 (s, 1H), 5.34 (s, 1H), 3.55 (d, *J* = 5.9 Hz, 1H), 2.92 (d, *J* = 6.0 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 200.9 (d, *J*_{CF} = 1.4 Hz, C_q), 158.8 (d, *J*_{CF} = 265.0 Hz, C_q), 156.5 (d, *J*_{CF} = 2.4 Hz, C_q), 145.2 (C_q), 144.5 (C_q), 137.5 (d, *J*_{CF} = 8.5 Hz, CH), 127.6 (CH), 127.4 (CH), 122.0 (d, *J*_{CF} = 4.2 Hz, CH), 120.0 (CH), 119.8 (CH), 115.5 (d, *J*_{CF} = 19.3 Hz, CH), 83.4 (CH), 82.4 (CH), 56.0 (CH), 48.6 (CH) ppm.

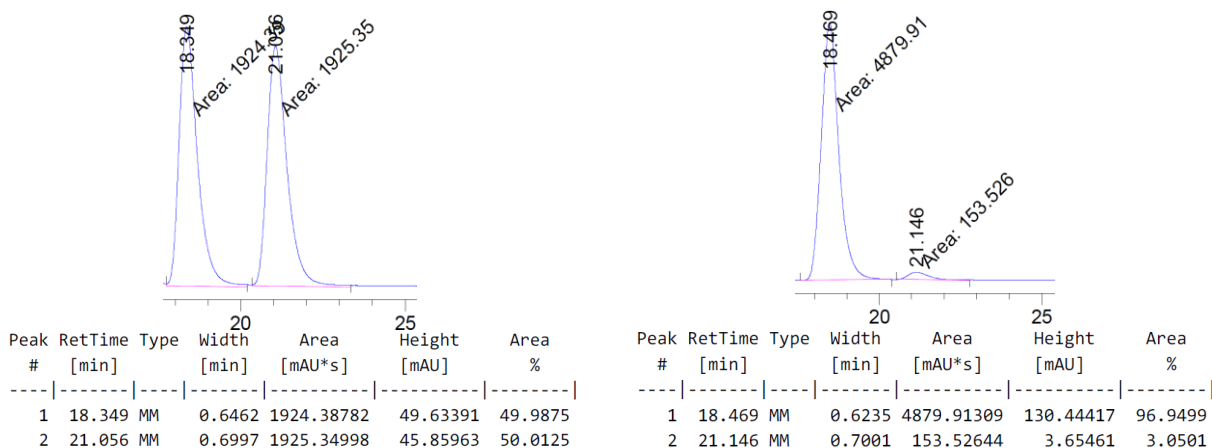
¹⁹F NMR (282 MHz, CDCl₃) δ –113.9 ppm.

IR (ATR): $\tilde{\nu}$ = 2996, 1710, 1615, 1475, 1142, 977, 855, 785, 769, 640 cm^{–1}.

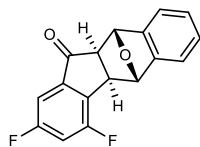
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₂O₂F: 267.0816; found: 267.0812.

[α]_D²⁰ = +92.40 (*c* = 0.25, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 85/15, 1.0 mL/min, 250.4 nm): tr(major) = 18.5 min, tr(minor) = 21.1 min, 97:3 e.r.



(4bR,5S,10R,10aR)-2,4-Difluoro-4b,5,10,10a-tetrahydro-11H-5,10-epoxybenzo[b]fluoren-11-one (52)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:4) afforded the title compound **52** as a sticky solid (46 mg, 0.16 mmol, 82%), with an enantiomeric ratio of 94.5:5.5.

¹H NMR (400 MHz, CDCl₃) δ 7.47 – 7.41 (m, 1H), 7.40 – 7.33 (m, 1H), 7.27 – 7.22 (m, 3H), 7.17 – 7.08 (m, 1H), 5.61 (s, 1H), 5.43 (s, 1H), 3.61 (d, *J* = 6.9 Hz, 1H), 2.95 (d, *J* = 5.8 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 202.2 (dd, *J*_{CF} = 2.9 Hz, C_q), 163.4 (dd, *J*_{CF} = 252.7, 9.4 Hz, C_q), 159.8 (dd, *J*_{CF} = 253.9, 11.6 Hz, C_q), 145.0 (C_q), 144.1 (C_q), 143.2 (dd, *J*_{CF} = 8.4, 5.8 Hz, C_q), 136.0 (dd, *J*_{CF} = 18.7, 2.7 Hz, C_q), 127.7 (CH), 127.6 (CH), 120.1 (CH), 119.9 (CH), 110.3 (dd, *J*_{CF} = 27.4, 23.7 Hz, CH), 106.4 (dd, *J*_{CF} = 22.1, 4.3 Hz, CH), 82.2 (CH), 81.5 (CH), 55.9 (CH), 44.9 (d, *J*_{CF} = 1.3 Hz, CH) ppm.

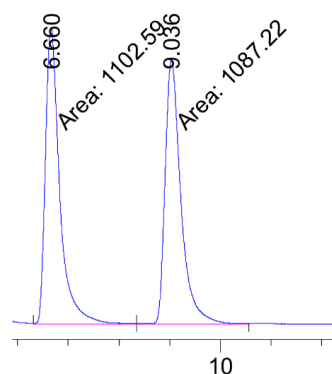
¹⁹F NMR (377 MHz, CDCl₃) δ -108.1, -115.0 ppm.

IR (ATR): $\tilde{\nu}$ = 1715, 1600, 1481, 1322, 1279, 1122, 1065, 860, 765, 653 cm⁻¹.

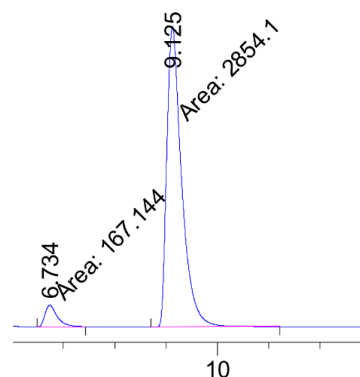
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₁F₂O₂: 285.0722; found: 285.0725.

[α]_D²⁰ = +83.8 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 9.1 min, tr(minor) = 6.7 min, 94.5:5.5 e.r.

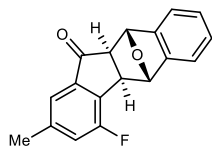


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.660	MF	0.3270	1102.58997	56.20037	50.3508
2	9.036	FM	0.3629	1087.22412	49.93872	49.6492



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.734	MM	0.2747	167.14439	10.13957	5.5323
2	9.125	MM	0.3343	2854.09570	142.30701	94.4677

(4bR,5S,10R,10aR)-4-Fluoro-2-methyl-4b,5,10,10a-tetrahydro-11H-5,10-epoxybenzo[b]fluoren-11-one (53)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:4) afforded the title compound **53** as a sticky solid (39 mg, 0.14 mmol, 70%), with an enantiomeric ratio of 94.5:5.5. Minor amount of the carboamination product was obtained (0.005 mmol).

¹H NMR (400 MHz, CDCl₃) δ 7.48 – 7.41 (m, 1H), 7.39 – 7.33 (m, 2H), 7.25 – 7.21 (m, 2H), 7.20 – 7.16 (m, 1H), 5.60 (s, 1H), 5.42 (s, 1H), 3.59 (d, *J* = 5.8 Hz, 1H), 2.90 (d, *J* = 5.8 Hz, 1H), 2.43 (s, 3H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 203.5 (d, *J*_{CF} = 2.7 Hz, C_q), 159.7 (d, *J*_{CF} = 250.2 Hz, C_q), 145.3 (C_q), 144.4 (C_q), 142.5 (d, *J*_{CF} = 5.1 Hz, C_q), 141.5 (d, *J*_{CF} = 6.2 Hz, C_q), 137.3 (d, *J*_{CF} = 18.7 Hz, C_q), 127.5 (CH), 127.4 (CH), 122.4 (d, *J*_{CF} = 19.6 Hz, CH), 120.1 (CH), 120.0 (CH), 119.8 (CH), 82.2 (CH), 81.6 (CH), 55.8 (CH), 44.9 (CH), 21.3 (d, *J*_{CF} = 1.5 Hz, CH₃) ppm.

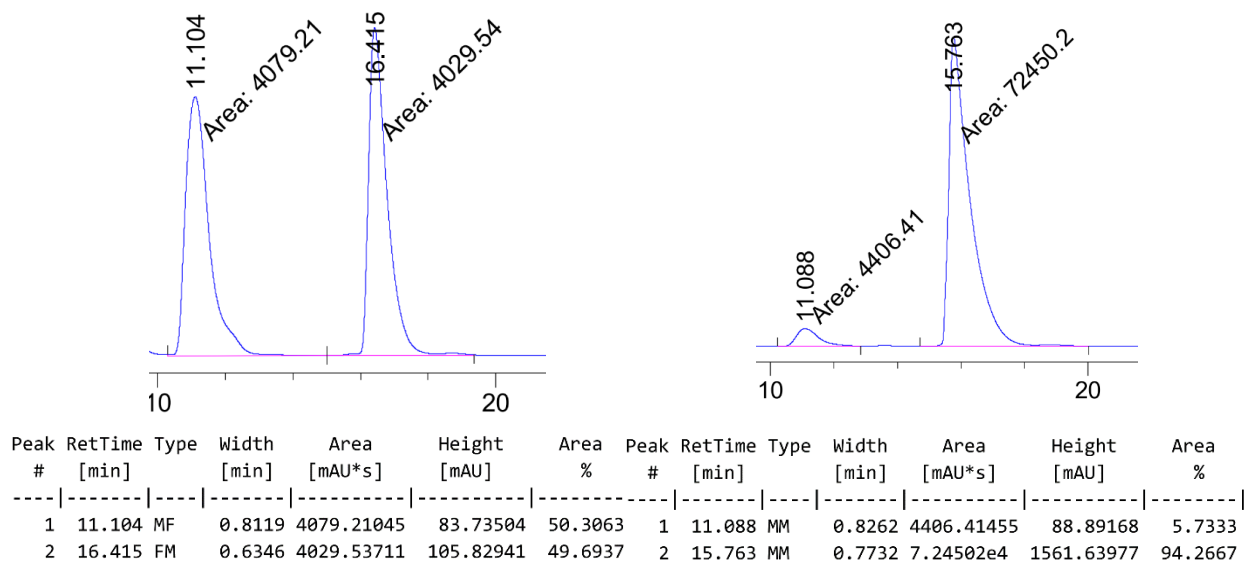
¹⁹F NMR (377 MHz, CDCl₃) δ -120.6 ppm.

IR (ATR): $\tilde{\nu}$ = 3006, 1715, 1487, 1309, 1153, 981, 859, 755, 654, 537 cm⁻¹.

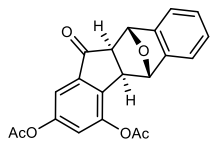
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₈H₁₄F₁O₂: 281.0972; found: 281.0971.

[α]_D²⁰ = +99.3 (c = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 95/5, 1.0 mL/min, 250.4 nm): tr(major) = 15.8 min, tr(minor) = 11.1 min, 94.5:5.5 e.r.



(4*R*,5*S*,10*R*,10*aR*)-11-Oxo-4*b*,10,10*a*,11-tetrahydro-5*H*-5,10-epoxybenzo[*b*]fluorene-2,4-diyl diacetate (54**)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 2:1) afforded the title compound **54** as a sticky solid (29 mg, 0.08 mmol, 40%), with an enantiomeric ratio of 94:6. Minor amount of the carboamination product was obtained (0.04 mmol).

¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, *J* = 1.9 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.33 – 7.29 (m, 1H), 7.26 – 7.21 (m, 2H), 5.62 (s, 1H), 5.34 (s, 1H), 3.45 (d, *J* = 5.9 Hz, 1H), 2.92 (d, *J* = 5.9 Hz, 1H), 2.45 (s, 3H), 2.32 (s, 3H) ppm.

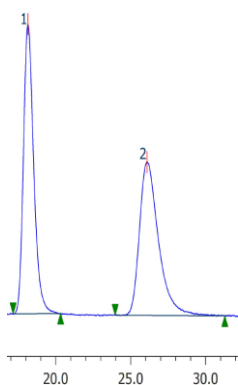
¹³C NMR (101 MHz, CDCl₃) δ 202.6 (C_q), 168.9 (C_q), 168.3 (C_q), 151.5 (C_q), 148.2 (C_q), 145.2 (C_q), 144.3 (C_q), 142.6 (C_q), 142.2 (C_q), 127.7 (CH), 127.4 (CH), 122.3 (CH), 120.0 (CH), 119.5 (CH), 114.4 (CH), 82.2 (CH), 81.4 (CH), 55.9 (CH), 45.9 (CH), 21.2 (CH₃), 21.1 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3004, 1772, 1716, 1476, 1370, 1301, 1190, 1122, 1023, 749 cm⁻¹.

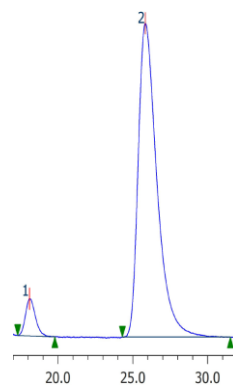
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₁H₁₇O₆: 365.1020; found: 365.1017.

[α]_D²⁰ = -6.80 (*c* = 1.0, CHCl₃).

R_t (IH column, *n*-hexane/*i*-PrOH 60/40, 1.0 mL/min, 250.0 nm): tr(major) = 25.8 min, tr(minor) = 18.1 min, 94:6 e.r.

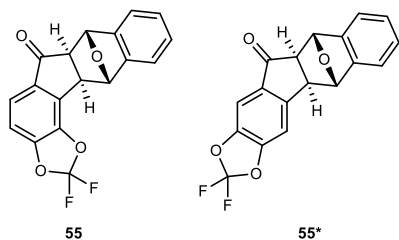


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	18.143	773228	16274	50.358	65.354	N/A	3546	4.655	1.285	
2	Unknown	9	26.093	762222	8627	49.642	34.646	N/A	2239	N/A	1.471	



#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	18.090	186040	4050	5.899	10.604	N/A	3623	4.574	1.283	
2	Unknown	9	25.830	2967741	34146	94.101	89.396	N/A	2224	N/A	1.578	

(6aR,7R,12S,12aR)-2,2-Difluoro-6a,7,12,12a-tetrahydro-6H-7,12-epoxybenzo[6,7]fluoreno[3,4-d][1,3]dioxol-6-one (55) and **(4bR,5S,10R,10aR)-2,2-difluoro-4b,5,10,10a-tetrahydro-11H-5,10-epoxybenzo[6,7]fluoreno[2,3-d][1,3]dioxol-11-one (55*)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:1) afforded the title compounds **55**, with an enantiomeric ratio of 91:9, and **55***, with an enantiomeric ratio of 89:11, (45 mg, 0.14 mmol, 69%) in a regioisomeric ratio of 2.3:1 (determined by ^1H NMR

spectroscopy) as sticky solid.

^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, $J = 8.2$ Hz, 1H, **55**), 7.48 – 7.35 (m, 5H, **55** and **55***), 7.33 (s, 1H, **55***), 7.28 – 7.22 (m, 4H, **55** and **55***), 7.18 (dd, $J = 8.2, 0.6$ Hz, 1H, **55**), 5.63 (s, 1H, **55**), 5.60 (s, 1H, **55***), 5.48 (s, 1H, **55**), 5.29 (s, 1H, **55***), 3.63 (d, $J = 5.9$ Hz, 1H, **55**), 3.52 (d, $J = 5.7$ Hz, 1H, **55***), 2.96 (d, $J = 6.0$ Hz, 1H, **55**), 2.92 (d, $J = 5.7$ Hz, 1H, **55***) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ 202.1 (C_q , **55***), 201.5 (C_q , **55**), 152.0 (C_q , **55***), 149.6 (C_q , **55***), 148.4 (C_q , **55**), 144.9 (C_q , **55***), 144.7 (C_q , **55**), 144.7 (C_q , **55***), 144.3 (C_q , **55***), 144.3 (C_q , **55**), 140.1 (C_q , **55**), 137.1 (C_q , **55**), 136.0 (C_q , **55***), 134.6 (C_q , **55**), 132.1 (t, $J_{\text{CF}} = 258.6$ Hz, C_q , **55**), 131.8 (t, $J_{\text{CF}} = 258.0$ Hz, C_q , **55***), 127.8 (CH, **55**), 127.7 (CH, **55***), 127.6 (CH, **55**), 127.4 (CH, **55***), 120.9 (CH, **55**), 120.0 (CH, **55**), 119.8 (CH, **55***), 119.8 (CH, **55** and **55***), 110.3 (CH, **55**), 106.7 (CH, **55***), 104.4 (CH, **55***), 82.9 (CH, **55***), 82.3 (CH, **55**), 82.2 (CH, **55***), 81.3 (CH, **55**), 55.9 (CH, **55**), 55.9 (CH, **55***), 48.5 (CH, **55***), 44.8 (CH, **55**) ppm.

^{19}F NMR (377 MHz, CDCl_3) δ -48.6 (d, $J_{\text{FF}} = 91.9$ Hz, **55**), -48.9 (d, $J_{\text{FF}} = 92.1$ Hz, **55**), -49.5 (d, $J_{\text{FF}} = 91.2$ Hz, **55***), -49.7 (d, $J_{\text{FF}} = 91.4$ Hz, **55***) ppm.

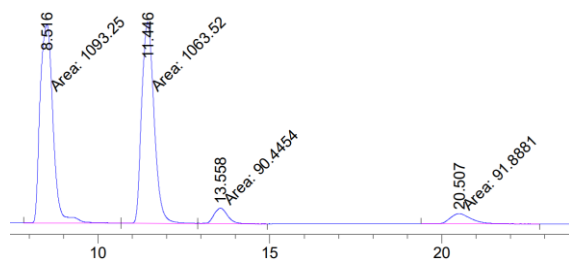
IR (ATR): $\tilde{\nu} = 3013, 1715, 1648, 1471, 1239, 1162, 1092, 860, 831, 756\text{ cm}^{-1}$.

HRMS (ESI): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{11}\text{F}_2\text{O}_4$: 329.0620; found: 329.0626.

$[\alpha]_{\text{D}}^{20}$ = +81.0 ($c = 1.0$, CHCl_3).

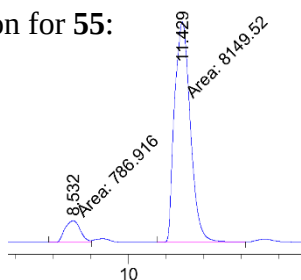
55: **R_t** (IE column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 273.4 nm): $\text{tr}(\text{major}) = 11.4$ min, $\text{tr}(\text{minor}) = 8.5$ min, 91:9 e.r.

55*: **R_t** (IE column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 273.4 nm): $\text{tr}(\text{major}) = 20.1$ min, $\text{tr}(\text{minor}) = 13.6$ min, 89:11 e.r.



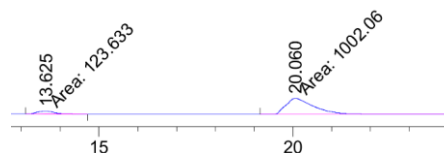
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.516	MF	0.4363	1093.25220	41.76331	46.7380
2	11.446	FM	0.4180	1063.52405	42.40996	45.4670
3	13.558	FM	0.4612	90.44543	3.26880	3.8667
4	20.507	MM	0.7146	91.88815	2.14308	3.9283

Integration for 55:



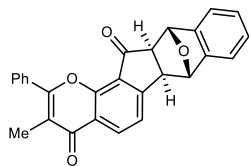
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.532	MM	0.4781	786.91559	27.43388	8.8057
2	11.429	MM	0.4859	8149.51807	279.53589	91.1943

Integration for 55*:



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.625	MM	0.5586	123.63319	3.68895	10.9828
2	20.060	MM	0.8467	1002.06195	19.72485	89.0172

(6b*R*,7*S*,12*R*,12a*R*)-3-Methyl-2-phenyl-6b,7,12,12a-tetrahydro-7,12-epoxybenzo[5,6]indeno[1,2-*h*]chromene-4,13-dione (56)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 3:1) afforded the title compound **56** as a sticky solid (33 mg, 0.08 mmol, 40%), with an enantiomeric ratio of 98:2.

¹H NMR (400 MHz, CDCl₃) δ 8.58 (d, *J* = 8.1 Hz, 1H), 7.85 – 7.80 (m, 2H), 7.65 (dd, *J* = 8.1, 0.7 Hz, 1H), 7.59 – 7.53 (m, 3H), 7.46 – 7.42 (m, 1H), 7.41 – 7.37 (m, 1H), 7.26 – 7.22 (m, 2H), 5.66 (s, 1H), 5.40 (s, 1H), 3.63 (d, *J* = 5.8 Hz, 1H), 2.98 (d, *J* = 5.8 Hz, 1H), 2.26 (s, 3H) ppm.

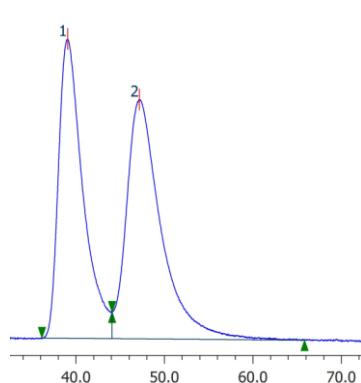
¹³C NMR (101 MHz, CDCl₃) δ 200.3 (C_q), 177.9 (C_q), 161.5 (C_q), 161.0 (C_q), 152.4 (C_q), 145.1 (C_q), 144.3 (C_q), 134.1 (CH), 132.9 (C_q), 130.8 (CH), 129.5 (CH), 128.7 (CH), 128.5 (C_q), 127.7 (CH), 127.5 (CH), 122.5 (C_q), 122.2 (CH), 120.0 (CH), 119.9 (CH), 118.9 (C_q), 82.9 (CH), 82.5 (CH), 56.2 (CH), 48.9 (CH), 12.1 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3004, 1714, 1611, 1433, 1309, 1142, 1053, 863, 753, 697 cm⁻¹.

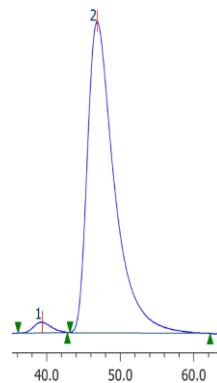
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₇H₁₉O₄: 407.1278; found: 407.1270.

[α]_D²⁰ = +23.20 (*c* = 0.5, CHCl₃).

R_t (IH column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 273.0 nm): tr(major) = 46.9 min, tr(minor) = 39.4 min, 98:2 e.r.

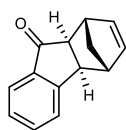


#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	10	39.040	1796840	10236	49.824	57.081	N/A	1154	1.526	1.475	
2	Unknown	10	47.160	1809564	7696	50.176	42.919	N/A	964	N/A	1.607	



#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	10	39.400	124897	755	2.238	3.398	N/A	1233	1.391	1.008	
2	Unknown	10	46.860	5456756	21474	97.762	96.602	N/A	895	N/A	1.785	

(1S,4R,4aR,9aS)-1,4,4a,9a-Tetrahydro-9H-1,4-methanofluoren-9-one (57)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:4) afforded the title compound **57** as a sticky solid (24 mg, 0.12 mmol, 61%), with an enantiomeric ratio of 93:7.

¹H NMR (300 MHz, CDCl₃) δ 7.71 (d, *J* = 7.7 Hz, 1H), 7.66 – 7.54 (m, 1H), 7.52 – 7.45 (m, 1H), 7.41 – 7.32 (m, 1H), 6.40 (dd, *J* = 5.7, 3.0 Hz, 1H), 6.30 (dd, *J* = 5.7, 3.0 Hz, 1H), 3.28 (d, *J* = 6.0 Hz, 1H), 3.14 (s, 1H), 2.92 (s, 1H), 2.64 – 2.59 (m, 1H), 1.40 – 1.30 (m, 1H), 1.00 (d, *J* = 9.3 Hz, 1H) ppm.

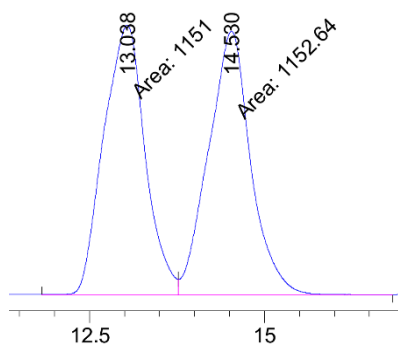
¹³C NMR (101 MHz, CDCl₃) δ 207.3 (C_q), 156.7 (C_q), 141.2 (C_q), 138.8 (CH), 137.9 (CH), 135.0 (CH), 127.8 (CH), 126.0 (CH), 123.8 (CH), 54.6 (CH), 47.4 (CH), 46.5 (CH), 45.6 (CH), 42.4 (CH₂) ppm.

IR (ATR): $\tilde{\nu}$ = 2968, 2930, 1707, 1602, 1463, 1324, 1283, 1207, 759, 697 cm⁻¹.

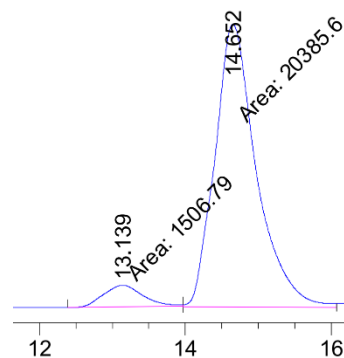
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₄H₁₃O₁: 197.0961; found: 197.0960.

[α]_D²⁰ = +123.0 (*c* = 0.5, CHCl₃).

R_t (IC column, *n*-hexane/*i*-PrOH 95/5, 1.0 mL/min, 250.4 nm): tr(major) = 14.7 min, tr(minor) = 13.1 min, 93:7 e.r.

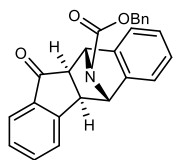


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.038	MF	0.6868	1150.99854	27.92971	49.9643
2	14.530	FM	0.7027	1152.64453	27.33951	50.0357



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.139	MF	0.6320	1506.79199	39.73765	6.8827
2	14.652	MM	0.6582	2.03856e4	516.21930	93.1173

Benzyl (4bR,5S,10R,10aR)-11-oxo-4b,10,10a,11-tetrahydro-5H-5,10-epiminobenzo[b]fluorene-12-carboxylate (58)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:4) afforded the title compound **58** as a sticky solid (43 mg, 0.11 mmol, 56%), with an enantiomeric ratio of 87.5:12.5.

¹H NMR (500 MHz, CDCl₃, 60 °C) δ 7.74 (d, *J* = 7.5 Hz, 1H), 7.70 – 7.62 (m, 2H), 7.46 – 7.40 (m, 2H), 7.38 – 7.34 (m, 1H), 7.25 – 7.23 (m, 3H), 7.22 – 7.18 (m, 2H), 7.08 – 7.00 (m, 2H), 5.53 (s, 1H), 5.27 (s, 1H), 4.86 – 4.70 (m, 2H), 3.50 (d, *J* = 5.9 Hz, 1H), 2.80 (dd, *J* = 5.8, 0.7 Hz, 1H) ppm.

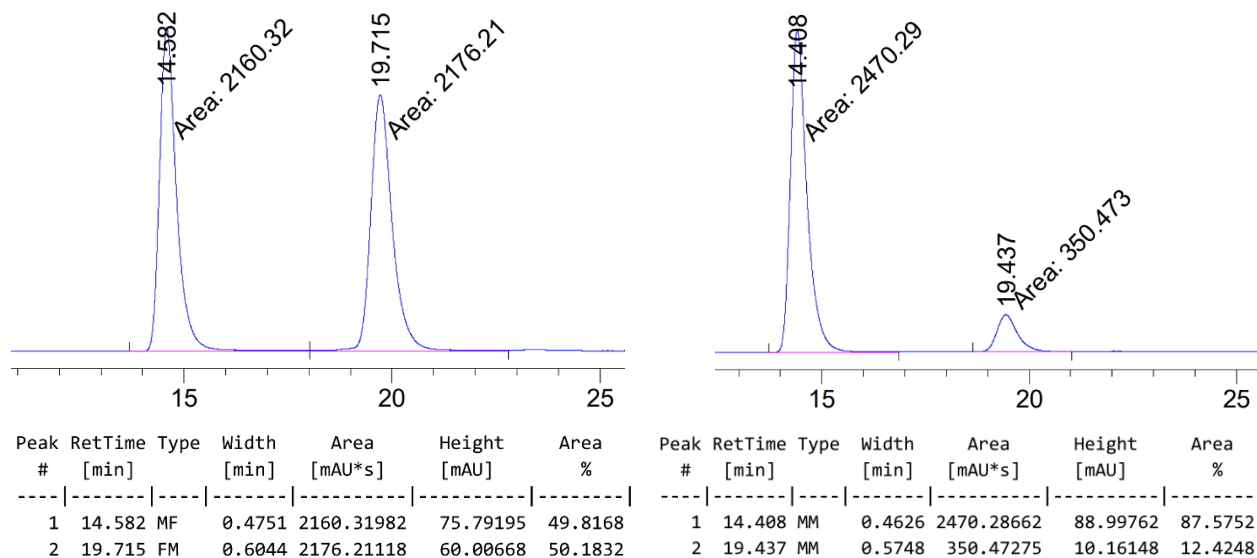
¹³C NMR (126 MHz, CDCl₃, 60 °C) δ 203.2 (C_q), 155.5 (C_q), 153.8 (C_q), 145.5 (C_q), 144.6 (C_q), 140.4 (C_q), 136.4 (C_q), 135.5 (CH), 128.7 (CH), 128.5 (CH), 128.0 (CH), 127.7 (CH), 127.5 (CH), 127.3 (CH), 126.6 (CH), 124.1 (CH), 120.6 (CH), 120.6 (CH), 67.2 (CH₂), 66.0 (CH), 64.6 (CH), 55.6 (CH), 49.0 (CH) ppm.

IR (ATR): $\tilde{\nu}$ = 3027, 1711, 1602, 1461, 1398, 1331, 1281, 1210, 1087, 758 cm⁻¹.

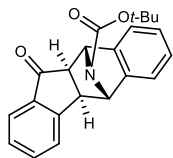
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₅H₂₀N₁O₃: 382.1438; found: 382.1434.

[α]_D²⁰ = +56.4 (*c* = 0.25, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 70/30, 1.0 mL/min, 250.4 nm): tr(major) = 14.4 min, tr(minor) = 19.4 min, 87.5:12.5 e.r.



***tert*-Butyl (4b*R*,5*S*,10*R*,10a*R*)-11-oxo-4b,10,10a,11-tetrahydro-5*H*-5,10-epiminobenzo[*b*]fluorene-12-carboxylate (**59**)**



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (ethyl acetate/*n*-hexane = 1:4) afforded the title compound **59** as a sticky solid (23 mg, 0.066 mmol, 23%), with an enantiomeric ratio of 95:5.

¹H NMR (500 MHz, CDCl₃, 60 °C) δ 7.75 (d, *J* = 7.7 Hz, 1H), 7.72 – 7.63 (m, 2H), 7.44 – 7.39 (m, 2H), 7.38 – 7.33 (m, 1H), 7.23 – 7.15 (m, 2H), 5.44 (s, 1H), 5.20 (s, 1H), 3.48 (d, *J* = 6.0 Hz, 1H), 2.78 (dd, *J* = 5.9, 0.7 Hz, 1H), 1.14 (s, 9H) ppm.

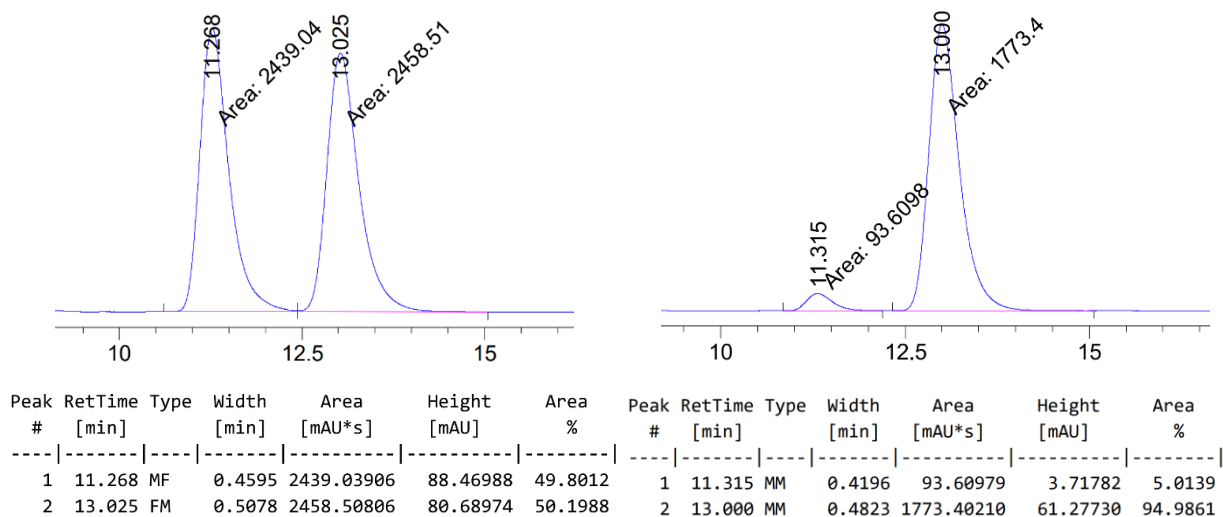
¹³C NMR (126 MHz, CDCl₃, 60 °C) δ 203.5 (C_q), 154.4 (C_q), 154.2 (C_q), 145.8 (C_q), 144.9 (C_q), 140.5 (C_q), 135.4 (CH), 128.6 (CH), 127.2 (CH), 127.0 (CH), 126.7 (CH), 124.2 (CH), 120.5 (CH), 120.4 (CH), 80.4 (C_q), 65.6 (CH), 64.5 (CH), 55.9 (CH), 49.2 (CH), 28.1 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 2972, 2926, 1706, 1466, 1404, 1284, 1176, 1142, 1091, 757 cm⁻¹.

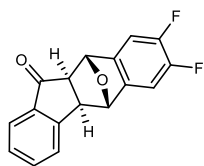
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₂₂H₂₂N₁O₃: 348.1594; found: 348.1590.

[α]_D²⁰ = +59.6 (c = 0.25, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 13.0 min, tr(minor) = 11.3 min, 95:5 e.r.



(4*bR*,5*S*,10*R*,10*aR*)-7,8-Difluoro-4*b*,5,10,10*a*-tetrahydro-11*H*-5,10-epoxybenzo[*b*]fluoren-11-one (60)



Prepared according to general procedure on a 0.2 mmol scale, column chromatography (*n*-hexane/ethyl acetate = 4:1) afforded the title compound **60** as a sticky solid (34 mg, 0.12 mmol, 60%), with an enantiomeric ratio of 95.5:4.5.

¹H NMR (600 MHz, CDCl₃) δ 7.77 (d, *J* = 7.6 Hz, 1H), 7.73 – 7.68 (m, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.50 – 7.42 (m, 1H), 7.29 – 7.23 (m, 1H), 7.19 (dd, *J* = 8.5, 6.9 Hz, 1H), 5.59 (s, 1H), 5.31 (s, 1H), 3.53 (d, *J* = 5.8 Hz, 1H), 2.86 (d, *J* = 5.8 Hz, 1H) ppm.

¹³C NMR (151 MHz, CDCl₃) δ 203.7 (C_q), 153.8 (C_q), 149.9 (dd, *J*_{CF} = 254.2, 19.0 Hz, C_q), 149.5 (*J*_{CF} = 247.2, 12.3 Hz, C_q), 141.4 (dd, *J*_{CF} = 6.3, 3.2 Hz, C_q), 140.7 (dd, *J*_{CF} = 6.3, 3.3 Hz, C_q), 139.9 (C_q), 135.7 (CH), 128.8 (CH), 126.1 (CH), 124.3 (CH), 110.0 (d, *J*_{CF} = 19.9 Hz, CH), 110.0 (d, *J*_{CF} = 20.0 Hz, CH), 82.9 (d, *J*_{CF} = 1.9 Hz, CH), 81.9 (d, *J*_{CF} = 2.2 Hz, CH), 55.2 (CH), 48.4 (CH) ppm.

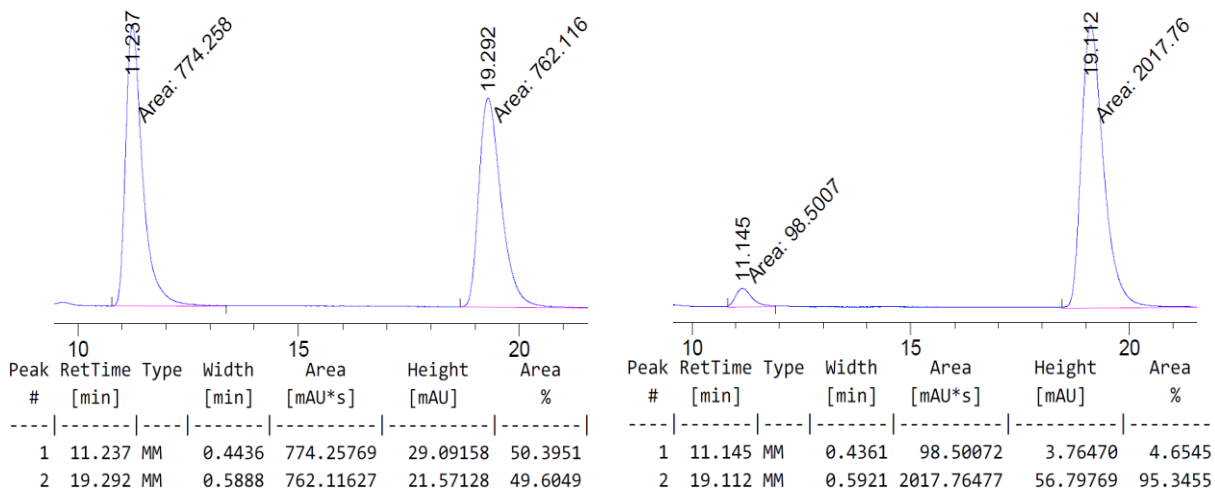
¹⁹F NMR (282 MHz, CDCl₃) δ -138.24 (d, *J*_{FF} = 18.7 Hz), -138.52 (d, *J*_{FF} = 18.7 Hz) ppm.

IR (ATR): $\tilde{\nu}$ = 1703, 1606, 1478, 1360, 1206, 1064, 851 791, 761, 630 cm⁻¹.

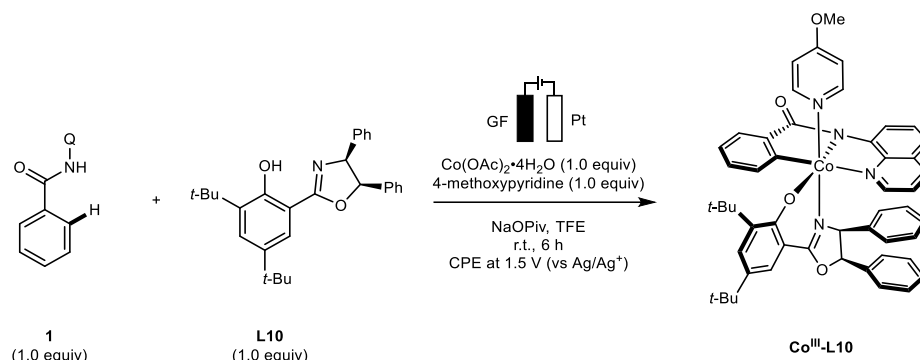
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₁₇H₁₁F₂O₂: 285.0722; found: 285.0699.

[α]_D²⁰ = +76.2 (*c* = 1.0, CHCl₃).

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 19.1 min, tr(minor) = 11.1 min, 95.5:4.5 e.r.



Synthesis of Cyclometalated Cobalt Complex



The electrolysis was carried out in an undivided cell setup. A GF anode (20 mm × 10 mm × 4 mm) and a platinum plate cathode (20 mm × 10 mm × 0.125 mm) with electrode holders made of stainless steel were used. The cell was charged with the amide **1** (25 mg, 0.10 mmol, 1.0 equiv), ligand **L10** (43 mg, 0.10 mmol, 1.0 equiv), Co(OAc)₂·4H₂O (25 mg, 0.10 mmol, 1.0 equiv), 4-methoxypyridine (10 μL, 11 mg, 0.10 mmol, 1.0 equiv), NaOPiv (0.20 mmol, 2.0 equiv), and a teflon-coated magnetic stirring bar (15 × 6 mm). Then, TFE (3.5 mL) was added, and the electrolysis was performed at room temperature with a constant potential of 1.5 V (vs Ag/Ag⁺, silver wire) maintained for 6 h with a stirring rate of 600 rpm. After completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by column chromatography (*n*-hexane/acetone = 3:1), yielding the title compound **Co^{III}-L10** as a yellow solid (50 mg, 60 μmol, 60% yield).

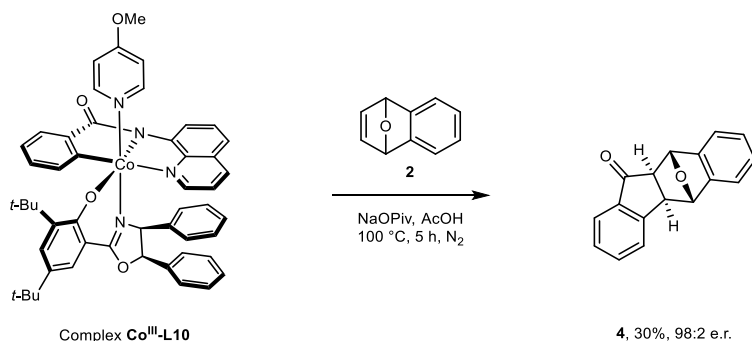
¹H NMR (400 MHz, CDCl₃) δ 9.51 (s, 1H), 9.02 (d, *J* = 8.4 Hz, 1H), 8.03 – 7.86 (m, 3H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.52 – 7.42 (m, 3H), 7.36 – 6.79 (m, 8H), 6.74 – 6.62 (m, 2H), 6.36 – 5.79 (m, 6H), 5.15 (d, *J* = 8.6 Hz, 1H), 4.48 (d, *J* = 8.6 Hz, 1H), 3.58 (s, 3H), 1.41 (s, 9H), 1.31 (s, 9H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ 176.2 (C_q), 168.8 (C_q), 167.3 (C_q), 166.0 (C_q), 164.6 (C_q), 153.0 (CH), 148.0 (C_q), 147.6 (CH), 146.7 (C_q), 146.6 (C_q), 140.9 (C_q), 136.7 (CH), 135.9 (CH), 134.9 (C_q), 134.1 (C_q), 134.0 (C_q), 130.0 (CH), 129.3 (CH), 128.9 (C_q), 128.3 (CH), 127.4 (CH), 127.3 (CH), 127.1 (CH), 126.1 (CH), 126.1 (CH), 125.7 (CH), 124.7 (CH), 123.9 (CH), 123.3 (CH), 121.8 (CH), 120.8 (CH), 117.8 (CH), 109.2 (CH), 109.2 (C_q), 84.7 (CH), 70.2 (CH), 55.3 (CH₃), 35.5 (C_q), 34.1 (C_q), 31.6 (CH₃), 29.8 (CH₃) ppm.

IR (ATR): $\tilde{\nu}$ = 3045, 2954, 1615, 1462, 1434, 1382, 1340, 1210, 1036, 696 cm⁻¹.

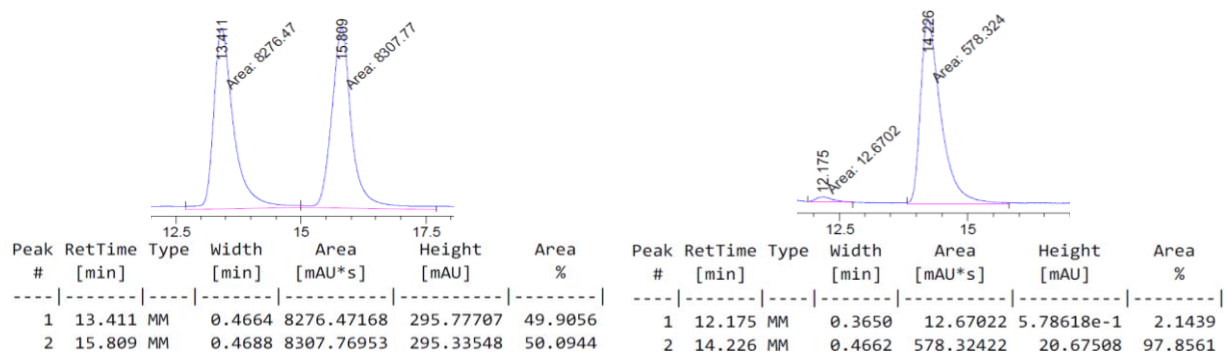
HRMS (ESI): *m/z* [M+H]⁺ calcd for C₅₁H₅₀N₄O₄Co: 841.3159; found: 841.3128.

Reaction Using Cyclometalated Cobalt Complex

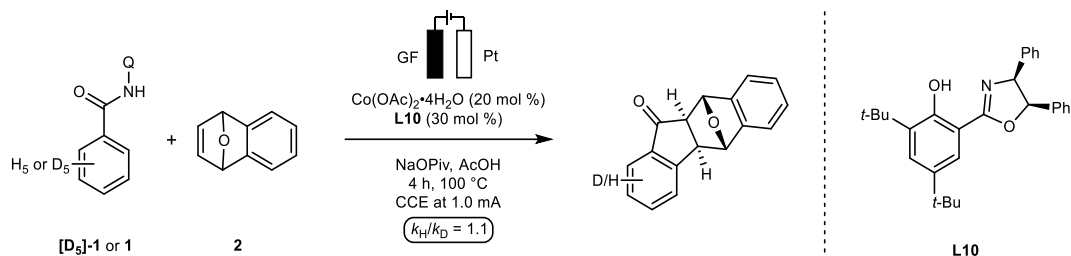


The complex **Co^{III}-L10** (17 mg, 0.020 mmol), alkene **2** (22 mg, 0.15 mmol, 0.06 M), and NaOPiv (0.30 mmol, 0.12 M) were dissolved in acetic acid (2.5 mL). The reaction mixture was heated for 5 h at 100 °C. Next, the solvent was removed under reduced, and triethylamine (1 mL) as added to the residue. Then, the mixture was filtered through a pad of silica and rinsed thoroughly with ethyl acetate (5 mL). After evaporation of the solvent under reduced pressure, the yield was examined with ¹H NMR spectroscopy, utilizing 1,3,5-trimethoxybenzene as the internal standard. Product **4** was obtained in 30% yield with an enantiomeric ratio of 98:2. Minor amount (<5%) of the carboamination product was obtained.

R_t (IA column, *n*-hexane/*i*-PrOH 80/20, 1.0 mL/min, 250.4 nm): tr(major) = 14.2 min, tr(minor) = 12.2 min, 98:2 e.r.



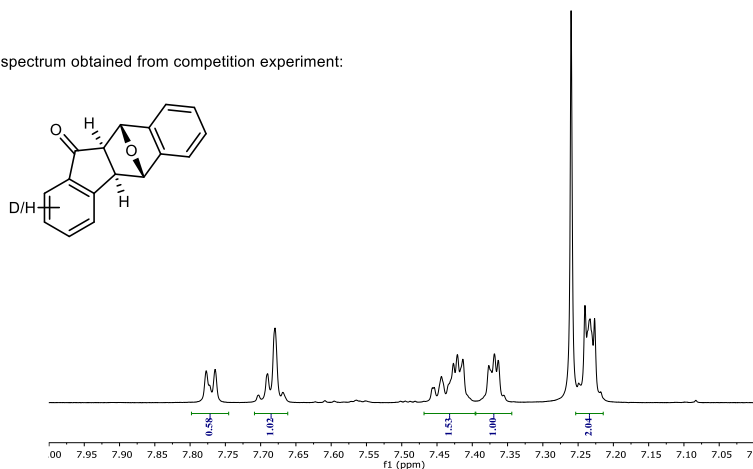
KIE Study for Cobalt Catalysis



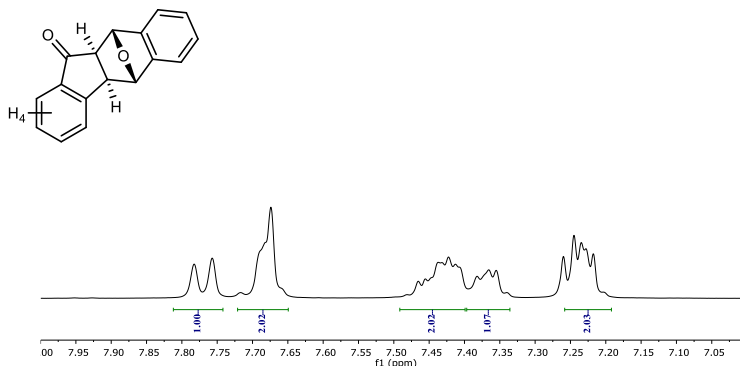
The KIE was determined in a competition experiment, utilizing both the deuterated and the non-deuterated benzamide **1** (0.1 mmol, respectively) in the catalytic reaction described in the general procedure with an altered reaction time of 4 h. After expiration of the selected reaction time, the solvent was removed under reduced pressure and the residue was purified by column chromatography (*n*-hexane/EtOAc = 3:1). Finally, the KIE was determined by ¹H NMR spectroscopy (in CDCl₃) and qualitatively verified by HR-MS.

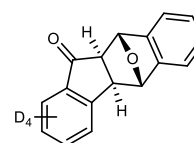
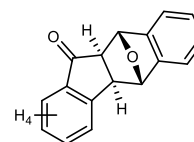
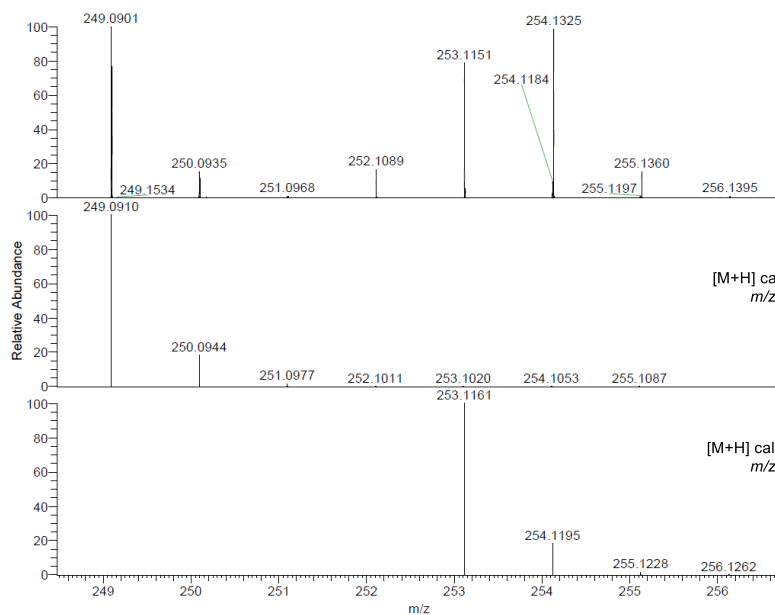
$$\text{KIE} \approx 0.53/(1.00 - 0.53) = 1.1$$

¹H NMR spectrum obtained from competition experiment:

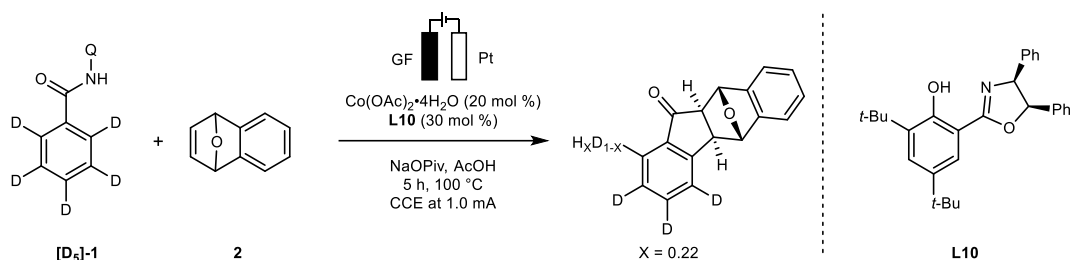


¹H NMR spectrum obtained from H₅-benzamide **1**:



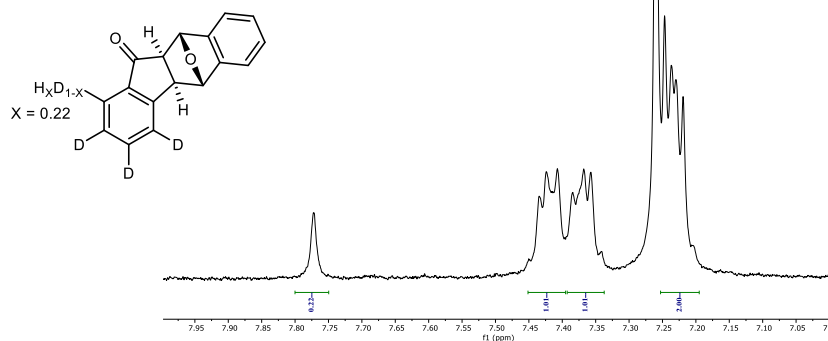


H/D Exchange Experiment for Cobalt Catalysis

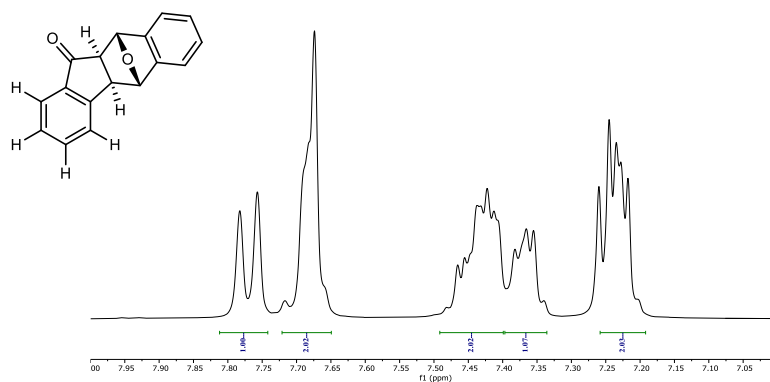


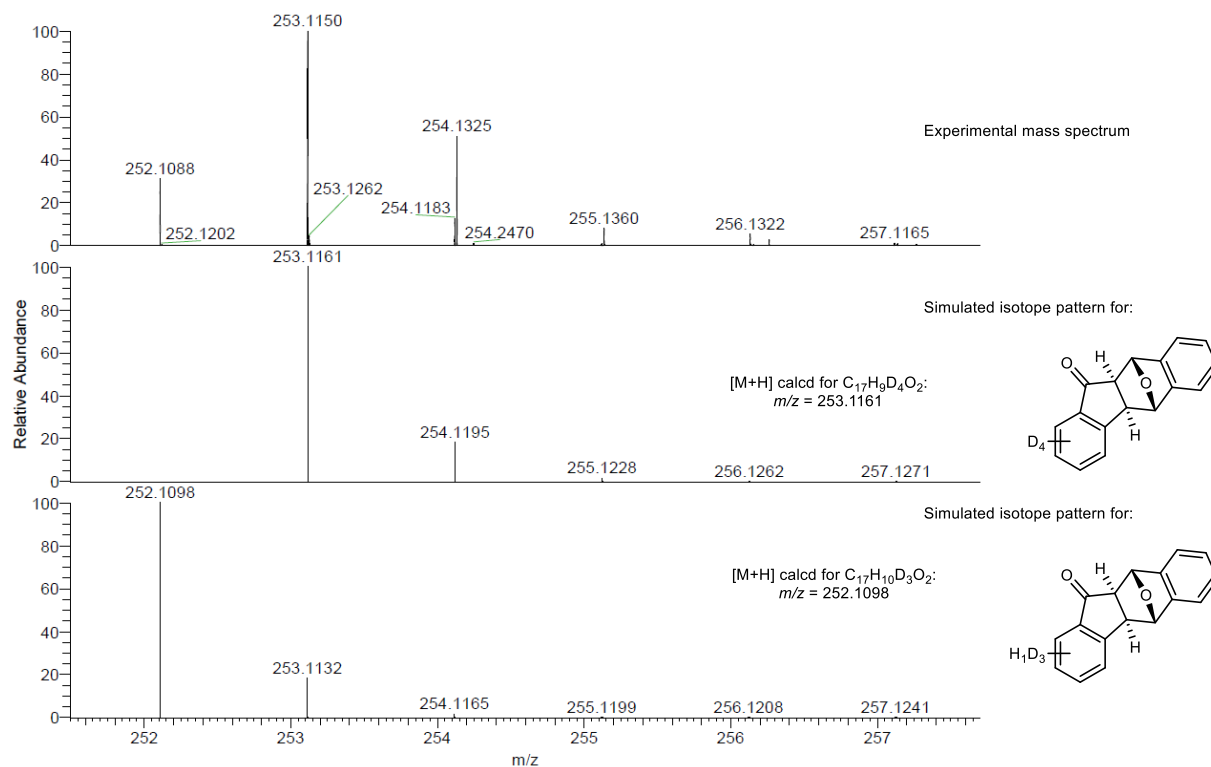
The catalytic reaction was conducted according to the general procedure on a 0.2 mmol scale with the deuterated benzamide **[D₅]-1** and an altered reaction time of 5 h. Next, the solvent was removed under reduced pressure and the residue was purified by column chromatography (*n*-hexane/EtOAc = 3:1). The product was analyzed by means of ^1H NMR spectroscopy (in CDCl_3), showing partial exchange in the formerly fully deuterated benzamide motif.

^1H NMR spectrum obtained from D_5 -benzamide **[D₅]-1**:

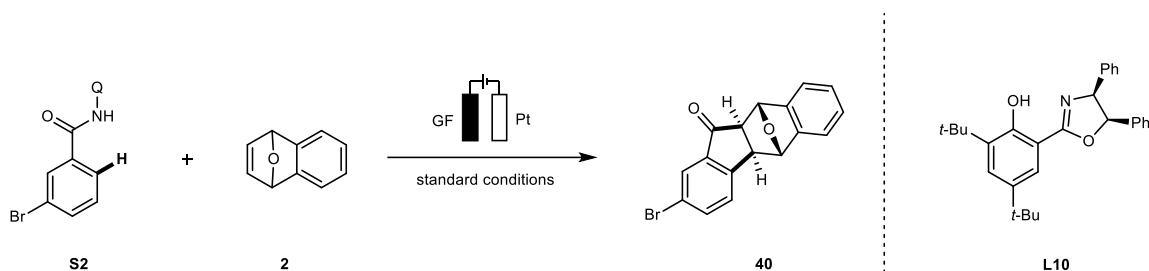


^1H NMR spectrum obtained from H_5 -benzamide **1**:

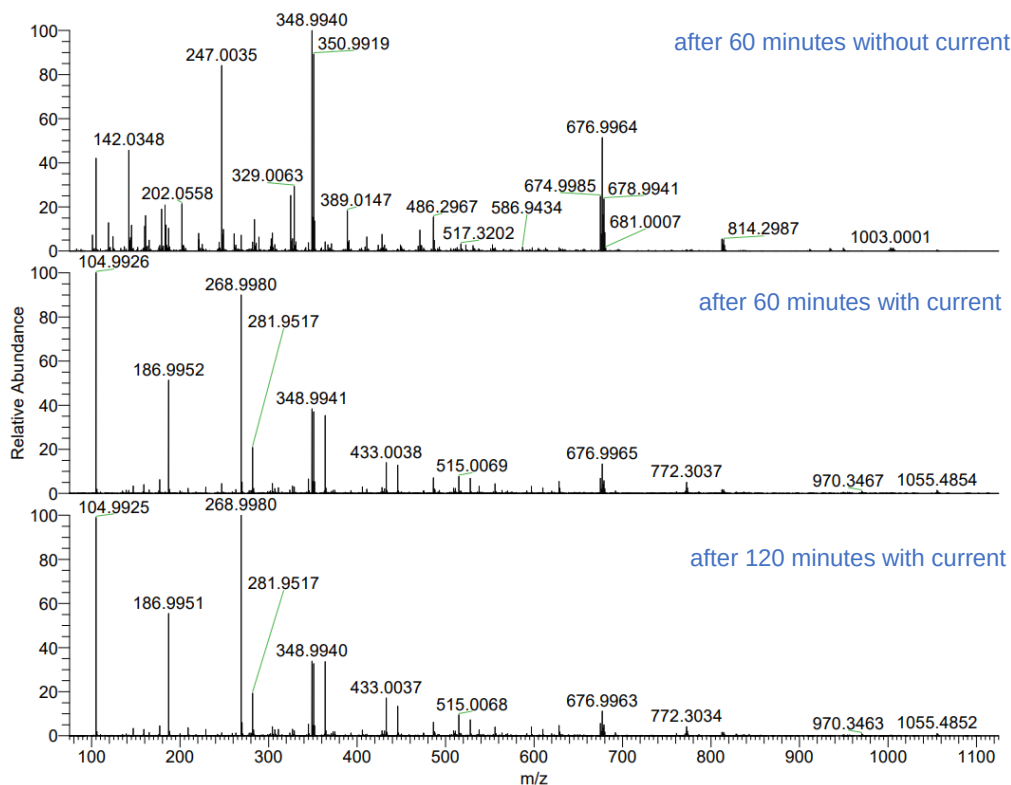




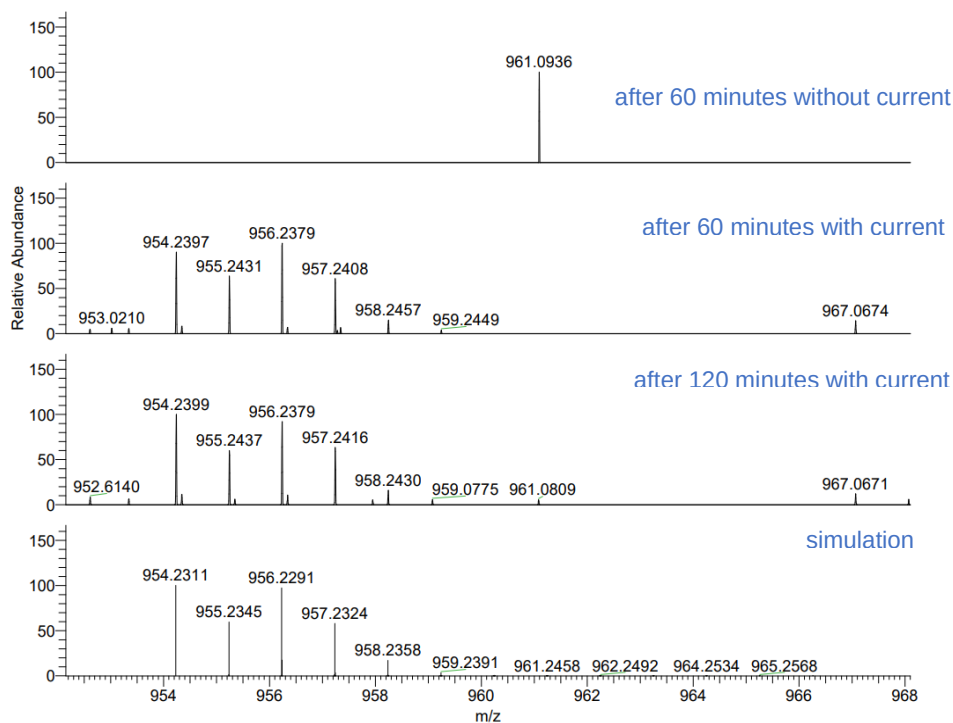
Monitoring the Cobalt Catalysis by Mass Spectrometry



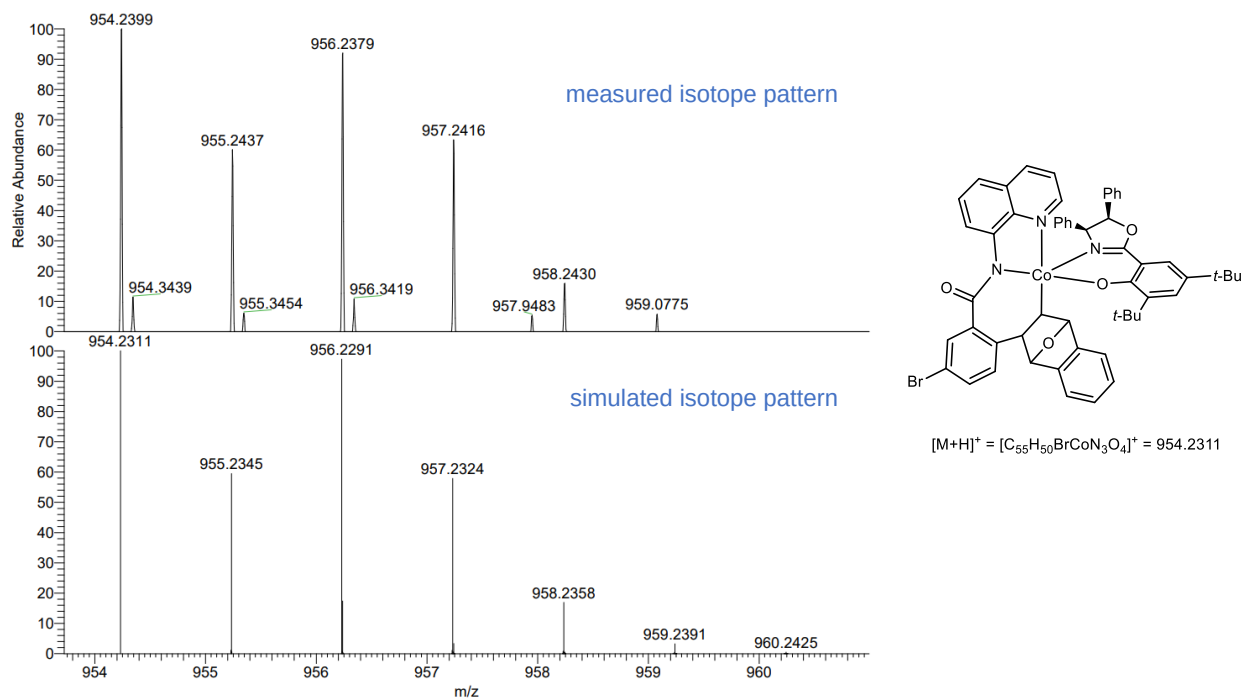
Electrocatalysis was performed according to the general procedure using benzamide **S2**. The first aliquot (50 μL) was taken after stirring the reactions mixture at 100 $^{\circ}\text{C}$ for 60 minutes without current. The aliquot was diluted with THF (500 μL), filtered through an HPLC filter, and directly analyzed via HR ESI MS. In an identical manner, aliquots were analyzed after 60 minutes and 120 minutes applying current.



Supplementary Figure 40. HR-ESI-mass spectrometric monitoring of the enantioselective electrochemical cobalt-catalyzed C–H activation with total m/z range.

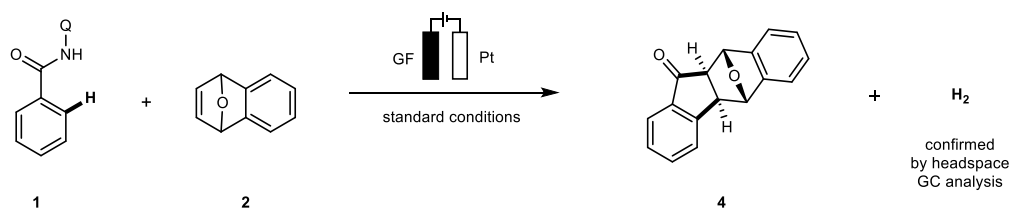


Supplementary Figure 41. HR-ESI-mass spectrometric monitoring of the enantioselective electrochemical cobalt-catalyzed C–H activation. m/z calculated for $[\text{C}_{55}\text{H}_{50}\text{BrCoN}_3\text{O}_4]^+ = 954.2311$.

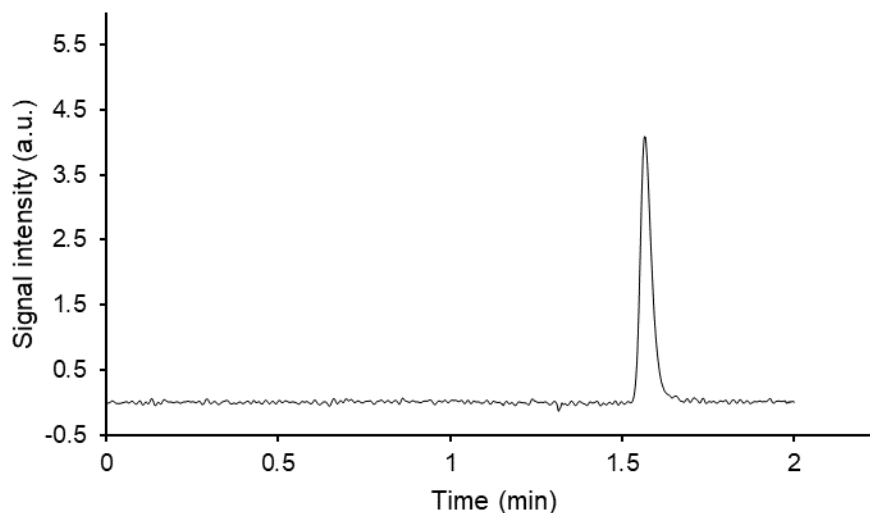


Supplementary Figure 42. Comparison of measured and simulated isotope pattern. m/z calculated for $[\text{C}_{55}\text{H}_{50}\text{BrCoN}_3\text{O}_4]^+ = 954.2311$.

Detection of Hydrogen Gas for Cobalt Catalysis



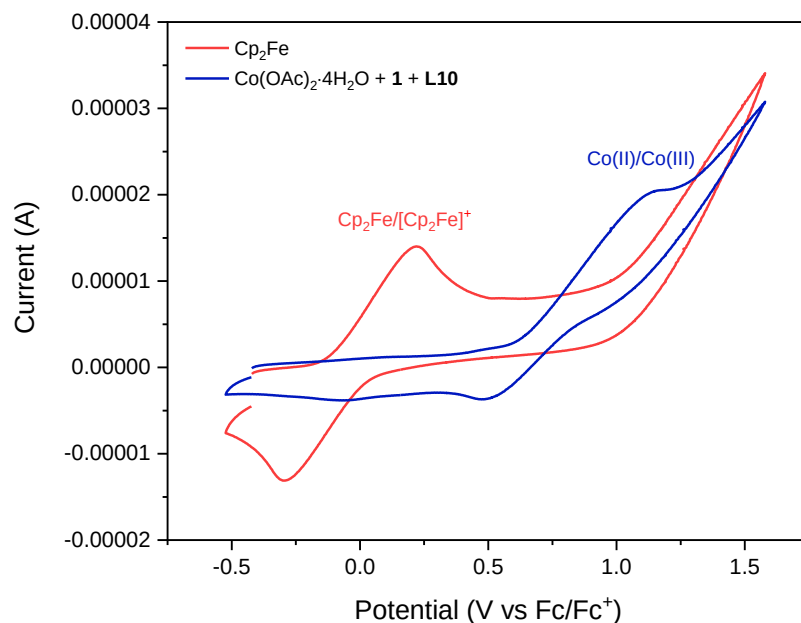
Electrocatalysis was performed according to the general procedure. A septum was used instead of a teflon cap. After completion of the reaction, 1 mL gas volume of the headspace was carefully collected using a gas syringe and directly analyzed. The peak at 1.56 min assigned to hydrogen gas is clearly visible.



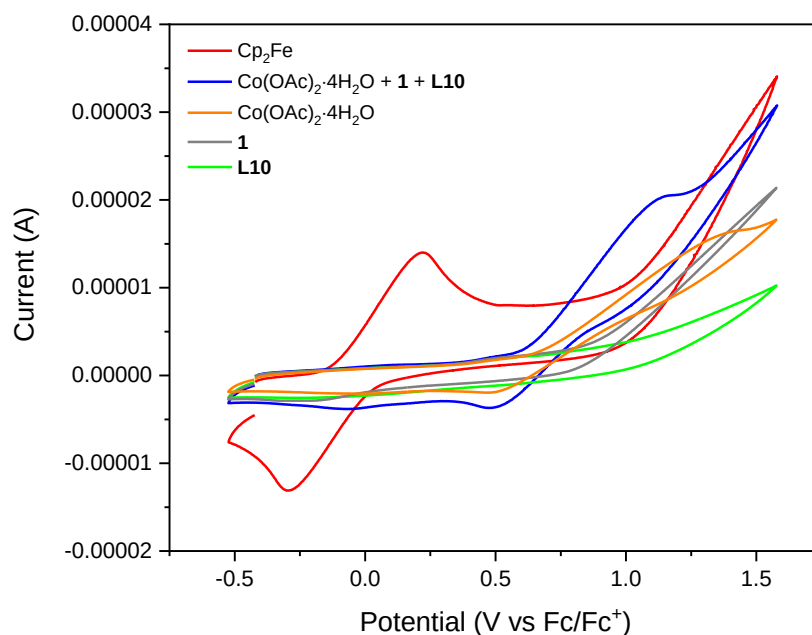
Supplementary Figure 43. Chromatogram detected via headspace GC analysis for enantioselective electrochemical cobalt-catalyzed C–H activation.

Electroanalytical Investigations for Cobalt Catalysis

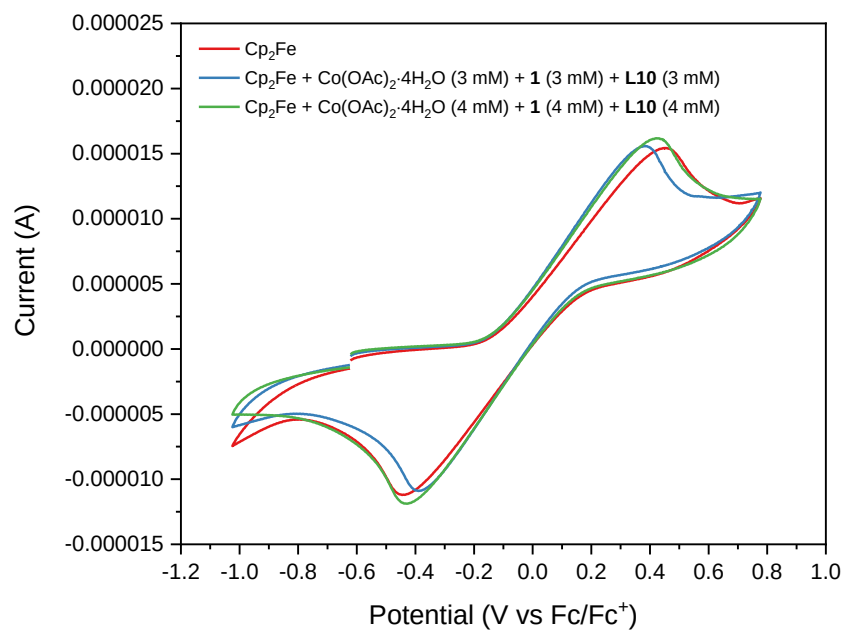
Cyclic Voltammetry (CV)



Supplementary Figure 44: Selected cyclic voltammograms at 100 mV·s⁻¹ using AcOH, NaOPiv (2 mM) as an additive, and *n*-Bu₄NPF₆ (0.05 M) as the electrolyte. All measurements were conducted at 40 °C. (red) Cp₂Fe (0.5 mM); (blue) Co(OAc)₂·4H₂O (2 mM) and **1** (2 mM) and **L10** (2 mM). Note: Cyclic voltammograms were measured using an SCE reference electrode. The data was then converted to V vs. Fc/Fc⁺.

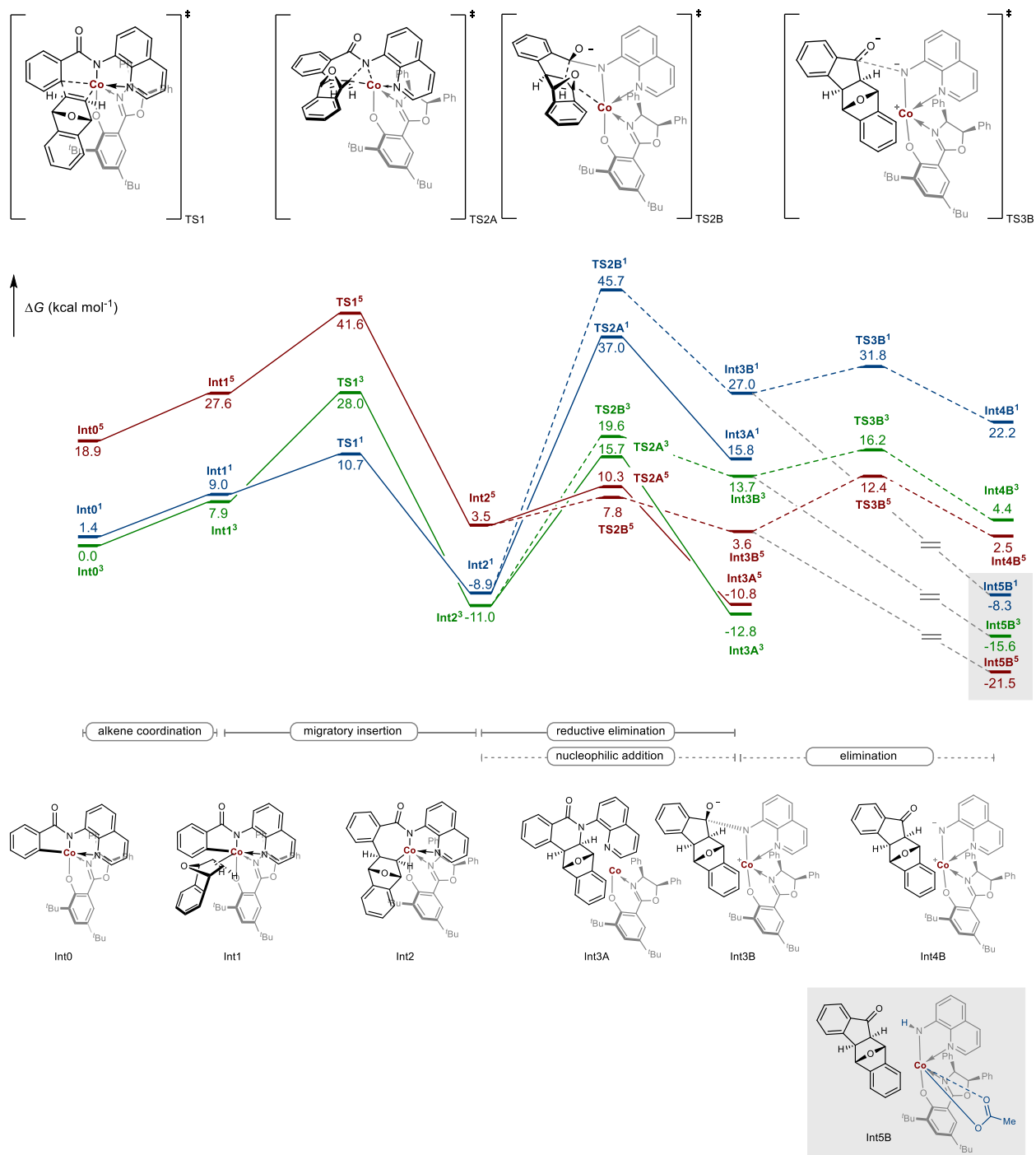


Supplementary Figure 45. Summary of cyclic voltammograms at 100 mV·s⁻¹ using AcOH, NaOPiv (2 mM) as an additive, and *n*-Bu₄NPF₆ (0.05 M) as the electrolyte. All measurements were conducted at 40 °C. (red) Cp₂Fe (0.5 mM); (blue) Co(OAc)₂·4H₂O (2 mM) and **1** (2 mM) and **L10** (2 mM); (orange) Co(OAc)₂·4H₂O (2 mM); (grey) **1** (2 mM); (green) **L10** (2 mM). Note: Cyclic voltammograms were measured using an SCE reference electrode. The data was then converted to V vs. Fc/Fc⁺.



Supplementary Figure 46. Cyclic voltammograms at 100 mV·s⁻¹ using AcOH, NaOPiv (2 mM) as an additive, and *n*-Bu₄NPF₆ (0.05 M) as the electrolyte. All measurements were conducted at 40 °C. (red) Cp₂Fe (0.5 mM); (blue) Cp₂Fe (0.5 mM) and Co(OAc)₂·4H₂O (3 mM) and **1** (3 mM) and **L10** (3 mM); (green) Cp₂Fe (0.5 mM) and Co(OAc)₂·4H₂O (4 mM) and **1** (4 mM) and **L10** (4 mM). Note: Cyclic voltammograms were measured using an SCE reference electrode. The data was then converted to V vs. Fc/Fc⁺.

Computational Studies for Cobalt Catalysis



Supplementary Figure 47. Computed Gibbs free energy ($\Delta G_{373.15}$) profile for the nickel-catalyzed carboamination (— A) and carboacylation (--- B) pathways in kcal mol^{-1} at the PW6B95-D4/def2-TZVPP+SMD(Acetic acid)//TPSS-D3(BJ)/def2-SVP level of theory. The superscripted numbers (1/3/5) in each stationary point labels represent the respective spin multiplicity.

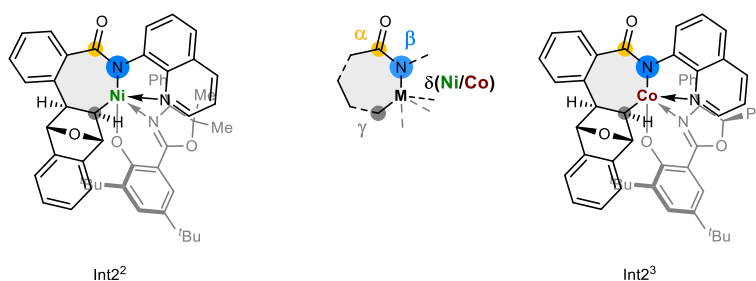
Supplementary Table 22. Calculated electronic and Gibbs free energies ($\Delta G_{373.15}$) at the PW6B95-D4/def2-TZVPP+SMD(Acetic acid)/TPSS-D3(BJ)/def2-SVP level of theory, for all structures involved in the cobalt catalysis reaction energy profile (all in Hartree).[#]

Structure	Electronic Energy	Total Gibbs Free Energy
alkene ¹	-461.8221189	-461.7238087
AcOH ¹	-229.4553923	-229.4319959
Int0 ¹	-3517.311569	-3516.711888
Int0 ³	-3517.312445	-3516.714165
Int0 ⁵	-3517.277599	-3516.684098
Int1 ¹	-3979.151510	-3978.423652
Int1 ³	-3979.146329	-3978.425369
Int1 ⁵	-3979.110827	-3978.393989
TS1 ¹	-3979.149883	-3978.420879
TS1 ³	-3979.117446	-3978.393290
TS1 ⁵	-3979.092079	-3978.371725
Int2 ¹	-3979.182866	-3978.452161
Int2 ³	-3979.184316	-3978.455568
Int2 ⁵	-3979.156996	-3978.432324
TS2A ¹	-3979.108021	-3978.378987
TS2A ³	-3979.141200	-3978.412931
TS2A ⁵	-3979.144031	-3978.421511
TS2B ¹	-3979.092657	-3978.365071
TS2B ³	-3979.129738	-3978.406799
TS2B ⁵	-3979.147816	-3978.425562
Int3A ¹	-3979.143594	-3978.412724
Int3A ³	-3979.185646	-3978.458348
Int3A ⁵	-3979.182137	-3978.455176
Int3B ¹	-3979.122626	-3978.394965
Int3B ³	-3979.140817	-3978.416183
Int3B ⁵	-3979.154635	-3978.432264
TS3B ¹	-3979.114158	-3978.387303
TS3B ³	-3979.137288	-3978.412210
TS3B ⁵	-3979.140023	-3978.418166
Int4B ¹	-3979.126579	-3978.402658
Int4B ³	-3979.152080	-3978.430876
Int4B ⁵	-3979.152402	-3978.433970
Int5B ¹	-4208.663659	-4207.883160
Int5B ³	-4208.672581	-4207.894781
Int5B ⁵	-4208.680095	-4207.904265

[#]Superscripted 1, 3, and 5 corresponds to the spin multiplicity as singlet, triplet and quintet, respectively.

NBO Charge Analysis

All the NBO analysis was performed at the PW6B95-D3(BJ)/def2-TZVPP level of theory with respective SMD solvation model (1,4-Dioxane for the nickel catalysis and Acetic acid for the cobalt catalysis) on the optimized geometries at the TPSS-D3(BJ)/def2-SVP level of theory.



Supplementary Figure 48. Indices used for the key atoms (α , β , γ , $\delta(\text{Ni})$, and $\delta(\text{Co})$) for the ground state involved in chemodivergent pathways (**Int2**, **TS2**, and **Int3**). Superscripted 2 and 3 represents doublet and triplet spin states, respectively.

Supplementary Table 23. Measured charge densities for primary chemodivergent pathways (**Int2**, **TS2**, and **Int3**) of key atoms.[#]

Reaction	System	NBO _{α}	NBO _{β}	NBO _{γ}	NBO _{$\delta(\text{Ni})$}	NBO _{$\delta(\text{Co})$}
Nickel	Int2 ²	0.33286	-0.29283	-0.23229	0.94243	-
	TS2A ²	0.33344	-0.27678	-0.06834	0.88803	-
	TS2B ⁴	0.23405	-0.18434	0.18429	1.36484	-
	Int3A ²	0.34498	-0.23448	-0.01610	0.83482	-
	Int3B ⁴	0.17620	-0.07944	-0.04141	1.36675	-
Cobalt	Int2 ³	0.34109	-0.29154	-0.27122	-	1.44815
	TS2A ⁵	0.34875	-0.27111	0.19089	-	1.90716
	TS2B ⁵	0.24231	-0.16518	0.17340	-	1.90046
	Int3A ³	0.35059	-0.23278	-0.01736	-	1.81499
	Int3B ⁵	0.18846	0.02010	-0.07902	-	1.91373

[#]Superscripted 1, 2, 4, and 6 corresponds to the spin multiplicity as singlet, doublet, quartet and sextet, respectively.

To calculate global nucleophilicities (N), tetracyanoethylene (TCE) was taken as reference for the nucleophilicity scale (Supplementary Equation 2)⁵².

$$N = (E_{\text{HOMO}} - E_{\text{HOMO}(\text{TCE})}) \quad (2)$$

Supplementary Table 24. Obtained frontier molecular orbitals energies for **Int2** (E_{HOMO} and E_{LUMO}) and **TCE** (E_{HOMO}), with the calculated N for nickel and cobalt catalysis (all in Hartree).[#]

Intermediate	E_{HOMO}	E_{LUMO}	$E_{HOMO(TCE)}$	N
Int2²_{Ni}	-0.208100	-0.076590	-0.343900	0.135800
Int2³_{Co}	-0.211120	-0.074860	-0.336180	0.125060

[#]Superscripted 2, and 3 corresponds to the spin multiplicity as doublet, and triplet, respectively.

For a neutral system (q_s^n) of n electrons, independent calculations were performed for its corresponding cationic (q_s^{n-1}), and anionic (q_s^{n+1}) electron system using the same optimized molecular geometry. The nucleophilicity (f_s^+) and electrophilicity (f_s^-) Fukui functions were calculated using Supplementary Equation 3 and 4 for an atom s ⁵³. Due to the change in spin states for the corresponding nickel/cobalt's cationic and anionic complex systems, the one with the lowest electronic energy (in Hartree) was taken for the NBO charges of studied atoms. Finally, the local nucleophilicity at atom γ were calculated from Supplementary Equation 5⁵⁴.

$$f_s^+ = |q_s^{n+1} - q_s^n| \quad (3)$$

$$f_s^- = |q_s^n - q_s^{n-1}| \quad (4)$$

$$N_s = N \cdot f_s^- \quad (5)$$

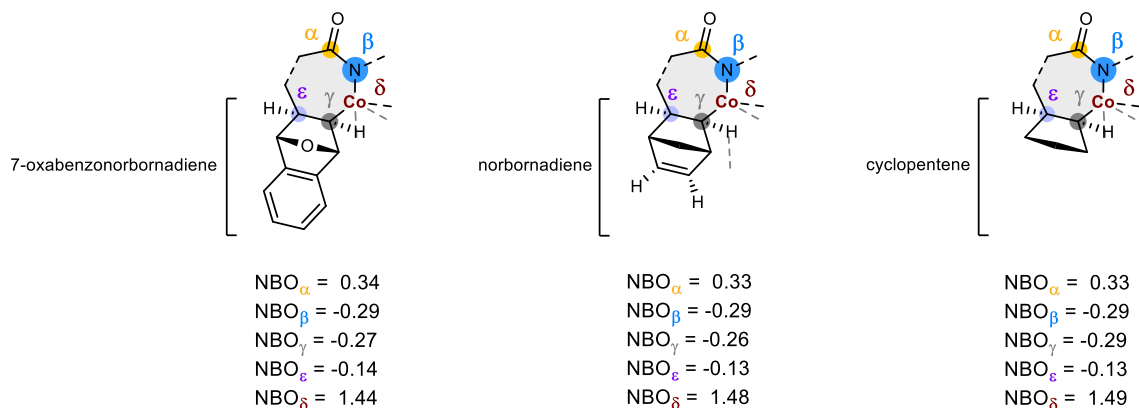
Supplementary Table 25. Calculated electronic energies at the PW6B95-D4/def2-TZVPP+SMD(Acetic acid)//TPSS-D3(BJ)/def2-SVP level of theory, for cationic, neutral, and anionic state of **Int2** in the nickel and cobalt catalysis (all in Hartree).

Intermediate	State	Spin	Electronic Energy	q_α	q_γ
Int2_{Ni}	Cationic ($n-1$)	Singlet	-3951.861376	-	-
		Triplet	-3951.883115	0.31855	-0.21988
		Quintet	-3951.826204	-	-
	Neutral (n)	Doublet	-3952.095341	0.33286	-0.23229
		Singlet	-3952.169077	-	-
		Triplet	-3952.170647	0.32893	-0.20470
	Anionic ($n+1$)	Quintet	-3952.098658	-	-
		Doublet	-3978.970384	-	-
		Quartet	-3978.986251	0.33296	-0.20582
Int2_{Co}	Cationic ($n-1$)	Sextet	-3978.926445	-	-
		Triplet	-3979.184315	0.34109	-0.27122
		Doublet	-3979.294744	0.33711	-0.23417
	Neutral (n)	Quartet	-3979.271869	-	-
		Sextet	-3979.212306	-	-
	Anionic ($n+1$)	Quartet	-3979.271869	-	-

Supplementary Table 26. Calculated nucleophilicity Fukui function of atom α , electrophilicity Fukui function and local nucleophilicity of atom γ from **Int2** in nickel and cobalt catalysis.[#]

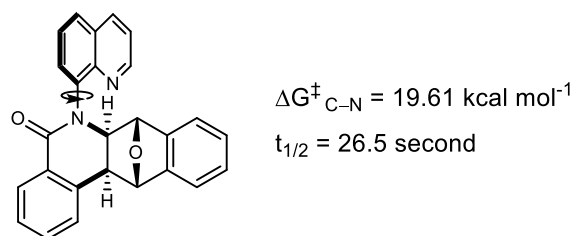
Intermediate	f_{α}^{+}	f_{γ}^{-}	N_{γ}
Int2 ² _{Ni}	0.00393	0.01241	0.001685
Int2 ³ _{Co}	0.00398	0.06540	0.008179

[#]Superscripted 2, and 3 corresponds to the spin multiplicity as doublet, and triplet, respectively.



Supplementary Figure 49. Comparison of measured charge densities of the key atoms (α , β , γ , and δ (Co)) from 7-oxabenzonorbornadiene **Int2** with other alkenes (norbornadiene and cyclopentene) in the triplet spin state as the ground state.

Rotational Barrier of the Quinoline Group



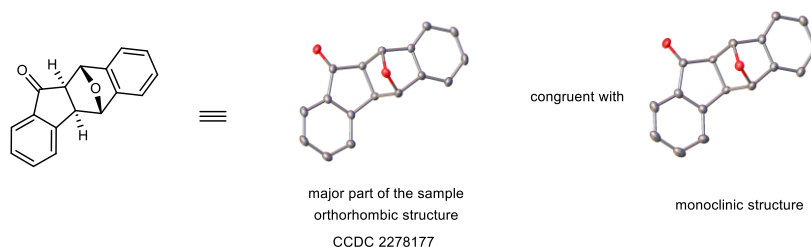
Supplementary Figure 50. Computed rotational barrier ($\Delta G^{\ddagger}_{373.15}$) in kcal mol⁻¹ along the C–N bond for the lactam product and the corresponding half-life ($t_{1/2}$). Calculations were performed at the PW6B95-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory.

Supplementary Table 27. Calculated electronic energies at the PW6B95-D4/def2-TZVPP+SMD(1,4-Dioxane)//TPSS-D3(BJ)/def2-SVP level of theory, Gibbs free energies ($\Delta G_{373.15}$) for the carboamination product and its transition state for rotation along the C–N bond for the lactam product (all in Hartree).

Structure	Electronic Energy	Total Gibbs Free Energy
Product	-1263.712103	-1263.435264
Transition State	-1263.682723	-1263.404006

X-Ray Crystallographic Data

Compound 4



CCDC number	2278177	-
Empirical formula	C ₁₇ H ₁₂ O ₂	C ₁₇ H ₁₂ O ₂
Formula weight	248.27	248.27
Temperature [K]	100.00	100.00
Crystal system	orthorhombic	monoclinic
Space group (number)	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (19)	<i>P</i> 2 ₁ (4)
<i>a</i> [Å]	5.6890(6)	7.4682(6)
<i>b</i> [Å]	10.6087(11)	6.0181(7)
<i>c</i> [Å]	19.937(2)	13.3169(11)
α [°]	90	90
β [°]	90	97.427(3)
γ [°]	90	90
Volume [Å ³]	1203.2(2)	593.50(10)
<i>Z</i>	4	2
ρ_{calc} [gcm ⁻³]	1.370	1.389
μ [mm ⁻¹]	0.713	0.723
<i>F</i> (000)	520	260
Crystal size [mm ³]	1.425×0.142×0.09	0.338×0.2×0.044
Crystal colour	colourless	colourless
Crystal shape	needle	plate
Radiation	CuK α (λ =1.54178 Å)	CuK α (λ =1.54178 Å)
2 θ range [°]	8.87 to 157.35 (0.79 Å)	6.69 to 159.14 (0.78 Å)
Index ranges	-7 ≤ <i>h</i> ≤ 6, -13 ≤ <i>k</i> ≤ 13, -25 ≤ <i>l</i> ≤ 25	-9 ≤ <i>h</i> ≤ 9, -6 ≤ <i>k</i> ≤ 7, -16 ≤ <i>l</i> ≤ 16
Reflections collected	48396	22495
Independent reflections	2591 [<i>R</i> _{int} = 0.0451, <i>R</i> _{sigma} = 0.0139]	2498 [<i>R</i> _{int} = 0.0546, <i>R</i> _{sigma} = 0.0282]
Completeness to θ = 67.679°	100.0 %	99.3 %
Data / Restraints / Parameters	2591/0/173	2498/1/172
Goodness-of-fit on <i>F</i> ²	1.055	1.041
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0264, <i>wR</i> ₂ = 0.0656	<i>R</i> ₁ = 0.0534, <i>wR</i> ₂ = 0.1415
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0266, <i>wR</i> ₂ = 0.0656	<i>R</i> ₁ = 0.0541, <i>wR</i> ₂ = 0.1437
Largest peak/hole [eÅ ⁻³]	0.22/-0.14	0.19/-0.23
Flack X parameter	0.07(5)	-0.1(4)
Extinction coefficient	0.0070(6)	-

Note:

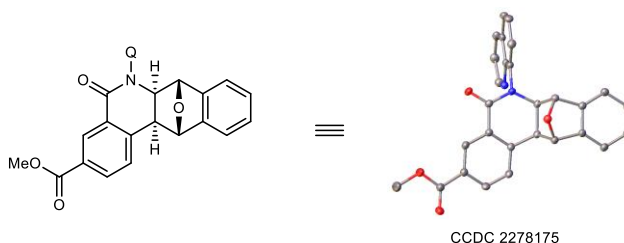
Alert level B from checkCIF/PLATON report:

CRYSS02_ALERT_3_B The value of _exptl_crystal_size_max is > 1.0
Maximum crystal size given = 1.425

Author Response:

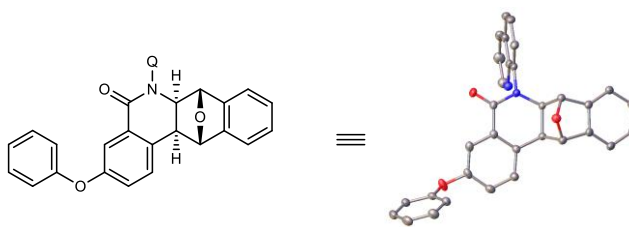
Long needle of good quality was found, however due to its brittleness it did not cut well, fraying out the edges. The long needle was used, so that the multicrystalline cutting edges were well outside the beam most of the time.

Compound 9



CCDC number	2278175
Empirical formula	C ₂₈ H ₂₀ N ₂ O ₄
Formula weight	448.46
Temperature [K]	100.00
Crystal system	orthorhombic
Space group (number)	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (19)
<i>a</i> [Å]	10.7336(6)
<i>b</i> [Å]	11.0877(11)
<i>c</i> [Å]	18.6465(12)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å ³]	2219.1(3)
<i>Z</i>	4
ρ_{calc} [gcm ⁻³]	1.342
μ [mm ⁻¹]	0.738
<i>F</i> (000)	936
Crystal size [mm ³]	0.56×0.294×0.066
Crystal colour	colourless
Crystal shape	plate
Radiation	CuK α (λ =1.54178 Å)
2 θ range [°]	9.28 to 159.06 (0.78 Å)
Index ranges	−13 ≤ <i>h</i> ≤ 13, −14 ≤ <i>k</i> ≤ 13, −23 ≤ <i>l</i> ≤ 23
Reflections collected	69318
Independent reflections	4790 [<i>R</i> _{int} = 0.0464, <i>R</i> _{sigma} = 0.0160]
Completeness to θ = 67.679°	100.0 %
Data / Restraints / Parameters	4790/0/309
Goodness-of-fit on <i>F</i> ²	1.041
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0277, <i>wR</i> ₂ = 0.0748
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0278, <i>wR</i> ₂ = 0.0749
Largest peak/hole [eÅ ⁻³]	0.20/−0.15
Flack <i>X</i> parameter	−0.04(4)
Extinction coefficient	0.0018(3)

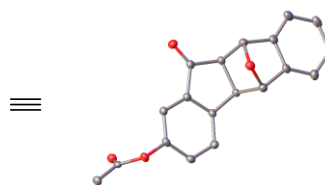
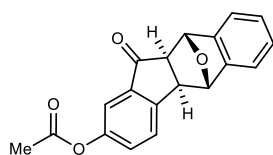
Compound 11



CCDC 2278176

CCDC number	2278176
Empirical formula	C ₃₂ H ₂₂ N ₂ O ₃
Formula weight	482.51
Temperature [K]	100.00
Crystal system	orthorhombic
Space group (number)	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (19)
<i>a</i> [Å]	10.4971(8)
<i>b</i> [Å]	10.9306(11)
<i>c</i> [Å]	20.2468(15)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å ³]	2323.1(3)
<i>Z</i>	4
ρ_{calc} [gcm ⁻³]	1.380
μ [mm ⁻¹]	0.714
<i>F</i> (000)	1008
Crystal size [mm ³]	0.452×0.406×0.182
Crystal colour	colourless
Crystal shape	block
Radiation	CuK α (λ =1.54178 Å)
2 θ range [°]	9.19 to 158.96 (0.78 Å)
Index ranges	−13 ≤ <i>h</i> ≤ 13, −11 ≤ <i>k</i> ≤ 13, −25 ≤ <i>l</i> ≤ 25
Reflections collected	65398
Independent reflections	5004 [<i>R</i> _{int} = 0.0500, <i>R</i> _{sigma} = 0.0188]
Completeness to θ = 67.679°	100.0 %
Data / Restraints / Parameters	5004/0/335
Goodness-of-fit on <i>F</i> ²	1.030
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0262, <i>wR</i> ₂ = 0.0682
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0265, <i>wR</i> ₂ = 0.0685
Largest peak/hole [eÅ ⁻³]	0.21/−0.14
Flack X parameter	0.04(4)
Extinction coefficient	0.0034(3)

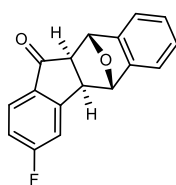
Compound 43



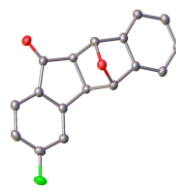
CCDC 2278179

CCDC number	2278179
Empirical formula	C ₁₉ H ₁₄ O ₄
Formula weight	306.30
Temperature [K]	100.00
Crystal system	monoclinic
Space group (number)	<i>P</i> 2 ₁ (4)
<i>a</i> [Å]	5.4650(6)
<i>b</i> [Å]	6.0943(8)
<i>c</i> [Å]	21.520(3)
α [°]	90
β [°]	90.365(5)
γ [°]	90
Volume [Å ³]	716.72(15)
<i>Z</i>	2
ρ_{calc} [gcm ⁻³]	1.419
μ [mm ⁻¹]	0.819
<i>F</i> (000)	320
Crystal size [mm ³]	0.233×0.224×0.096
Crystal colour	colourless
Crystal shape	block
Radiation	CuK α (λ =1.54178 Å)
2 θ range [°]	8.22 to 157.86 (0.79 Å)
Index ranges	−6 ≤ <i>h</i> ≤ 6, −7 ≤ <i>k</i> ≤ 7, −27 ≤ <i>l</i> ≤ 27
Reflections collected	29137
Independent reflections	3049 [<i>R</i> _{int} = 0.0447, <i>R</i> _{sigma} = 0.0221]
Completeness to θ = 67.679°	99.7 %
Data / Restraints / Parameters	3049/1/210
Goodness-of-fit on <i>F</i> ²	1.045
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0370, <i>wR</i> ₂ = 0.1006
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0371, <i>wR</i> ₂ = 0.1007
Largest peak/hole [eÅ ⁻³]	0.27/−0.17
Flack <i>X</i> parameter	0.00(19)
Extinction coefficient	0.011(3)

Compound 46



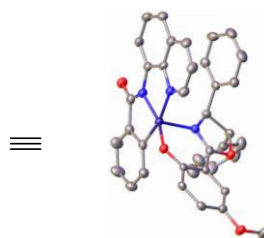
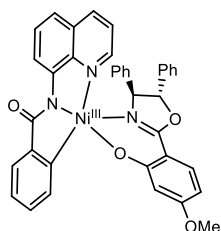
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CCDC 2278178

CCDC number	2278178
Empirical formula	C ₁₇ H ₁₁ FO ₂
Formula weight	266.26
Temperature [K]	100.00
Crystal system	orthorhombic
Space group (number)	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (19)
<i>a</i> [Å]	6.1688(6)
<i>b</i> [Å]	7.5501(9)
<i>c</i> [Å]	25.816(3)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å ³]	1202.4(2)
<i>Z</i>	4
ρ_{calc} [gcm ⁻³]	1.471
μ [mm ⁻¹]	0.879
<i>F</i> (000)	552
Crystal size [mm ³]	0.436×0.426×0.226
Crystal colour	colourless
Crystal shape	block
Radiation	CuK α (λ =1.54178 Å)
2 θ range [°]	6.85 to 157.32 (0.79 Å)
Index ranges	−7 ≤ <i>h</i> ≤ 7, −9 ≤ <i>k</i> ≤ 9, −32 ≤ <i>l</i> ≤ 31
Reflections collected	27208
Independent reflections	2583 [<i>R</i> _{int} = 0.0450, <i>R</i> _{sigma} = 0.0212]
Completeness to θ = 67.679°	99.7 %
Data / Restraints / Parameters	2583/0/182
Goodness-of-fit on <i>F</i> ²	1.050
Final <i>R</i> indexes, [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0277, <i>wR</i> ₂ = 0.0746
Final <i>R</i> indexes, [all data]	<i>R</i> ₁ = 0.0277, <i>wR</i> ₂ = 0.0747
Largest peak/hole [eÅ ⁻³]	0.21/−0.14
Flack <i>X</i> parameter	−0.04(4)
Extinction coefficient	0.0106(13)

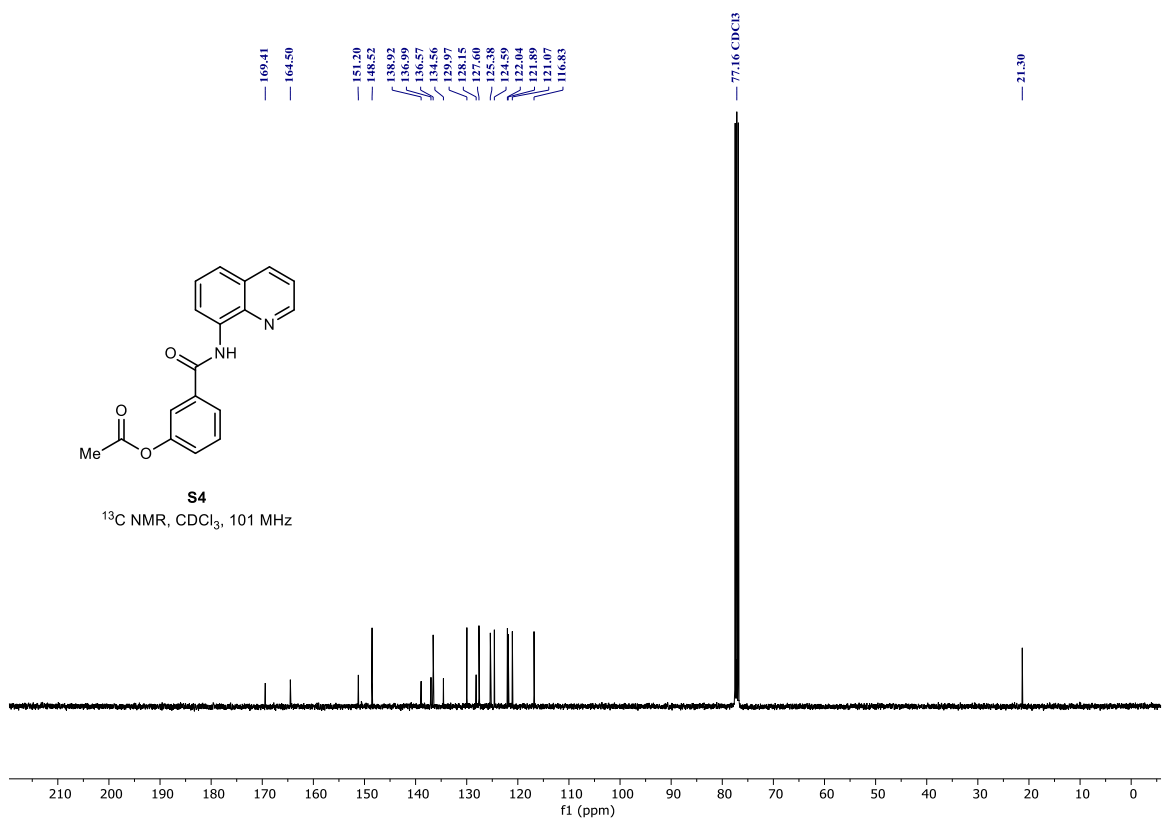
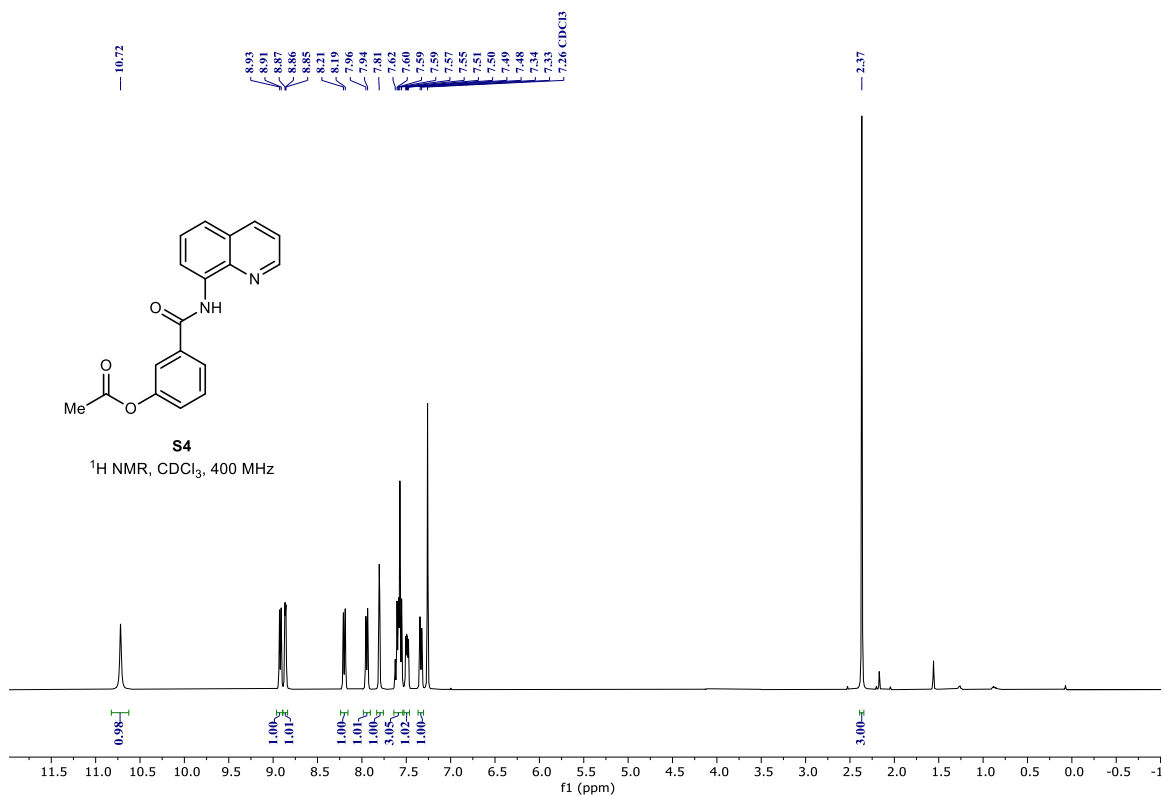
Compound Ni^{III}-L11

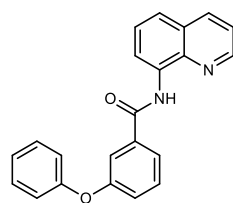


CCDC 2278180

CCDC number	2278180
Empirical formula	C ₃₈ H ₂₈ N ₃ NiO ₄
Formula weight	649.34
Temperature [K]	100.00
Crystal system	orthorhombic
Space group (number)	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (19)
<i>a</i> [Å]	8.973(3)
<i>b</i> [Å]	11.113(4)
<i>c</i> [Å]	30.773(11)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å ³]	3068.6(18)
<i>Z</i>	4
ρ_{calc} [gcm ⁻³]	1.406
μ [mm ⁻¹]	0.680
<i>F</i> (000)	1348
Crystal size [mm ³]	0.18×0.047×0.024
Crystal colour	red
Crystal shape	needle
Radiation	MoK α (λ =0.71073 Å)
2 θ range [°]	3.90 to 52.76 (0.80 Å)
Index ranges	−11 ≤ <i>h</i> ≤ 11, −10 ≤ <i>k</i> ≤ 13, −38 ≤ <i>l</i> ≤ 38
Reflections collected	40259
Independent reflections	6267 [<i>R</i> _{int} = 0.0548, <i>R</i> _{sigma} = 0.0375]
Completeness to θ = 25.242°	100.0 %
Data / Restraints / Parameters	6267/51/459
Goodness-of-fit on <i>F</i> ²	1.049
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0350, <i>wR</i> ₂ = 0.0753
Final <i>R</i> indexes, [all data]	<i>R</i> ₁ = 0.0425, <i>wR</i> ₂ = 0.0791
Largest peak/hole [eÅ ⁻³]	0.37/−0.34
Flack X parameter	−0.026(6)

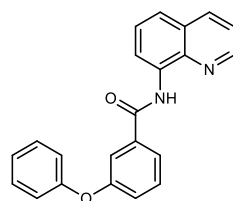
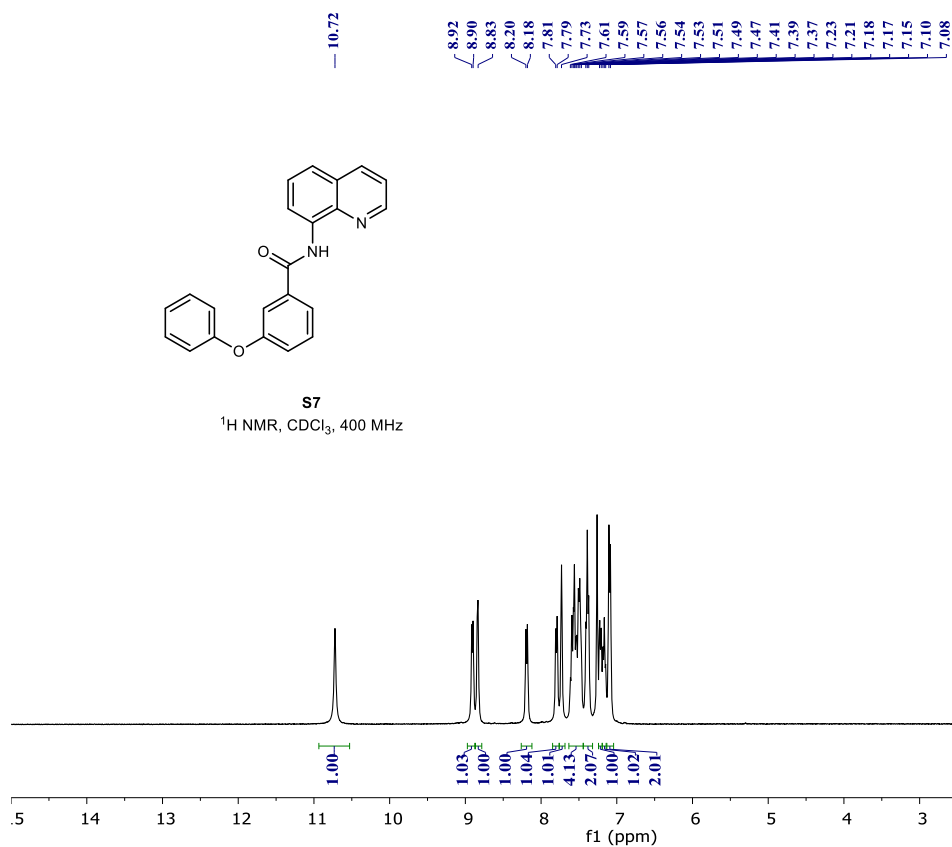
NMR Spectra





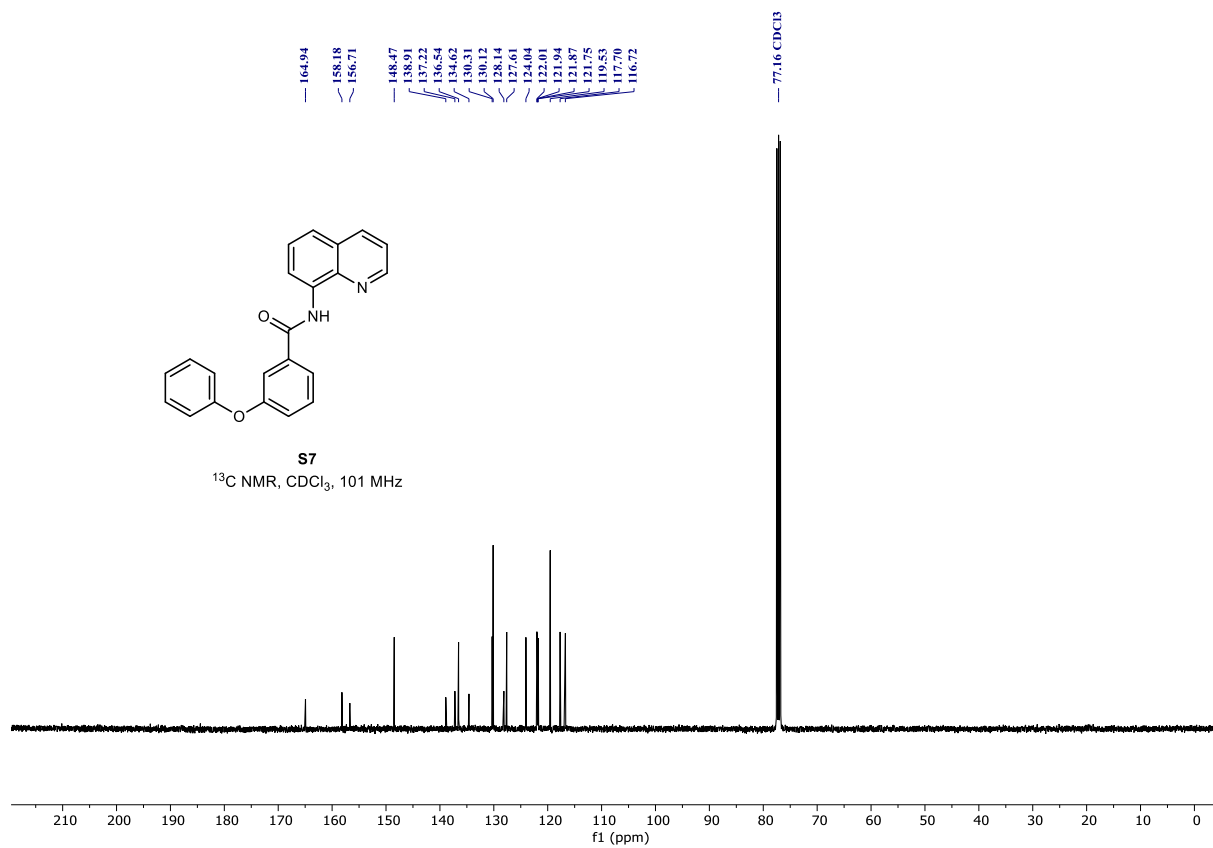
S7

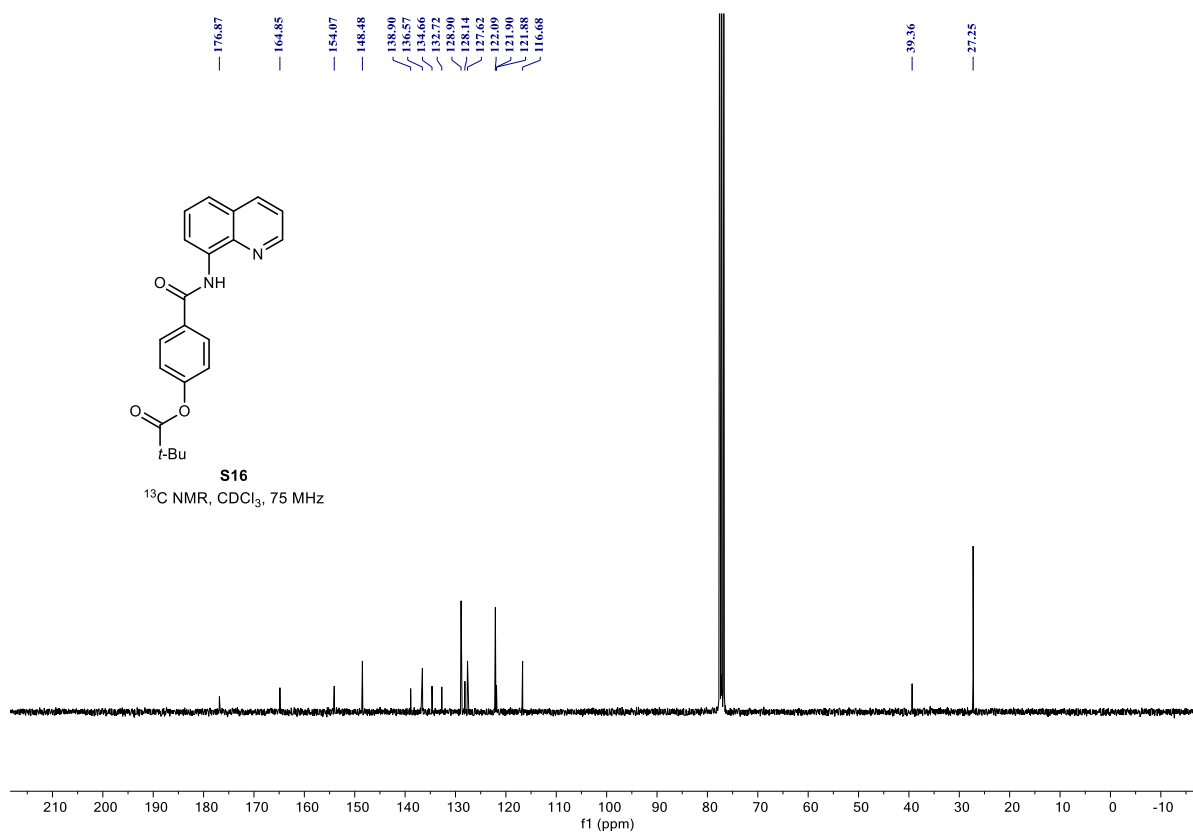
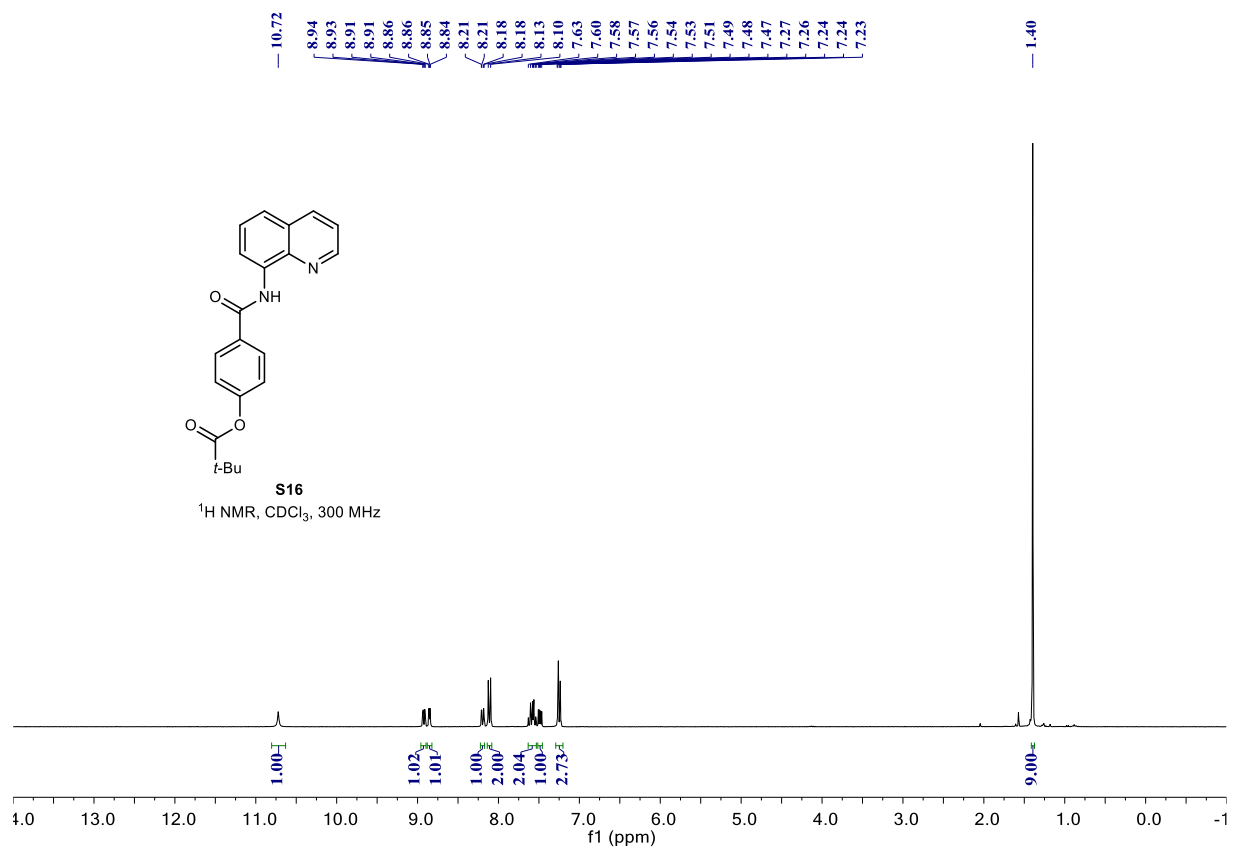
^1H NMR, CDCl_3 , 400 MHz

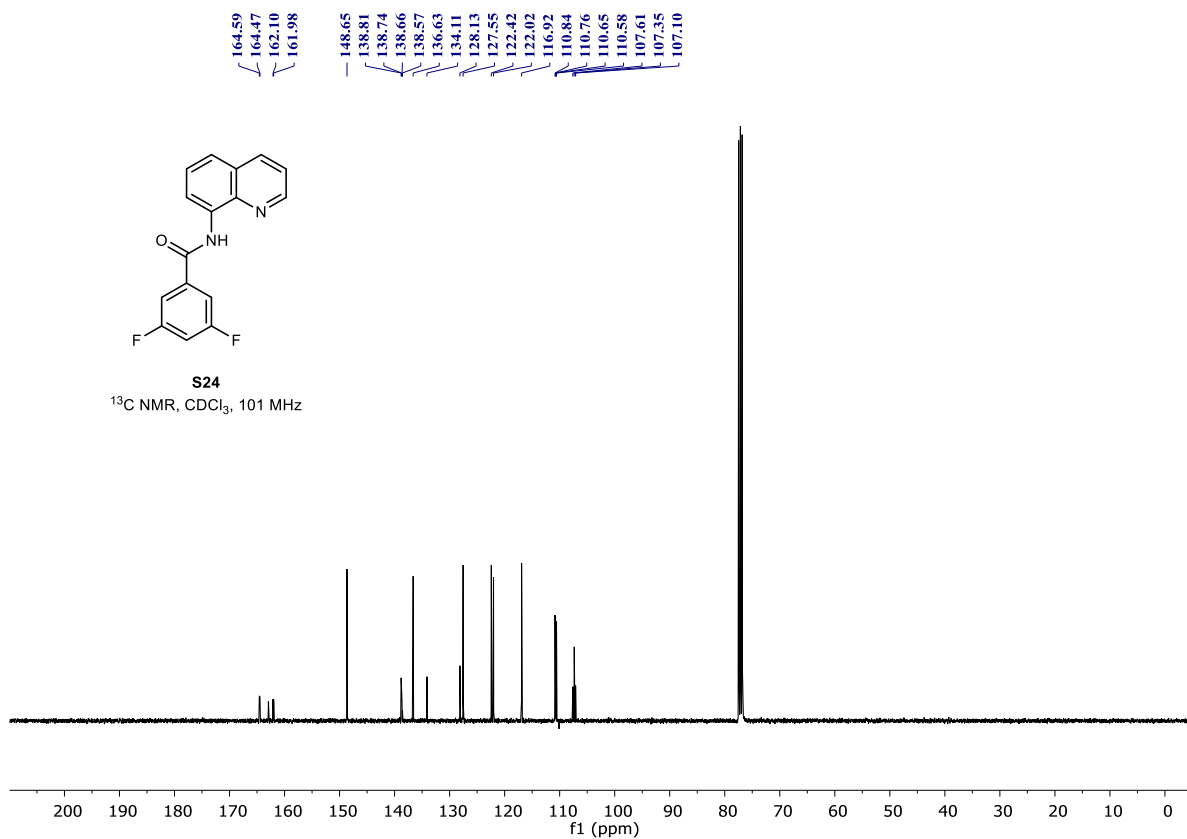
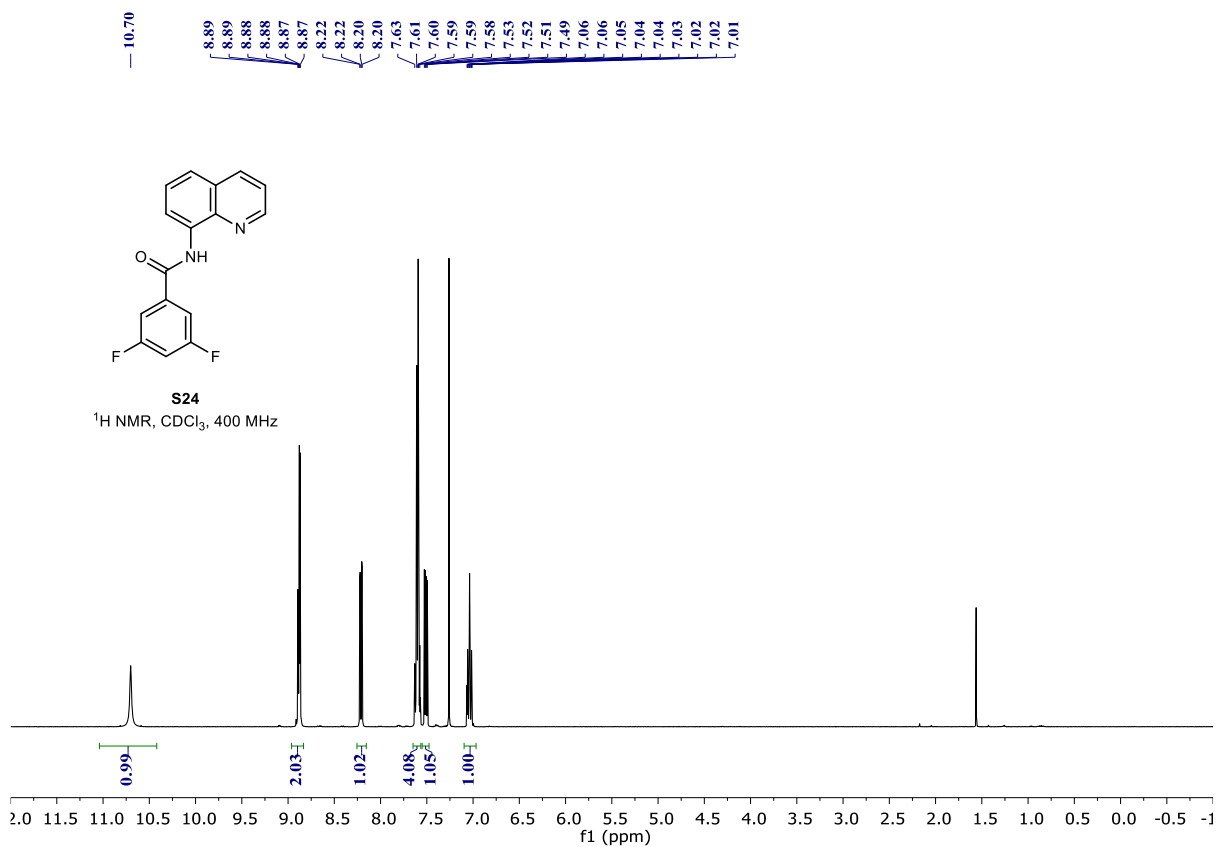


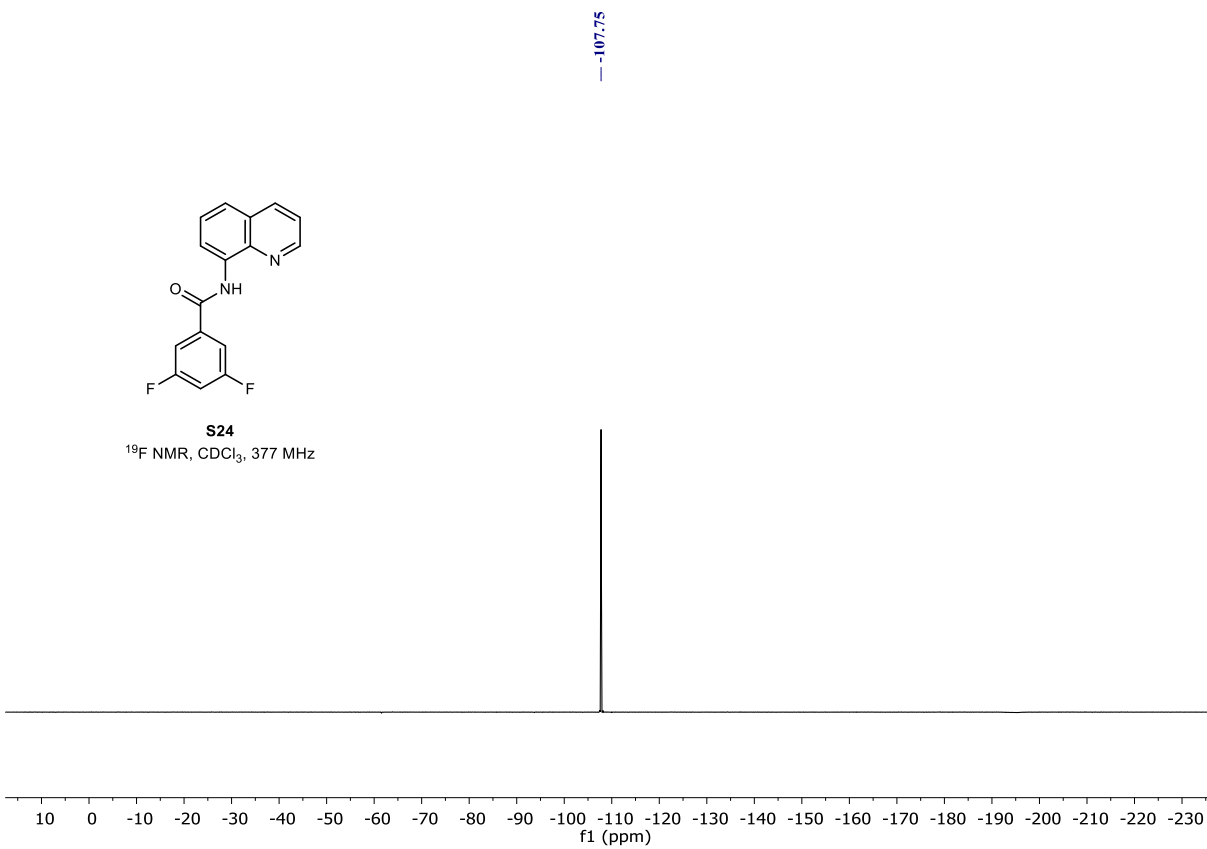
S7

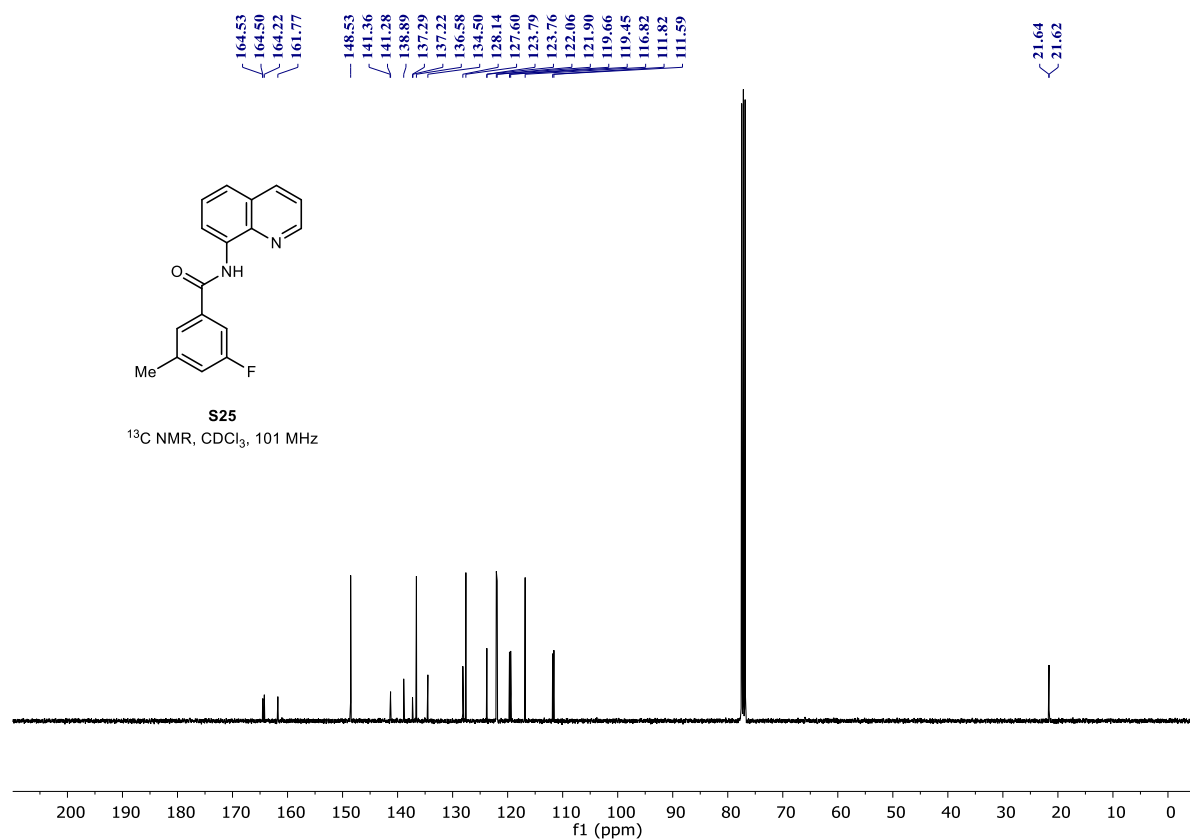
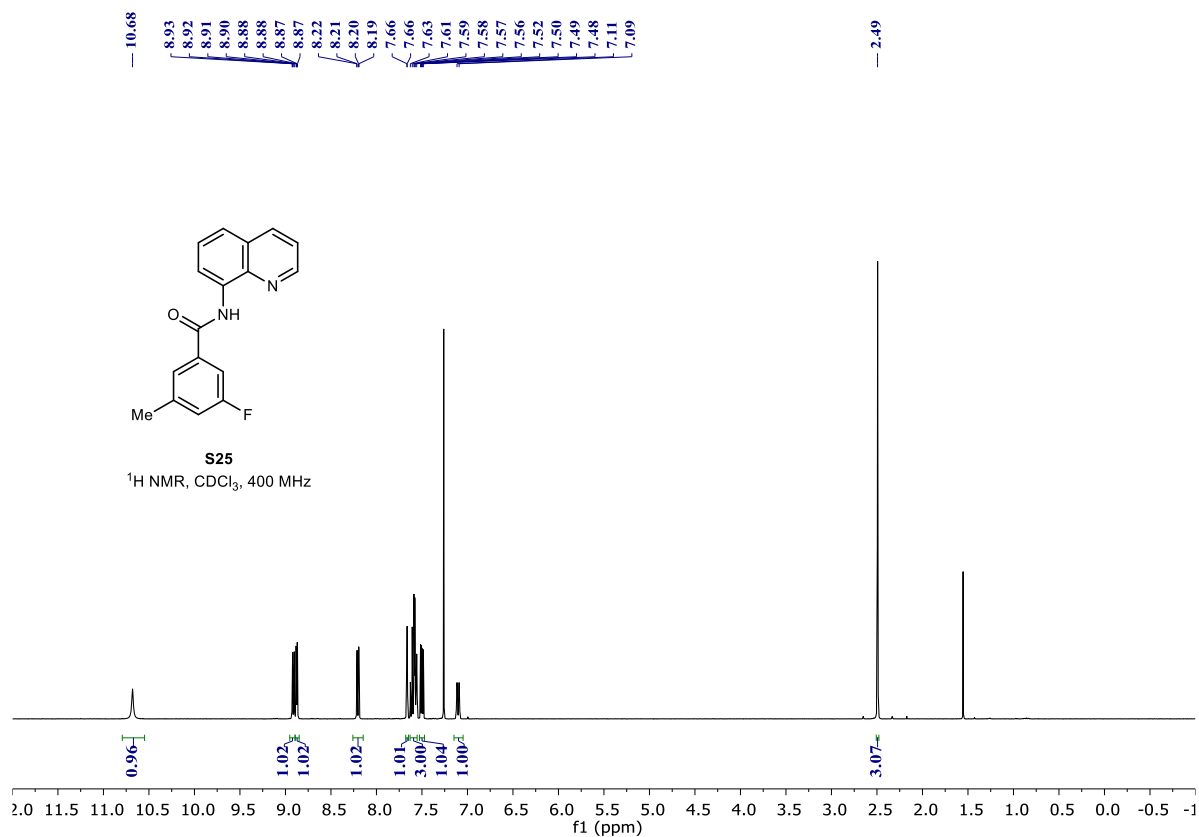
^{13}C NMR, CDCl_3 , 101 MHz

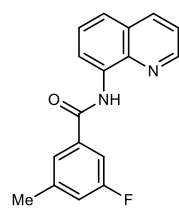






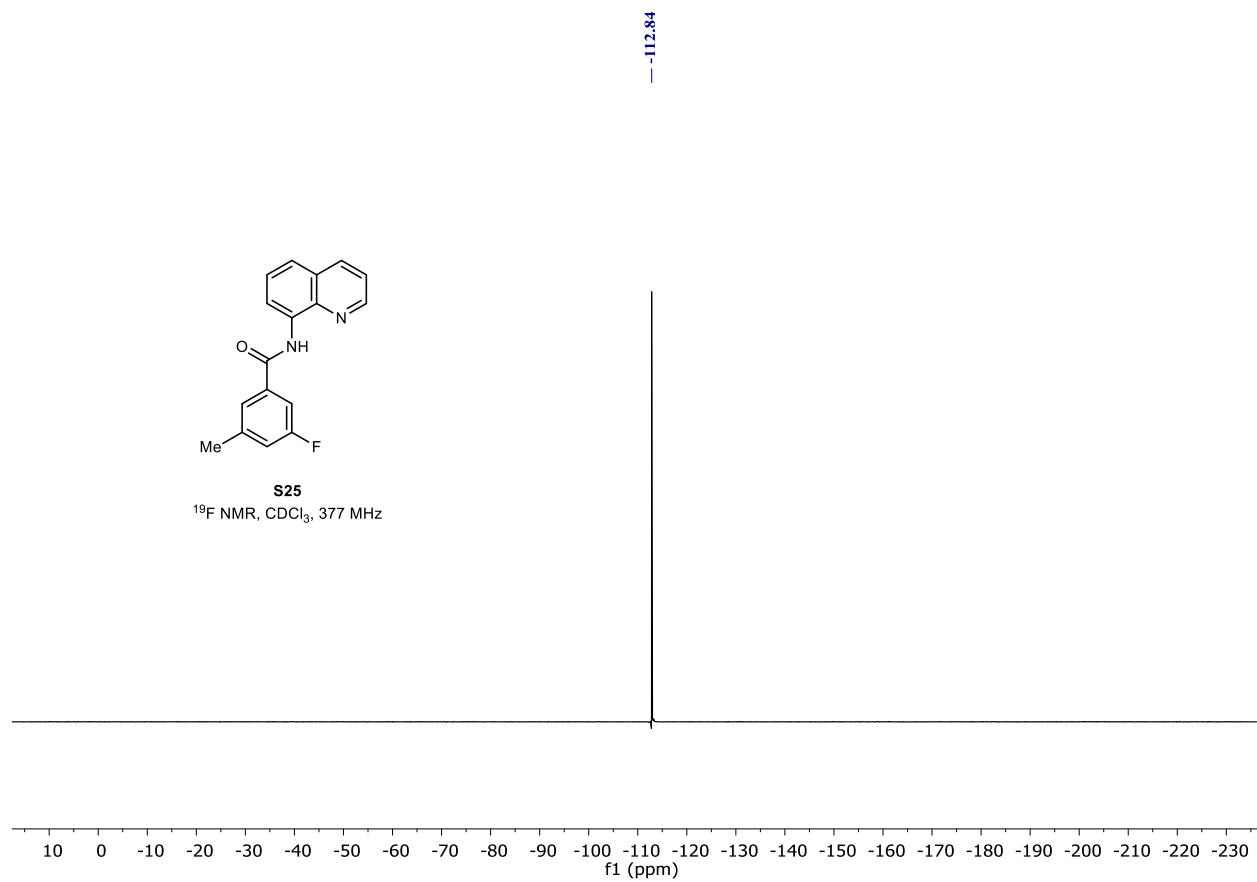


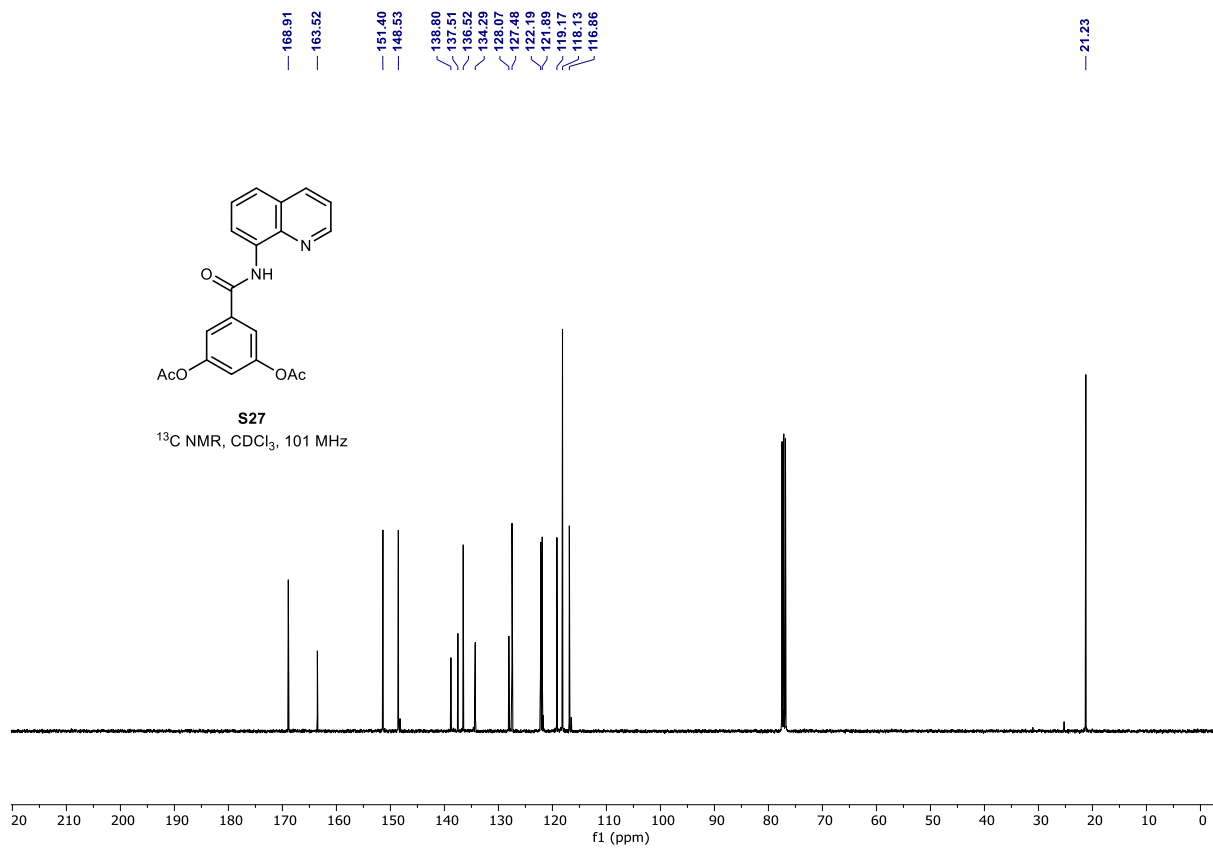
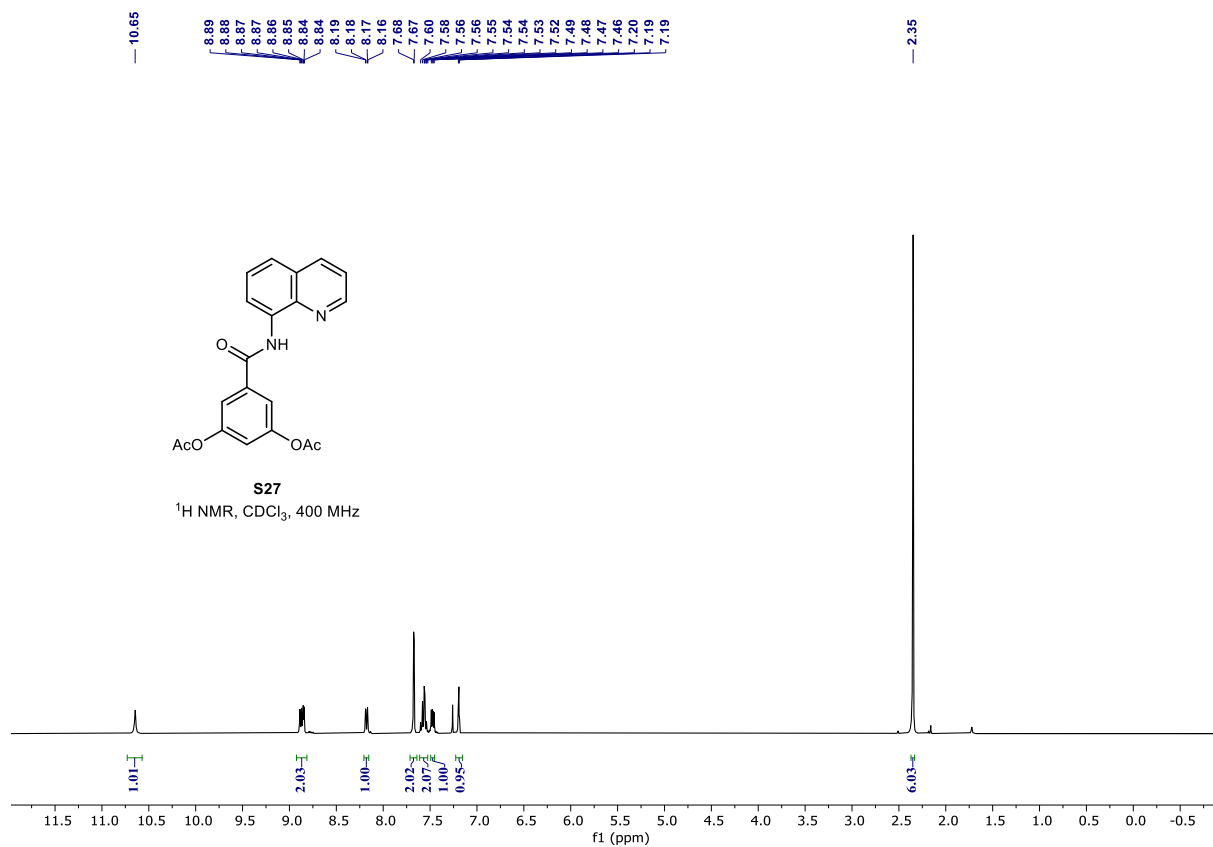


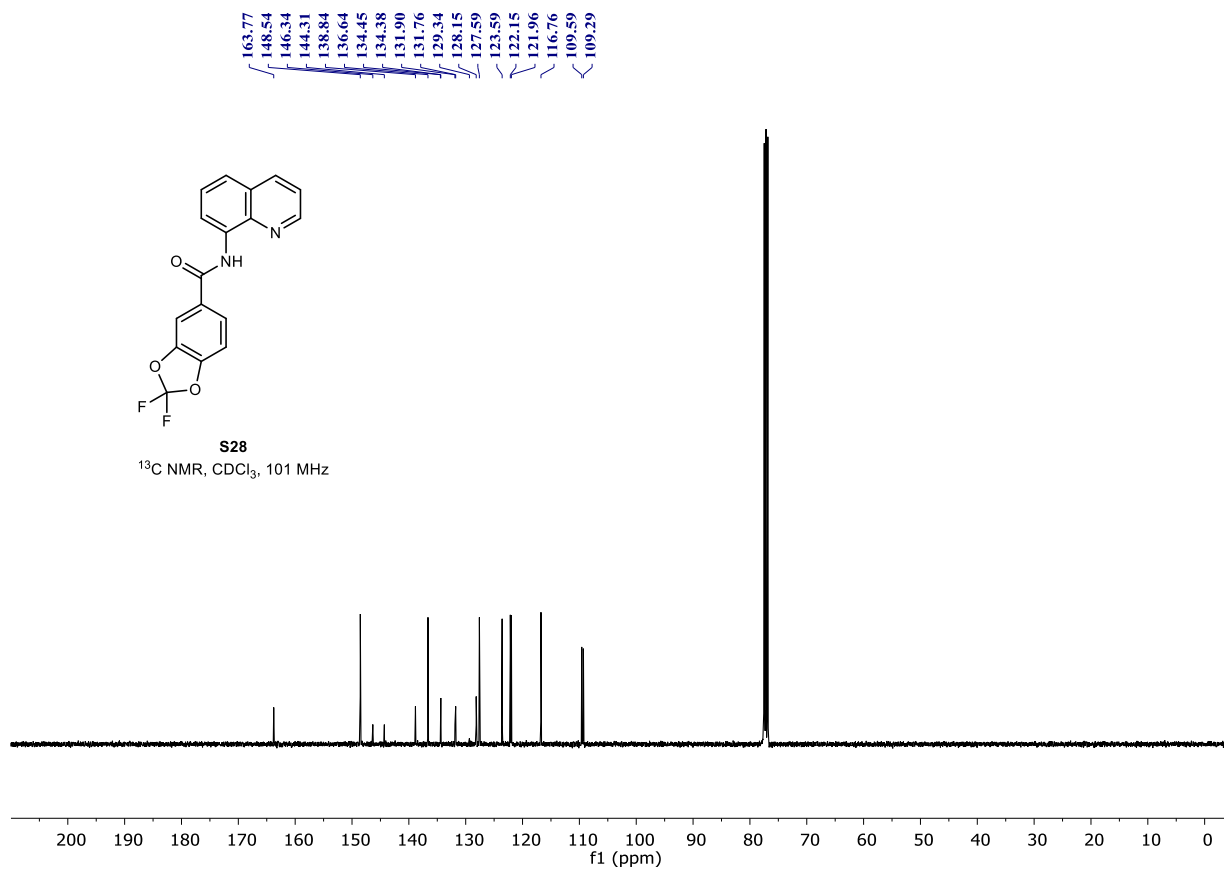
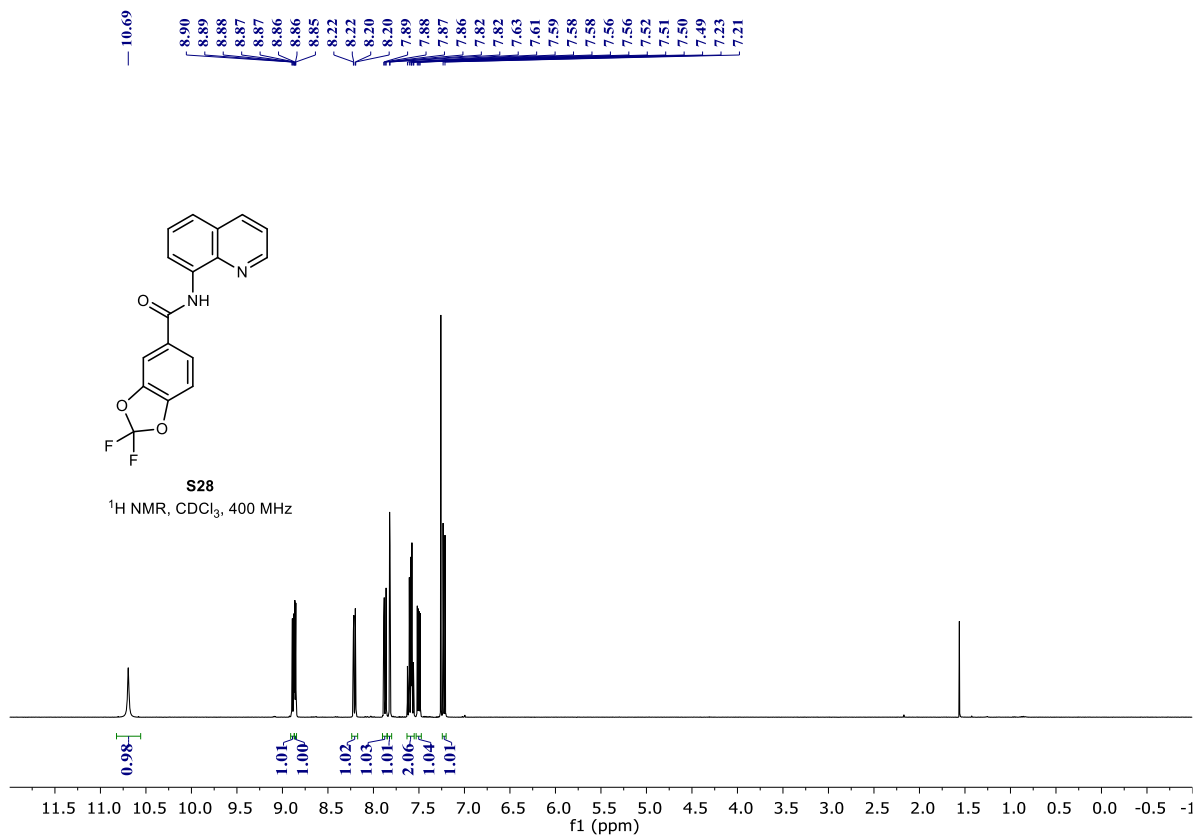


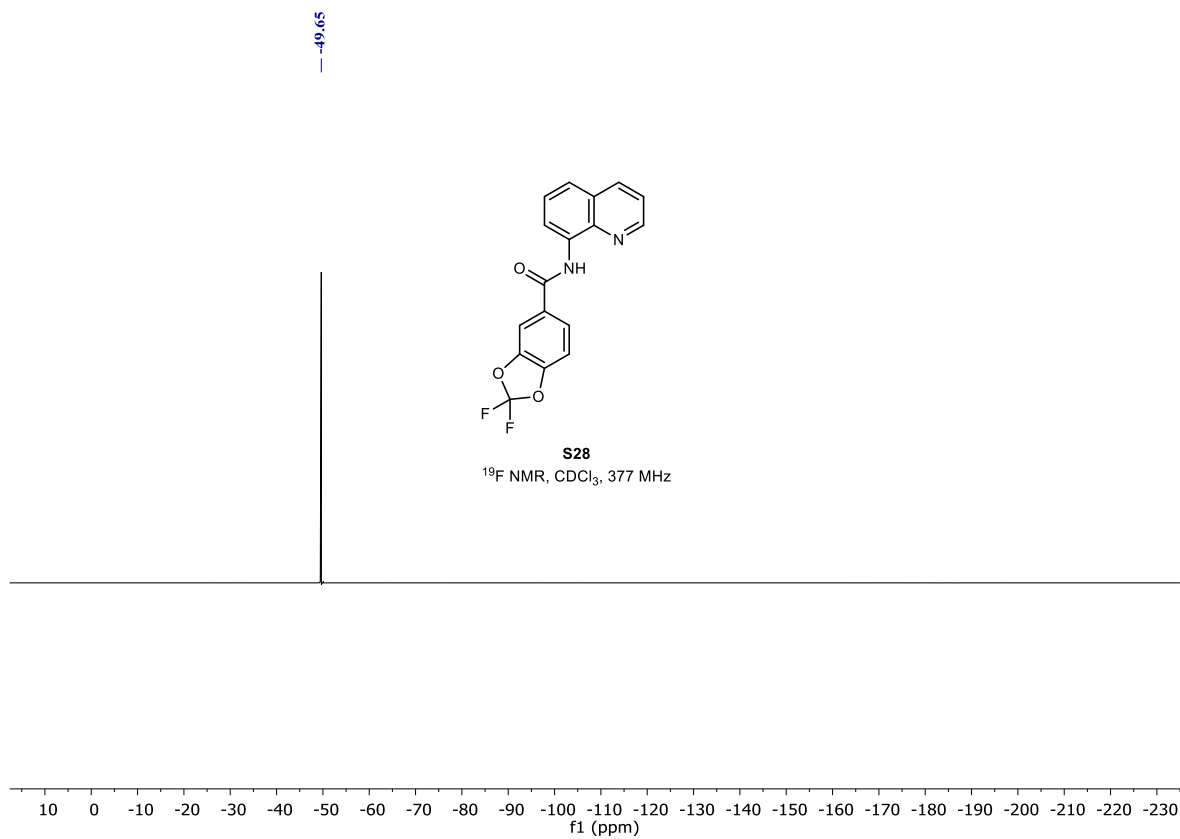
S25

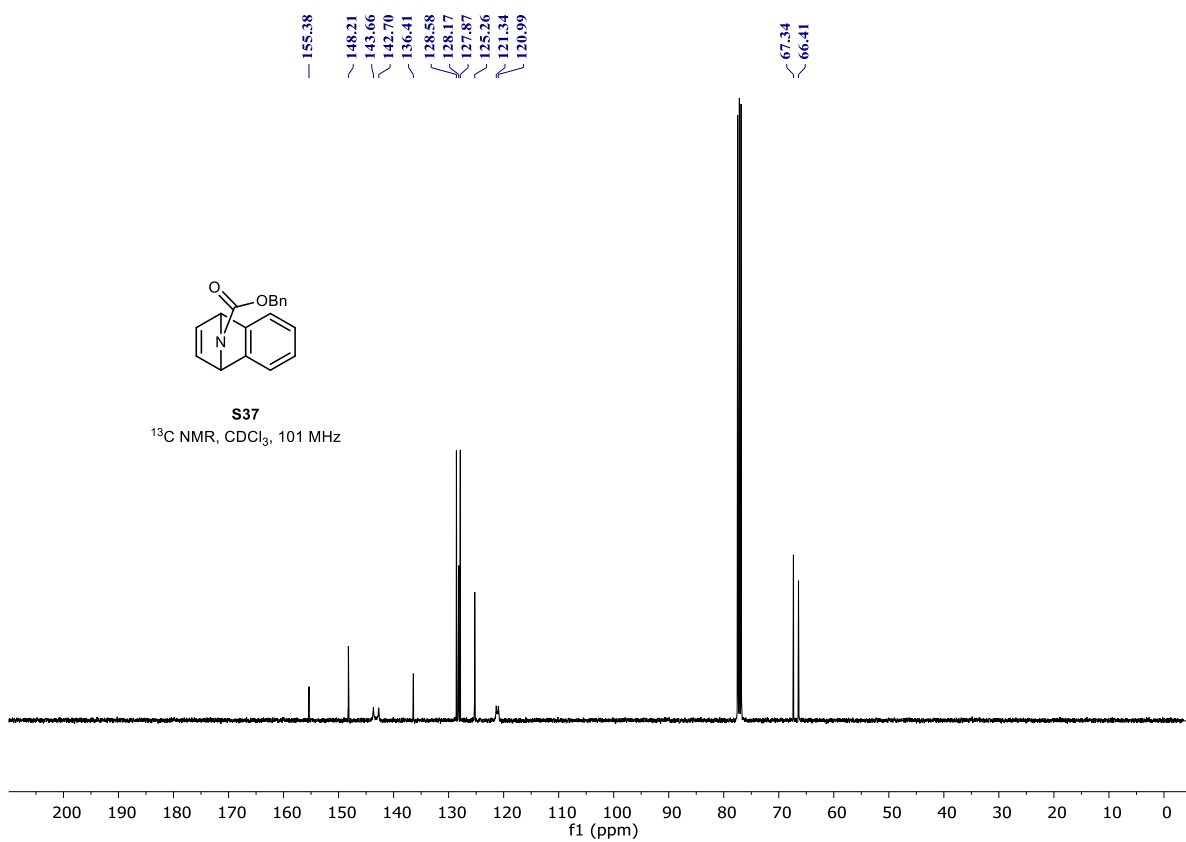
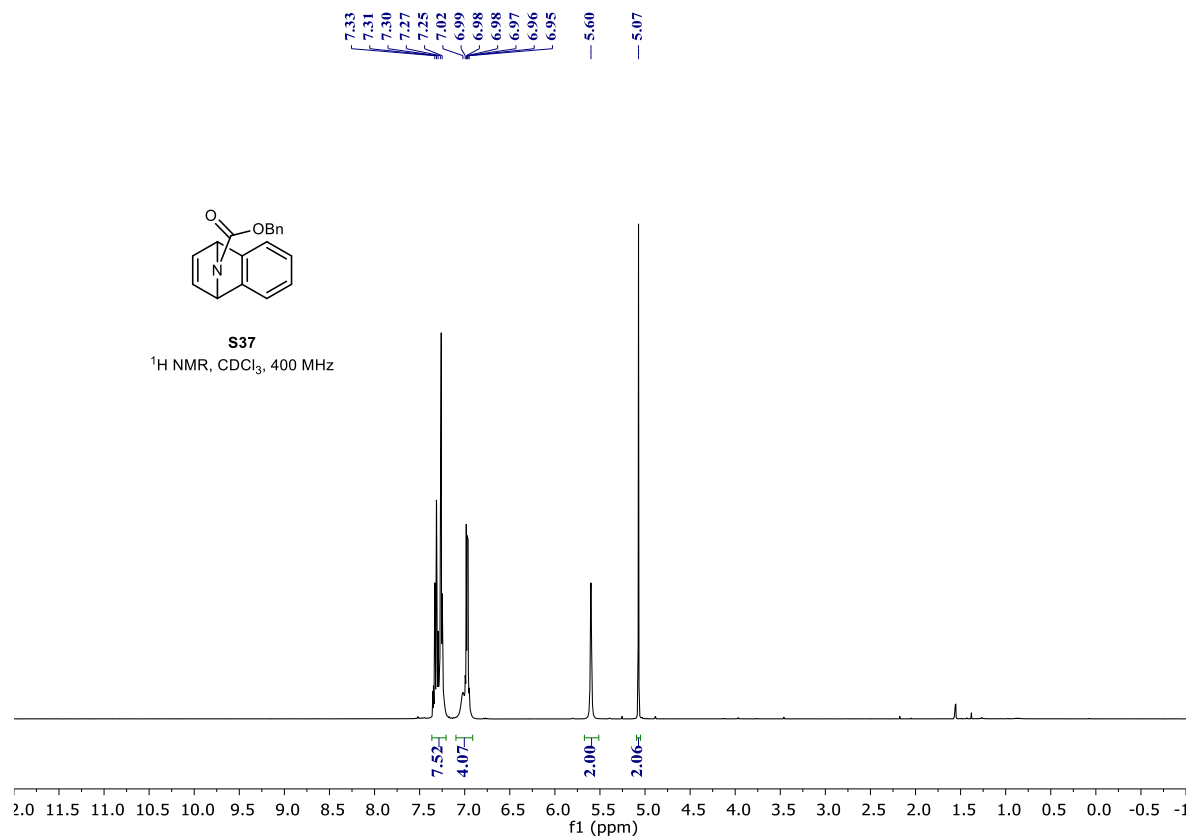
^{19}F NMR, CDCl_3 , 377 MHz

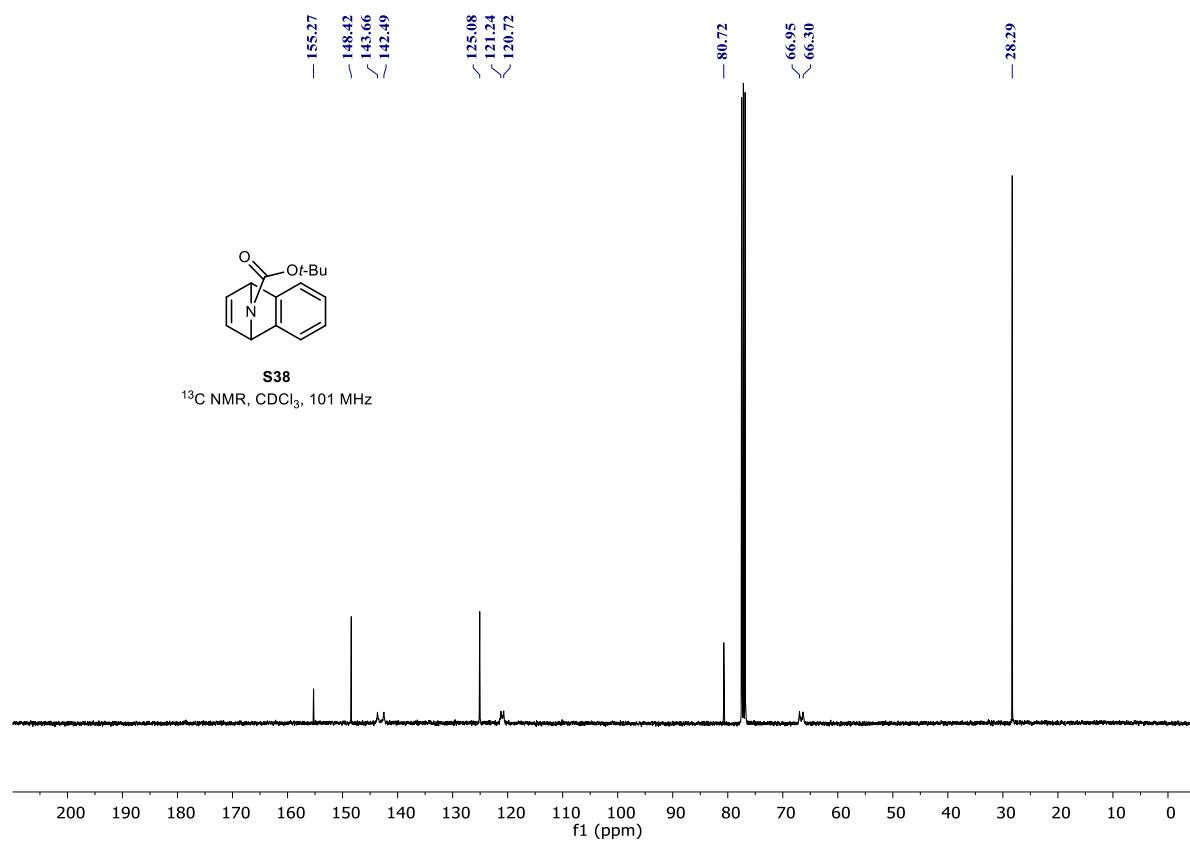
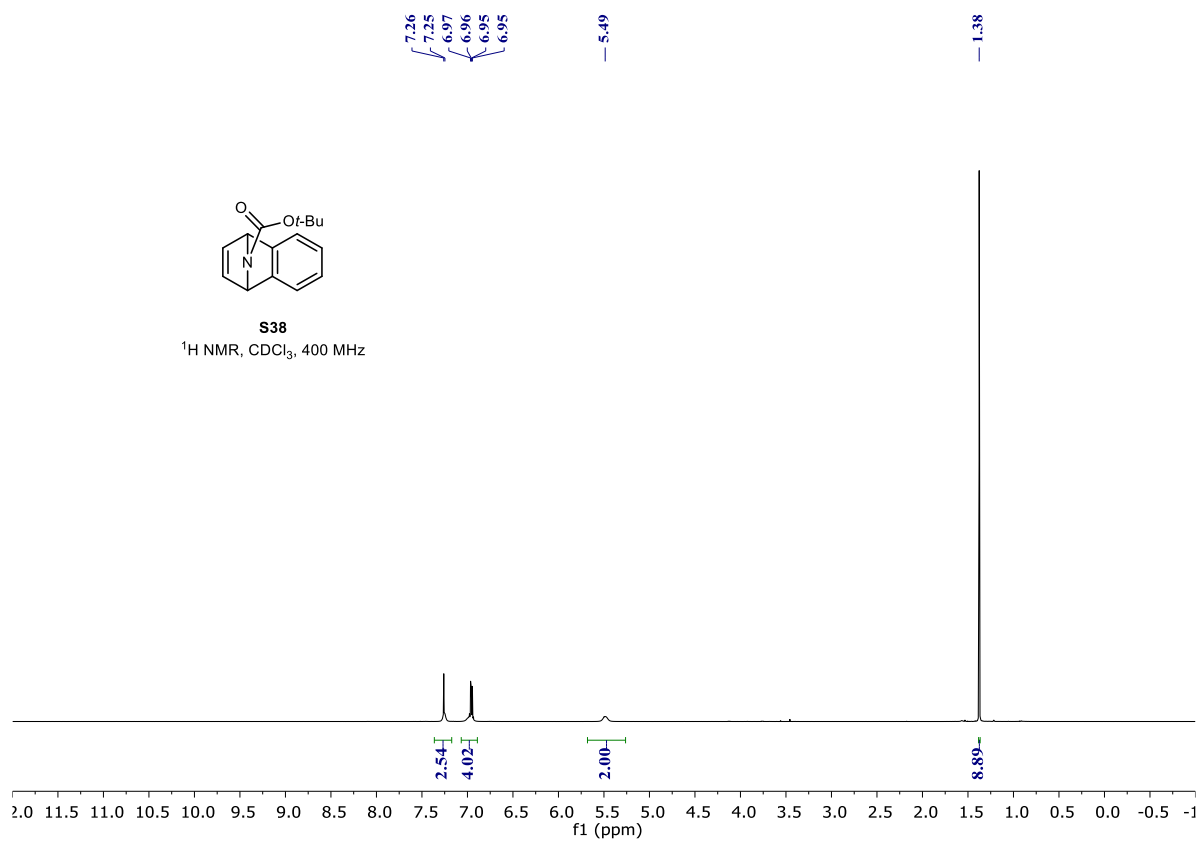


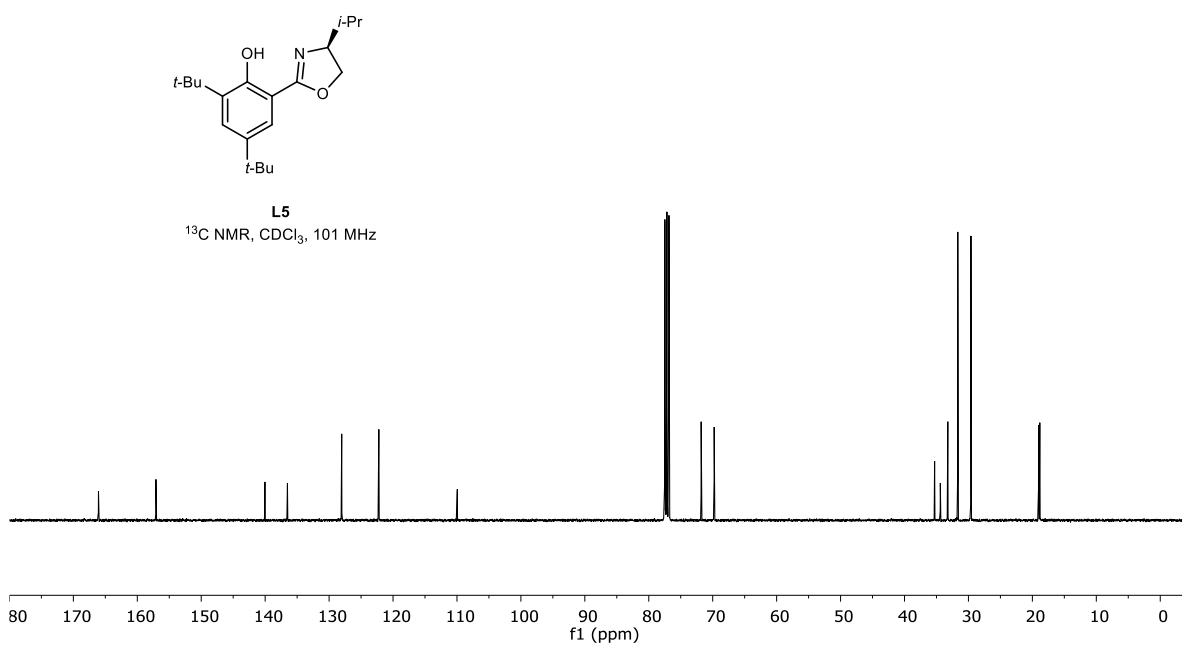
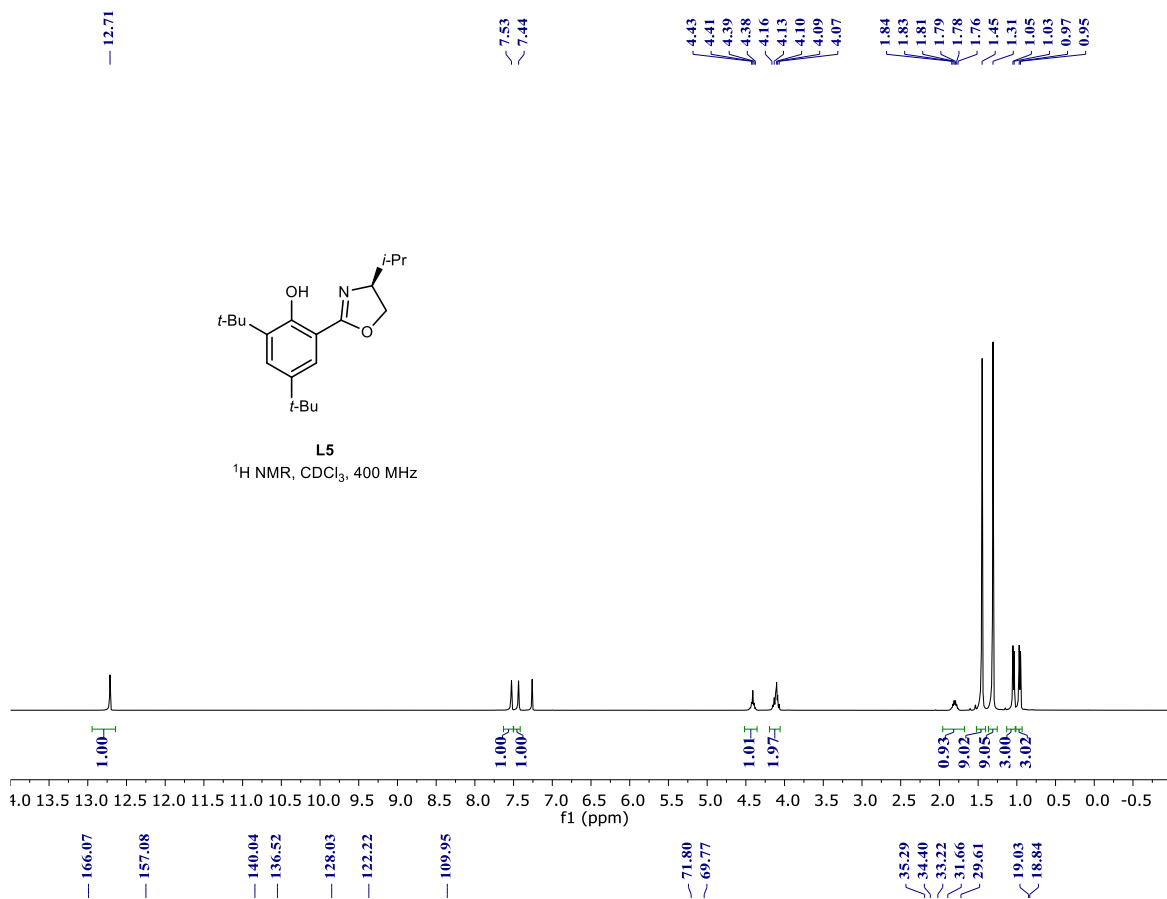


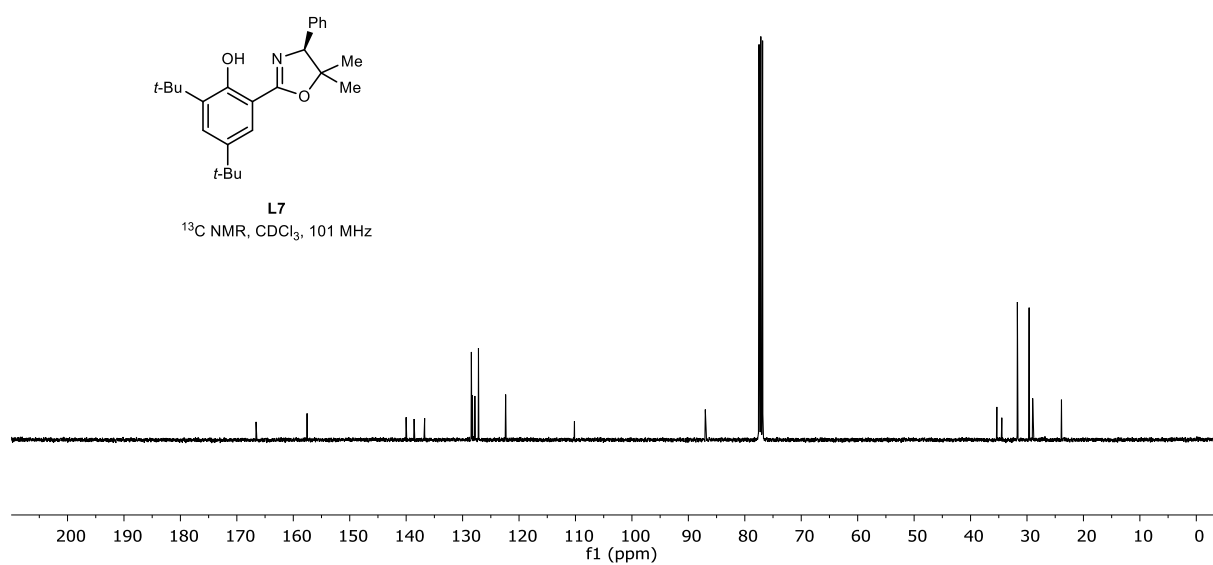
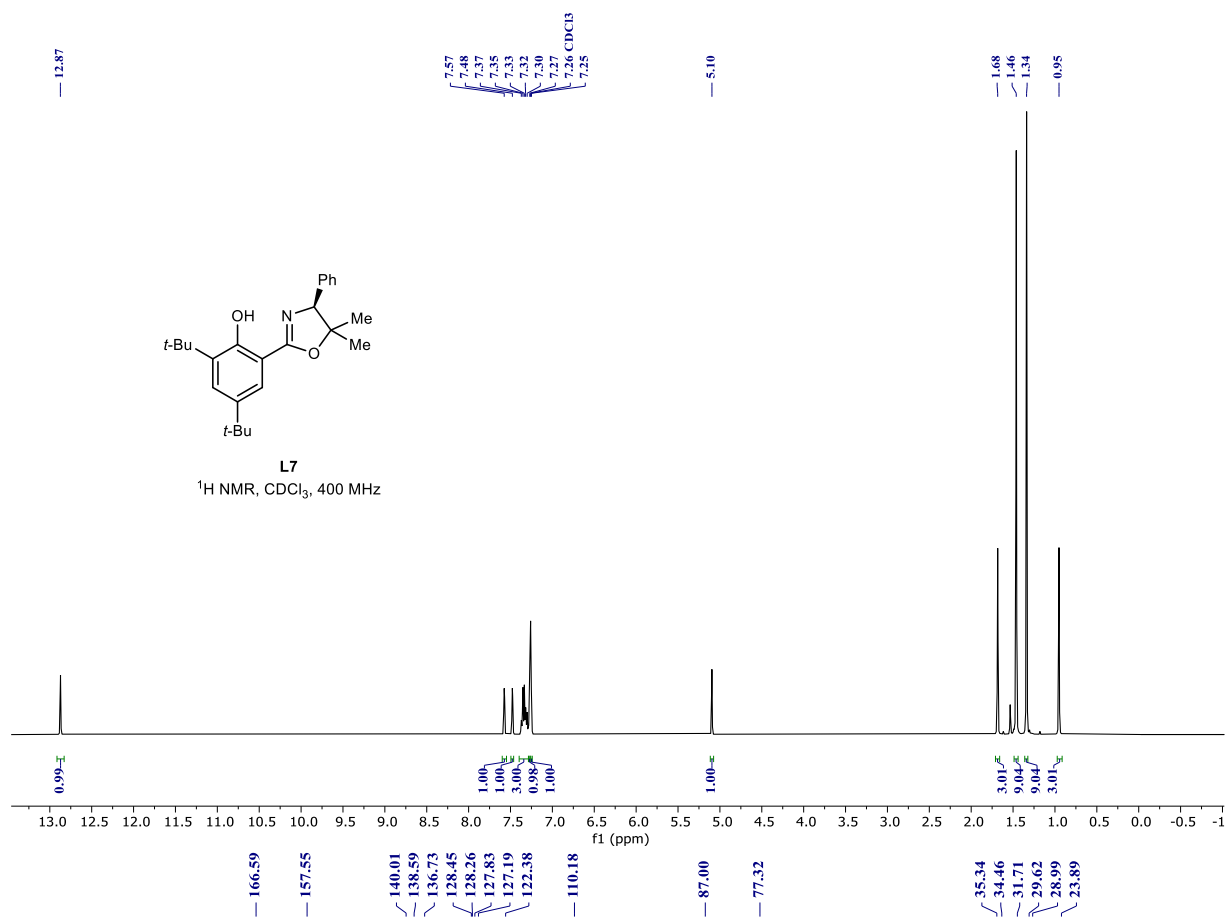


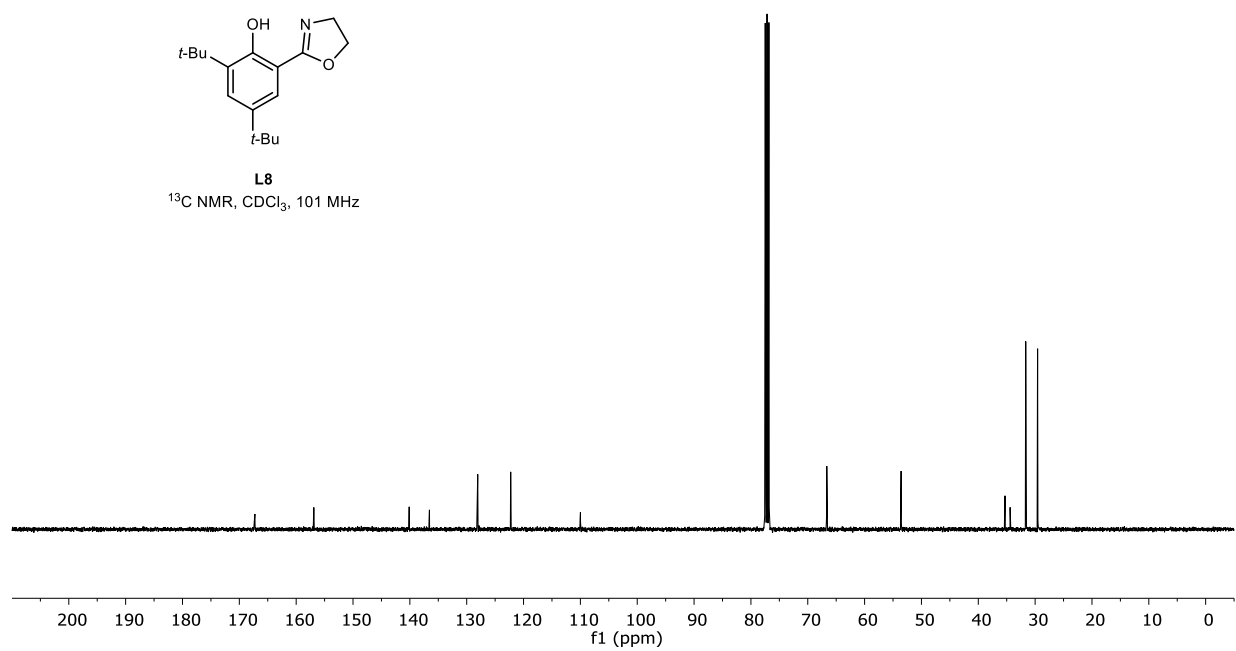
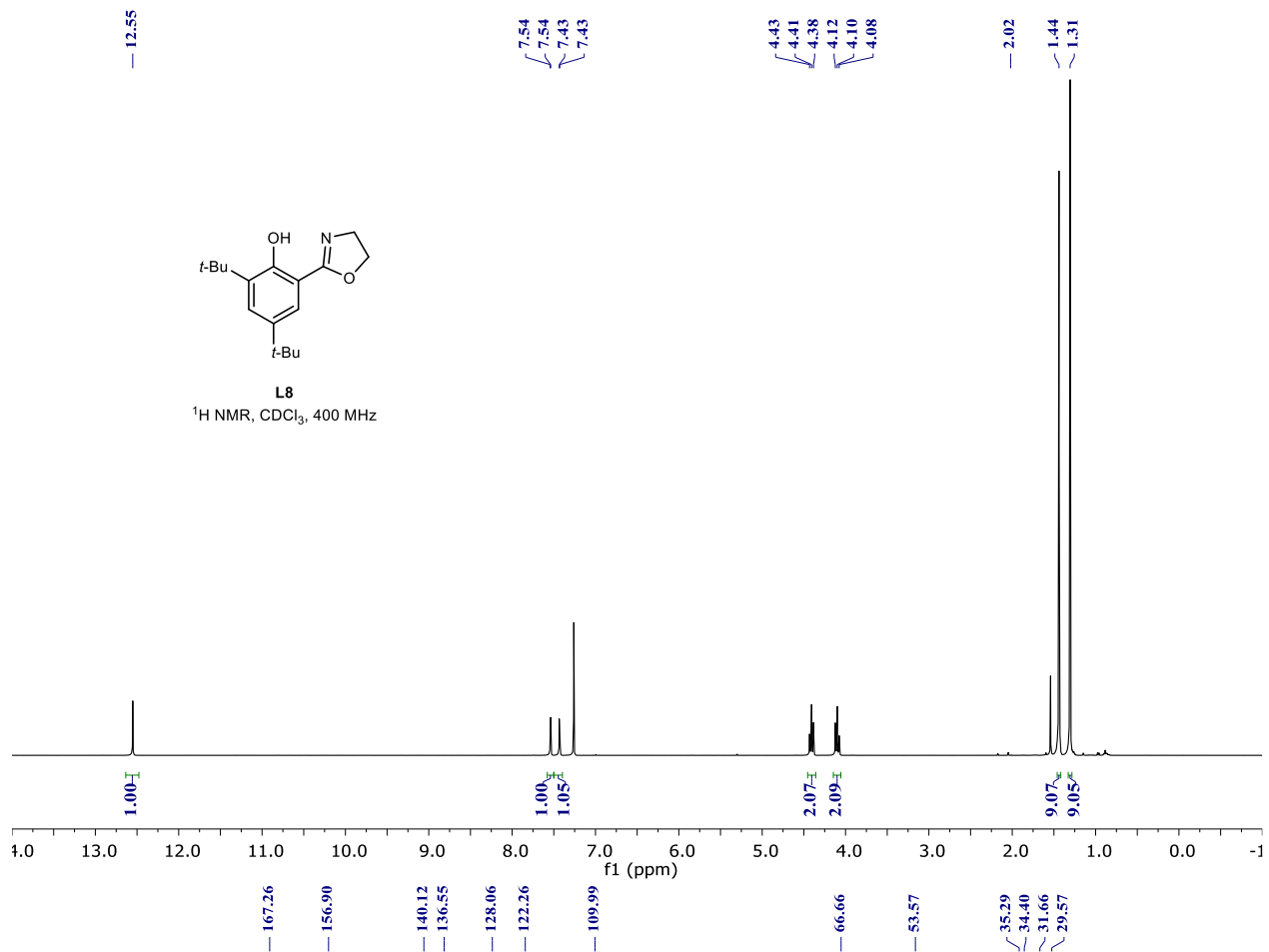


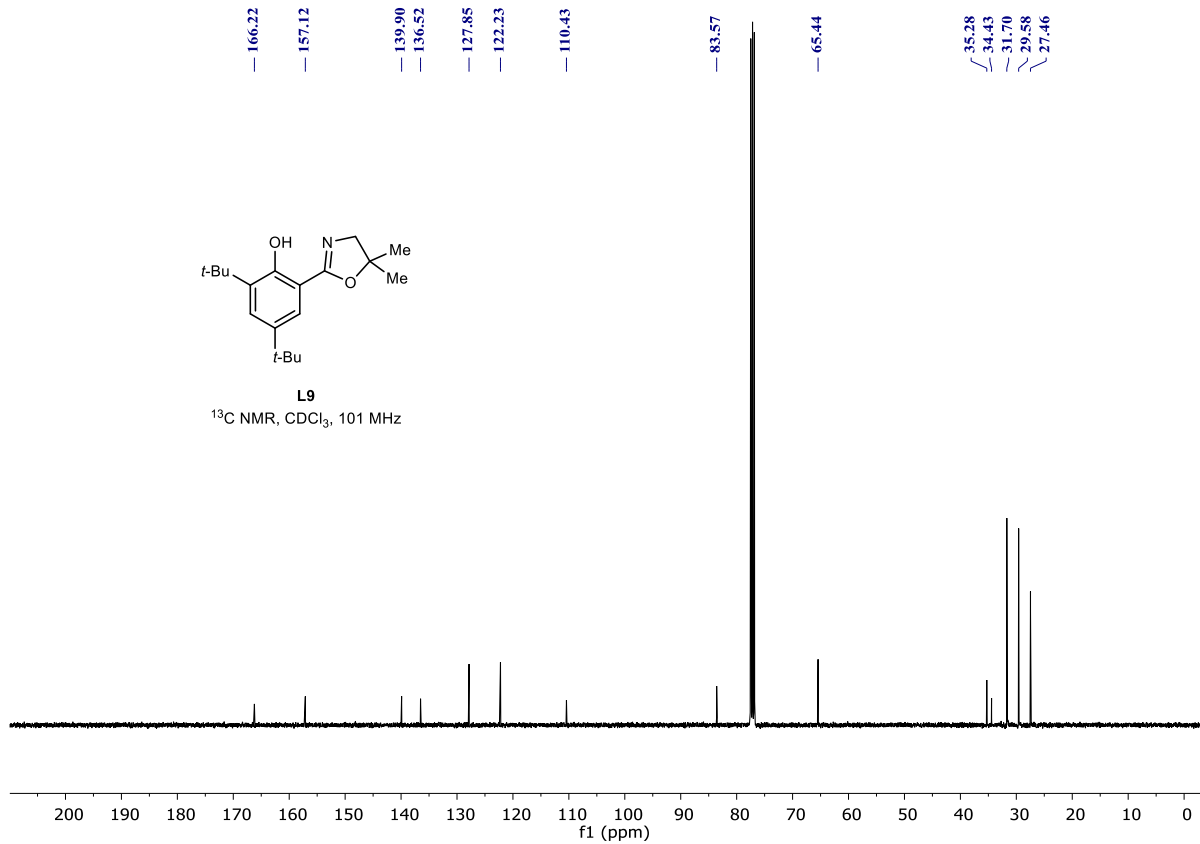
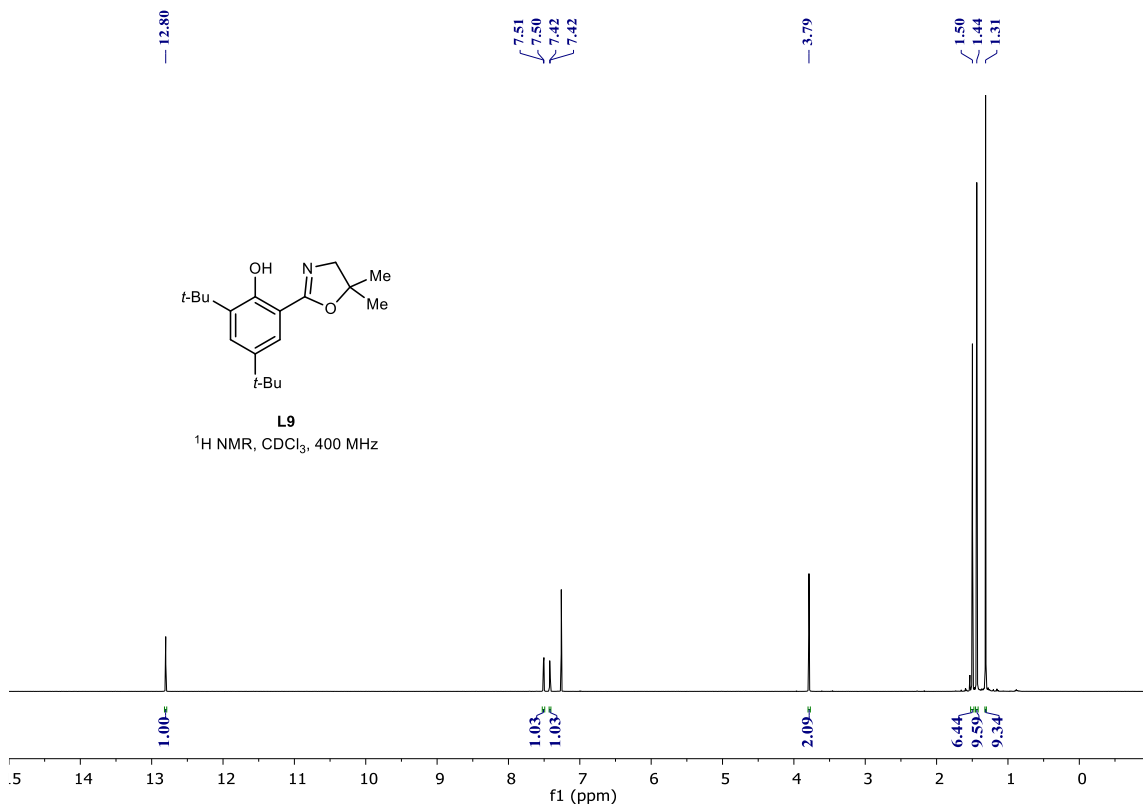


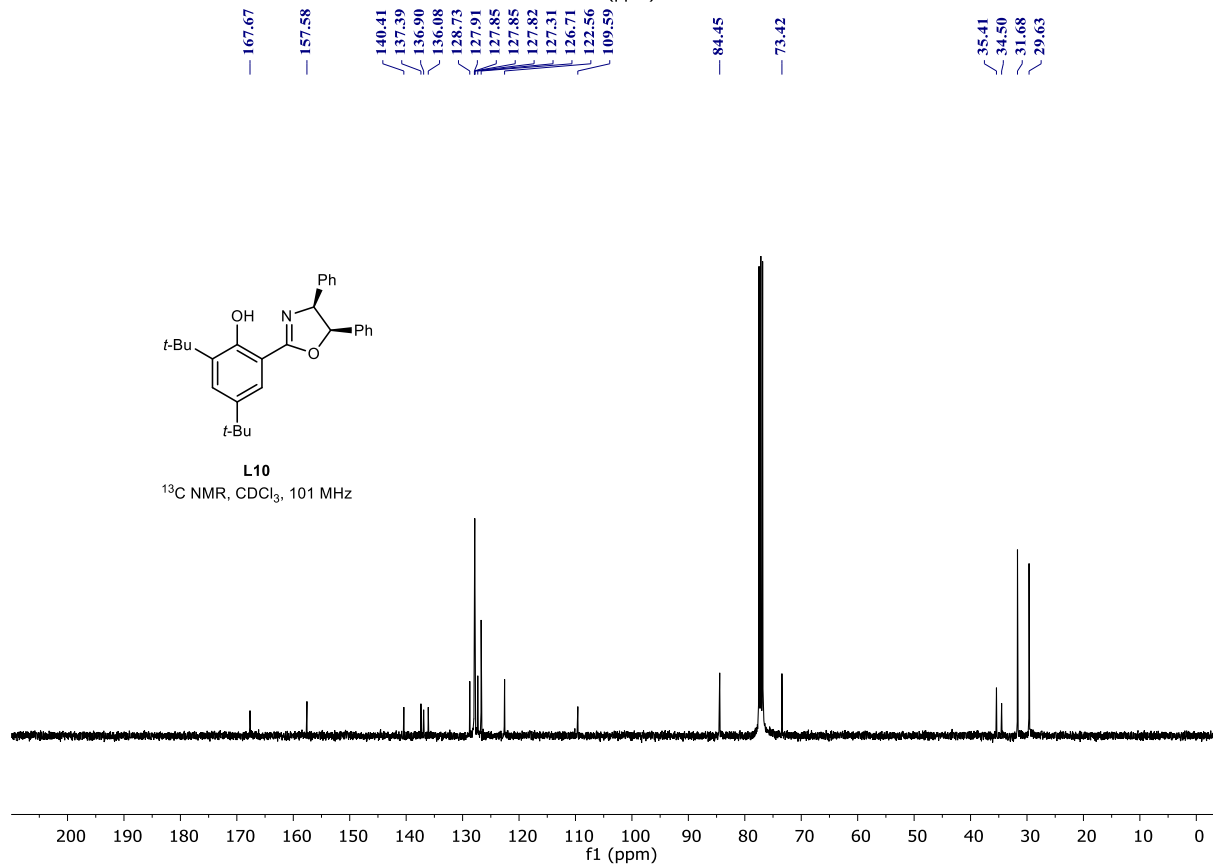
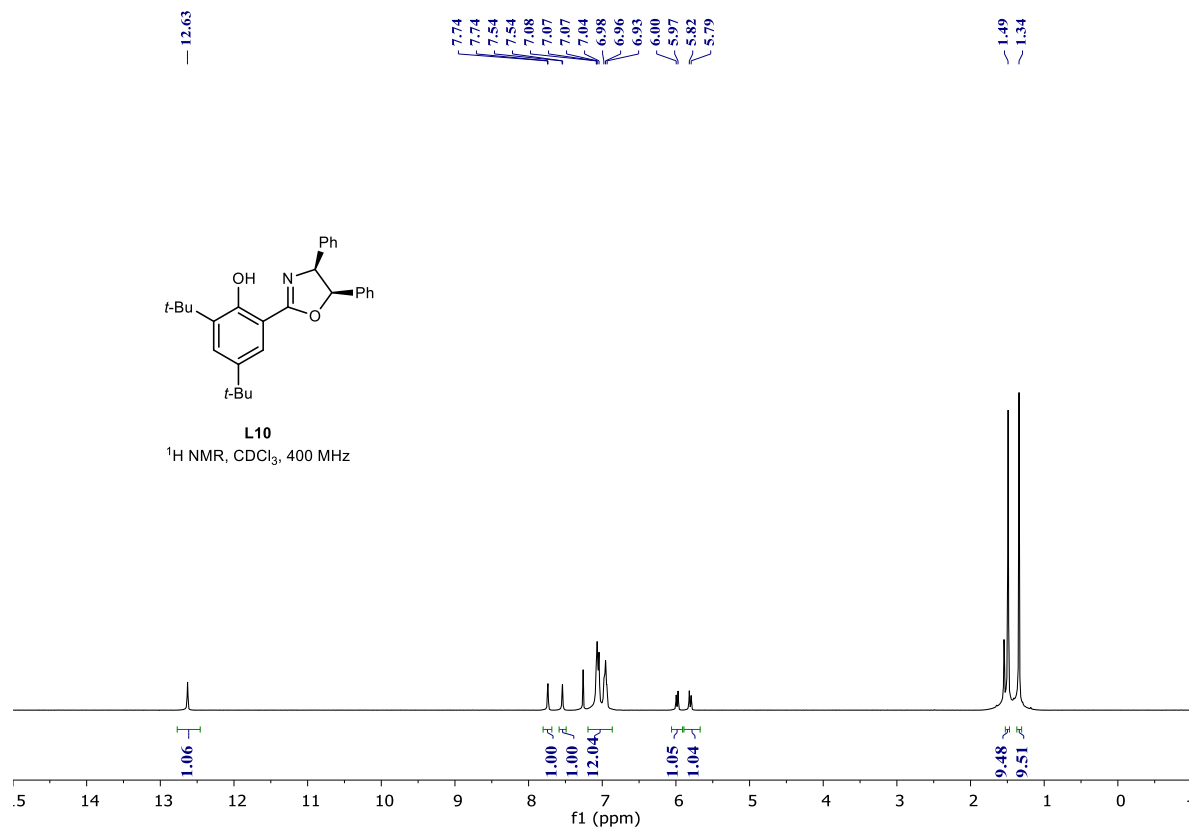


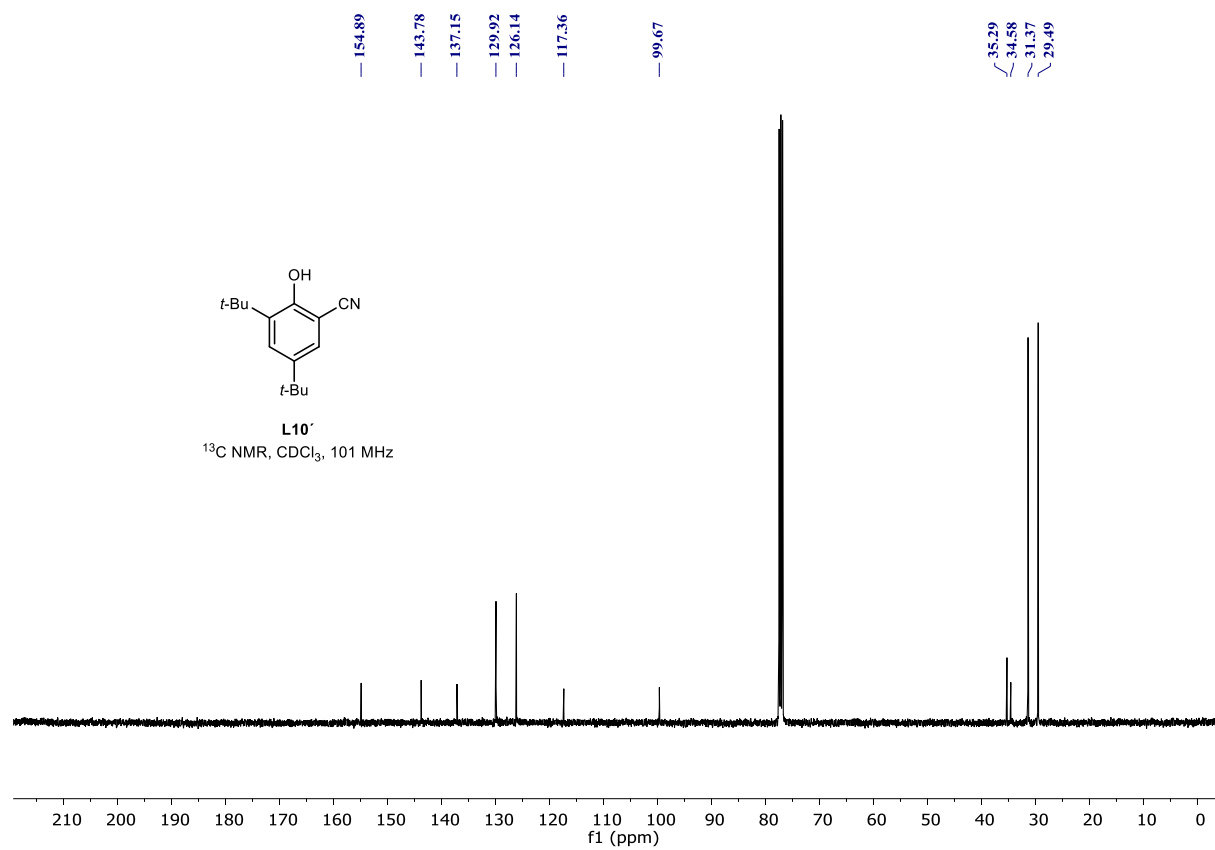
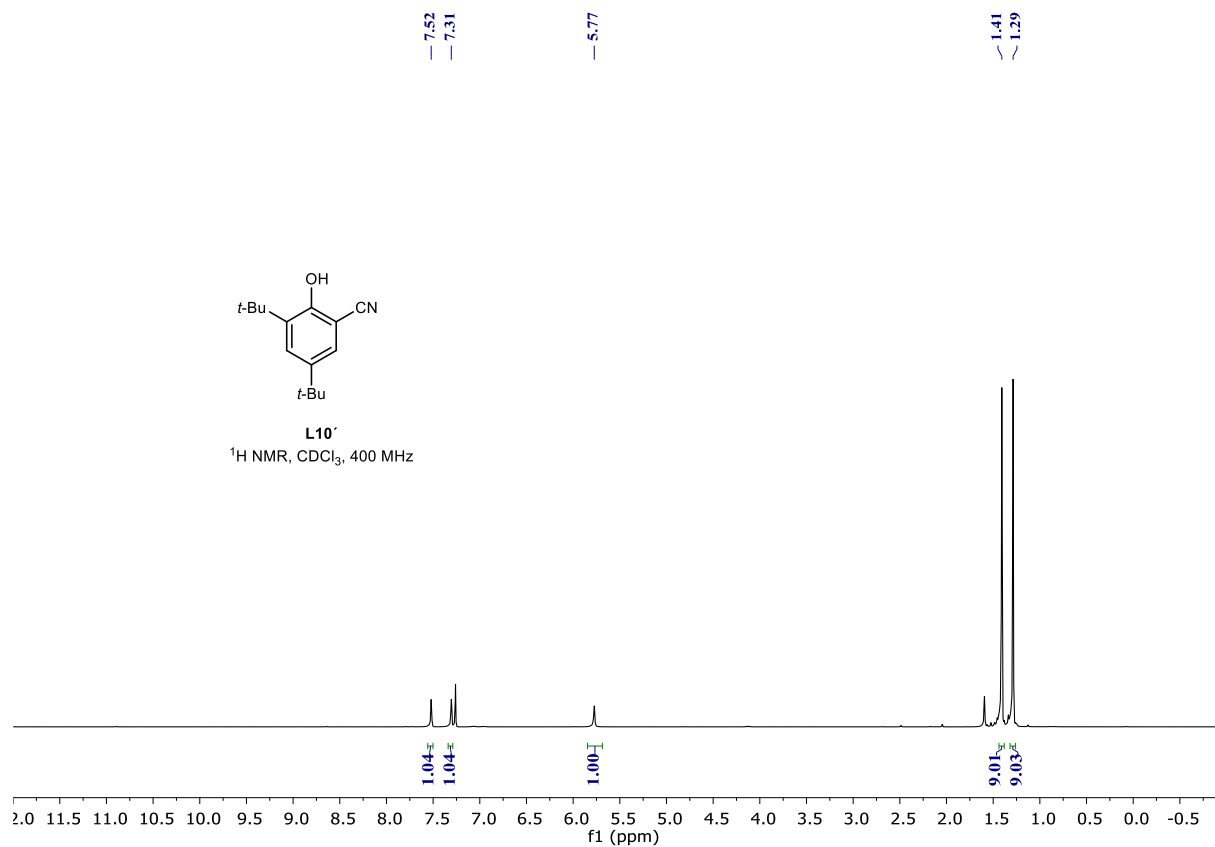


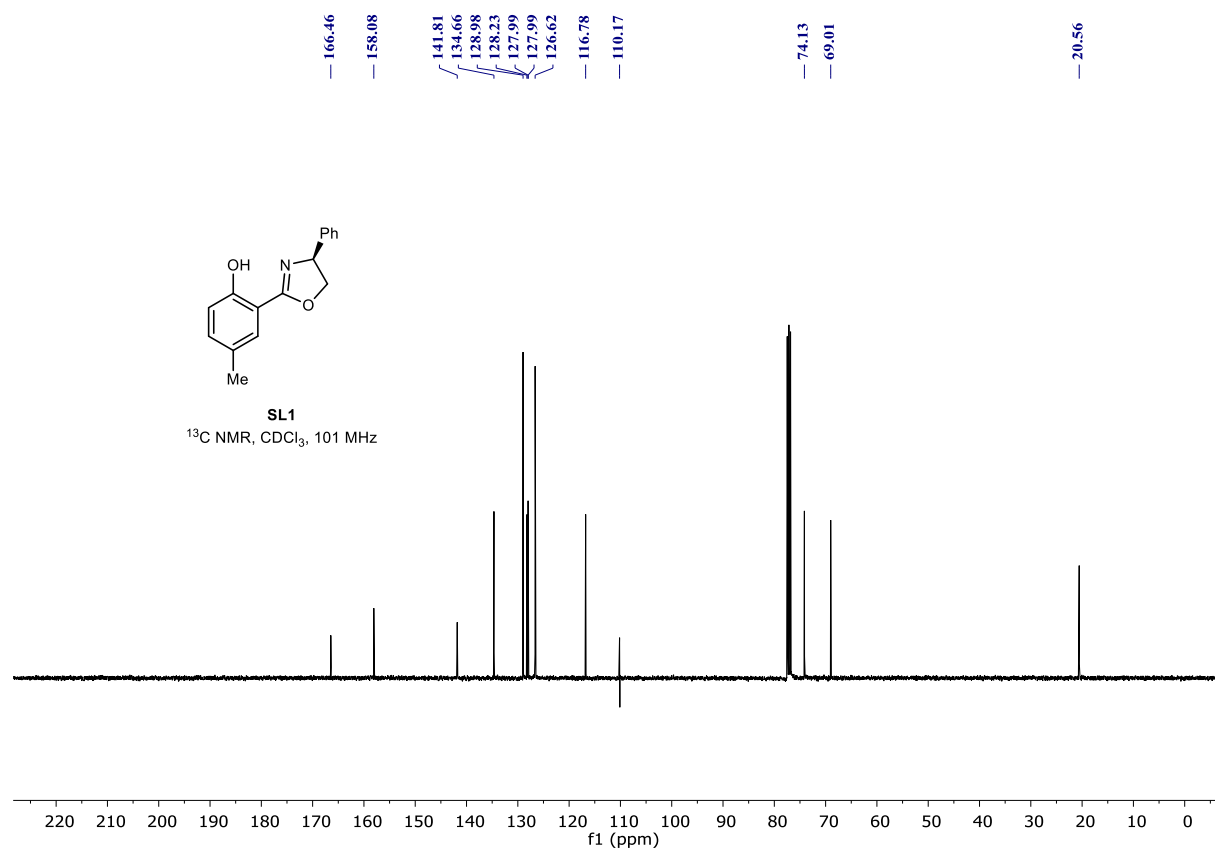
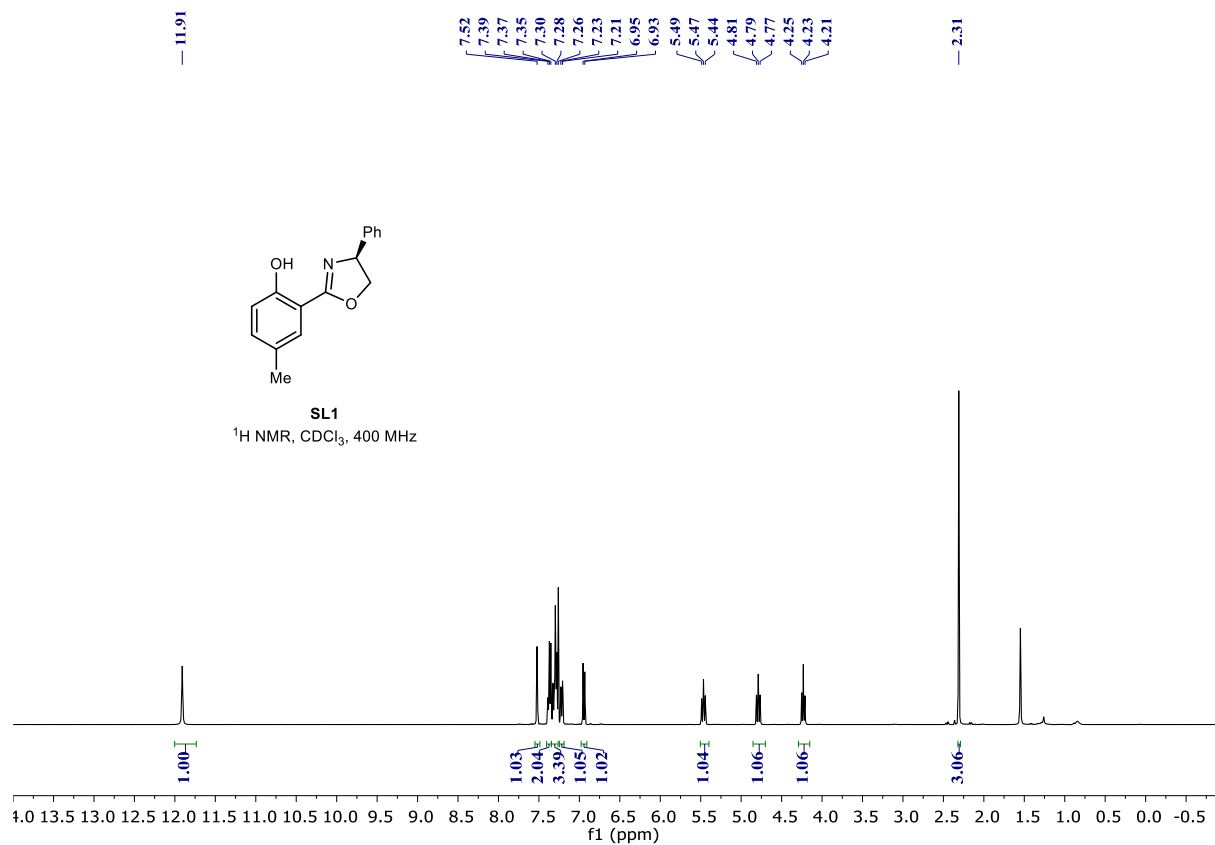


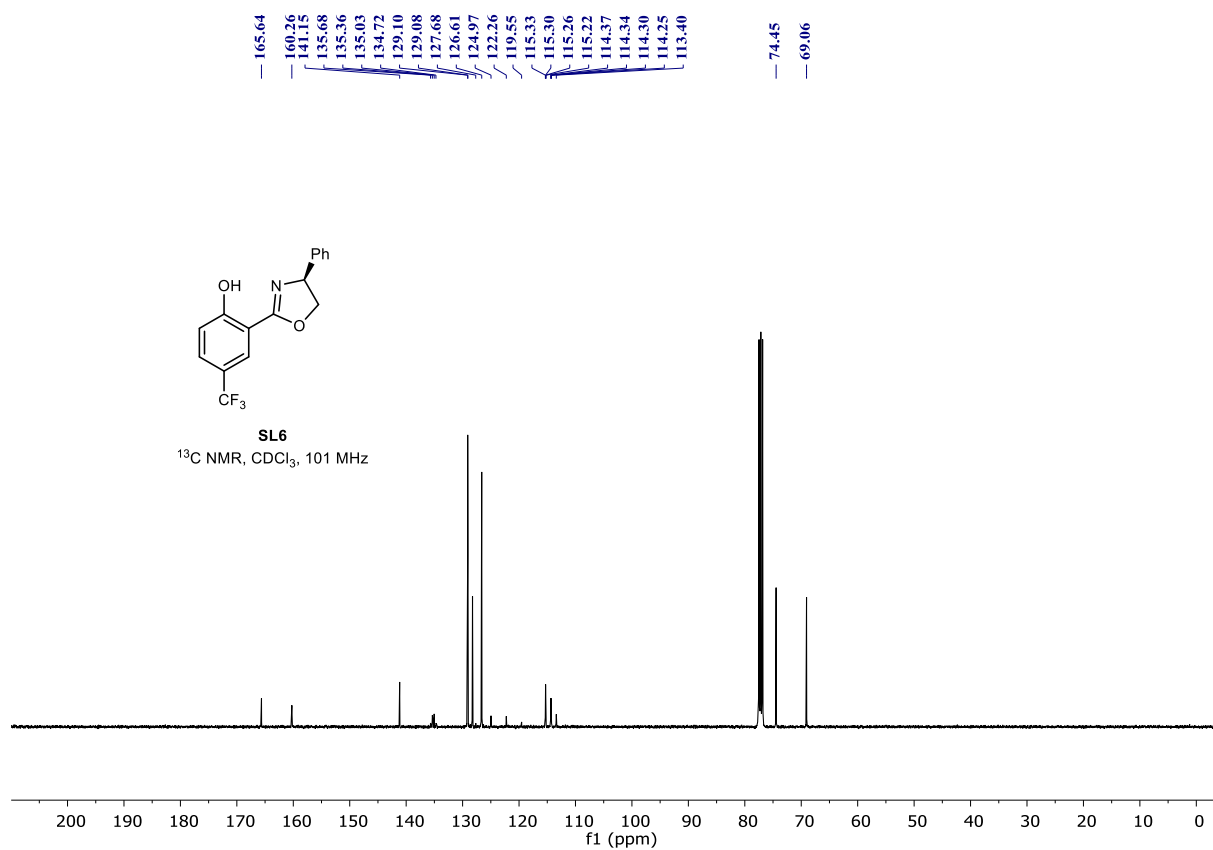
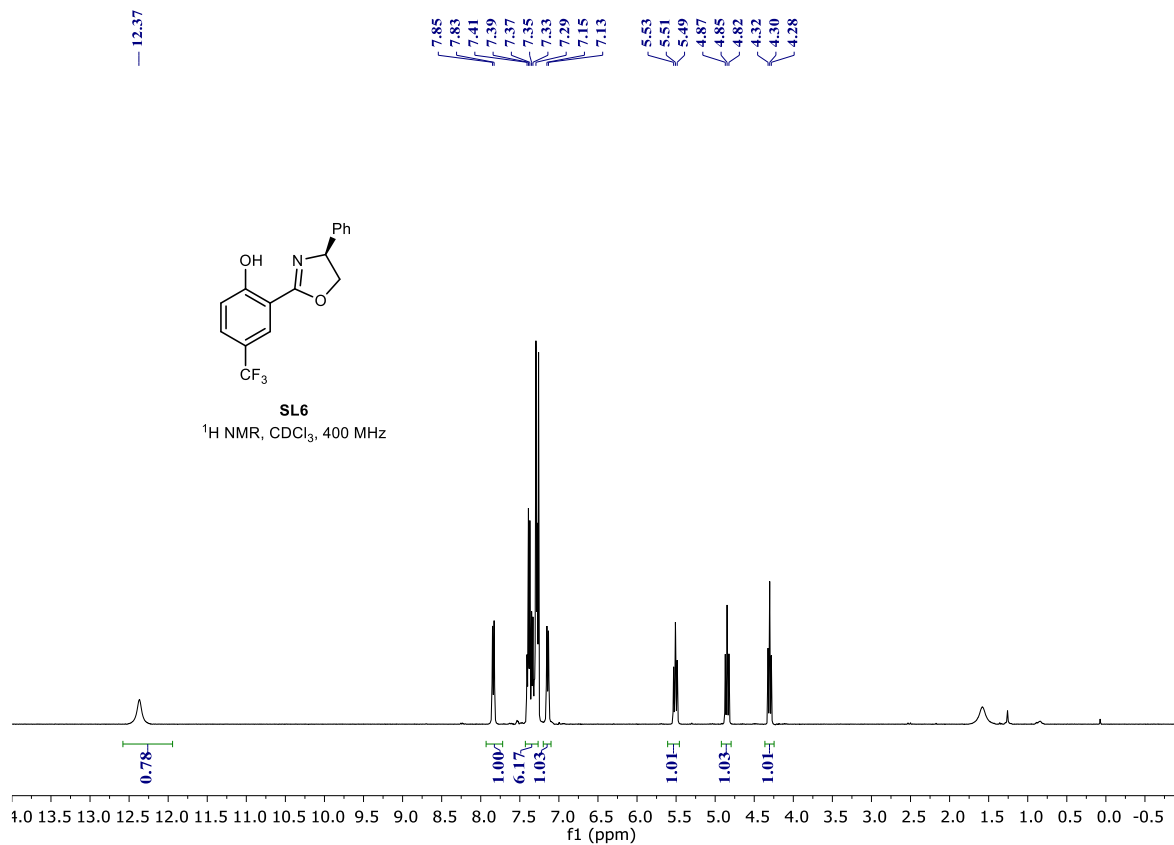


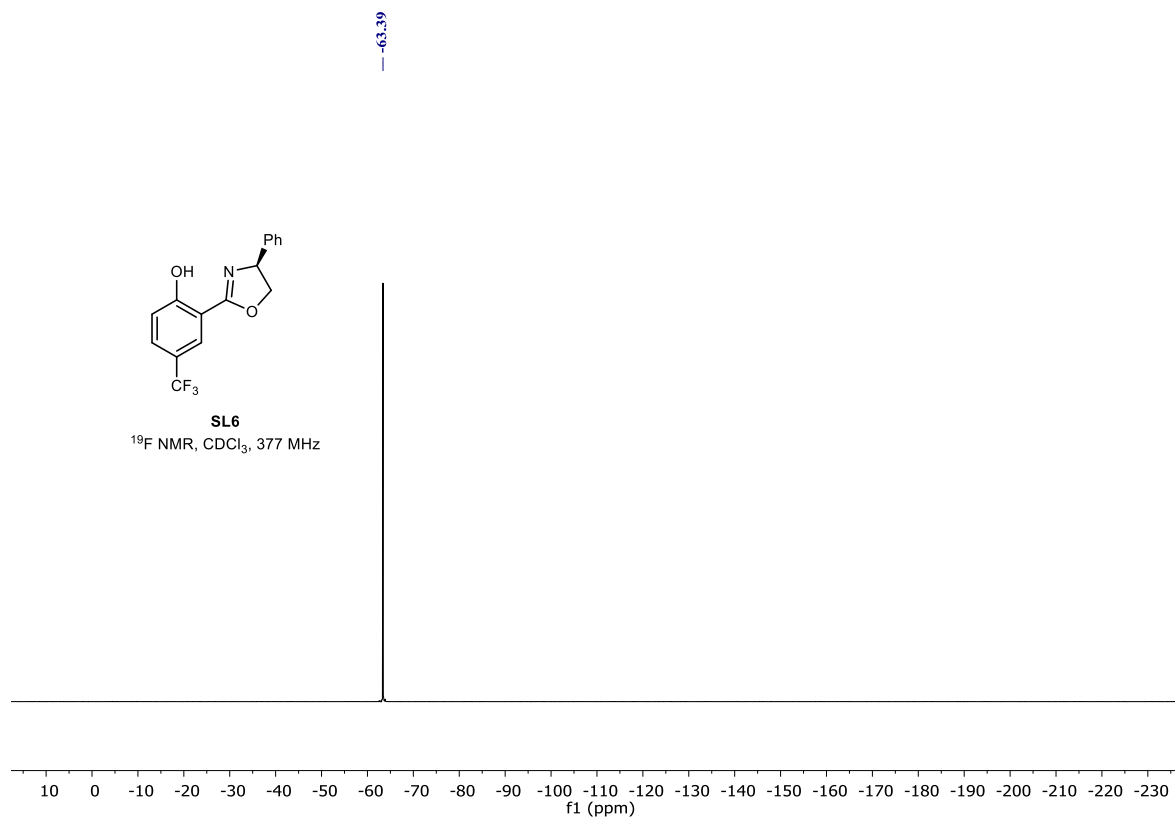


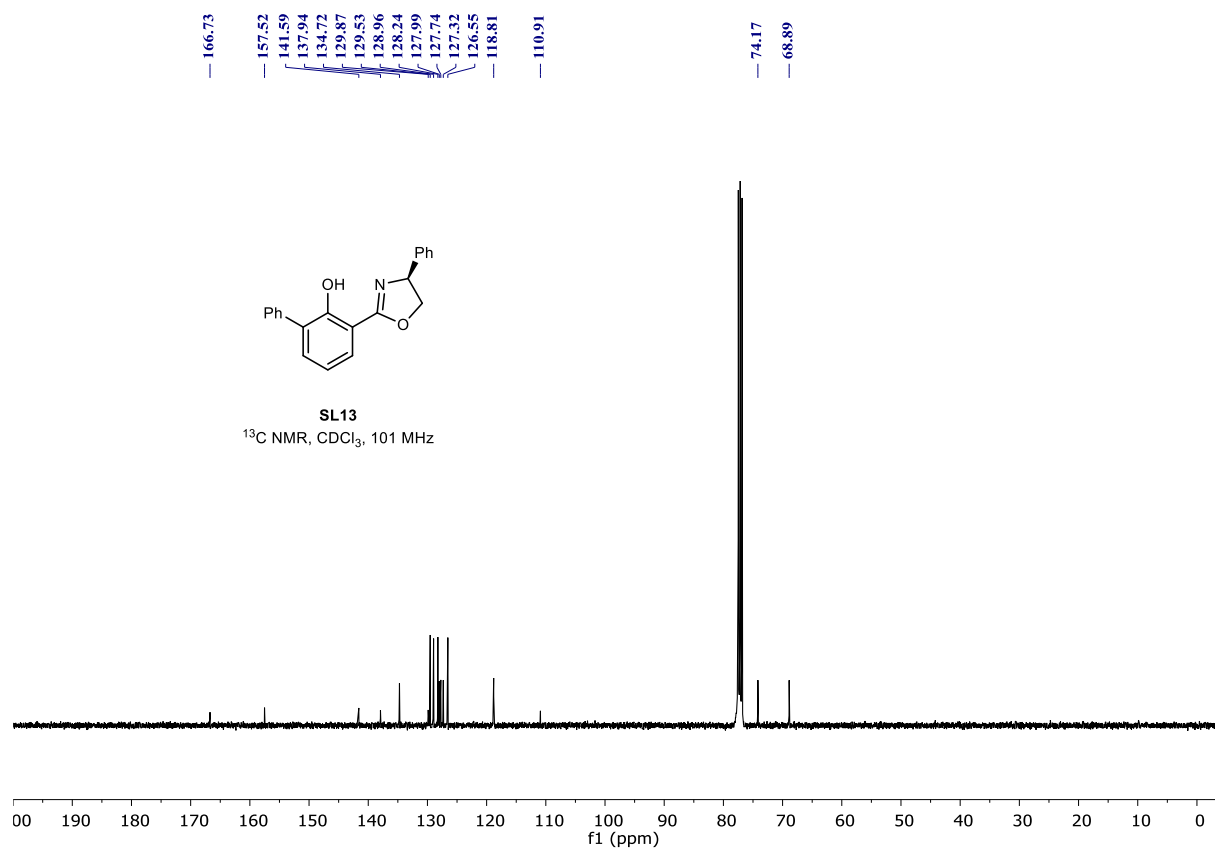
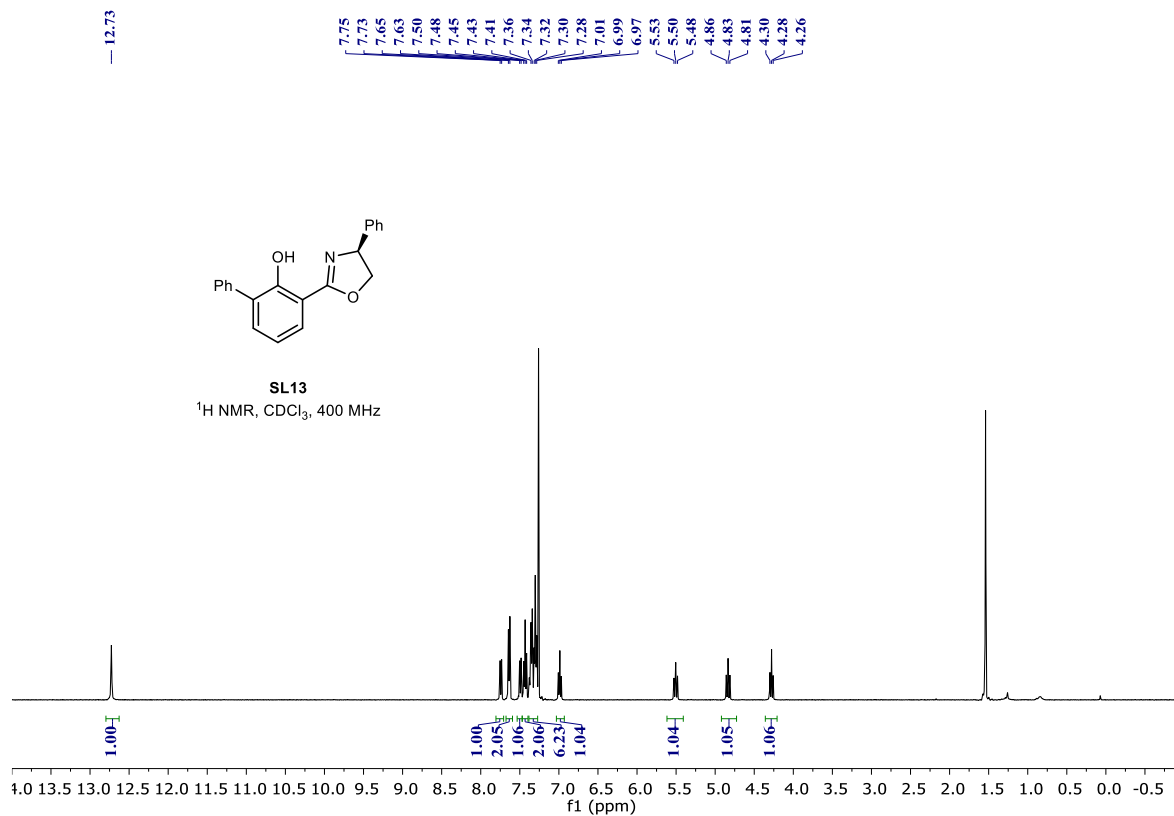


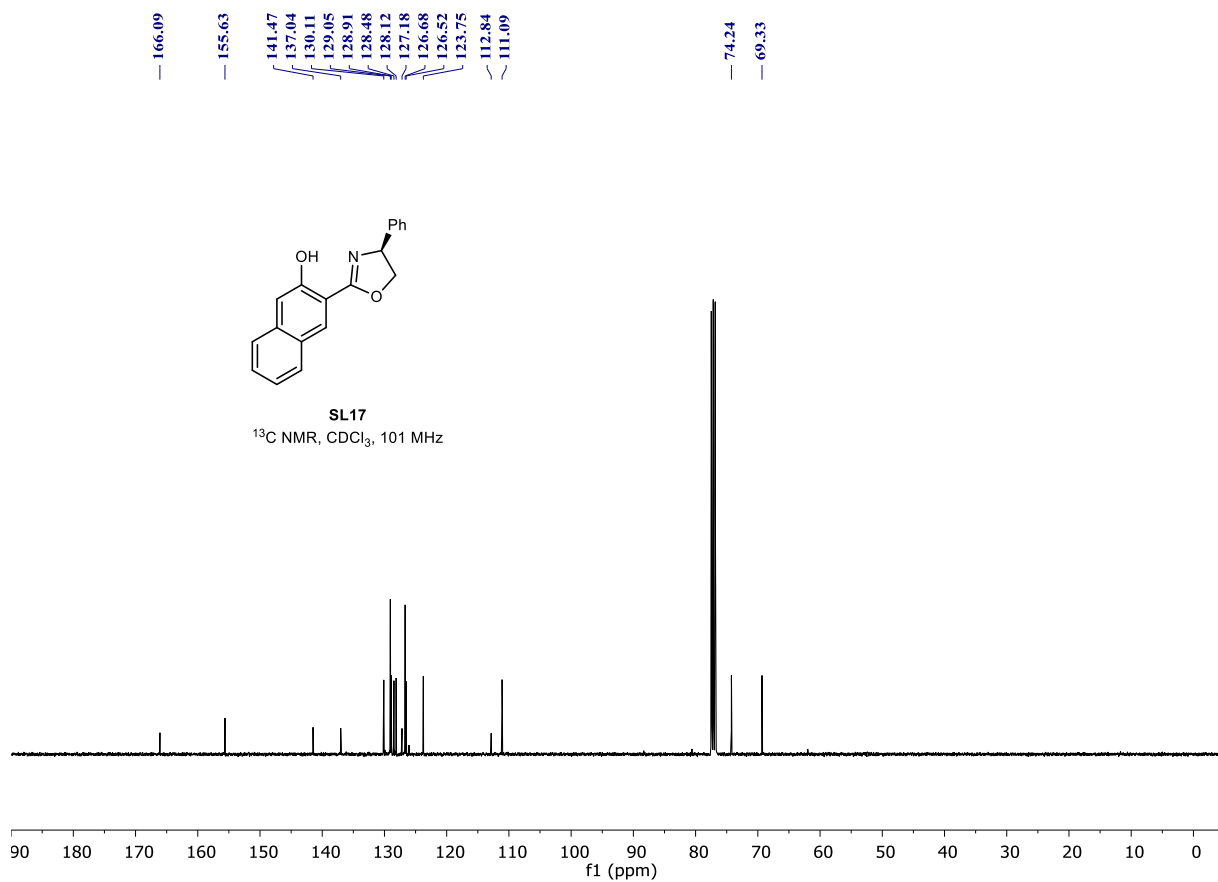
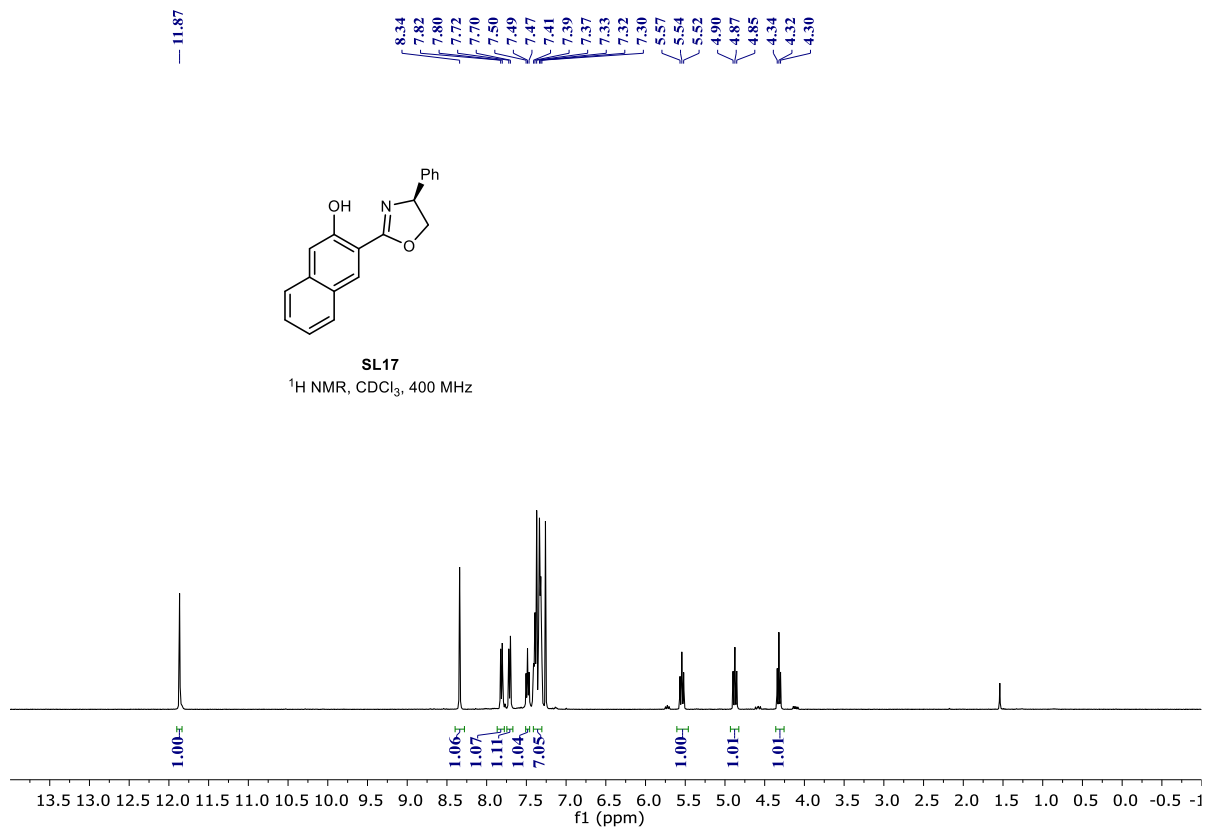


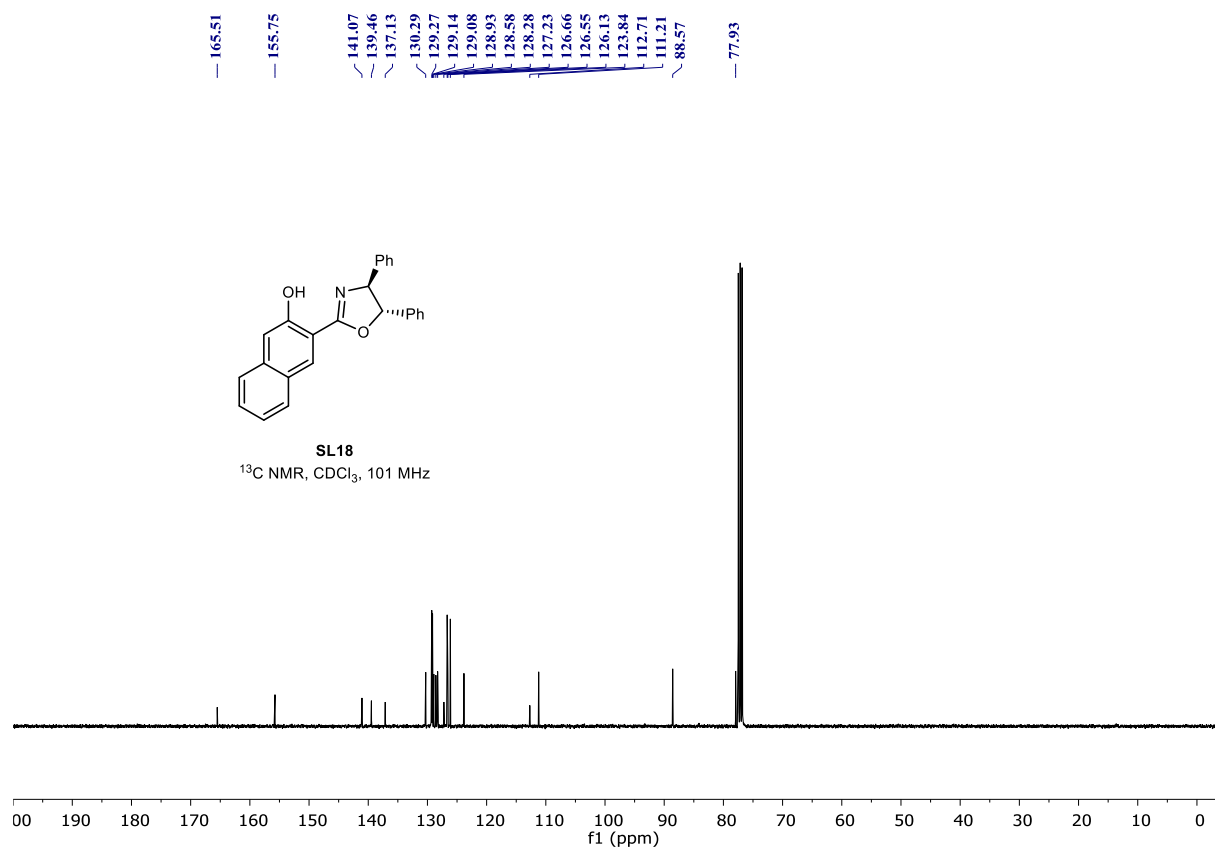
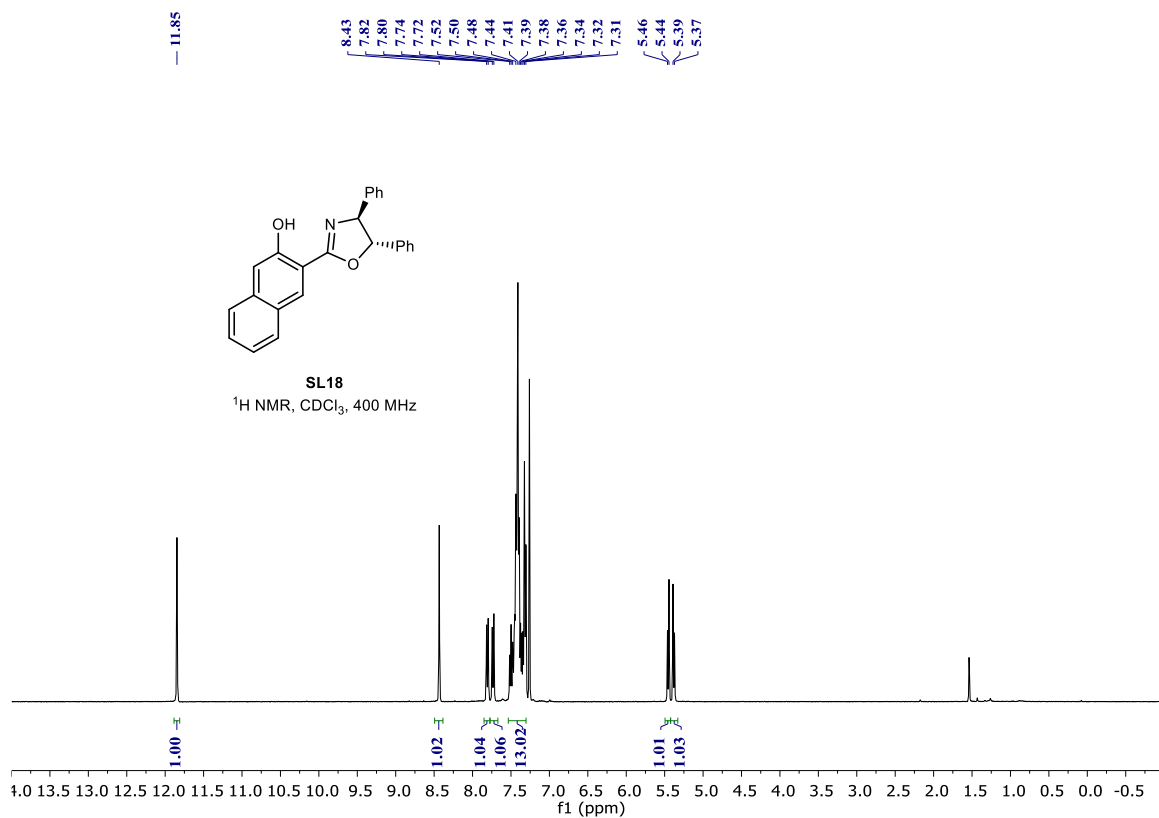


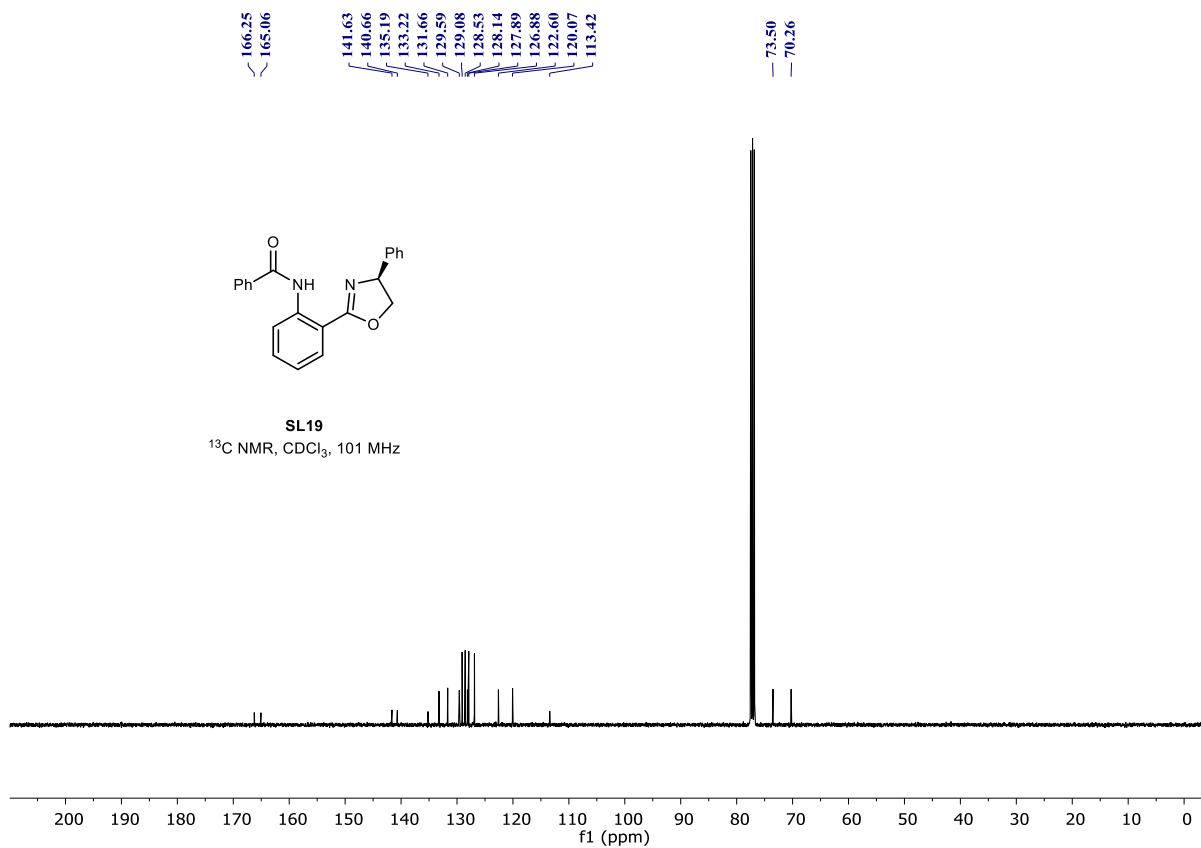
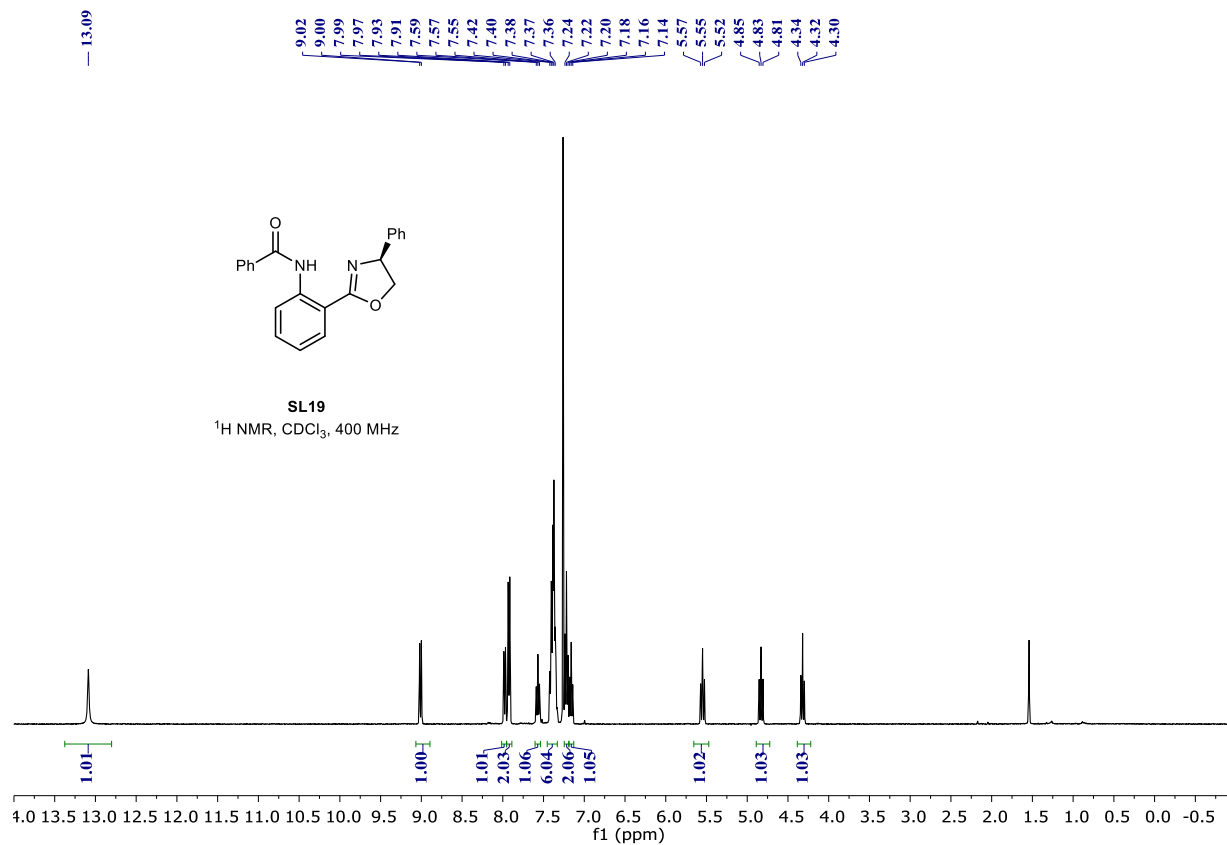


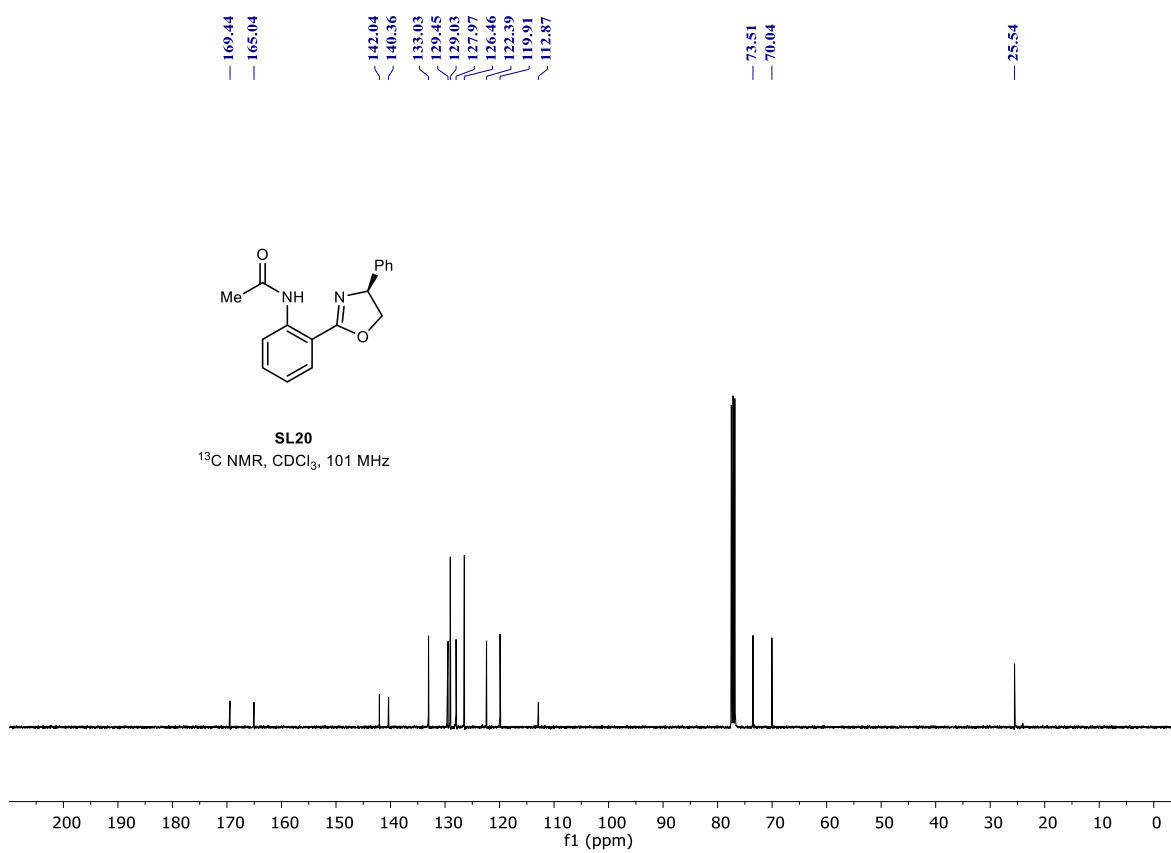
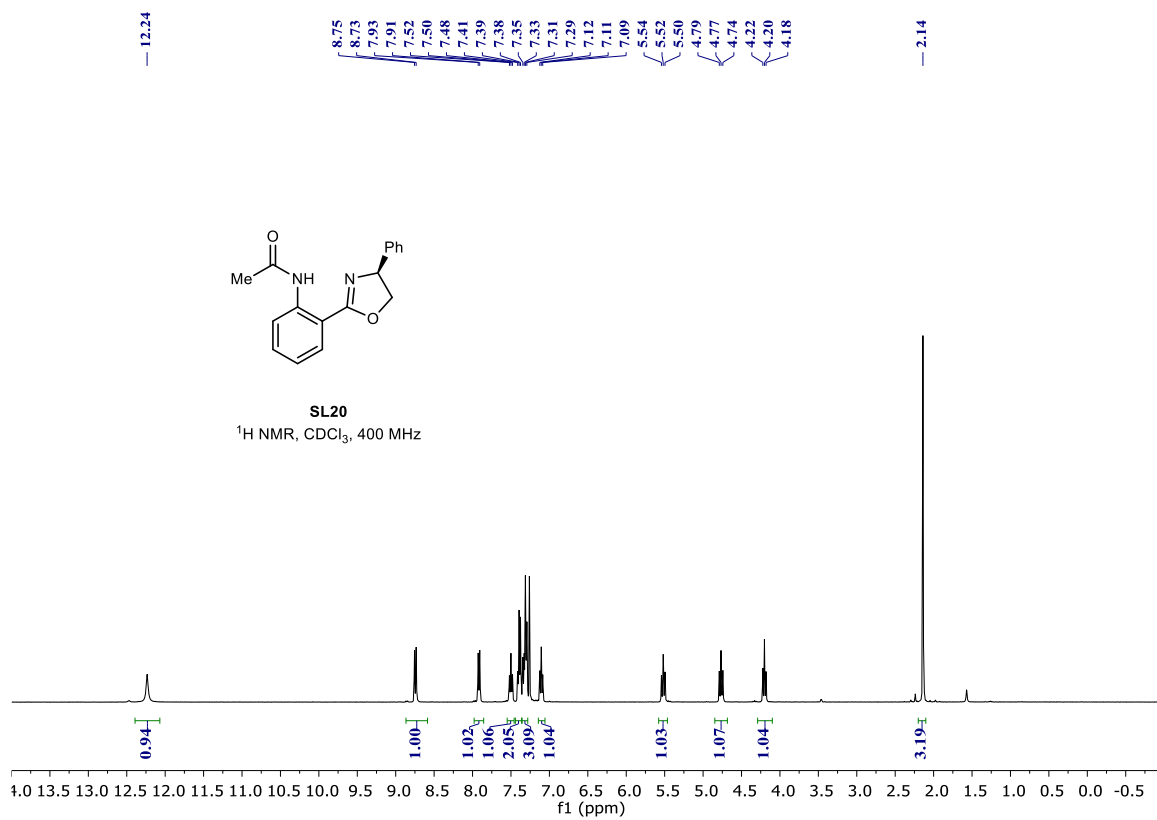


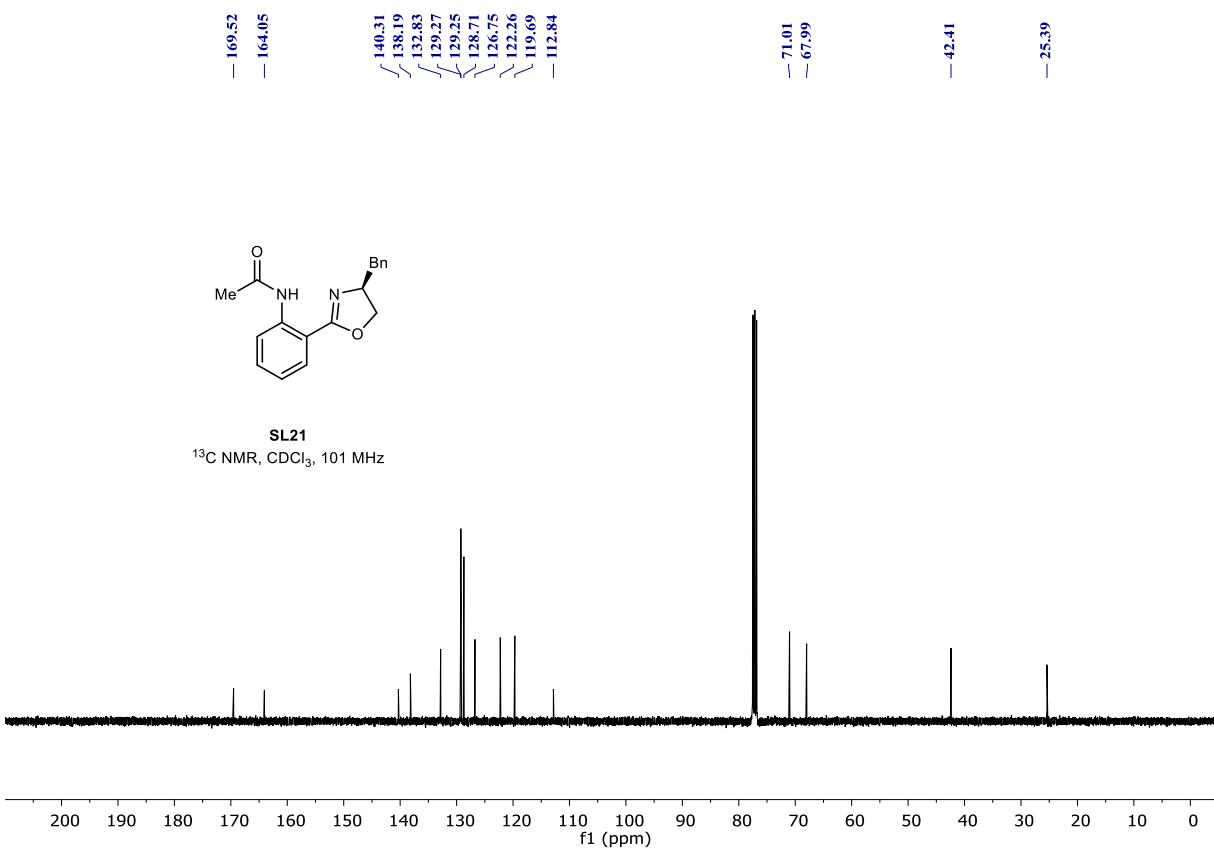
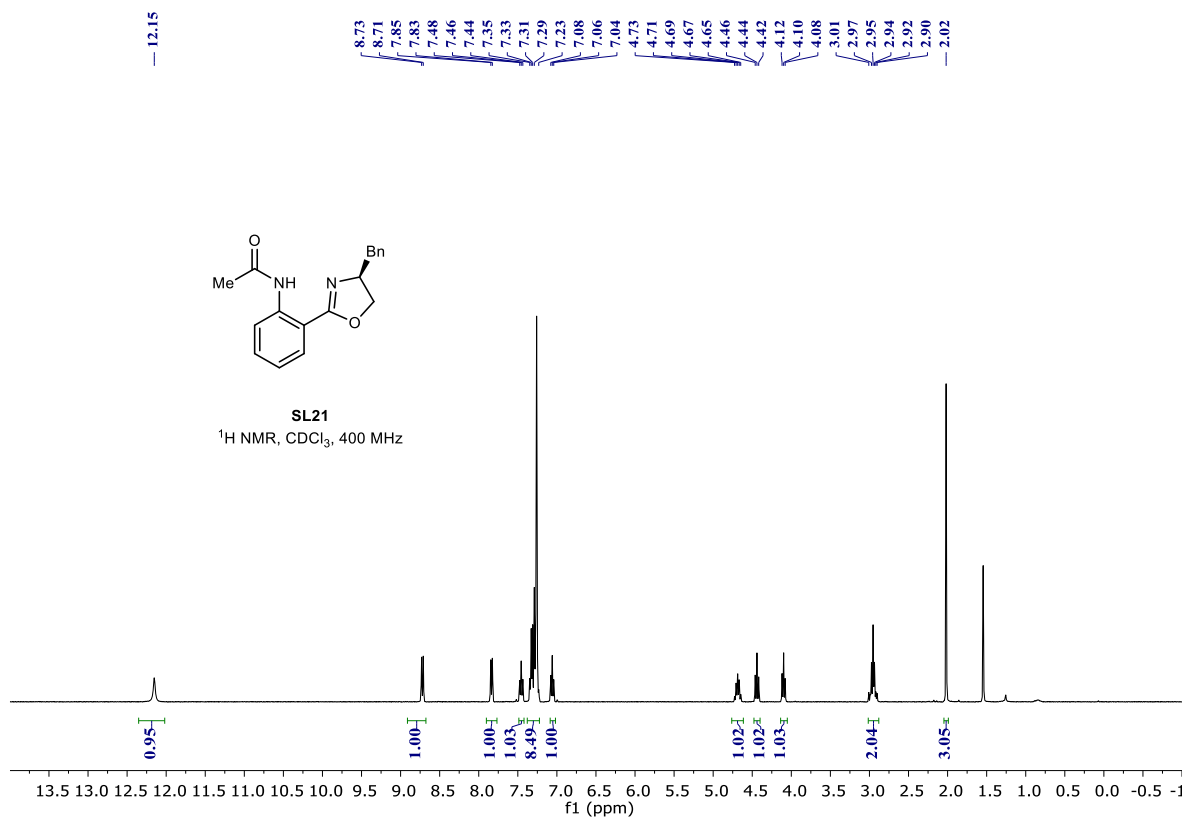


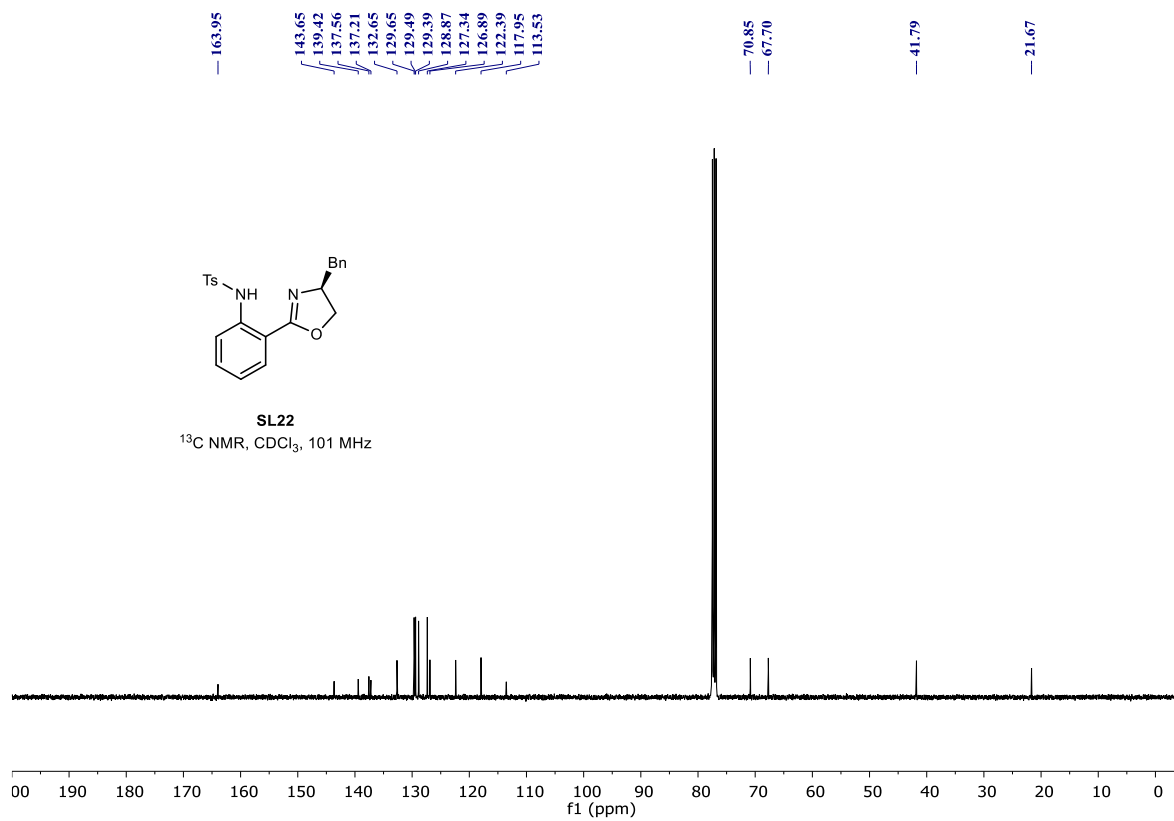
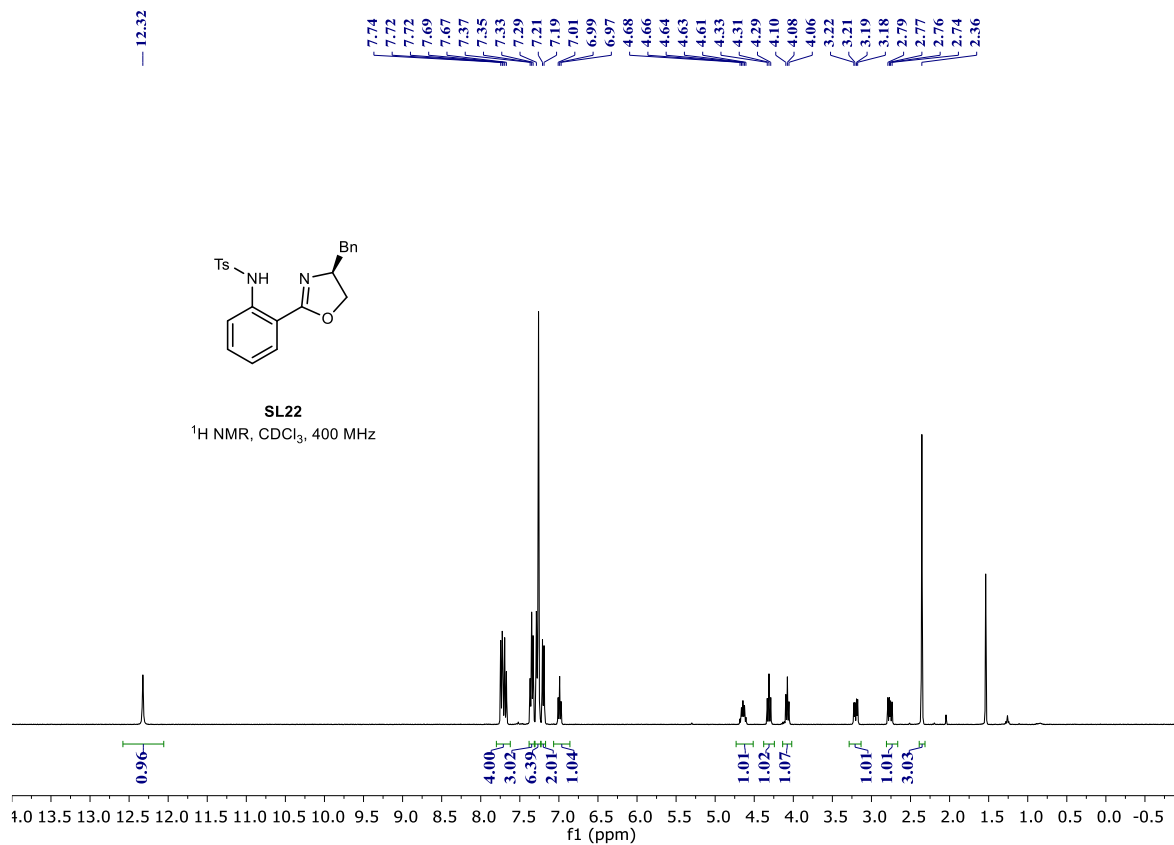


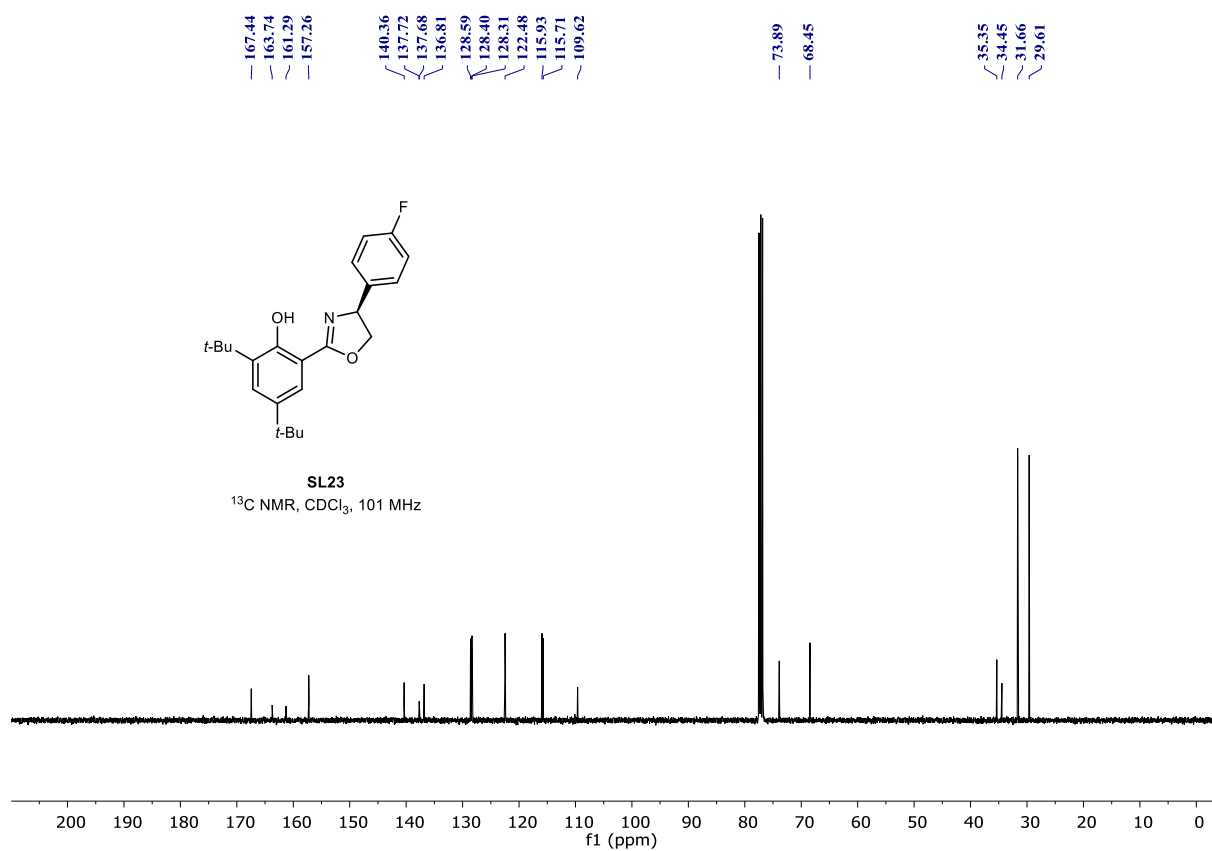
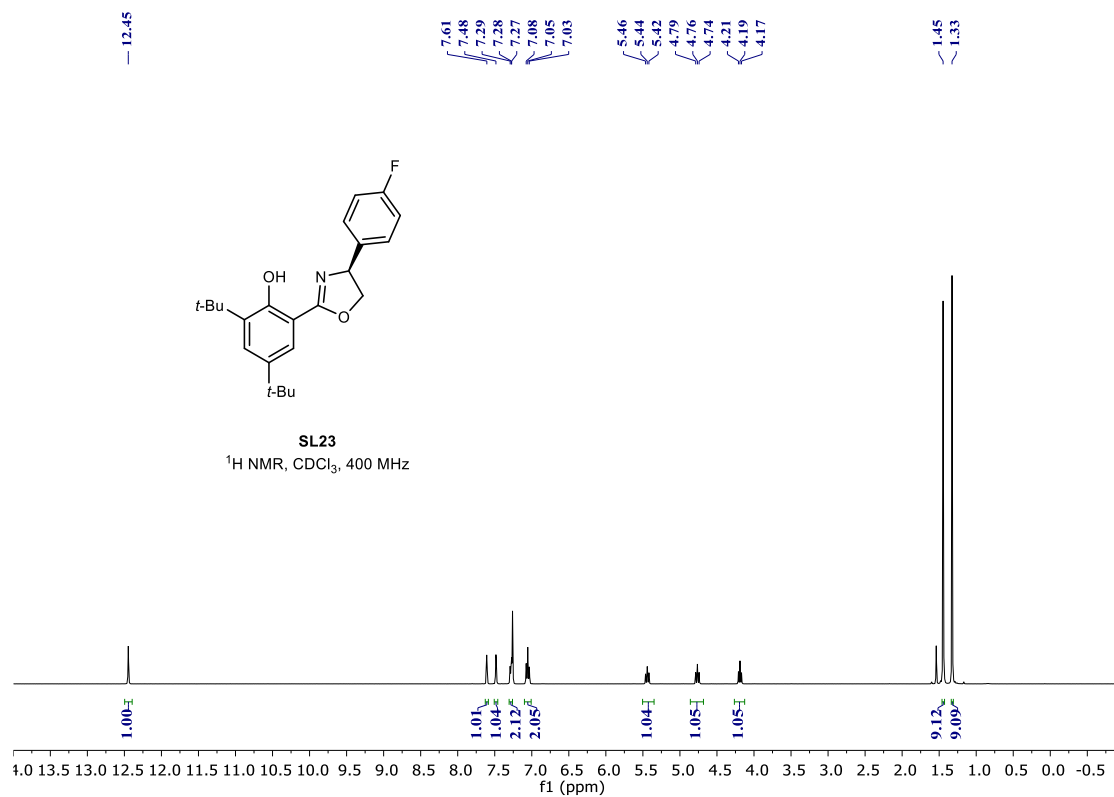


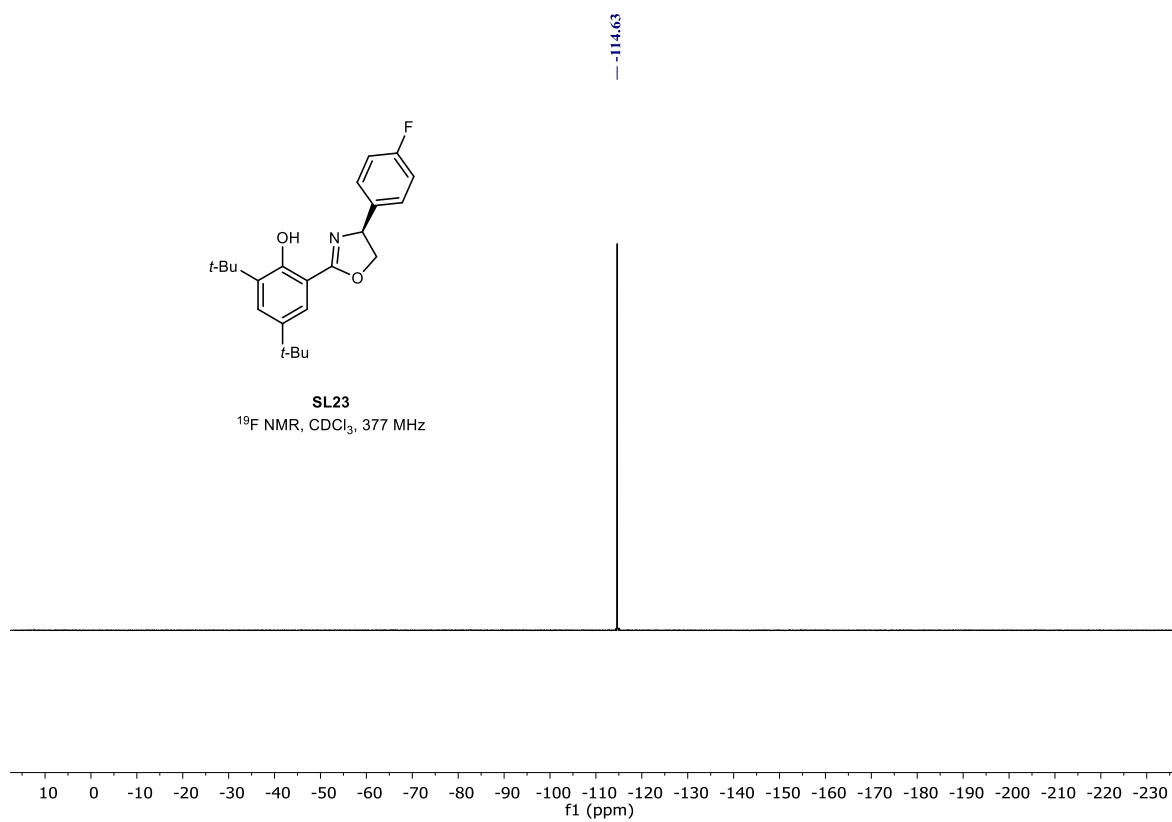


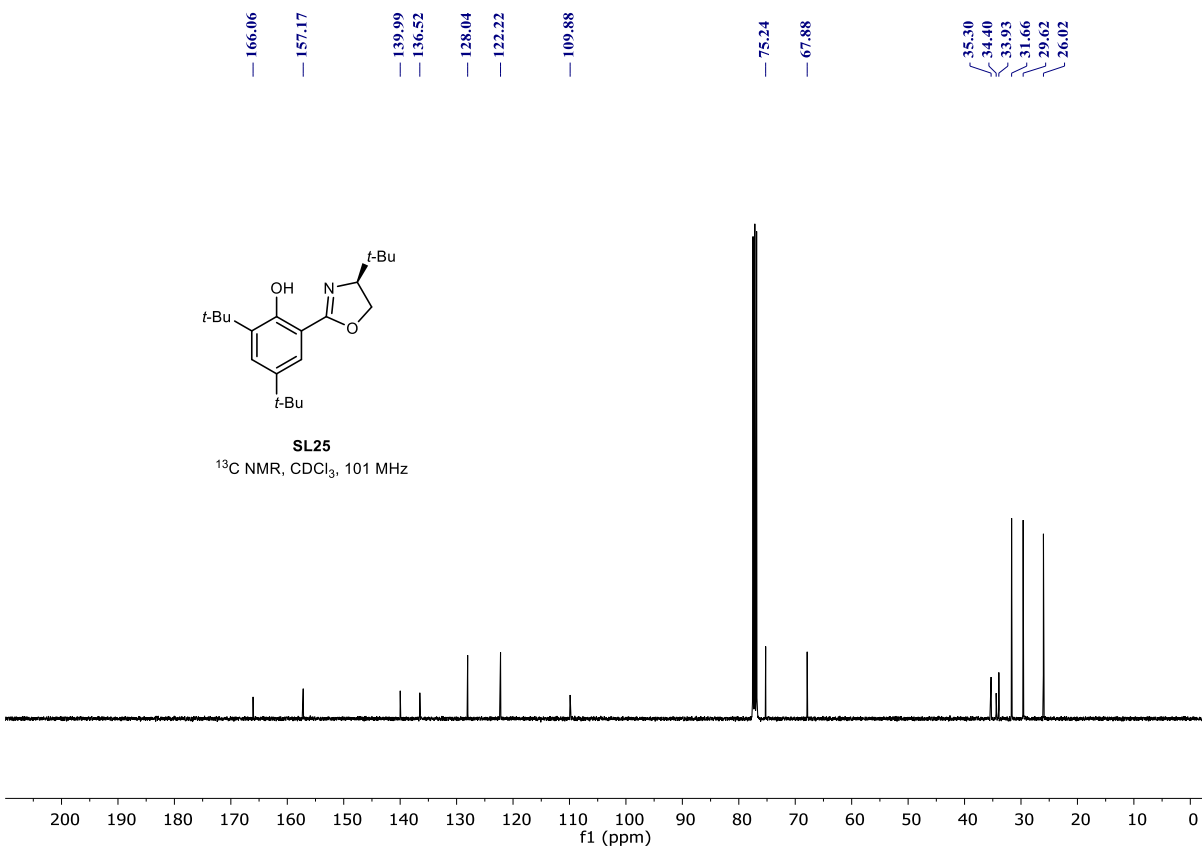
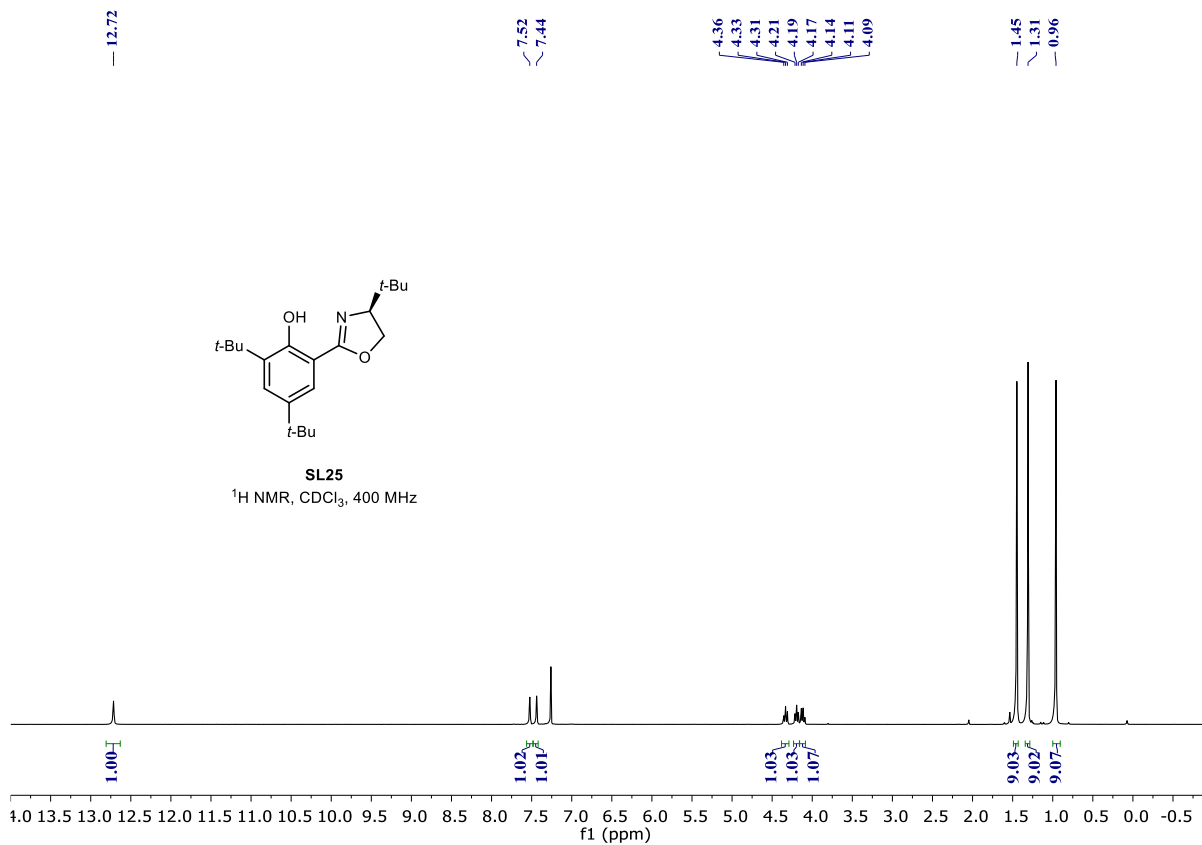


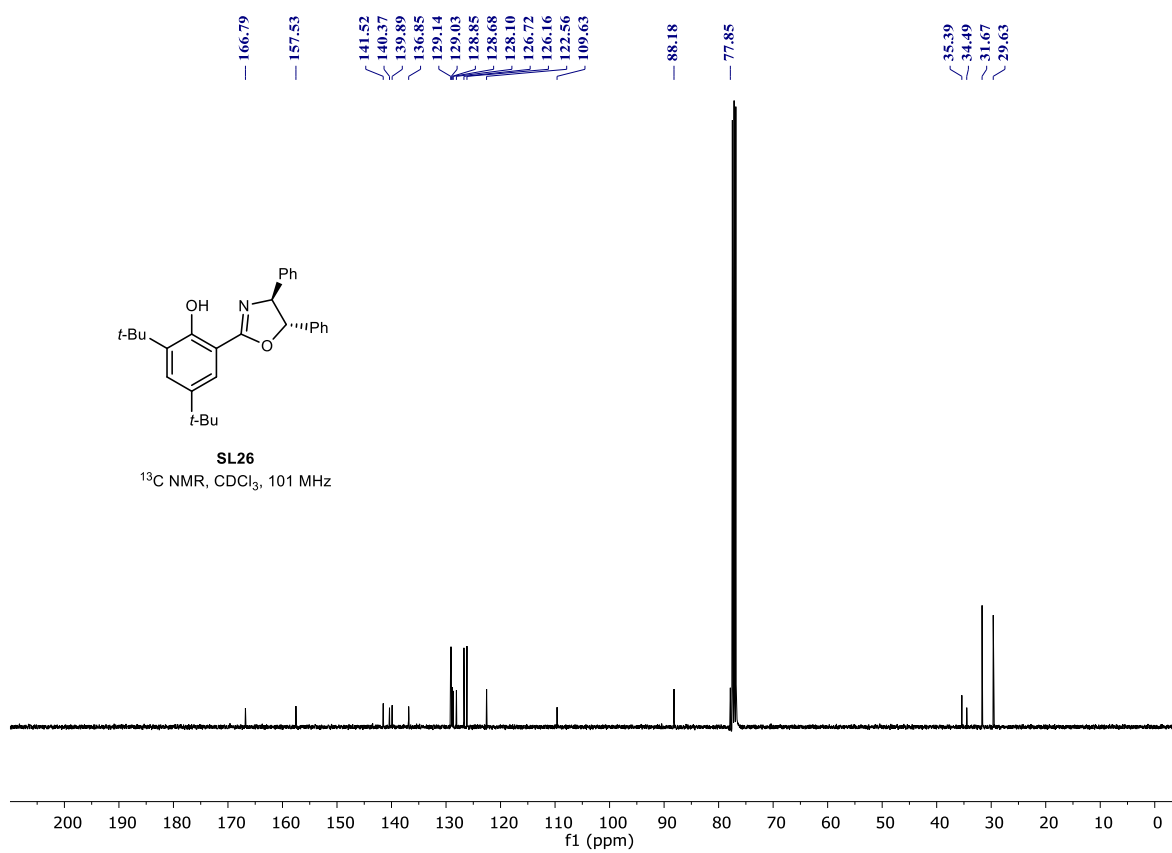
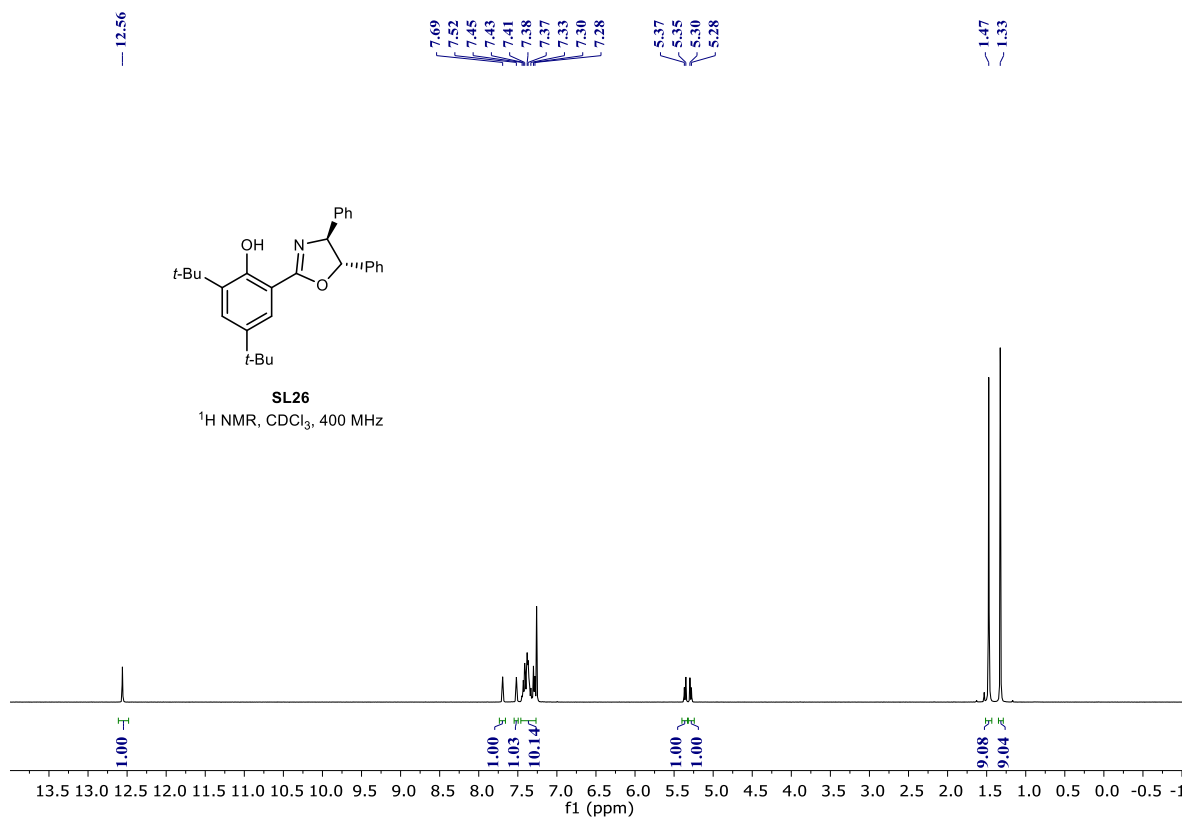


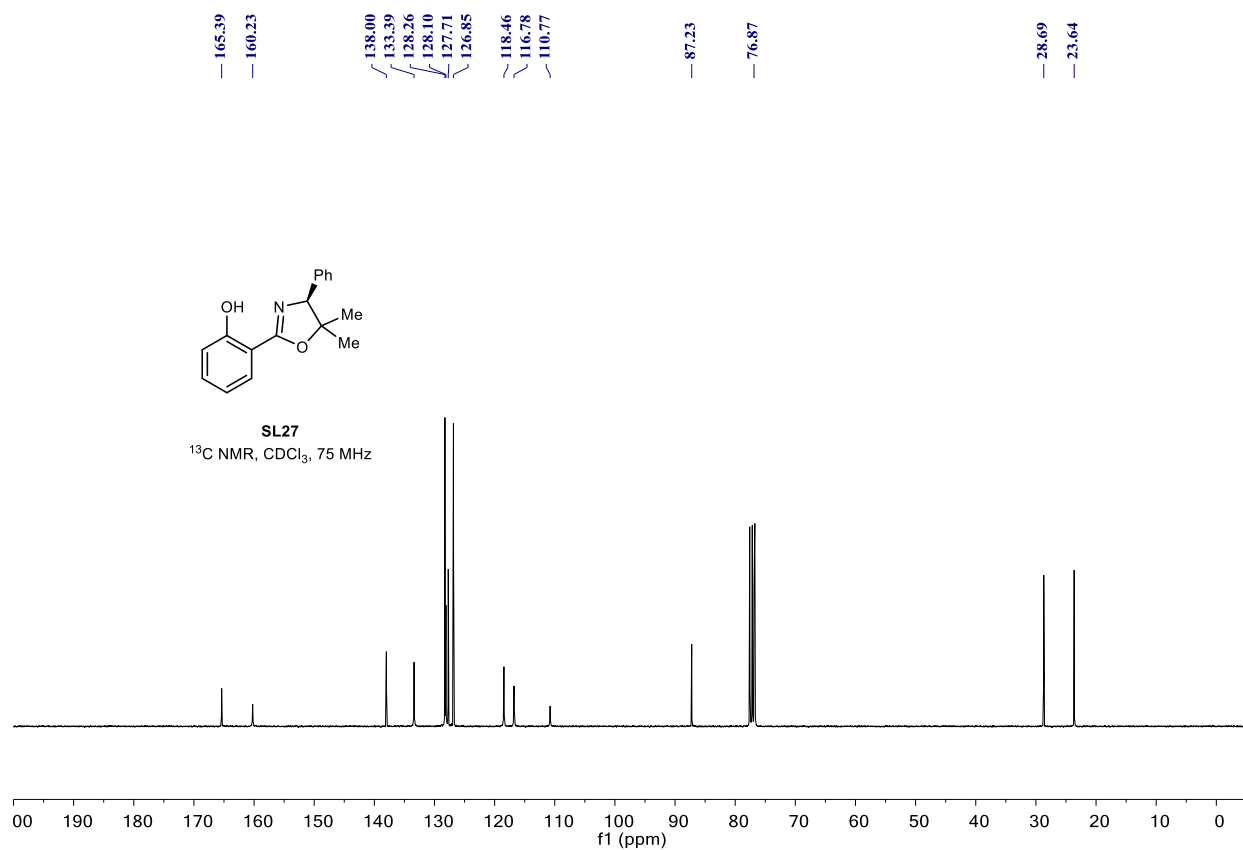
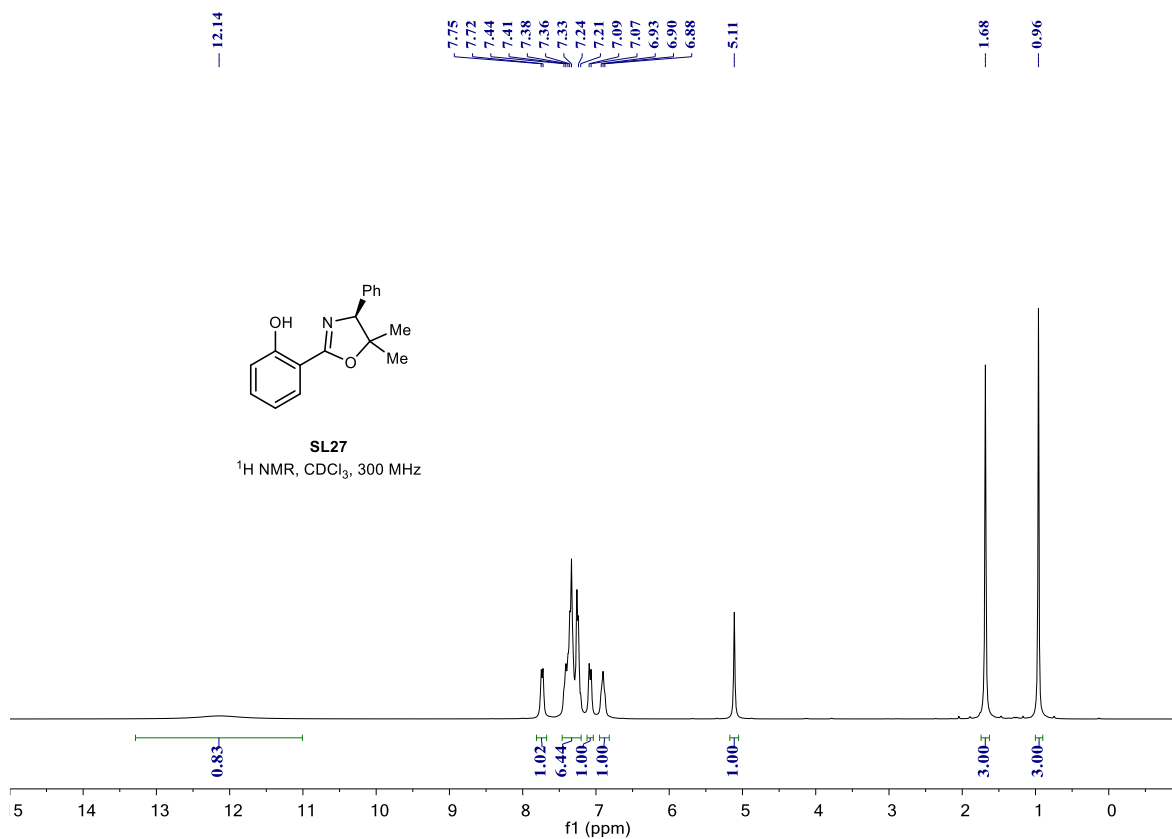


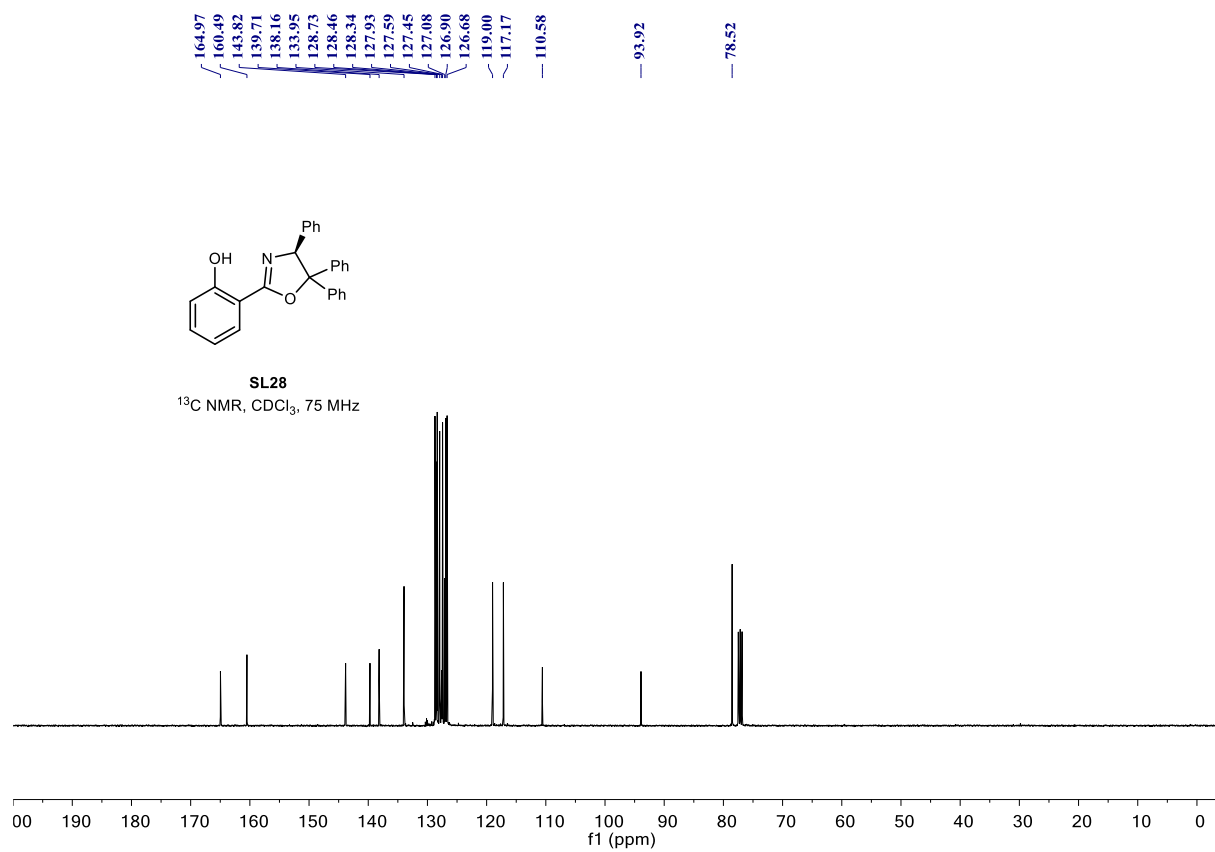
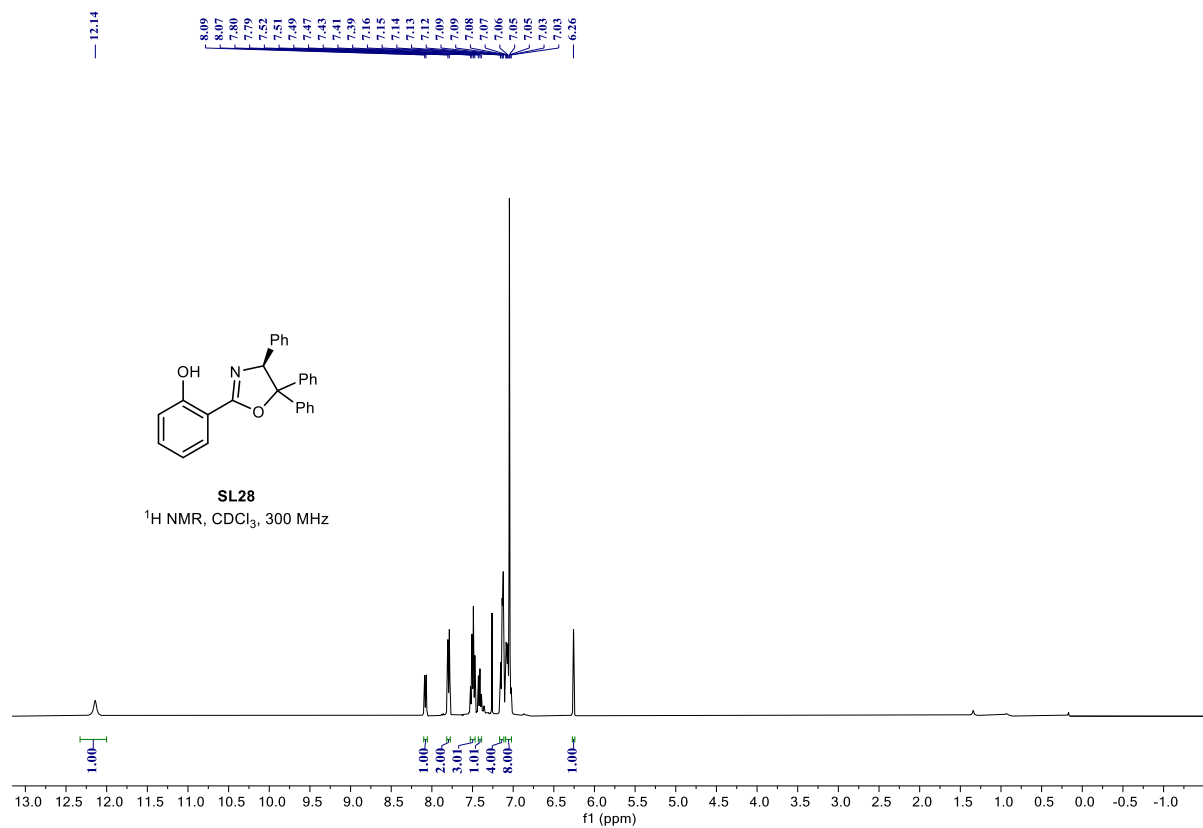


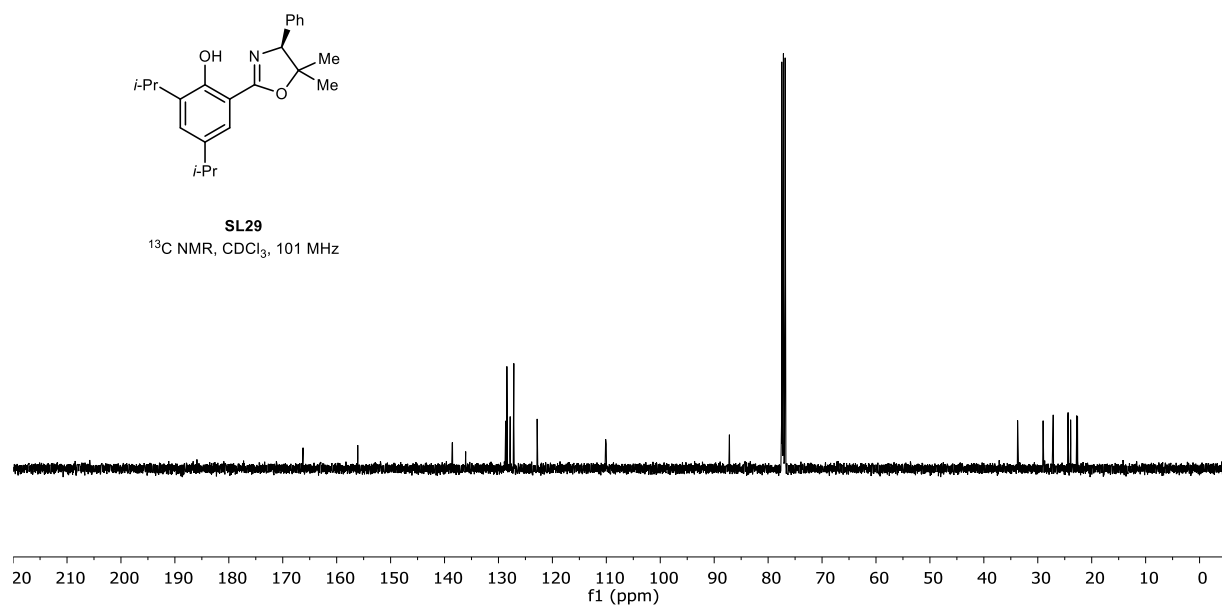
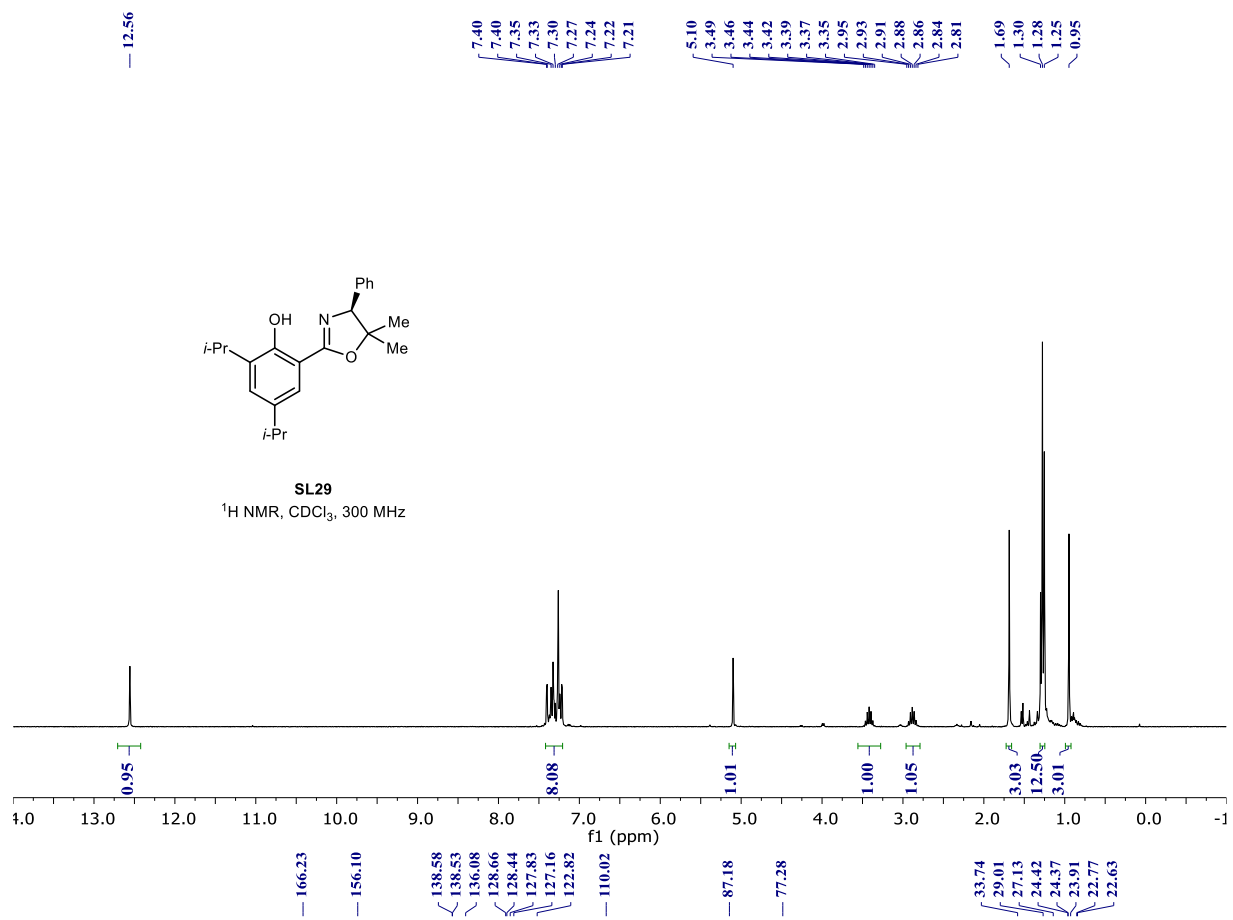




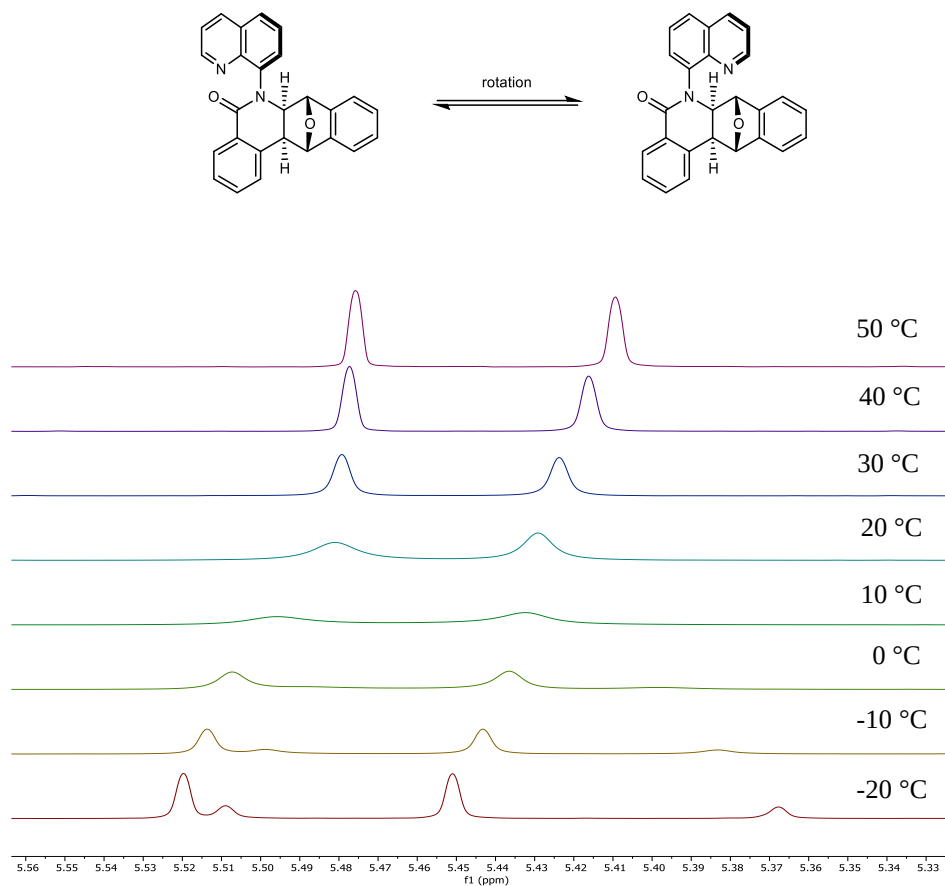


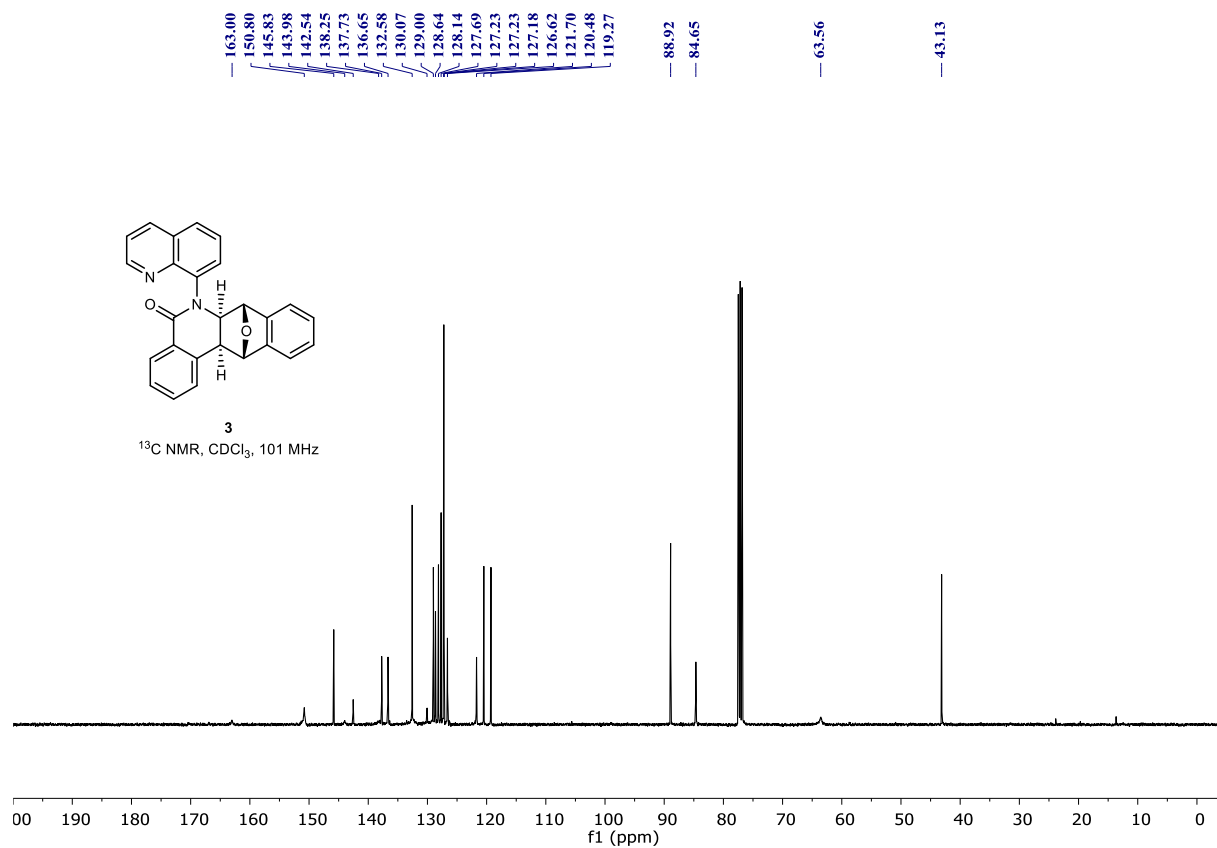
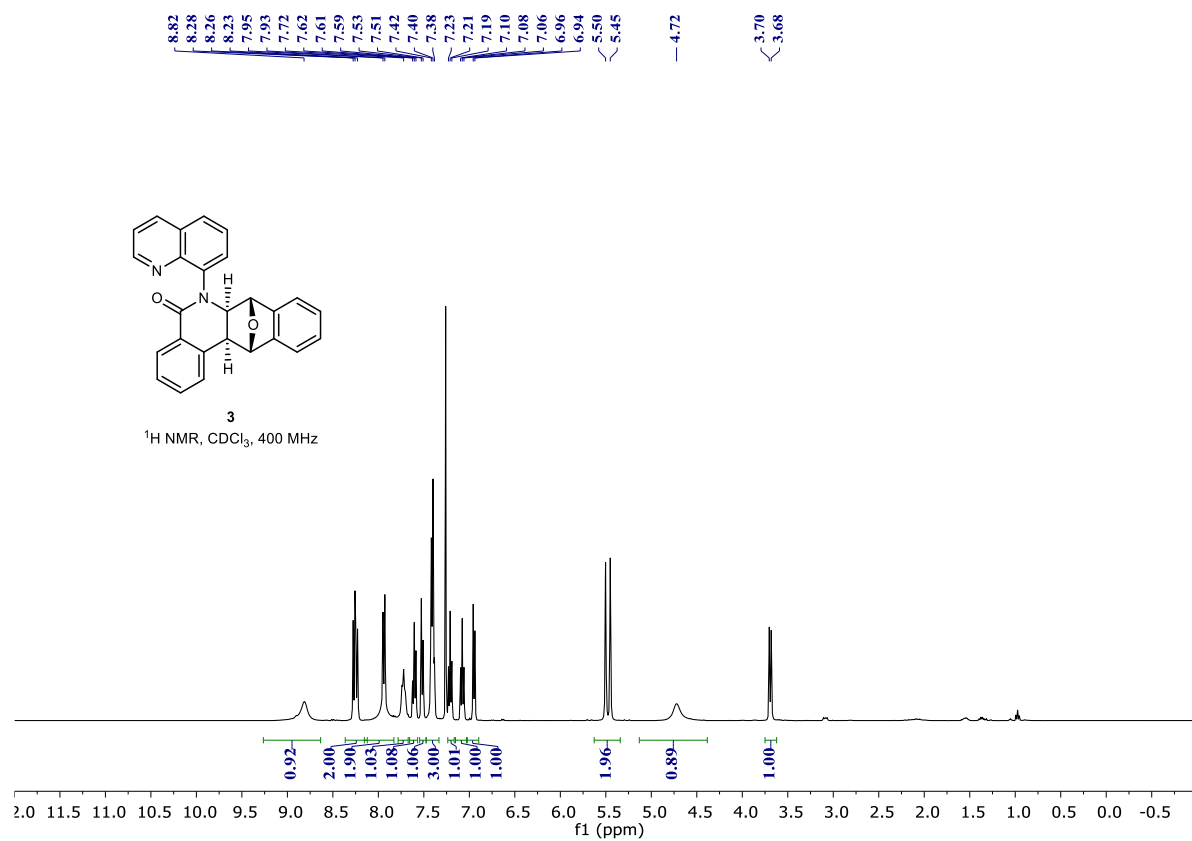


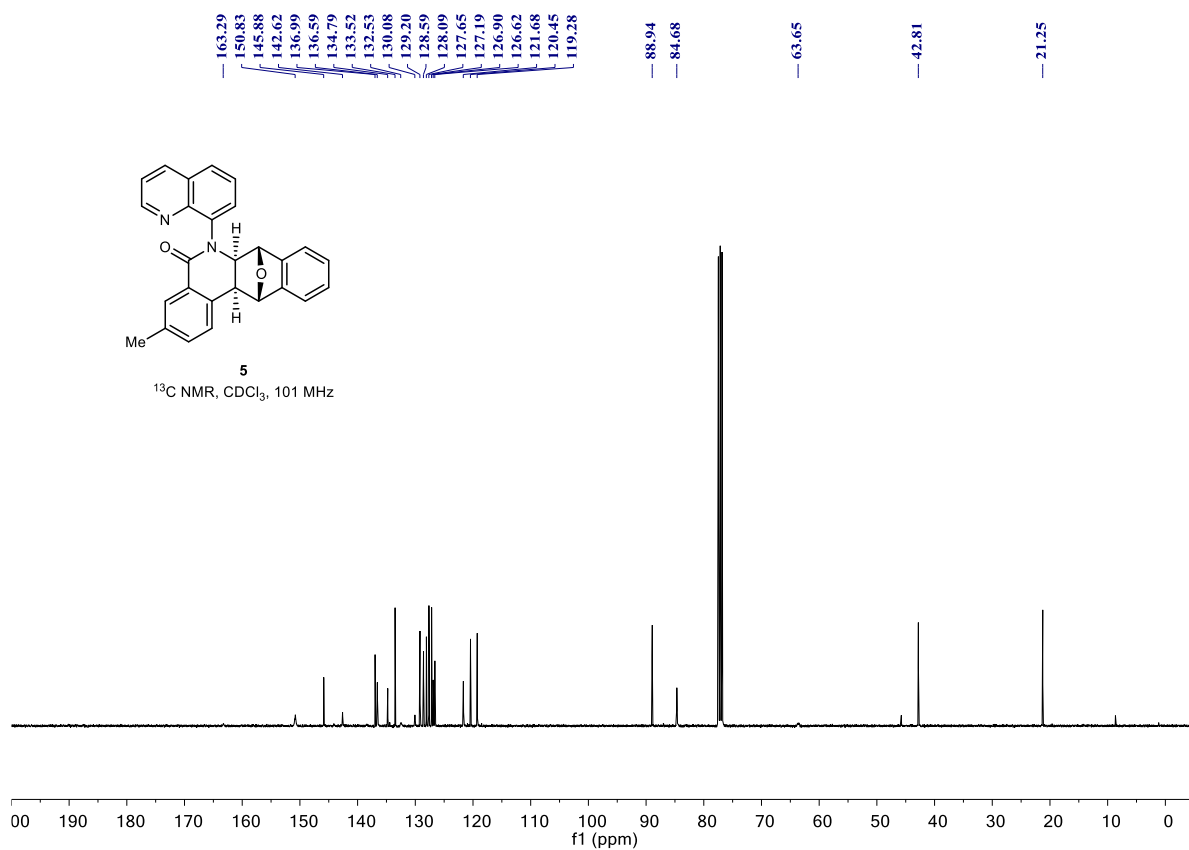
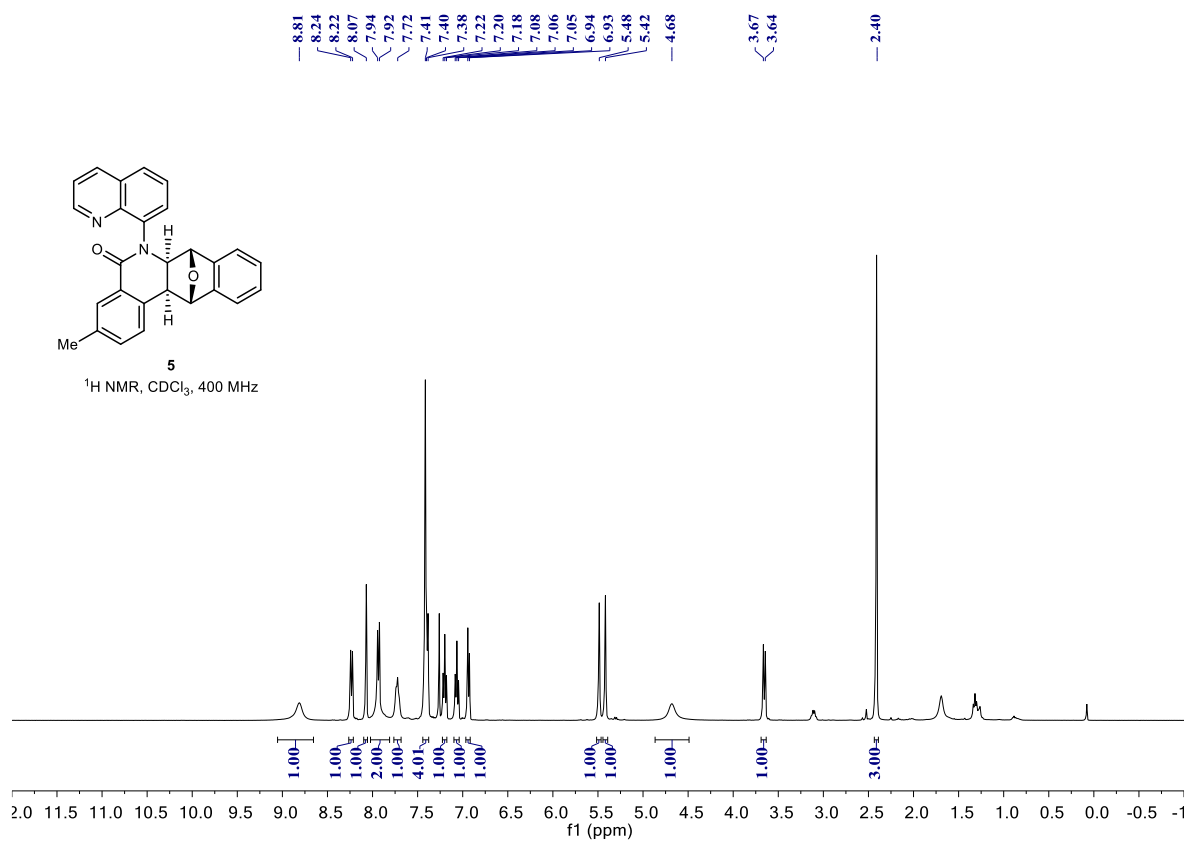


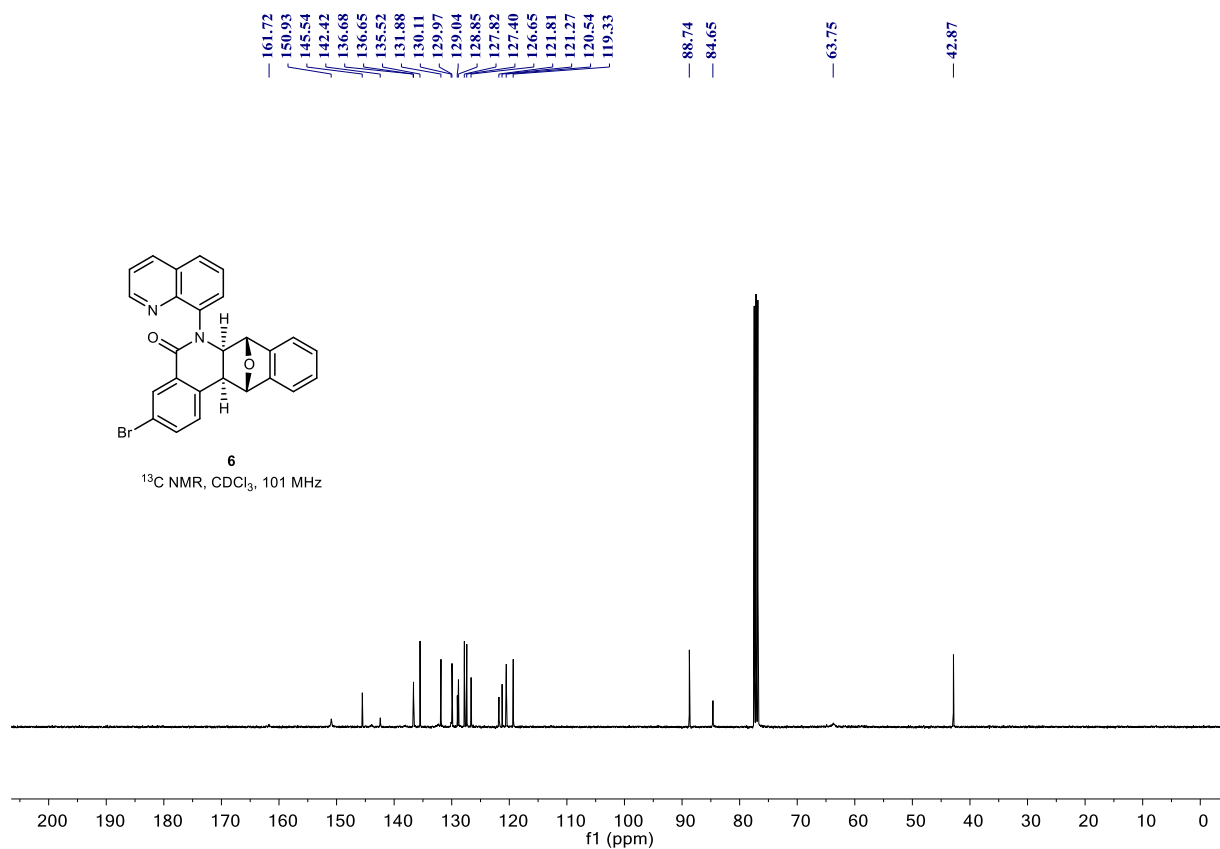
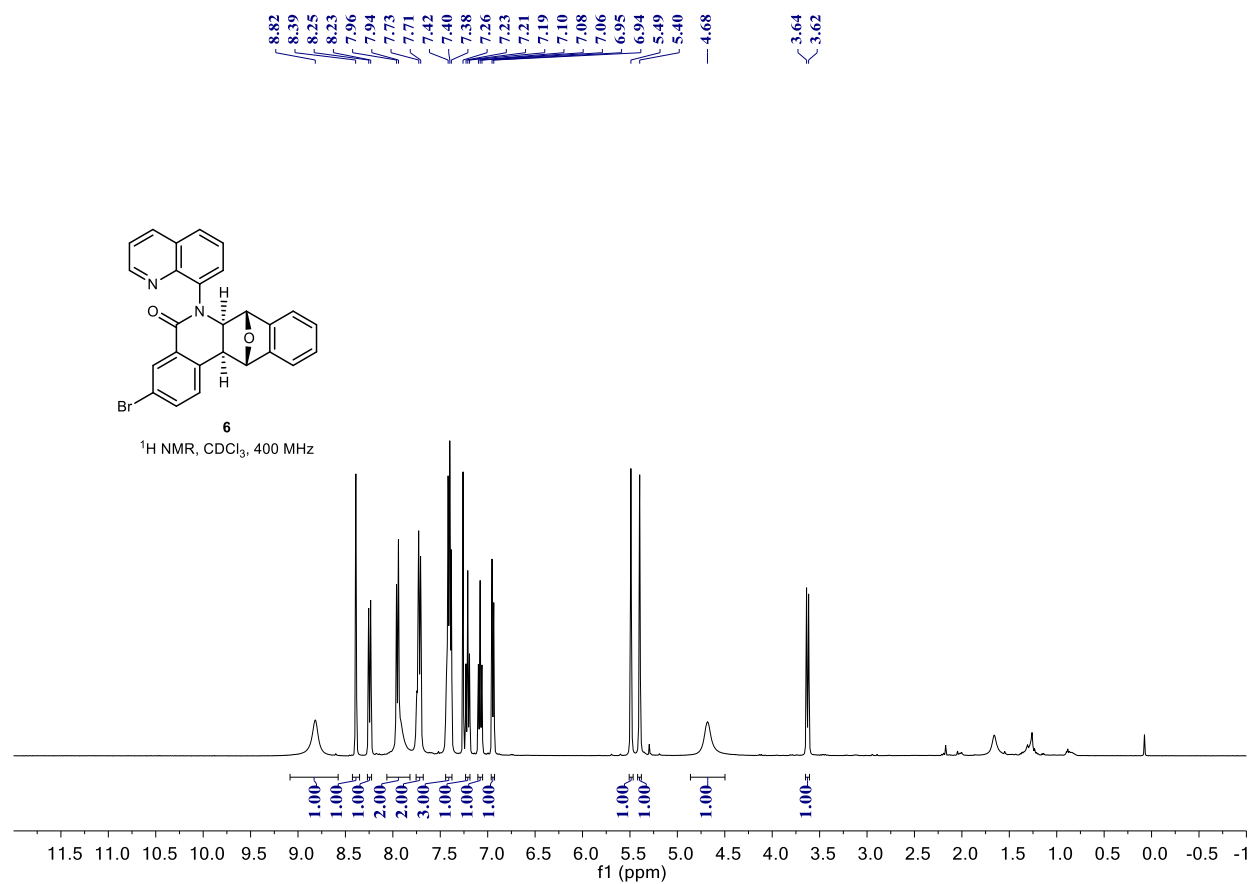


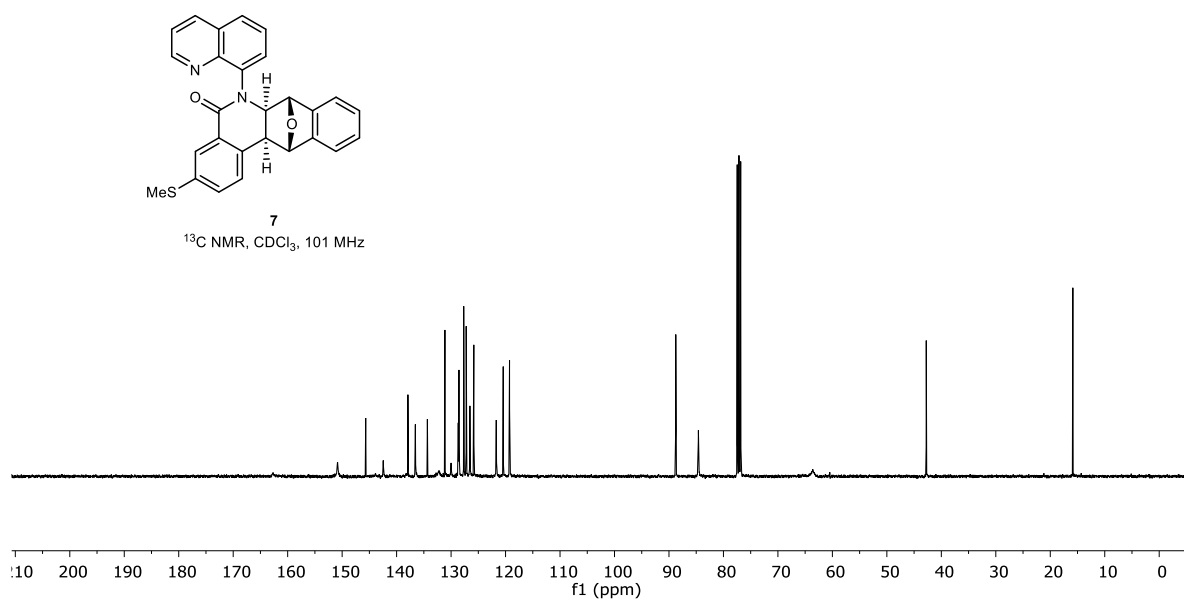
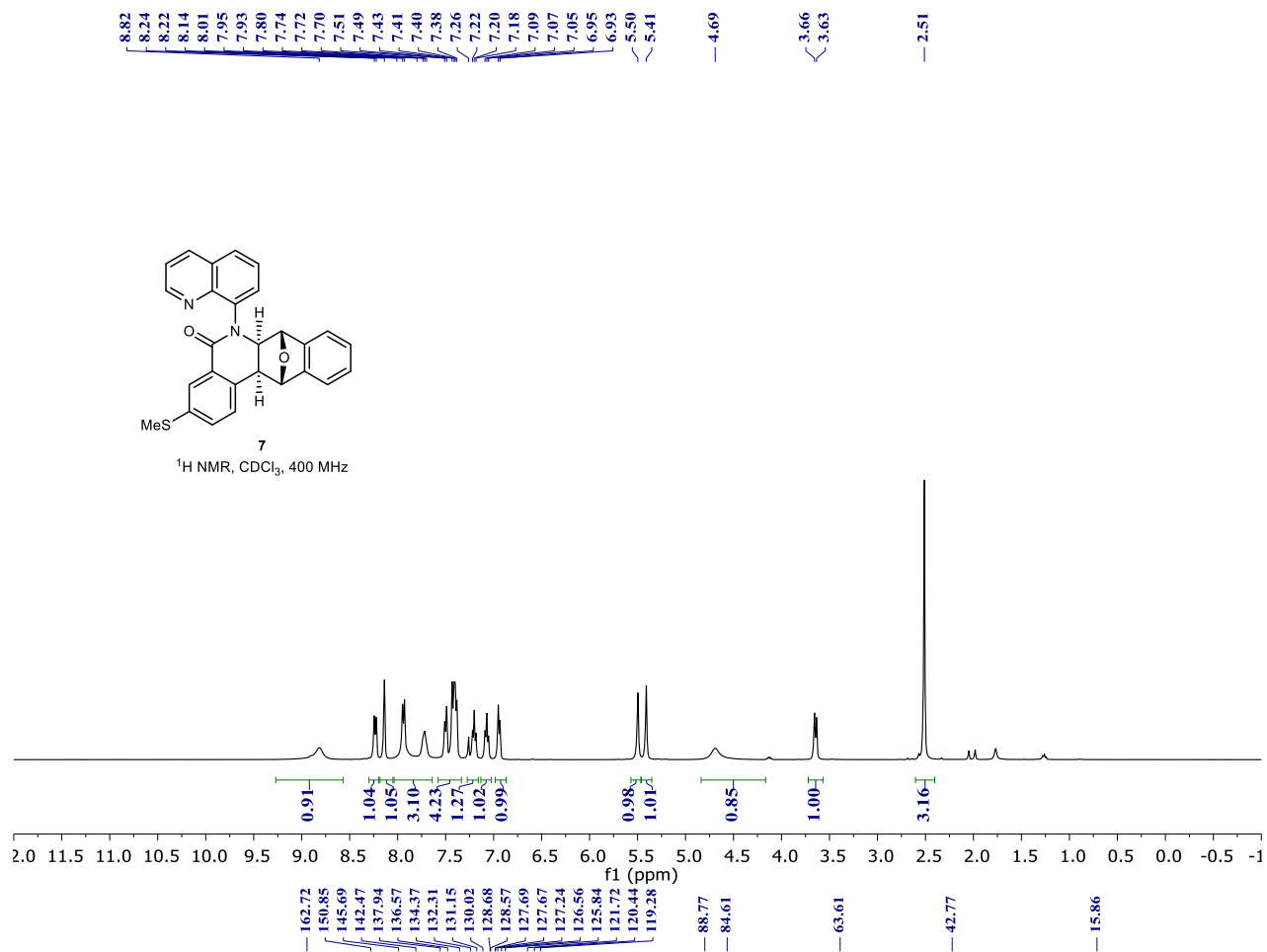
Note: The quinoline group has restricted rotation at the C–N axis, resulting in signal broadening in the ^1H NMR and ^{13}C NMR spectra. This effect could be confirmed by temperature-dependent NMR measurements.

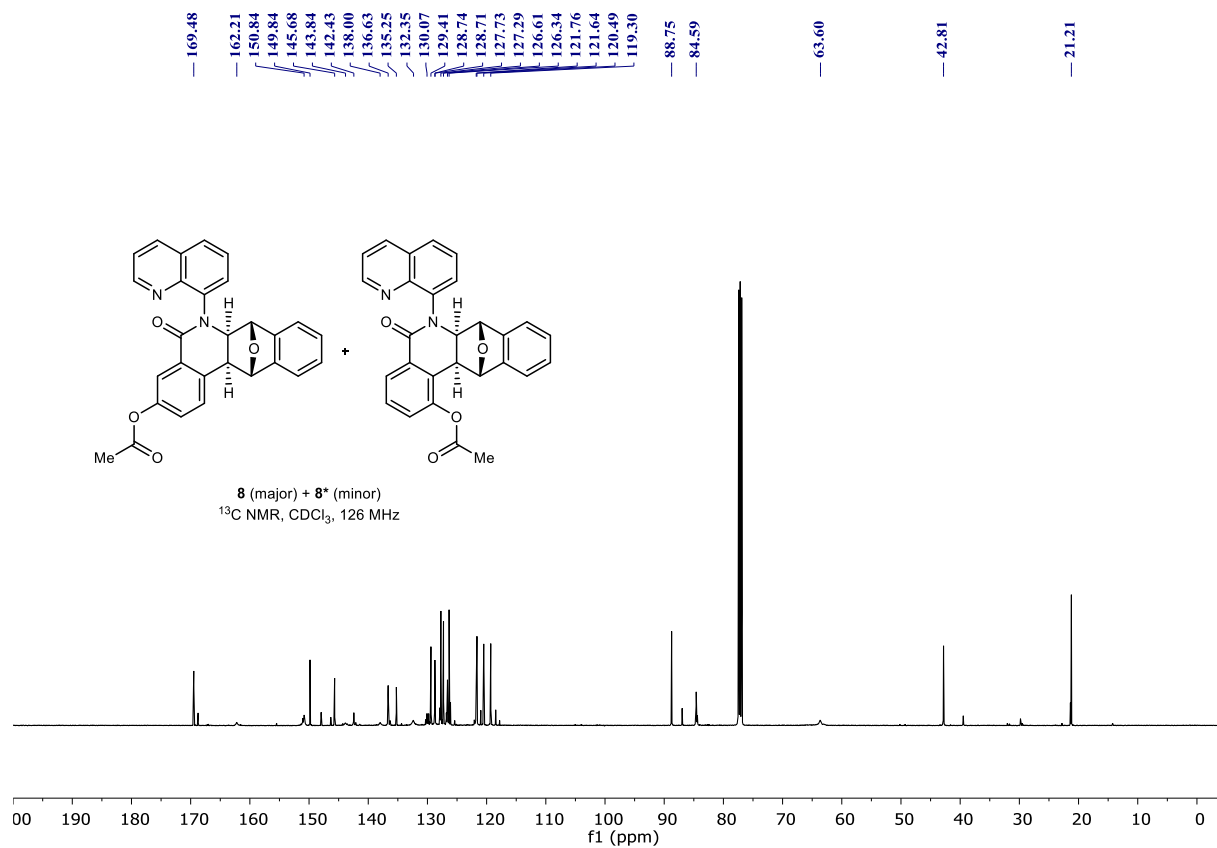
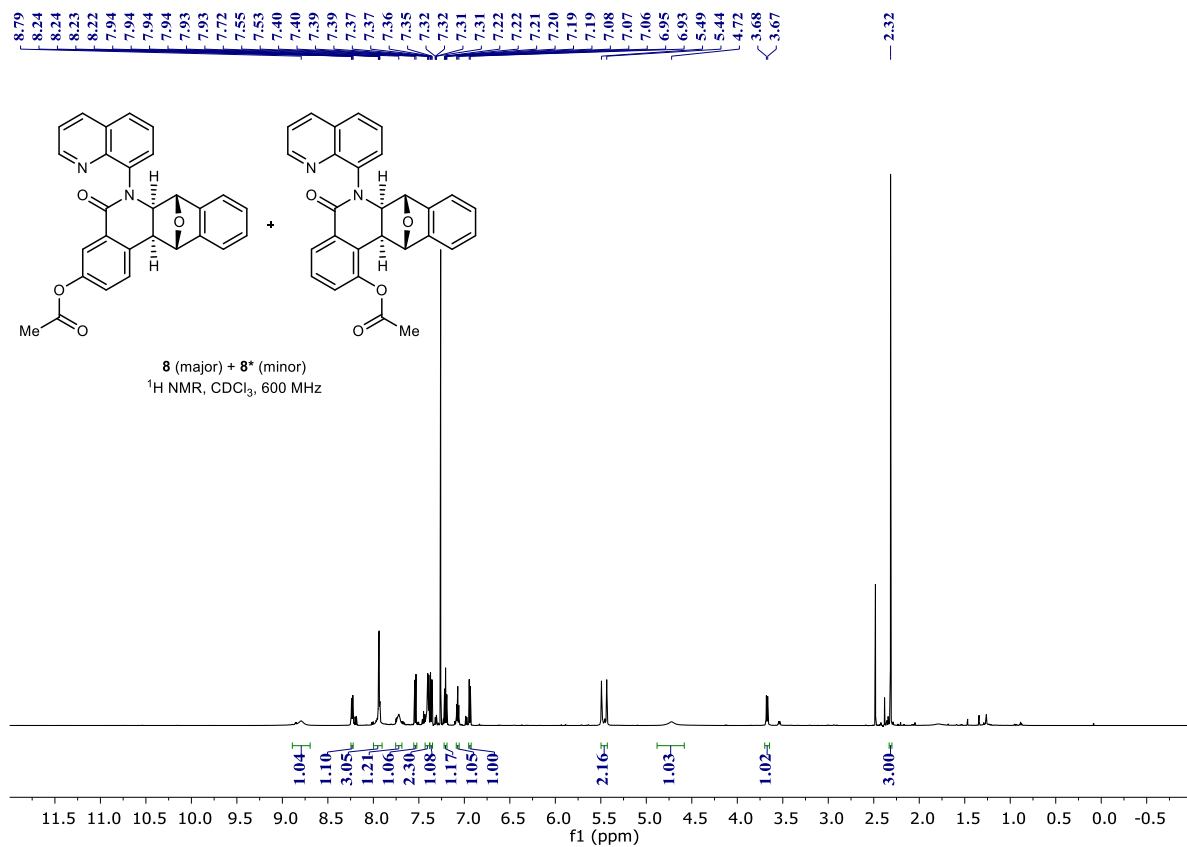


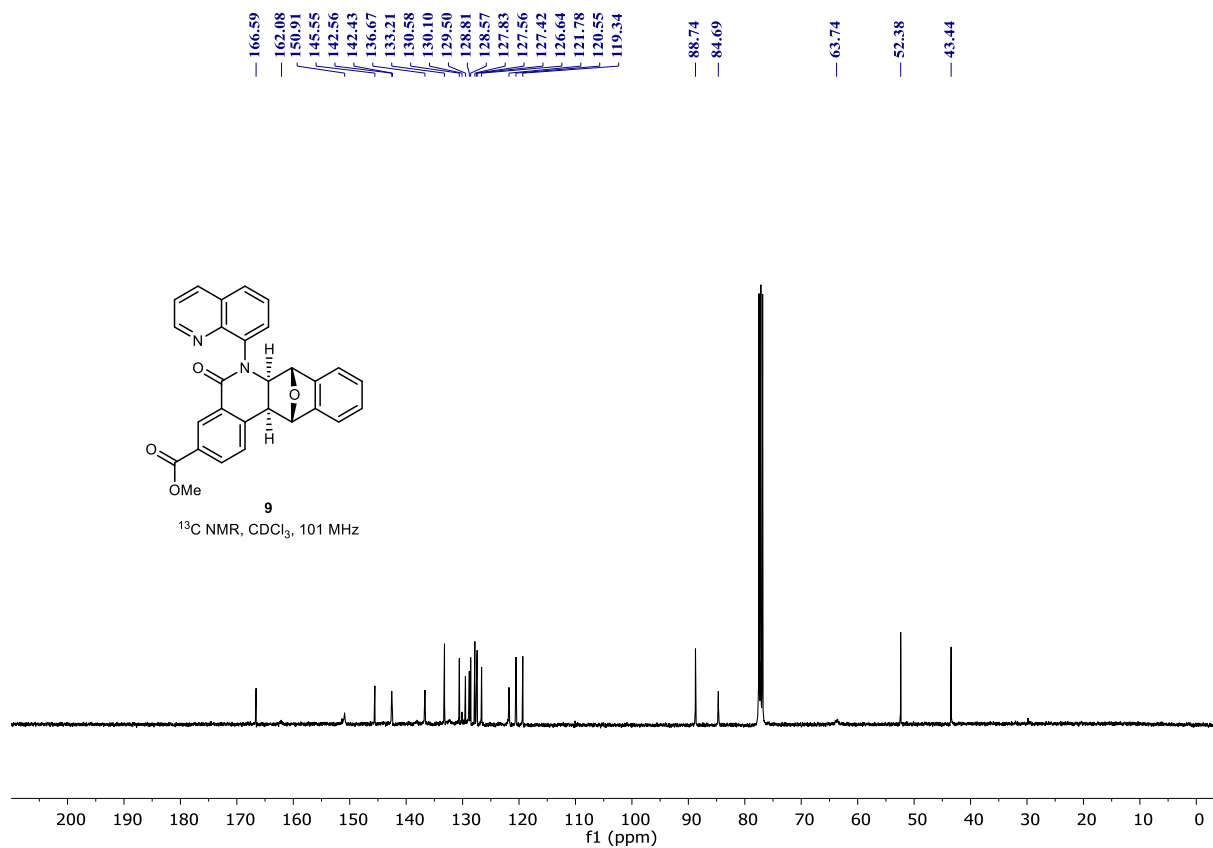
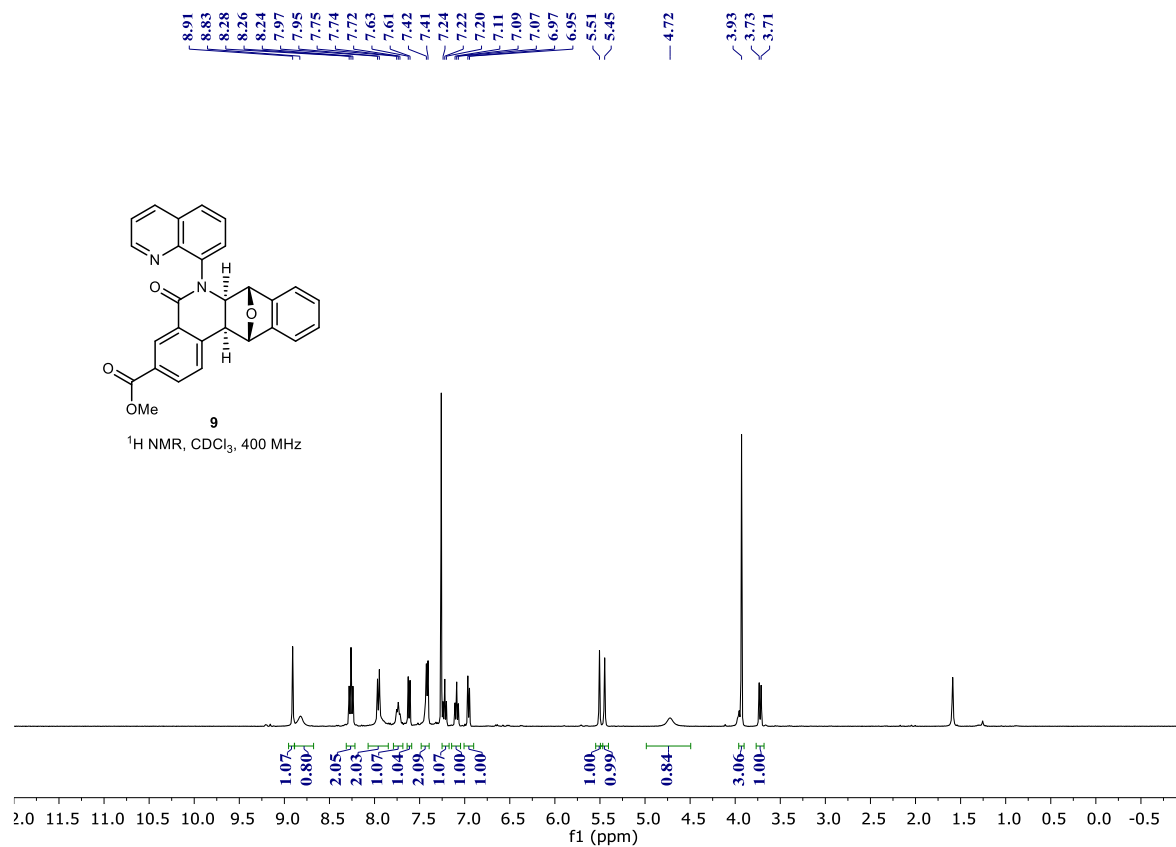


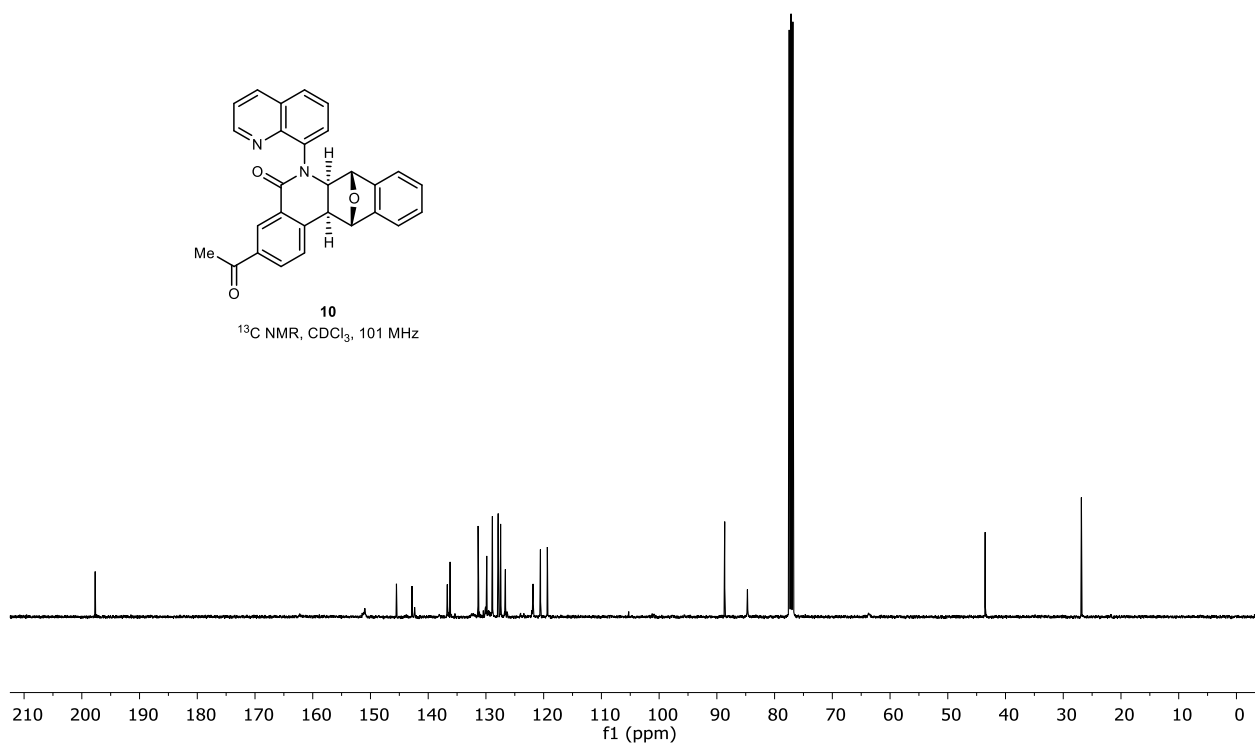
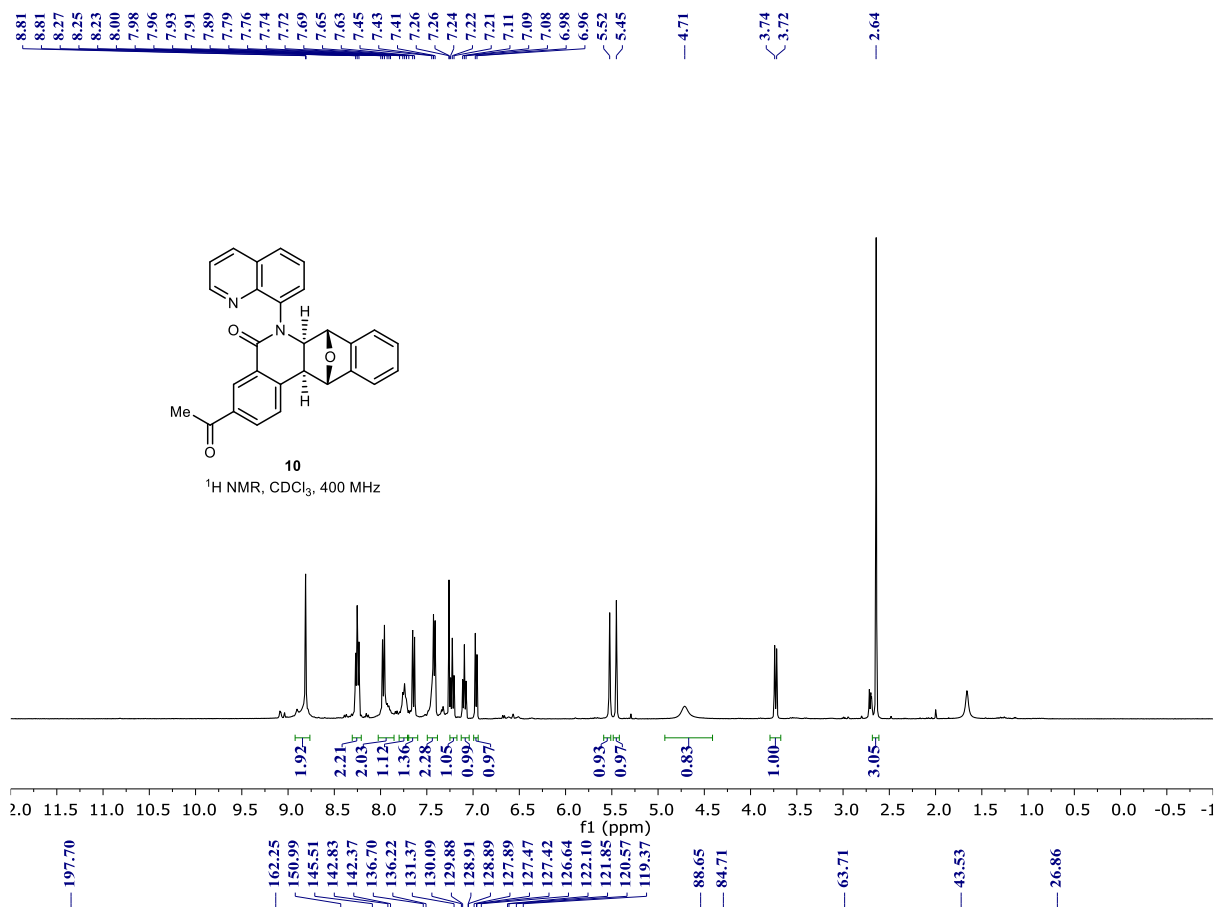


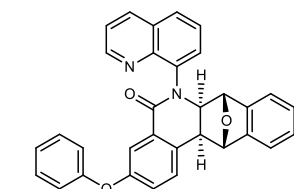




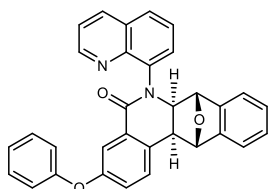




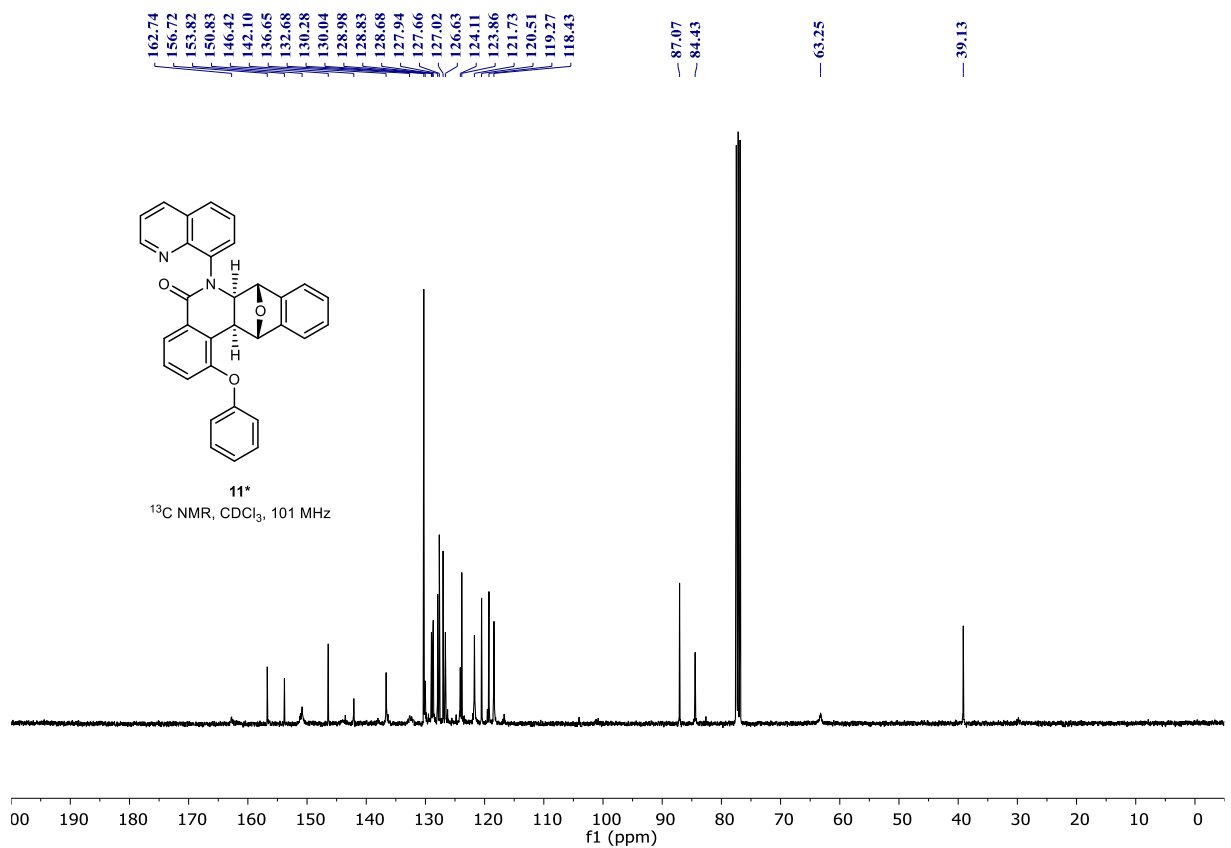
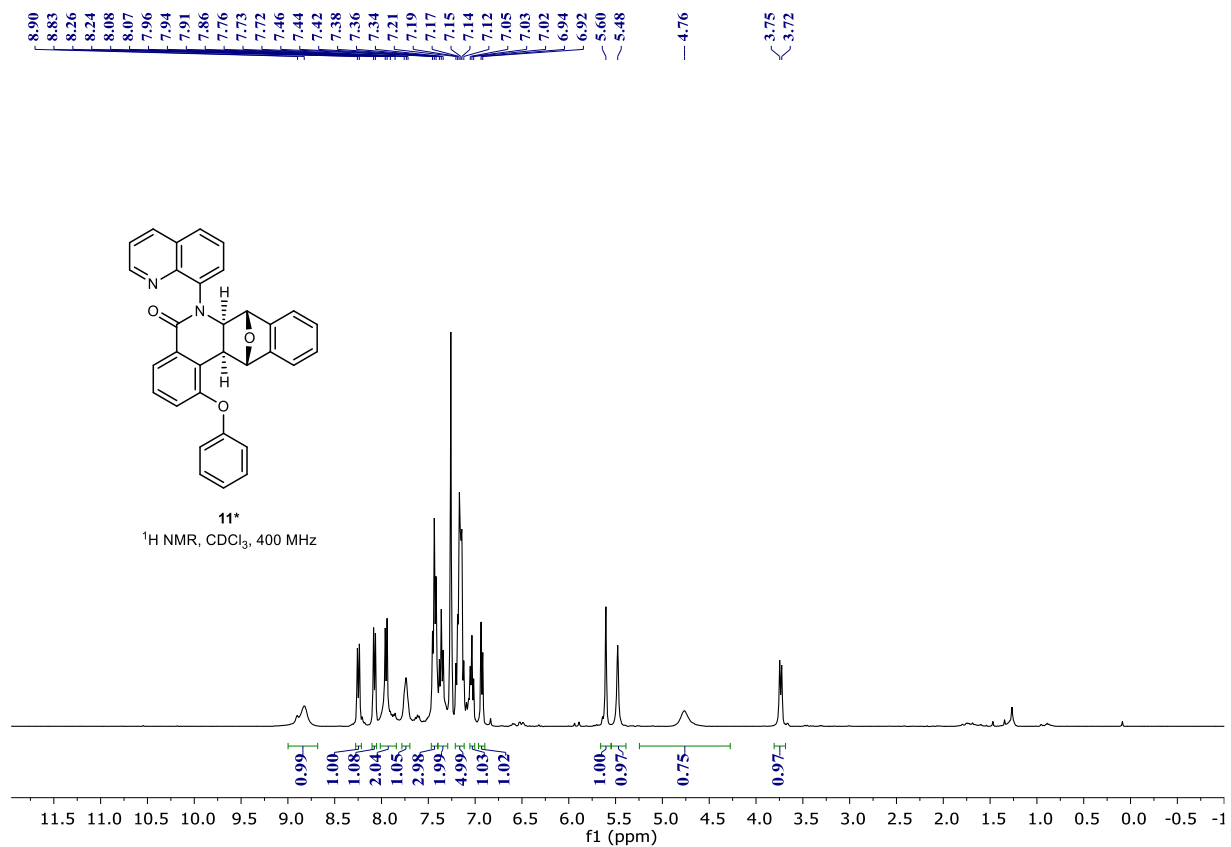


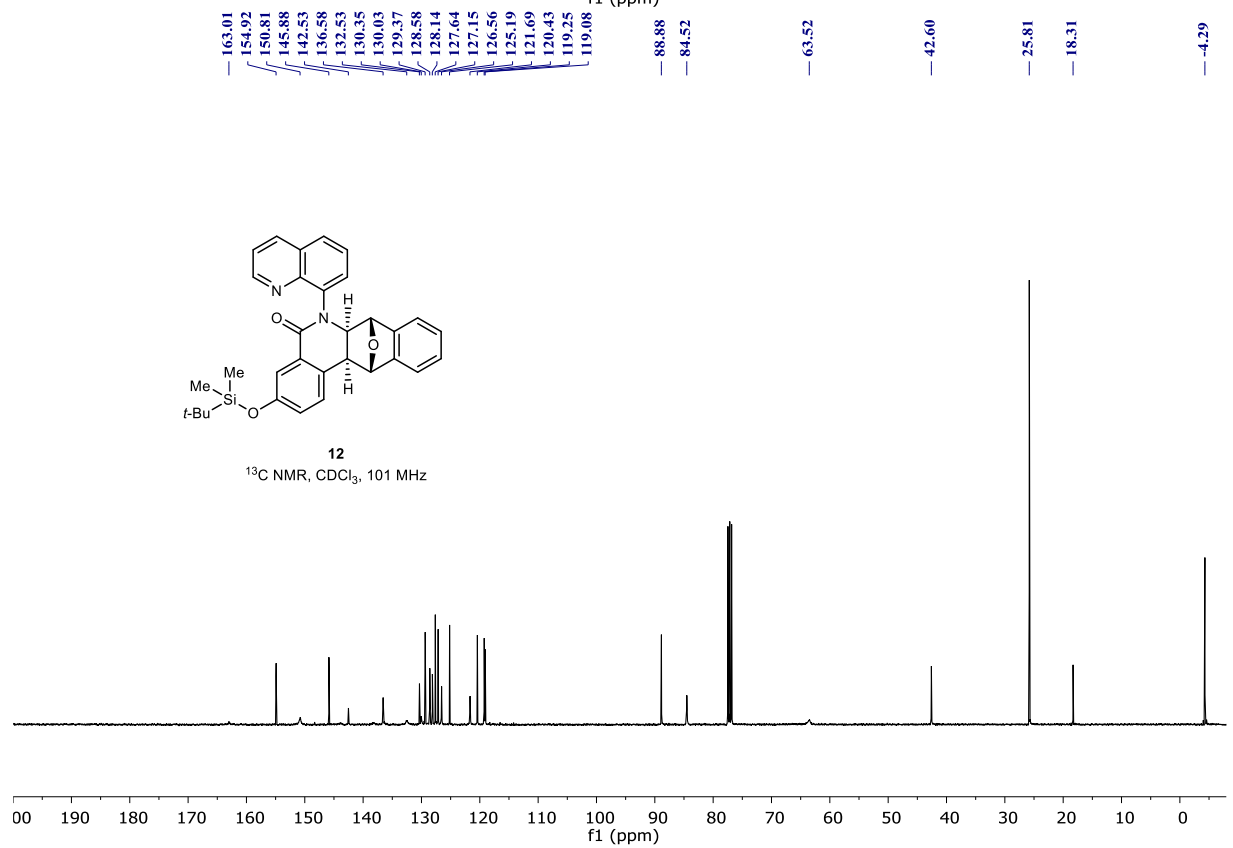
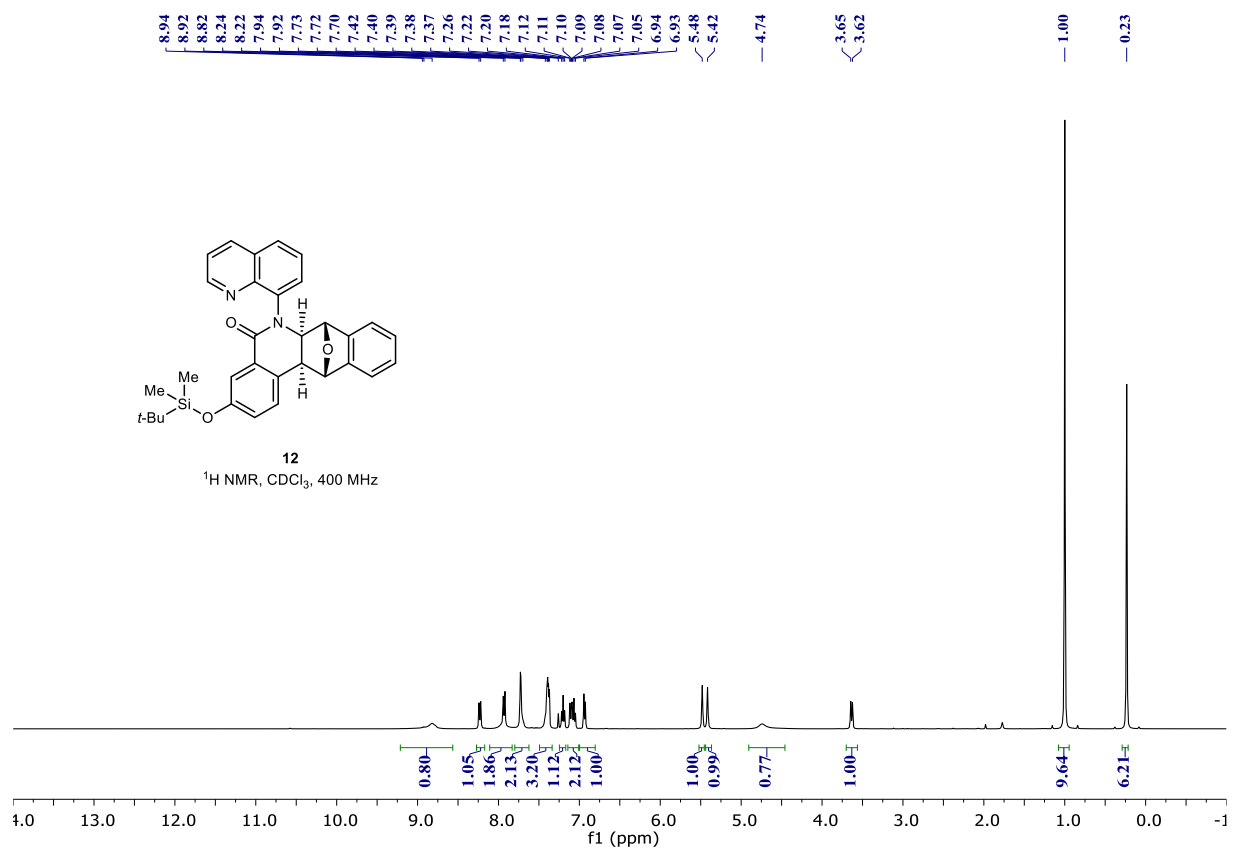


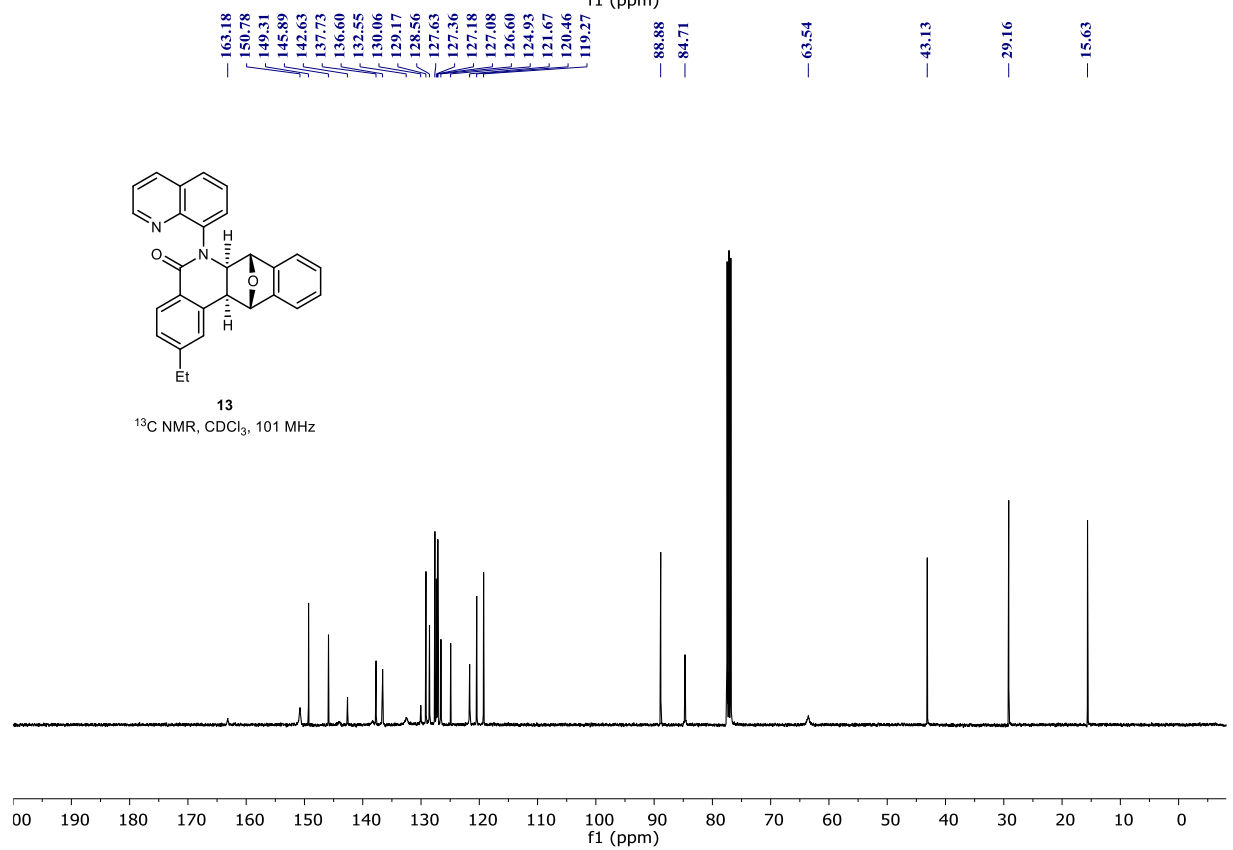
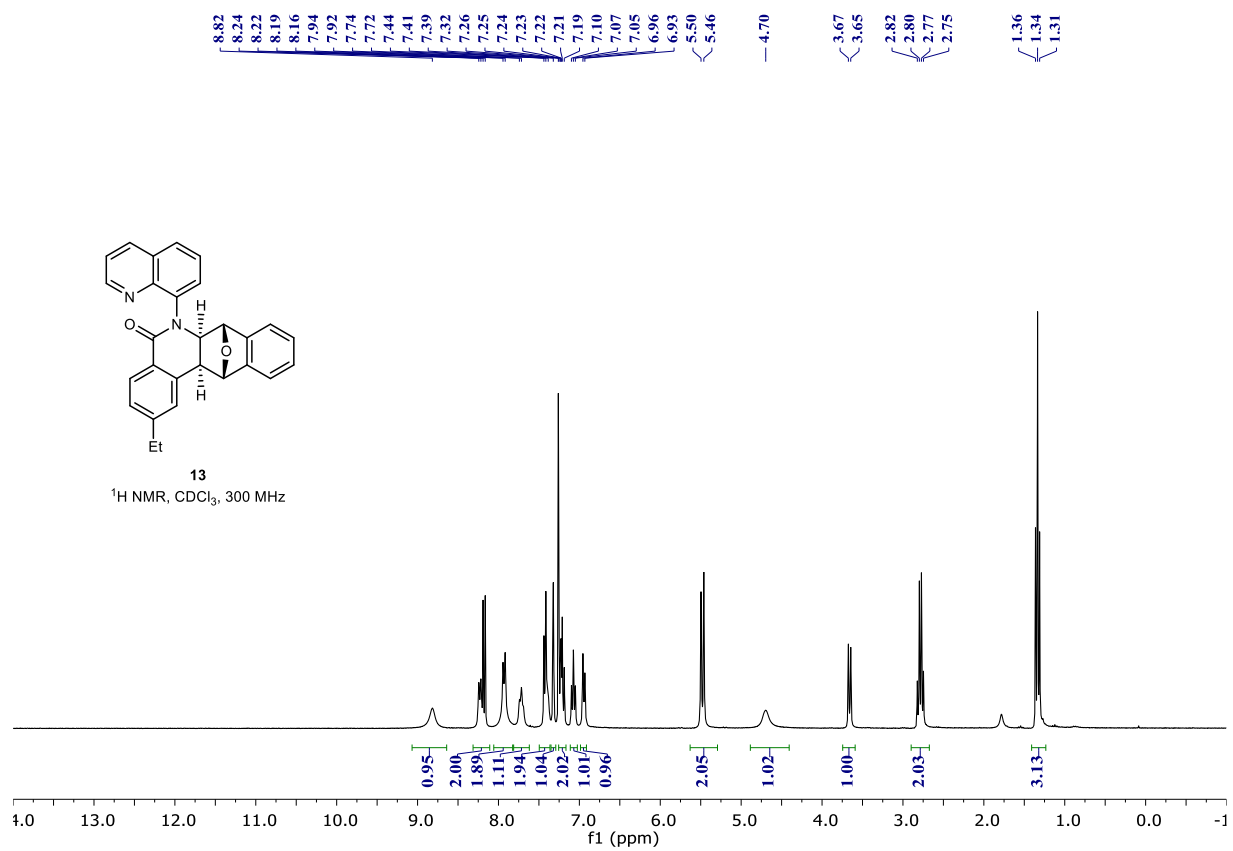
11
¹H NMR, CDCl₃, 400 MHz

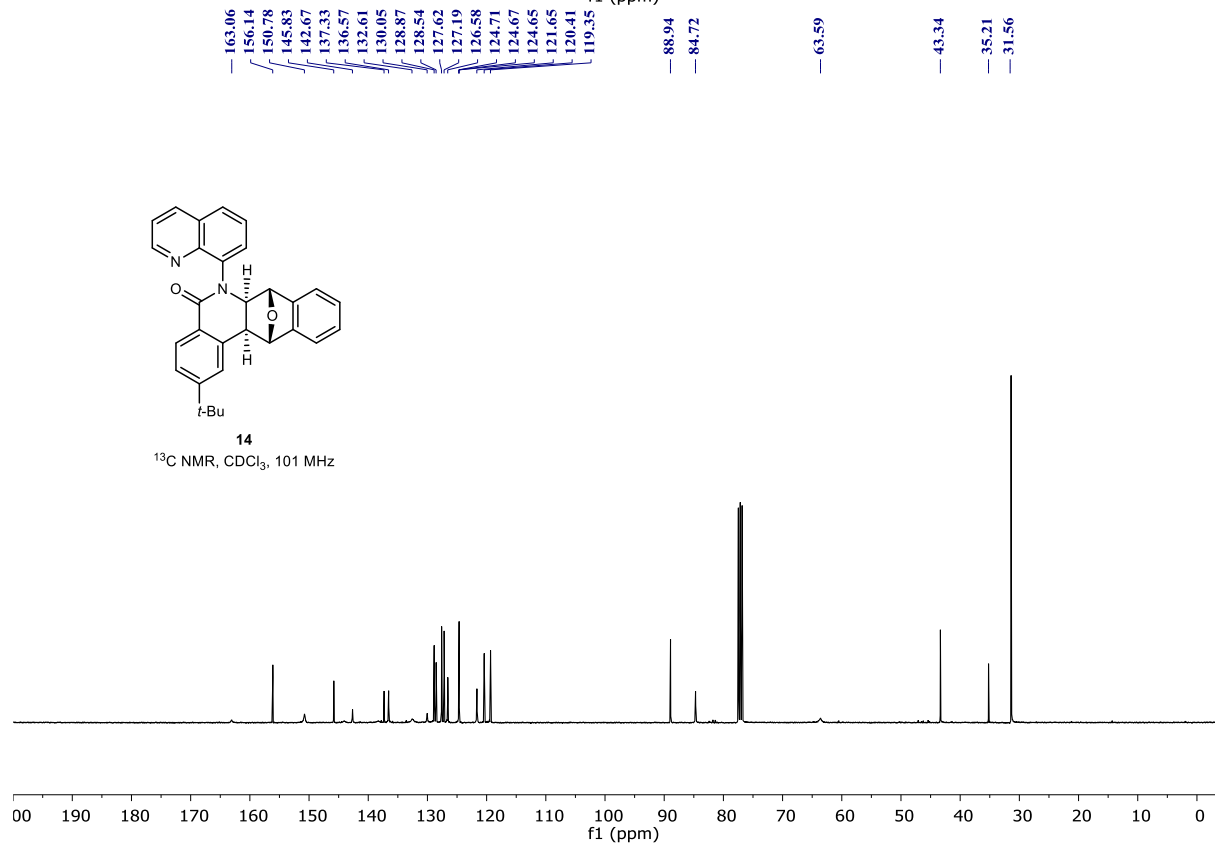
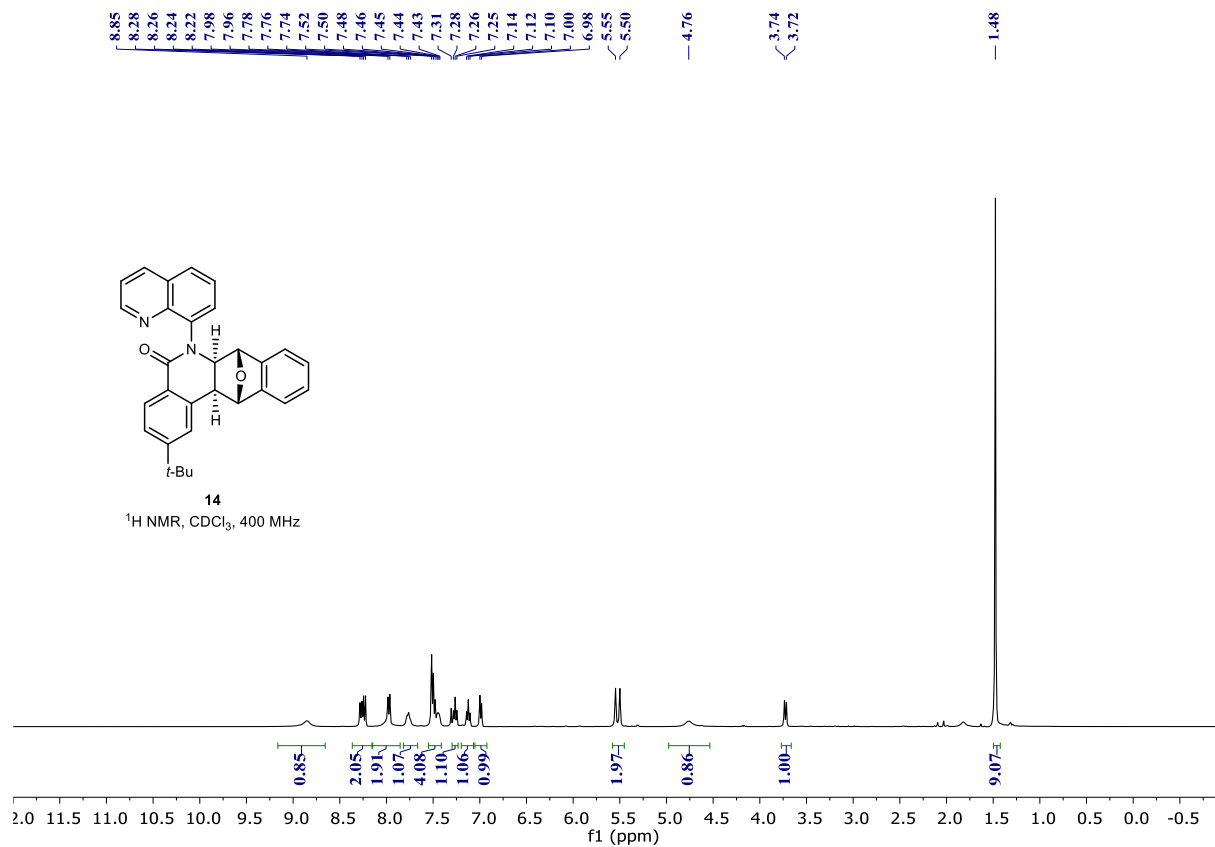


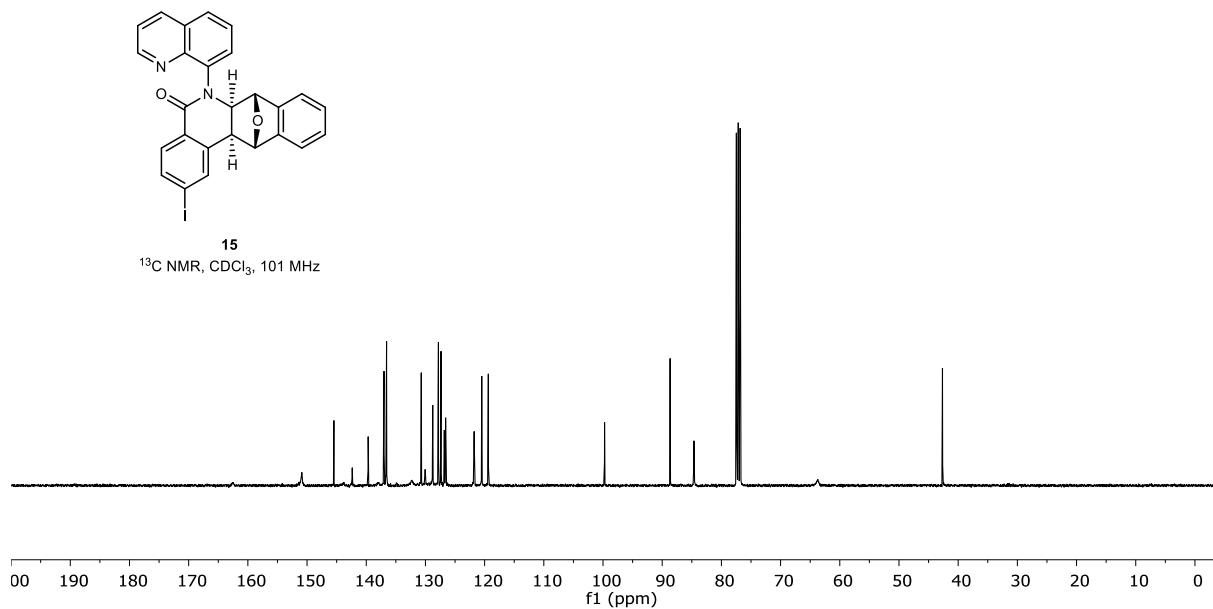
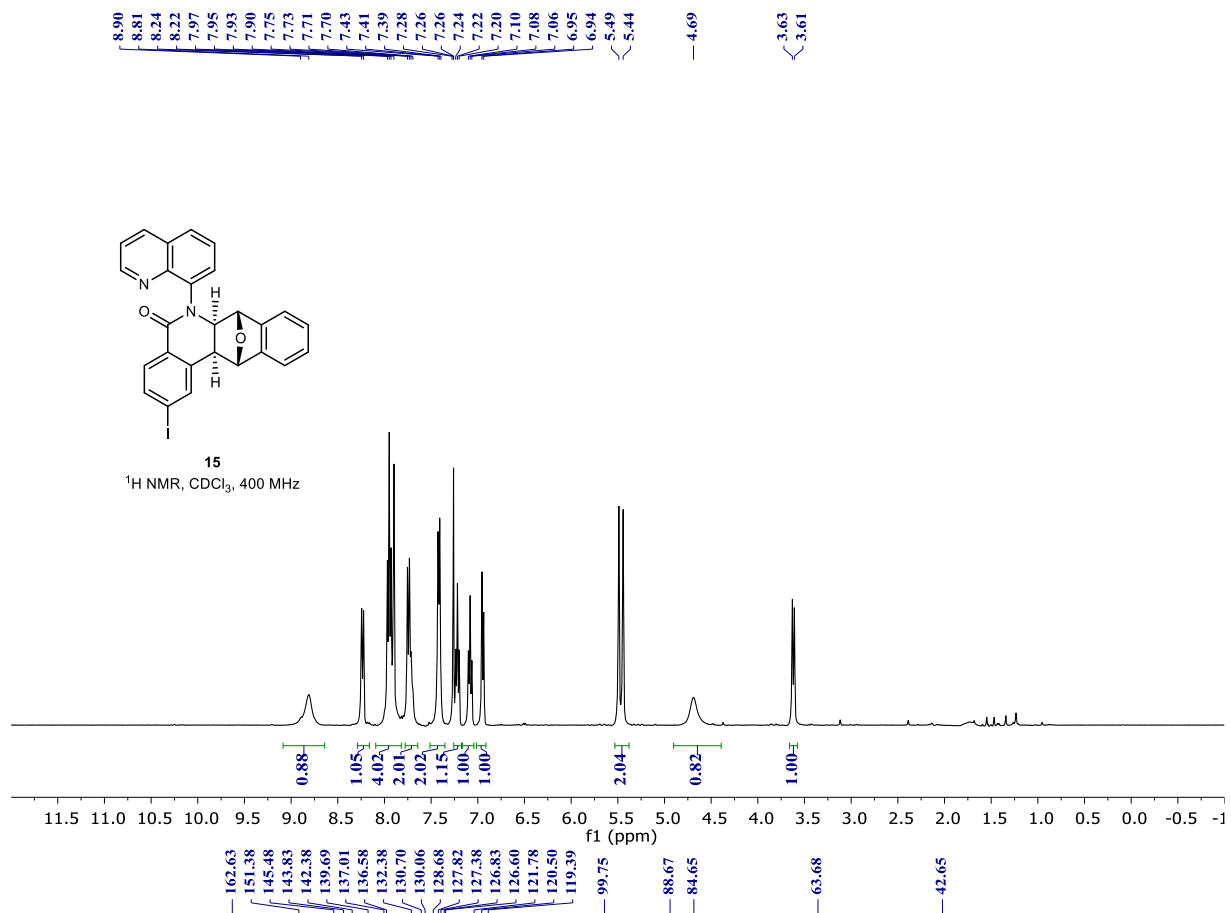
11
¹³C NMR, CDCl₃, 101 MHz

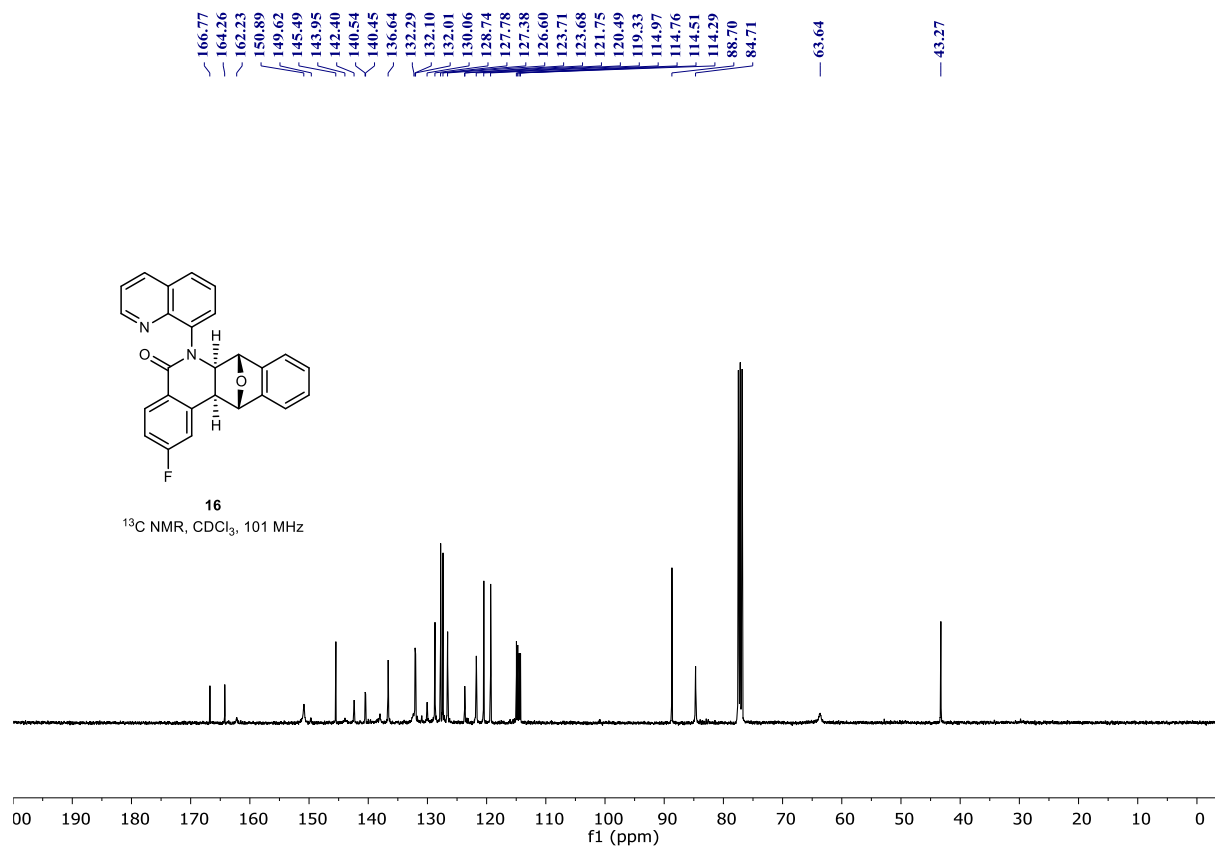
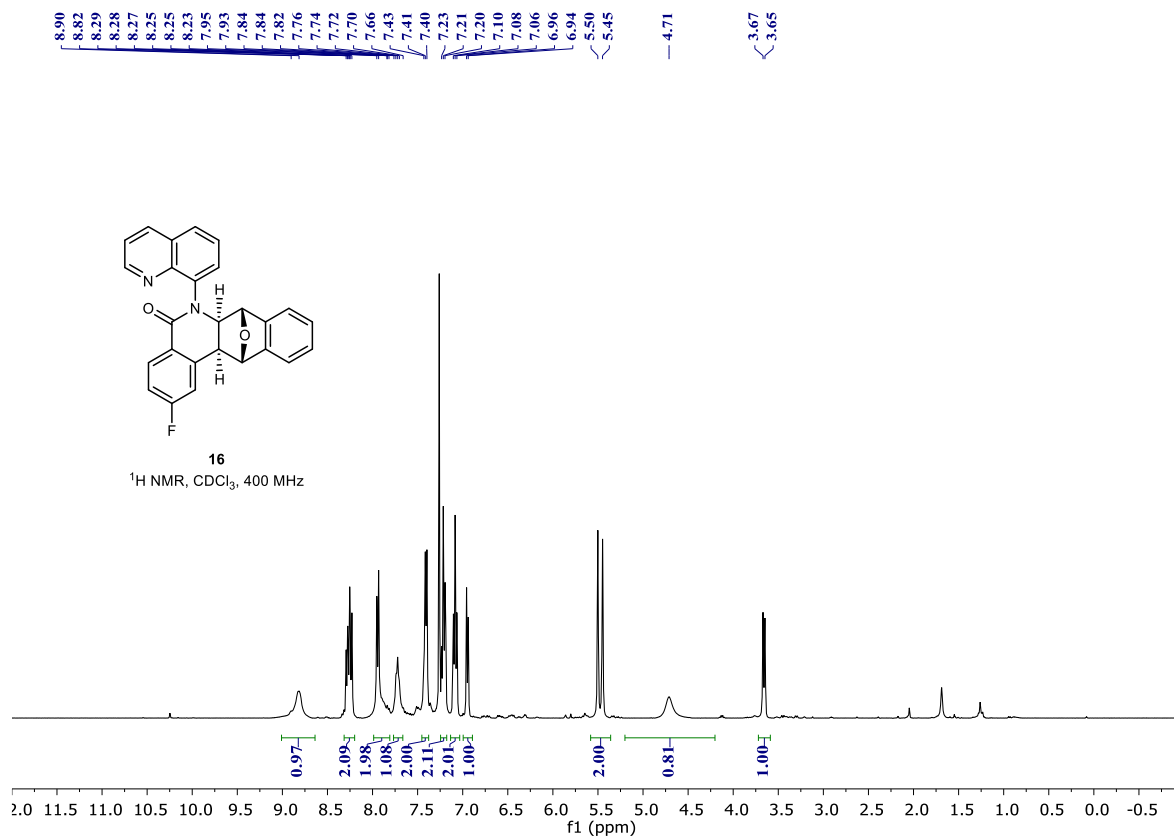


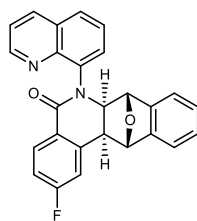






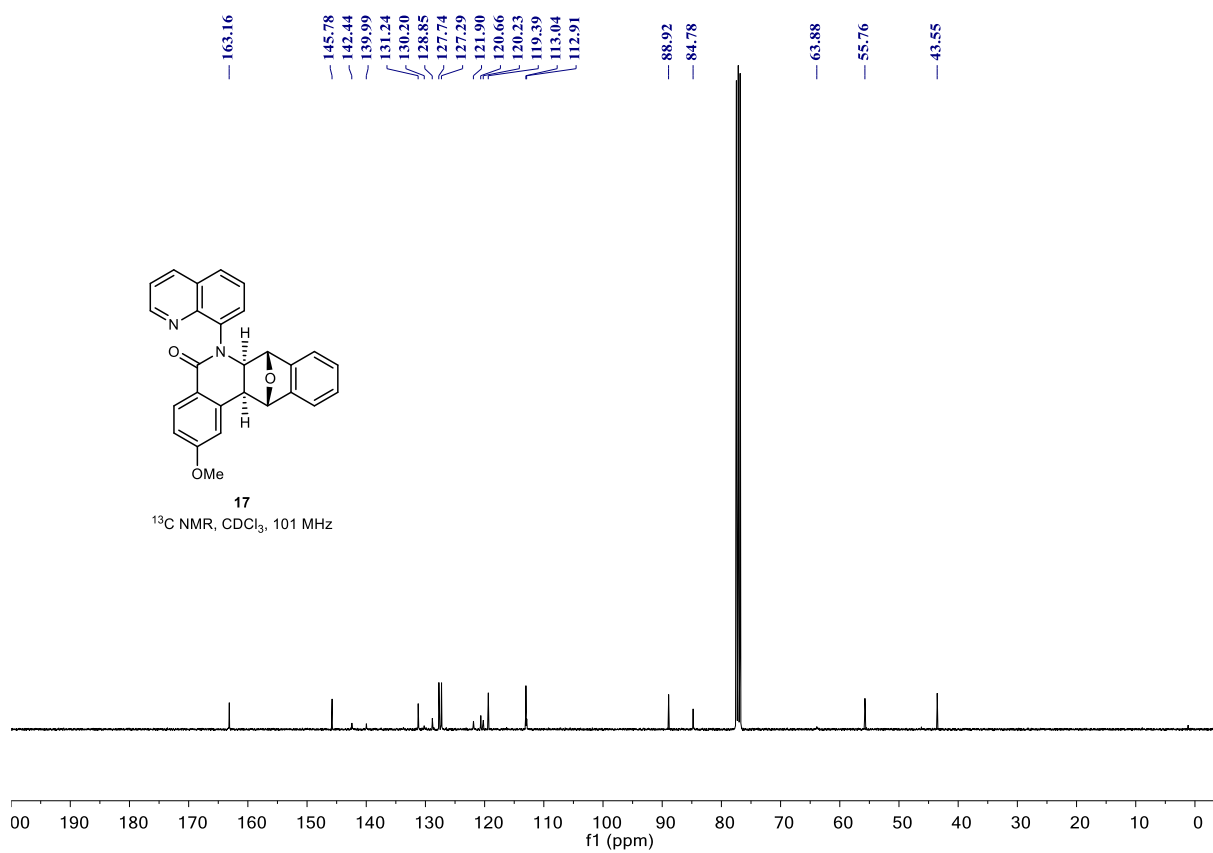
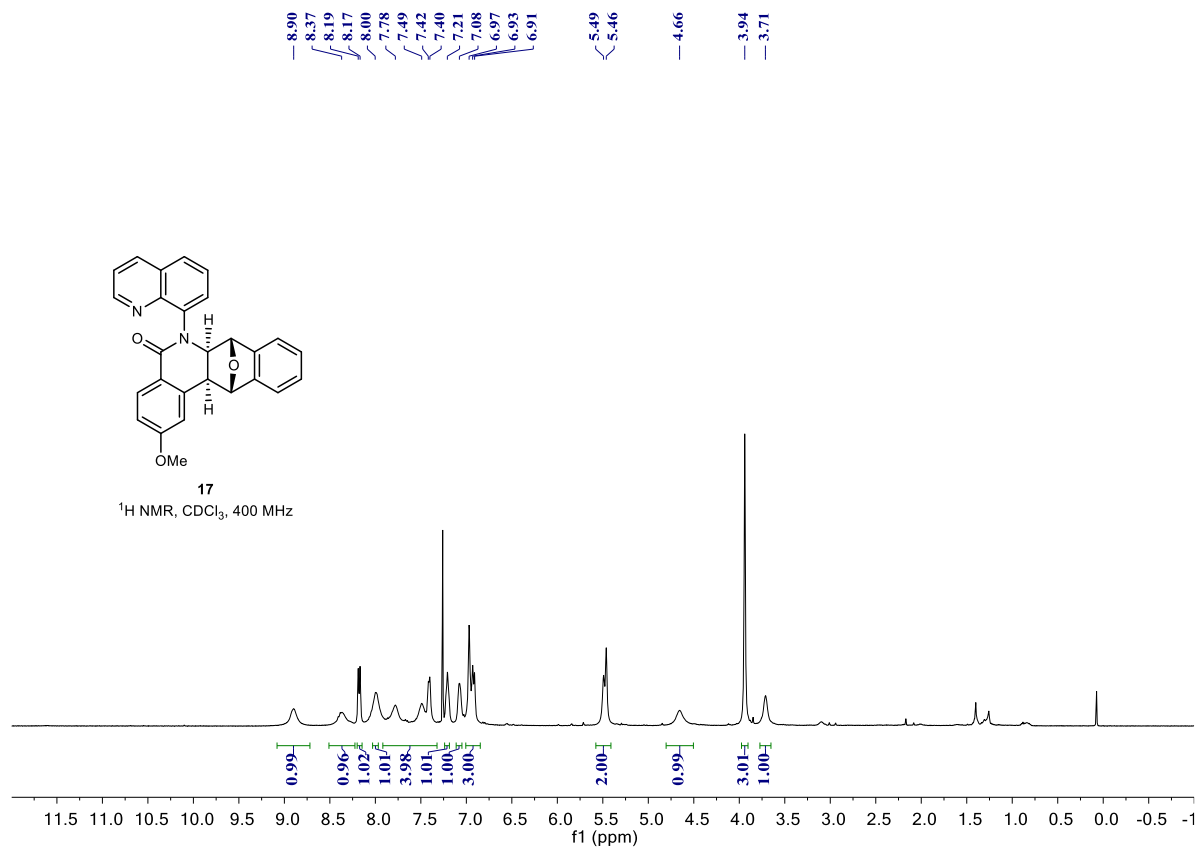


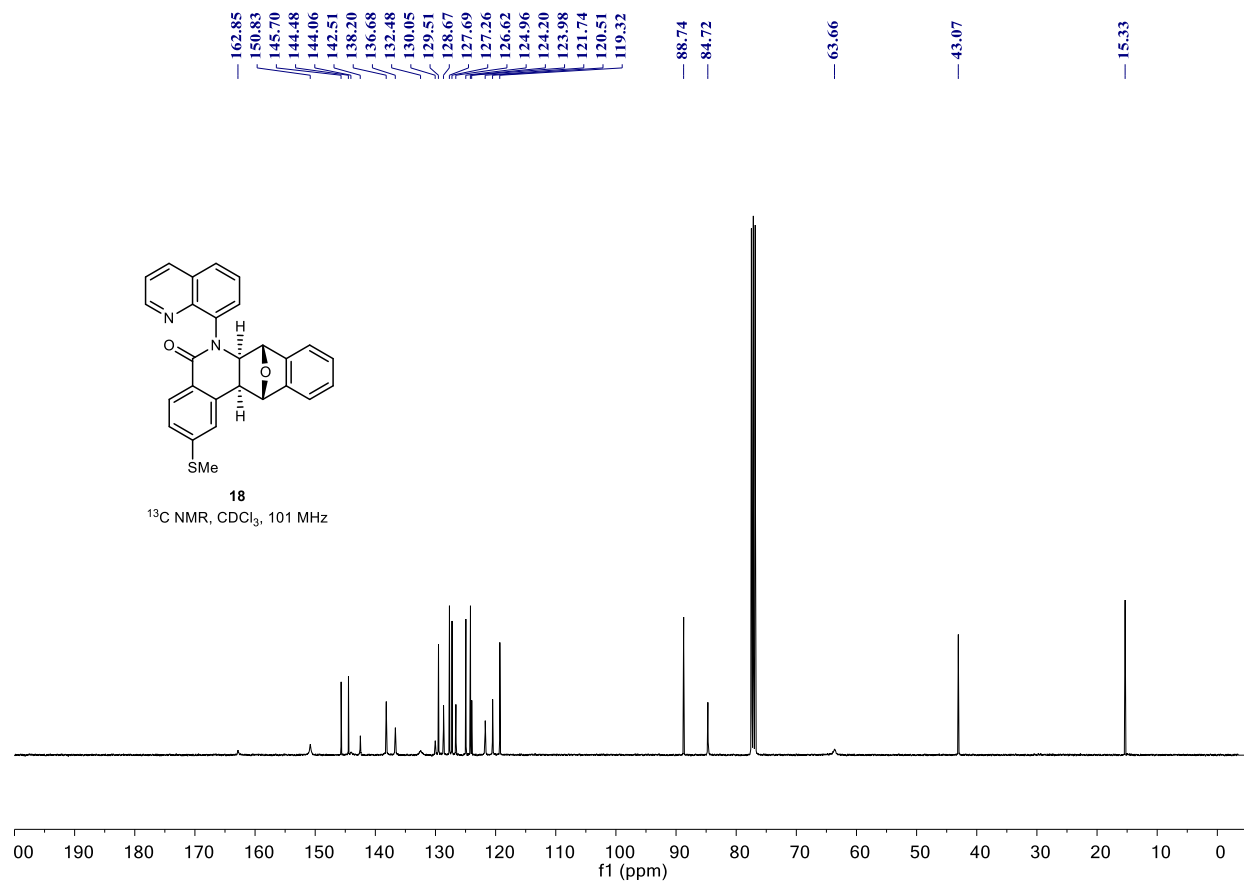
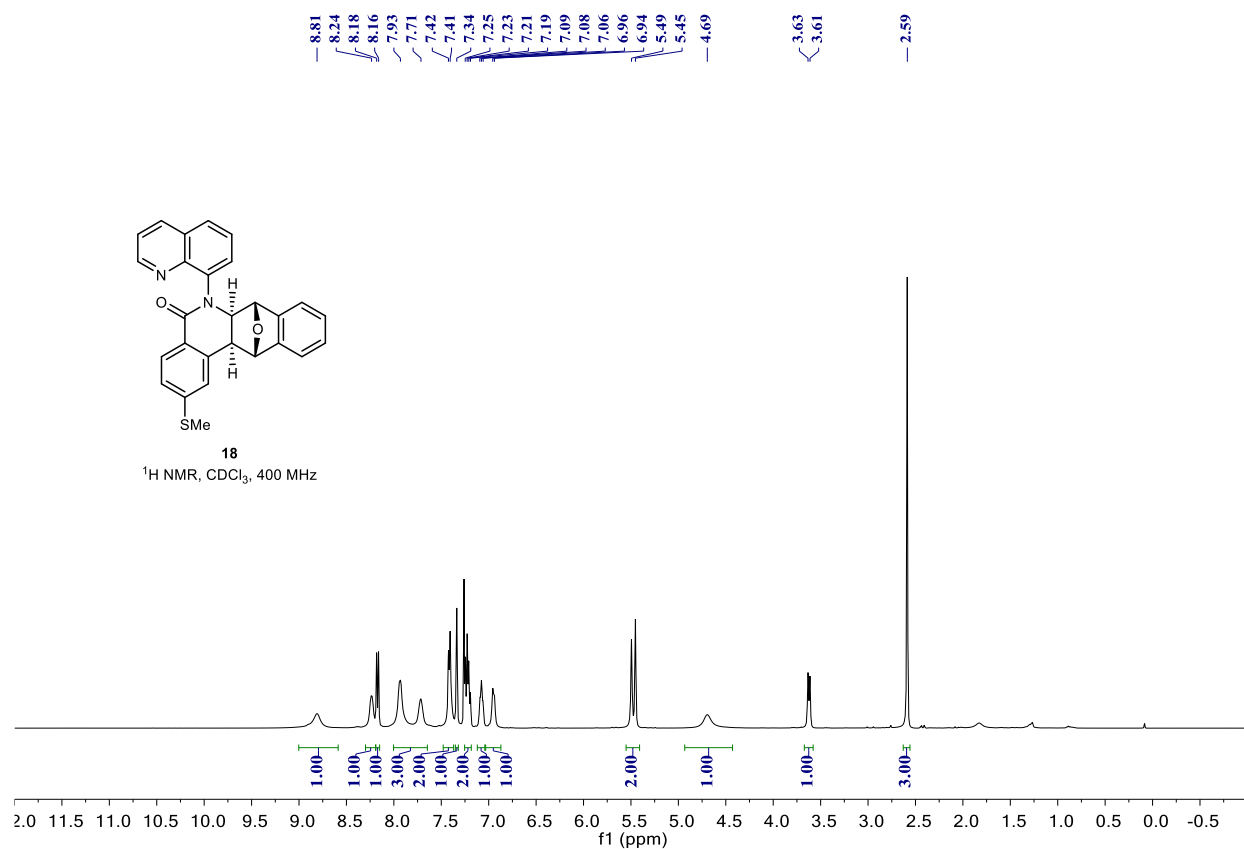


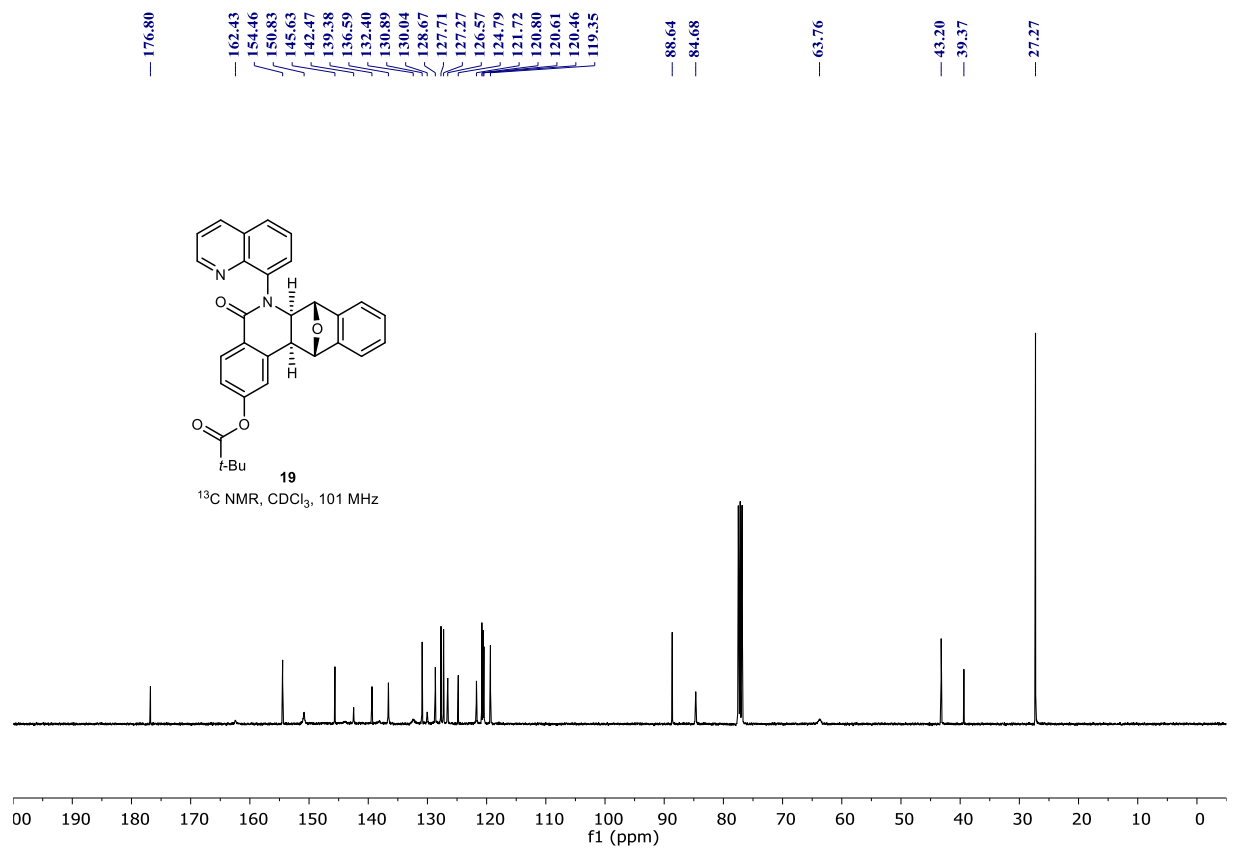
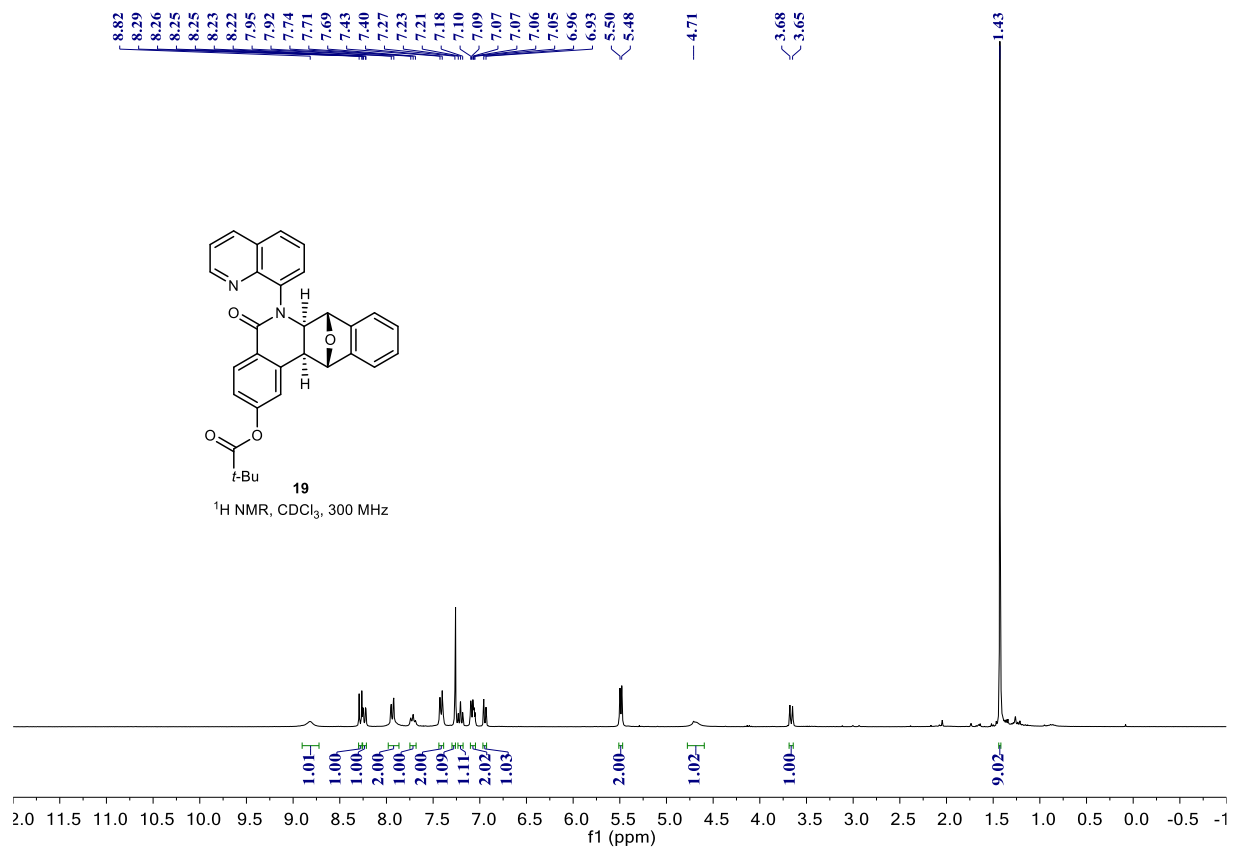


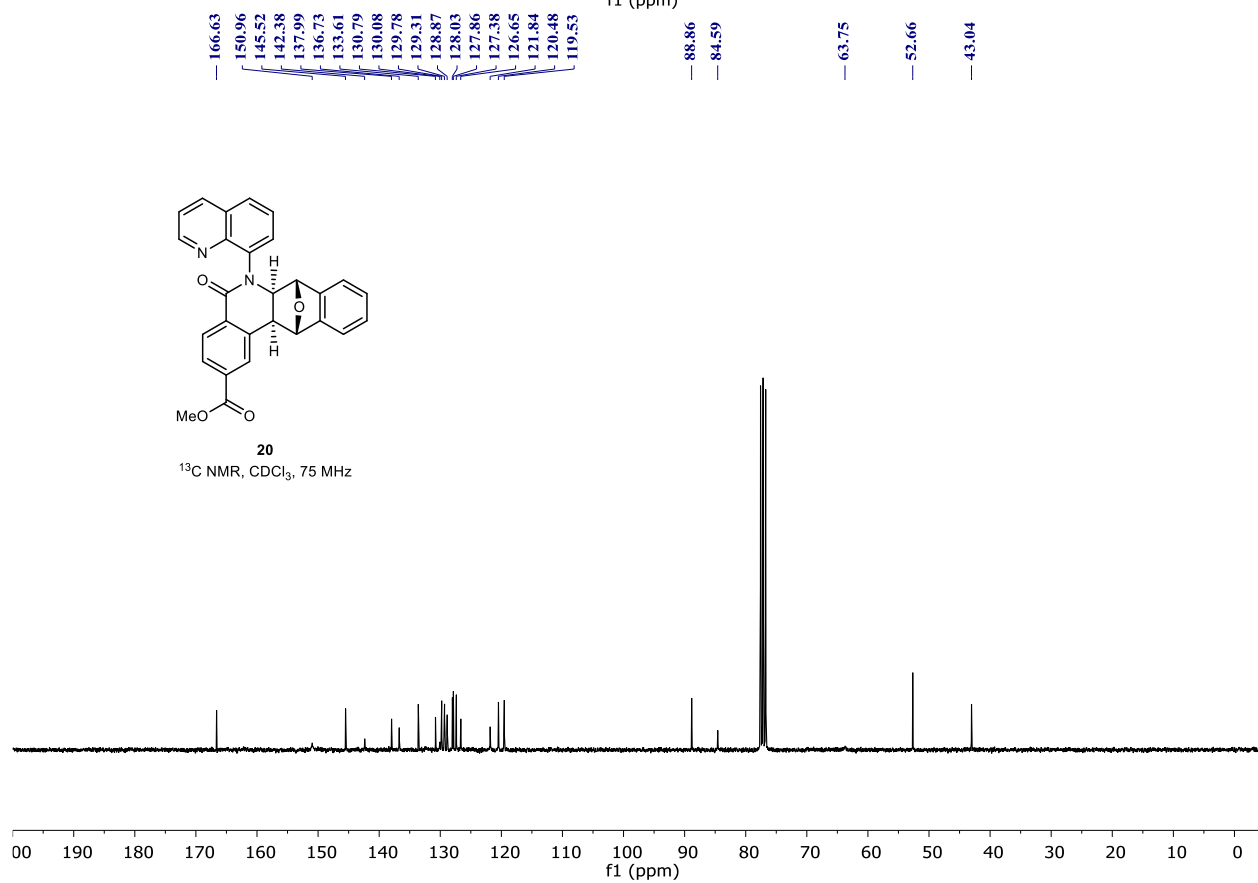
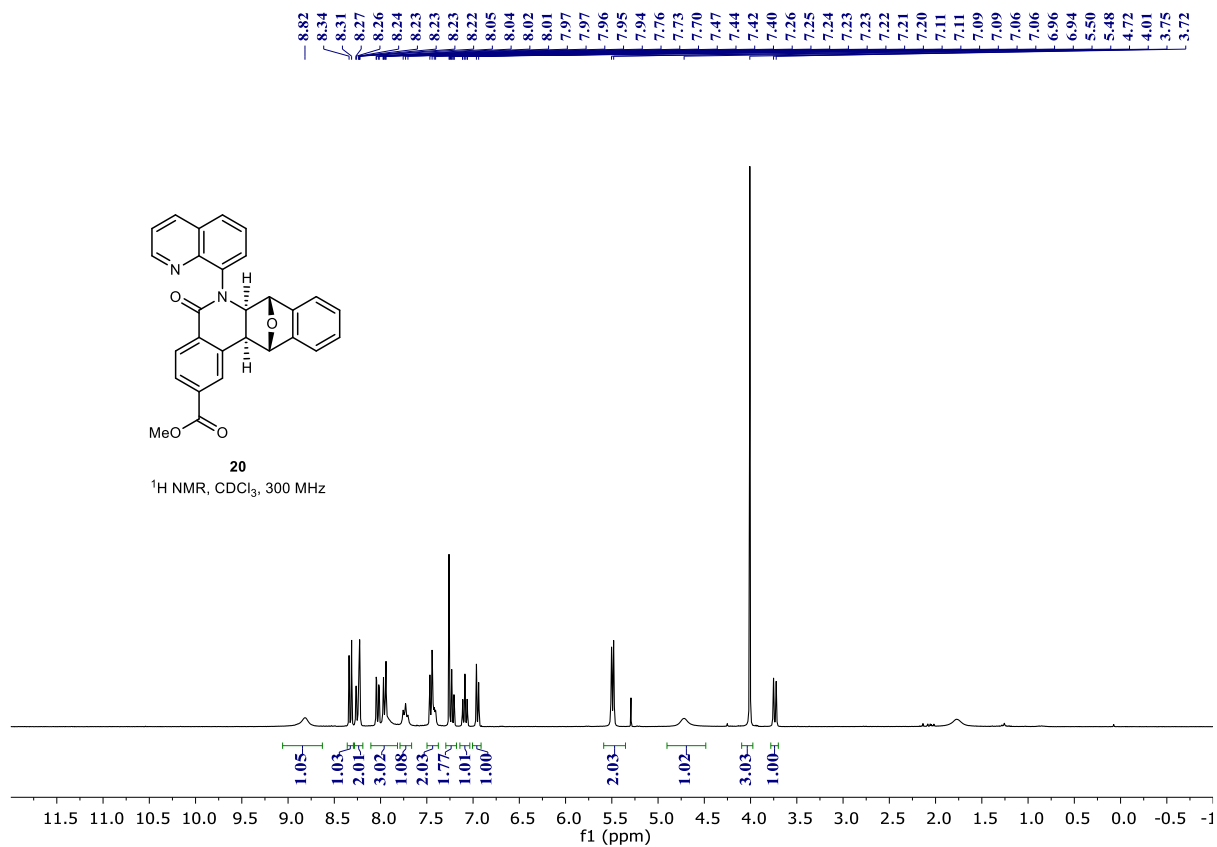
16
 ^{19}F NMR, CDCl_3 , 377 MHz

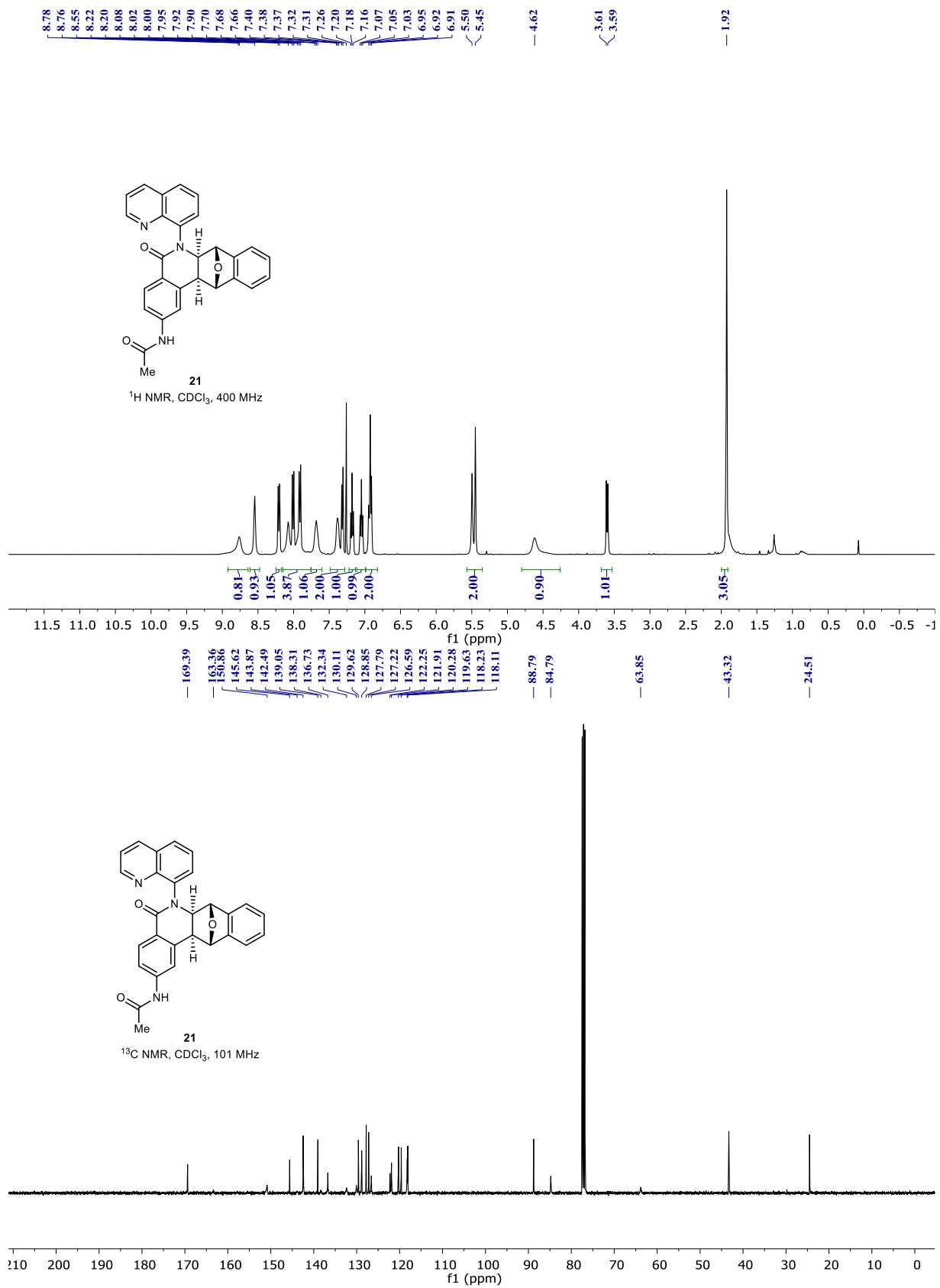


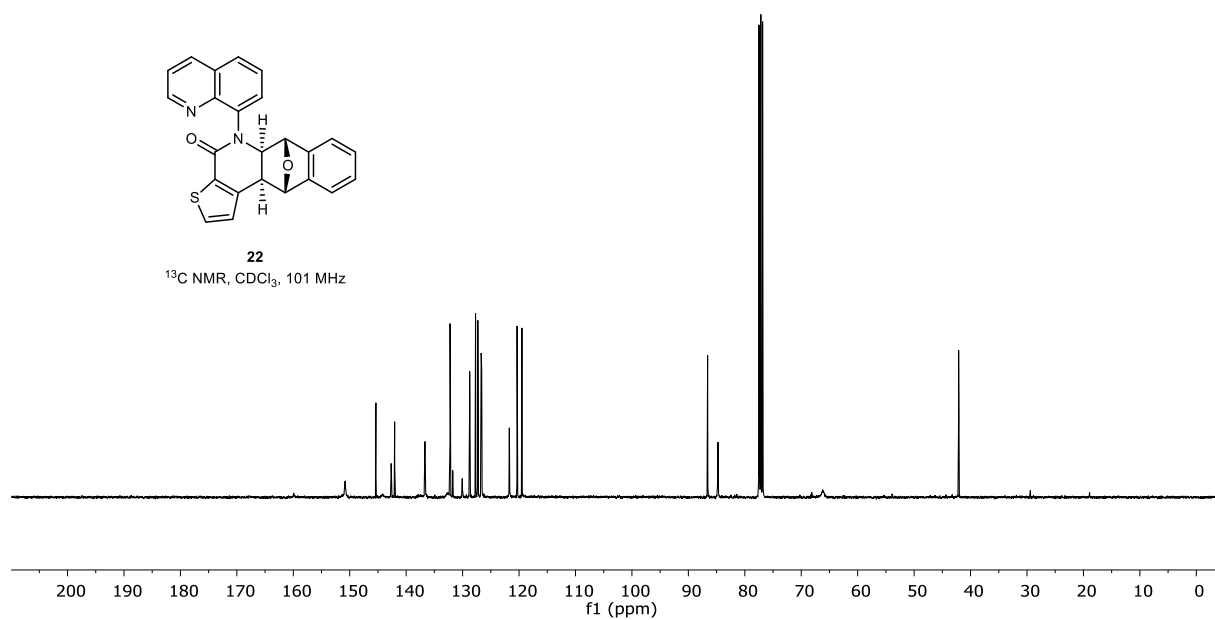
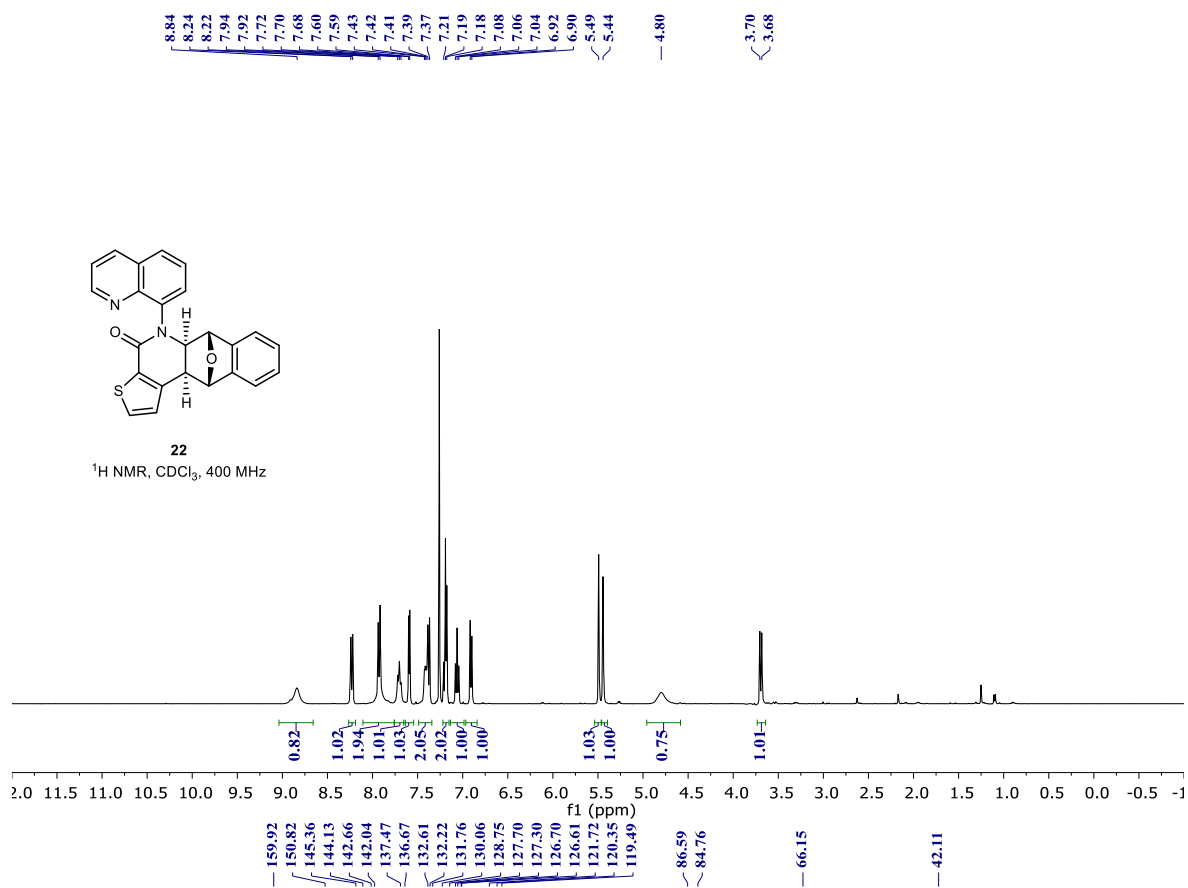


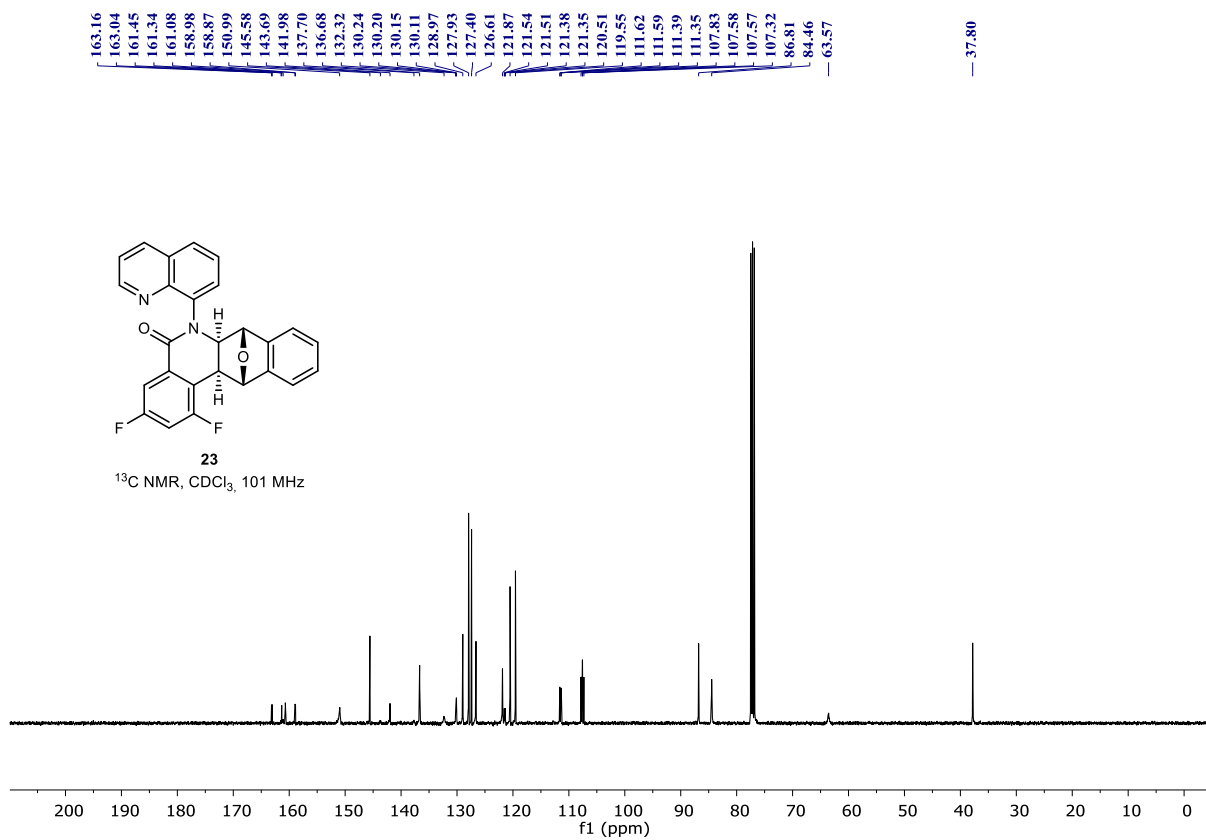
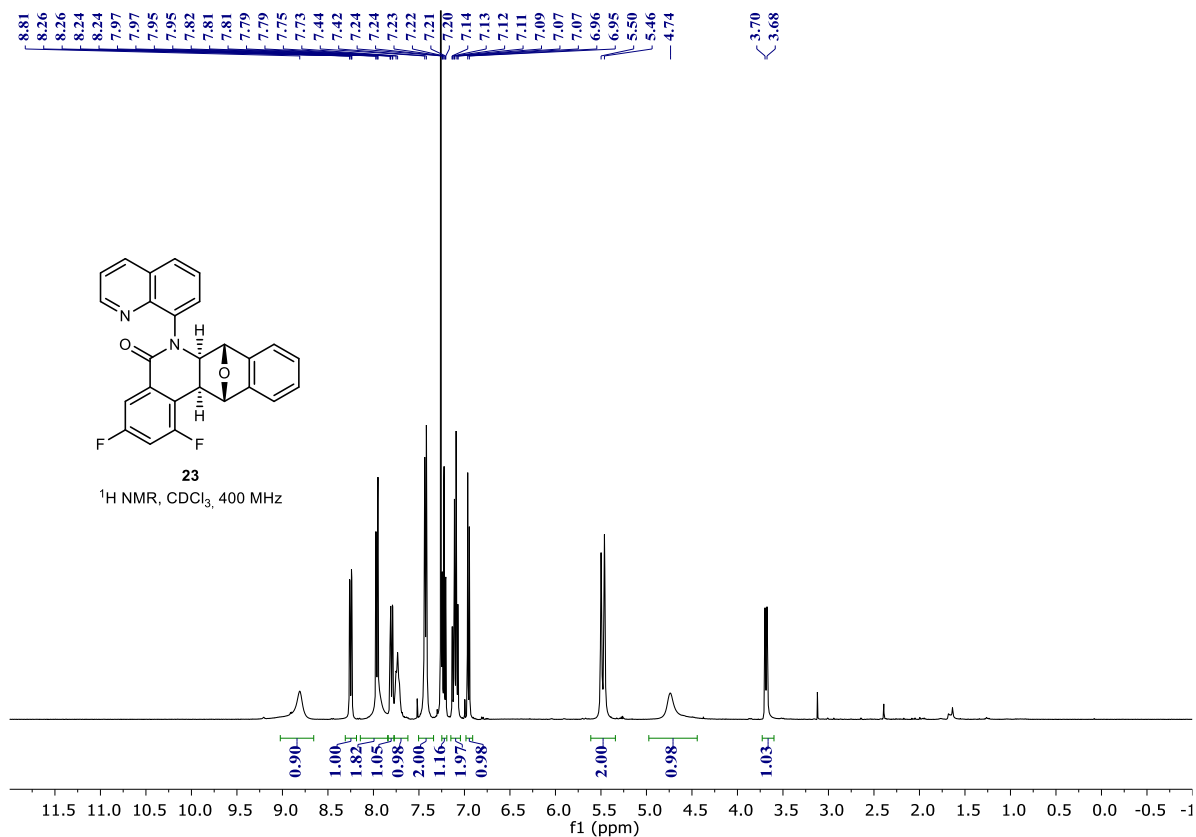


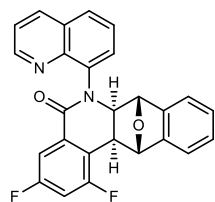




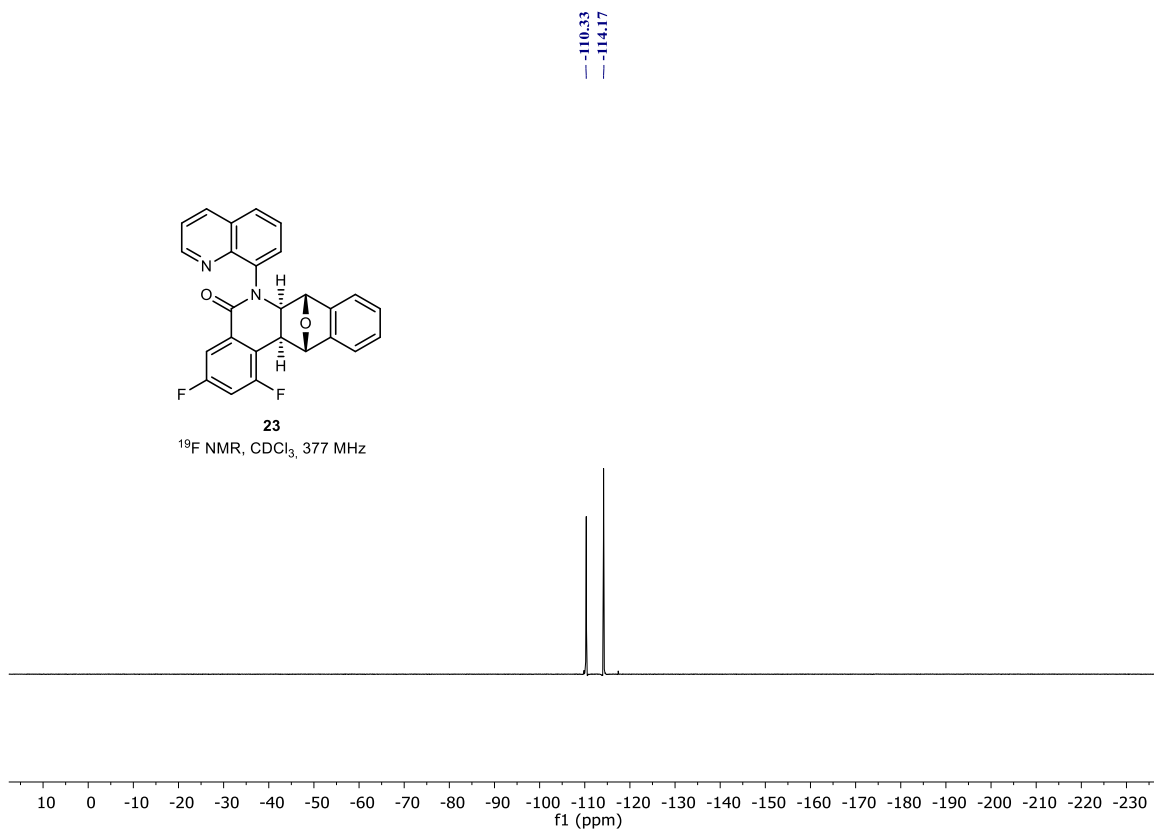


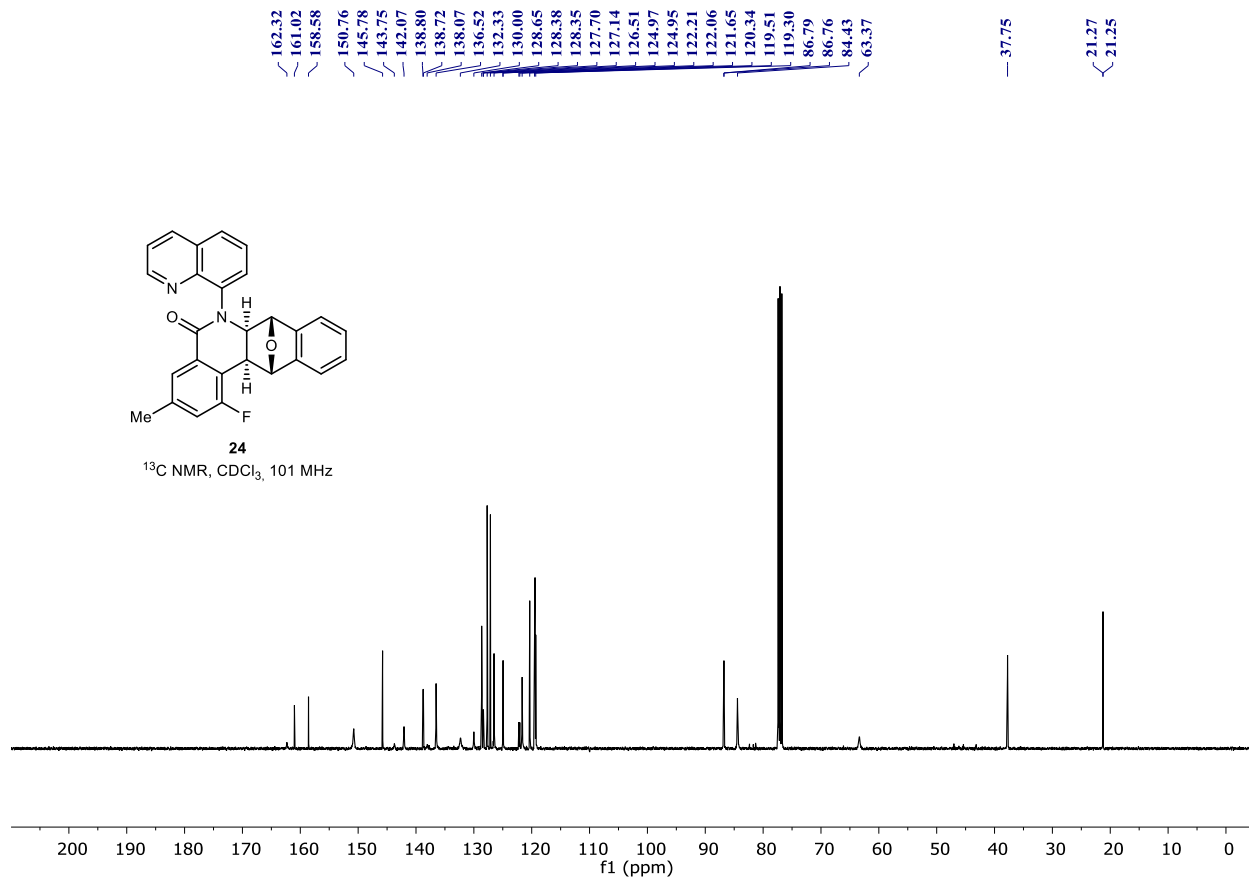
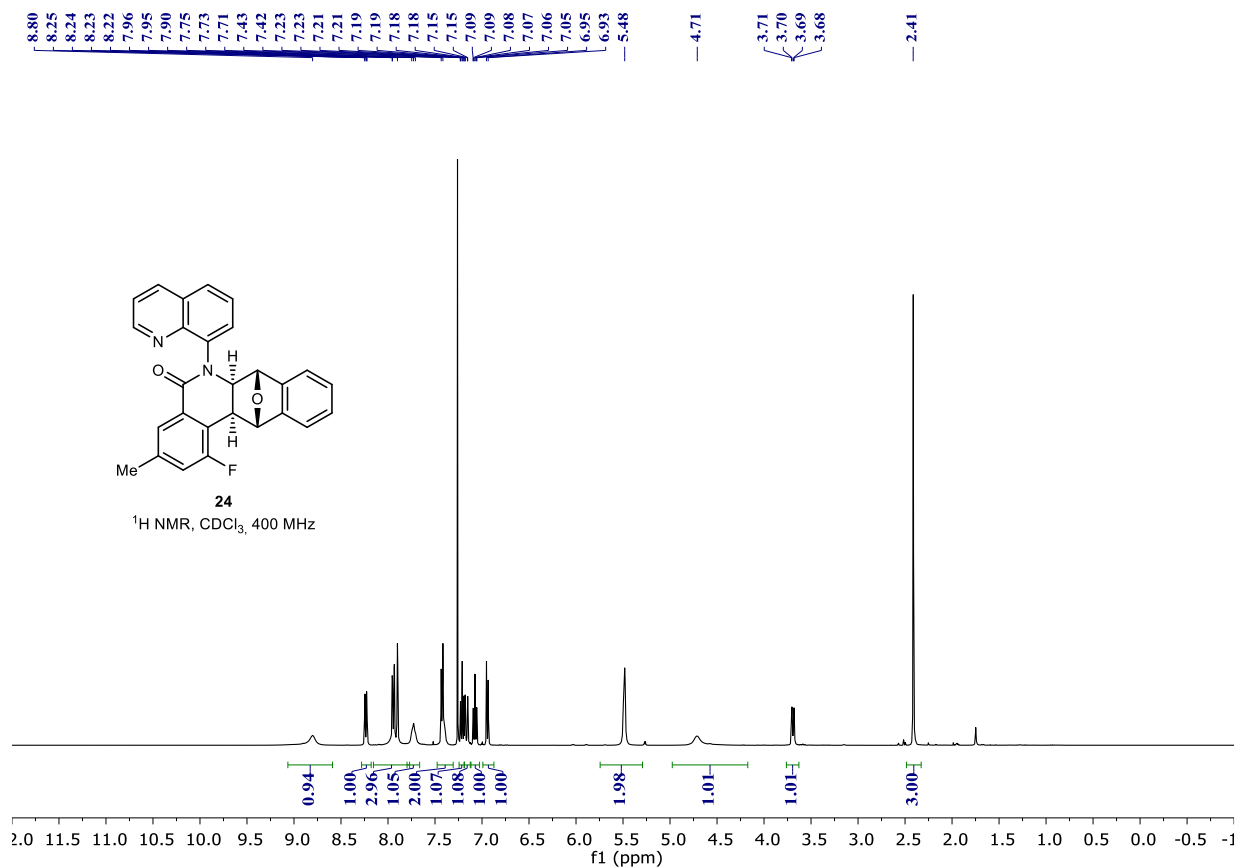


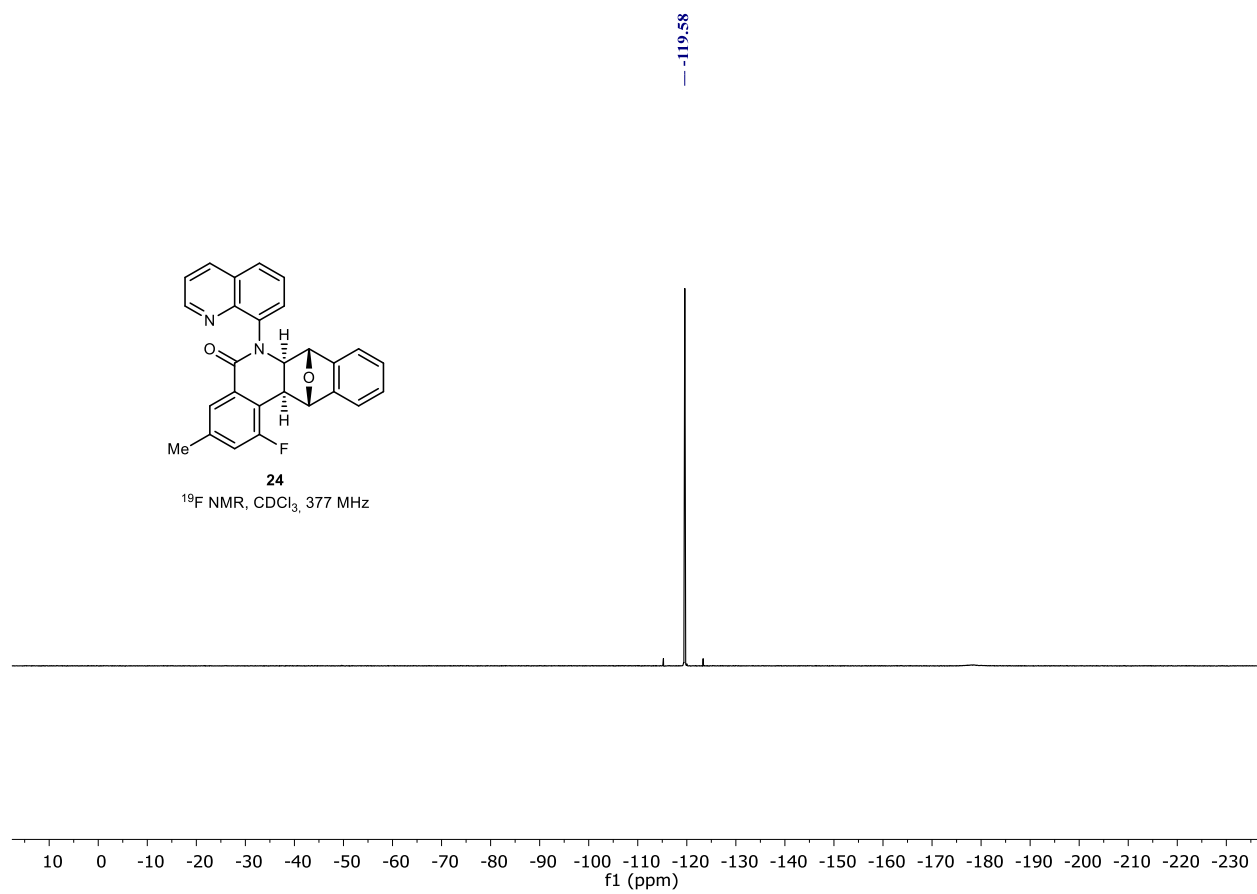


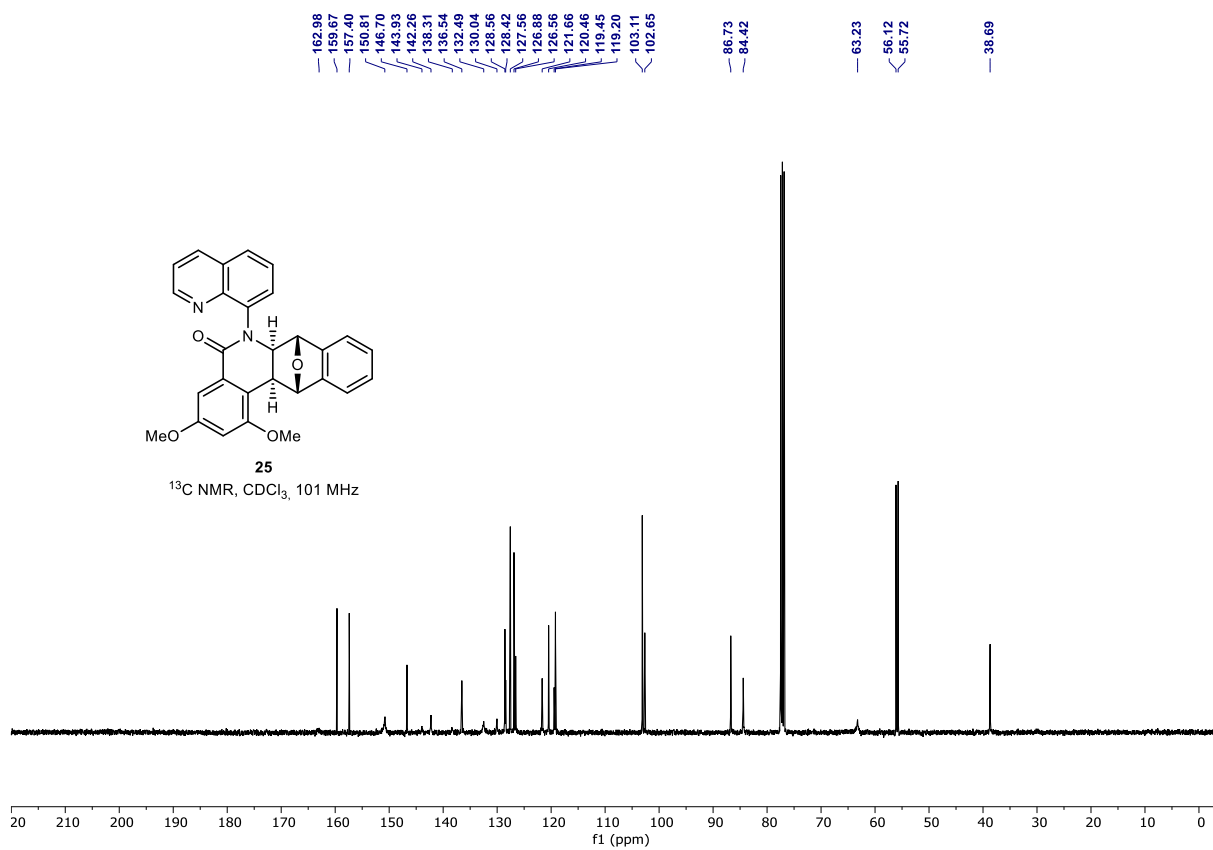
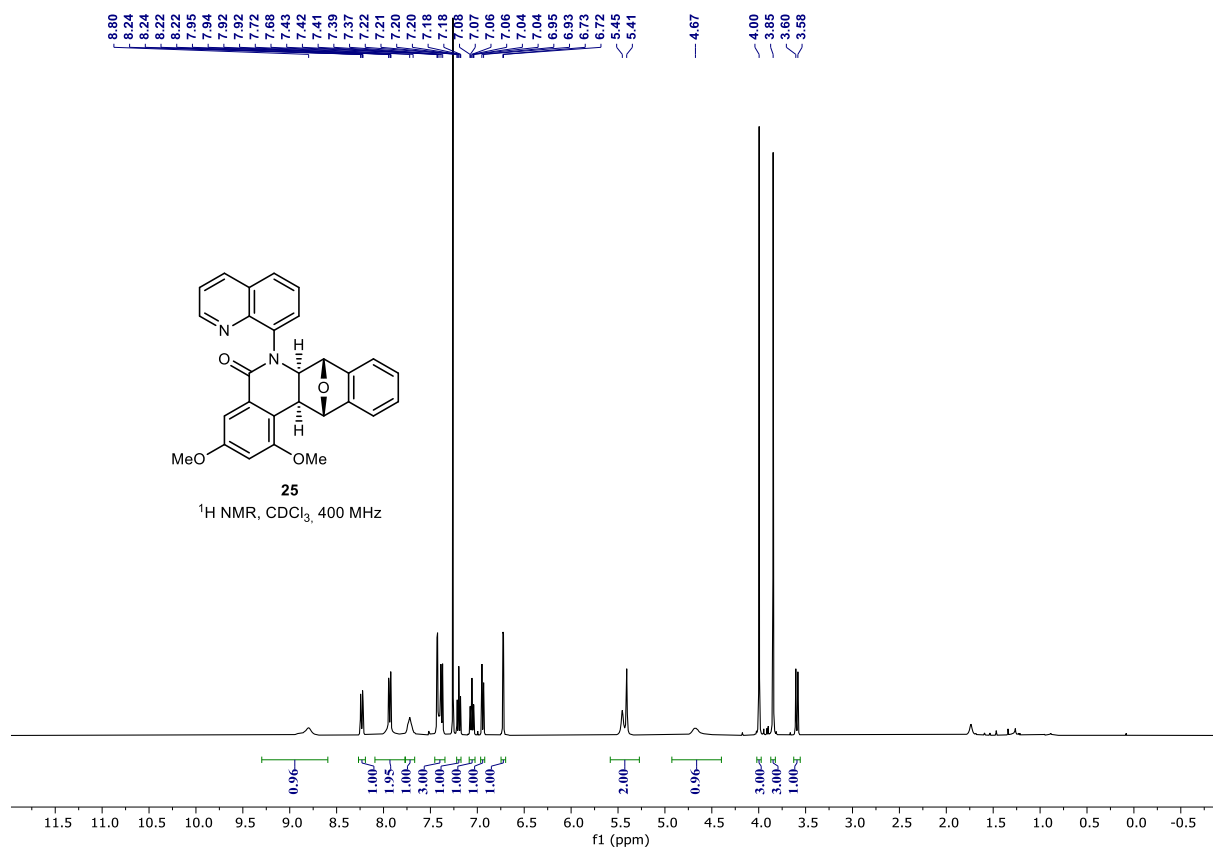


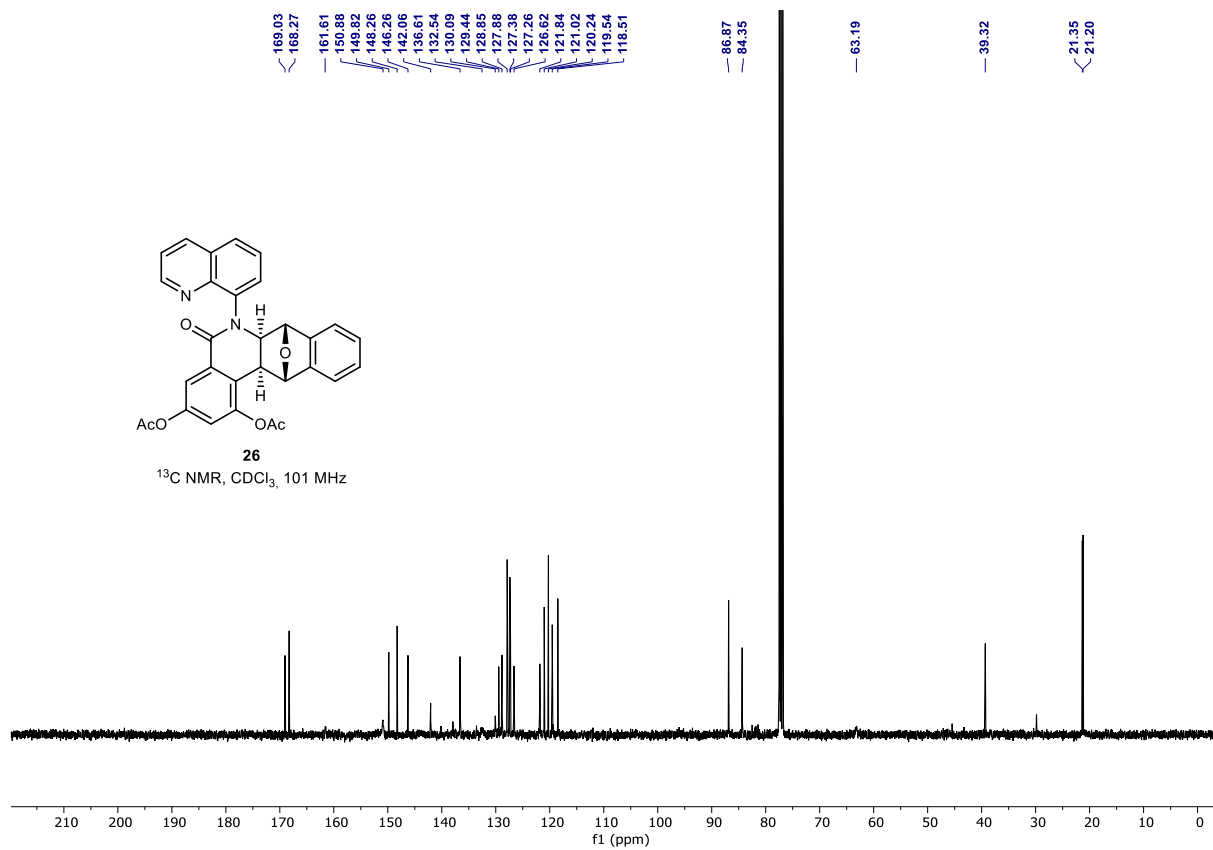
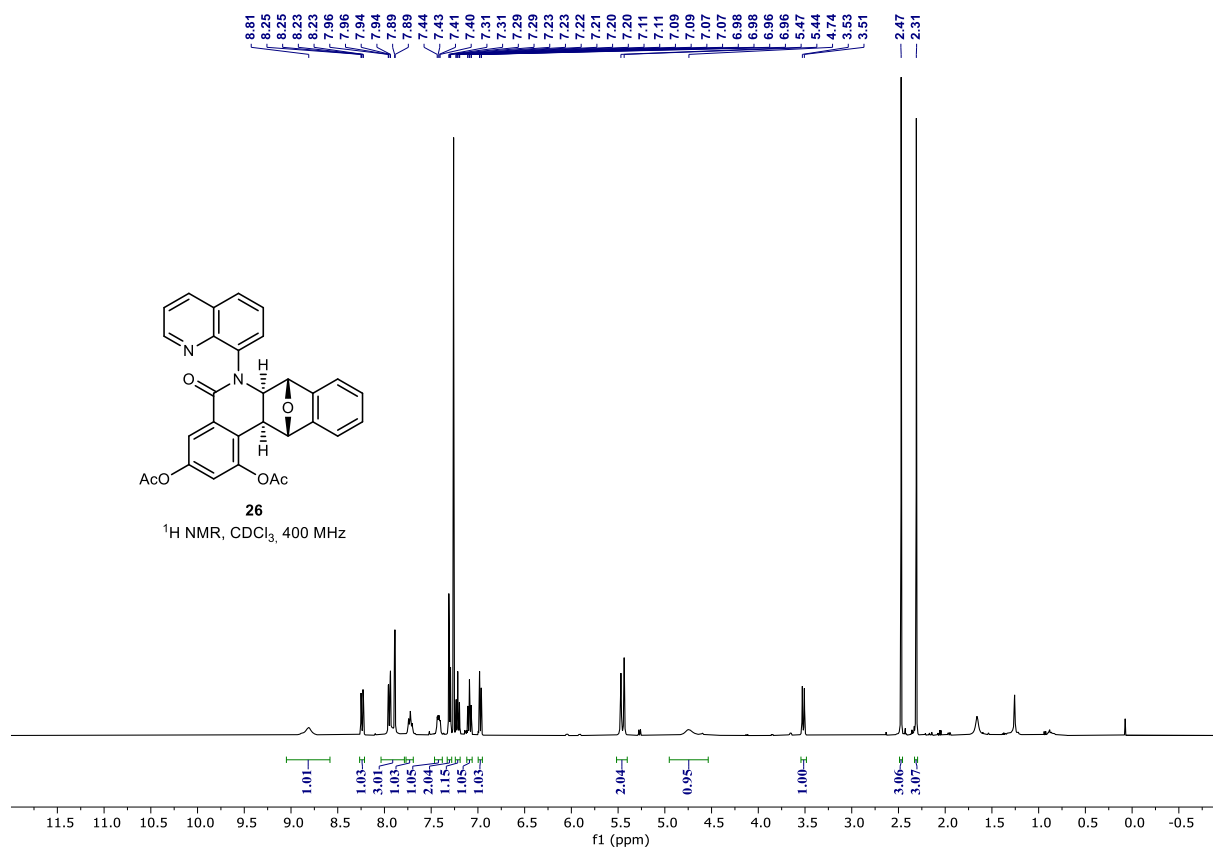
23
 ^{19}F NMR, CDCl_3 , 377 MHz

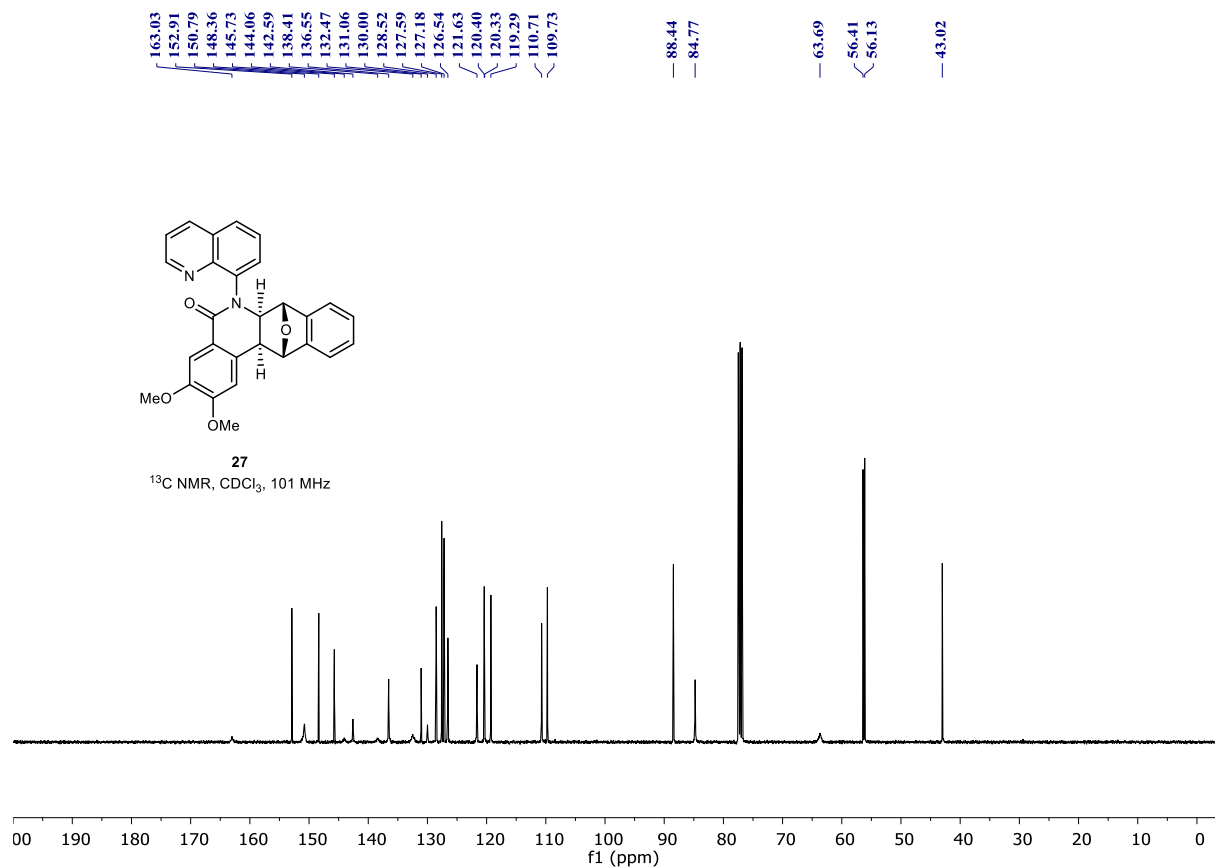
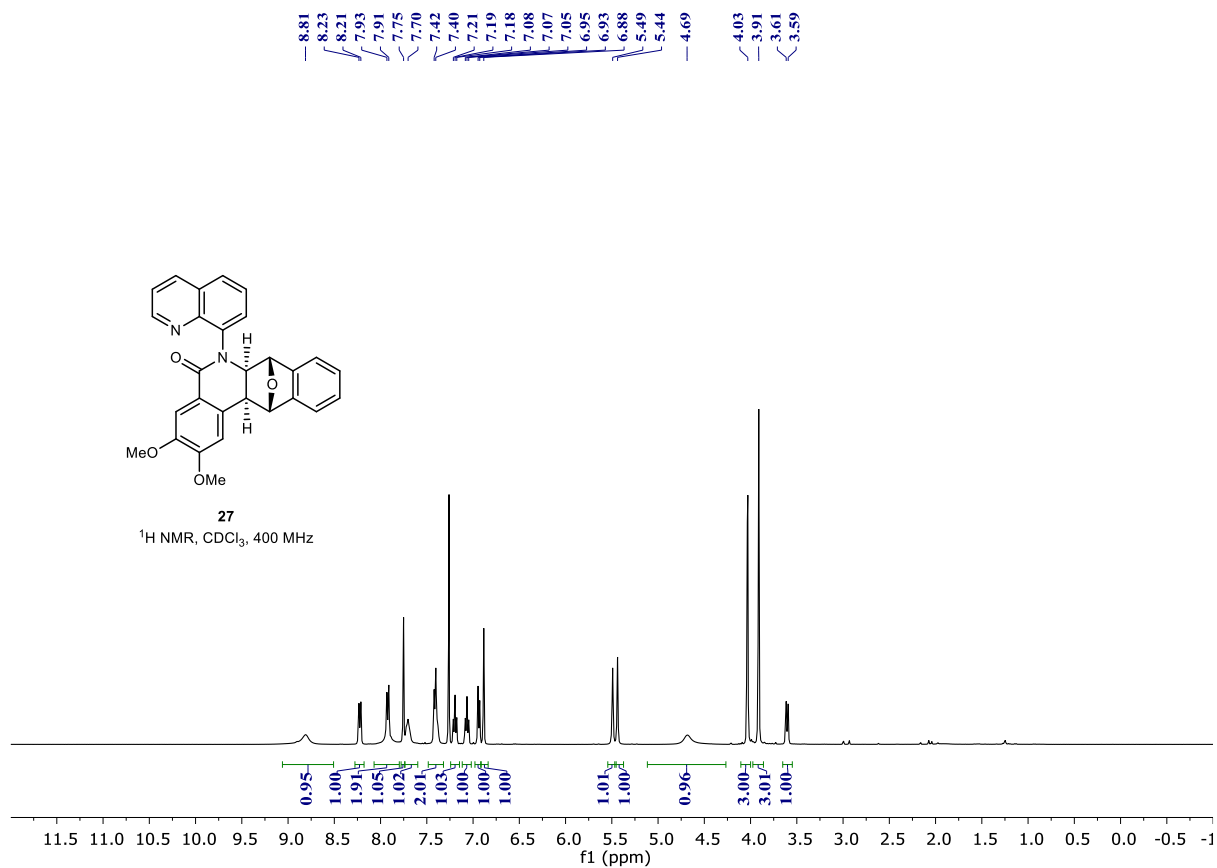


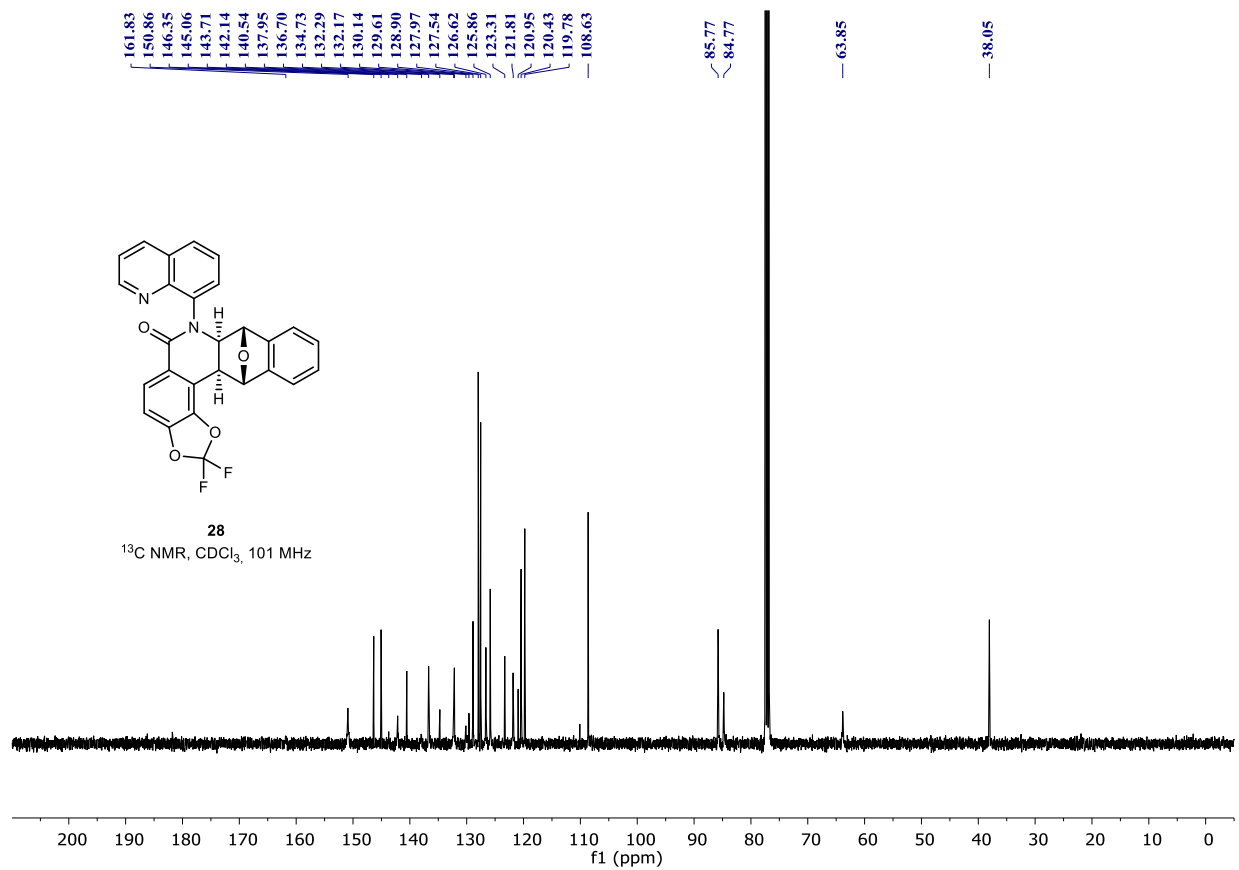
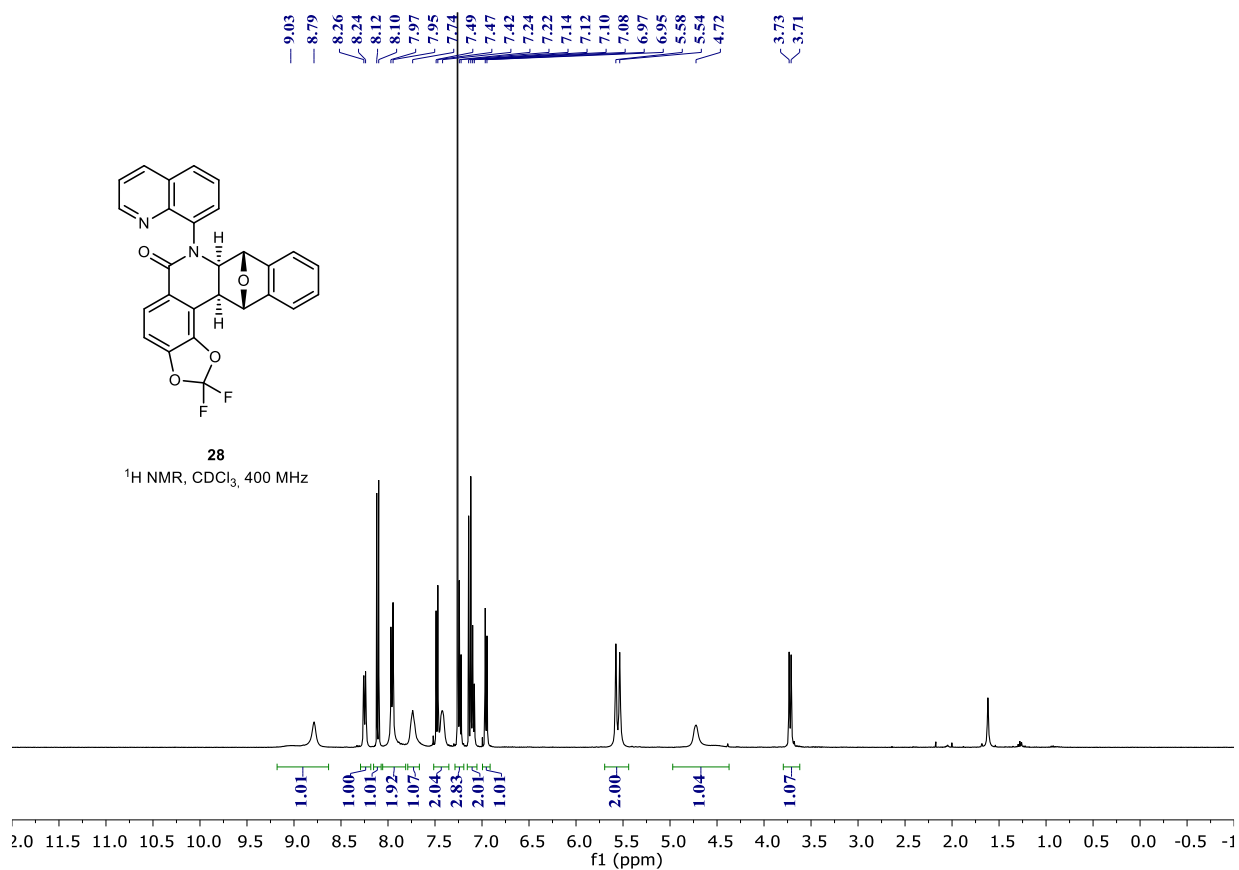


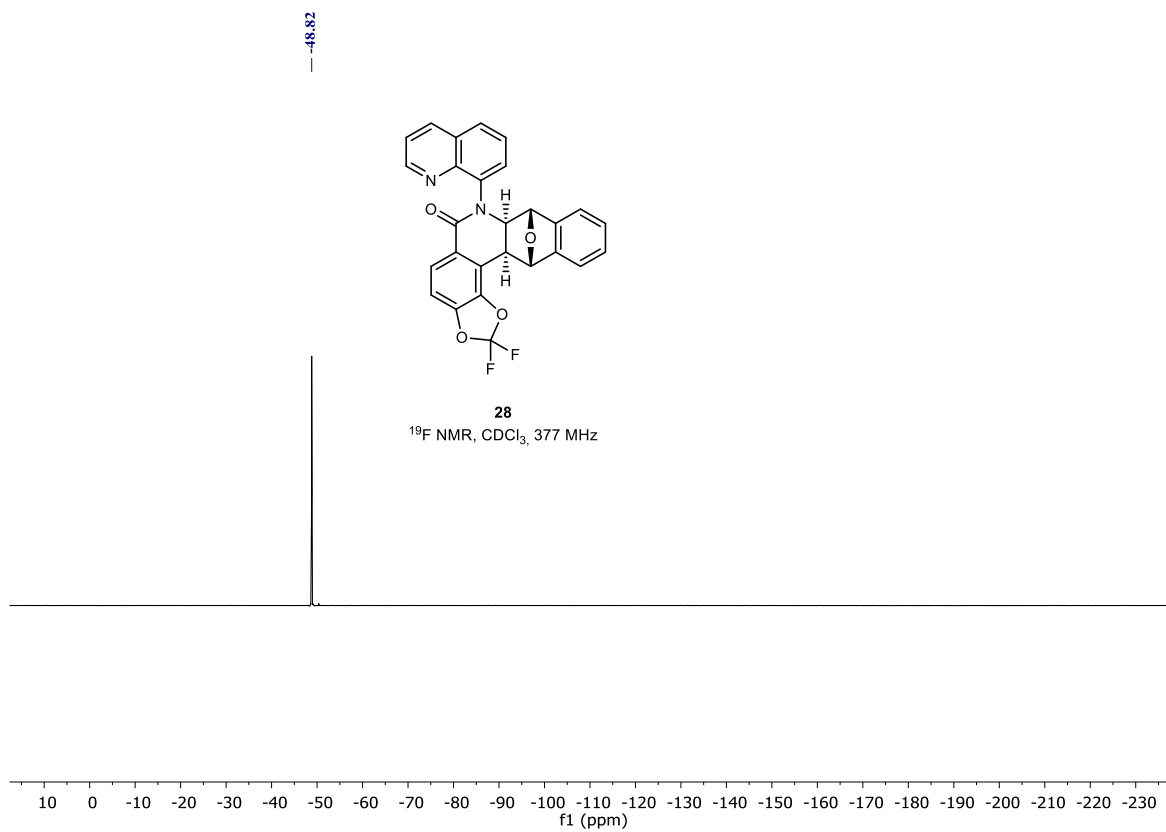


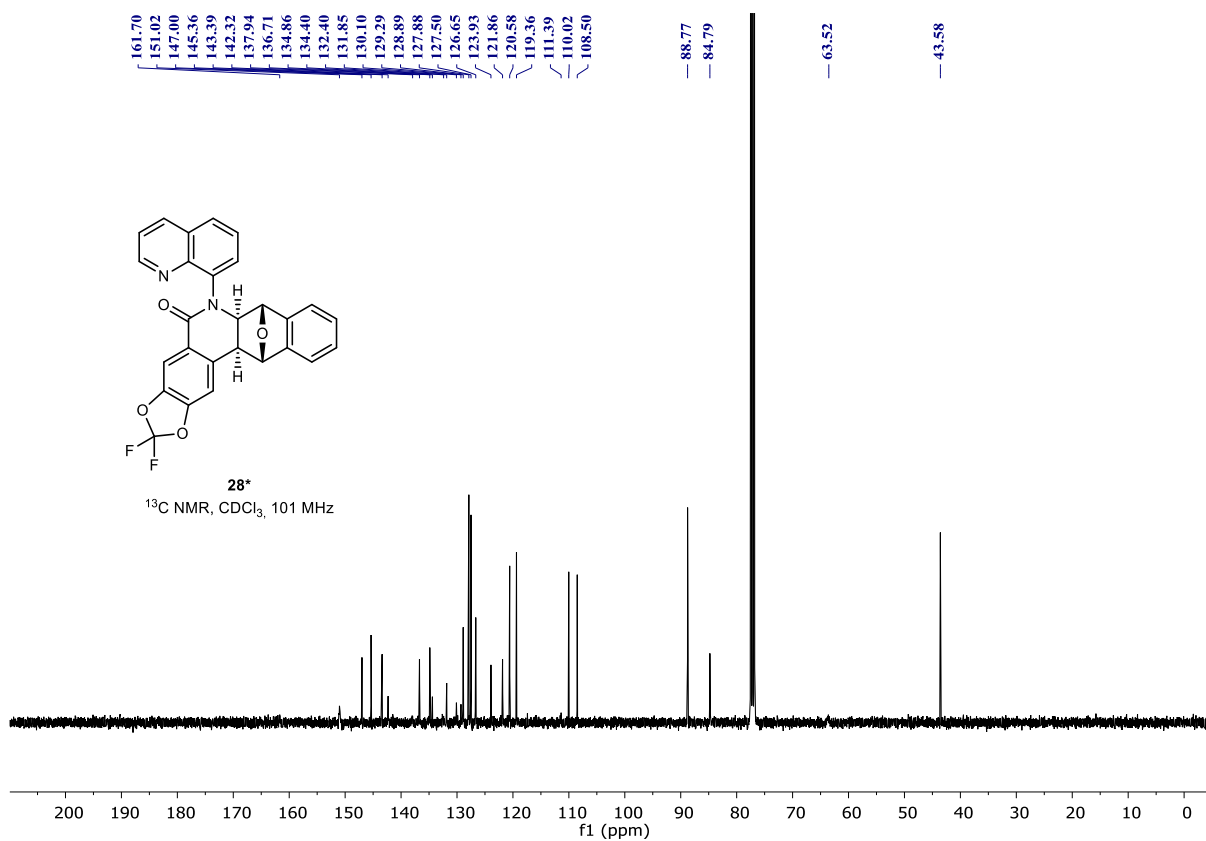
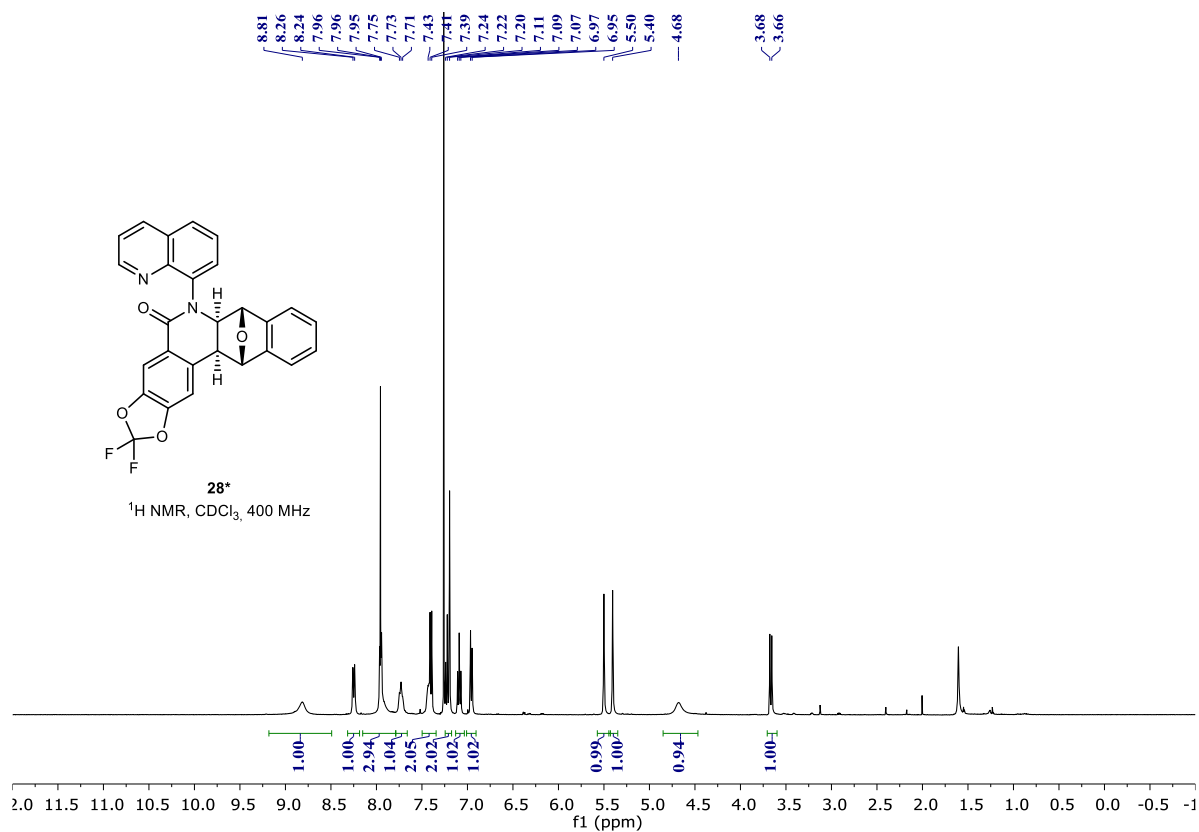


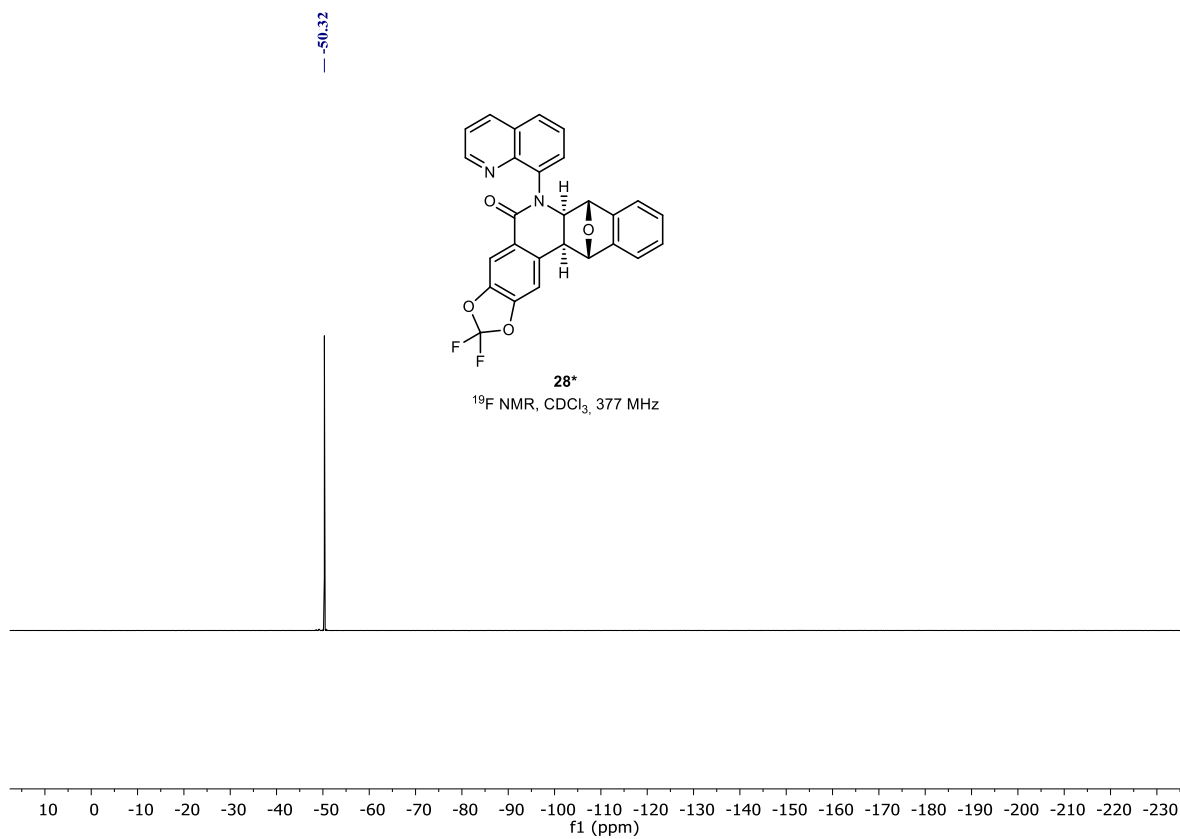


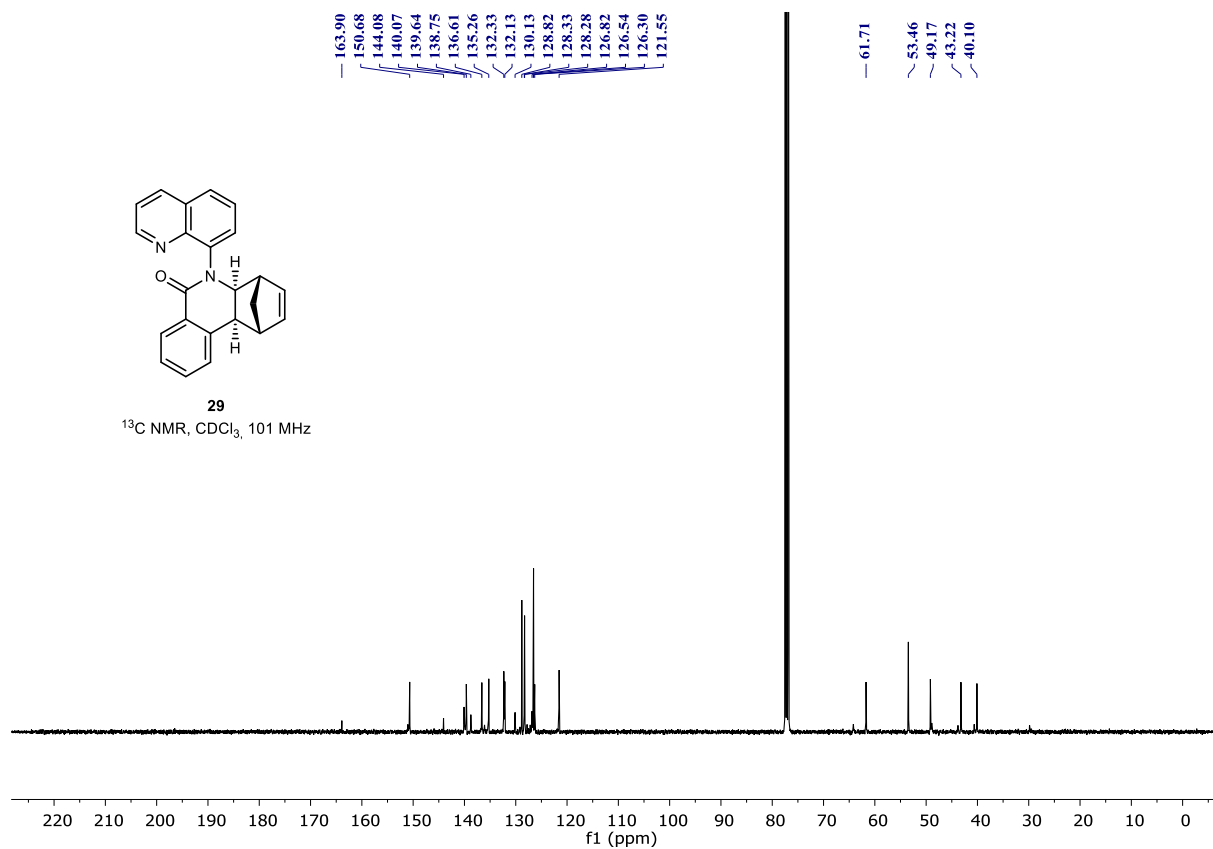
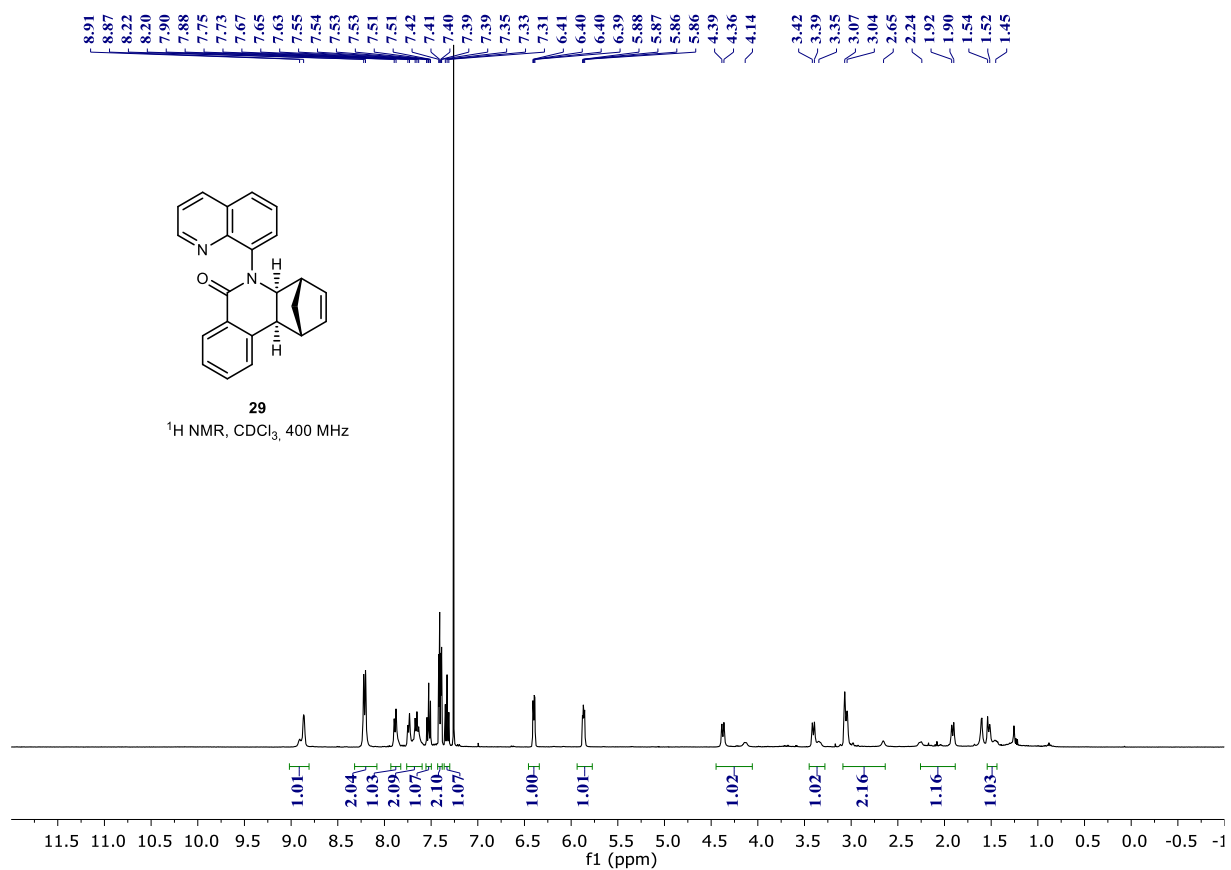


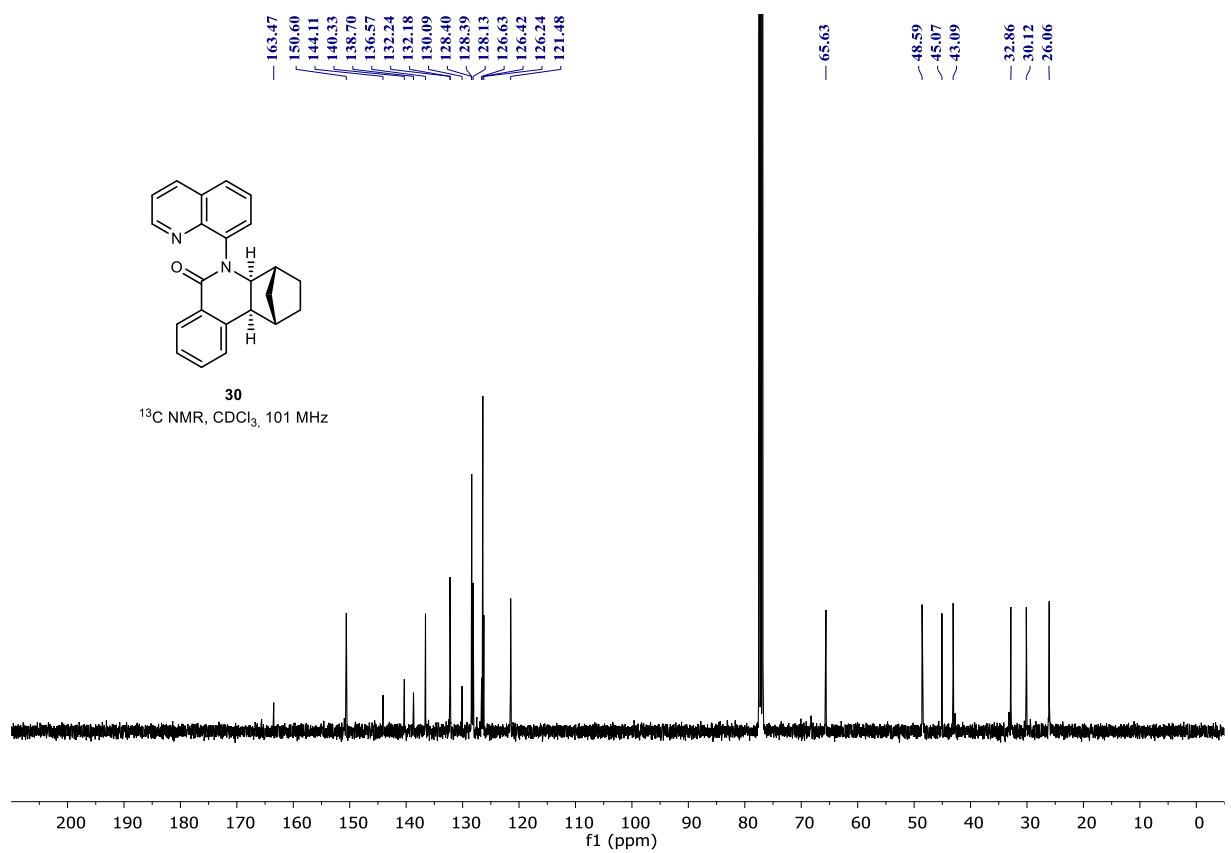
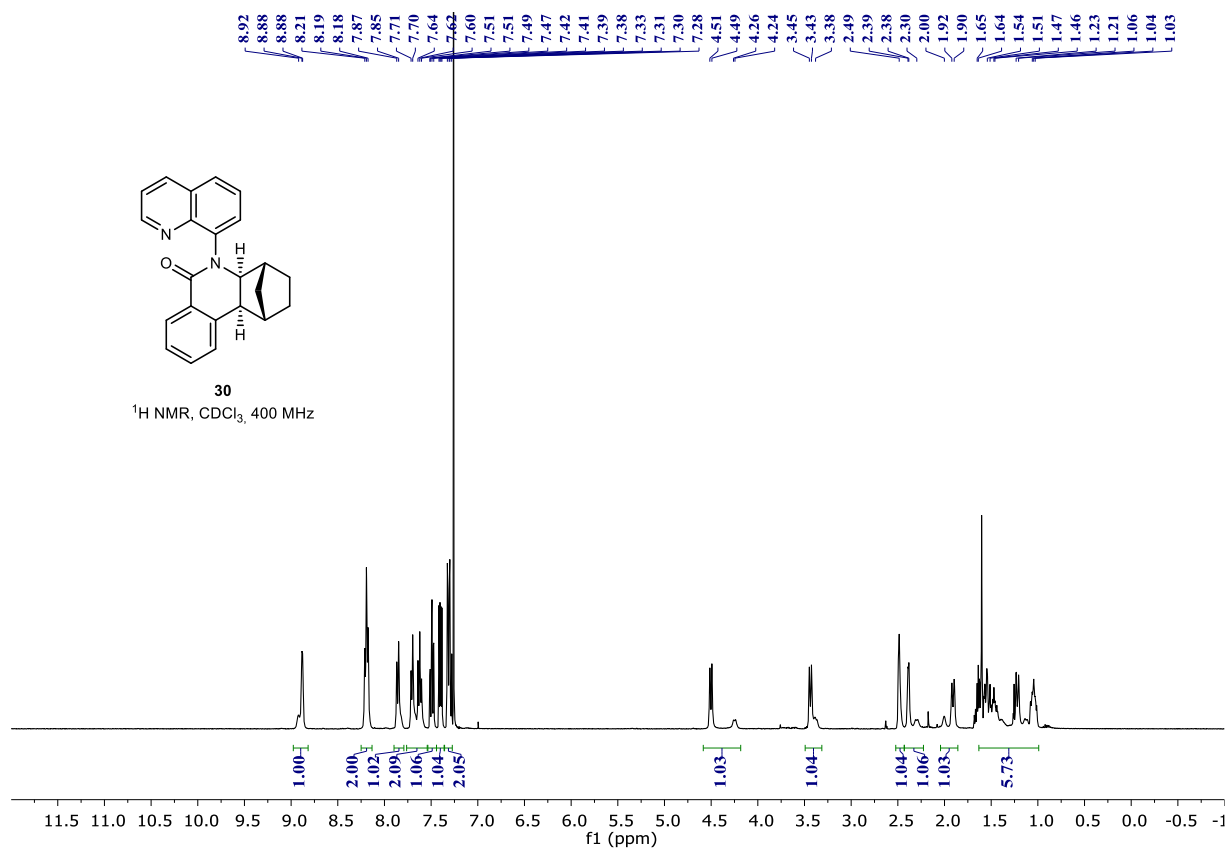


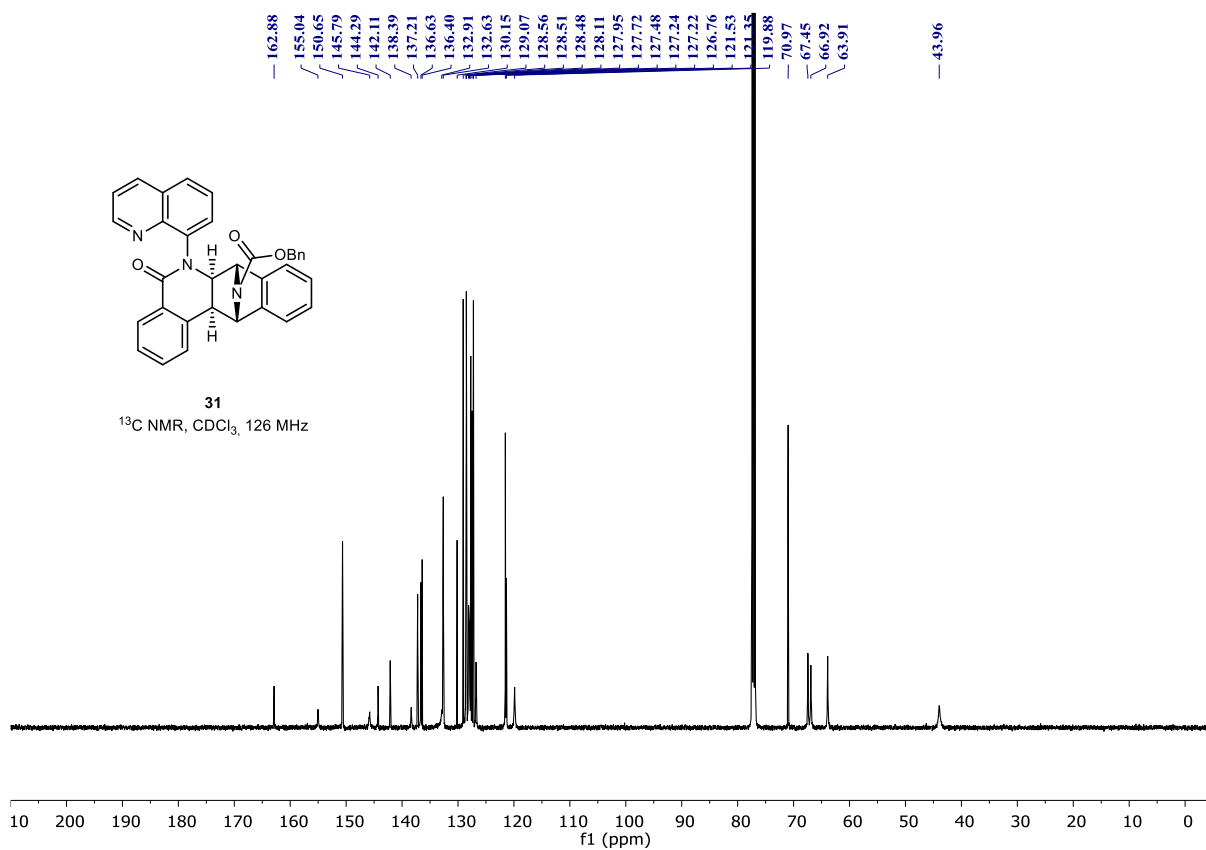
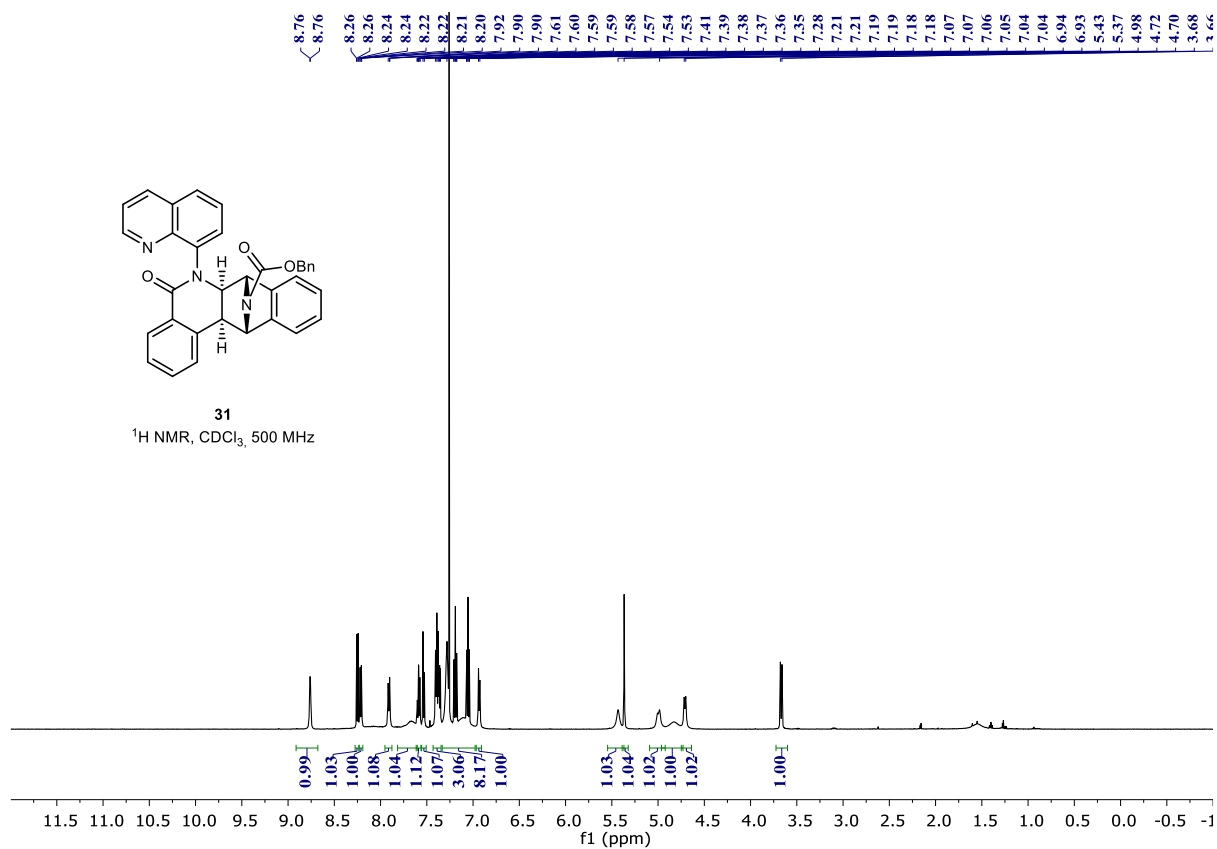


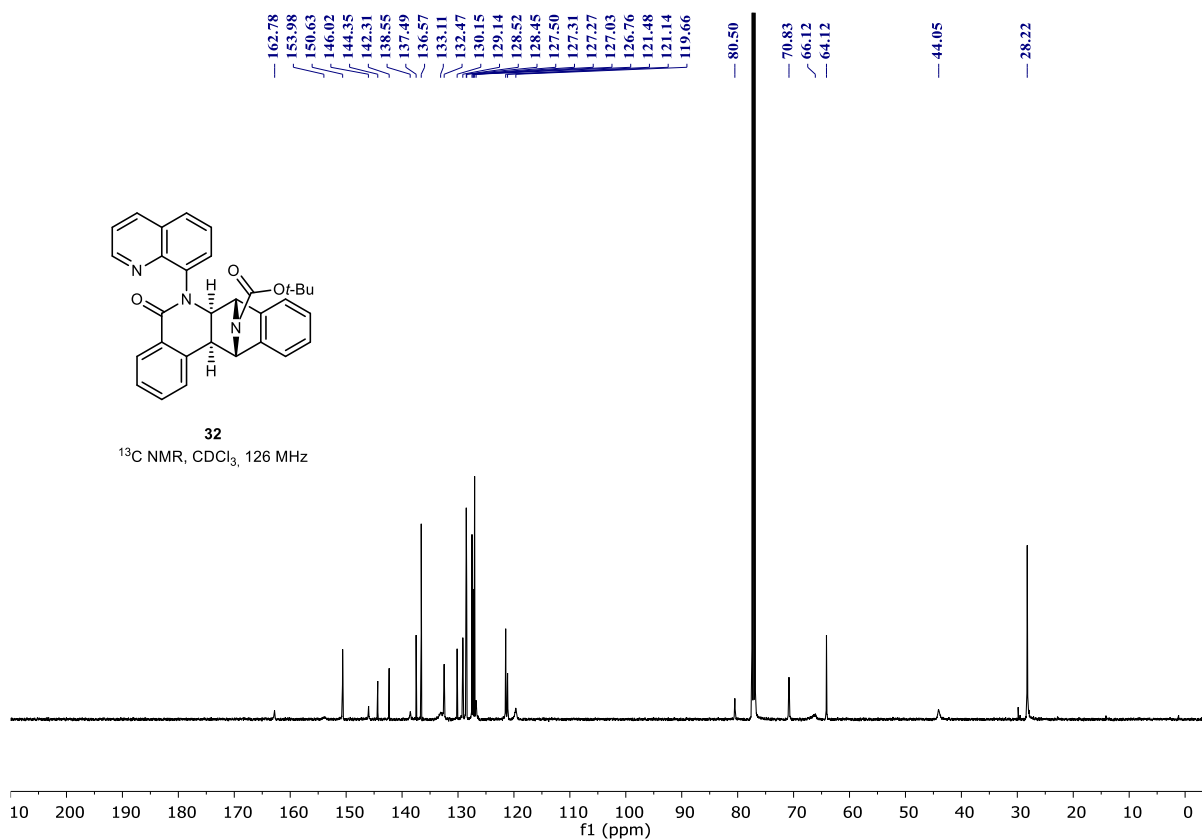
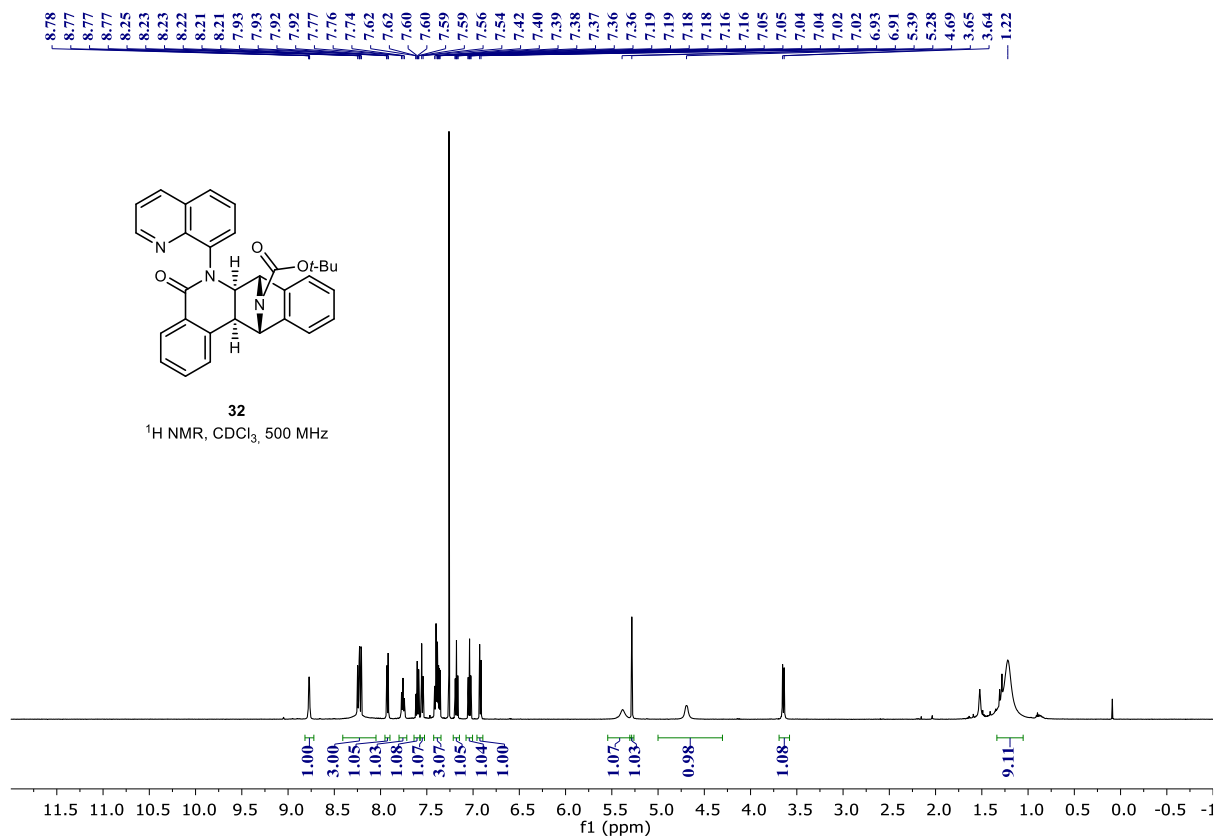


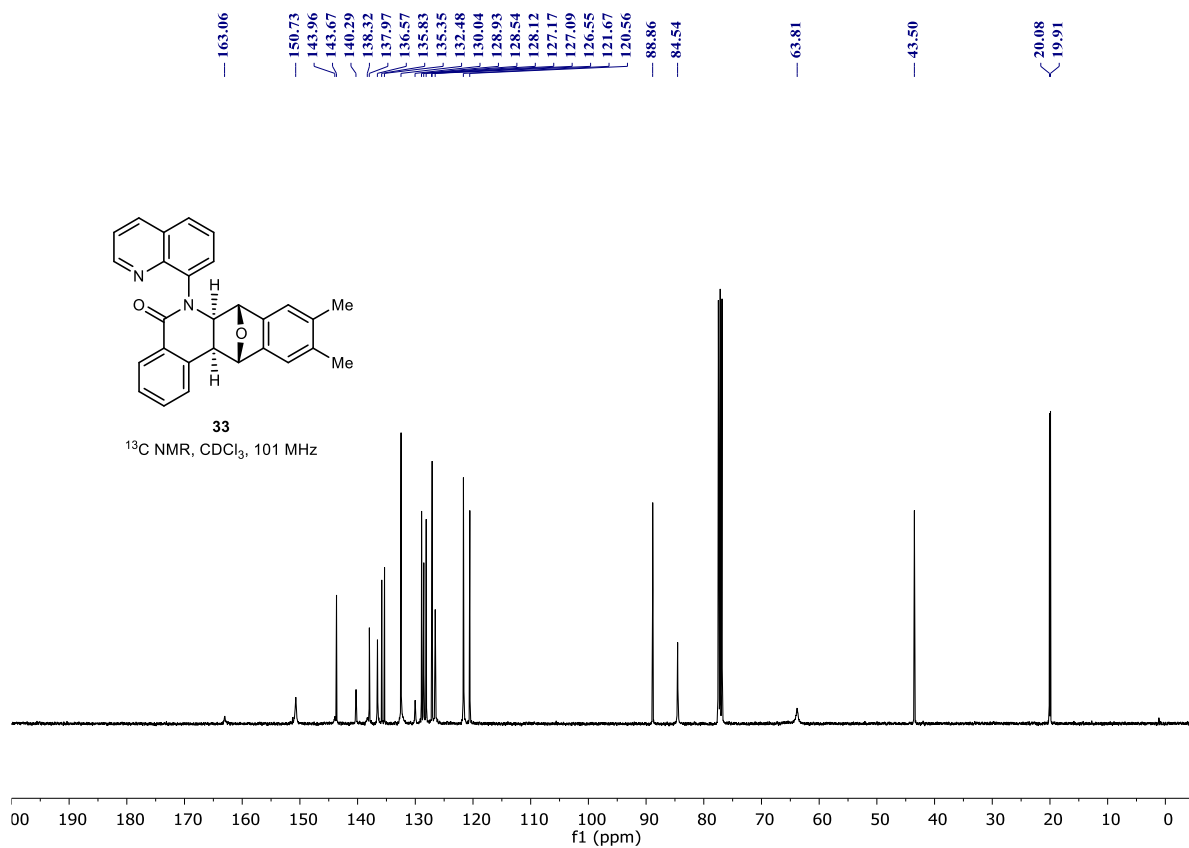
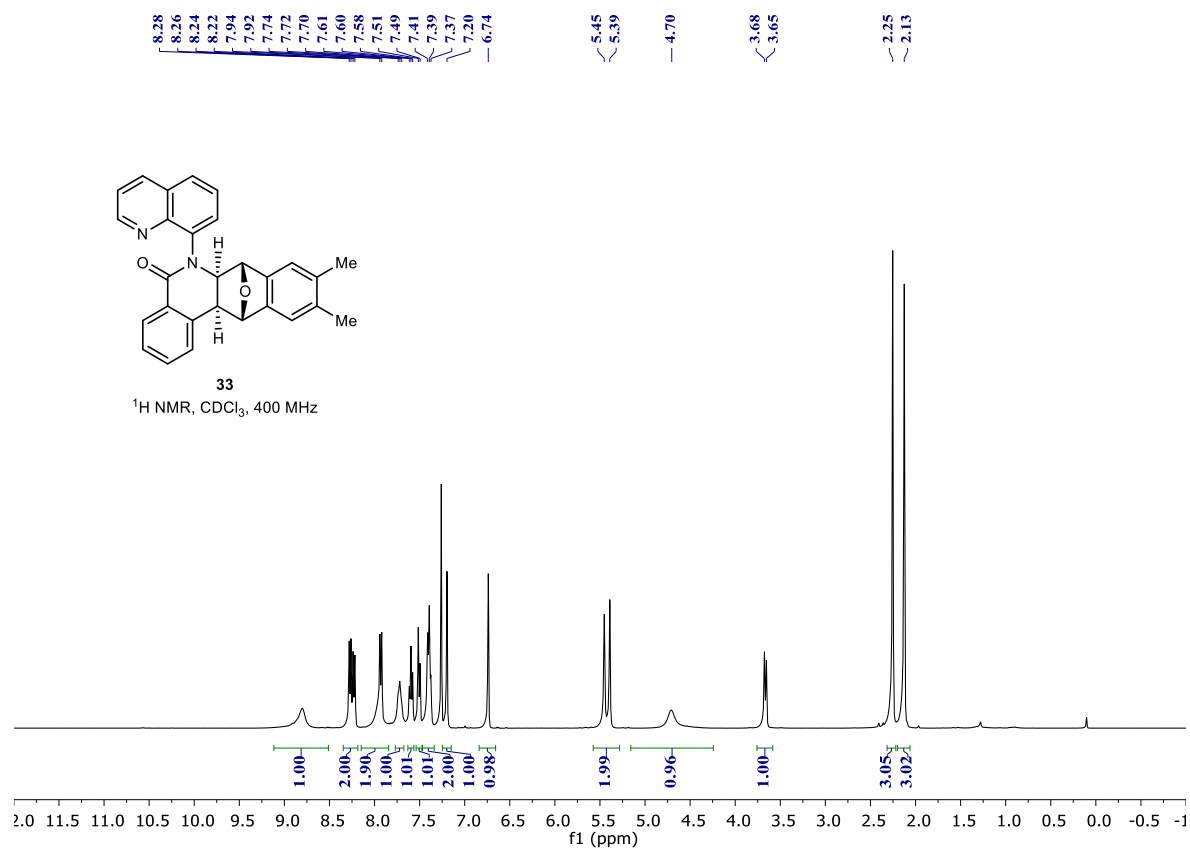


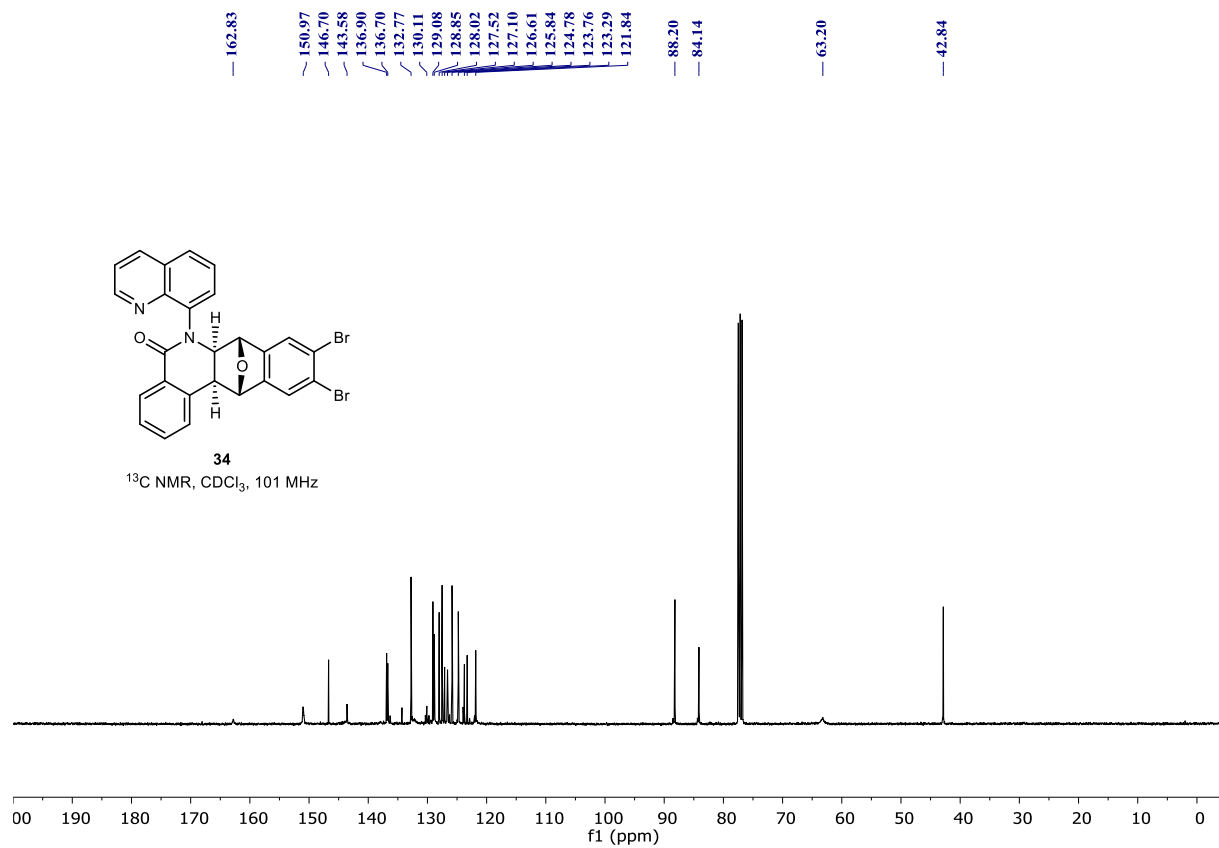
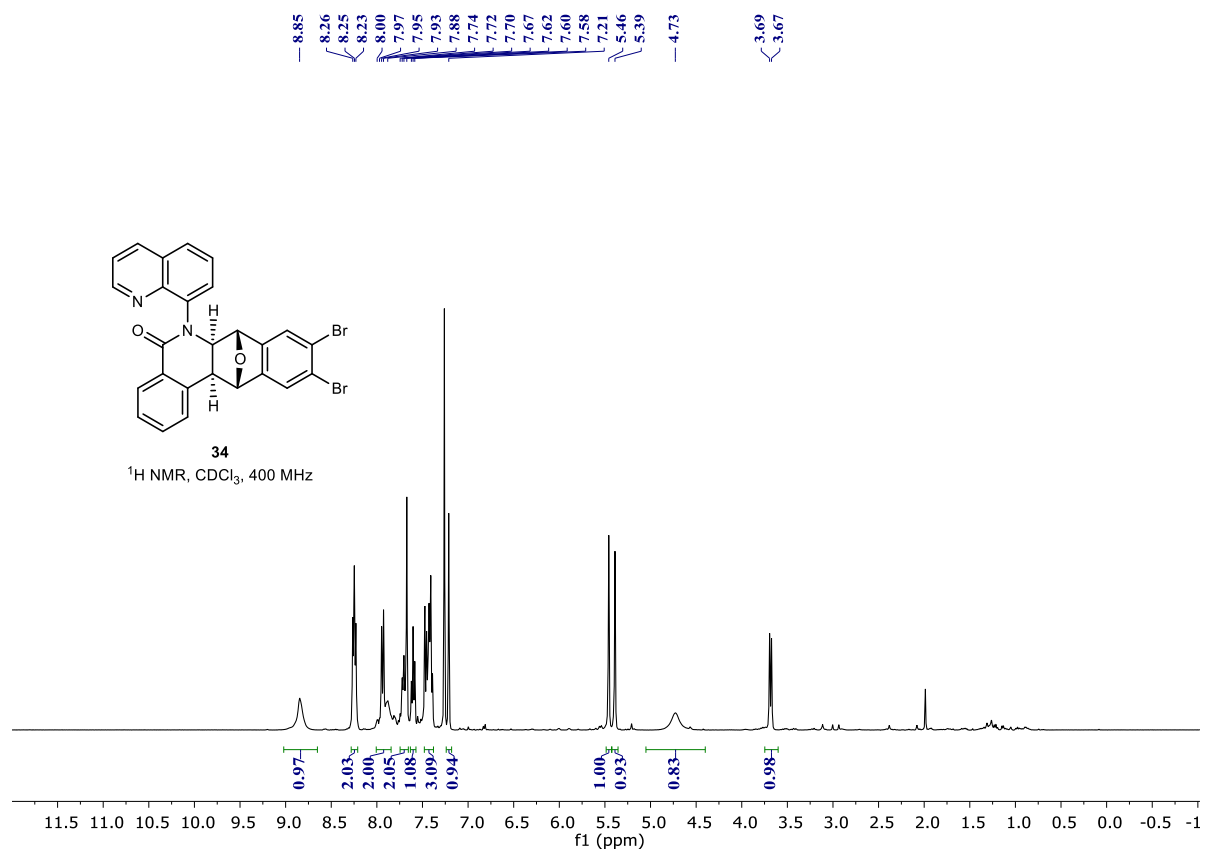


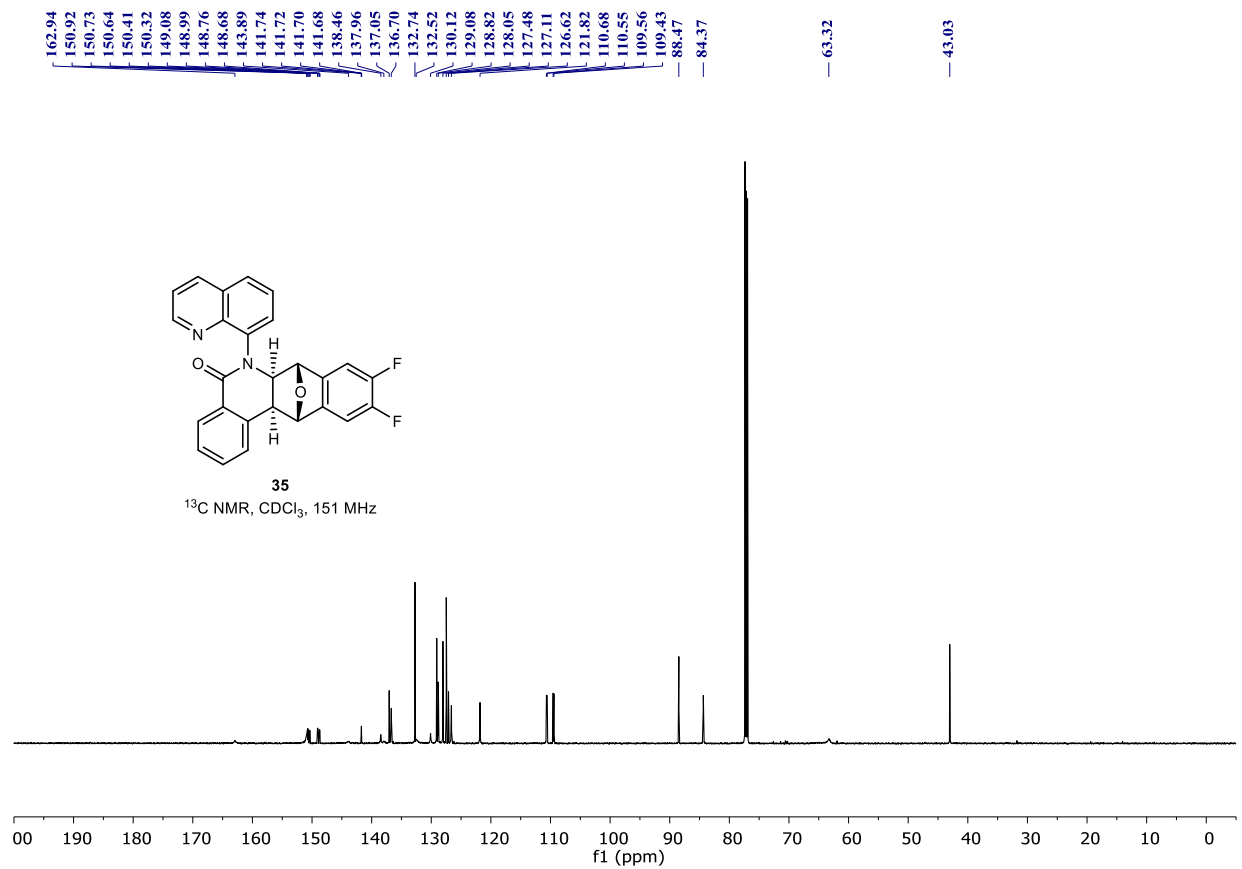
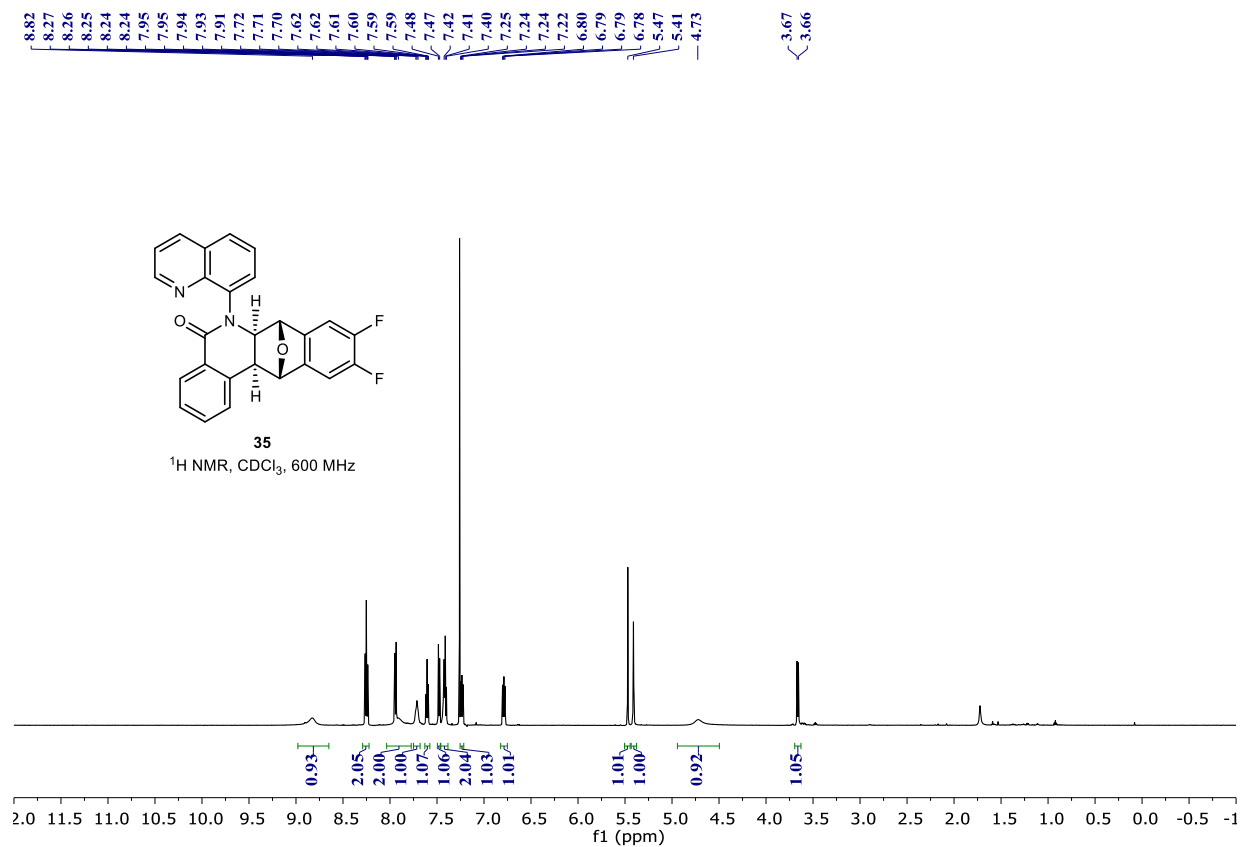


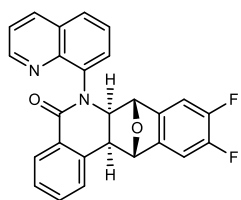




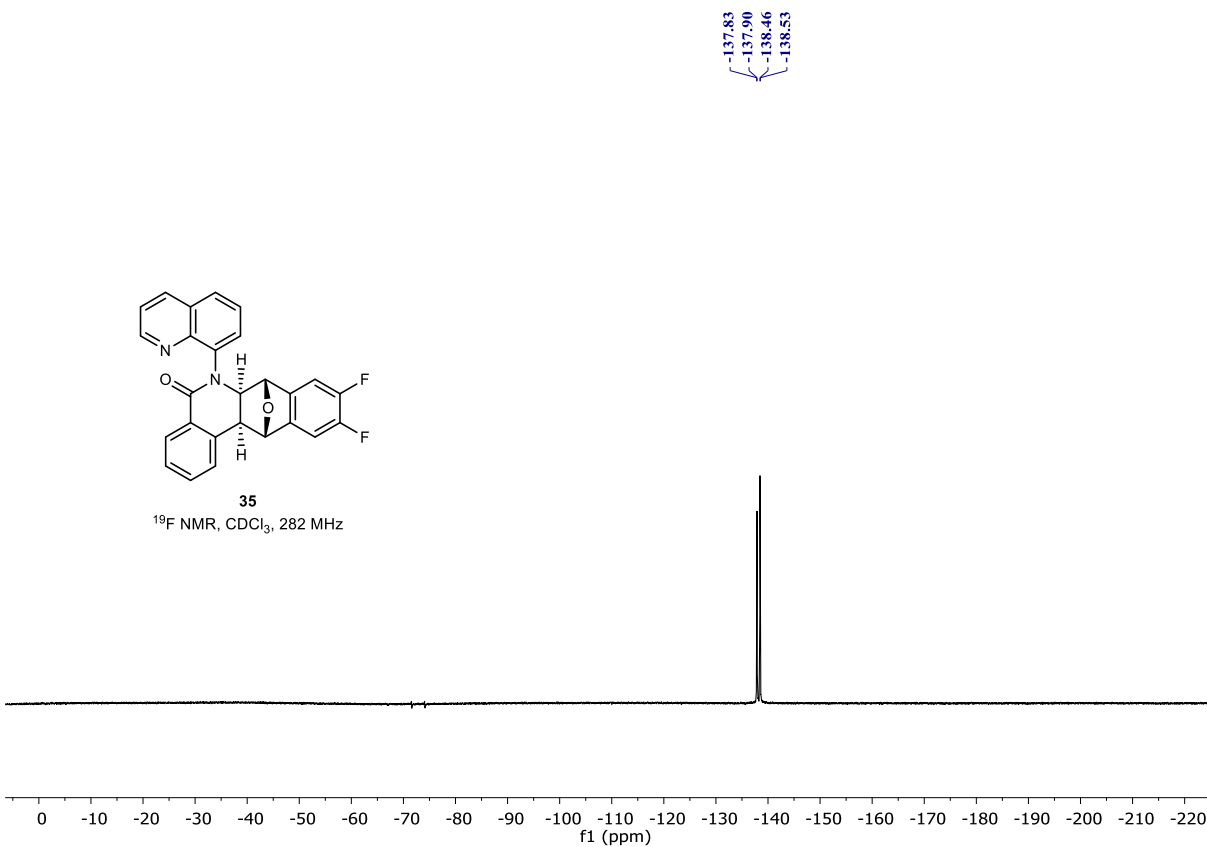


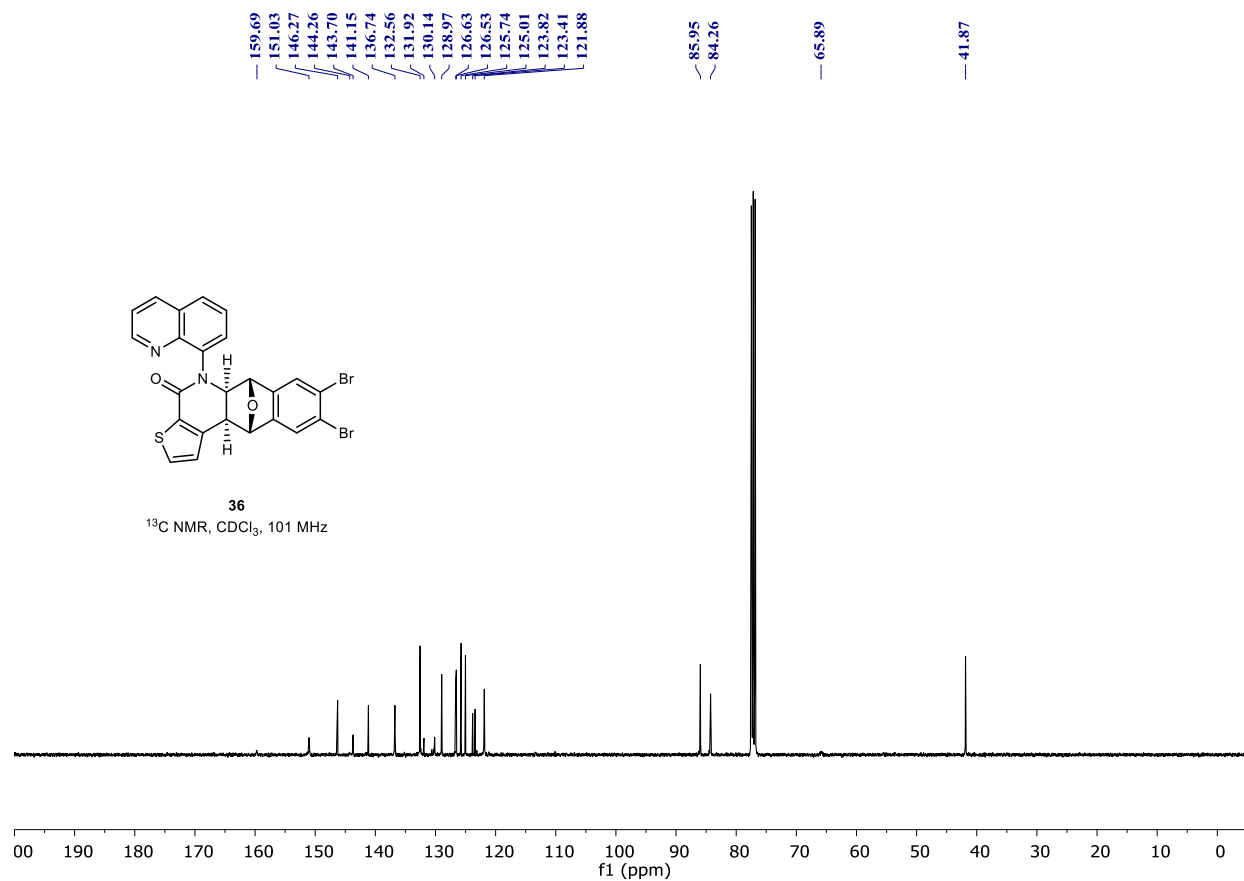
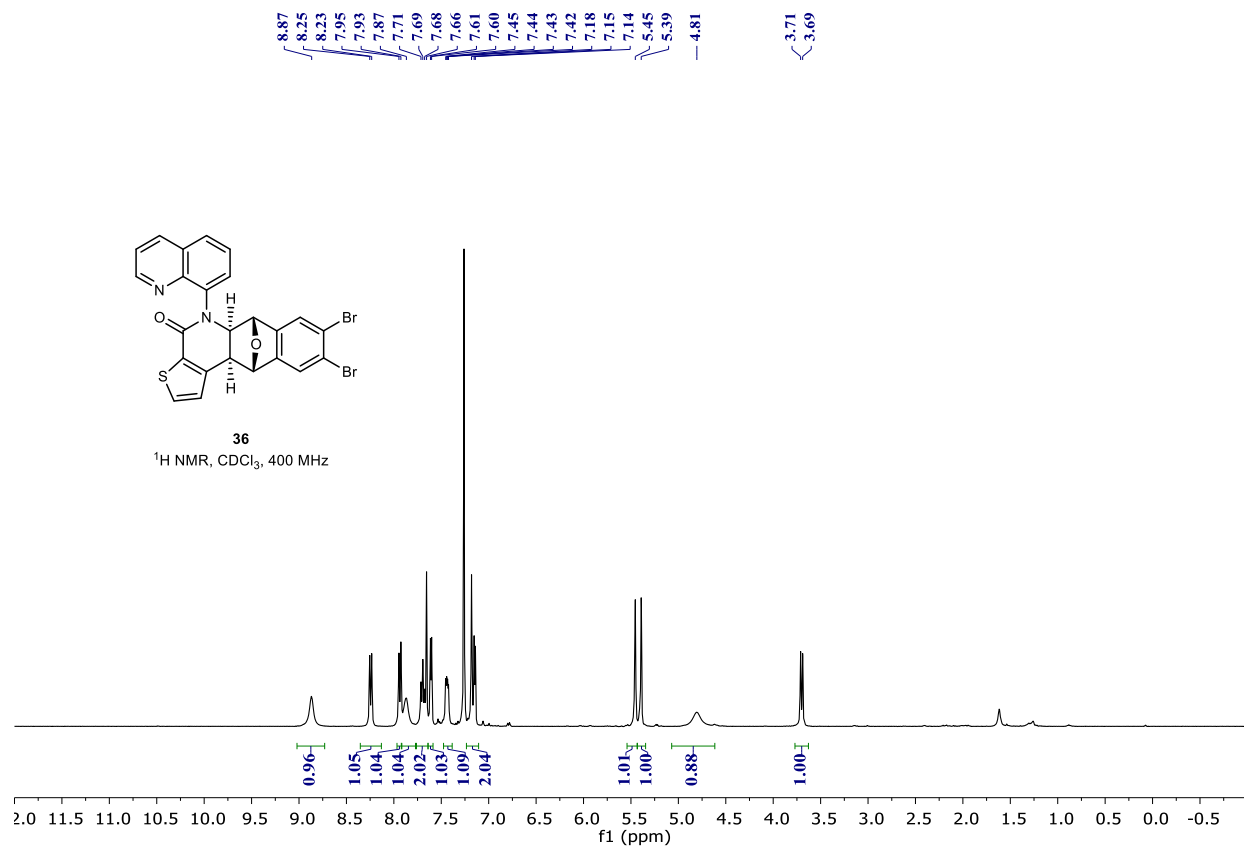


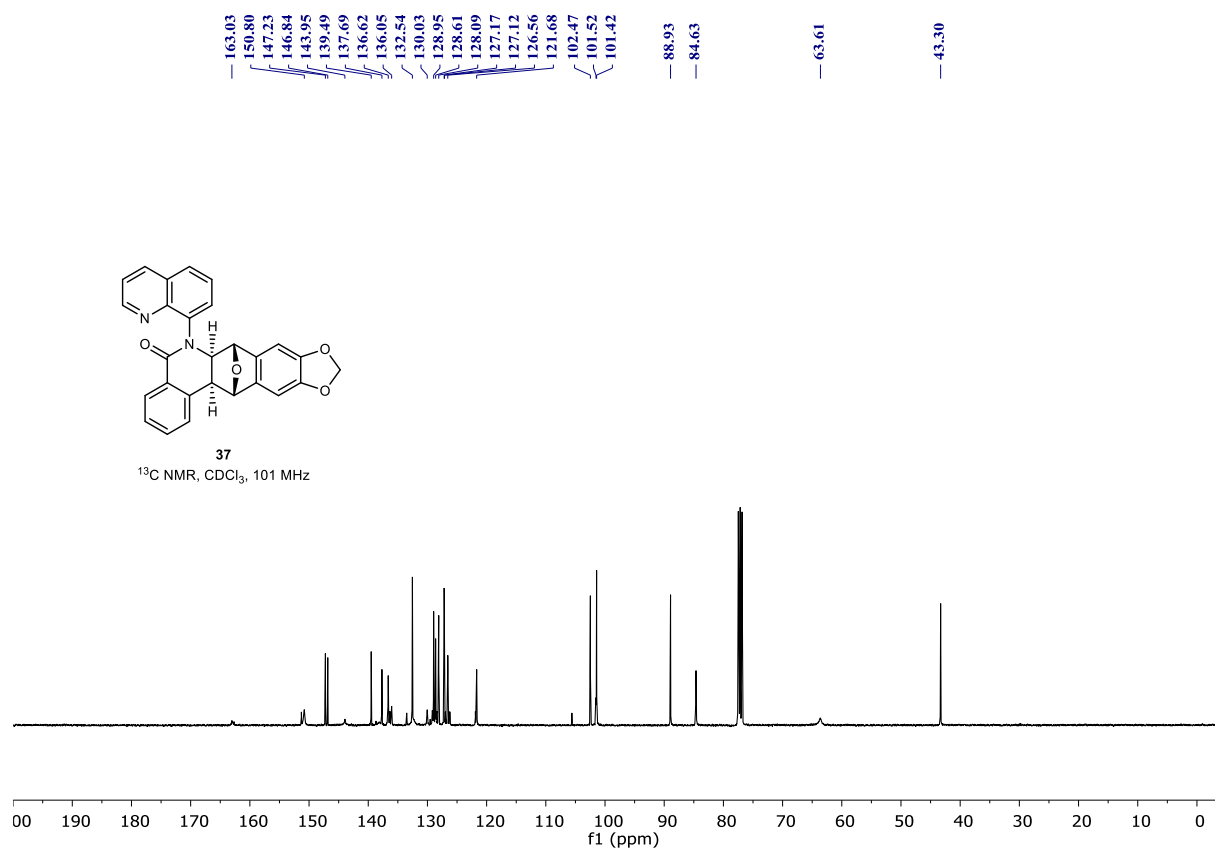
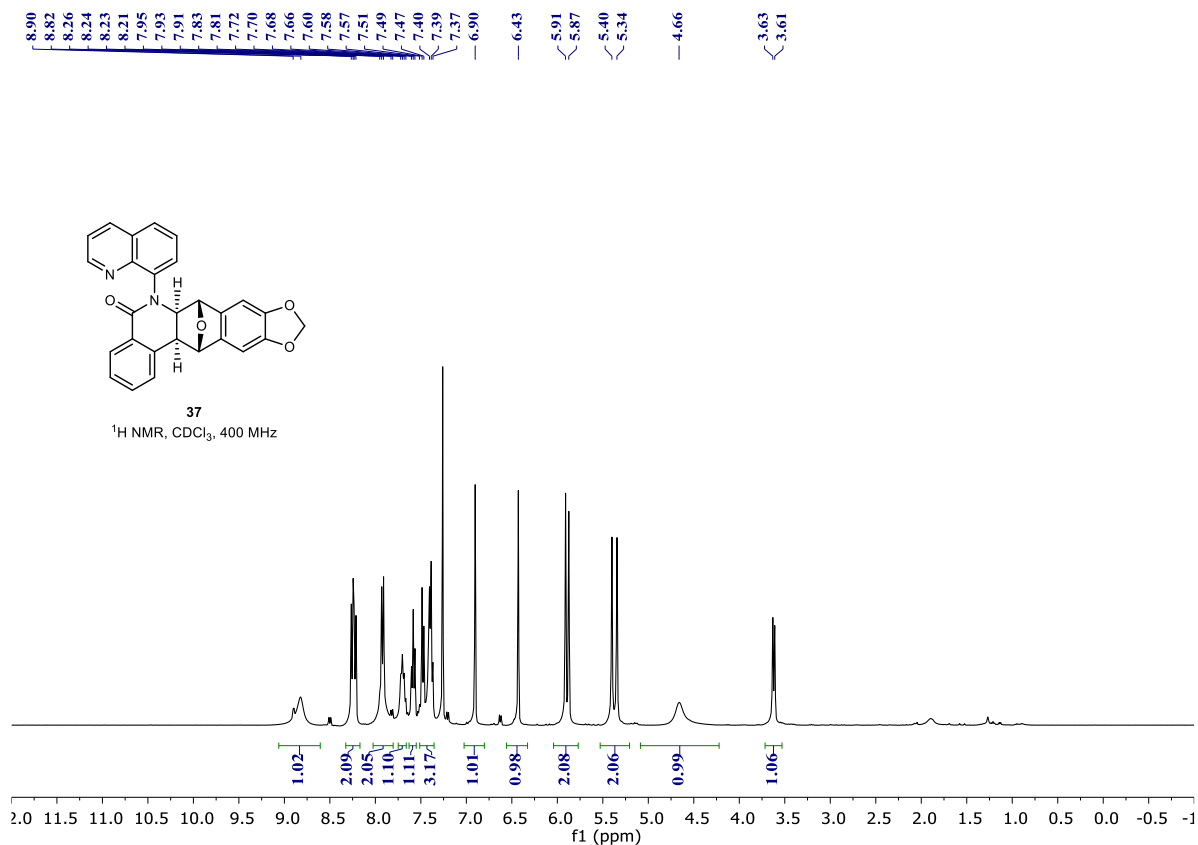


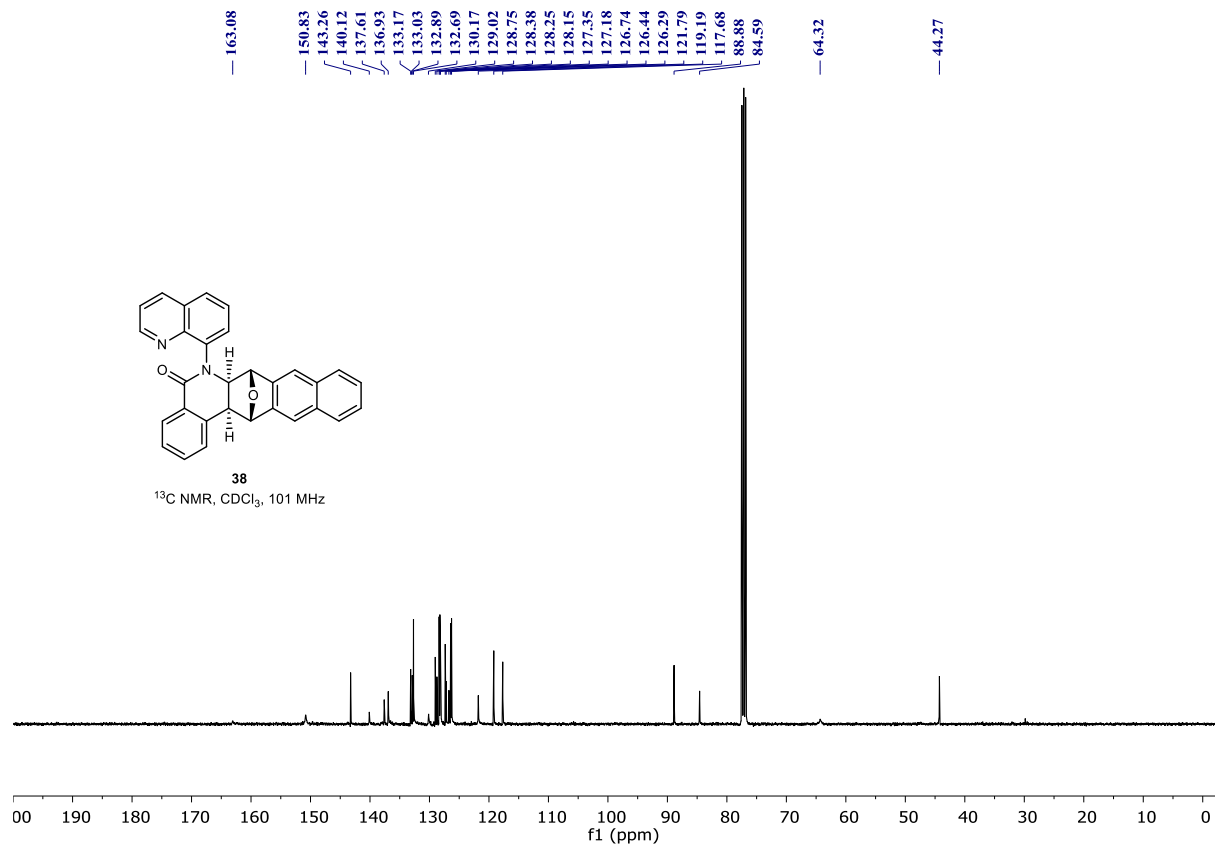
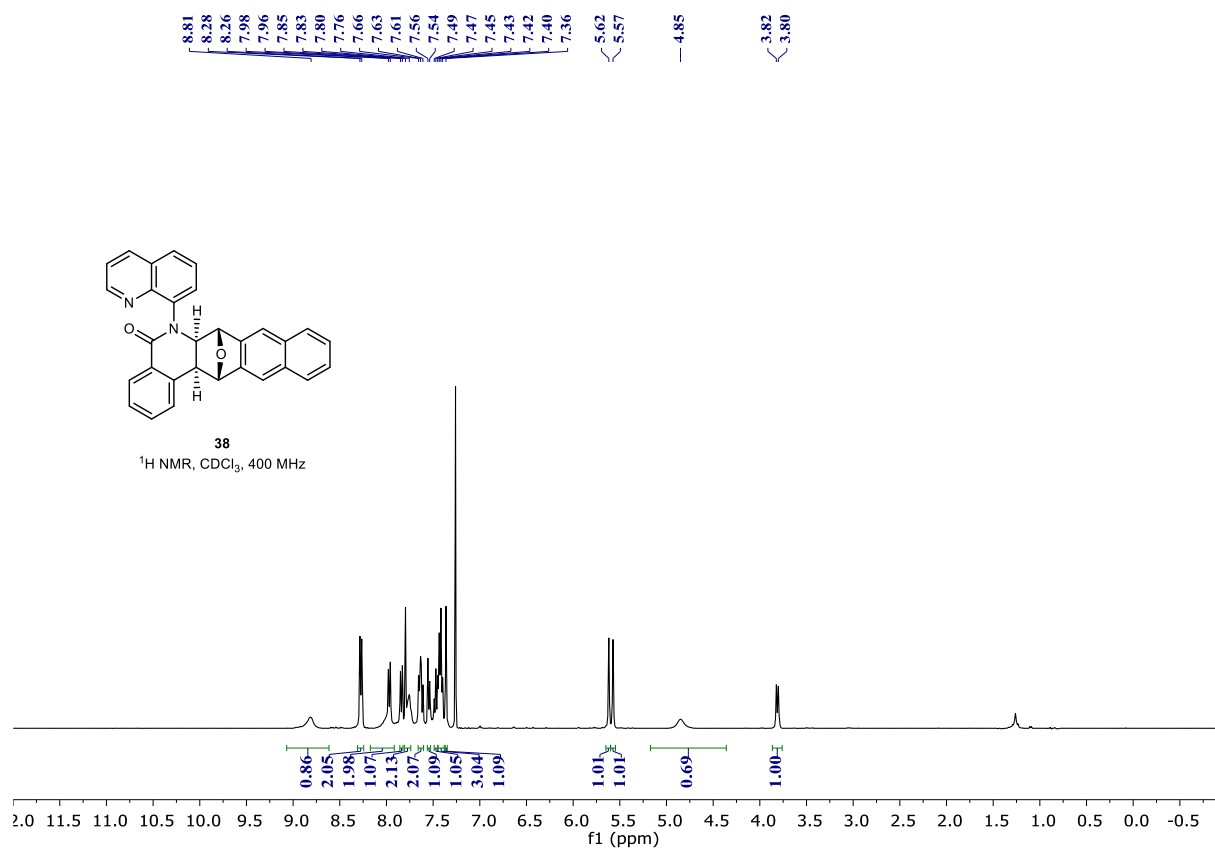


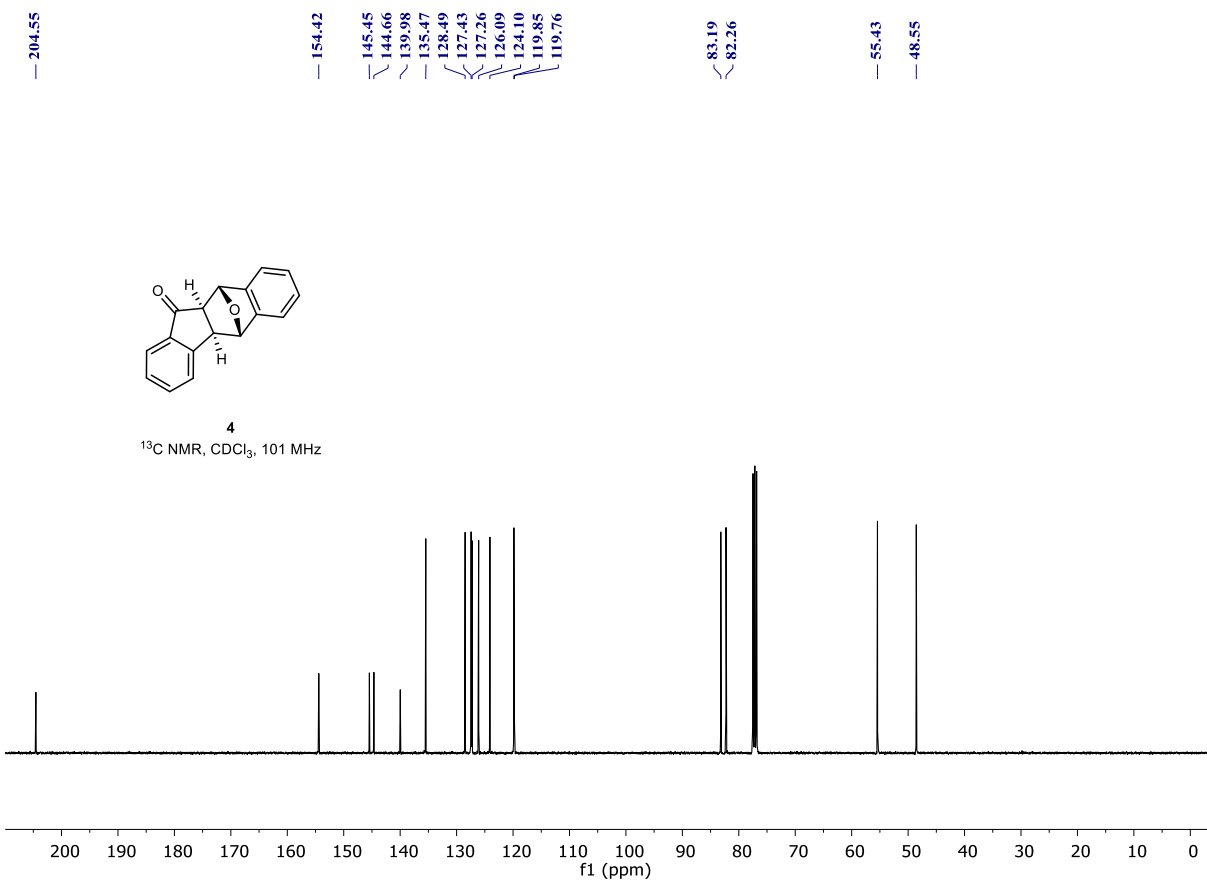
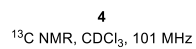
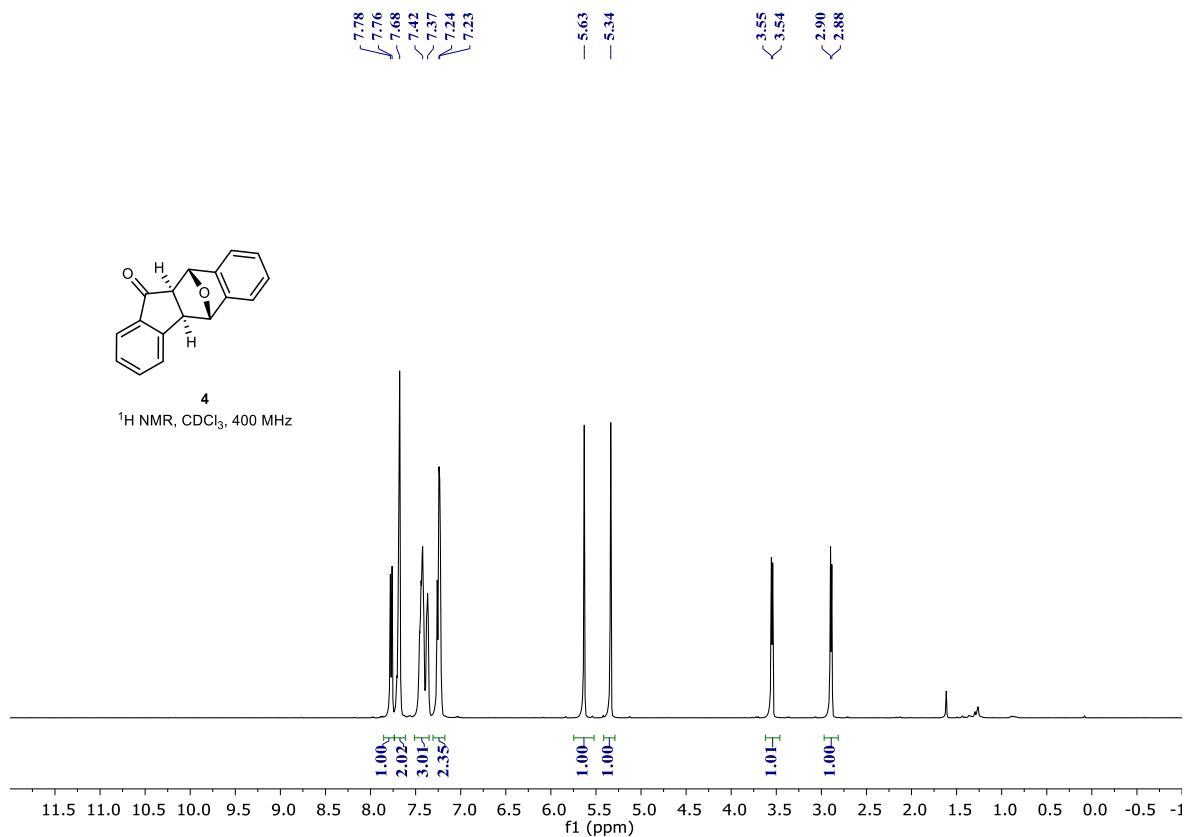
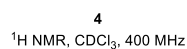
35
¹⁹F NMR, CDCl₃, 282 MHz

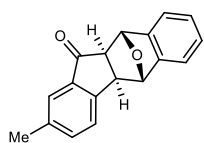






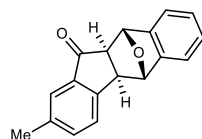
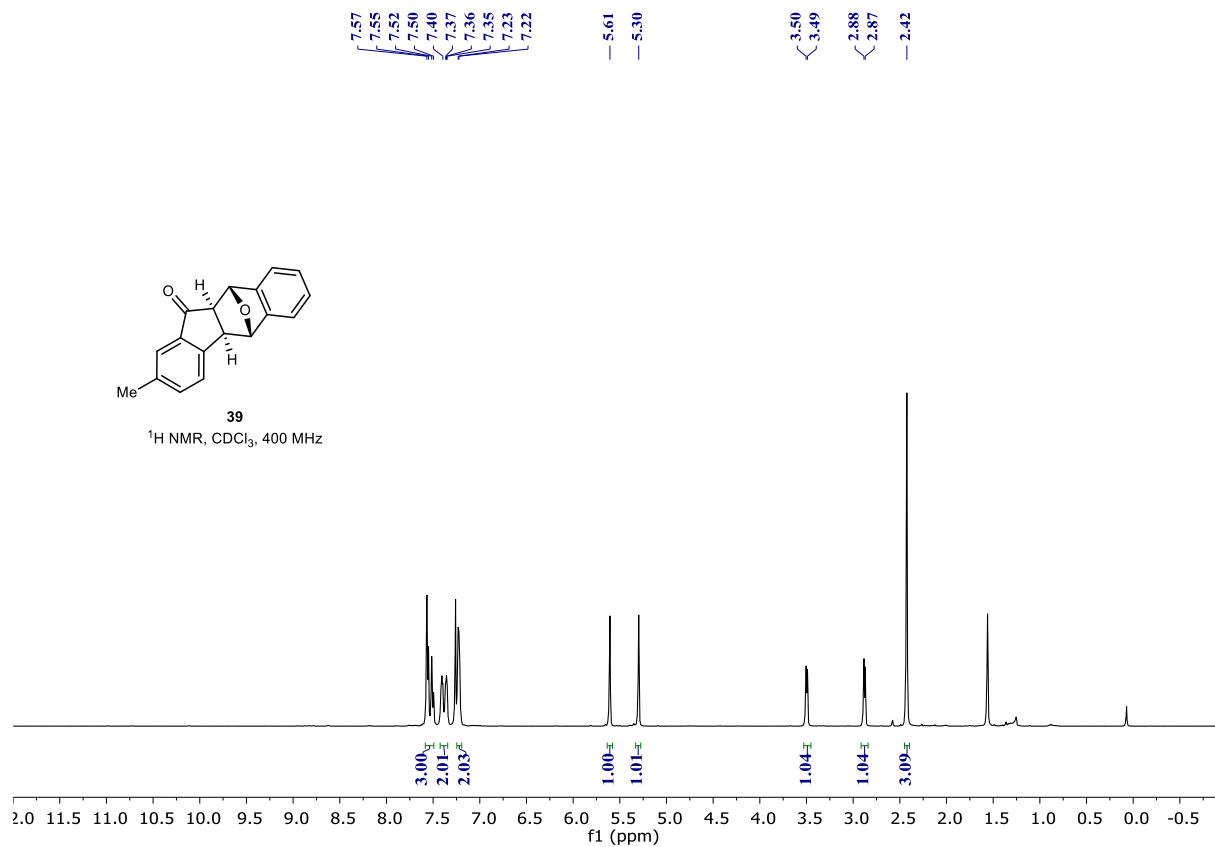






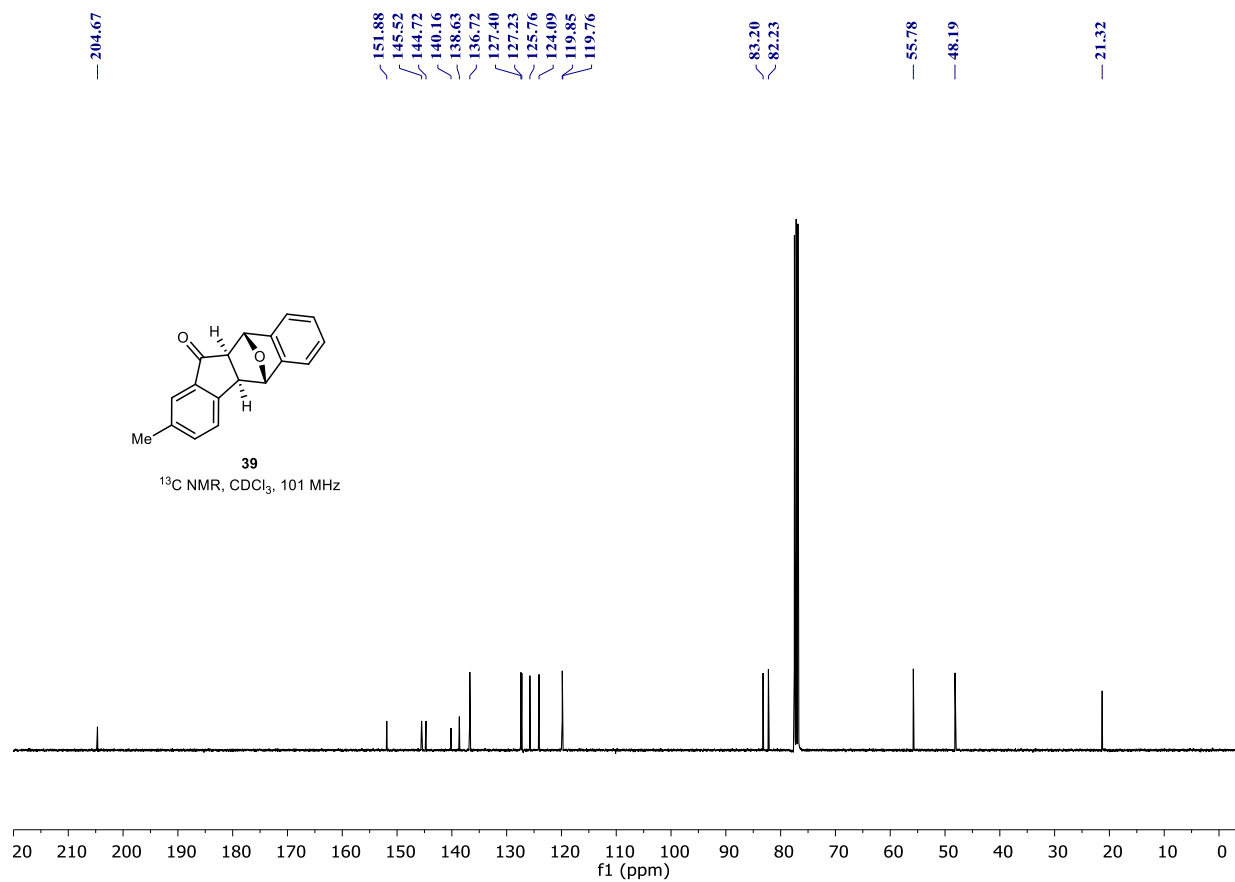
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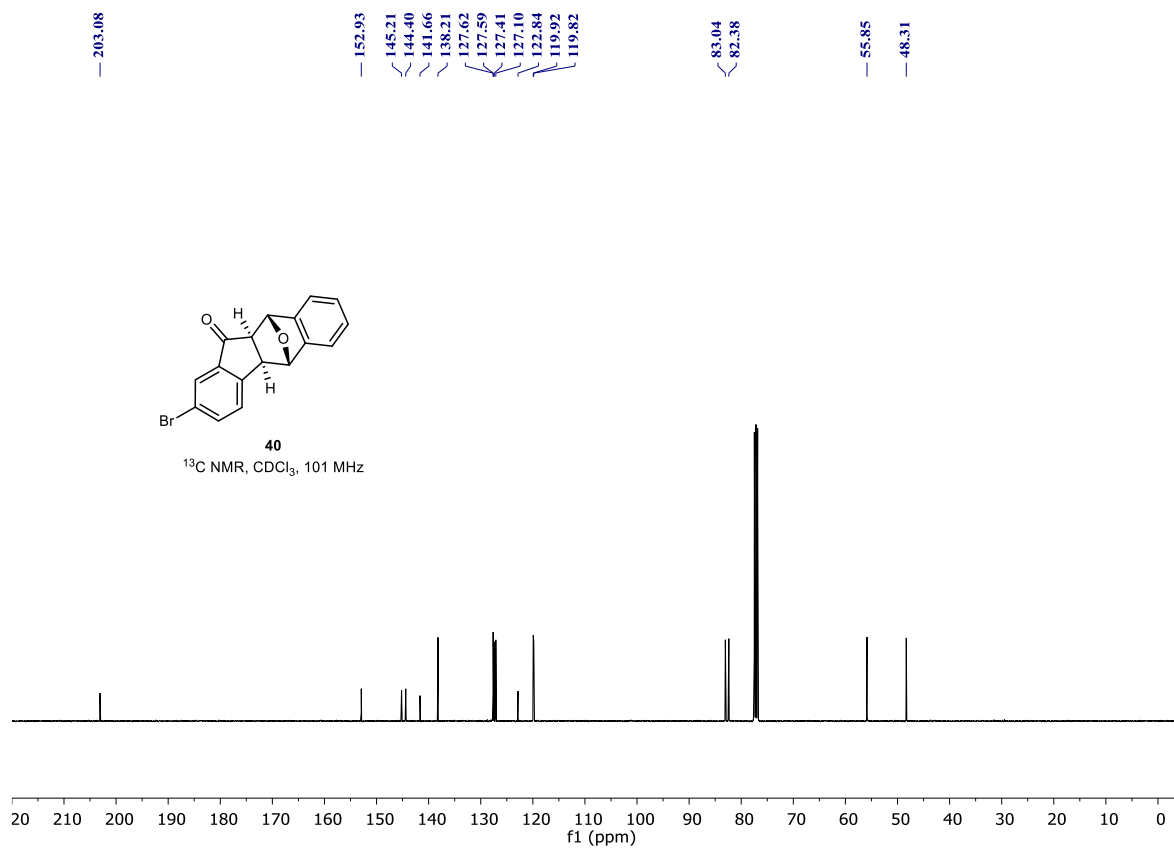
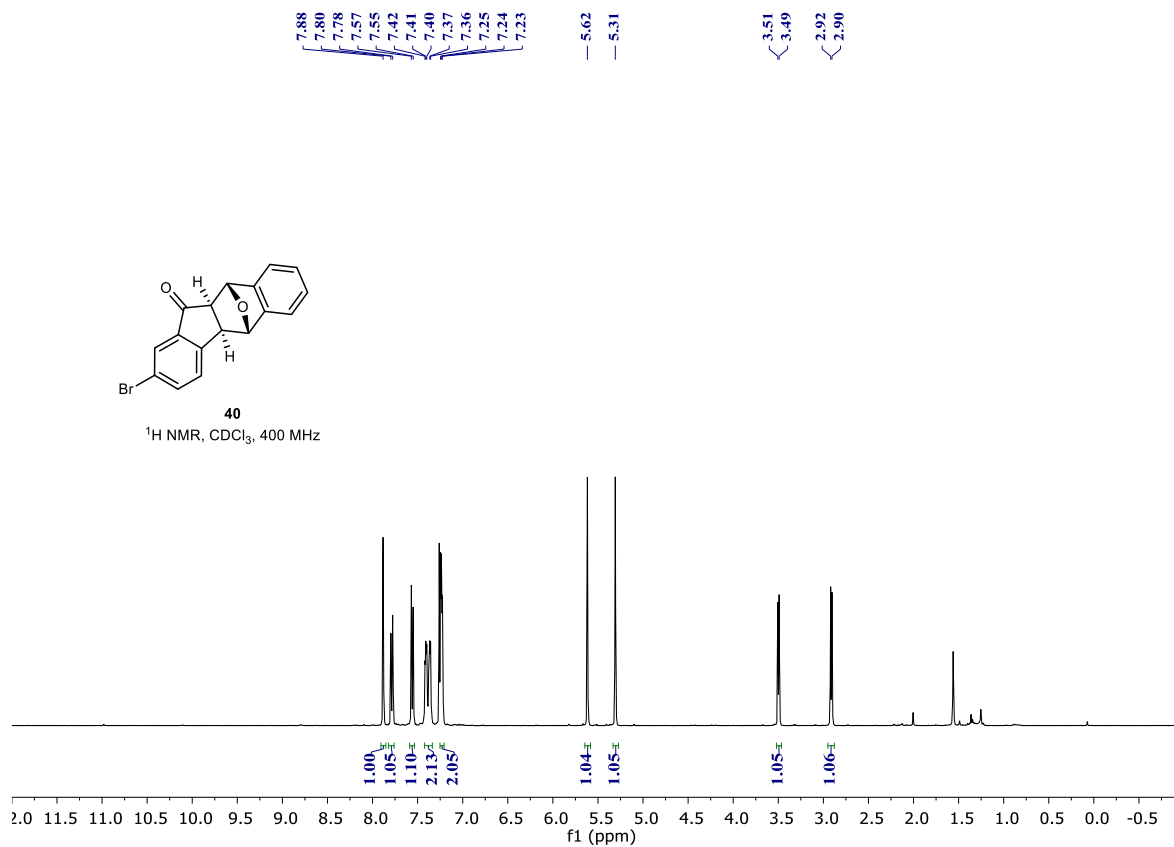
^1H NMR, CDCl_3 , 400 MHz

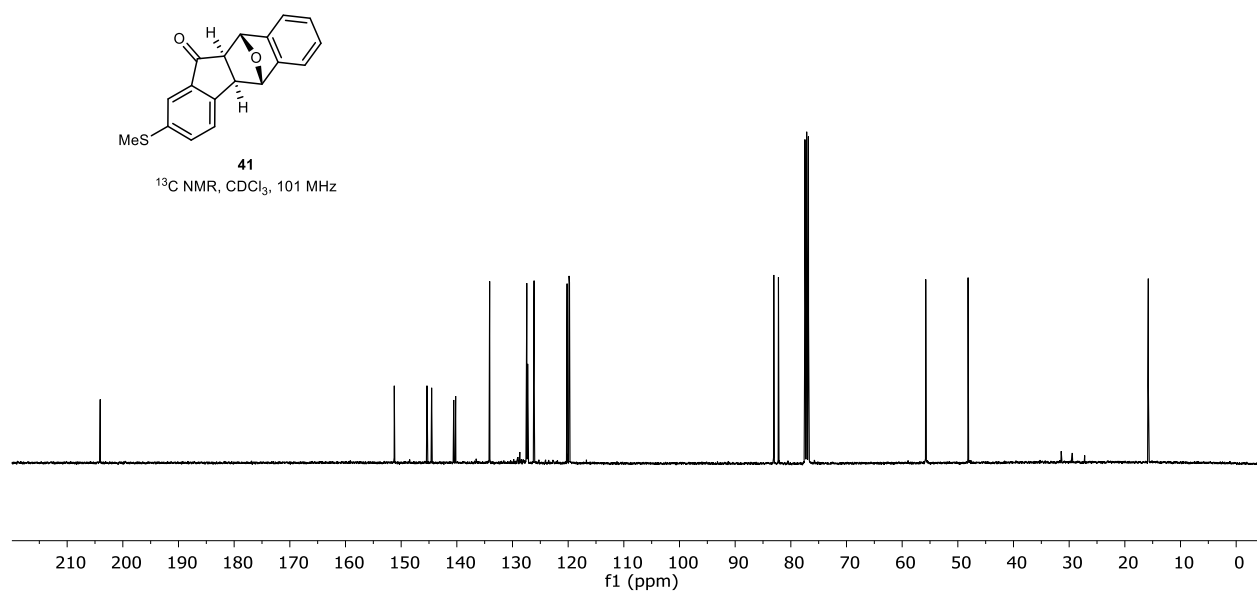
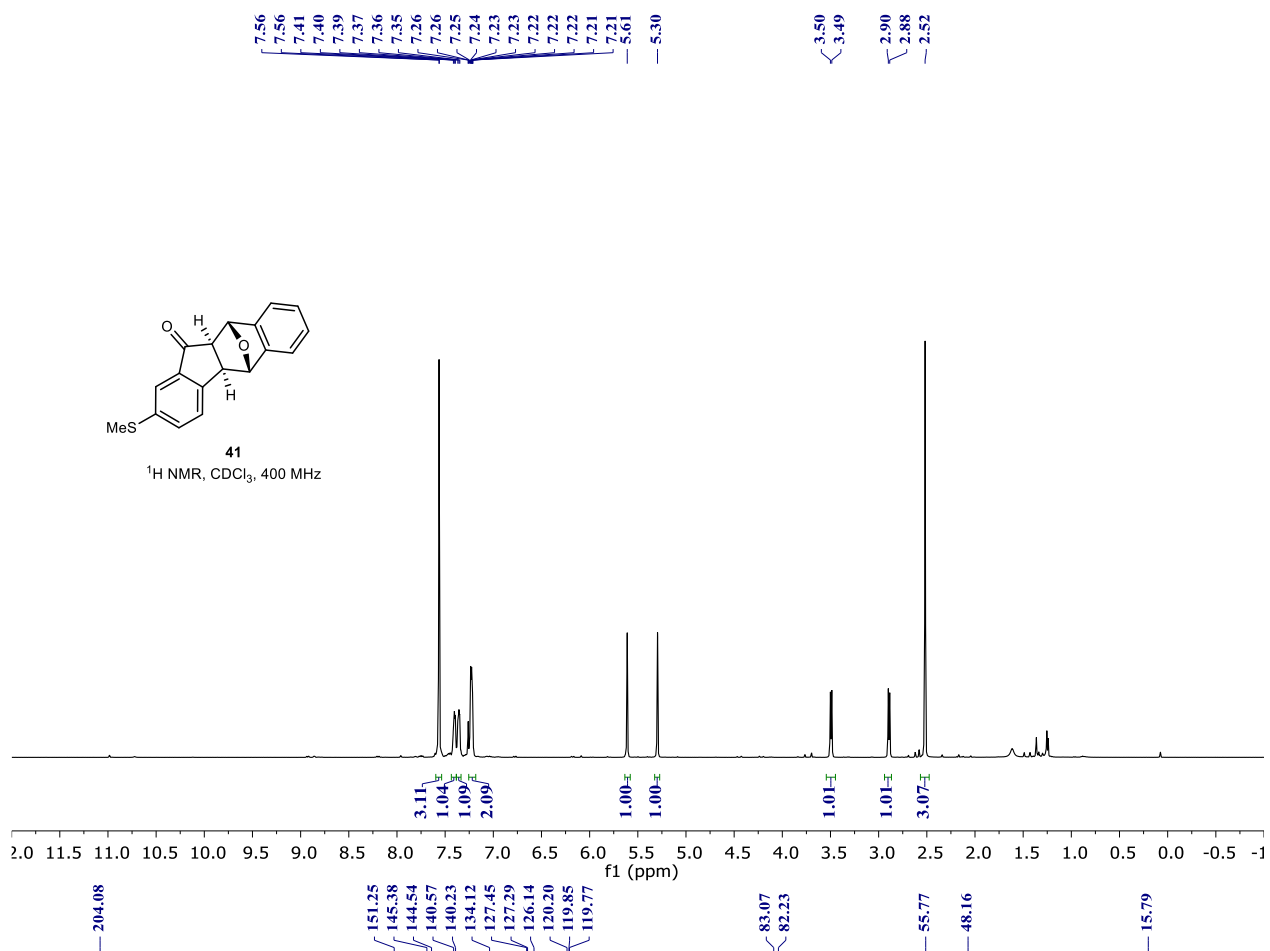


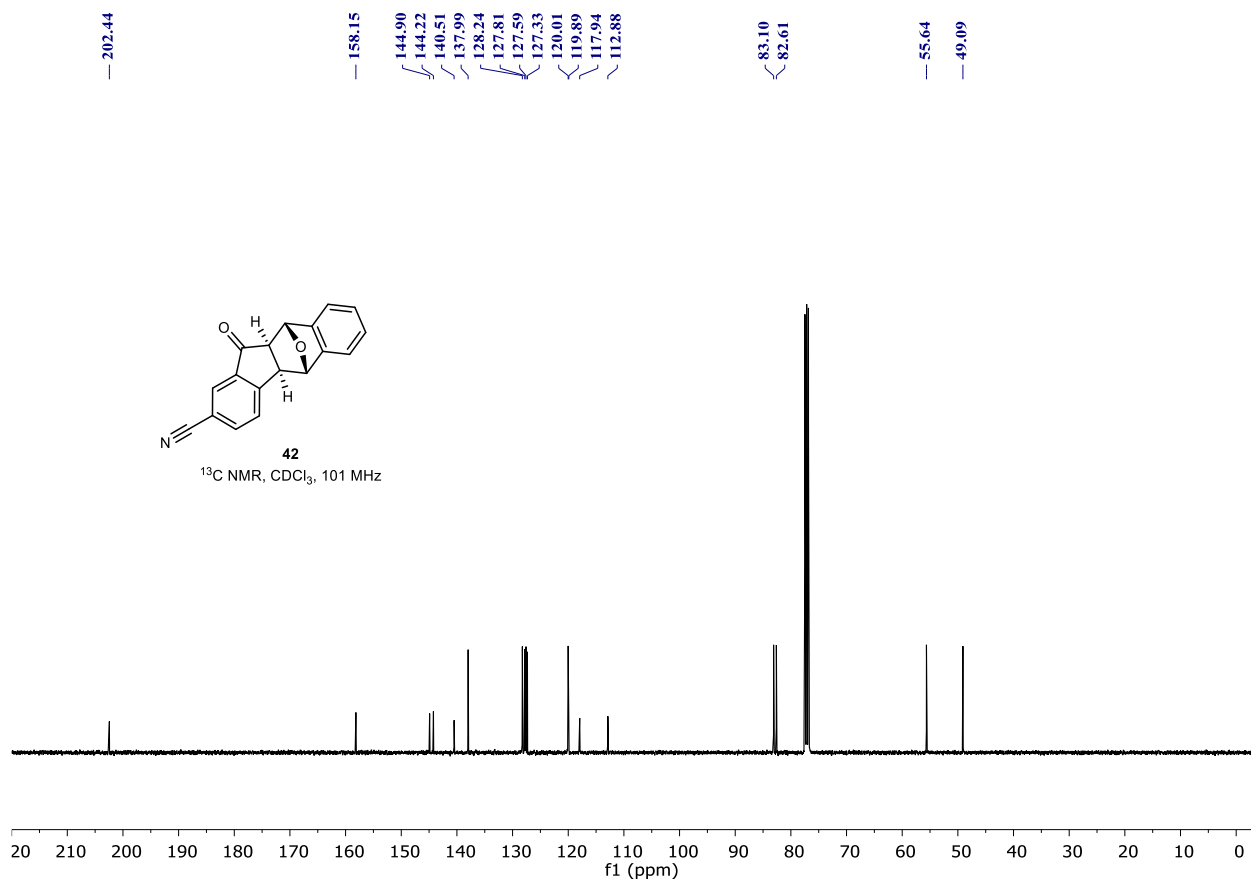
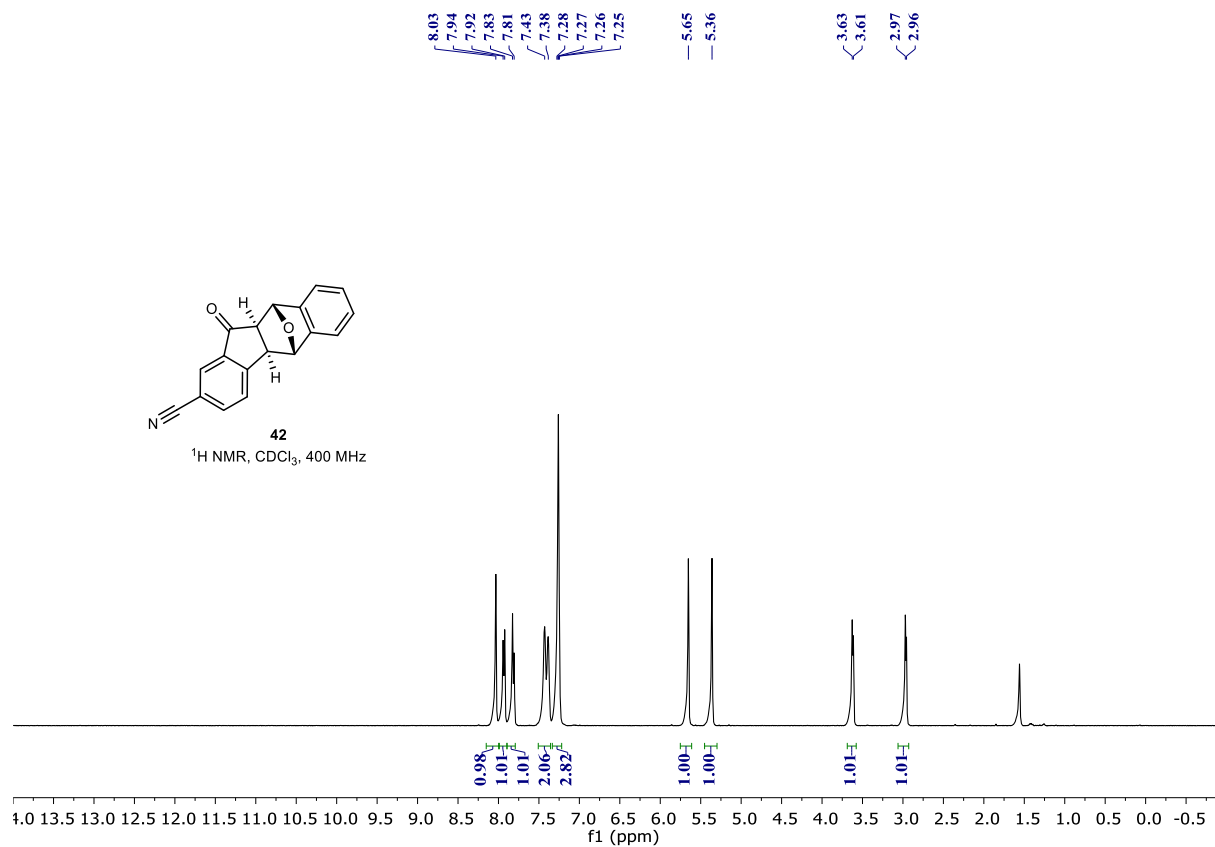
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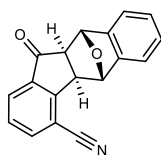
^{13}C NMR, CDCl_3 , 101 MHz





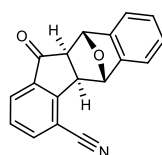
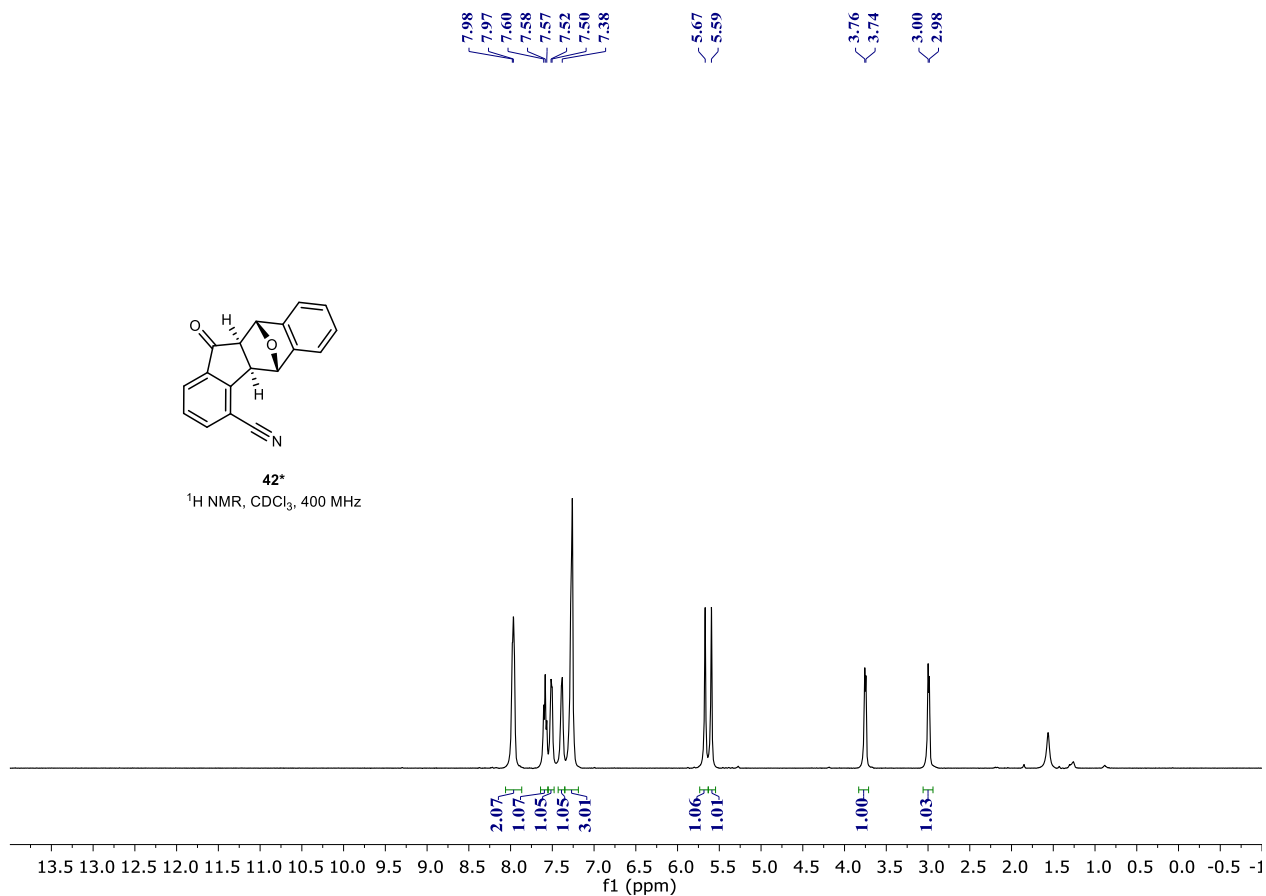






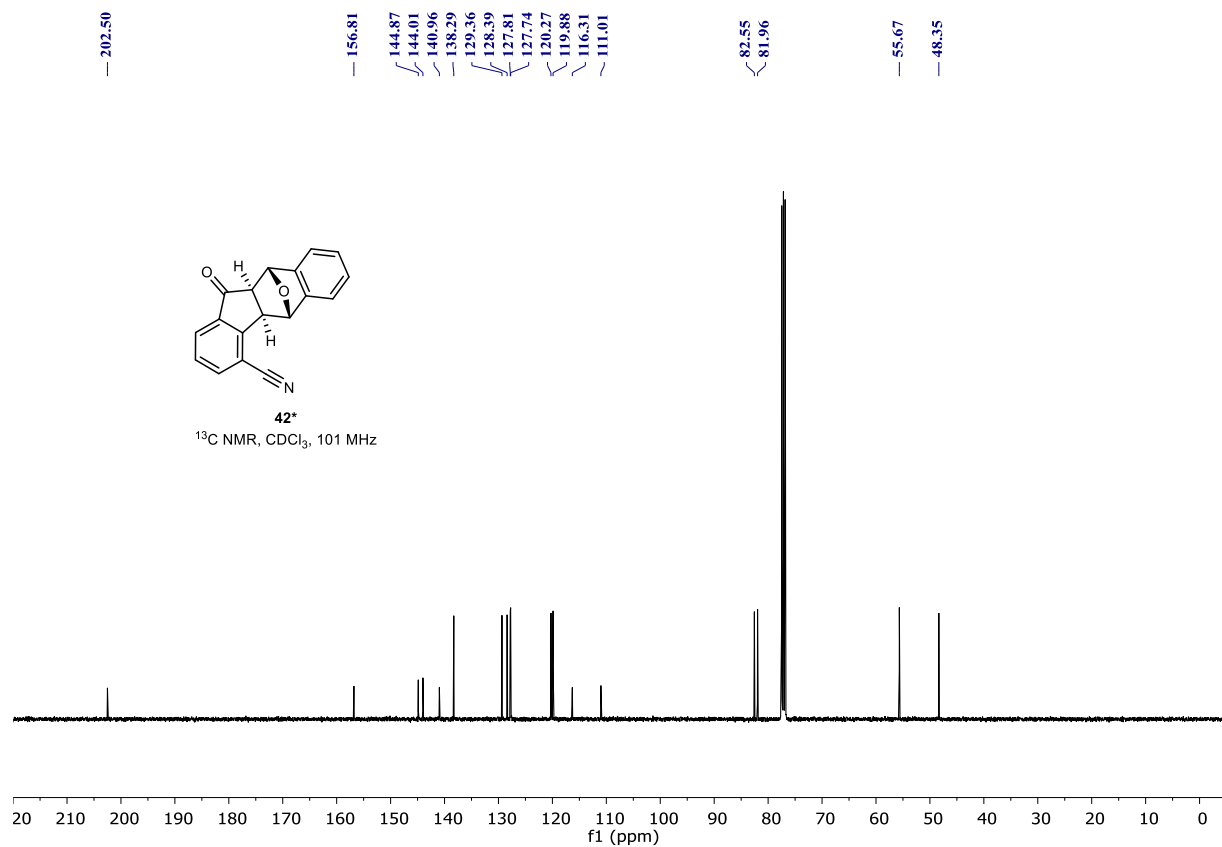
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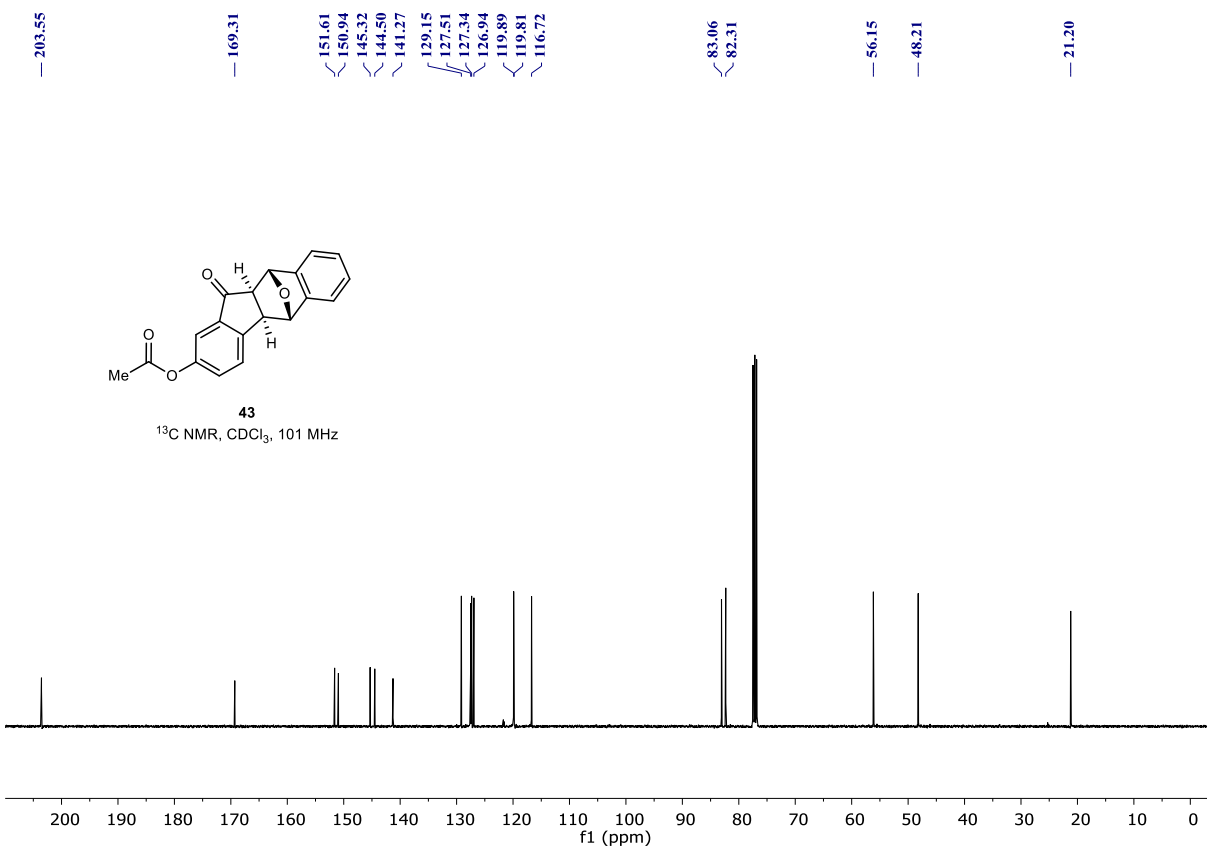
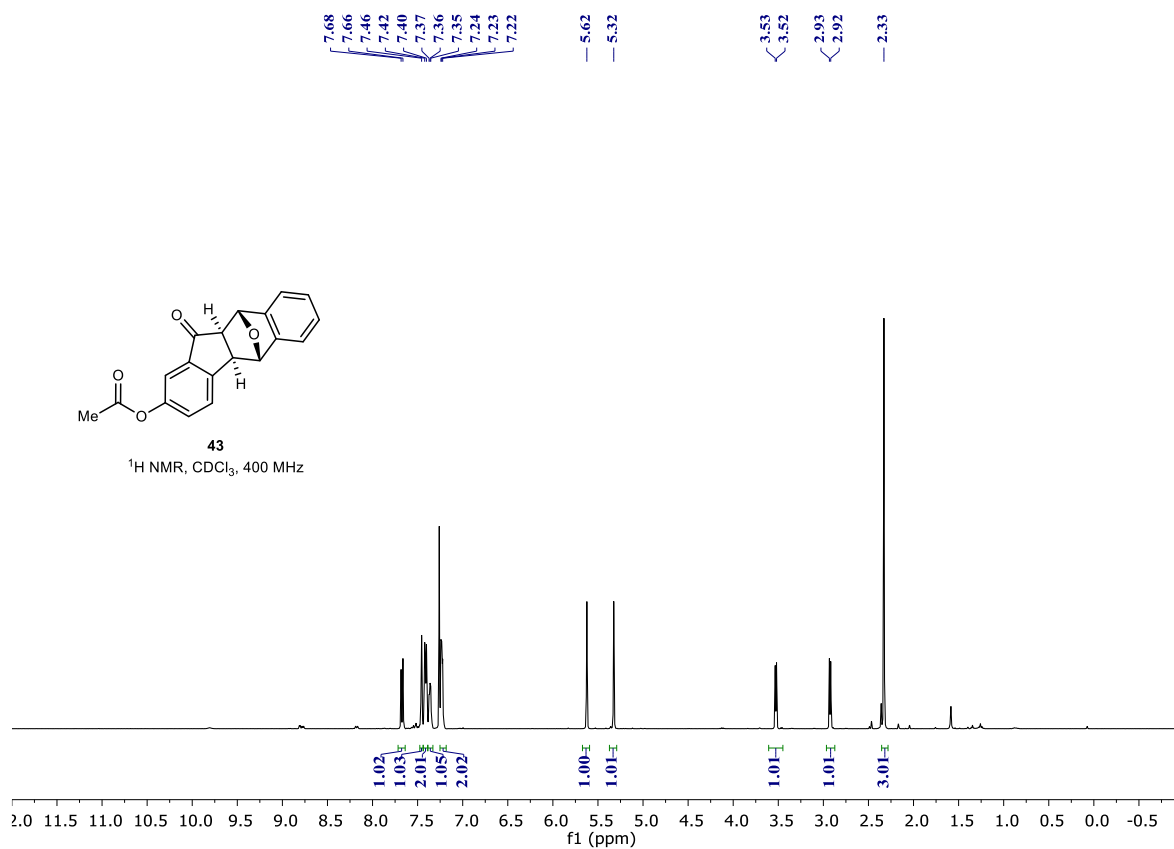
^1H NMR, CDCl_3 , 400 MHz

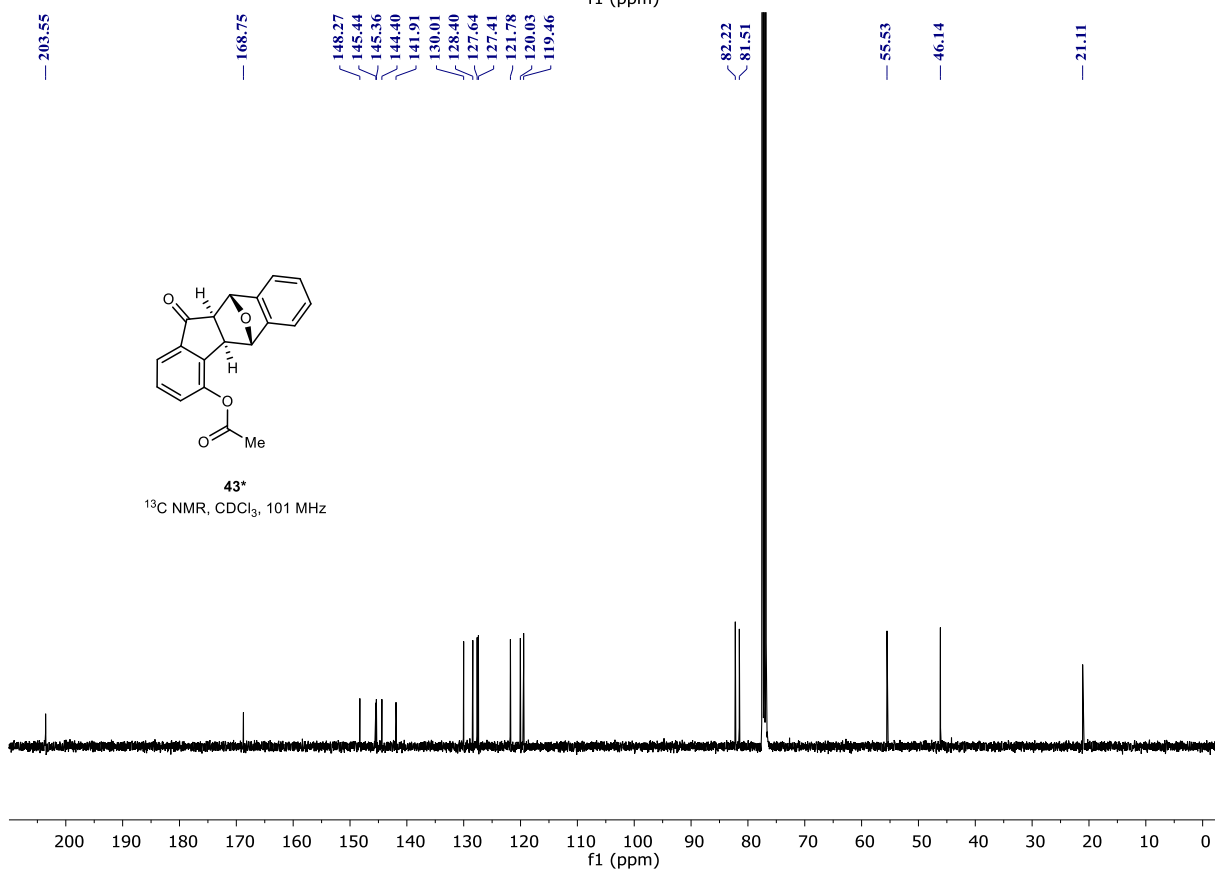
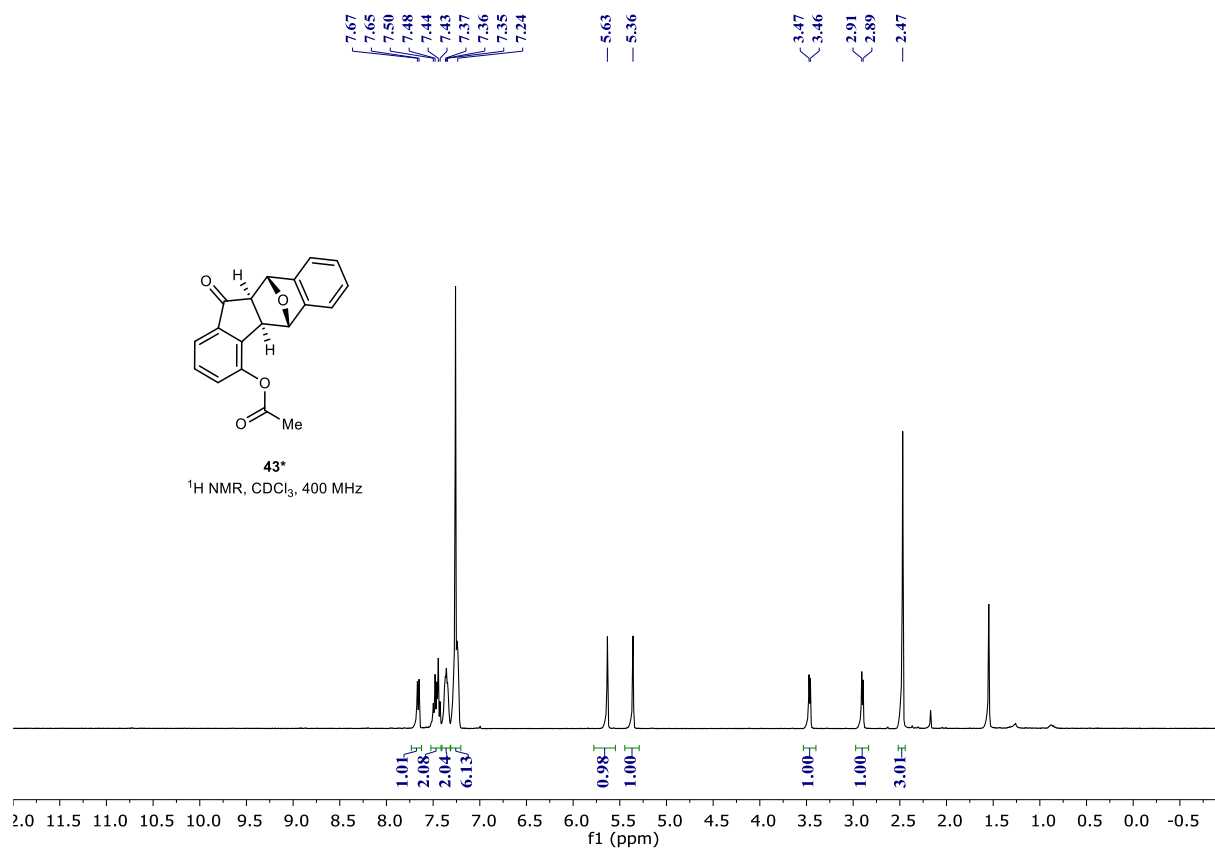


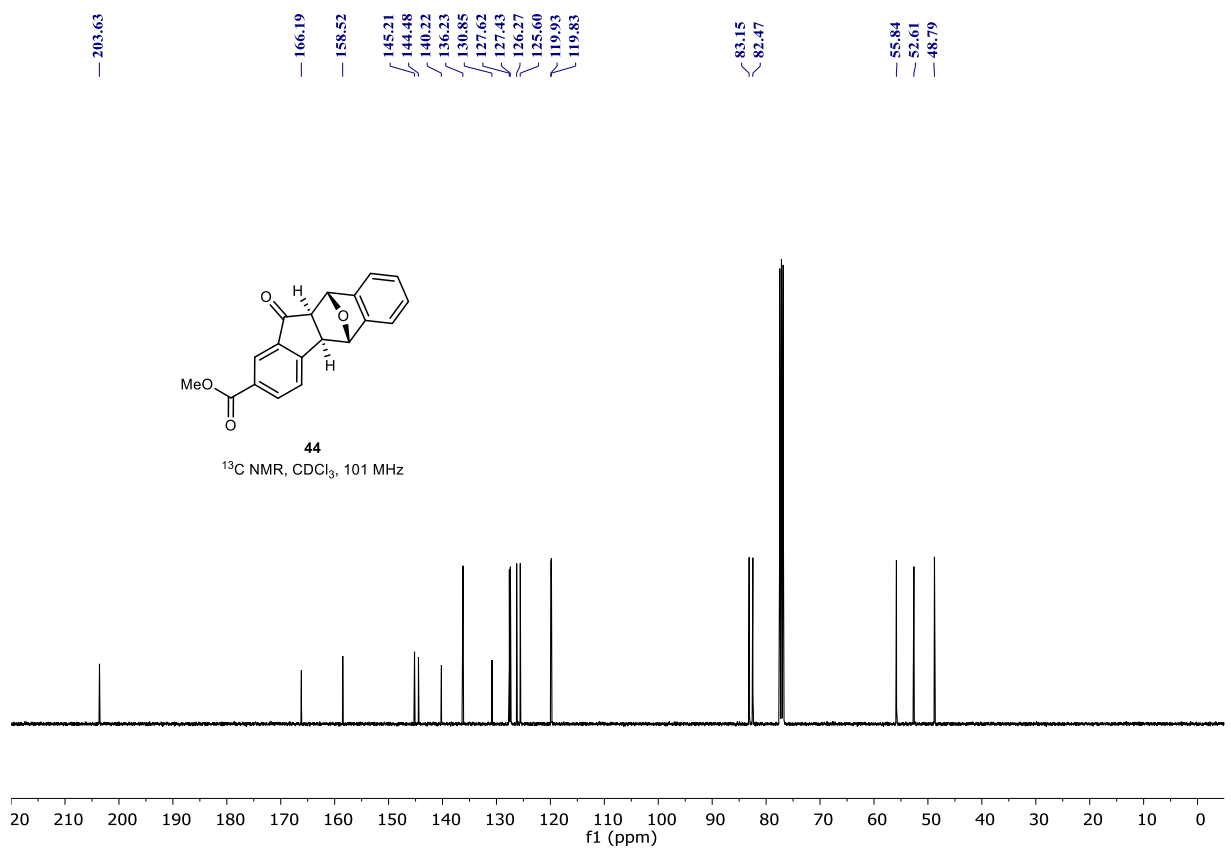
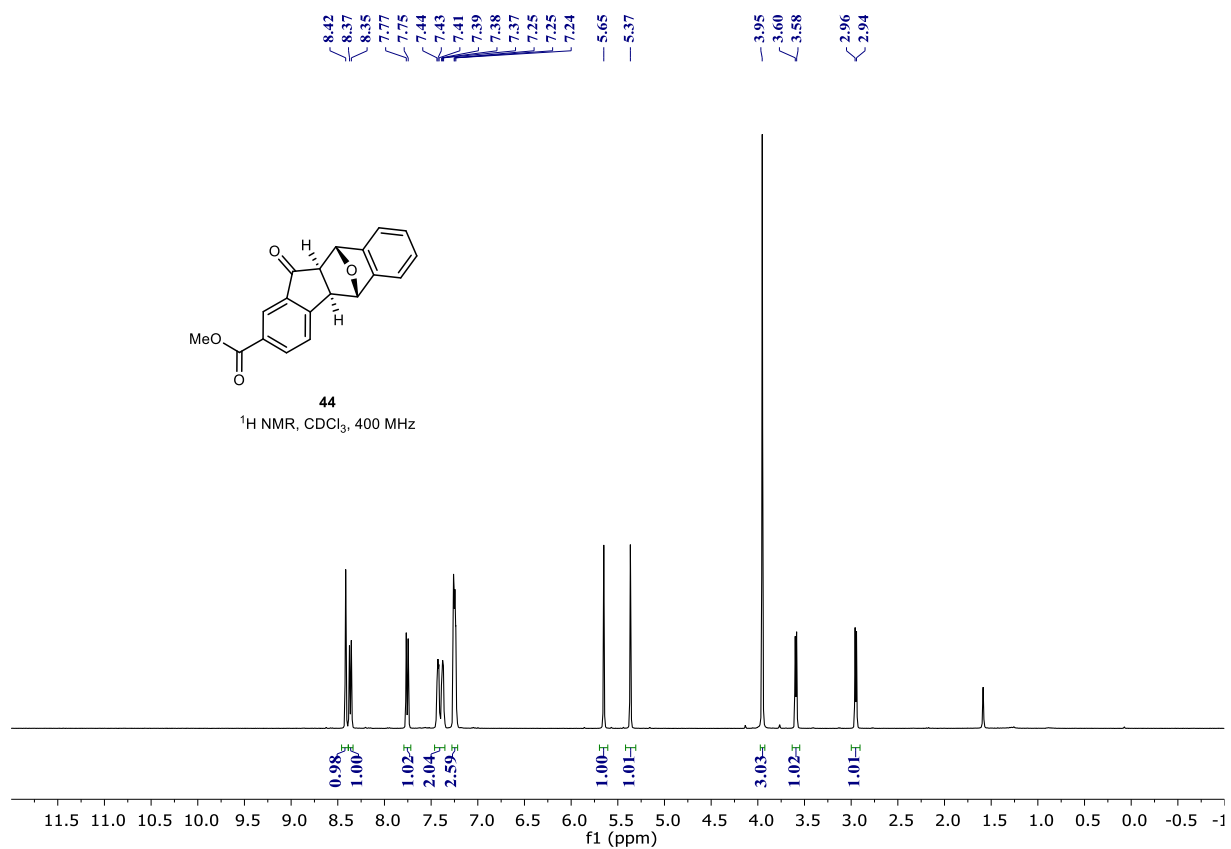
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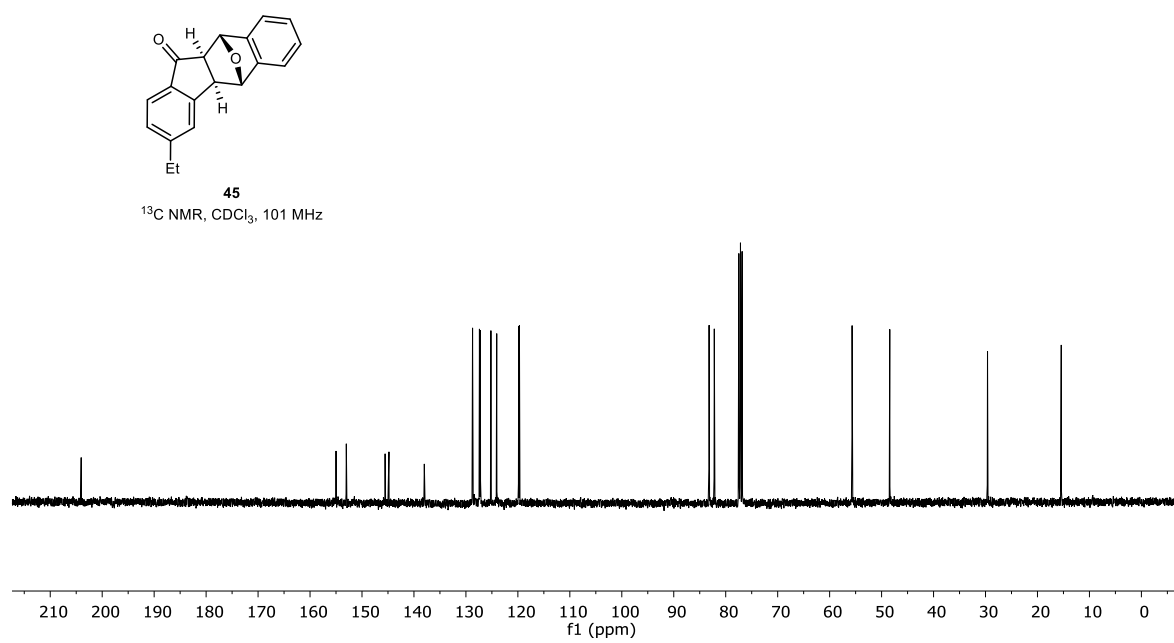
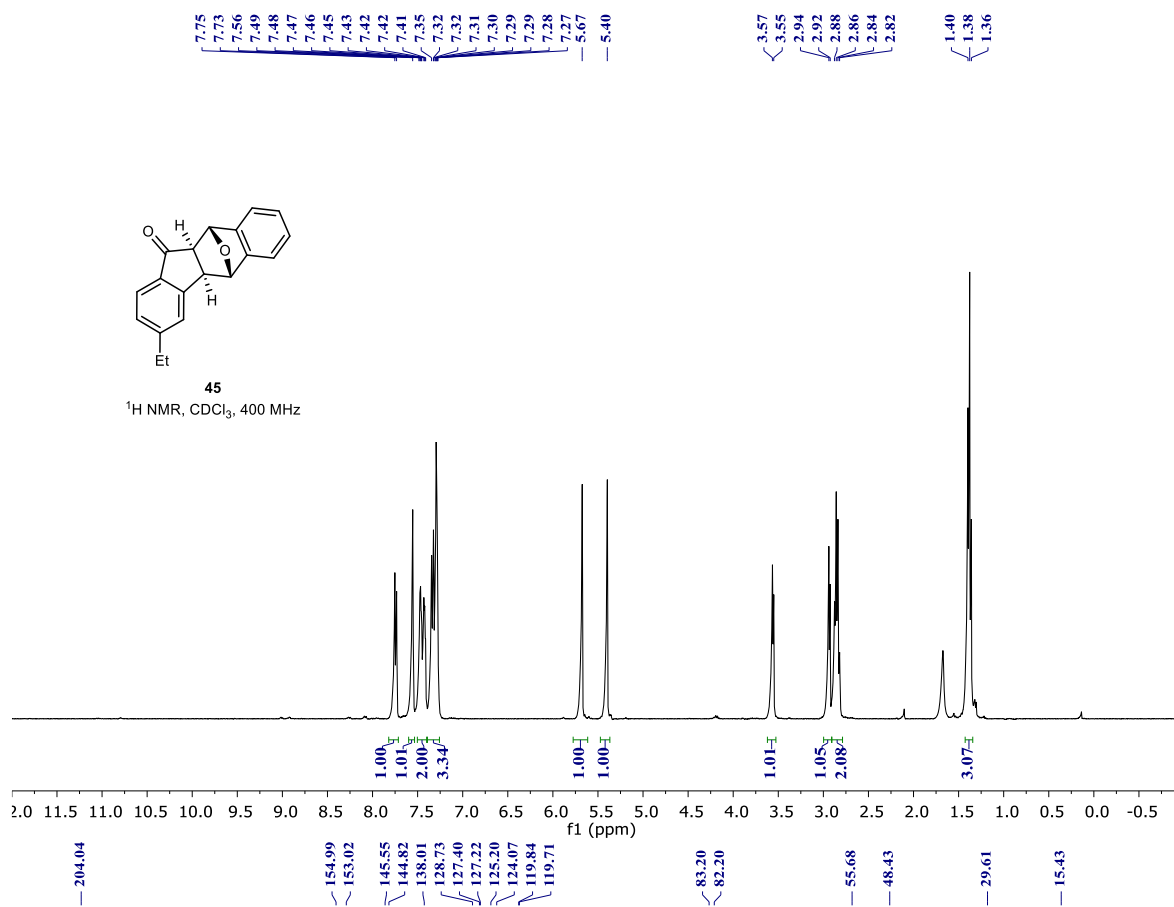
^{13}C NMR, CDCl_3 , 101 MHz

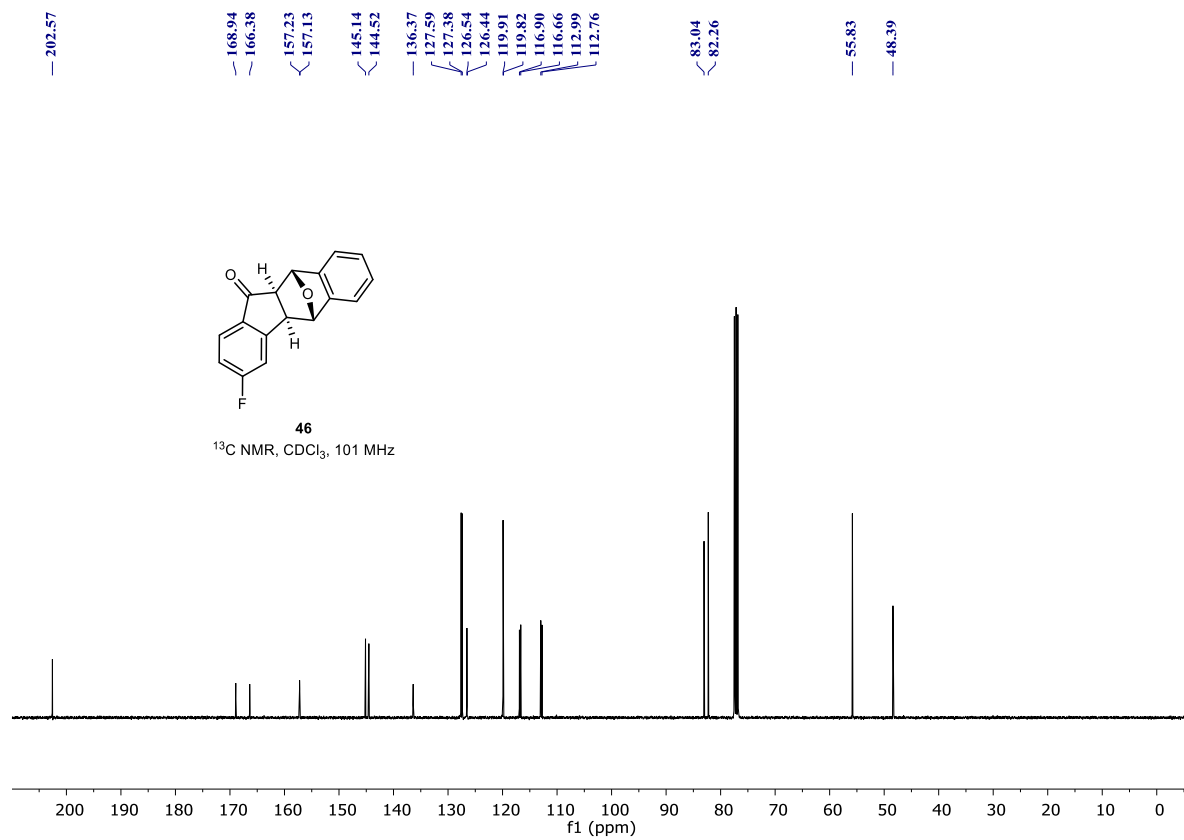
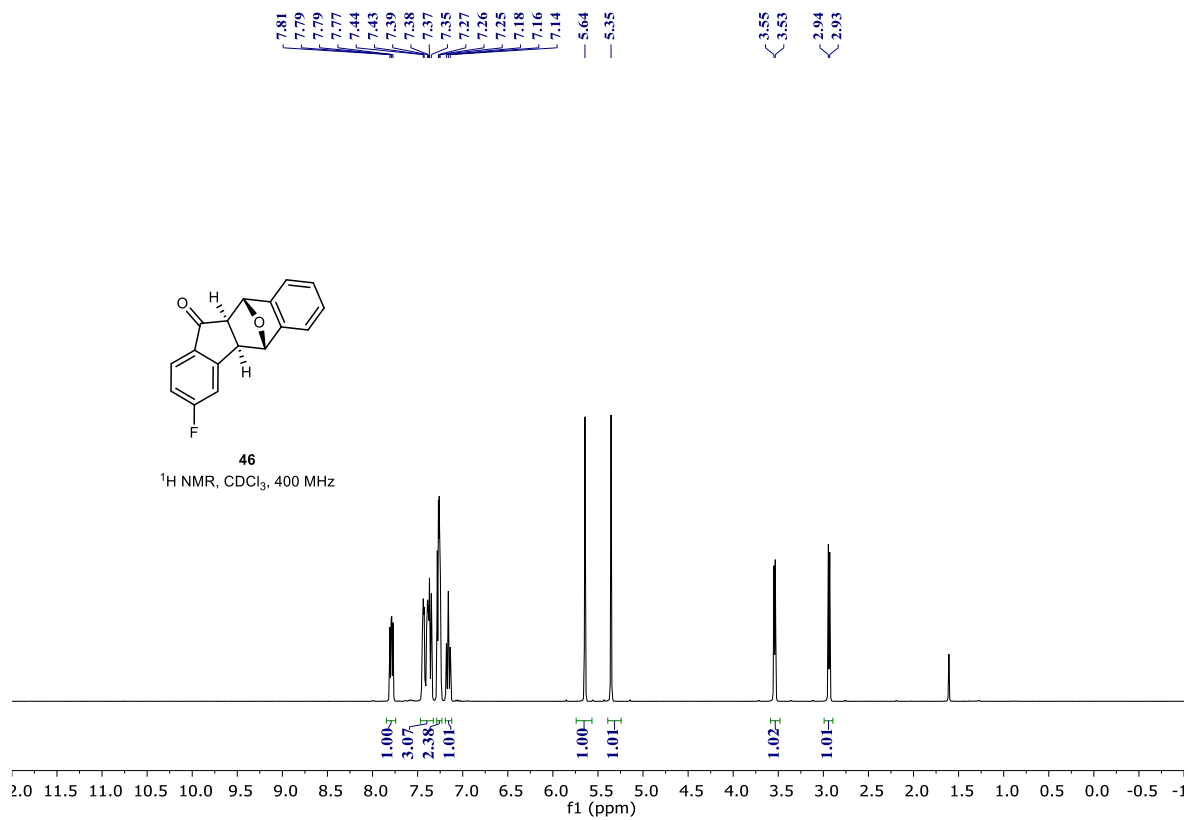


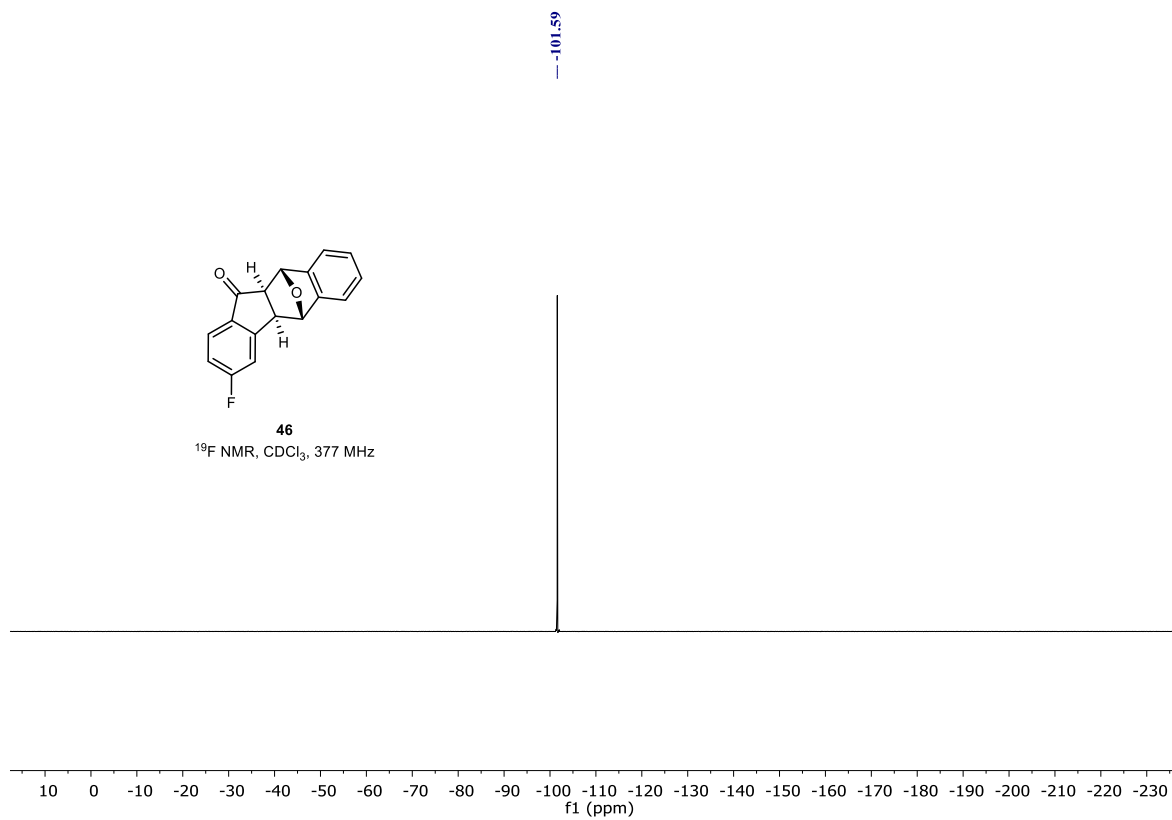


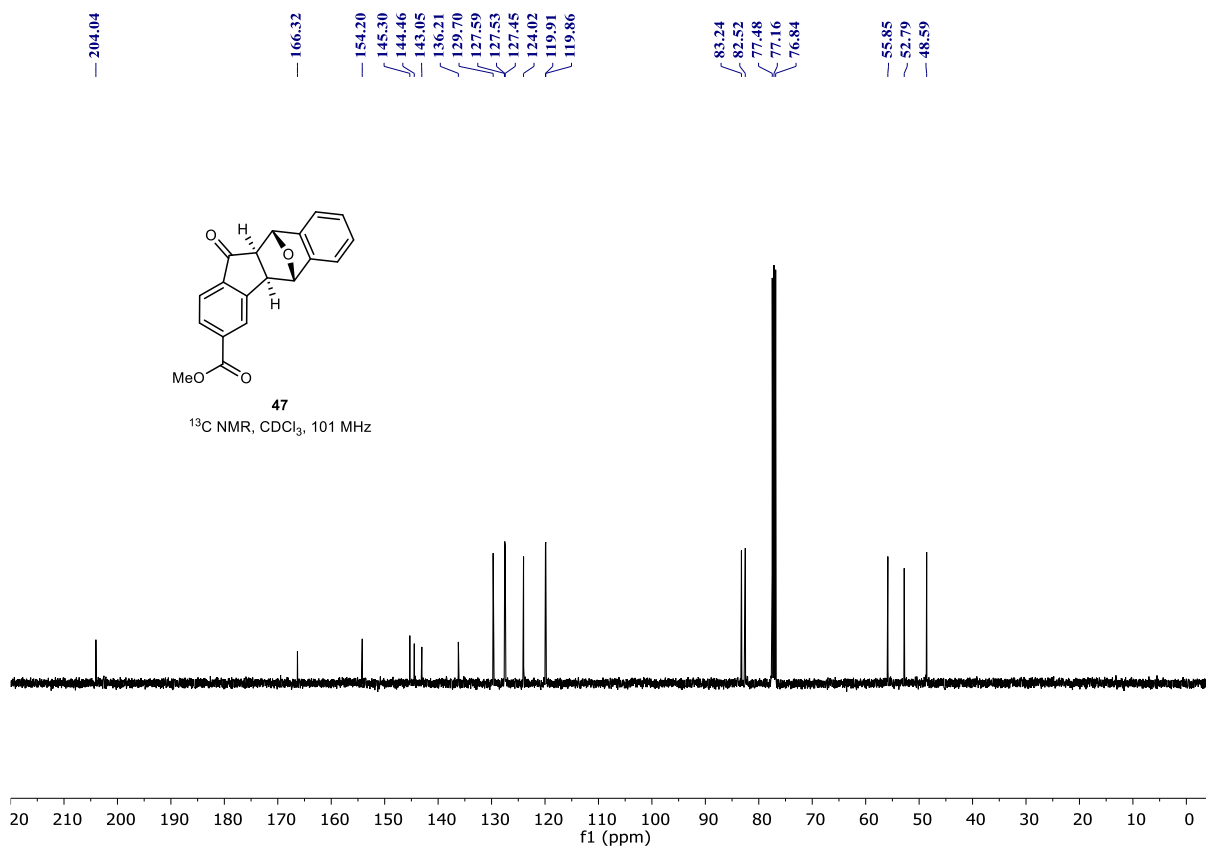
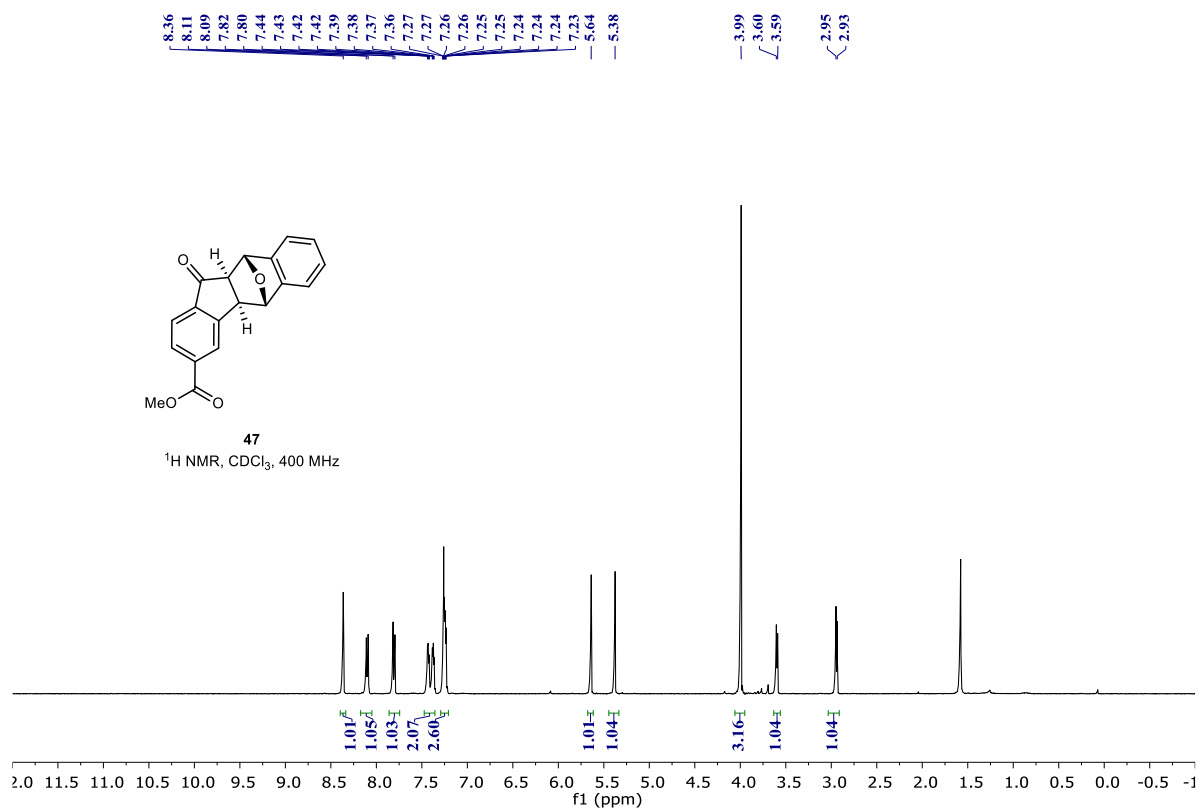


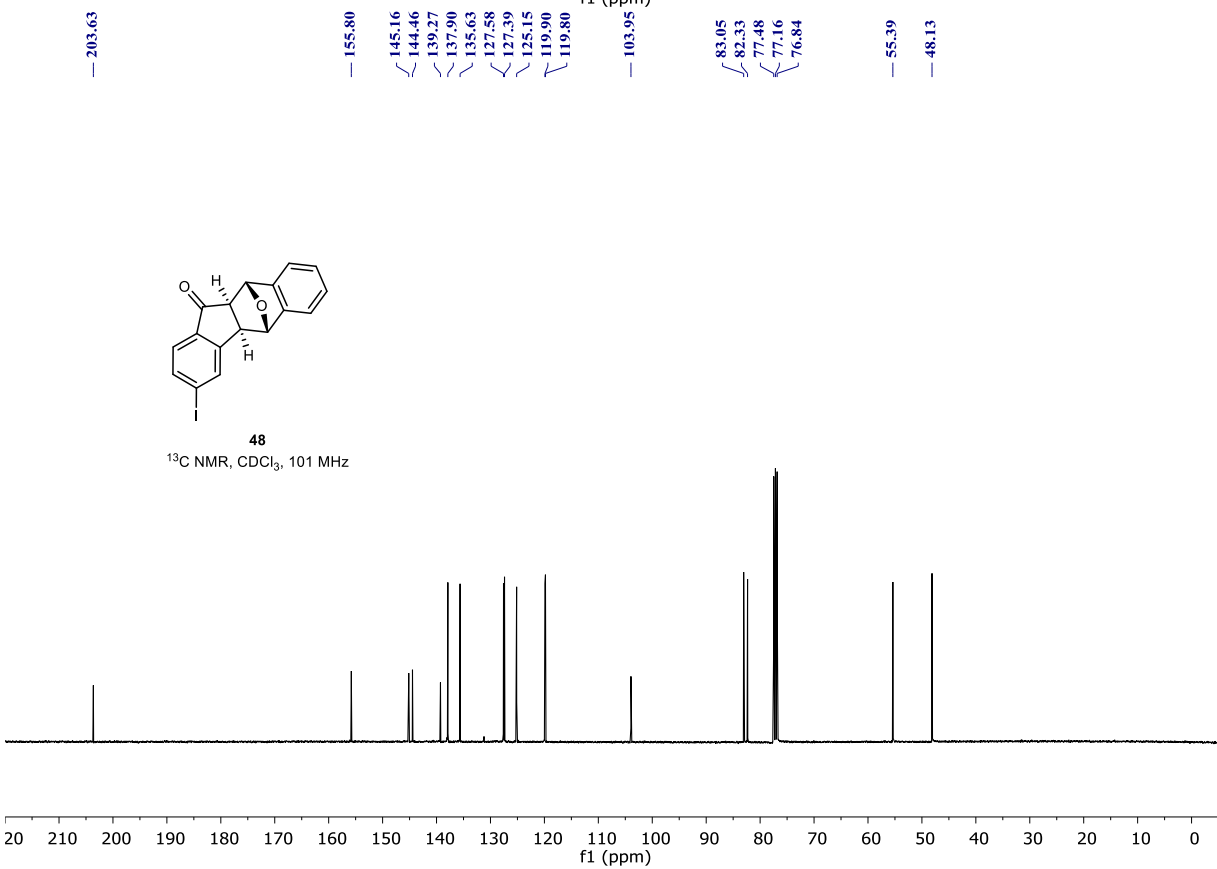
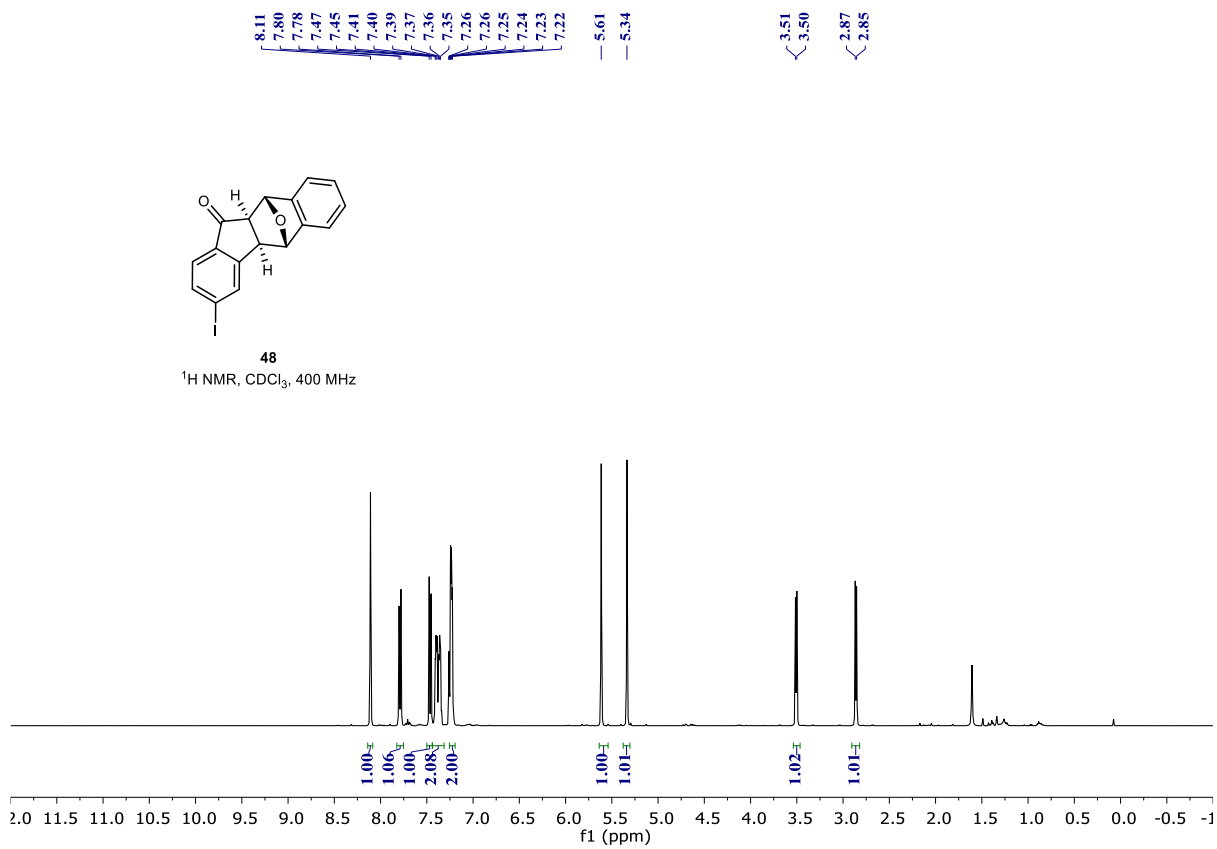


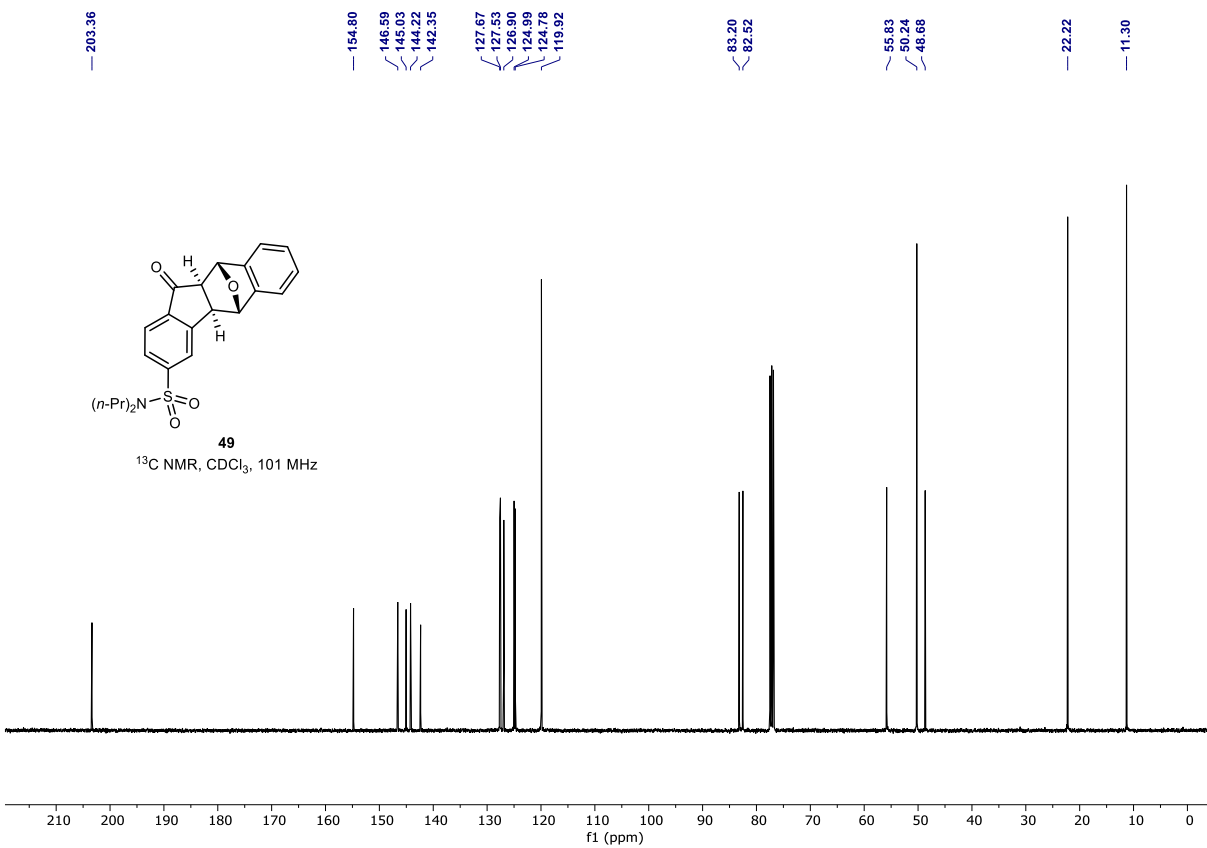
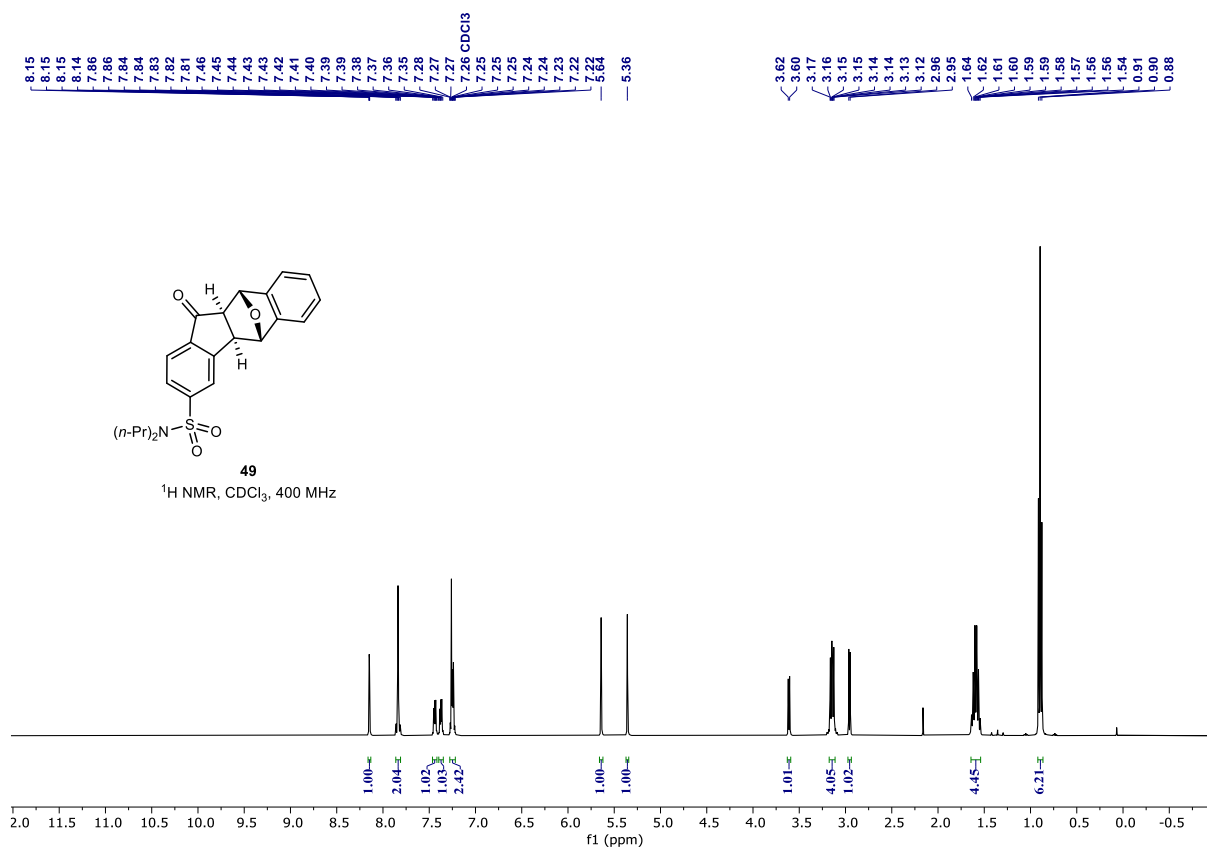


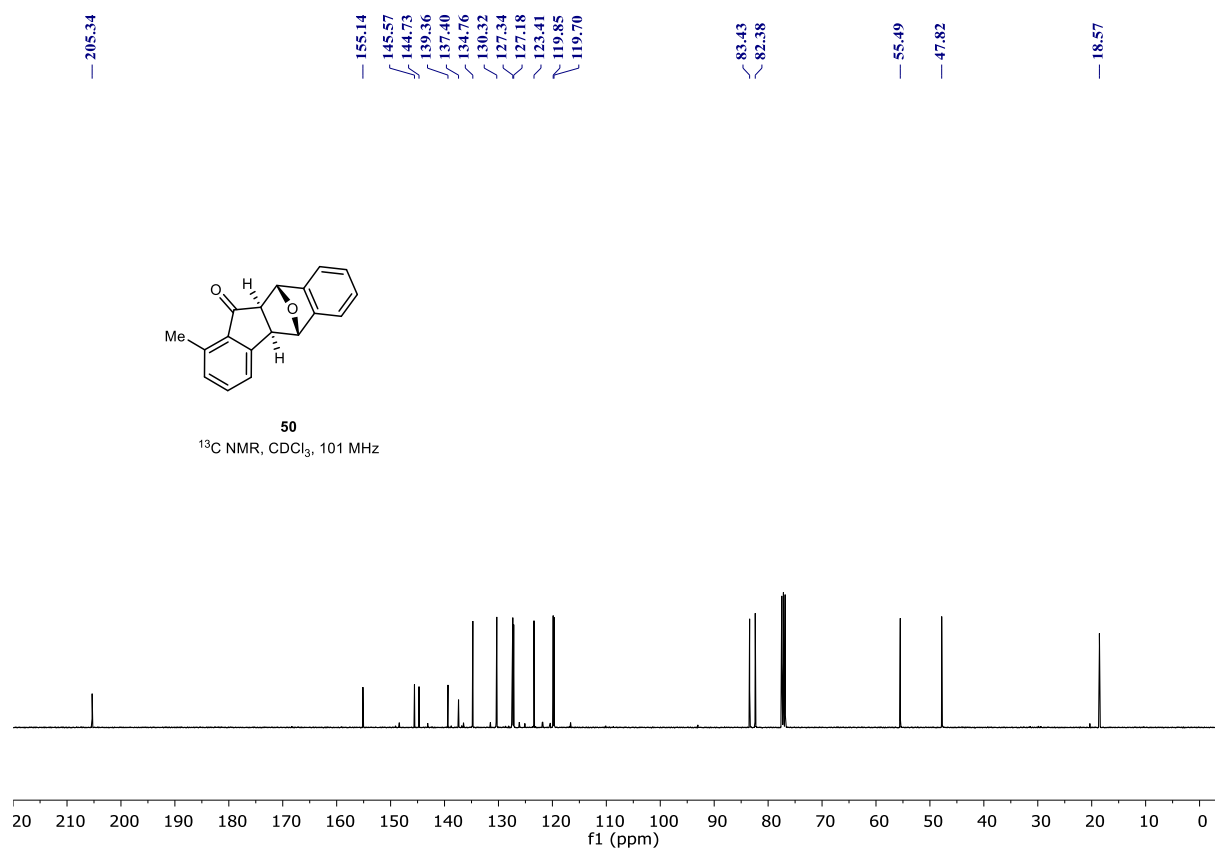
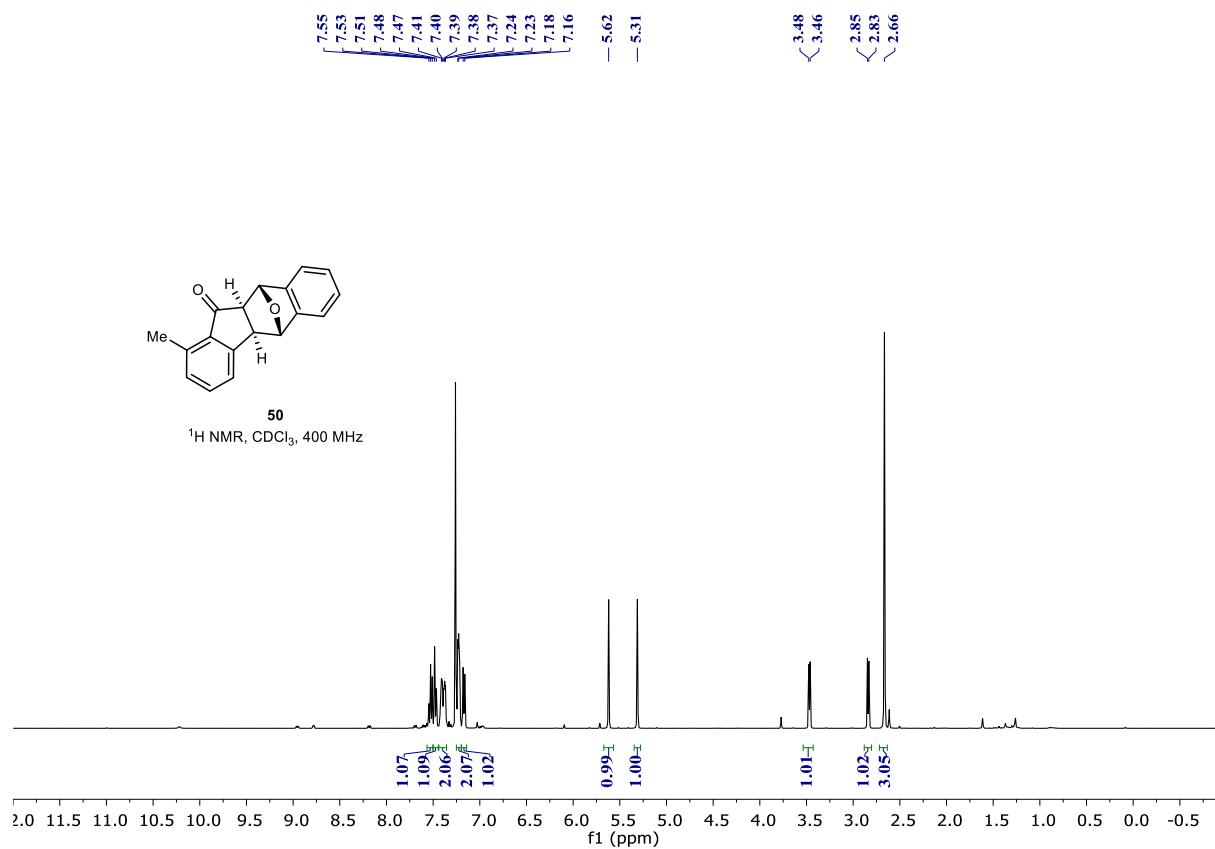


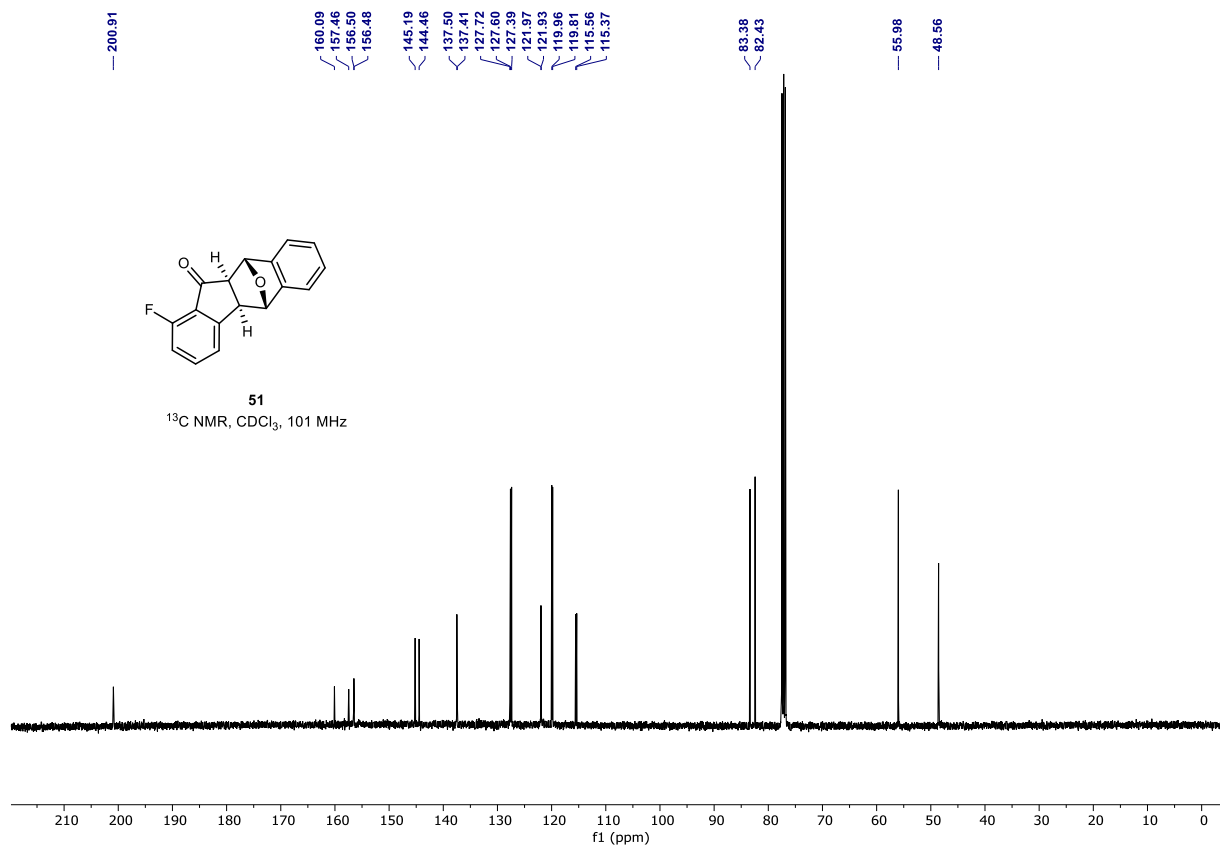
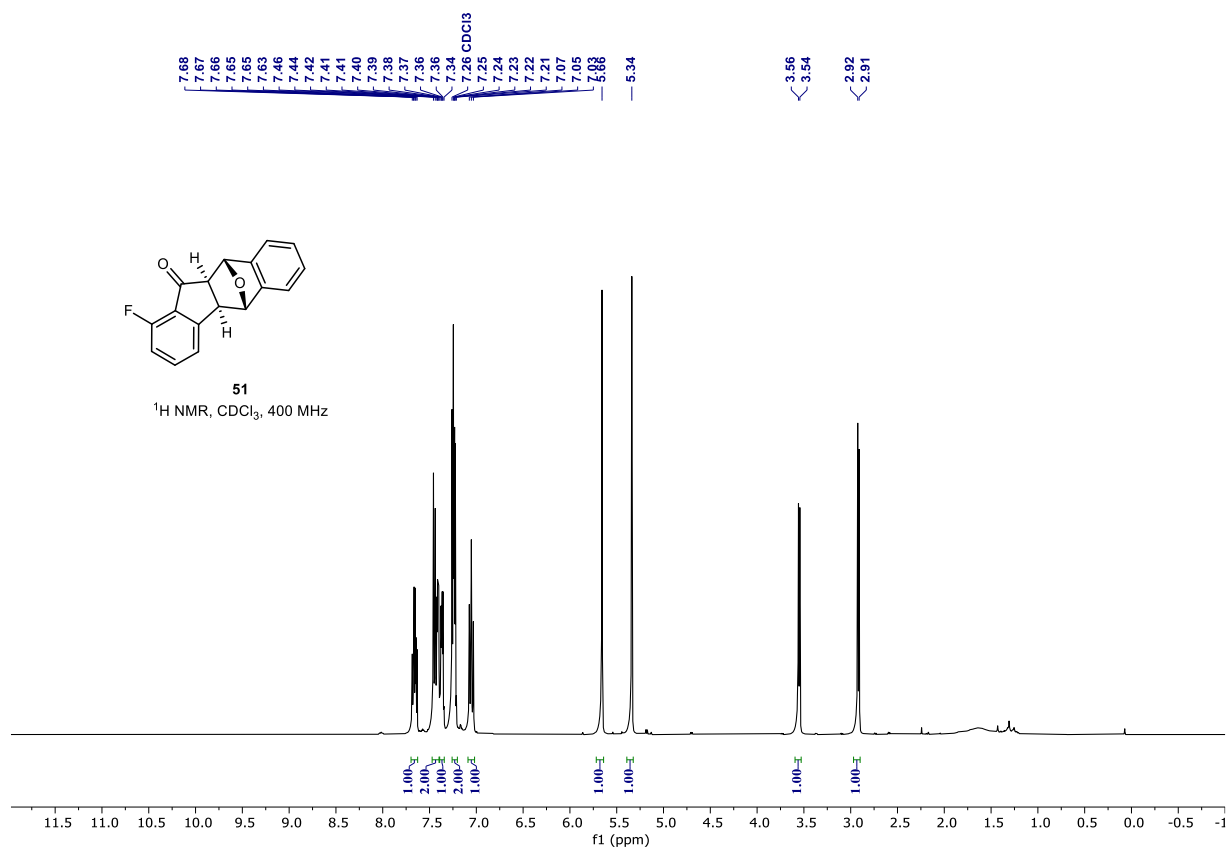


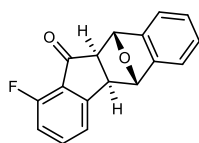






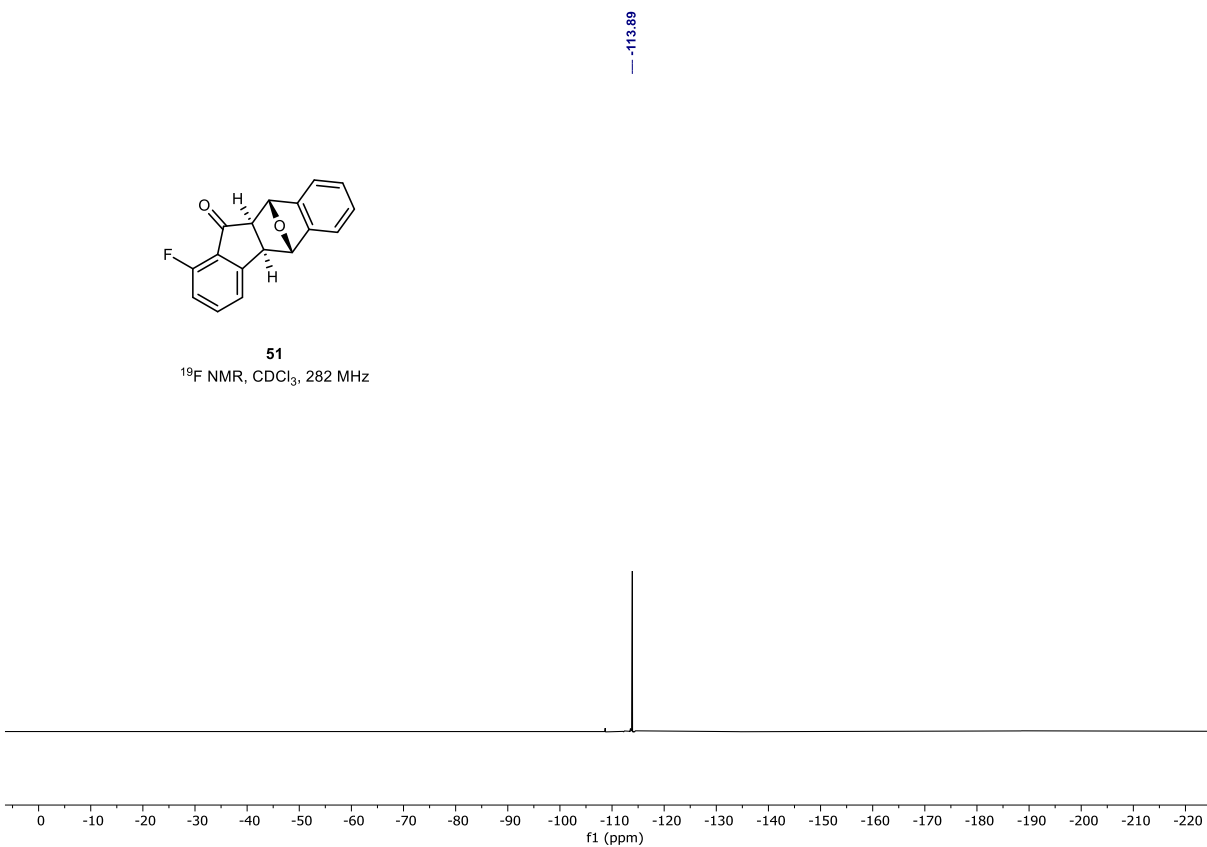


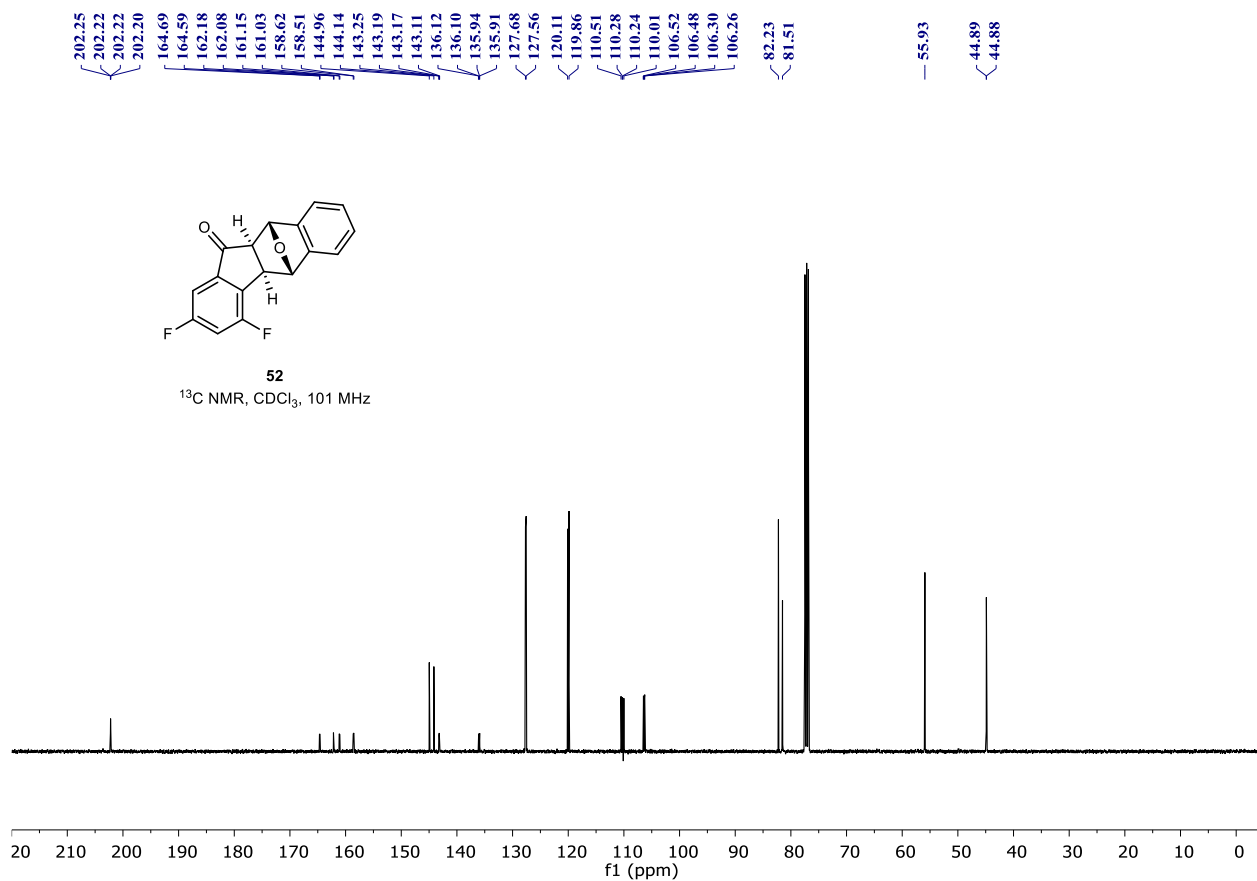
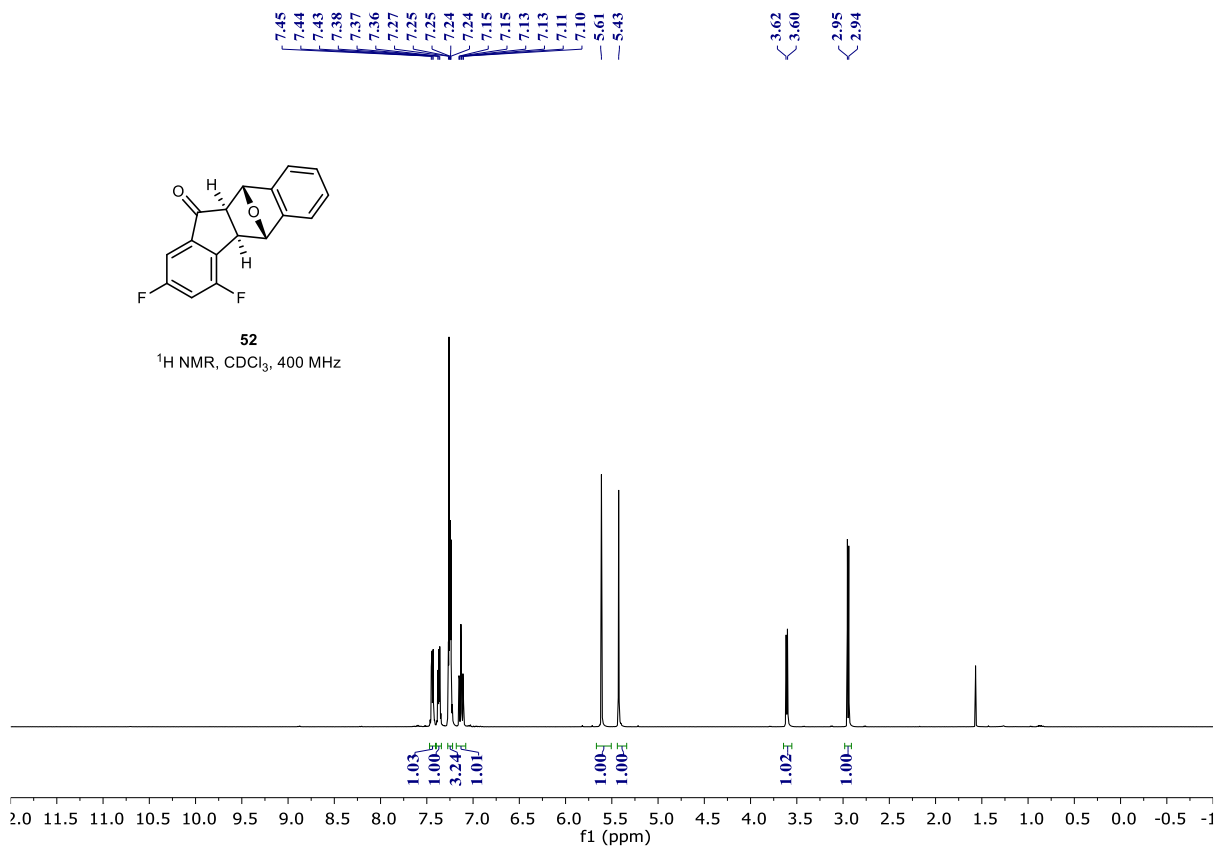


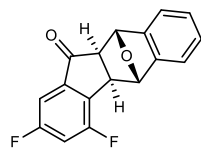


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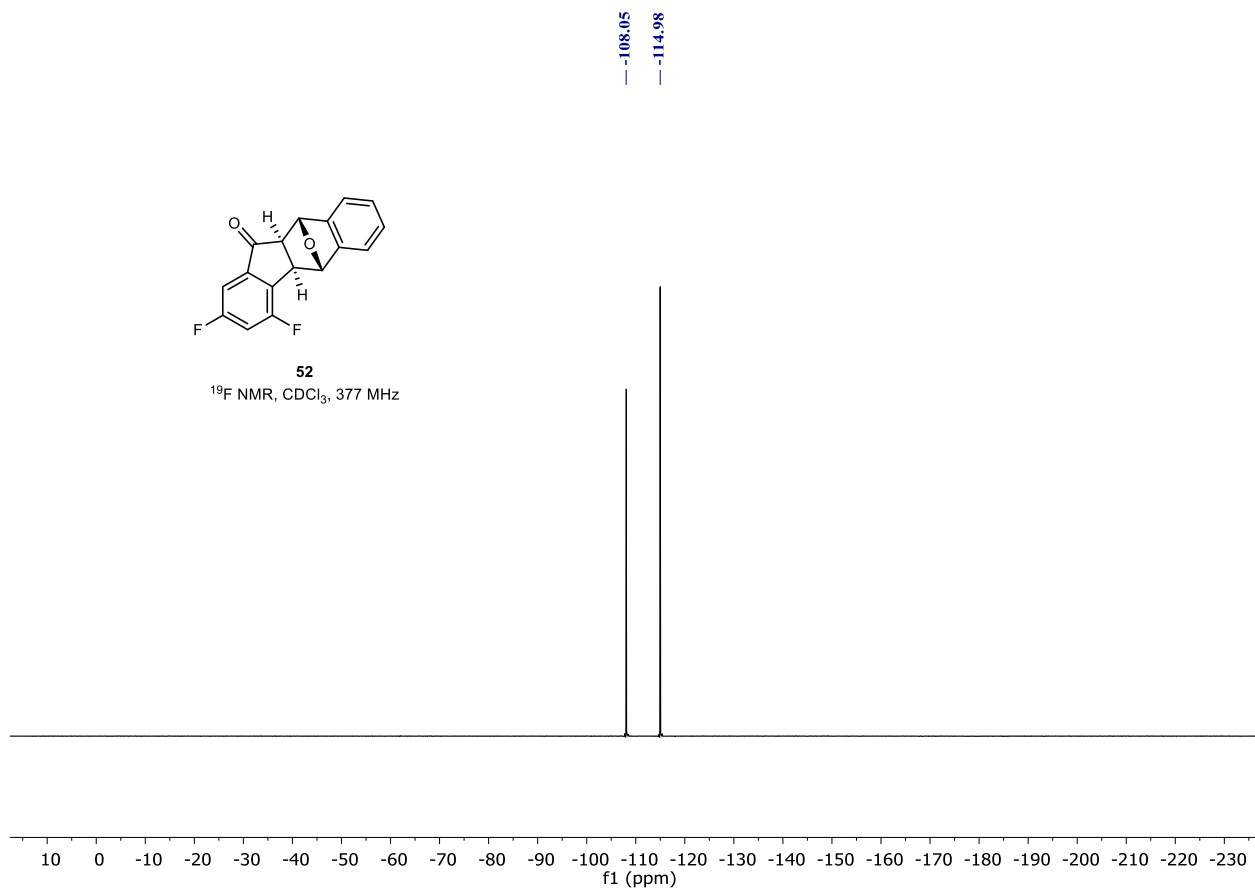
^{19}F NMR, CDCl_3 , 282 MHz

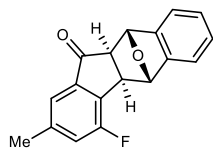






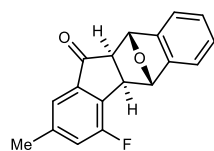
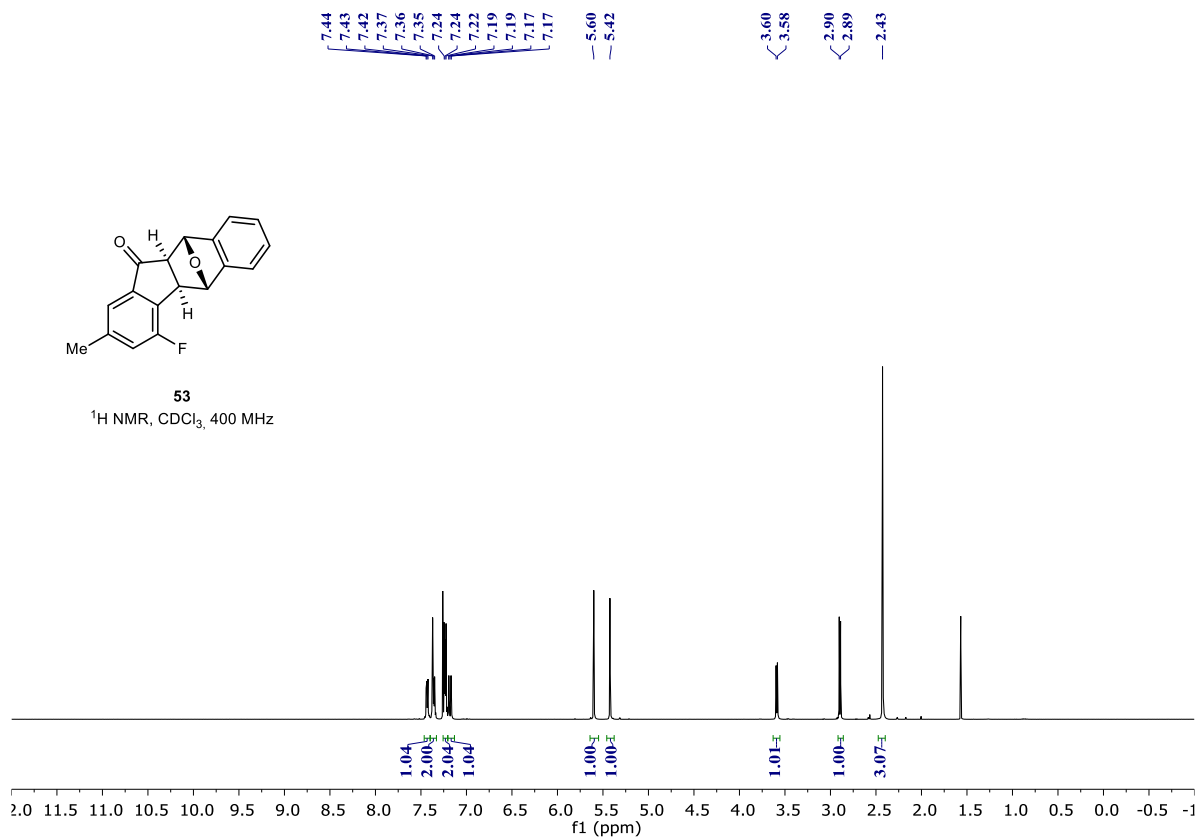
52
 ^{19}F NMR, CDCl_3 , 377 MHz





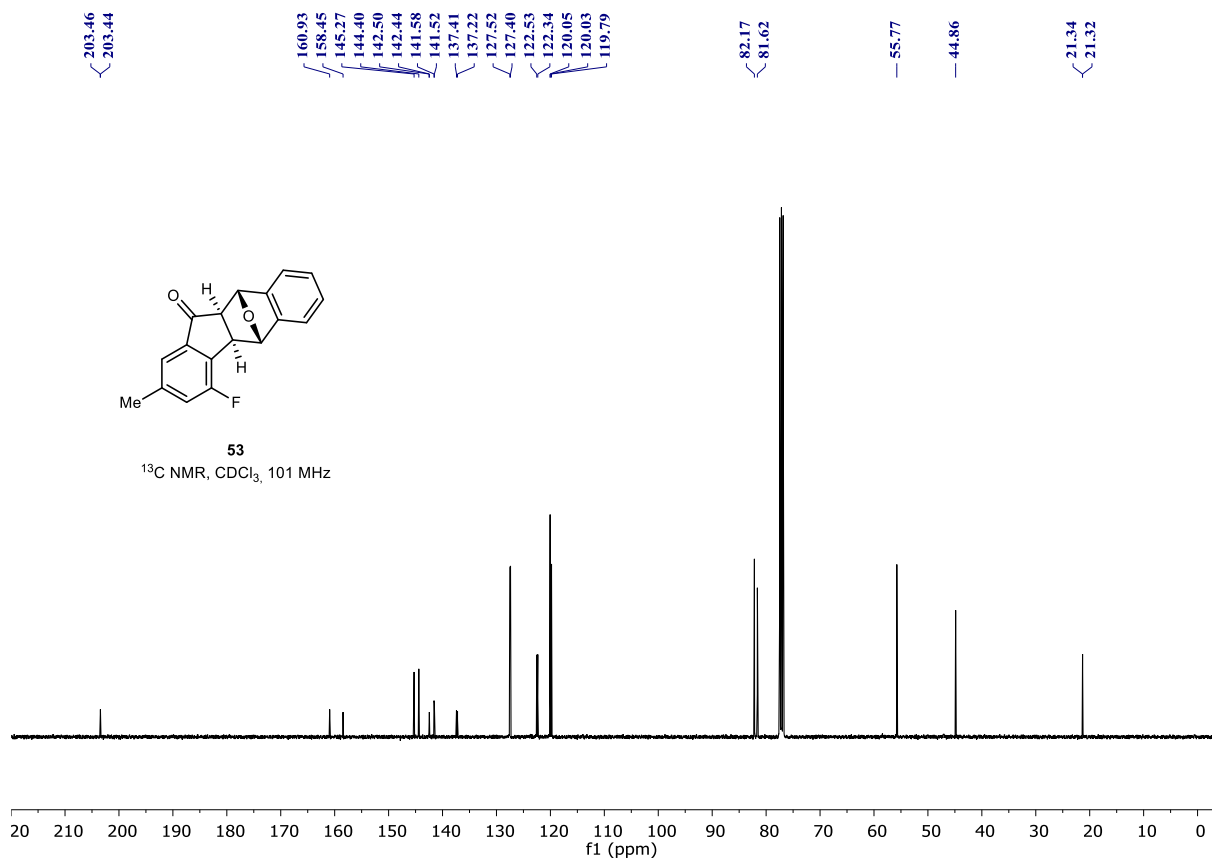
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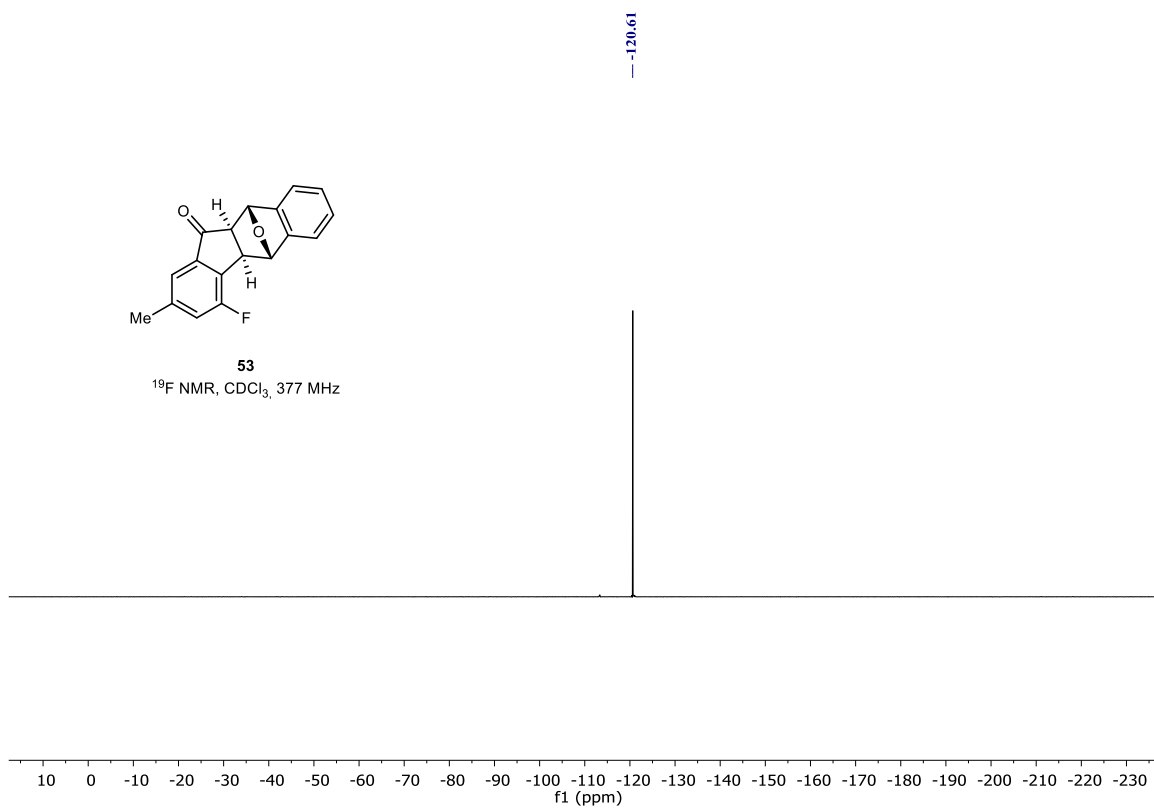
^1H NMR, CDCl_3 , 400 MHz

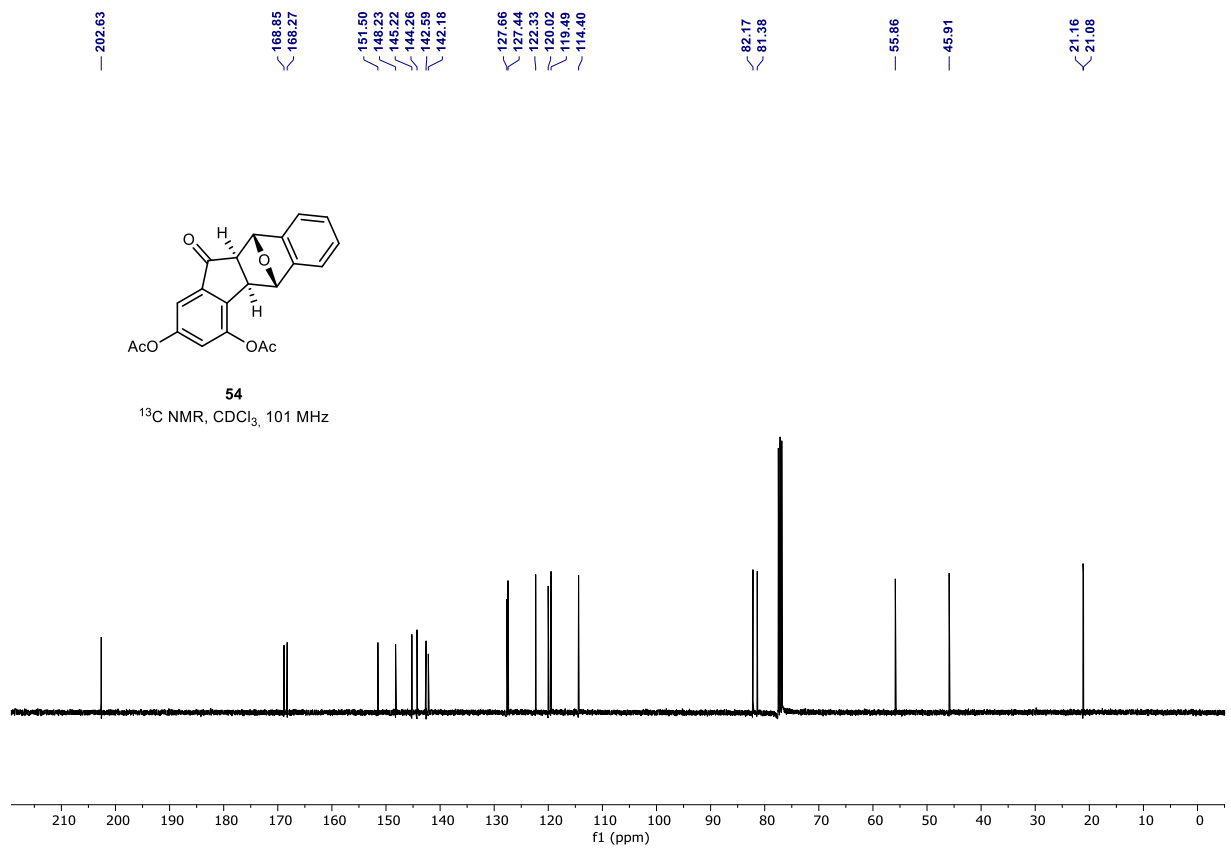
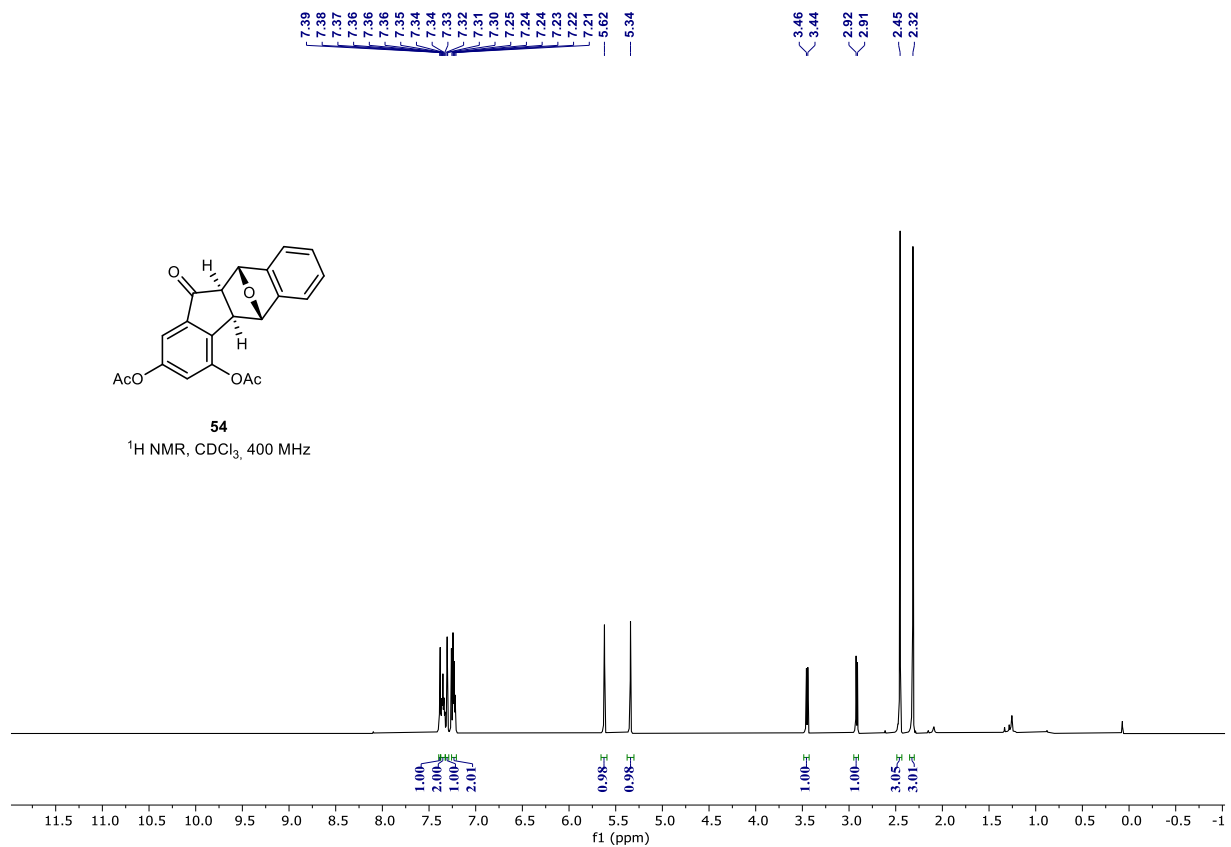


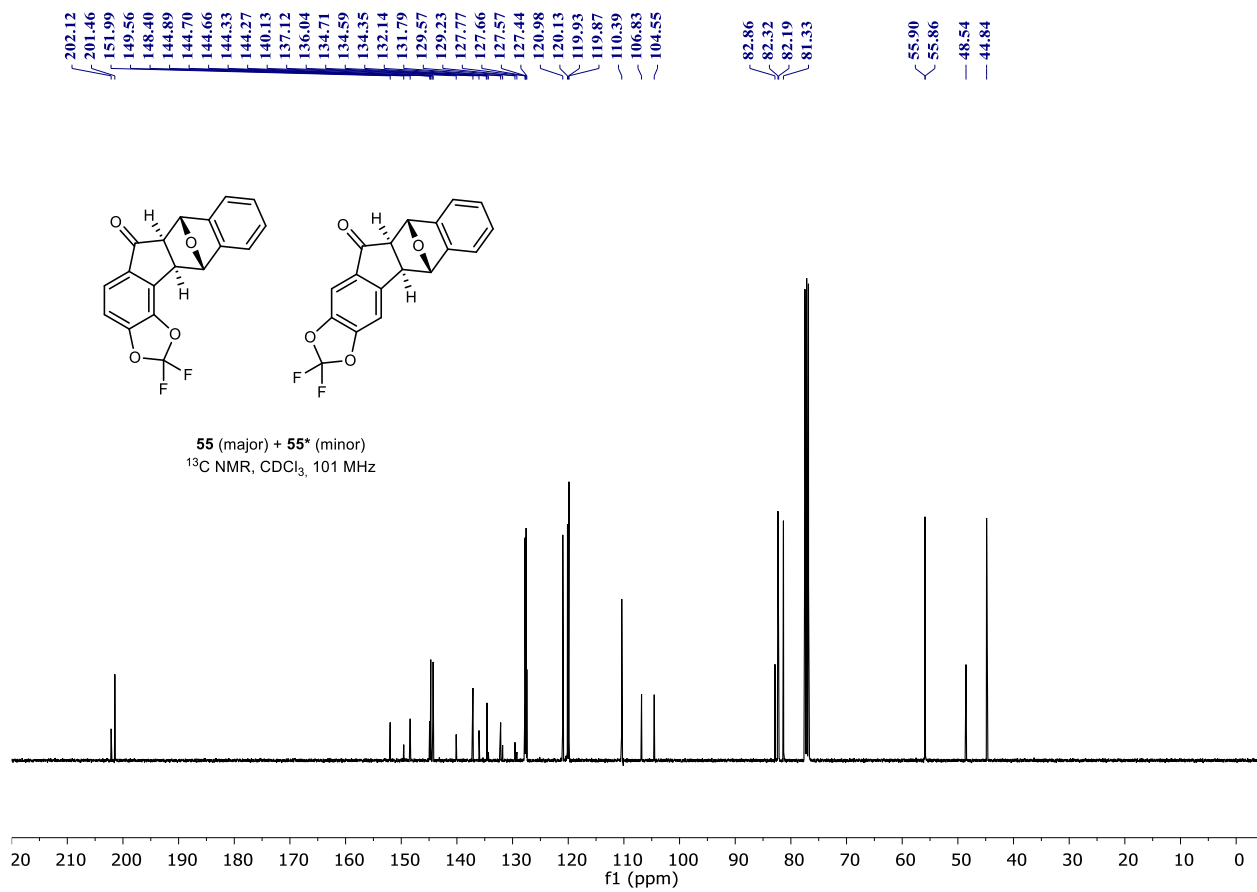
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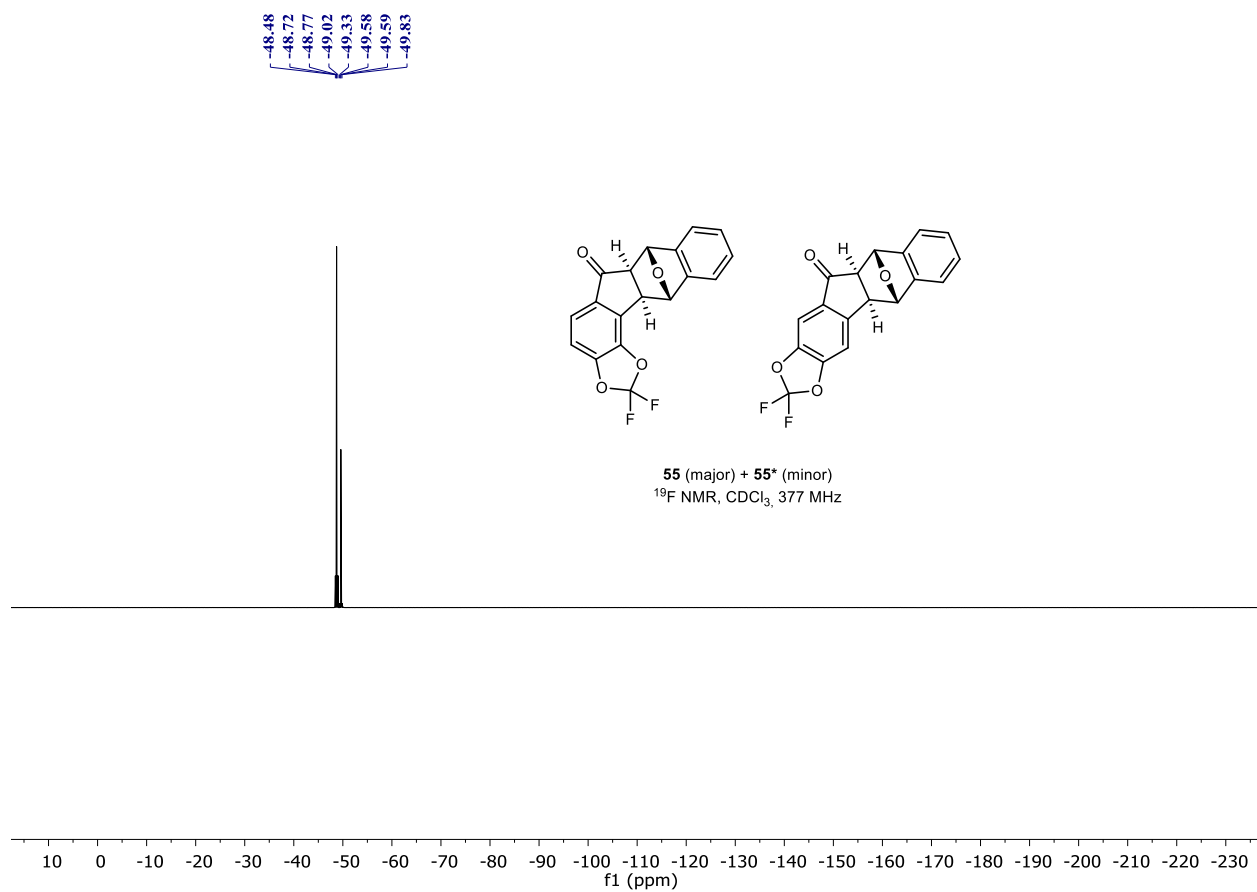
^{13}C NMR, CDCl_3 , 101 MHz

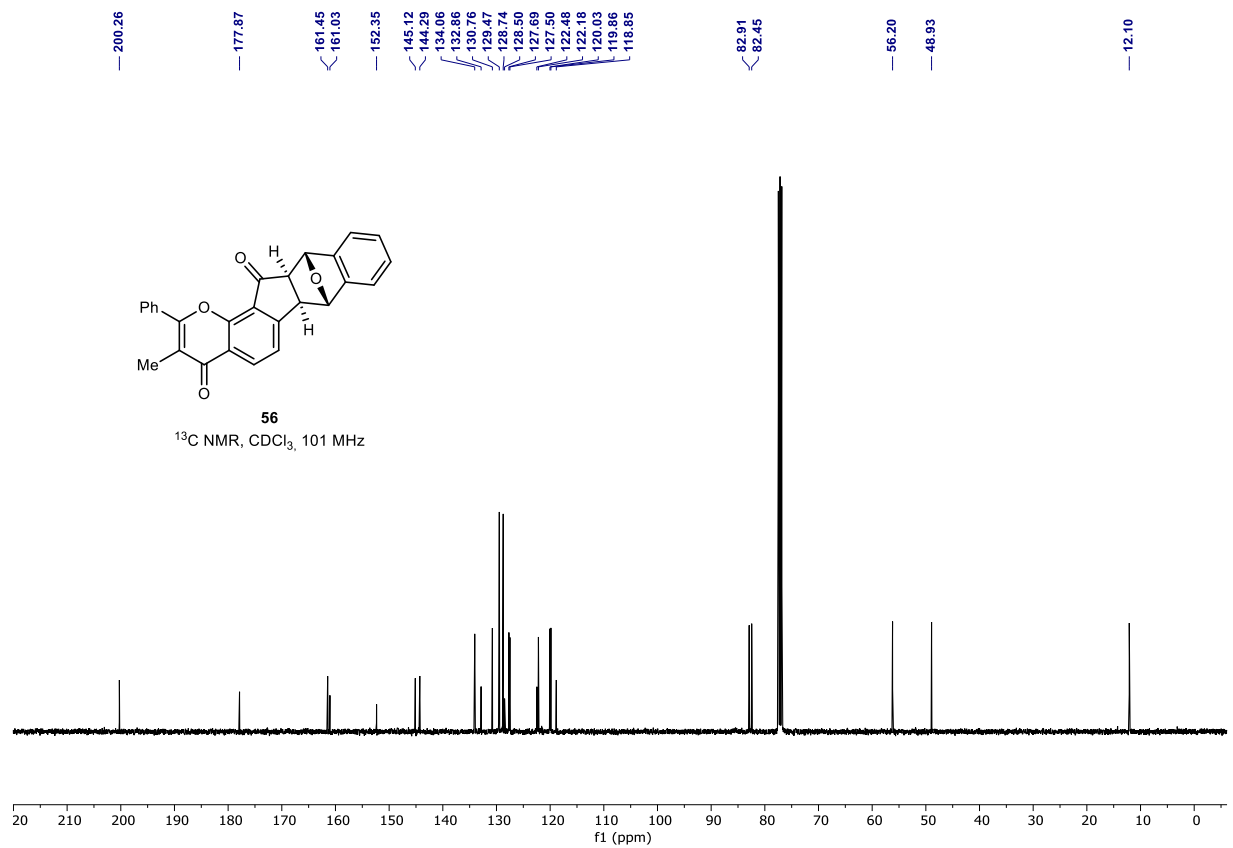
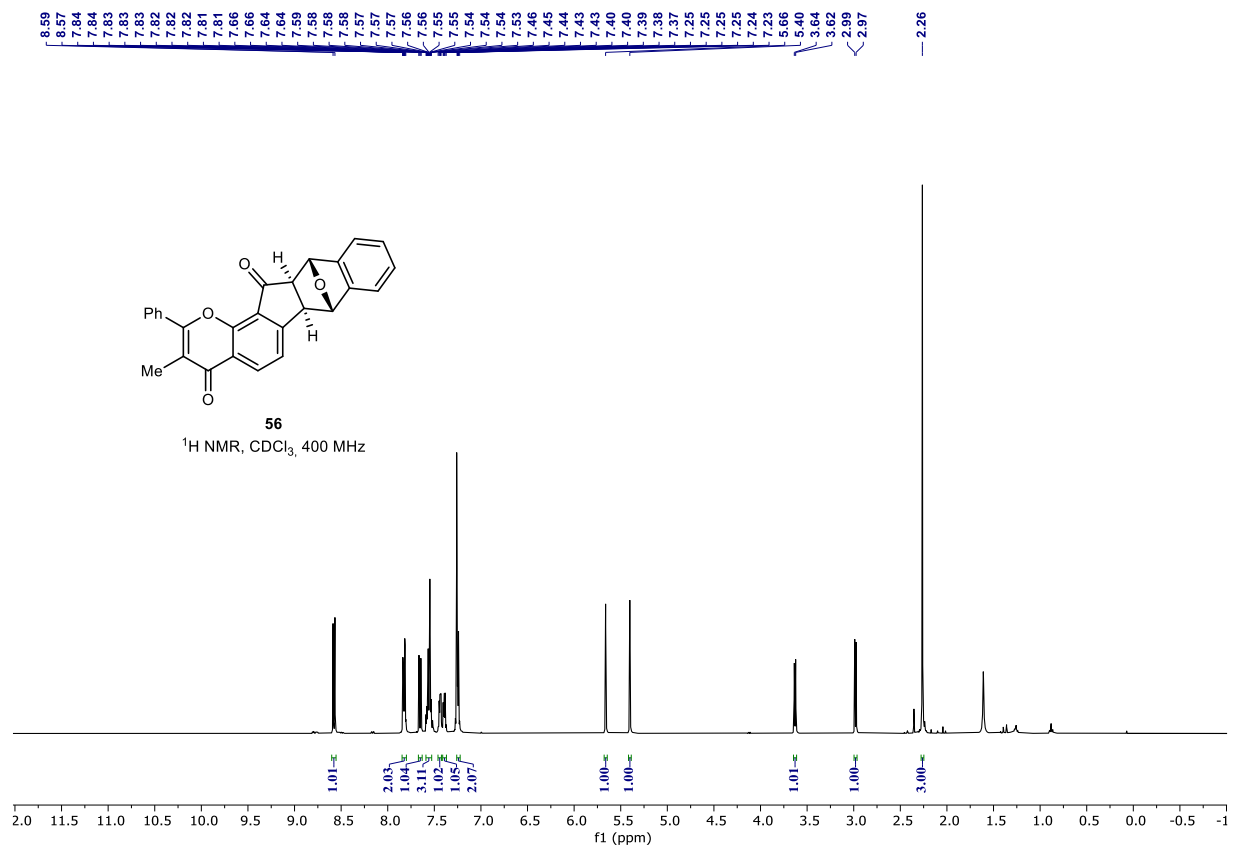


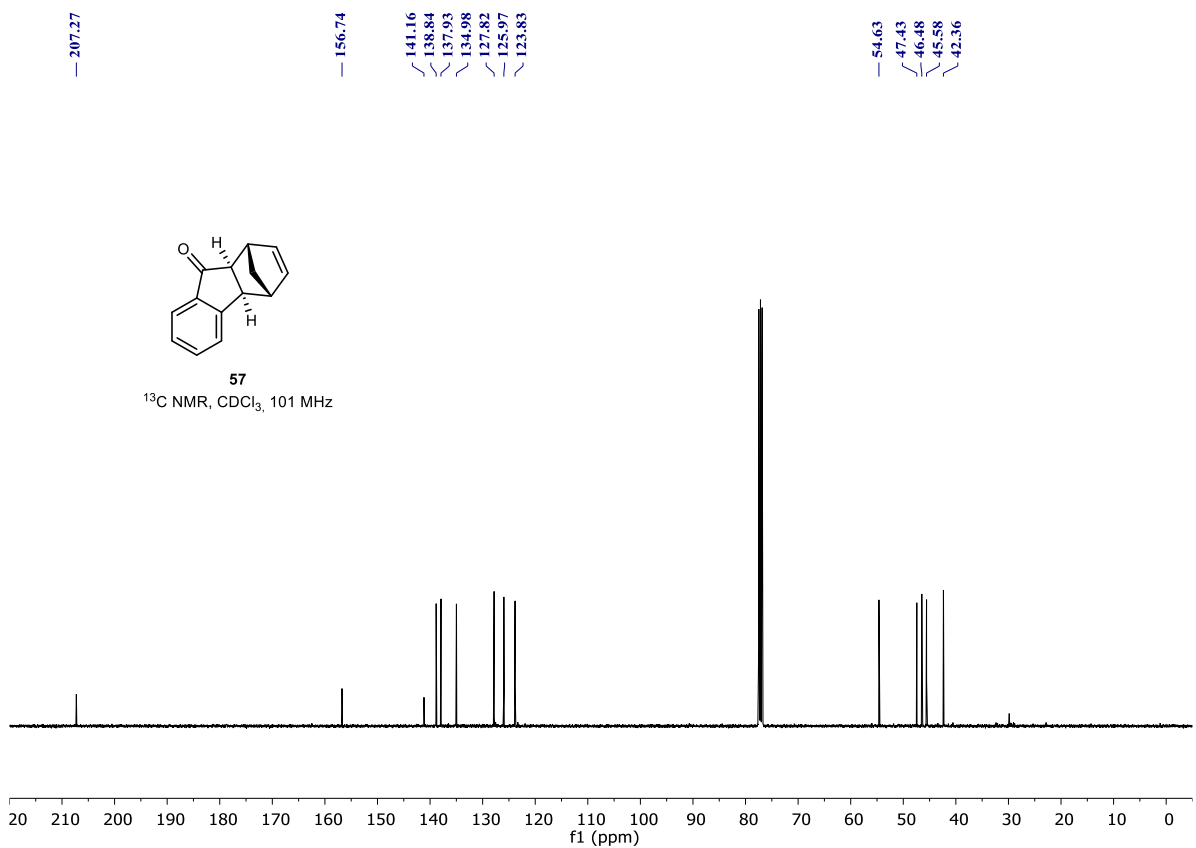
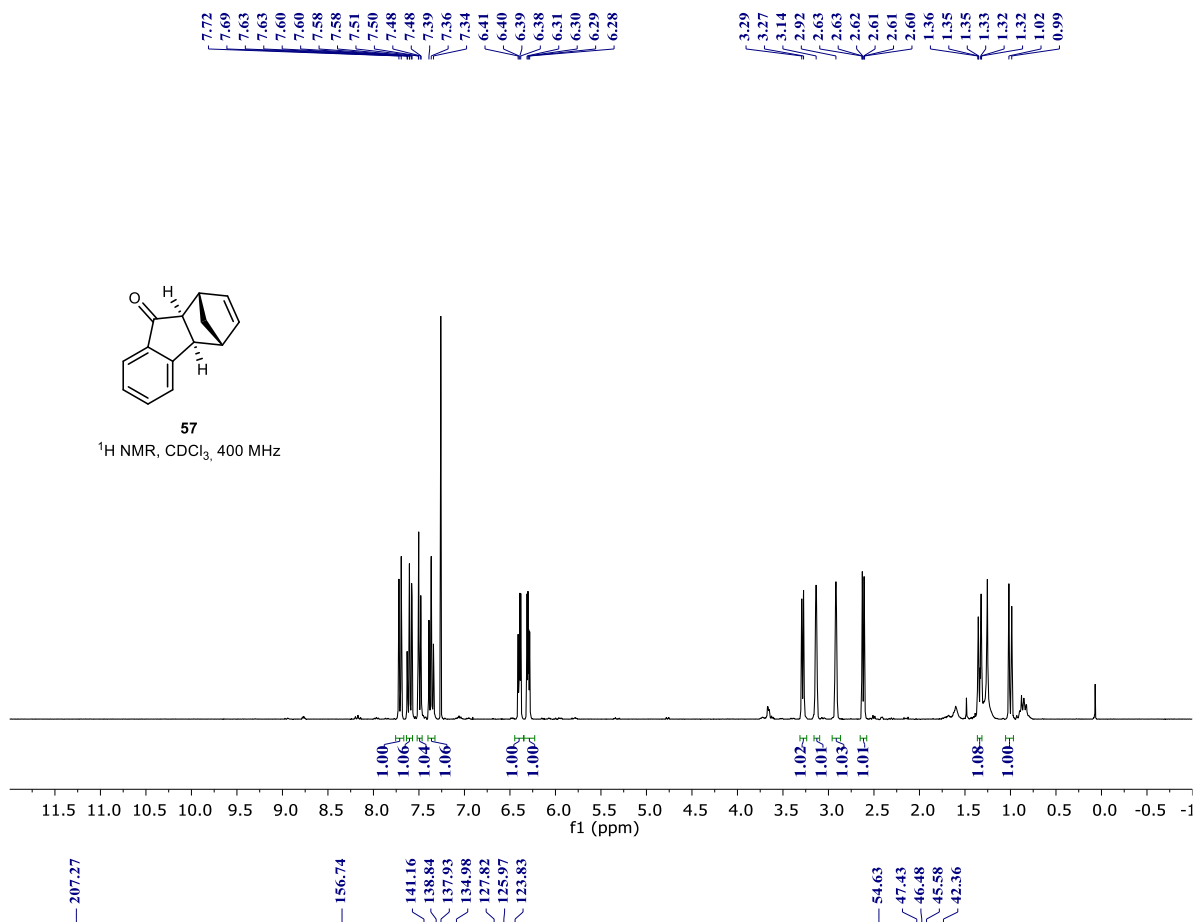


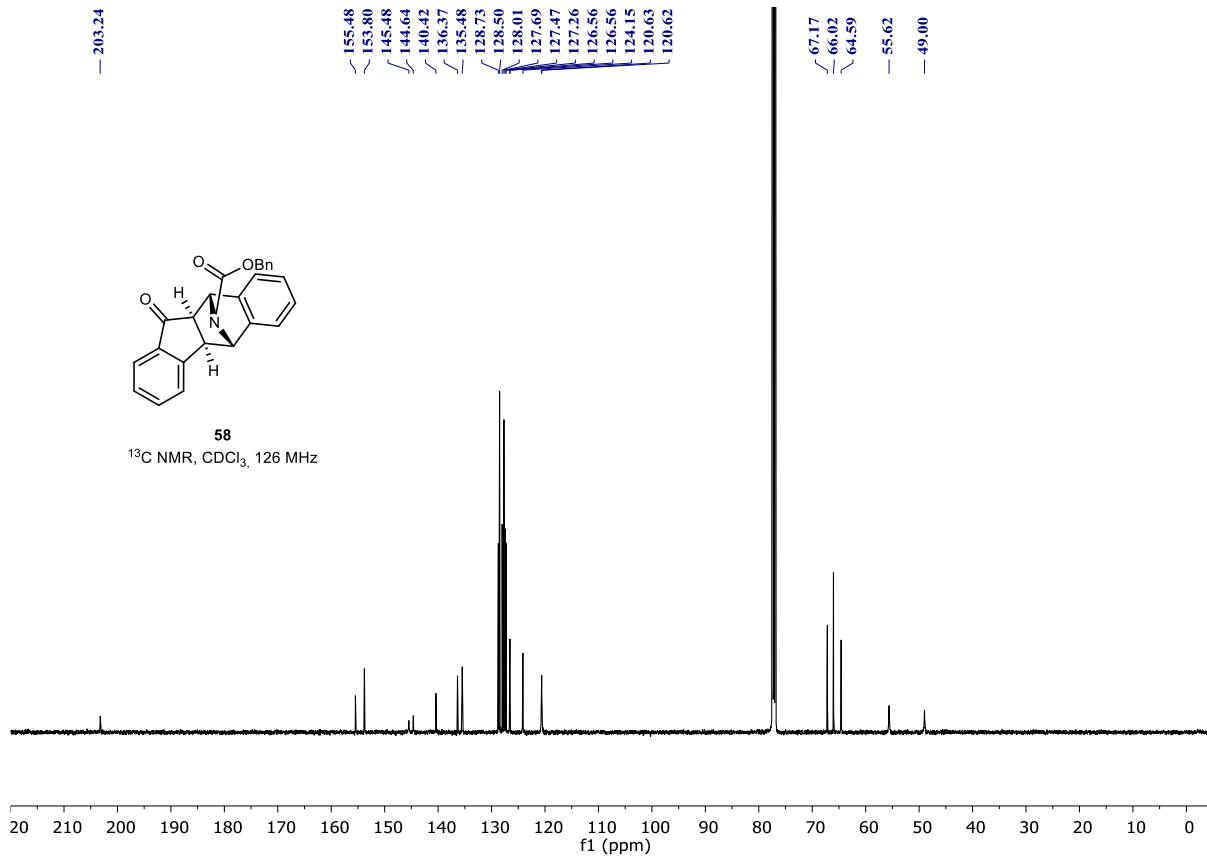
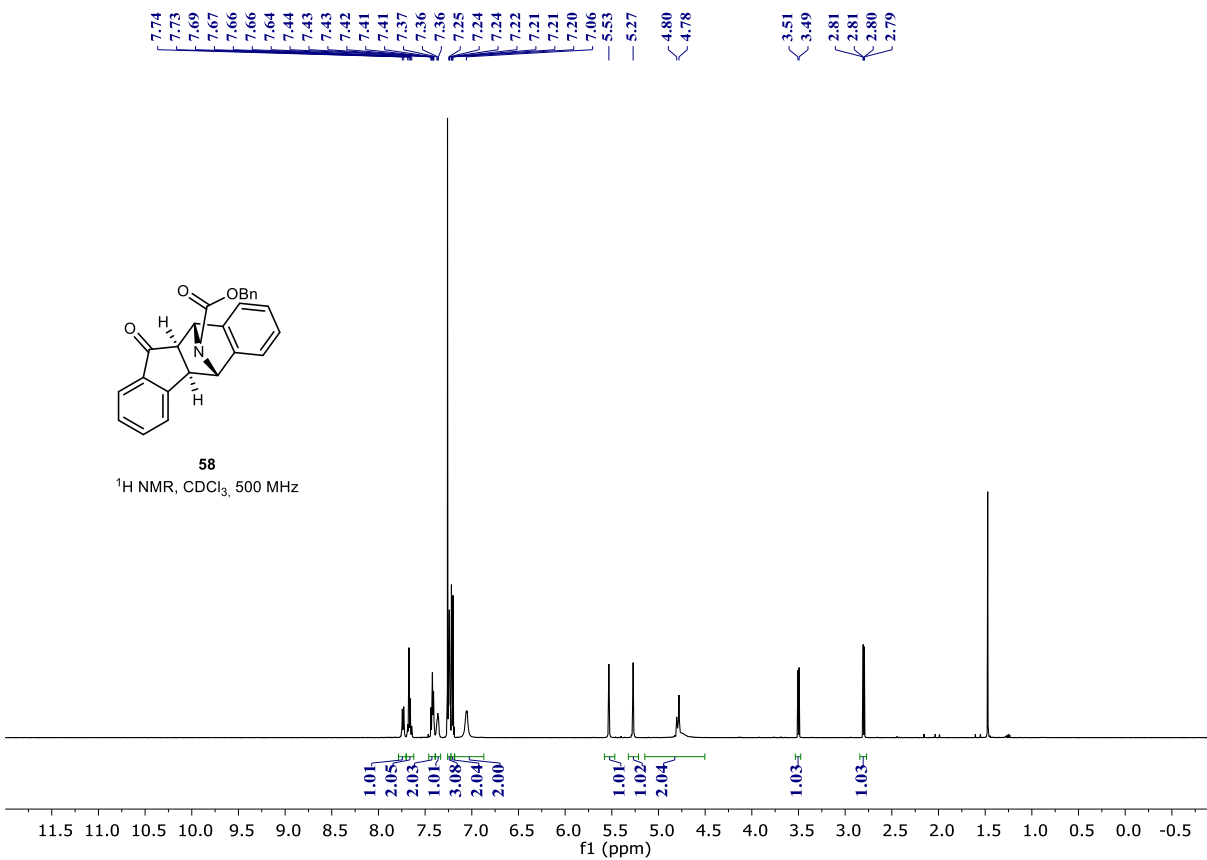


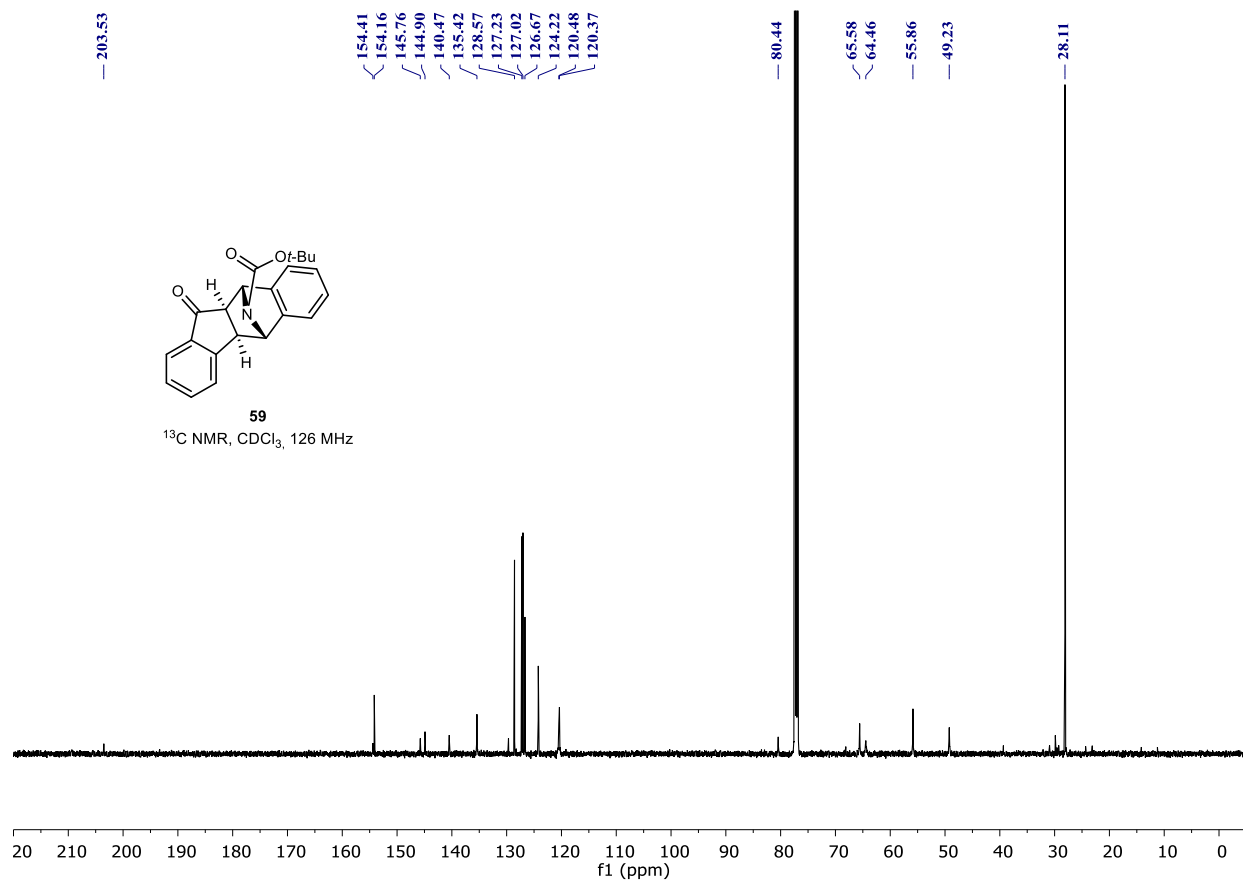
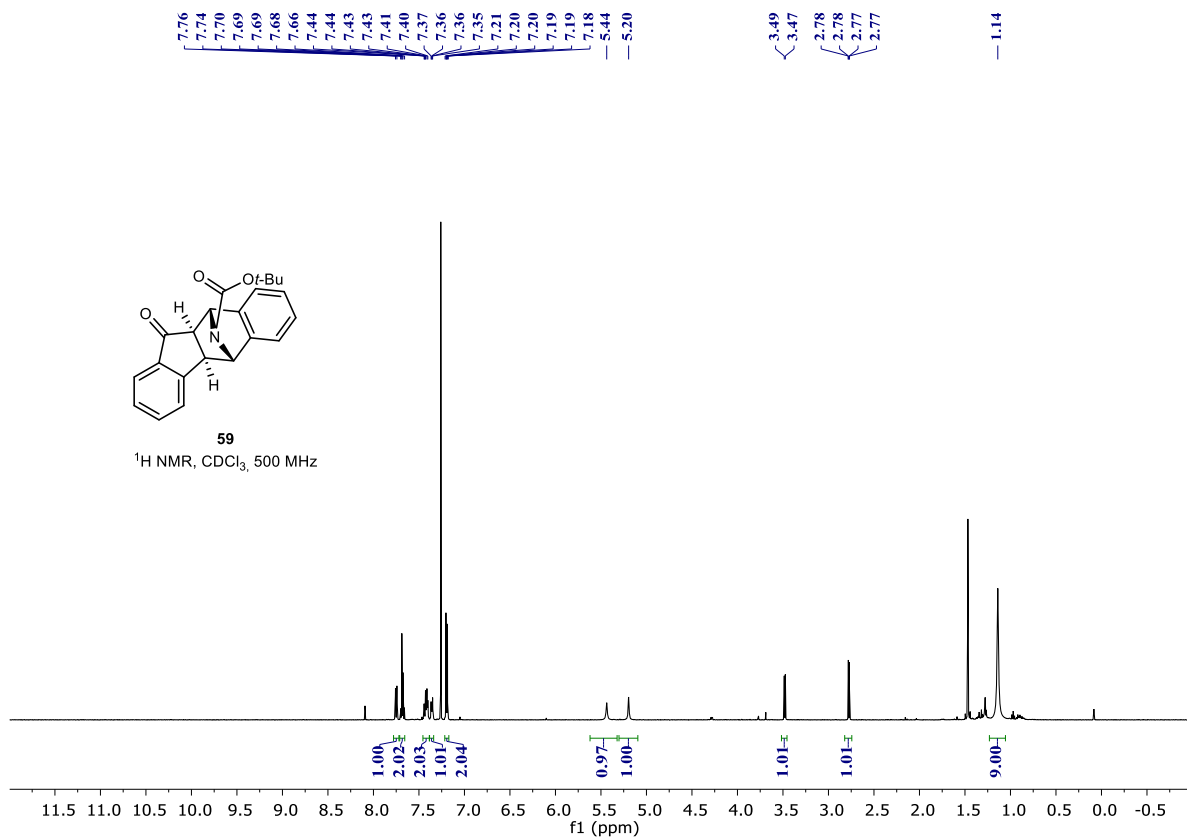


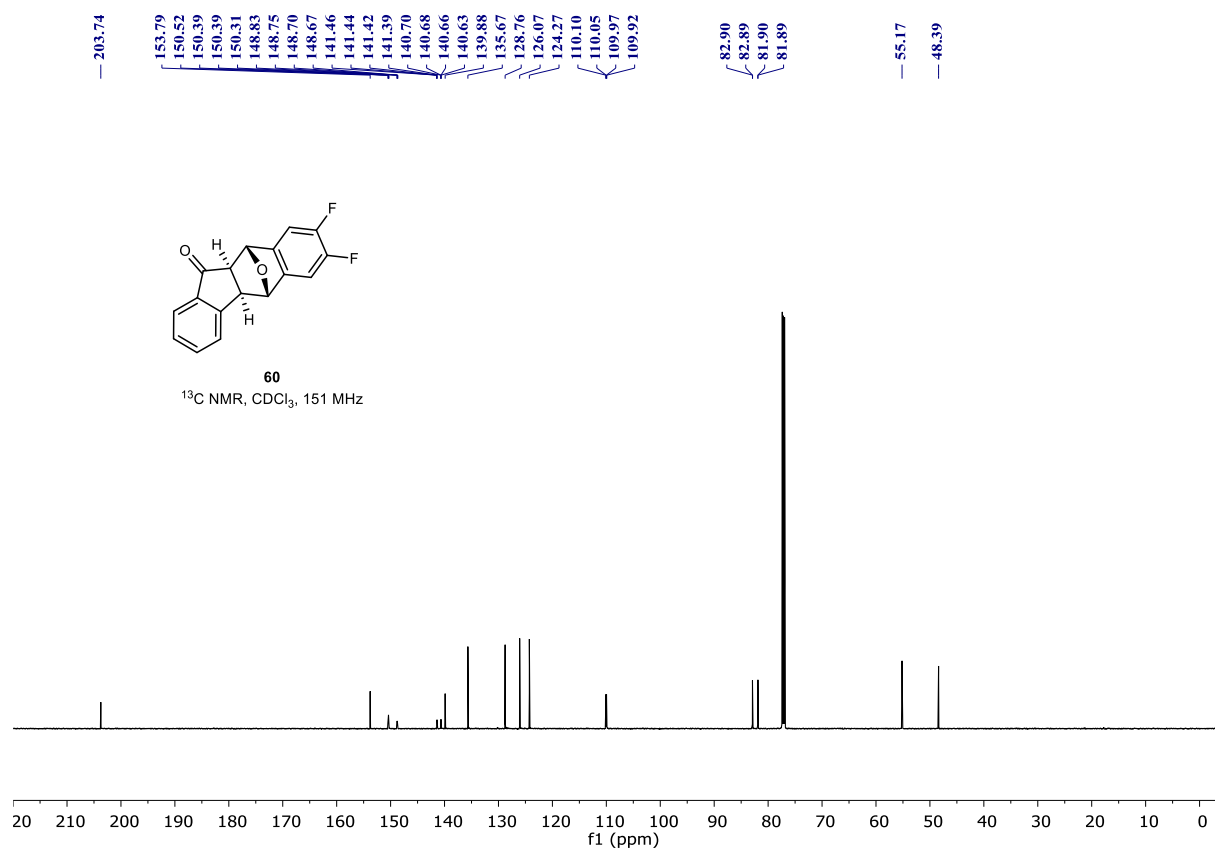
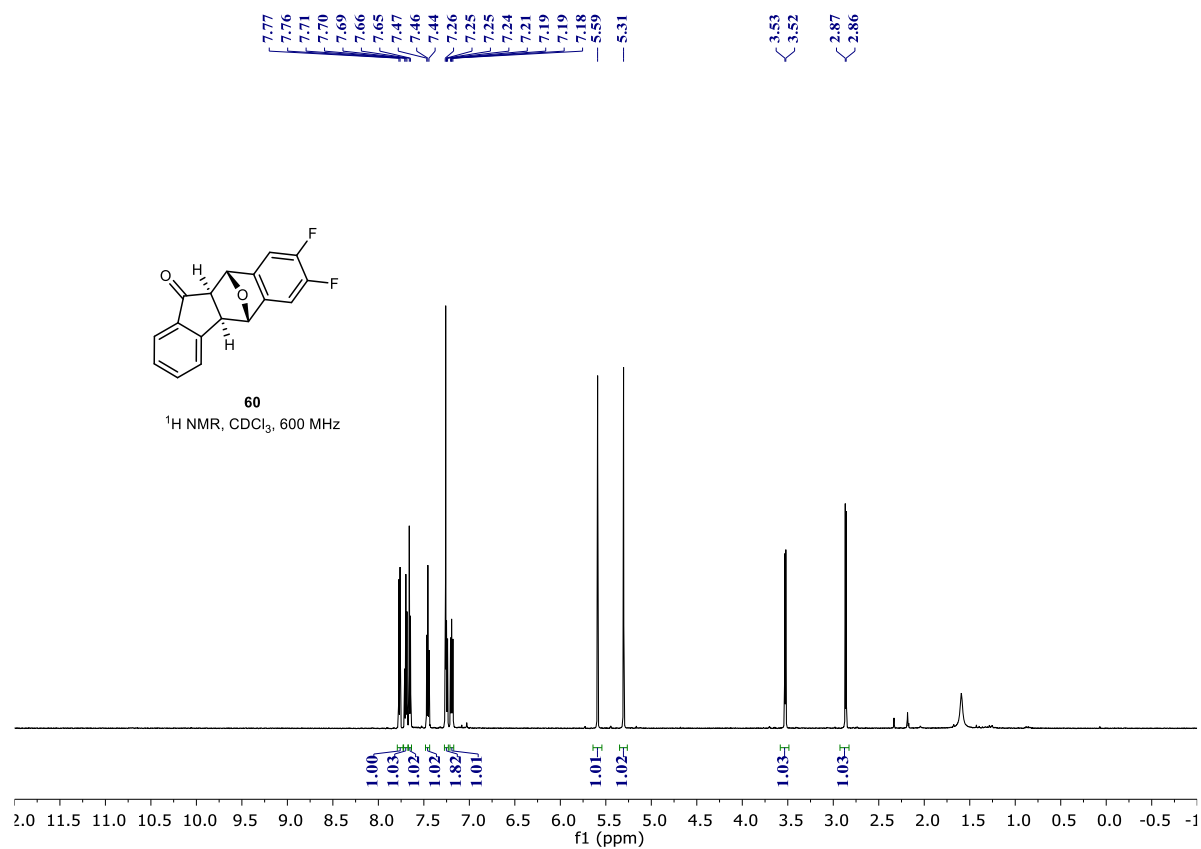


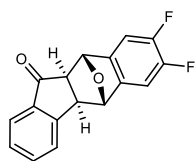






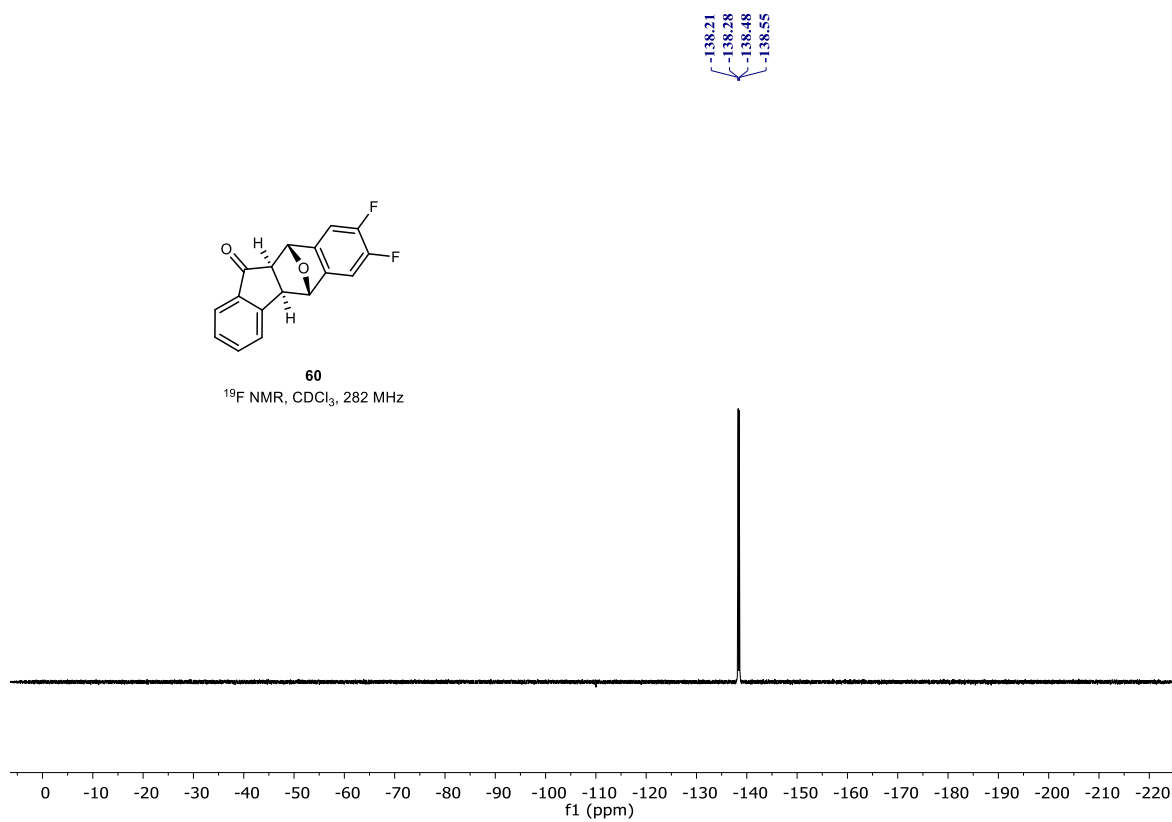


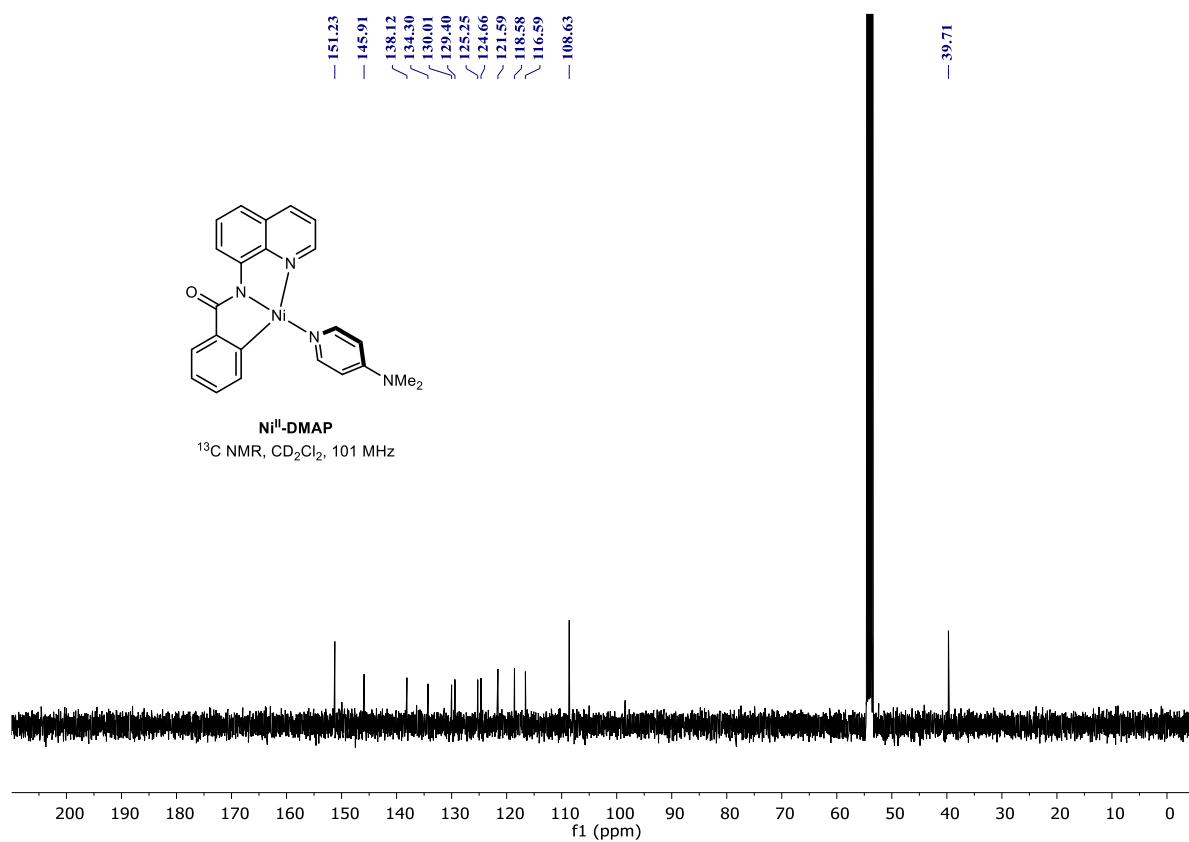
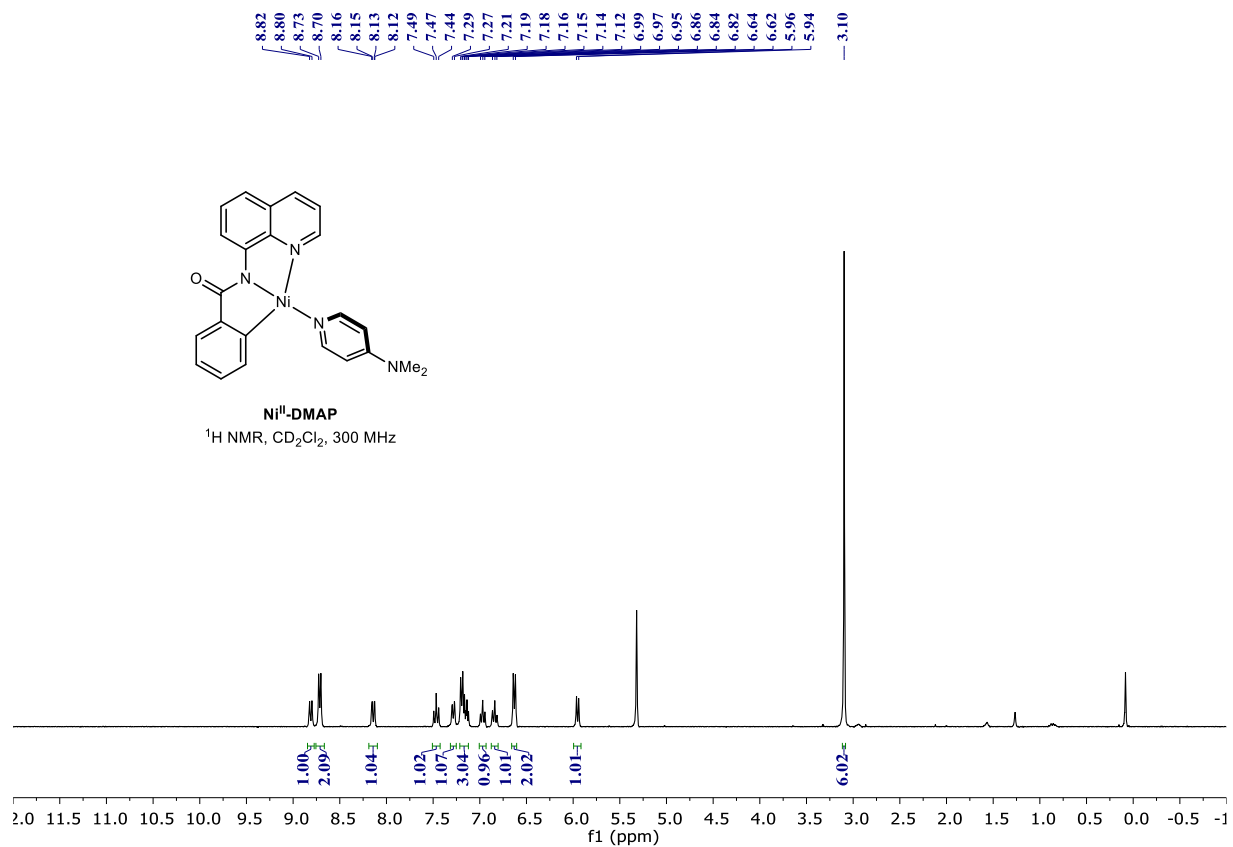


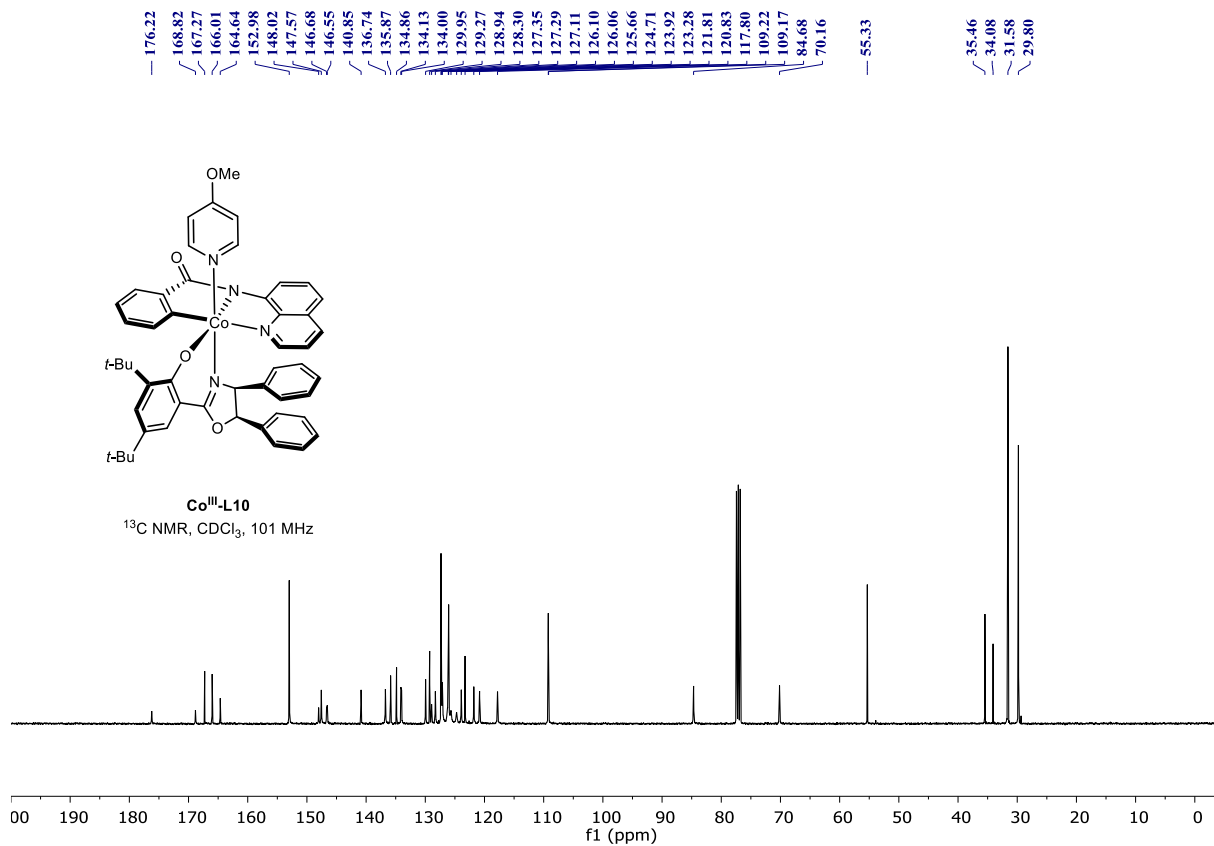
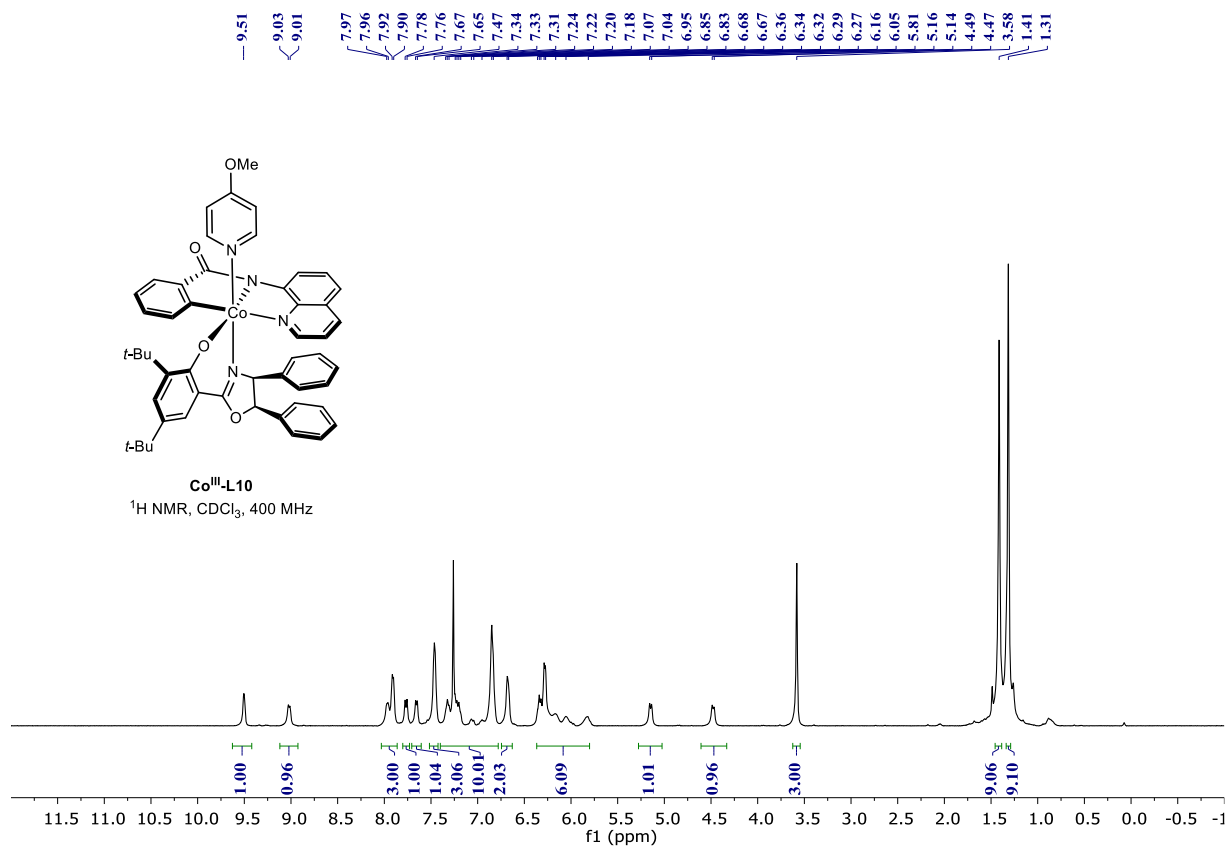


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^{19}F NMR, CDCl_3 , 282 MHz







Cartesian Coordinates of the Optimized Structures

Nickel catalysis

Alkene: In Ni and Co catalyzed reaction energy profile

Alkene¹: $\nu_{\text{lowest}} = 133.5694 \text{ cm}^{-1}$

19

C	1.338508	1.154844	0.457477
O	1.543043	0.319029	1.620280
C	2.253752	0.454195	-0.569596
C	2.195677	-0.850396	-0.257093
C	1.245945	-0.931487	0.956904
C	-0.165648	-0.617443	0.424313
C	-0.104474	0.753961	0.096220
C	-1.201074	1.417401	-0.436184
C	-2.390612	0.675566	-0.631399
C	-2.451380	-0.684117	-0.306104
C	-1.324762	-1.354870	0.227092
H	1.531716	2.211922	0.684512
H	2.747978	0.938951	-1.414446
H	2.630119	-1.704329	-0.781535
H	1.354164	-1.783918	1.640983
H	-1.161362	2.481915	-0.692218
H	-3.276916	1.174353	-1.038187
H	-3.384580	-1.236241	-0.461426
H	-1.380093	-2.419336	0.480408

Intermediate-0: In Ni catalyzed reaction energy profile

Int0²: $\nu_{\text{lowest}} = 13.2583 \text{ cm}^{-1}$

Int0⁴: $\nu_{\text{lowest}} = 12.0558 \text{ cm}^{-1}$

Int0⁶: $\nu_{\text{lowest}} = 9.7182 \text{ cm}^{-1}$

90				90				90			
Ni	-0.676334	0.033935	-1.155258	Ni	-0.659800	-0.271694	-1.071962	Ni	-0.655114	0.135446	-1.110683
C	-1.228102	2.613759	-1.991124	C	-1.333882	2.170709	-2.418645	C	-1.679796	2.786615	-1.683259
C	1.171216	2.227621	-1.940049	C	1.048919	1.820112	-2.641805	C	0.655446	2.664907	-2.338551
C	-1.030820	3.956462	-2.349465	C	-1.219409	3.458037	-2.975878	C	-1.679644	4.182824	-1.874140
C	1.366858	3.573588	-2.305827	C	1.171888	3.106326	-3.202422	C	0.655989	4.058316	-2.538795
H	2.039105	1.581857	-1.778343	H	1.949752	1.206148	-2.514451	H	1.576535	2.096236	-2.510796
C	0.275552	4.437096	-2.505219	C	0.040874	3.925708	-3.368306	C	-0.508186	4.814912	-2.305205
H	-1.909961	4.593227	-2.500211	H	-2.123869	4.067536	-3.084335	H	-2.602897	4.740003	-1.679325
H	2.388909	3.949174	-2.432763	H	2.158384	3.472333	-3.513437	H	1.571113	4.558263	-2.878665
H	0.449772	5.481861	-2.783953	H	0.147795	4.925651	-3.803342	H	-0.494860	5.898906	-2.464169
N	-2.431378	0.668373	-1.491728	N	-2.531044	0.379782	-1.427778	N	-2.652523	0.712596	-1.118244
C	-3.009633	-1.481548	-0.718196	C	-3.135748	-1.634638	-0.373314	C	-2.951988	-1.580251	-0.824713
C	-1.139041	-2.800720	-0.228534	C	-1.319951	-2.960798	0.260344	C	-0.966957	-2.864413	-0.756938
C	-3.920644	-2.510594	-0.325178	C	-4.077328	-2.543464	0.205284	C	-3.759338	-2.738959	-0.595282
C	-3.462347	-0.201585	-1.182523	C	-3.564328	-0.412063	-1.014614	C	-3.554177	-0.275561	-0.943419
C	-1.965432	-3.872213	0.181856	C	-2.174128	-3.905587	0.871141	C	-1.679722	-4.023592	-0.513818
H	-0.045925	-2.860485	-0.211721	H	-0.231713	-3.082164	0.257621	H	0.123315	-2.848461	-0.827827

C	-3.345168	-3.727348	0.134894	C	-3.546541	-3.698058	0.842485	C	-3.098218	-3.985584	-0.437576
C	-5.315616	-2.246209	-0.417006	C	-5.465825	-2.245765	0.100462	C	-5.172952	-2.551128	-0.530362
C	-4.846111	0.018689	-1.263612	C	-4.949977	-0.174240	-1.117402	C	-4.998173	-0.139667	-0.884348
H	-1.505410	-4.800784	0.532070	H	-1.743696	-4.788893	1.352208	H	-1.139373	-4.966873	-0.387460
H	-4.002713	-4.544162	0.452086	H	-4.231014	-4.416326	1.307176	H	-3.678667	-4.894605	-0.253161
C	-5.743934	-1.007956	-0.881664	C	-5.870212	-1.089533	-0.559943	C	-5.769716	-1.266876	-0.681955
H	-6.031765	-3.019129	-0.121308	H	-6.197427	-2.938435	0.528433	H	-5.808060	-3.427500	-0.359616
H	-5.205493	0.987115	-1.612195	H	-5.284236	0.739431	-1.610288	H	-5.423001	0.859849	-0.985275
H	-6.818483	-0.806461	-0.954409	H	-6.940165	-0.869768	-0.647452	H	-6.859974	-1.178885	-0.631814
N	-1.652627	-1.652950	-0.663786	N	-1.791062	-1.870424	-0.346719	N	-1.594001	-1.646974	-0.926017
C	-2.580557	2.013486	-1.808225	C	-2.664599	1.652498	-1.964247	C	-2.910586	2.078614	-1.233197
O	-3.654101	2.613739	-1.904114	O	-3.719986	2.296788	-2.038814	O	-3.988853	2.632681	-0.973269
O	0.999496	-0.822021	-1.275441	O	1.047153	-1.163067	-0.959943	O	1.139093	-0.503195	-1.383884
C	2.077173	-0.643742	-0.546937	C	2.144512	-0.804916	-0.360720	C	2.201943	-0.439461	-0.640324
C	2.077433	0.050069	0.712816	C	2.176434	0.231736	0.645623	C	2.179203	0.115429	0.693565
C	3.331681	-1.175832	-1.020363	C	3.390875	-1.460472	-0.698290	C	3.465604	-0.928650	-1.153021
C	3.269721	0.202596	1.464491	C	3.382520	0.577550	1.293158	C	3.355709	0.173786	1.475130
C	0.863808	0.639045	1.234254	C	0.967781	0.934254	1.022335	C	0.953210	0.628840	1.262884
C	4.464292	-1.000807	-0.224903	C	4.543792	-1.064493	-0.025388	C	4.582378	-0.841735	-0.327410
C	4.478008	-0.319300	1.020169	C	4.582374	-0.057000	0.976624	C	4.570411	-0.301894	0.988688
H	3.197634	0.749741	2.406125	H	3.338726	1.365531	2.046743	H	3.274580	0.606869	2.473225
N	-0.314934	0.629017	0.672240	N	-0.216726	0.787436	0.489562	N	-0.231064	0.664521	0.698935
O	0.912551	1.290022	2.419850	O	1.033743	1.844537	2.017922	O	0.997296	1.134465	2.512822
H	5.411106	-1.407231	-0.589609	H	5.485136	-1.554239	-0.286195	H	5.536276	-1.208762	-0.713573
C	-1.285728	1.332572	1.512007	C	-1.181165	1.655784	1.167445	C	-1.214065	1.196482	1.649785
C	-0.349828	2.059189	2.543673	C	-0.246987	2.597272	2.008533	C	-0.297304	1.816744	2.762353
H	-1.803691	2.094199	0.905193	H	-1.702441	2.261336	0.407493	H	-1.781000	2.005602	1.160435
C	-2.324104	0.366847	2.050006	C	-2.217428	0.823881	1.898267	C	-2.190385	0.115998	2.073042
C	-1.942085	-0.877319	2.585775	C	-1.842798	-0.311145	2.641362	C	-1.756236	-1.200374	2.313490
C	-3.688943	0.690222	1.977638	C	-3.578547	1.156289	1.795326	C	-3.554614	0.424812	2.202076
C	-2.909022	-1.774115	3.055524	C	-2.813026	-1.092336	3.280586	C	-2.673922	-2.191399	2.680662
H	-0.882039	-1.151006	2.615323	H	-0.787214	-0.597896	2.697309	H	-0.701315	-1.459974	2.179015
C	-4.658942	-0.207891	2.444532	C	-4.550898	0.375609	2.435584	C	-4.473249	-0.565822	2.574020
H	-3.994161	1.639114	1.522634	H	-3.879756	2.007721	1.174963	H	-3.903962	1.436191	1.965585
C	-4.270480	-1.439884	2.987012	C	-4.170172	-0.748987	3.179695	C	-4.034555	-1.875300	2.812364
H	-2.600775	-2.741815	3.464736	H	-2.511227	-1.979146	3.847480	H	-2.329538	-3.217723	2.841061
H	-5.720046	0.047831	2.364118	H	-5.609452	0.632347	2.329670	H	-5.537049	-0.319428	2.648448
H	-5.028137	-2.146764	3.341217	H	-4.931020	-1.367956	3.666542	H	-4.754794	-2.654943	3.081083
C	-0.134437	1.748510	-1.786538	C	-0.209121	1.333339	-2.256429	C	-0.515443	2.019852	-1.913113
C	3.403438	-1.902218	-2.377624	C	3.424047	-2.533234	-1.800922	C	3.553369	-1.509745	-2.575347
C	5.796091	-0.180808	1.798848	C	5.918439	0.292471	1.648112	C	5.872643	-0.262039	1.801394
C	2.974184	-0.934793	-3.510284	C	2.960751	-1.908056	-3.142719	C	3.141164	-0.429562	-3.608812
H	1.946451	-0.574790	-3.355856	H	1.936063	-1.515306	-3.066154	H	2.101290	-0.107907	-3.451695
H	3.651167	-0.062809	-3.549302	H	3.632811	-1.082039	-3.435661	H	3.801816	0.452313	-3.532143
H	3.024957	-1.451528	-4.486114	H	2.988121	-2.671806	-3.940976	H	3.231648	-0.837777	-4.631568
C	2.477114	-3.144772	-2.366367	C	2.497820	-3.717541	-1.422400	C	2.621289	-2.741835	-2.704335
H	2.772844	-3.840925	-1.560709	H	2.810054	-4.163145	-0.460799	H	2.895473	-3.516105	-1.965663

H	1.428652	-2.849266	-2.214737	H	1.453142	-3.384942	-1.339811	H	1.570093	-2.459106	-2.549690
H	2.555771	-3.681643	-3.329349	H	2.557209	-4.501163	-2.199212	H	2.720220	-3.180503	-3.713551
C	4.833377	-2.388331	-2.691045	C	4.845284	-3.096037	-2.006728	C	4.987052	-1.966186	-2.915310
H	5.550298	-1.550188	-2.748457	H	5.558261	-2.311691	-2.316637	H	5.706595	-1.129179	-2.876862
H	5.199199	-3.108175	-1.937244	H	5.234060	-3.579663	-1.092811	H	5.339481	-2.761292	-2.234402
H	4.836144	-2.898047	-3.670269	H	4.820489	-3.858281	-2.804586	H	5.002718	-2.373157	-3.941015
C	6.826288	0.583875	0.931569	C	6.918878	0.778825	0.569657	C	6.922543	0.586269	1.040898
H	7.786104	0.684797	1.470426	H	7.890456	1.027888	1.033459	H	7.870502	0.618906	1.607670
H	7.025667	0.057830	-0.018106	H	7.098248	0.004622	-0.196112	H	7.139400	0.166100	0.043711
H	6.456126	1.595106	0.688027	H	6.535603	1.679694	0.059719	H	6.563525	1.621088	0.903811
C	6.347592	-1.589546	2.129286	C	6.485184	-0.970269	2.343940	C	6.406645	-1.705558	1.977961
H	6.533044	-2.176581	1.213094	H	6.649630	-1.790904	1.624518	H	6.607158	-2.186254	1.004965
H	7.302738	-1.511266	2.680077	H	7.454109	-0.740858	2.823150	H	7.350835	-1.696282	2.551850
H	5.631393	-2.151981	2.753581	H	5.790191	-1.332965	3.121226	H	5.675459	-2.328778	2.521628
C	5.602311	0.589458	3.118978	C	5.758531	1.403276	2.703726	C	5.660940	0.356278	3.196553
H	5.232102	1.614090	2.939849	H	5.379586	2.338131	2.255207	H	5.300941	1.397728	3.128754
H	4.888198	0.076179	3.786548	H	5.067275	1.100959	3.509717	H	4.933989	-0.223566	3.791638
H	6.566558	0.667244	3.651361	H	6.737696	1.623044	3.163796	H	6.617047	0.365617	3.748225
C	-0.044122	3.476764	2.055461	C	0.015803	3.891211	1.236488	C	-0.067652	3.303875	2.488938
H	0.764007	3.924486	2.657246	H	0.817651	4.473012	1.720654	H	0.725248	3.698672	3.145523
H	0.264646	3.458717	0.995723	H	0.310043	3.665154	0.196839	H	0.224210	3.461668	1.436367
H	-0.945890	4.107202	2.143166	H	-0.902236	4.503290	1.208984	H	-0.998526	3.866202	2.676582
C	-0.783226	2.002502	3.999754	C	-0.655409	2.823980	3.455253	C	-0.699367	1.520707	4.198379
H	-0.033913	2.501457	4.636877	H	0.091434	3.454466	3.966178	H	0.037146	1.955227	4.894846
H	-1.750213	2.518428	4.121105	H	-1.632291	3.334189	3.489838	H	-1.687664	1.962782	4.406683
H	-0.904498	0.961293	4.334708	H	-0.748556	1.867511	3.991922	H	-0.765699	0.435725	4.370518

Intermediate-1: In Ni catalyzed reaction energy profile

Int1 ² : $\nu_{\text{lowest}} = 15.5844 \text{ cm}^{-1}$				Int1 ⁴ : $\nu_{\text{lowest}} = 9.0946 \text{ cm}^{-1}$				Int1 ⁶ : $\nu_{\text{lowest}} = 11.4371 \text{ cm}^{-1}$			
109				109				109			
Ni	0.408542	0.000211	0.323828	Ni	-0.504794	0.095017	0.236990	Ni	-0.420890	0.040665	0.277267
C	0.785234	0.227215	3.064328	C	-1.365369	-0.474174	2.926712	C	-1.702666	-0.613559	2.833099
C	-1.104931	-1.222257	2.581820	C	0.560056	0.981132	3.049008	C	-0.036463	1.108208	3.195187
C	0.562655	0.098364	4.444564	C	-1.386393	-0.599276	4.330365	C	-1.931854	-0.709268	4.222208
C	-1.325090	-1.351159	3.967120	C	0.549864	0.860133	4.450225	C	-0.258248	1.015315	4.582183
H	-1.767329	-1.739211	1.881871	H	1.332877	1.599071	2.571532	H	0.709910	1.817801	2.815275
C	-0.500181	-0.693923	4.896523	C	-0.425125	0.072466	5.092883	C	-1.208570	0.110051	5.094154
H	1.232091	0.627825	5.132172	H	-2.153227	-1.232162	4.791272	H	-2.673561	-1.430571	4.583238
H	-2.155749	-1.973562	4.319891	H	1.305070	1.383942	5.049545	H	0.312137	1.652405	5.269391
H	-0.690135	-0.804054	5.969584	H	-0.424910	-0.016258	6.184903	H	-1.377454	0.049115	6.174966
N	1.831736	0.995145	1.120845	N	-2.087468	-1.036568	0.732766	N	-2.028289	-1.237687	0.566810
C	2.271591	1.521456	-1.132171	C	-2.262889	-1.402953	-1.590989	C	-1.905523	-1.410284	-1.760247
C	0.791228	0.485034	-2.622154	C	-0.500630	-0.534968	-2.845903	C	-0.076253	-0.302994	-2.762435
C	2.969840	2.185313	-2.189025	C	-2.867319	-1.998957	-2.743761	C	-2.349387	-1.914502	-3.024887
C	2.636605	1.695309	0.244459	C	-2.840868	-1.561640	-0.272398	C	-2.597731	-1.752838	-0.543814
C	1.422343	1.100634	-3.727066	C	-1.014615	-1.097569	-4.036624	C	-0.425710	-0.774778	-4.015867

H	-0.067307	-0.185977	-2.730587	H	0.425781	0.049232	-2.837359	H	0.802767	0.326376	-2.598604
C	2.503363	1.944585	-3.510856	C	-2.195552	-1.824495	-3.984549	C	-1.582677	-1.581832	-4.174967
C	4.062684	3.029652	-1.848112	C	-4.090622	-2.710368	-2.584120	C	-3.527439	-2.717071	-3.035458
C	3.722008	2.532521	0.539289	C	-4.069543	-2.248787	-0.172080	C	-3.800219	-2.558494	-0.611826
H	1.047296	0.907369	-4.736308	H	-0.478751	-0.951334	-4.979229	H	0.196266	-0.515261	-4.878373
H	3.004473	2.435505	-4.352316	H	-2.619881	-2.270701	-4.890752	H	-1.880630	-1.955646	-5.159241
C	4.414077	3.180804	-0.511703	C	-4.668150	-2.807701	-1.321293	C	-4.237864	-3.017346	-1.840716
H	4.610692	3.548395	-2.640770	H	-4.569448	-3.158398	-3.460742	H	-3.889272	-3.102718	-3.995216
H	4.012110	2.668183	1.581309	H	-4.525865	-2.350417	0.812469	H	-4.318869	-2.784187	0.319940
H	5.258752	3.828471	-0.251313	H	-5.618580	-3.340649	-1.206765	H	-5.146832	-3.624907	-1.900610
N	1.214546	0.688948	-1.377486	N	-1.113659	-0.679416	-1.674174	N	-0.819256	-0.600228	-1.642011
C	1.887812	1.058823	2.500138	C	-2.340635	-1.234242	2.086191	C	-2.431876	-1.492236	1.881381
O	2.705627	1.706837	3.164058	O	-3.218678	-1.973920	2.550981	O	-3.239536	-2.368106	2.222264
O	-0.834296	-1.177789	-0.533985	O	0.956928	1.190927	-0.507771	O	0.971451	1.334984	-0.126214
C	-2.147822	-1.145917	-0.528113	C	2.252301	1.071925	-0.471731	C	2.267445	1.243874	-0.201472
C	-2.913829	0.006074	-0.136337	C	2.915661	-0.088974	0.073871	C	2.985273	0.052525	0.186553
C	-2.881930	-2.321409	-0.937098	C	3.090679	2.132085	-1.000013	C	3.044089	2.377508	-0.666203
C	-4.330971	-0.015171	-0.141646	C	4.323473	-0.161852	0.142905	C	4.394022	-0.001913	0.126057
C	-2.260419	1.222153	0.296858	C	2.152044	-1.234642	0.529621	C	2.276628	-1.119010	0.659146
C	-4.276256	-2.270142	-0.933232	C	4.473914	1.993163	-0.902513	C	4.429800	2.248848	-0.717247
C	-5.039704	-1.141439	-0.540471	C	5.129817	0.871548	-0.331773	C	5.142052	1.082054	-0.331187
H	-4.842115	0.893070	0.181939	H	4.756176	-1.064138	0.577954	H	4.874279	-0.927706	0.446376
N	-0.976424	1.432398	0.397706	N	0.856326	-1.372501	0.503712	N	0.982585	-1.297779	0.678315
O	-3.035695	2.276271	0.649045	O	2.838340	-2.297056	1.015649	O	3.009817	-2.158465	1.117751
H	-4.820168	-3.165797	-1.244242	H	5.099490	2.801729	-1.288445	H	5.012120	3.102680	-1.071449
C	-0.733608	2.809787	0.835666	C	0.503901	-2.713818	0.979070	C	0.697378	-2.669673	1.120731
C	-2.153416	3.240800	1.346005	C	1.842910	-3.205223	1.632288	C	2.061038	-3.102646	1.759582
H	-0.033191	2.804643	1.686345	H	-0.258276	-2.619376	1.769216	H	-0.075087	-2.638077	1.906093
C	-0.121517	3.633431	-0.282369	C	-0.084598	-3.547416	-0.142725	C	0.179359	-3.504233	-0.035320
C	-0.581006	3.508532	-1.606184	C	0.493390	-3.549798	-1.425565	C	0.753957	-3.402572	-1.315526
C	0.931195	4.521635	-0.004943	C	-1.249497	-4.299907	0.083799	C	-0.910222	-4.368179	0.161799
C	-0.004011	4.268333	-2.631592	C	-0.077787	-4.300762	-2.460281	C	0.244994	-4.153090	-2.381616
H	-1.381591	2.797766	-1.835665	H	1.382748	-2.940386	-1.618274	H	1.581163	-2.706966	-1.488909
C	1.512016	5.280289	-1.030319	C	-1.823696	-5.051097	-0.951272	C	-1.419655	-5.121321	-0.904769
H	1.316138	4.597001	1.017862	H	-1.731760	-4.262620	1.067023	H	-1.395399	-4.412288	1.143174
C	1.043092	5.157198	-2.345424	C	-1.238468	-5.054066	-2.224604	C	-0.844272	-5.013686	-2.178073
H	-0.365259	4.157813	-3.659420	H	0.376062	-4.288381	-3.456795	H	0.683645	-4.046953	-3.378707
H	2.344386	5.953851	-0.803515	H	-2.743273	-5.615478	-0.767013	H	-2.286232	-5.770629	-0.745164
H	1.502933	5.741798	-3.149306	H	-1.693968	-5.630220	-3.036975	H	-1.256374	-5.584494	-3.016691
C	-0.043331	-0.428691	2.131270	C	-0.405517	0.325083	2.267365	C	-0.762533	0.295925	2.312174
C	3.506760	-1.742362	1.033613	C	-2.894141	2.294413	1.390245	C	-3.140659	2.139001	1.286384
C	4.344211	-2.987752	0.684760	C	-3.609982	3.574829	0.917273	C	-4.031749	3.247881	0.692775
H	3.704065	-1.230370	1.983524	H	-2.868379	2.070629	2.463430	H	-3.109091	2.016753	2.375644
O	3.841063	-0.904462	-0.096005	O	-3.658434	1.309254	0.662554	O	-3.728379	0.988725	0.642307
C	3.427781	-1.836129	-1.116549	C	-3.436976	1.862899	-0.650764	C	-3.561566	1.454805	-0.714671
C	4.291552	-3.051477	-0.725564	C	-3.969314	3.292171	-0.420181	C	-4.309991	2.798261	-0.618057
C	5.033324	-3.939528	1.423161	C	-3.904759	4.800035	1.498552	C	-4.526402	4.457981	1.158872

H	3.555252	-1.412499	-2.121479	H	-3.913386	1.250578	-1.427702	H	-3.915465	0.710938	-1.439903
C	4.925480	-4.068224	-1.425952	C	-4.630095	4.229719	-1.202073	C	-5.086887	3.550204	-1.488523
C	5.692750	-4.972968	0.716168	C	-4.590449	5.756460	0.712387	C	-5.330199	5.224697	0.282079
H	5.077912	-3.895963	2.516659	H	-3.627737	5.025094	2.534100	H	-4.314783	4.811916	2.173681
C	5.639910	-5.036305	-0.680975	C	-4.945938	5.476639	-0.612063	C	-5.604798	4.779524	-1.016297
H	4.887859	-4.123698	-2.519377	H	-4.910533	4.018108	-2.239719	H	-5.304912	3.207637	-2.505867
H	6.255395	-5.731665	1.270618	H	-4.849645	6.727340	1.148130	H	-5.746726	6.177484	0.626212
H	6.161921	-5.843615	-1.205768	H	-5.479891	6.231444	-1.199411	H	-6.233027	5.388728	-1.675051
C	2.049198	-2.123305	0.702673	C	-1.558591	2.277209	0.621457	C	-1.800789	2.252054	0.535712
H	1.312822	-2.474638	1.425997	H	-0.632573	2.712666	0.995247	H	-0.926842	2.795309	0.893037
C	2.002681	-2.179150	-0.647387	C	-1.903642	2.012813	-0.672570	C	-2.068338	1.834119	-0.729898
H	1.185089	-2.524613	-1.279191	H	-1.292252	2.145924	-1.565526	H	-1.465339	1.960619	-1.629073
C	-2.133761	-3.601743	-1.355568	C	2.460140	3.385818	-1.633569	C	2.347590	3.689641	-1.066574
C	-6.575027	-1.211370	-0.563284	C	6.663932	0.837733	-0.267993	C	6.674225	1.062156	-0.426874
C	-1.272400	-4.109238	-0.171634	C	1.619538	4.139715	-0.573482	C	1.619867	4.274097	0.170862
H	-0.572173	-3.333050	0.166035	H	0.815937	3.496258	-0.191062	H	0.898973	3.549114	0.574738
H	-1.919810	-4.388720	0.678332	H	2.255587	4.453666	0.272895	H	2.346831	4.523615	0.963534
H	-0.695247	-5.002549	-0.472565	H	1.165206	5.043226	-1.019145	H	1.077839	5.196175	-0.105995
C	-1.244293	-3.305780	-2.588881	C	1.560332	2.976760	-2.827141	C	1.337273	3.430704	-2.212452
H	-1.868642	-3.014891	-3.452297	H	2.154217	2.457876	-3.600748	H	1.855456	3.029405	-3.101452
H	-0.545418	-2.483721	-2.375494	H	0.755759	2.306979	-2.491300	H	0.567427	2.712047	-1.900781
H	-0.664698	-4.204313	-2.869198	H	1.107129	3.874490	-3.285194	H	0.843427	4.376263	-2.499724
C	-3.099642	-4.738898	-1.746952	C	3.527545	4.362593	-2.168439	C	3.353020	4.748776	-1.563376
H	-3.755019	-5.029238	-0.906973	H	4.182319	4.739591	-1.363171	H	4.086684	5.020704	-0.784161
H	-3.736209	-4.463018	-2.606286	H	4.161328	3.897000	-2.943955	H	3.903319	4.406209	-2.457591
H	-2.512899	-5.628380	-2.036281	H	3.024428	5.233369	-2.623662	H	2.803824	5.665720	-1.838589
C	-7.051090	-2.343661	0.379772	C	7.166389	2.043080	0.565397	C	7.255393	2.188993	0.463564
H	-8.154013	-2.417065	0.370368	H	8.270449	2.041763	0.615535	H	8.358524	2.194867	0.400384
H	-6.644680	-3.323125	0.073186	H	6.848866	3.002694	0.122125	H	6.893518	3.183016	0.149068
H	-6.724206	-2.150178	1.416433	H	6.771339	1.996897	1.595163	H	6.968343	2.039986	1.518995
C	-7.054526	-1.508432	-2.005374	C	7.238734	0.930098	-1.703499	C	7.094856	1.300085	-1.898851
H	-6.647225	-2.464283	-2.378196	H	6.923284	1.859847	-2.207720	H	6.725805	2.269760	-2.275098
H	-8.157435	-1.573921	-2.040640	H	8.343527	0.917779	-1.676380	H	8.196359	1.299910	-1.986167
H	-6.731474	-0.709617	-2.695690	H	6.896589	0.077765	-2.316125	H	6.694271	0.505970	-2.552697
C	-7.214202	0.111357	-0.099150	C	7.183194	-0.457920	0.384294	C	7.262383	-0.283252	0.039712
H	-6.922547	0.360954	0.936030	H	6.817687	-0.564834	1.420471	H	7.009997	-0.493039	1.093741
H	-6.922956	0.952861	-0.751848	H	6.873288	-1.351454	-0.185205	H	6.896587	-1.122279	-0.577459
H	-8.314725	0.025687	-0.128737	H	8.286751	-0.443371	0.415157	H	8.362746	-0.257285	-0.044693
C	-2.279385	2.946575	2.842483	C	1.832230	-2.894215	3.130300	C	2.064393	-2.780679	3.255401
H	-3.328174	3.049301	3.166943	H	2.836131	-3.043438	3.561689	H	3.081199	-2.883170	3.669444
H	-1.933972	1.921305	3.061658	H	1.514886	-1.851424	3.303885	H	1.704299	-1.751856	3.429117
H	-1.656292	3.652204	3.418679	H	1.119117	-3.560186	3.646044	H	1.390691	-3.473756	3.787951
C	-2.607857	4.640229	0.963753	C	2.261963	-4.631860	1.313500	C	2.531681	-4.513013	1.443151
H	-3.633192	4.818314	1.329110	H	3.235030	-4.855149	1.782469	H	3.518543	-4.695404	1.900756
H	-1.936460	5.387996	1.417738	H	1.510749	-5.337235	1.706039	H	1.813251	-5.244273	1.849228
H	-2.585746	4.775204	-0.128370	H	2.342067	-4.785116	0.226486	H	2.601474	-4.667829	0.355779

Transition State (1-2): In Ni catalyzed reaction energy profile

TS1 ² : $\nu_{\text{lowest}} = -186.9021 \text{ cm}^{-1}$				TS1 ⁴ : $\nu_{\text{lowest}} = -230.1097 \text{ cm}^{-1}$				TS1 ⁶ : $\nu_{\text{lowest}} = -295.5137 \text{ cm}^{-1}$			
109				109				109			
Ni	-0.629489	0.177506	0.120814	Ni	-0.596844	0.178003	0.026087	Ni	-0.451011	0.009307	0.191149
C	-1.319838	0.057281	2.829976	C	-1.194858	0.061408	2.823310	C	-1.679114	-0.330074	2.766332
C	0.938677	0.957834	2.603221	C	1.013732	1.045599	2.631606	C	-0.008288	1.432241	2.966912
C	-1.144117	-0.030989	4.221321	C	-0.980255	-0.166387	4.196336	C	-1.616799	-0.543884	4.160109
C	1.108597	0.845805	3.992558	C	1.243431	0.781687	3.990374	C	0.091131	1.175828	4.342827
H	1.755435	1.341545	1.982598	H	1.795441	1.539643	2.040211	H	0.609547	2.219496	2.517727
C	0.063242	0.370616	4.806023	C	0.237154	0.196045	4.782956	C	-0.735013	0.204091	4.944959
H	-1.969937	-0.447713	4.809043	H	-1.775394	-0.657516	4.768330	H	-2.249406	-1.330669	4.586476
H	2.064421	1.138798	4.441201	H	2.206888	1.048216	4.440682	H	0.801448	1.746068	4.952599
H	0.202488	0.299082	5.889874	H	0.413596	0.013105	5.848220	H	-0.677386	0.030689	6.025008
N	-2.350282	-0.540025	0.815540	N	-2.285797	-0.476728	0.782538	N	-2.084644	-1.111277	0.574299
C	-2.669870	-1.023883	-1.457950	C	-2.782861	-0.989197	-1.465626	C	-2.008058	-1.444343	-1.737106
C	-0.803124	-0.531829	-2.788171	C	-1.015176	-0.646519	-2.946617	C	-0.163396	-0.469137	-2.833795
C	-3.399636	-1.552071	-2.570767	C	-3.638222	-1.471182	-2.503951	C	-2.496843	-2.008906	-2.957961
C	-3.219380	-1.016311	-0.125686	C	-3.236716	-0.914670	-0.093460	C	-2.695205	-1.672768	-0.489536
C	-1.443746	-1.054690	-3.935225	C	-1.789110	-1.100651	-4.038510	C	-0.554990	-1.005498	-4.051437
H	0.206352	-0.109194	-2.809675	H	0.024058	-0.321484	-3.064834	H	0.737295	0.141363	-2.724331
C	-2.733788	-1.553611	-3.828355	C	-3.094881	-1.517400	-3.817972	C	-1.739087	-1.778282	-4.136989
C	-4.716030	-2.041253	-2.344629	C	-4.965153	-1.864781	-2.165372	C	-3.708374	-2.760394	-2.897167
C	-4.529481	-1.497837	0.049327	C	-4.565171	-1.299243	0.189329	C	-3.934185	-2.420386	-0.485307
H	-0.912959	-1.053296	-4.891655	H	-1.347359	-1.126919	-5.039150	H	0.055211	-0.819164	-4.940673
H	-3.250528	-1.957484	-4.705938	H	-3.715246	-1.883278	-4.643334	H	-2.068425	-2.202115	-5.090682
C	-5.250964	-1.995120	-1.060426	C	-5.401005	-1.767539	-0.846370	C	-4.409385	-2.944473	-1.674987
H	-5.288744	-2.450911	-3.182462	H	-5.632946	-2.229044	-2.952844	H	-4.103660	-3.193529	-3.822662
H	-4.952602	-1.496385	1.054825	H	-4.915971	-1.236187	1.219416	H	-4.447807	-2.559522	0.466140
H	-6.267241	-2.369362	-0.892442	H	-6.426497	-2.061502	-0.597470	H	-5.344000	-3.514954	-1.679701
N	-1.406986	-0.519293	-1.603319	N	-1.502623	-0.595001	-1.708906	N	-0.890529	-0.672046	-1.689716
C	-2.547180	-0.505408	2.172084	C	-2.425595	-0.480058	2.172278	C	-2.463976	-1.255211	1.912626
O	-3.522631	-0.943482	2.794527	O	-3.380624	-0.954306	2.795027	O	-3.252751	-2.109543	2.344486
O	1.020901	0.915706	-0.838535	O	1.042583	0.789046	-0.935532	O	0.966178	1.281508	-0.244223
C	2.274563	0.586846	-0.693147	C	2.295846	0.493347	-0.763686	C	2.258012	1.157973	-0.290817
C	2.690754	-0.615767	-0.018450	C	2.731666	-0.684533	-0.048495	C	2.947943	-0.033603	0.147746
C	3.320046	1.433819	-1.232334	C	3.325428	1.347857	-1.328560	C	3.066555	2.260031	-0.778261
C	4.063397	-0.921634	0.173149	C	4.103063	-0.959284	0.142593	C	4.360205	-0.112680	0.118555
C	1.716597	-1.566053	0.464657	C	1.767080	-1.645215	0.451473	C	2.212340	-1.171664	0.650502
C	4.647952	1.070414	-1.013780	C	4.659376	1.020006	-1.095472	C	4.449419	2.107098	-0.793767
C	5.064362	-0.088333	-0.305843	C	5.091389	-0.113719	-0.358064	C	5.135477	0.941964	-0.352643
H	4.298438	-1.842008	0.710196	H	4.358613	-1.863797	0.696928	H	4.817036	-1.035750	0.478905
N	0.410619	-1.458254	0.466665	N	0.470034	-1.535196	0.422224	N	0.911222	-1.319040	0.684569
O	2.181729	-2.732543	0.972713	O	2.245308	-2.789122	1.000488	O	2.917457	-2.216824	1.141268
H	5.428734	1.723403	-1.412589	H	5.429283	1.677038	-1.507514	H	5.053757	2.937973	-1.166190
C	-0.185416	-2.689899	1.000581	C	-0.133035	-2.735498	1.001980	C	0.592102	-2.666679	1.175010
C	1.050866	-3.399199	1.651843	C	1.101484	-3.490706	1.621752	C	1.950715	-3.116273	1.814554

H	-0.902034	-2.431591	1.795583	H	-0.800189	-2.428287	1.825758	H	-0.170148	-2.587980	1.967731
C	-0.927973	-3.454722	-0.077405	C	-0.977435	-3.473385	-0.018851	C	0.034262	-3.525386	0.055948
C	-0.379975	-3.609245	-1.363878	C	-0.526766	-3.652934	-1.339303	C	0.611400	-3.505075	-1.227165
C	-2.190134	-4.005969	0.199351	C	-2.251102	-3.947070	0.338548	C	-1.094569	-4.328010	0.288559
C	-1.080253	-4.310301	-2.353423	C	-1.332060	-4.303234	-2.282272	C	0.068633	-4.278157	-2.259904
H	0.591056	-3.158683	-1.594821	H	0.449531	-3.253123	-1.633279	H	1.469966	-2.856274	-1.428302
C	-2.893661	-4.706125	-0.790393	C	-3.060121	-4.597148	-0.604073	C	-1.638876	-5.102790	-0.745009
H	-2.638250	-3.853605	1.187501	H	-2.625714	-3.769237	1.352980	H	-1.579942	-4.306647	1.270666
C	-2.339234	-4.861009	-2.068058	C	-2.601585	-4.776979	-1.916115	C	-1.058856	-5.078518	-2.020430
H	-0.647731	-4.417416	-3.353717	H	-0.974897	-4.428372	-3.309826	H	0.512219	-4.237727	-3.259680
H	-3.885786	-5.111490	-0.568225	H	-4.058659	-4.942474	-0.317821	H	-2.534314	-5.704059	-0.558690
H	-2.893533	-5.397129	-2.845679	H	-3.237742	-5.272547	-2.657130	H	-1.496037	-5.667314	-2.833550
C	-0.285201	0.587299	2.023563	C	-0.210447	0.704000	2.030758	C	-0.890985	0.686329	2.167423
C	-1.882906	2.956864	1.691593	C	-1.882475	2.896025	1.689408	C	-3.168703	2.158129	1.417725
C	-2.242574	4.278385	0.993254	C	-2.164268	4.289371	1.122143	C	-3.869509	3.361099	0.774627
H	-1.711752	2.959751	2.774728	H	-1.765460	2.792057	2.774872	H	-3.243773	2.033605	2.504687
O	-3.020915	2.154535	1.340562	O	-3.038748	2.175693	1.219108	O	-3.817370	1.074988	0.722704
C	-2.943152	2.340573	-0.087310	C	-2.892297	2.510178	-0.182770	C	-3.528558	1.533374	-0.620980
C	-2.946892	3.875979	-0.164337	C	-2.844864	4.040123	-0.092439	C	-4.121231	2.949307	-0.554671
C	-1.992424	5.619730	1.256025	C	-1.860209	5.582093	1.529484	C	-4.222477	4.629722	1.216319
H	-3.734287	1.783013	-0.603528	H	-3.692798	2.047134	-0.776466	H	-3.923784	0.834357	-1.370213
C	-3.413736	4.807869	-1.083308	C	-3.234186	5.087102	-0.921860	C	-4.727243	3.803761	-1.469148
C	-2.484331	6.573846	0.336727	C	-2.270349	6.650893	0.699740	C	-4.856063	5.497041	0.296581
H	-1.441741	5.936907	2.147974	H	-1.327896	5.776707	2.467031	H	-4.028046	4.953395	2.244634
C	-3.182020	6.175297	-0.811014	C	-2.944560	6.405556	-0.503965	C	-5.102839	5.090655	-1.021455
H	-3.952867	4.502849	-1.986519	H	-3.756333	4.905551	-1.867706	H	-4.920212	3.494702	-2.502135
H	-2.319772	7.639967	0.525515	H	-2.062164	7.682533	1.003034	H	-5.161200	6.498057	0.619767
H	-3.555004	6.934563	-1.506587	H	-3.256296	7.249787	-1.128778	H	-5.598813	5.779070	-1.714292
C	-0.790946	2.352500	0.792791	C	-0.770956	2.308885	0.785256	C	-1.752526	2.104751	0.786895
H	0.238768	2.708932	0.800253	H	0.235820	2.731975	0.834418	H	-0.979185	2.826933	1.058201
C	-1.475939	1.984170	-0.386057	C	-1.438094	2.109624	-0.465066	C	-2.018358	1.768178	-0.556804
H	-1.045066	2.098210	-1.383590	H	-0.962040	2.327387	-1.424812	H	-1.404973	2.046392	-1.414955
C	2.967668	2.701368	-2.036715	C	2.943793	2.588568	-2.157500	C	2.395746	3.557612	-1.263743
C	6.563789	-0.366750	-0.113153	C	6.593293	-0.361655	-0.154444	C	6.669545	0.898167	-0.410862
C	2.182045	3.697402	-1.149609	C	2.149024	3.587912	-1.281177	C	1.605332	4.202191	-0.096733
H	1.234225	3.248998	-0.822878	H	1.214903	3.131997	-0.926591	H	0.835309	3.510757	0.273403
H	2.772473	3.975039	-0.258231	H	2.747450	3.900360	-0.406927	H	2.284388	4.456559	0.736230
H	1.956635	4.620004	-1.715259	H	1.897237	4.490938	-1.866356	H	1.113417	5.130787	-0.438356
C	2.109014	2.318890	-3.268124	C	2.081997	2.163322	-3.373793	C	1.439908	3.247884	-2.443795
H	2.657496	1.616899	-3.921233	H	2.638663	1.457786	-4.016314	H	1.999054	2.810961	-3.290277
H	1.169596	1.844545	-2.947923	H	1.152453	1.681393	-3.037817	H	0.657331	2.539346	-2.137238
H	1.865691	3.221323	-3.858503	H	1.822796	3.050304	-3.980122	H	0.957423	4.178363	-2.793712
C	4.227011	3.427395	-2.553074	C	4.187230	3.323674	-2.698968	C	3.429454	4.590084	-1.757956
H	4.871927	3.773370	-1.726007	H	4.830071	3.702514	-1.884793	H	4.129344	4.888714	-0.957558
H	4.830099	2.784025	-3.217860	H	4.798032	2.675357	-3.352025	H	4.017685	4.208051	-2.611105
H	3.920980	4.316240	-3.132299	H	3.861207	4.192110	-3.297426	H	2.900487	5.498182	-2.095570
C	7.205922	0.803891	0.671254	C	7.209513	0.840456	0.603938	C	7.246776	2.042858	0.458768

H	8.288901	0.630415	0.810150	H	8.294047	0.687189	0.752073	H	8.351239	2.033673	0.421199
H	7.082584	1.762759	0.138331	H	7.073599	1.783276	0.046435	H	6.904885	3.031596	0.107134
H	6.739891	0.907072	1.666913	H	6.736725	0.960110	1.594381	H	6.933568	1.929078	1.511212
C	7.247724	-0.492930	-1.496692	C	7.282359	-0.506016	-1.534245	C	7.130275	1.084636	-1.878047
H	7.129849	0.429231	-2.091920	H	7.151007	0.400487	-2.149993	H	6.783326	2.046808	-2.292825
H	8.330377	-0.682495	-1.377985	H	8.367262	-0.673962	-1.406338	H	8.233597	1.067890	-1.938927
H	6.809694	-1.326748	-2.072764	H	6.861649	-1.360427	-2.092607	H	6.734442	0.276096	-2.517035
C	6.806624	-1.670447	0.670947	C	6.858828	-1.641879	0.660574	C	7.226237	-0.440406	0.110553
H	6.355598	-1.627067	1.677811	H	6.405337	-1.583973	1.665461	H	6.944839	-0.613937	1.163883
H	6.387027	-2.544592	0.142993	H	6.458698	-2.536544	0.152387	H	6.862150	-1.292614	-0.489425
H	7.891380	-1.837675	0.793125	H	7.946312	-1.784019	0.788279	H	8.328733	-0.433401	0.052526
C	1.145852	-3.029739	3.132924	C	1.183645	-3.216301	3.123385	C	1.974863	-2.754205	3.301303
H	2.114066	-3.355070	3.548668	H	2.136504	-3.591060	3.533340	H	2.991419	-2.875975	3.710686
H	1.048017	-1.938695	3.262528	H	1.109541	-2.133185	3.318419	H	1.648582	-1.710383	3.449483
H	0.332353	-3.518588	3.696093	H	0.349650	-3.718362	3.644086	H	1.284914	-3.411516	3.857966
C	1.178397	-4.893386	1.397338	C	1.225045	-4.966984	1.273057	C	2.382191	-4.547385	1.536270
H	2.101873	-5.277424	1.862434	H	2.148879	-5.382555	1.709529	H	3.367838	-4.741635	1.991591
H	0.315523	-5.422071	1.835286	H	0.361639	-5.520778	1.677761	H	1.648615	-5.247871	1.968757
H	1.202359	-5.108511	0.318366	H	1.245557	-5.113787	0.182435	H	2.439807	-4.735878	0.453585

Intermediate-2: In Ni catalyzed reaction energy profile

Int2 ² : $\nu_{\text{lowest}} = 9.0219 \text{ cm}^{-1}$				Int2 ⁴ : $\nu_{\text{lowest}} = 12.0338 \text{ cm}^{-1}$				Int2 ⁶ : $\nu_{\text{lowest}} = 7.3002 \text{ cm}^{-1}$			
109				109				109			
Ni	-0.532144	0.041644	0.070209	Ni	-0.346208	-0.249119	-0.038943	Ni	-0.361724	-0.179862	-0.178438
C	-1.331557	0.099322	2.861701	C	-1.490708	0.061045	2.669352	C	-1.226515	0.145443	2.679158
C	0.311154	1.855229	3.209669	C	-0.164525	2.064913	3.028617	C	0.170578	2.125316	2.868405
C	-0.837125	-0.541248	4.014701	C	-0.834458	-0.523661	3.770892	C	-0.542894	-0.389362	3.791703
C	0.835648	1.175801	4.314316	C	0.532233	1.445351	4.071509	C	0.898361	1.544112	3.911965
H	0.748794	2.812990	2.906878	H	0.080893	3.096927	2.753967	H	0.429691	3.134380	2.529096
C	0.239648	-0.020107	4.738590	C	0.175026	0.148862	4.466504	C	0.514140	0.288596	4.403746
H	-1.320352	-1.475972	4.316990	H	-1.135062	-1.535995	4.061053	H	-0.860354	-1.374606	4.148355
H	1.692357	1.592350	4.854435	H	1.332130	1.984533	4.589735	H	1.739655	2.084391	4.358198
H	0.617638	-0.547782	5.620675	H	0.681340	-0.335794	5.308073	H	1.040076	-0.161812	5.252196
N	-2.122499	-0.758875	0.768283	N	-2.090694	-0.966336	0.597933	N	-2.019544	-0.895055	0.655624
C	-2.441642	-1.261984	-1.520472	C	-2.196854	-1.721198	-1.642319	C	-2.347096	-1.587403	-1.562136
C	-0.684609	-0.545614	-2.894950	C	-0.375085	-1.060660	-2.961452	C	-0.591138	-1.060210	-3.064515
C	-3.164698	-1.814114	-2.626194	C	-2.815359	-2.402316	-2.739551	C	-3.110434	-2.201793	-2.605060
C	-2.953009	-1.320116	-0.175979	C	-2.810961	-1.674094	-0.338007	C	-2.846627	-1.537548	-0.212202
C	-1.317061	-1.086479	-4.039181	C	-0.912317	-1.711186	-4.094669	C	-1.267390	-1.645760	-4.119380
H	0.279225	-0.029035	-2.949354	H	0.577423	-0.521214	-2.999988	H	0.393838	-0.597479	-3.178385
C	-2.548492	-1.711596	-3.905046	C	-2.123944	-2.379520	-3.981834	C	-2.546817	-2.227142	-3.909572
C	-4.428827	-2.414302	-2.376598	C	-4.066256	-3.045218	-2.523211	C	-4.381318	-2.746463	-2.252288
C	-4.215454	-1.903664	0.021954	C	-4.056261	-2.305428	-0.177501	C	-4.146705	-2.092382	0.092866
H	-0.829833	-0.997292	-5.014576	H	-0.368339	-1.678173	-5.043111	H	-0.808688	-1.653061	-5.112910
H	-3.059812	-2.129732	-4.779051	H	-2.560022	-2.893480	-4.845633	H	-3.095518	-2.694189	-4.733039
C	-4.926884	-2.436437	-1.077804	C	-4.657738	-2.979514	-1.266155	C	-4.879094	-2.682762	-0.921439

H	-4.994140	-2.846318	-3.208248	H	-4.549866	-3.574023	-3.350656	H	-4.982406	-3.221965	-3.035286
H	-4.615636	-1.945074	1.034964	H	-4.530894	-2.274251	0.803562	H	-4.507518	-2.032365	1.119397
H	-5.906846	-2.888591	-0.888603	H	-5.625422	-3.467178	-1.103665	H	-5.865420	-3.104933	-0.702689
N	-1.238159	-0.640518	-1.689852	N	-1.000091	-1.073580	-1.784767	N	-1.123164	-1.025290	-1.794936
C	-2.391213	-0.678057	2.110878	C	-2.438668	-0.861660	1.926292	C	-2.198339	-0.808273	2.031178
O	-3.286893	-1.287854	2.705438	O	-3.287914	-1.528125	2.524246	O	-2.919168	-1.557520	2.702557
O	0.955678	1.093359	-0.478589	O	0.966848	1.109196	-0.535676	O	0.995939	1.065305	-0.632934
C	2.241862	0.845989	-0.468873	C	2.271404	1.083599	-0.496628	C	2.301495	0.991440	-0.574762
C	2.813846	-0.380757	0.006331	C	3.024917	-0.024504	0.035805	C	2.983450	-0.137150	-0.002512
C	3.146052	1.861933	-0.959106	C	3.016341	2.215810	-1.001339	C	3.101226	2.075399	-1.090042
C	4.217069	-0.591958	-0.005692	C	4.444897	-0.010368	0.037956	C	4.400517	-0.187884	0.036716
C	1.967102	-1.433713	0.513794	C	2.354616	-1.168640	0.607404	C	2.242461	-1.244475	0.562237
C	4.512537	1.588787	-0.948341	C	4.407446	2.163082	-0.970216	C	4.488513	1.962131	-1.019922
C	5.089458	0.377428	-0.481292	C	5.160171	1.068282	-0.463508	C	5.176242	0.848437	-0.467672
H	4.580773	-1.547845	0.374888	H	4.951451	-0.881604	0.457094	H	4.856643	-1.072117	0.484940
N	0.659709	-1.425070	0.613793	N	1.060518	-1.349504	0.738349	N	0.939929	-1.363891	0.678985
O	2.565428	-2.572671	0.933942	O	3.114179	-2.186741	1.079227	O	2.950914	-2.293159	1.037366
H	5.190701	2.360071	-1.322608	H	4.962234	3.021102	-1.359526	H	5.090716	2.784224	-1.415741
C	0.210154	-2.748008	1.077780	C	0.801457	-2.680052	1.307044	C	0.613920	-2.682326	1.244157
C	1.538697	-3.383918	1.619412	C	2.224332	-3.108580	1.816420	C	2.015415	-3.198661	1.737995
H	-0.499711	-2.623299	1.910824	H	0.127672	-2.571399	2.172821	H	-0.041233	-2.541940	2.119589
C	-0.485691	-3.508216	-0.034520	C	0.113004	-3.571059	0.290487	C	-0.129160	-3.542103	0.240622
C	0.055258	-3.545110	-1.333392	C	0.629738	-3.723012	-1.010676	C	0.330337	-3.677039	-1.082542
C	-1.689603	-4.183588	0.222885	C	-1.084751	-4.221840	0.627635	C	-1.316376	-4.188515	0.621973
C	-0.592746	-4.253139	-2.352480	C	-0.031498	-4.523730	-1.948698	C	-0.379376	-4.454520	-2.004261
H	0.979769	-3.000000	-1.551093	H	1.543656	-3.190183	-1.295946	H	1.231481	-3.142506	-1.402227
C	-2.341726	-4.891354	-0.796545	C	-1.752930	-5.019776	-0.312185	C	-2.030998	-4.965923	-0.300507
H	-2.137054	-4.122165	1.221144	H	-1.521258	-4.067740	1.620771	H	-1.708076	-4.042368	1.634903
C	-1.793720	-4.928817	-2.085414	C	-1.226152	-5.174669	-1.600629	C	-1.562833	-5.100338	-1.614127
H	-0.166536	-4.267932	-3.360919	H	0.376447	-4.628559	-2.959337	H	-0.023895	-4.534798	-3.036111
H	-3.291048	-5.394367	-0.587584	H	-2.698945	-5.499466	-0.042971	H	-2.968842	-5.442244	0.001875
H	-2.309250	-5.470257	-2.885536	H	-1.753882	-5.786509	-2.339444	H	-2.130108	-5.689817	-2.341757
C	-0.782429	1.355746	2.470594	C	-1.191297	1.408709	2.318145	C	-0.908796	1.467170	2.243551
C	-2.869096	2.694954	1.738987	C	-3.539154	2.332748	1.671047	C	-3.275545	2.405023	1.742579
C	-3.190528	3.866469	0.825743	C	-4.091032	3.489788	0.854037	C	-3.881968	3.567194	0.974076
H	-3.118402	2.776336	2.805187	H	-3.793093	2.272762	2.737204	H	-3.454041	2.338533	2.823435
O	-3.612154	1.629751	1.122140	O	-4.067426	1.198650	0.957677	O	-3.852559	1.274295	1.060616
C	-3.081800	1.794033	-0.212114	C	-3.582559	1.571380	-0.353406	C	-3.463177	1.659227	-0.282715
C	-3.330226	3.279565	-0.449774	C	-4.117621	2.999390	-0.471278	C	-4.000449	3.087729	-0.349596
C	-3.276146	5.245514	0.998241	C	-4.450188	4.802685	1.142887	C	-4.223011	4.876734	1.298542
H	-3.550928	1.084443	-0.905179	H	-3.887941	0.835989	-1.110411	H	-3.821015	0.931756	-1.022814
C	-3.550775	4.061346	-1.582138	C	-4.495053	3.818368	-1.535077	C	-4.450179	3.913897	-1.379530
C	-3.534854	6.038602	-0.139053	C	-4.866267	5.625758	0.074589	C	-4.710408	5.707285	0.267101
H	-3.157135	5.707852	1.984252	H	-4.423518	5.190645	2.167047	H	-4.127589	5.256417	2.321564
C	-3.669056	5.455426	-1.408782	C	-4.886262	5.140682	-1.242406	C	-4.820056	5.233081	-1.049885
H	-3.641865	3.613085	-2.577558	H	-4.503784	3.449292	-2.566389	H	-4.530380	3.551562	-2.409936
H	-3.634935	7.123946	-0.030661	H	-5.180068	6.655738	0.275224	H	-5.009061	6.735693	0.496501

H	-3.872362	6.093096	-2.275938	H	-5.216542	5.798370	-2.053791	H	-5.204892	5.897349	-1.831126
C	-1.379804	2.284960	1.417605	C	-1.993161	2.253301	1.330246	C	-1.757385	2.316912	1.296664
H	-0.741218	3.181461	1.387257	H	-1.554691	3.267180	1.359098	H	-1.305950	3.325230	1.300751
C	-1.551592	1.702855	-0.007773	C	-2.098360	1.761291	-0.099361	C	-1.964395	1.840349	-0.126286
H	-0.983906	2.241597	-0.779581	H	-1.386714	2.055036	-0.879021	H	-1.297905	2.107493	-0.954610
C	2.600305	3.210269	-1.468323	C	2.264112	3.441598	-1.553228	C	2.417167	3.314469	-1.697213
C	6.615618	0.197084	-0.518145	C	6.696171	1.128184	-0.484138	C	6.713451	0.838134	-0.447493
C	1.850062	3.934117	-0.321383	C	1.376412	4.051147	-0.437399	C	1.530211	3.995785	-0.623680
H	1.024847	3.311776	0.052335	H	0.665241	3.304009	-0.056495	H	0.774995	3.293938	-0.241524
H	2.539623	4.146702	0.514977	H	2.002981	4.401053	0.402421	H	2.149263	4.340908	0.223661
H	1.436559	4.893871	-0.681616	H	0.811256	4.916317	-0.830313	H	1.015846	4.873689	-1.055751
C	1.642324	2.980158	-2.664940	C	1.386719	3.022960	-2.761060	C	1.552997	2.895165	-2.914201
H	2.175971	2.484089	-3.495631	H	2.018791	2.623576	-3.574667	H	2.187316	2.446073	-3.699166
H	0.789515	2.352903	-2.367484	H	0.661332	2.249953	-2.466775	H	0.788175	2.160654	-2.621003
H	1.257255	3.948557	-3.033372	H	0.836594	3.898567	-3.152159	H	1.049733	3.780458	-3.344345
C	3.729613	4.143768	-1.950441	C	3.230492	4.541457	-2.037364	C	3.443049	4.355895	-2.188211
H	4.439991	4.383706	-1.139625	H	3.874572	4.911917	-1.220191	H	4.081326	4.724386	-1.365608
H	4.296382	3.705423	-2.791085	H	3.879675	4.187354	-2.857918	H	4.096617	3.948278	-2.979741
H	3.289520	5.093500	-2.301604	H	2.646147	5.397632	-2.417792	H	2.906560	5.223553	-2.610544
C	7.284499	1.299933	0.338810	C	7.174983	2.343576	0.347585	C	7.224981	2.052758	0.365597
H	8.384563	1.193413	0.316403	H	8.278351	2.410894	0.335063	H	8.330111	2.068615	0.382584
H	7.035150	2.308668	-0.033592	H	6.774084	3.290858	-0.052809	H	6.880215	3.006237	-0.070735
H	6.949829	1.233763	1.388829	H	6.843827	2.251920	1.396811	H	6.861760	2.005203	1.407129
C	7.111403	0.312263	-1.980681	C	7.184084	1.282689	-1.945700	C	7.245503	0.930638	-1.898901
H	6.855380	1.292710	-2.418459	H	6.782033	2.199314	-2.411118	H	6.900134	1.852372	-2.398393
H	8.209872	0.197291	-2.027165	H	8.287468	1.340629	-1.981722	H	8.350851	0.935670	-1.905803
H	6.653006	-0.470503	-2.610125	H	6.860851	0.422014	-2.557134	H	6.897832	0.070111	-2.496816
C	7.042674	-1.176011	0.034828	C	7.327192	-0.146370	0.108163	C	7.269192	-0.447309	0.194671
H	6.731744	-1.303469	1.086529	H	7.030494	-0.293330	1.161446	H	6.937463	-0.552946	1.242460
H	6.609997	-2.002783	-0.555290	H	7.034121	-1.045768	-0.461282	H	6.951857	-1.347471	-0.360242
H	8.142124	-1.270573	-0.006392	H	8.428309	-0.069047	0.074951	H	8.373070	-0.419842	0.191072
C	1.694339	-3.115190	3.116921	C	2.379295	-2.770153	3.300567	C	2.191747	-2.935498	3.233929
H	2.706373	-3.396838	3.452153	H	3.428540	-2.896902	3.614779	H	3.230104	-3.144761	3.540458
H	1.526888	-2.047774	3.334310	H	2.071490	-1.728048	3.487309	H	1.953546	-1.884983	3.466536
H	0.954029	-3.704805	3.685173	H	1.742313	-3.436138	3.908483	H	1.512184	-3.584869	3.813004
C	1.783916	-4.841361	1.255626	C	2.658508	-4.530956	1.492070	C	2.379525	-4.625106	1.349665
H	2.759318	-5.168825	1.652952	H	3.681649	-4.706312	1.864853	H	3.393246	-4.865266	1.711966
H	0.993617	-5.473635	1.693397	H	1.976918	-5.248479	1.978601	H	1.663628	-5.329409	1.804883
H	1.773095	-4.984336	0.164879	H	2.635179	-4.717507	0.408346	H	2.345698	-4.761267	0.258804

Transition State (2-3) – reductive elimination^A pathway: In Ni catalyzed reaction energy profile

TS2A ² : $v_{\text{lowest}} = -438.7138 \text{ cm}^{-1}$				TS2A ⁴ : $v_{\text{lowest}} = -409.4987 \text{ cm}^{-1}$				TS2A ⁶ : $v_{\text{lowest}} = -682.6306 \text{ cm}^{-1}$			
109				109				109			
Ni	-0.517562	-0.167789	-0.230349	Ni	0.551965	-0.297134	0.718392	Ni	0.397417	-0.095638	0.357642
C	-1.162517	-0.192089	2.837108	C	0.063272	0.382458	-2.300806	C	0.558273	0.376843	-2.357213
C	0.889194	1.065863	3.170742	C	-1.890132	1.738720	-1.814843	C	-1.222863	1.901720	-1.601258

C	-0.818400	-1.011528	3.928114	C	-0.734451	-0.426831	-3.134178	C	-0.294180	-0.049110	-3.406856
C	1.252281	0.211364	4.218948	C	-2.688775	0.888663	-2.588216	C	-2.088737	1.370761	-2.552404
H	1.549866	1.890331	2.880737	H	-2.341254	2.598994	-1.310116	H	-1.569124	2.705774	-0.941353
C	0.379692	-0.812208	4.621580	C	-2.104504	-0.188796	-3.271049	C	-1.601523	0.413744	-3.491670
H	-1.507566	-1.818803	4.194272	H	-0.245667	-1.257413	-3.652656	H	0.102001	-0.789562	-4.109882
H	2.207787	0.356652	4.733776	H	-3.765514	1.071580	-2.660599	H	-3.131027	1.702027	-2.595212
H	0.643144	-1.464030	5.460969	H	-2.717736	-0.848436	-3.893230	H	-2.264733	0.042931	-4.280924
N	-2.294943	-0.255316	0.681766	N	1.936360	0.127230	-0.762877	N	2.118853	-0.170125	-0.693867
C	-2.911887	-0.611628	-1.598766	C	3.345340	-0.632847	0.998577	C	2.831002	-1.147817	1.331819
C	-1.161492	-0.308582	-3.125539	C	2.265893	-0.945016	3.074908	C	1.255824	-1.033543	3.099923
C	-3.838820	-0.937670	-2.639692	C	4.625985	-0.966878	1.559751	C	3.811225	-1.762837	2.179976
C	-3.314908	-0.607401	-0.223839	C	3.220363	-0.280337	-0.382971	C	3.121143	-0.887940	-0.043034
C	-2.007647	-0.622627	-4.209670	C	3.477259	-1.263867	3.698328	C	2.160513	-1.603281	3.984233
H	-0.106552	-0.050545	-3.263489	H	1.317117	-0.931902	3.621126	H	0.242147	-0.745072	3.391981
C	-3.340879	-0.934226	-3.975061	C	4.658446	-1.282562	2.950291	C	3.450304	-1.978235	3.540610
C	-5.174456	-1.263169	-2.277620	C	5.756192	-0.965685	0.702380	C	5.058104	-2.117274	1.593665
C	-4.645911	-0.913545	0.092251	C	4.376012	-0.272619	-1.200059	C	4.383644	-1.260696	-0.599196
H	-1.601159	-0.611047	-5.225575	H	3.484320	-1.499309	4.766916	H	1.862462	-1.762822	5.025289
H	-4.015944	-1.181776	-4.801026	H	5.613869	-1.539726	3.419372	H	4.166949	-2.440594	4.226579
C	-5.553589	-1.245161	-0.939606	C	5.616902	-0.626555	-0.651183	C	5.323073	-1.873173	0.222979
H	-5.890466	-1.532519	-3.060975	H	6.735314	-1.233535	1.112835	H	5.818700	-2.592869	2.222099
H	-4.957940	-0.929620	1.135622	H	4.281822	-0.017868	-2.256343	H	4.563721	-1.085897	-1.661040
H	-6.583577	-1.498171	-0.666293	H	6.498450	-0.638054	-1.301425	H	6.288758	-2.177204	-0.194867
N	-1.601432	-0.303094	-1.859893	N	2.203205	-0.636439	1.755906	N	1.589745	-0.789898	1.790717
C	-2.361724	-0.598817	2.043252	C	1.471516	-0.078050	-2.076007	C	1.787451	-0.354863	-2.072411
O	-3.240849	-1.323598	2.514418	O	2.074020	-0.748180	-2.913644	O	2.375695	-1.150581	-2.828139
O	1.007630	0.802712	-0.900581	O	-1.077695	0.470103	1.317907	O	-1.103364	0.538712	1.368522
C	2.277793	0.536421	-0.750658	C	-2.320585	0.132837	1.063379	C	-2.358745	0.444575	1.039110
C	2.768288	-0.690460	-0.169441	C	-2.665462	-1.033091	0.296015	C	-2.841047	-0.568118	0.121972
C	3.263599	1.496040	-1.201302	C	-3.397491	0.956816	1.554557	C	-3.319310	1.360751	1.610611
C	4.160197	-0.952285	-0.077065	C	-4.011158	-1.303707	-0.054057	C	-4.199930	-0.620806	-0.228361
C	1.858667	-1.701790	0.321806	C	-1.647621	-1.946516	-0.172202	C	-1.948460	-1.568467	-0.438476
C	4.613878	1.181237	-1.063072	C	-4.698601	0.641617	1.163332	C	-4.651102	1.263212	1.200976
C	5.105008	-0.032587	-0.511966	C	-5.044500	-0.463777	0.342407	C	-5.125755	0.299290	0.277889
H	4.457743	-1.905904	0.363128	H	-4.200205	-2.191736	-0.659159	H	-4.511147	-1.401706	-0.927079
N	0.573552	-1.566915	0.547569	N	-0.350358	-1.853753	0.006018	N	-0.643120	-1.580333	-0.372445
O	2.359469	-2.935619	0.586753	O	-2.038557	-3.022561	-0.894157	O	-2.503646	-2.605099	-1.093647
H	5.349446	1.915132	-1.403352	H	-5.509519	1.285247	1.514049	H	-5.367240	1.972575	1.615859
C	0.011015	-2.863000	0.953194	C	0.307510	-2.891928	-0.805037	C	-0.115120	-2.745047	-1.094447
C	1.294133	-3.729115	1.229822	C	-0.854717	-3.903079	-1.067014	C	-1.418516	-3.521361	-1.532412
H	-0.541675	-2.739449	1.899081	H	0.569921	-2.435501	-1.777122	H	0.395936	-2.384041	-2.003620
C	-0.970858	-3.347529	-0.099053	C	1.590830	-3.400088	-0.193237	C	0.909728	-3.497829	-0.273958
C	-0.618604	-3.356486	-1.463230	C	1.688260	-3.702995	1.177242	C	0.703742	-3.766066	1.092123
C	-2.269530	-3.733171	0.271235	C	2.733060	-3.521565	-1.004483	C	2.109386	-3.904744	-0.882990
C	-1.543090	-3.758223	-2.433255	C	2.900415	-4.143324	1.720704	C	1.669569	-4.458801	1.829583
H	0.378192	-3.018235	-1.767396	H	0.820161	-3.553526	1.826562	H	-0.201052	-3.398283	1.587396
C	-3.201182	-4.127164	-0.701011	C	3.947840	-3.960519	-0.460792	C	3.076409	-4.600493	-0.144305

H	-2.569447	-3.679121	1.323138	H	2.678254	-3.218316	-2.055004	H	2.301111	-3.624971	-1.924123
C	-2.839399	-4.143120	-2.053719	C	4.031962	-4.275906	0.901580	C	2.856077	-4.882309	1.209967
H	-1.260102	-3.752618	-3.490798	H	2.969486	-4.360201	2.791325	H	1.508545	-4.647236	2.895472
H	-4.218153	-4.397741	-0.399885	H	4.835675	-4.025707	-1.097234	H	4.016451	-4.894137	-0.621696
H	-3.569668	-4.436853	-2.814810	H	4.985177	-4.599396	1.332517	H	3.619522	-5.408403	1.792497
C	-0.325596	0.892463	2.484925	C	-0.509480	1.509387	-1.667086	C	0.112040	1.437625	-1.457077
C	-1.780096	2.960138	2.356951	C	1.030474	3.513168	-2.060117	C	1.816495	3.300812	-1.947084
C	-1.990559	4.169486	1.467028	C	1.516575	4.719839	-1.281704	C	2.594266	4.379883	-1.212472
H	-1.520812	3.114795	3.411730	H	0.453256	3.671073	-2.979986	H	1.149011	3.594501	-2.767443
O	-3.032604	2.260301	2.233567	O	2.257581	2.812119	-2.338879	O	2.864870	2.439501	-2.423101
C	-3.082651	2.242036	0.795024	C	2.748860	2.777088	-0.977754	C	3.533794	2.260851	-1.155459
C	-2.837253	3.701189	0.442237	C	2.627495	4.235346	-0.557118	C	3.714918	3.700787	-0.685674
C	-1.466957	5.459797	1.436678	C	1.050087	6.018892	-1.105128	C	2.369100	5.723949	-0.933610
H	-4.001240	1.764405	0.430170	H	3.734058	2.295835	-0.915592	H	4.424007	1.624904	-1.254736
C	-3.179620	4.509647	-0.640229	C	3.294191	5.042391	0.366232	C	4.631068	4.351467	0.141239
C	-1.836286	6.293988	0.361979	C	1.739770	6.850018	-0.196620	C	3.306108	6.395568	-0.116192
H	-0.794219	5.824535	2.220134	H	0.181590	6.395449	-1.656432	H	1.499568	6.254619	-1.336499
C	-2.678969	5.826698	-0.659438	C	2.842109	6.366993	0.527395	C	4.415864	5.719056	0.411973
H	-3.821649	4.143197	-1.448320	H	4.149176	4.669392	0.940189	H	5.497367	3.828227	0.559937
H	-1.461209	7.322112	0.322489	H	1.413187	7.885728	-0.055220	H	3.165642	7.458622	0.106828
H	-2.950751	6.496458	-1.482145	H	3.362171	7.033510	1.223905	H	5.129985	6.263529	1.039298
C	-0.805243	1.986397	1.562180	C	0.344212	2.554607	-0.987290	C	1.139699	2.388838	-0.831295
H	0.061234	2.528409	1.156411	H	-0.295209	3.145469	-0.311499	H	0.631581	3.017767	-0.078967
C	-1.744466	1.548746	0.431069	C	1.597971	2.064210	-0.278583	C	2.396877	1.723848	-0.292565
H	-1.412208	1.793274	-0.585629	H	1.611124	1.982143	0.816163	H	2.555302	1.635151	0.789097
C	2.813546	2.833122	-1.824349	C	-3.107011	2.132148	2.508270	C	-2.867684	2.418367	2.633577
C	6.621434	-0.267496	-0.417528	C	-6.511522	-0.685440	-0.058713	C	-6.590153	0.241652	-0.183393
C	1.952121	3.629107	-0.811628	C	-2.215520	3.191383	1.816161	C	-1.832380	3.377289	1.992166
H	1.052219	3.056506	-0.545379	H	-1.263066	2.742499	1.501200	H	-0.945855	2.824508	1.648734
H	2.527593	3.838245	0.108153	H	-2.725357	3.610074	0.930003	H	-2.276822	3.909908	1.132559
H	1.637975	4.594495	-1.249123	H	-2.003923	4.023448	2.512087	H	-1.511664	4.132193	2.732331
C	1.987659	2.563082	-3.107538	C	-2.387633	1.594062	3.772062	C	-2.238192	1.715397	3.864665
H	2.595420	2.014313	-3.849088	H	-3.024349	0.858180	4.294438	H	-2.968109	1.034134	4.336632
H	1.094068	1.967847	-2.869091	H	-1.436320	1.110027	3.503182	H	-1.348856	1.137132	3.574461
H	1.668171	3.518870	-3.562825	H	-2.177471	2.425272	4.469824	H	-1.939055	2.471272	4.613064
C	4.012689	3.720740	-2.215476	C	-4.401546	2.834301	2.966411	C	-4.051245	3.272354	3.133097
H	4.636823	3.978140	-1.341249	H	-4.952300	3.278597	2.118230	H	-4.529164	3.836130	2.312457
H	4.656315	3.234738	-2.969963	H	-5.079432	2.142603	3.497035	H	-4.822520	2.657153	3.629208
H	3.639527	4.664351	-2.651219	H	-4.143987	3.652181	3.661805	H	-3.681670	4.005556	3.870564
C	7.258846	0.832185	0.467008	C	-7.007571	0.544462	-0.858736	C	-7.461306	1.312623	0.501315
H	8.352941	0.688894	0.537410	H	-8.065830	0.416291	-1.150910	H	-8.500920	1.230615	0.139577
H	7.075440	1.839190	0.053673	H	-6.929466	1.471485	-0.264703	H	-7.475953	1.186144	1.598014
H	6.837765	0.802945	1.487332	H	-6.408575	0.678358	-1.776952	H	-7.107040	2.333340	0.274329
C	7.241054	-0.207162	-1.835463	C	-7.378666	-0.856099	1.212567	C	-7.178331	-1.153279	0.144394
H	7.058048	0.770180	-2.314852	H	-7.321148	0.032294	1.864956	H	-7.153683	-1.342070	1.231759
H	8.334848	-0.361661	-1.788240	H	-8.439024	-1.006517	0.939325	H	-8.227972	-1.214133	-0.195419
H	6.806758	-0.988717	-2.483193	H	-7.043139	-1.729710	1.798215	H	-6.613369	-1.959149	-0.354244

C	6.951031	-1.640304	0.199145	C	-6.680865	-1.939173	-0.937933	C	-6.637377	0.473871	-1.715160
H	6.553435	-1.729063	1.225391	H	-6.096695	-1.860608	-1.871620	H	-6.221665	1.463916	-1.972479
H	6.533822	-2.465484	-0.404137	H	-6.360890	-2.852764	-0.407112	H	-6.054596	-0.290777	-2.256735
H	8.046024	-1.776176	0.247843	H	-7.743080	-2.062689	-1.212974	H	-7.680198	0.429745	-2.078153
C	1.609797	-3.756577	2.726106	C	-0.864413	-4.426776	-2.495882	C	-1.513941	-3.639626	-3.049682
H	2.596460	-4.217166	2.900963	H	-1.741735	-5.071069	-2.672688	H	-2.471391	-4.099690	-3.346686
H	1.613964	-2.732057	3.132216	H	-0.885880	-3.590463	-3.212387	H	-1.432271	-2.644463	-3.513861
H	0.843641	-4.341231	3.264898	H	0.048897	-5.020094	-2.673518	H	-0.688104	-4.270105	-3.421890
C	1.312881	-5.117646	0.603873	C	-0.988523	-5.017385	-0.031541	C	-1.661867	-4.852025	-0.828244
H	2.271164	-5.617293	0.824851	H	-1.910691	-5.589937	-0.225719	H	-2.633608	-5.266126	-1.145644
H	0.491885	-5.726003	1.018830	H	-0.123041	-5.697860	-0.084152	H	-0.864328	-5.567020	-1.088557
H	1.181647	-5.063606	-0.487000	H	-1.043125	-4.602728	0.987699	H	-1.667706	-4.730311	0.265397

Transition State (2-3) – nucleophilic addition^B pathway: In Ni catalyzed reaction energy profile

TS2B ² : $\nu_{\text{lowest}} = -387.4039 \text{ cm}^{-1}$				TS2B ⁴ : $\nu_{\text{lowest}} = -395.6481 \text{ cm}^{-1}$				TS2B ⁶ : $\nu_{\text{lowest}} = -430.2025 \text{ cm}^{-1}$			
109				109				109			
Ni	0.308473	0.379069	-0.025355	Ni	0.343378	0.308028	-0.075897	Ni	0.453942	0.372548	-0.497557
C	1.952385	0.088467	2.296003	C	1.879795	-0.032931	2.356381	C	0.786720	-0.659869	2.214440
C	0.393429	-1.744048	2.675561	C	0.239263	-1.806443	2.672122	C	-1.270137	-1.828676	1.638967
C	1.485600	0.744985	3.441385	C	1.427694	0.613539	3.513009	C	0.125647	0.052567	3.222133
C	-0.109827	-1.062877	3.792202	C	-0.245490	-1.134701	3.802226	C	-1.948882	-1.063023	2.596316
H	-0.020152	-2.716829	2.389202	H	-0.211902	-2.752859	2.355625	H	-1.812137	-2.570011	1.044256
C	0.457539	0.159648	4.194514	C	0.368892	0.052178	4.241322	C	-1.250656	-0.149876	3.405988
H	1.928319	1.705018	3.726843	H	1.906327	1.546451	3.828685	H	0.684966	0.760652	3.841886
H	-0.930584	-1.500012	4.370788	H	-1.089384	-1.551563	4.362178	H	-3.028359	-1.190618	2.723274
H	0.085481	0.662061	5.094056	H	0.009707	0.546000	5.150788	H	-1.789057	0.411081	4.176959
N	2.092767	1.131424	0.180894	N	2.108471	1.103692	0.289587	N	2.140443	0.402722	0.561386
C	1.566500	2.114798	-1.905686	C	1.732402	2.073392	-1.834019	C	2.893441	1.434223	-1.414390
C	-0.472693	1.402885	-2.808013	C	-0.248554	1.376786	-2.874323	C	1.255879	1.690482	-3.119028
C	1.837029	2.958732	-3.027177	C	2.082016	2.918684	-2.934002	C	3.891610	2.055384	-2.228323
C	2.498121	1.990130	-0.803729	C	2.589742	1.940824	-0.671995	C	3.206318	0.955124	-0.093732
C	-0.283727	2.202571	-3.957390	C	0.016884	2.185851	-4.000952	C	2.168161	2.306085	-3.954116
H	-1.363211	0.778656	-2.675967	H	-1.147167	0.754395	-2.805008	H	0.214421	1.516293	-3.406300
C	0.862330	2.979871	-4.062202	C	1.173888	2.953497	-4.027861	C	3.511495	2.501592	-3.526636
C	3.049430	3.706734	-3.038183	C	3.301604	3.650777	-2.868485	C	5.198108	2.186984	-1.675958
C	3.691904	2.738536	-0.868765	C	3.800033	2.670591	-0.666678	C	4.550771	1.090811	0.411683
H	-1.041514	2.200307	-4.746272	H	-0.689761	2.195830	-4.835920	H	1.846631	2.637058	-4.946695
H	1.027707	3.613920	-4.940323	H	1.399921	3.590586	-4.890115	H	4.248027	2.982533	-4.177204
C	3.939708	3.582504	-1.975537	C	4.125802	3.509760	-1.754027	C	5.510055	1.706730	-0.376780
H	3.269022	4.362571	-3.886678	H	3.580412	4.306494	-3.699422	H	5.974770	2.671924	-2.277954
H	4.398228	2.646784	-0.042312	H	4.455704	2.565093	0.198780	H	4.765304	0.728218	1.417089
H	4.872970	4.156626	-1.991386	H	5.067237	4.069318	-1.713536	H	6.528255	1.829946	0.007221
N	0.424556	1.372518	-1.824182	N	0.585881	1.333004	-1.835598	N	1.606486	1.249245	-1.858308
C	2.916906	0.741045	1.300599	C	2.889435	0.601016	1.391823	C	2.219778	-0.375427	1.775654
O	3.956048	1.351701	1.667911	O	3.960090	1.133207	1.799725	O	3.152018	-0.234248	2.632706
O	-0.800736	-1.145817	-0.497440	O	-0.843347	-1.139199	-0.548064	O	-1.098406	-0.397116	-1.361274

C	-2.096881	-1.287412	-0.430729	C	-2.145525	-1.218150	-0.468210	C	-2.354923	-0.303338	-1.010105
C	-2.967187	-0.318263	0.189110	C	-2.957468	-0.206268	0.159984	C	-2.840813	0.688279	-0.081795
C	-2.711767	-2.466239	-1.001059	C	-2.821920	-2.366998	-1.027031	C	-3.319634	-1.220342	-1.574626
C	-4.373700	-0.512387	0.222029	C	-4.370868	-0.332430	0.211765	C	-4.208340	0.738674	0.282327
C	-2.430572	0.864286	0.822659	C	-2.358031	0.953844	0.781659	C	-1.947488	1.657096	0.519439
C	-4.097458	-2.590152	-0.936668	C	-4.211341	-2.423701	-0.944926	C	-4.647189	-1.123049	-1.161708
C	-4.964882	-1.636896	-0.336778	C	-5.023061	-1.428343	-0.336576	C	-5.131108	-0.165621	-0.230828
H	-4.971556	0.259034	0.710737	H	-4.924472	0.467805	0.705934	H	-4.506876	1.511697	0.992365
N	-1.168922	1.210710	0.924690	N	-1.081742	1.247229	0.866927	N	-0.649159	1.738763	0.367699
O	-3.299553	1.736212	1.391314	O	-3.182310	1.861655	1.358420	O	-2.478022	2.590807	1.340451
H	-4.552802	-3.480970	-1.377759	H	-4.714956	-3.292468	-1.377233	H	-5.367960	-1.828900	-1.582370
C	-1.067780	2.522364	1.585130	C	-0.917026	2.554602	1.520997	C	-0.116796	2.807026	1.220515
C	-2.508655	2.703940	2.181191	C	-2.343074	2.801434	2.132598	C	-1.412734	3.566197	1.681508
H	-0.343507	2.443332	2.411681	H	-0.184493	2.448302	2.337442	H	0.333917	2.323503	2.106245
C	-0.552684	3.565174	0.611011	C	-0.384921	3.582754	0.541233	C	0.974222	3.608784	0.545788
C	-1.221076	3.829760	-0.600545	C	-1.036678	3.829441	-0.682791	C	0.854345	4.044262	-0.786485
C	0.647447	4.240570	0.885009	C	0.798273	4.279581	0.833096	C	2.159620	3.884807	1.248115
C	-0.712719	4.771350	-1.501707	C	-0.526637	4.772188	-1.581976	C	1.890349	4.760332	-1.395319
H	-2.135340	3.278518	-0.846697	H	-1.940422	3.265423	-0.938725	H	-0.037029	3.781513	-1.363872
C	1.168971	5.172862	-0.023736	C	1.320163	5.214958	-0.071941	C	3.203149	4.594598	0.638376
H	1.195441	4.011183	1.805507	H	1.332494	4.064527	1.765033	H	2.278903	3.507486	2.270180
C	0.485697	5.445439	-1.215169	C	0.655150	5.467397	-1.278201	C	3.067526	5.037169	-0.683830
H	-1.242365	4.968365	-2.439315	H	-1.042253	4.954301	-2.530348	H	1.792611	5.072647	-2.439243
H	2.118040	5.672409	0.193674	H	2.256535	5.732021	0.159136	H	4.130651	4.779653	1.189411
H	0.894221	6.167491	-1.929389	H	1.065444	6.190866	-1.990051	H	3.888086	5.574501	-1.170227
C	1.449704	-1.180140	1.938932	C	1.326197	-1.268222	1.961124	C	0.110072	-1.638051	1.456141
C	3.142589	-3.009146	1.601379	C	2.951617	-3.153986	1.582547	C	1.088486	-3.957934	1.403693
C	3.993167	-3.685101	0.540574	C	3.784211	-3.825651	0.505827	C	2.064143	-4.835211	0.639008
H	2.597370	-3.642807	2.313888	H	2.378301	-3.788987	2.271420	H	0.107998	-4.374959	1.669555
O	4.106348	-2.187402	2.283321	O	3.938346	-2.388305	2.295331	O	1.838595	-3.624005	2.583360
C	4.644863	-1.536447	1.112647	C	4.509326	-1.721204	1.150173	C	3.027079	-3.156409	1.912243
C	4.984404	-2.729515	0.225013	C	4.810920	-2.896398	0.226700	C	3.334652	-4.319447	0.974704
C	3.919757	-4.899404	-0.135799	C	3.670394	-5.013237	-0.211400	C	1.925981	-5.875360	-0.275325
H	5.420204	-0.807766	1.380883	H	5.306550	-1.028488	1.447360	H	3.786069	-2.819319	2.628481
C	5.918347	-2.967411	-0.782985	C	5.741334	-3.134724	-0.784641	C	4.496249	-4.825626	0.391951
C	4.885109	-5.160144	-1.130957	C	4.631501	-5.275898	-1.209948	C	3.100518	-6.416615	-0.839701
H	3.144032	-5.637488	0.095887	H	2.866853	-5.729664	-0.008214	H	0.941896	-6.271092	-0.548822
C	5.868109	-4.209275	-1.448034	C	5.650225	-4.351329	-1.490549	C	4.363684	-5.899776	-0.510988
H	6.678062	-2.223509	-1.045676	H	6.528652	-2.410406	-1.019237	H	5.483065	-4.416724	0.633234
H	4.869208	-6.117424	-1.662936	H	4.584316	-6.213929	-1.773440	H	3.026652	-7.251688	-1.544358
H	6.608498	-4.437797	-2.222297	H	6.386504	-4.581014	-2.268383	H	5.259497	-6.339737	-0.962001
C	2.265953	-1.902973	0.882534	C	2.122222	-1.994278	0.892090	C	1.036287	-2.550893	0.675833
H	1.656812	-2.316771	0.063229	H	1.506217	-2.361877	0.055234	H	0.781401	-2.647229	-0.392139
C	3.393821	-0.963194	0.435651	C	3.284482	-1.078559	0.482817	C	2.479261	-2.092141	0.952375
H	3.488815	-0.698283	-0.622018	H	3.402660	-0.797280	-0.568771	H	3.130047	-1.807810	0.118197
C	-1.834194	-3.544214	-1.665614	C	-2.005992	-3.488597	-1.698255	C	-2.874678	-2.271321	-2.609969
C	-6.481428	-1.888448	-0.327555	C	-6.549853	-1.605514	-0.307174	C	-6.616907	-0.167833	0.160975

C	-0.851176	-4.128409	-0.619214	C	-1.039235	-4.116987	-0.662404	C	-1.835007	-3.230819	-1.978931
H	-0.231910	-3.328761	-0.188197	H	-0.371406	-3.349348	-0.245821	H	-0.960967	-2.668164	-1.621113
H	-1.406687	-4.624226	0.196788	H	-1.607437	-4.577863	0.165225	H	-2.279769	-3.780738	-1.129599
H	-0.188898	-4.877055	-1.091984	H	-0.424701	-4.902348	-1.139901	H	-1.497658	-3.971852	-2.726365
C	-1.044011	-2.927771	-2.848756	C	-1.201754	-2.915764	-2.893617	C	-2.254481	-1.560403	-3.840486
H	-1.740548	-2.531844	-3.609806	H	-1.887290	-2.488271	-3.647470	H	-2.996466	-0.891422	-4.311448
H	-0.395728	-2.109219	-2.503198	H	-0.509180	-2.129417	-2.559368	H	-1.376648	-0.965193	-3.548404
H	-0.416642	-3.701478	-3.328387	H	-0.619174	-3.720836	-3.377973	H	-1.942702	-2.310234	-4.590470
C	-2.675219	-4.710901	-2.221979	C	-2.910012	-4.614705	-2.239369	C	-4.058147	-3.125916	-3.107835
H	-3.248128	-5.221565	-1.427691	H	-3.496616	-5.094355	-1.435848	H	-4.532181	-3.693540	-2.287273
H	-3.383781	-4.373393	-2.999207	H	-3.611314	-4.245554	-3.008709	H	-4.832869	-2.509788	-3.597439
H	-2.002960	-5.456228	-2.682143	H	-2.280810	-5.393267	-2.705292	H	-3.691145	-3.855602	-3.850576
C	-6.779410	-3.209343	0.423773	C	-6.901931	-2.908931	0.451264	C	-6.971396	-1.532170	0.802763
H	-7.865783	-3.413770	0.432053	H	-7.996755	-3.060081	0.473761	H	-8.039916	-1.561577	1.083951
H	-6.277607	-4.068515	-0.054141	H	-6.448764	-3.792484	-0.030779	H	-6.781179	-2.368015	0.107417
H	-6.428502	-3.150277	1.468913	H	-6.535343	-2.865025	1.491758	H	-6.368511	-1.703188	1.712102
C	-6.992290	-2.000935	-1.785112	C	-7.083948	-1.695735	-1.757943	C	-7.484741	0.046524	-1.103605
H	-6.494358	-2.824637	-2.325543	H	-6.634005	-2.544012	-2.302403	H	-7.312627	-0.745987	-1.852247
H	-8.080495	-2.195054	-1.800584	H	-8.180438	-1.836196	-1.759065	H	-8.558289	0.036273	-0.840893
H	-6.798105	-1.065665	-2.338940	H	-6.851157	-0.772273	-2.316637	H	-7.251466	1.016501	-1.576292
C	-7.246634	-0.747824	0.370264	C	-7.249562	-0.427632	0.397448	C	-6.944351	0.946956	1.172697
H	-6.936499	-0.637518	1.424165	H	-6.921148	-0.330657	1.447102	H	-6.367420	0.828959	2.106747
H	-7.086335	0.218545	-0.139205	H	-7.049137	0.528873	-0.116380	H	-6.728537	1.947055	0.757900
H	-8.330078	-0.961095	0.357390	H	-8.342123	-0.588081	0.398774	H	-8.017049	0.913035	1.432087
C	-2.547822	2.212535	3.630263	C	-2.391120	2.326706	3.586090	C	-1.443353	3.784011	3.189153
H	-3.588786	2.173191	3.991478	H	-3.429192	2.339664	3.957476	H	-2.404032	4.225385	3.502915
H	-2.103607	1.206606	3.702302	H	-1.993160	1.302317	3.664099	H	-1.298123	2.830083	3.719974
H	-1.970951	2.895509	4.277814	H	-1.776741	2.988364	4.221140	H	-0.630690	4.474132	3.474664
C	-3.149135	4.075689	2.021510	C	-2.925985	4.197338	1.961788	C	-1.735587	4.841866	0.906829
H	-4.164478	4.067386	2.452192	H	-3.936091	4.237909	2.402841	H	-2.712519	5.232651	1.237122
H	-2.546624	4.830461	2.554003	H	-2.285909	4.932514	2.477536	H	-0.961789	5.606202	1.084972
H	-3.212174	4.371895	0.964656	H	-2.987085	4.481486	0.901382	H	-1.785006	4.645959	-0.175384

Intermediate-3 from reductive elimination^A pathway: In Ni catalyzed reaction energy profile

Int3A ² : $\nu_{\text{lowest}} = 12.4900 \text{ cm}^{-1}$				Int3A ⁴ : $\nu_{\text{lowest}} = 6.8274 \text{ cm}^{-1}$				Int3A ⁶ : $\nu_{\text{lowest}} = 16.6194 \text{ cm}^{-1}$			
109				109				109			
Ni	0.576828	-0.399273	0.615790	Ni	0.570485	-0.264789	0.759821	Ni	-0.373948	-0.032707	0.428810
C	0.296512	0.007595	-2.561734	C	-0.258303	0.501737	-2.249734	C	-0.334059	-1.126214	-1.976915
C	-1.774346	1.168873	-2.053977	C	-2.022053	2.024908	-1.574031	C	0.728782	-2.928657	-0.672956
C	-0.401267	-0.854774	-3.425751	C	-1.188413	-0.210843	-3.039711	C	0.847153	-1.036901	-2.762412
C	-2.474172	0.275589	-2.874916	C	-2.947904	1.298983	-2.334066	C	1.920528	-2.742757	-1.374797
H	-2.314003	1.953822	-1.514517	H	-2.350894	2.901713	-1.008005	H	0.662561	-3.705957	0.094598
C	-1.784439	-0.720629	-3.585063	C	-2.525499	0.184226	-3.079696	C	1.959334	-1.803848	-2.447155
H	0.162221	-1.645414	-3.930606	H	-0.831339	-1.083754	-3.593386	H	0.879314	-0.306249	-3.574863
H	-3.562305	0.358678	-2.958382	H	-3.999572	1.600159	-2.340259	H	2.806641	-3.335071	-1.129766
H	-2.330949	-1.404871	-4.242129	H	-3.247324	-0.383697	-3.675455	H	2.884324	-1.679001	-3.019445

N	2.119489	0.255347	-0.971140	N	1.791938	0.381979	-0.906549	N	-2.106591	-0.071856	-0.771896
C	3.325889	-0.312392	1.060441	C	3.364785	-0.540629	0.689504	C	-2.615377	1.541340	0.924139
C	2.098780	-0.204720	3.061300	C	2.553895	-0.777620	2.905617	C	-1.340133	1.321862	2.923895
C	4.529077	-0.638549	1.765421	C	4.690376	-0.930192	1.088919	C	-3.437707	2.562367	1.510086
C	3.353529	-0.170095	-0.356963	C	3.110527	-0.179504	-0.653720	C	-2.866184	1.104298	-0.398330
C	3.244952	-0.494579	3.821149	C	3.824586	-1.089805	3.375124	C	-2.135497	2.258981	3.567131
H	1.125606	-0.030324	3.531480	H	1.681681	-0.744232	3.566524	H	-0.489825	0.836322	3.411595
C	4.461606	-0.727557	3.186041	C	4.903231	-1.193039	2.475585	C	-3.181726	2.906716	2.872856
C	5.714117	-0.871123	1.012152	C	5.682802	-1.032634	0.079729	C	-4.430629	3.155547	0.686310
C	4.528062	-0.400802	-1.066953	C	4.111657	-0.297655	-1.640058	C	-3.850883	1.715988	-1.201751
H	3.161132	-0.537975	4.911392	H	3.966290	-1.283336	4.442893	H	-1.920929	2.510372	4.610591
H	5.363088	-0.973578	3.755930	H	5.901912	-1.474209	2.824018	H	-3.790389	3.673971	3.360503
C	5.705304	-0.767222	-0.371590	C	5.385929	-0.741711	-1.260963	C	-4.615633	2.751858	-0.648015
H	6.631486	-1.143851	1.544649	H	6.691284	-1.351384	0.364545	H	-5.052532	3.952151	1.108919
H	4.525435	-0.320377	-2.154898	H	3.881805	-0.066183	-2.681597	H	-3.981429	1.394969	-2.237200
H	6.620301	-0.960455	-0.940795	H	6.164622	-0.846586	-2.023776	H	-5.373929	3.248332	-1.262843
N	2.114237	-0.131366	1.711690	N	2.314647	-0.514419	1.582260	N	-1.574190	0.954561	1.620078
C	1.683381	-0.359087	-2.178712	C	1.094548	-0.055963	-2.094460	C	-1.375952	-0.120426	-2.060659
O	2.322869	-1.258226	-2.718837	O	1.548581	-0.967752	-2.784213	O	-1.546964	0.739290	-2.929691
O	-0.977041	0.423949	1.408079	O	-1.054700	0.465863	1.353273	O	1.169416	-0.594703	1.402495
C	-2.229794	0.197455	1.110340	C	-2.293813	0.135011	1.066752	C	2.389607	-0.612389	0.951457
C	-2.677848	-0.952236	0.359443	C	-2.612346	-1.008102	0.257734	C	2.800227	0.240237	-0.168757
C	-3.246347	1.127336	1.555199	C	-3.382971	0.931936	1.571061	C	3.384171	-1.431092	1.608235
C	-4.048077	-1.142732	0.050813	C	-3.946232	-1.264973	-0.141140	C	4.129727	0.168144	-0.633160
C	-1.734262	-1.932119	-0.122528	C	-1.584224	-1.932837	-0.164806	C	1.911805	1.206093	-0.751067
C	-4.571776	0.896846	1.189887	C	-4.672699	0.631821	1.131424	C	4.680474	-1.450024	1.086035
C	-5.014247	-0.220779	0.432352	C	-4.991063	-0.437817	0.254443	C	5.071091	-0.686348	-0.048905
H	-4.308453	-2.034805	-0.522460	H	-4.118256	-2.134289	-0.777459	H	4.400349	0.801057	-1.481926
N	-0.432173	-1.799976	-0.155318	N	-0.290369	-1.840732	0.043284	N	0.616589	1.360412	-0.501957
O	-2.195782	-3.111785	-0.612522	O	-1.966069	-3.032944	-0.852391	O	2.431288	2.117743	-1.604172
H	-5.326633	1.619141	1.512560	H	-5.495503	1.255880	1.489620	H	5.427319	-2.077291	1.569964
C	0.173001	-2.990631	-0.761452	C	0.380602	-2.934126	-0.684798	C	0.131092	2.592164	-1.125958
C	-1.032404	-3.994789	-0.855255	C	-0.789748	-3.935447	-0.949171	C	1.357236	3.051798	-2.012935
H	0.494087	-2.738005	-1.787798	H	0.702321	-2.533349	-1.662567	H	-0.712503	2.343842	-1.796766
C	1.412713	-3.386898	0.015444	C	1.618151	-3.444201	0.012161	C	-0.358514	3.601363	-0.107301
C	1.423603	-3.333109	1.424168	C	1.656909	-3.647295	1.403450	C	0.220341	3.697288	1.170664
C	2.596903	-3.719921	-0.662624	C	2.778490	-3.678675	-0.747242	C	-1.400852	4.476778	-0.458061
C	2.589516	-3.632274	2.137590	C	2.827672	-4.102052	2.020058	C	-0.226359	4.665028	2.077160
H	0.518487	-3.027209	1.958783	H	0.776282	-3.408173	2.008143	H	1.002463	2.987951	1.460505
C	3.769724	-4.007965	0.051399	C	3.951409	-4.134188	-0.130783	C	-1.843697	5.449757	0.446347
H	2.610423	-3.703221	-1.756669	H	2.767843	-3.460962	-1.820151	H	-1.884068	4.373790	-1.435777
C	3.767082	-3.968886	1.451595	C	3.976253	-4.350990	1.253606	C	-1.257647	5.546024	1.716616
H	2.587043	-3.579934	3.230889	H	2.852812	-4.238783	3.105736	H	0.217562	4.719298	3.076485
H	4.691746	-4.242269	-0.490527	H	4.853852	-4.292411	-0.729442	H	-2.665633	6.117031	0.167202
H	4.685441	-4.179858	2.009640	H	4.896835	-4.688562	1.740906	H	-1.613859	6.295628	2.431065
C	-0.382445	1.055882	-1.902957	C	-0.671145	1.642887	-1.527788	C	-0.404125	-2.126878	-0.921631
C	0.797419	3.257381	-2.250359	C	0.818416	3.661646	-1.840995	C	-2.544753	-3.448000	-1.448576

C	1.313764	4.431682	-1.441915	C	1.572541	4.680956	-1.009194	C	-3.732468	-4.027631	-0.702659
H	0.044691	3.442661	-3.026993	H	0.037105	4.014396	-2.526229	H	-1.907404	-4.120902	-2.036257
O	2.001321	2.714171	-2.821239	O	1.872661	2.999925	-2.559841	O	-3.165456	-2.461572	-2.293338
C	2.747252	2.629731	-1.591704	C	2.699043	2.707397	-1.417233	C	-3.911860	-1.789622	-1.257449
C	2.590117	4.020588	-1.010209	C	2.800053	4.051689	-0.725030	C	-4.619537	-2.940454	-0.567396
C	0.765550	5.642362	-1.023222	C	1.258033	5.926572	-0.469556	C	-4.014689	-5.264147	-0.125469
H	3.761425	2.247302	-1.766301	H	3.626769	2.201554	-1.710801	H	-4.519644	-0.973891	-1.668596
C	3.351360	4.808058	-0.148843	C	3.744627	4.647550	0.108145	C	-5.807805	-3.060382	0.150007
C	1.544540	6.459340	-0.179456	C	2.223144	6.550927	0.346176	C	-5.230823	-5.401289	0.574462
H	-0.233858	5.959423	-1.339544	H	0.299608	6.415730	-0.674118	H	-3.325675	-6.110687	-0.217338
C	2.816764	6.049342	0.250469	C	3.445790	5.921793	0.630971	C	-6.112330	-4.317300	0.710990
H	4.336125	4.483789	0.204225	H	4.691834	4.152002	0.345726	H	-6.491694	-2.213494	0.269804
H	1.152685	7.428841	0.145872	H	2.017967	7.542550	0.763363	H	-5.493947	-6.368371	1.016123
H	3.401067	6.704266	0.905434	H	4.177821	6.430266	1.267266	H	-7.051134	-4.451721	1.258620
C	0.403345	2.126473	-1.205845	C	0.348207	2.513862	-0.847553	C	-1.765061	-2.535768	-0.407316
H	-0.178154	2.548288	-0.376114	H	-0.079543	2.951806	0.065213	H	-1.668904	-3.057490	0.558150
C	1.823666	1.694168	-0.733891	C	1.724276	1.837988	-0.547130	C	-2.754753	-1.334769	-0.310174
H	1.955575	1.866417	0.342929	H	1.990451	1.896594	0.520878	H	-3.099237	-1.147382	0.717758
C	-2.857109	2.331457	2.436022	C	-3.122798	2.047142	2.602910	C	3.031744	-2.194597	2.897458
C	-6.501965	-0.355828	0.070044	C	-6.447264	-0.652334	-0.188498	C	6.482494	-0.774675	-0.647658
C	-1.834875	3.237491	1.705688	C	-2.213064	3.151783	2.013732	C	1.898038	-3.220016	2.651402
H	-0.913798	2.674357	1.497363	H	-1.257982	2.722122	1.679346	H	0.987316	-2.722129	2.289370
H	-2.254180	3.609922	0.753118	H	-2.704851	3.646296	1.157245	H	2.213795	-3.973763	1.908949
H	-1.583290	4.112942	2.332094	H	-2.007995	3.921878	2.779350	H	1.664205	-3.746173	3.594548
C	-2.233495	1.812710	3.757141	C	-2.440461	1.425685	3.849155	C	2.585862	-1.174268	3.979246
H	-2.966209	1.203346	4.315308	H	-3.090711	0.655705	4.300642	H	3.391524	-0.446361	4.180178
H	-1.347929	1.194730	3.543963	H	-1.479994	0.960887	3.578528	H	1.688156	-0.625681	3.656672
H	-1.932013	2.663073	4.396807	H	-2.253701	2.207951	4.607490	H	2.357297	-1.704762	4.921268
C	-4.077263	3.202132	2.798347	C	-4.432123	2.716947	3.067341	C	4.246188	-2.967141	3.453094
H	-4.558677	3.629755	1.900589	H	-4.960432	3.212033	2.233115	H	4.610960	-3.727348	2.739941
H	-4.837699	2.632314	3.360865	H	-5.121774	1.991907	3.534194	H	5.084064	-2.293641	3.704070
H	-3.748703	4.042320	3.435329	H	-4.197389	3.490184	3.819595	H	3.948325	-3.490728	4.377904
C	-6.928303	0.859627	-0.789892	C	-6.948568	0.613116	-0.926676	C	7.396253	-1.736698	0.136406
H	-7.999597	0.793863	-1.055627	H	-8.003311	0.490112	-1.233031	H	8.393671	-1.765540	-0.335527
H	-6.769831	1.809843	-0.250928	H	-6.884198	1.508887	-0.285037	H	7.528610	-1.410736	1.182754
H	-6.340981	0.898870	-1.724700	H	-6.345810	0.799450	-1.832879	H	6.996988	-2.765864	0.141261
C	-7.352566	-0.392336	1.363293	C	-7.333421	-0.905314	1.056090	C	7.132626	0.631609	-0.645972
H	-7.213514	0.522571	1.964903	H	-7.300021	-0.053386	1.757102	H	7.221906	1.018930	0.383804
H	-8.427588	-0.476392	1.118900	H	-8.386618	-1.055668	0.756287	H	8.144166	0.582204	-1.087842
H	-7.069456	-1.256014	1.990002	H	-6.994301	-1.804907	1.598691	H	6.540321	1.354302	-1.231987
C	-6.781368	-1.641101	-0.732070	C	-6.583965	-1.856415	-1.139771	C	6.365099	-1.287009	-2.106523
H	-6.218937	-1.655618	-1.682281	H	-5.976251	-1.721458	-2.051795	H	5.893935	-2.285290	-2.132747
H	-6.508288	-2.543478	-0.157680	H	-6.270286	-2.796076	-0.652706	H	5.755953	-0.605707	-2.724558
H	-7.856885	-1.705870	-0.974760	H	-7.637756	-1.971775	-1.448599	H	7.367015	-1.363454	-2.566329
C	-1.181738	-4.578669	-2.255516	C	-0.755161	-4.508995	-2.358443	C	1.079184	2.824508	-3.497240
H	-2.090389	-5.199934	-2.325706	H	-1.640942	-5.137660	-2.549547	H	2.011870	2.913268	-4.079476
H	-1.245195	-3.769578	-3.000659	H	-0.721436	-3.698161	-3.103574	H	0.620968	1.837328	-3.664106

H	-0.306182	-5.208367	-2.490758	H	0.148968	-5.130602	-2.476403	H	0.364535	3.584936	-3.856423
C	-1.063574	-5.067719	0.230896	C	-0.978708	-5.008528	0.120500	C	1.880545	4.455328	-1.725756
H	-1.997047	-5.649278	0.149476	H	-1.904293	-5.572606	-0.082531	H	2.773357	4.651838	-2.343301
H	-0.202992	-5.748744	0.123017	H	-0.123816	-5.704257	0.120643	H	1.108529	5.204378	-1.965445
H	-1.020433	-4.613989	1.233285	H	-1.056647	-4.556094	1.122091	H	2.145066	4.566054	-0.662964

Intermediate-3 from nucleophilic addition^B pathway: In Ni catalyzed reaction energy profile

Int3B ² : $\nu_{\text{lowest}} = 9.9580 \text{ cm}^{-1}$				Int3B ⁴ : $\nu_{\text{lowest}} = 8.3987 \text{ cm}^{-1}$				Int3B ⁶ : $\nu_{\text{lowest}} = 12.5856 \text{ cm}^{-1}$			
109				109				109			
Ni	0.295825	0.359588	-0.045493	Ni	0.322276	0.276242	-0.099636	Ni	0.387764	-0.389710	0.559012
C	2.005488	0.074247	2.243094	C	1.962840	-0.026512	2.308831	C	0.786865	0.768864	-2.136815
C	0.403686	-1.699626	2.693228	C	0.309209	-1.766482	2.694106	C	-1.188195	2.041048	-1.529415
C	1.584749	0.792135	3.363674	C	1.550177	0.672830	3.443460	C	0.088644	0.069767	-3.123998
C	-0.055318	-0.964261	3.796186	C	-0.138574	-1.051408	3.814474	C	-1.915535	1.299271	-2.471596
H	-0.045235	-2.667575	2.446521	H	-0.163765	-2.714061	2.415333	H	-1.685454	2.810644	-0.932047
C	0.551633	0.255747	4.148704	C	0.496976	0.142285	4.205181	C	-1.279617	0.340216	-3.281841
H	2.066062	1.743455	3.612321	H	2.051257	1.605805	3.720289	H	0.607297	-0.665102	-3.746422
H	-0.875609	-1.357856	4.406047	H	-0.974053	-1.439750	4.406810	H	-2.988661	1.480566	-2.587347
H	0.207049	0.793999	5.038564	H	0.158457	0.665581	5.106144	H	-1.862965	-0.202762	-4.032591
N	2.091954	1.041951	0.089396	N	2.089274	1.047794	0.202644	N	2.047065	-0.436555	-0.502115
C	1.503759	2.123593	-1.927597	C	1.625414	2.094374	-1.861930	C	2.777687	-1.600216	1.402992
C	-0.563240	1.461473	-2.798071	C	-0.372175	1.400724	-2.867097	C	1.155893	-1.860771	3.118406
C	1.763001	2.989275	-3.032550	C	1.947223	2.957755	-2.953716	C	3.761667	-2.294526	2.170503
C	2.462638	1.948798	-0.850210	C	2.515874	1.937368	-0.721328	C	3.087830	-1.075183	0.101056
C	-0.387900	2.284786	-3.932053	C	-0.137003	2.229617	-3.985346	C	2.056594	-2.547621	3.911377
H	-1.459260	0.846371	-2.660359	H	-1.265411	0.771883	-2.787086	H	0.126850	-1.660927	3.433250
C	0.767305	3.048801	-4.045207	C	1.015543	3.004396	-4.026789	C	3.384284	-2.779192	3.456517
C	2.987452	3.720438	-3.048570	C	3.166013	3.695232	-2.901161	C	5.053072	-2.449866	1.586538
C	3.660657	2.700708	-0.911754	C	3.713540	2.697929	-0.718709	C	4.412941	-1.240577	-0.437416
H	-1.162468	2.311544	-4.703995	H	-0.862216	2.249044	-4.804063	H	1.735211	-2.907268	4.894072
H	0.922214	3.700182	-4.912430	H	1.218836	3.655055	-4.884490	H	4.110075	-3.314855	4.075535
C	3.896917	3.562680	-2.005071	C	4.012868	3.547651	-1.802898	C	5.363690	-1.925548	0.305814
H	3.197539	4.397460	-3.882754	H	3.421292	4.369711	-3.724586	H	5.820986	-2.989487	2.152266
H	4.370345	2.589258	-0.090074	H	4.367857	2.605575	0.149895	H	4.622532	-0.851836	-1.437090
H	4.833486	4.131181	-2.025114	H	4.945988	4.121381	-1.770598	H	6.369845	-2.070744	-0.101242
N	0.356541	1.395808	-1.835883	N	0.488019	1.344893	-1.849190	N	1.503755	-1.377258	1.873114
C	3.012183	0.548313	1.165470	C	2.981426	0.455832	1.245462	C	2.224859	0.503564	-1.639143
O	4.026242	1.268282	1.547078	O	4.008673	1.139175	1.672616	O	3.036212	0.140155	-2.627982
O	-0.820258	-1.153456	-0.515675	O	-0.856318	-1.178625	-0.531672	O	-1.155304	0.412744	1.392488
C	-2.115544	-1.297466	-0.435559	C	-2.158194	-1.262768	-0.449963	C	-2.405269	0.383348	1.017779
C	-2.979426	-0.329244	0.192588	C	-2.969739	-0.250229	0.176330	C	-2.909344	-0.558178	0.045959
C	-2.733215	-2.478041	-0.997941	C	-2.830554	-2.417628	-0.999151	C	-3.340726	1.324028	1.594076
C	-4.385638	-0.522837	0.237681	C	-4.382386	-0.380317	0.232955	C	-4.267285	-0.538689	-0.346560
C	-2.433435	0.847375	0.828372	C	-2.369113	0.909361	0.798950	C	-2.038299	-1.541983	-0.566304
C	-4.118319	-2.601981	-0.921351	C	-4.219719	-2.477802	-0.913635	C	-4.661444	1.296185	1.151649
C	-4.981004	-1.647807	-0.315798	C	-5.032517	-1.480902	-0.309128	C	-5.162372	0.388928	0.179404

H	-4.979215	0.248139	0.732266	H	-4.937170	0.419599	0.726255	H	-4.583512	-1.273528	-1.088682
N	-1.169325	1.187740	0.924356	N	-1.093413	1.208317	0.876607	N	-0.750689	-1.682962	-0.377053
O	-3.294425	1.717391	1.410844	O	-3.193778	1.807971	1.389454	O	-2.583138	-2.419030	-1.437391
H	-4.576936	-3.494015	-1.356523	H	-4.721843	-3.350698	-1.339279	H	-5.362193	2.017387	1.579543
C	-1.058246	2.490722	1.602339	C	-0.932417	2.510895	1.542705	C	-0.237237	-2.742412	-1.254877
C	-2.494159	2.669091	2.211032	C	-2.352950	2.738000	2.173792	C	-1.549017	-3.428552	-1.781619
H	-0.329268	2.395669	2.422447	H	-0.188744	2.402450	2.348121	H	0.259942	-2.245162	-2.106361
C	-0.545120	3.546993	0.642038	C	-0.425321	3.556759	0.568691	C	0.796954	-3.617832	-0.583673
C	-1.229949	3.851070	-0.550958	C	-1.105191	3.822878	-0.635922	C	0.617420	-4.105877	0.723348
C	0.669649	4.197895	0.911470	C	0.760003	4.255039	0.848260	C	1.988666	-3.916896	-1.265643
C	-0.724501	4.809399	-1.435977	C	-0.621595	4.787338	-1.526610	C	1.599226	-4.899673	1.325383
H	-2.155959	3.318936	-0.795099	H	-2.011264	3.258570	-0.882662	H	-0.276409	-3.825034	1.288420
C	1.188351	5.146425	0.017986	C	1.255319	5.212385	-0.048857	C	2.976875	-4.707091	-0.662884
H	1.230271	3.937014	1.815690	H	1.316460	4.024417	1.763236	H	2.158802	-3.491967	-2.261321
C	0.487608	5.460171	-1.152971	C	0.561623	5.485146	-1.234351	C	2.780329	-5.204270	0.632040
H	-1.268036	5.038744	-2.358165	H	-1.159665	4.985538	-2.459168	H	1.456927	-5.253268	2.350820
H	2.147703	5.627550	0.231805	H	2.192767	5.731756	0.172522	H	3.910534	-4.911545	-1.196291
H	0.892489	6.196626	-1.854516	H	0.950289	6.227034	-1.939405	H	3.558503	-5.805038	1.113877
C	1.463478	-1.186237	1.927101	C	1.388574	-1.260289	1.950483	C	0.183614	1.785832	-1.371119
C	3.124756	-3.037112	1.547323	C	3.013529	-3.136077	1.520793	C	1.416356	3.980673	-1.306903
C	4.018497	-3.656835	0.487977	C	3.890569	-3.743954	0.441532	C	2.521330	4.718035	-0.572832
H	2.553262	-3.711099	2.200435	H	2.430458	-3.815248	2.158105	H	0.490643	4.527025	-1.534784
O	4.060130	-2.256837	2.313311	O	3.965186	-2.393562	2.302558	O	2.076051	3.568092	-2.515521
C	4.648575	-1.547463	1.200615	C	4.564102	-1.666659	1.206956	C	3.219833	2.947507	-1.887386
C	5.028300	-2.693775	0.275812	C	4.917498	-2.794482	0.250316	C	3.703523	4.055933	-0.966323
C	3.972536	-4.832356	-0.257532	C	3.818091	-4.897244	-0.336061	C	2.549216	5.758635	0.352524
H	5.409782	-0.835971	1.541957	H	5.339032	-0.978499	1.565278	H	3.897955	2.527106	-2.639456
C	6.013982	-2.887278	-0.690290	C	5.894329	-2.980090	-0.726322	C	4.940917	4.418546	-0.437927
C	4.987806	-5.048155	-1.212298	C	4.824198	-5.105943	-1.301925	C	3.802953	6.151783	0.864558
H	3.181354	-5.575184	-0.106969	H	3.013466	-5.628682	-0.201623	H	1.632676	6.267503	0.670644
C	5.993041	-4.091408	-1.423447	C	5.846533	-4.162902	-1.492113	C	4.979162	5.492518	0.474694
H	6.790492	-2.136481	-0.872224	H	6.684026	-2.239383	-0.892050	H	5.860353	3.897306	-0.725110
H	4.994821	-5.975679	-1.794958	H	4.810659	-6.017049	-1.909830	H	3.860980	6.984270	1.573906
H	6.773191	-4.285089	-2.167670	H	6.619148	-4.350805	-2.245635	H	5.940875	5.819309	0.884588
C	2.278110	-1.895812	0.864320	C	2.188072	-1.959391	0.869427	C	1.206621	2.585560	-0.596748
H	1.691692	-2.261950	0.007060	H	1.594598	-2.296434	0.004061	H	0.988460	2.696529	0.477506
C	3.419735	-0.892009	0.507046	C	3.345742	-0.965041	0.538949	C	2.570532	1.898024	-0.934973
H	3.589267	-0.748815	-0.568125	H	3.517359	-0.797072	-0.532925	H	3.209683	1.698347	-0.063249
C	-1.859324	-3.556665	-1.665798	C	-2.010536	-3.539462	-1.664553	C	-2.870723	2.318934	2.671627
C	-6.497309	-1.899957	-0.293296	C	-6.558768	-1.661926	-0.275108	C	-6.636331	0.468046	-0.245067
C	-0.862748	-4.132237	-0.627134	C	-1.031964	-4.151771	-0.629648	C	-1.777482	3.252409	2.092795
H	-0.237273	-3.330514	-0.209029	H	-0.362340	-3.378336	-0.226656	H	-0.922251	2.667552	1.724937
H	-1.407887	-4.622857	0.198964	H	-1.591400	-4.606276	0.207437	H	-2.183845	3.855478	1.260713
H	-0.206914	-4.884345	-1.103336	H	-0.419714	-4.940459	-1.104565	H	-1.421631	3.947580	2.874648
C	-1.084760	-2.943295	-2.860787	C	-1.219026	-2.970444	-2.870223	C	-2.307812	1.540299	3.888995
H	-1.791242	-2.556131	-3.617169	H	-1.913117	-2.557693	-3.624475	H	-3.086244	0.886066	4.320152
H	-0.437295	-2.119032	-2.527291	H	-0.532430	-2.173669	-2.548273	H	-1.447113	0.920721	3.596671

H	-0.457903	-3.716505	-3.341798	H	-0.630675	-3.774176	-3.349708	H	-1.984333	2.251068	4.671099
C	-2.703107	-4.728757	-2.206346	C	-2.910354	-4.676526	-2.189380	C	-4.026646	3.207200	3.175222
H	-3.266090	-5.236070	-1.402854	H	-3.489147	-5.151728	-1.377580	H	-4.459615	3.820690	2.365084
H	-3.420778	-4.397860	-2.978061	H	-3.618456	-4.319613	-2.958289	H	-4.836275	2.609733	3.630313
H	-2.033826	-5.475036	-2.669212	H	-2.278985	-5.455676	-2.651273	H	-3.643795	3.896405	3.947822
C	-6.788215	-3.220033	0.462252	C	-6.905527	-2.962651	0.490383	C	-6.912942	1.865441	-0.854075
H	-7.874411	-3.424641	0.480281	H	-7.999910	-3.116157	0.516481	H	-7.971639	1.950028	-1.159593
H	-6.290482	-4.079705	-0.018970	H	-6.451656	-3.847422	0.011297	H	-6.703888	2.671556	-0.129771
H	-6.428211	-3.159606	1.504204	H	-6.536328	-2.912989	1.529678	H	-6.280628	2.035150	-1.743400
C	-7.020471	-2.014467	-1.746314	C	-7.095866	-1.760411	-1.724242	C	-7.542058	0.257903	0.993645
H	-6.526696	-2.838512	-2.290012	H	-6.644919	-2.610032	-2.265750	H	-7.353652	1.020818	1.768519
H	-8.108619	-2.209292	-1.752165	H	-8.191945	-1.903821	-1.722048	H	-8.607055	0.323746	0.706078
H	-6.831711	-1.079729	-2.302917	H	-6.866983	-0.838934	-2.287819	H	-7.363835	-0.734499	1.443054
C	-7.256950	-0.758780	0.409689	C	-7.259943	-0.482556	0.425586	C	-6.989555	-0.601603	-1.296093
H	-6.938178	-0.647338	1.460891	H	-6.929596	-0.379857	1.474082	H	-6.387824	-0.482745	-2.214189
H	-7.101244	0.207122	-0.102110	H	-7.063259	0.472092	-0.093133	H	-6.827771	-1.621873	-0.906677
H	-8.340377	-0.972385	0.406060	H	-8.352043	-0.645900	0.430039	H	-8.053567	-0.511939	-1.576563
C	-2.527182	2.154261	3.652107	C	-2.384901	2.234692	3.618153	C	-1.540678	-3.593859	-3.296031
H	-3.566194	2.116650	4.019052	H	-3.419436	2.237236	3.999476	H	-2.509077	-3.980647	-3.654794
H	-2.089759	1.144399	3.705186	H	-1.982986	1.210488	3.672764	H	-1.335093	-2.631330	-3.789975
H	-1.941353	2.822540	4.306819	H	-1.766441	2.885901	4.259907	H	-0.750454	-4.310412	-3.579131
C	-3.130373	4.045907	2.080267	C	-2.946016	4.133420	2.037767	C	-1.951309	-4.714313	-1.063204
H	-4.141616	4.033775	2.520341	H	-3.950933	4.158712	2.491582	H	-2.932509	-5.050710	-1.437843
H	-2.520073	4.788755	2.620580	H	-2.304281	4.861667	2.561236	H	-1.205129	-5.504856	-1.244181
H	-3.202362	4.361422	1.029730	H	-3.021448	4.439232	0.984433	H	-2.027645	-4.554062	0.023271

Transition State (3B-4B) –elimination^B pathway: In Ni catalyzed reaction energy profile

TS3B ² : $\nu_{\text{lowest}} = -288.1430 \text{ cm}^{-1}$				TS3B ⁴ : $\nu_{\text{lowest}} = -304.0824 \text{ cm}^{-1}$				TS3B ⁶ : $\nu_{\text{lowest}} = -389.2686 \text{ cm}^{-1}$			
109				109				109			
Ni	0.282521	0.335413	-0.138928	Ni	0.474458	0.277421	-0.444517	Ni	0.302407	0.276778	0.174149
C	1.869670	-0.154686	2.407576	C	1.011742	-0.694702	2.474431	C	2.305347	0.489372	2.334309
C	0.130627	-1.857948	2.409100	C	-1.178566	-1.588170	1.897359	C	0.870861	-1.374514	2.957904
C	1.321660	0.458919	3.534287	C	0.465294	0.079452	3.498140	C	1.830498	1.263942	3.394281
C	-0.442929	-1.228602	3.525473	C	-1.740144	-0.787263	2.904025	C	0.371684	-0.593206	4.012070
H	-0.328431	-2.757533	1.986205	H	-1.817422	-2.238728	1.291908	H	0.496592	-2.390364	2.794305
C	0.165467	-0.098836	4.103999	C	-0.922382	0.020591	3.714494	C	0.860236	0.707002	4.242458
H	1.809865	1.343788	3.957259	H	1.122723	0.702487	4.114317	H	2.216198	2.278641	3.538488
H	-1.358827	-1.637339	3.965876	H	-2.822585	-0.804107	3.067103	H	-0.399201	-1.005626	4.671898
H	-0.269259	0.346424	5.005717	H	-1.377026	0.600754	4.525365	H	0.469535	1.288306	5.084835
N	2.004342	0.955487	0.163159	N	2.132913	0.356112	0.500897	N	1.867080	1.380844	0.022417
C	1.662332	2.105475	-1.882368	C	2.837218	1.439093	-1.486061	C	1.052537	1.824951	-2.112260
C	-0.349329	1.579283	-2.942031	C	1.227683	1.530703	-3.176759	C	-1.043557	0.844905	-2.595008
C	2.066759	2.984218	-2.928006	C	3.815055	2.095383	-2.288180	C	1.099122	2.481965	-3.376435
C	2.496596	1.842778	-0.721305	C	3.128225	0.984781	-0.127848	C	2.104334	2.013108	-1.136905
C	-0.044606	2.448216	-4.013689	C	2.131088	2.182312	-4.043378	C	-1.074377	1.457065	-3.839734
H	-1.274328	0.993039	-2.914941	H	0.202230	1.291901	-3.478798	H	-1.853509	0.197950	-2.244185

C	1.157403	3.148181	-4.007667	C	3.418705	2.466884	-3.601642	C	-0.001492	2.283592	-4.261264
C	3.339356	3.621284	-2.809908	C	5.106041	2.324194	-1.720422	C	2.238187	3.296931	-3.647196
C	3.759184	2.490670	-0.662323	C	4.438086	1.234659	0.381370	C	3.237237	2.842130	-1.460511
H	-0.754692	2.553441	-4.839133	H	1.806784	2.455930	-5.051633	H	-1.937251	1.290381	-4.492292
H	1.411409	3.825285	-4.830782	H	4.133785	2.974396	-4.258416	H	-0.011001	2.768387	-5.242074
C	4.149898	3.358230	-1.703627	C	5.387637	1.893213	-0.420080	C	3.281033	3.464083	-2.700824
H	3.668471	4.310810	-3.593975	H	5.867076	2.838470	-2.316108	H	2.297690	3.807770	-4.614778
H	4.398423	2.285636	0.200938	H	4.658358	0.899502	1.398095	H	4.020972	2.950032	-0.706761
H	5.126445	3.850565	-1.634846	H	6.385956	2.077130	-0.007481	H	4.136312	4.097757	-2.958050
N	0.481401	1.429409	-1.910375	N	1.580552	1.175512	-1.938380	N	0.015059	1.011468	-1.736245
C	3.068386	0.296742	1.590643	C	2.460266	-0.744720	2.008746	C	3.246675	0.906548	1.223616
O	3.932804	1.103770	1.999997	O	3.430543	-0.372619	2.706576	O	4.031127	1.891212	1.303148
O	-0.907990	-1.061614	-0.691554	O	-1.070361	-0.564060	-1.206878	O	-0.689200	-1.352300	0.038838
C	-2.201821	-1.179394	-0.549640	C	-2.337729	-0.395506	-0.922800	C	-1.983951	-1.504469	-0.062055
C	-3.006261	-0.207593	0.143870	C	-2.814326	0.659057	-0.064751	C	-2.909651	-0.517337	0.443376
C	-2.872853	-2.328637	-1.112182	C	-3.316620	-1.302805	-1.473735	C	-2.513633	-2.700246	-0.667501
C	-4.412323	-0.368326	0.257060	C	-4.193813	0.784882	0.240835	C	-4.303895	-0.744426	0.374772
C	-2.396924	0.942256	0.769987	C	-1.905029	1.620318	0.521474	C	-2.435845	0.722971	1.019815
C	-4.254612	-2.424055	-0.963139	C	-4.655297	-1.123936	-1.128416	C	-3.899864	-2.857536	-0.706578
C	-5.061359	-1.467200	-0.288753	C	-5.135058	-0.097985	-0.271715	C	-4.823022	-1.907176	-0.194318
H	-4.960789	0.404621	0.798353	H	-4.484683	1.603040	0.901742	H	-4.958800	0.029767	0.777829
N	-1.117827	1.232850	0.829855	N	-0.603799	1.682727	0.370973	N	-1.190678	1.135841	1.115551
O	-3.203493	1.836878	1.384638	O	-2.423829	2.577973	1.321218	O	-3.353929	1.591970	1.508236
H	-4.756377	-3.294209	-1.394717	H	-5.388402	-1.821040	-1.542615	H	-4.303463	-3.764336	-1.163325
C	-0.924147	2.508454	1.539255	C	-0.057311	2.777441	1.178133	C	-1.183630	2.532591	1.592495
C	-2.351040	2.773873	2.149310	C	-1.347700	3.527666	1.684174	C	-2.605242	2.644557	2.238143
H	-0.207063	2.341439	2.358858	H	0.459229	2.326862	2.045026	H	-0.411274	2.638400	2.370521
C	-0.342822	3.560259	0.614963	C	0.956117	3.604190	0.415751	C	-0.852726	3.473344	0.448556
C	-0.981917	3.910381	-0.590435	C	0.727864	3.998435	-0.915822	C	-1.648102	3.514772	-0.714685
C	0.877854	4.173372	0.940196	C	2.161565	3.973567	1.035755	C	0.293915	4.280516	0.517620
C	-0.428282	4.880165	-1.433219	C	1.672919	4.769238	-1.602540	C	-1.312194	4.363230	-1.774095
H	-1.911076	3.405658	-0.877450	H	-0.186181	3.672619	-1.422354	H	-2.521445	2.860326	-0.803710
C	1.443336	5.135020	0.090089	C	3.115517	4.736034	0.347297	C	0.639149	5.123479	-0.548696
H	1.407395	3.868864	1.849511	H	2.365400	3.633166	2.056957	H	0.941512	4.222175	1.399295
C	0.786710	5.496844	-1.092834	C	2.870155	5.141076	-0.971505	C	-0.166883	5.170979	-1.692998
H	-0.936980	5.146355	-2.365352	H	1.482847	5.067323	-2.638732	H	-1.929553	4.374243	-2.677252
H	2.405462	5.588900	0.346984	H	4.058150	4.999302	0.837541	H	1.549731	5.727997	-0.490759
H	1.228535	6.244727	-1.759360	H	3.617108	5.730880	-1.513128	H	0.109072	5.816560	-2.532866
C	1.313604	-1.330256	1.867425	C	0.209836	-1.548619	1.694113	C	1.858644	-0.828221	2.120958
C	2.946576	-3.218763	1.457685	C	1.052233	-3.920307	1.398212	C	3.672240	-2.543553	1.630897
C	3.892836	-3.776885	0.410913	C	1.949244	-4.766500	0.515181	C	4.429194	-3.168064	0.473989
H	2.281361	-3.919925	1.980459	H	0.062561	-4.316461	1.664076	H	3.261141	-3.207715	2.403555
O	3.855422	-2.593926	2.383441	O	1.863632	-3.742791	2.573415	O	4.651562	-1.652837	2.193116
C	4.579079	-1.807031	1.410884	C	3.051021	-3.273433	1.897256	C	5.003581	-0.981985	0.963254
C	4.968921	-2.863807	0.390757	C	3.257463	-4.357847	0.852808	C	5.309421	-2.152540	0.045125
C	3.843980	-4.856347	-0.467911	C	1.720158	-5.699342	-0.493581	C	4.348677	-4.386346	-0.196422
H	5.360483	-1.205275	1.892543	H	3.851893	-3.050053	2.613662	H	5.773758	-0.219230	1.136601

C	6.020541	-3.014149	-0.511176	C	4.365607	-4.878109	0.186844	C	6.130707	-2.334978	-1.065807
C	4.921965	-5.030897	-1.360241	C	2.840303	-6.252682	-1.147519	C	5.201127	-4.587957	-1.301324
H	3.002217	-5.557845	-0.466079	H	0.704836	-6.005066	-0.769656	H	3.653978	-5.171096	0.122851
C	5.993573	-4.124603	-1.379899	C	4.141986	-5.849227	-0.810789	C	6.078649	-3.578685	-1.727652
H	6.851552	-2.301132	-0.543539	H	5.383078	-4.554799	0.432212	H	6.804333	-1.545064	-1.414906
H	4.925858	-5.886357	-2.044454	H	2.694211	-7.009918	-1.925473	H	5.180897	-5.545236	-1.833164
H	6.821828	-4.284691	-2.078849	H	4.996163	-6.298000	-1.329608	H	6.733028	-3.761452	-2.586781
C	2.234998	-1.957659	0.834066	C	1.052276	-2.455546	0.813753	C	2.644177	-1.515146	1.016697
H	1.743488	-2.196564	-0.122568	H	0.760655	-2.444429	-0.250022	H	2.009702	-1.991436	0.250970
C	3.444009	-0.973928	0.729485	C	2.526772	-2.031969	1.101690	C	3.623893	-0.419574	0.480817
H	3.724763	-0.700970	-0.296187	H	3.140495	-1.861984	0.207012	H	3.614338	-0.283935	-0.608768
C	-2.061434	-3.402141	-1.862241	C	-2.873543	-2.445263	-2.408762	C	-1.555055	-3.751568	-1.255205
C	-6.579479	-1.687693	-0.188977	C	-6.636672	-0.010065	0.045047	C	-6.330261	-2.186667	-0.295033
C	-1.009554	-4.026598	-0.910074	C	-1.926775	-3.407121	-1.647345	C	-0.634785	-4.310372	-0.138663
H	-0.326332	-3.254437	-0.528500	H	-1.042421	-2.868603	-1.278618	H	-0.046207	-3.503424	0.322084
H	-1.506607	-4.515546	-0.053169	H	-2.448845	-3.862436	-0.786533	H	-1.234638	-4.803384	0.647061
H	-0.417537	-4.790584	-1.446815	H	-1.591040	-4.221701	-2.315158	H	0.058933	-5.058876	-0.563457
C	-1.352360	-2.763730	-3.084457	C	-2.147259	-1.861570	-3.647560	C	-0.698264	-3.106069	-2.376038
H	-2.097000	-2.339747	-3.782178	H	-2.823767	-1.193332	-4.209998	H	-1.344290	-2.733718	-3.190525
H	-0.668215	-1.963122	-2.765969	H	-1.256957	-1.291062	-3.343748	H	-0.105252	-2.263126	-1.992211
H	-0.771400	-3.531265	-3.627950	H	-1.833369	-2.679672	-4.321628	H	-0.009211	-3.858632	-2.800568
C	-2.960139	-4.542268	-2.382260	C	-4.072305	-3.272412	-2.916219	C	-2.320253	-4.939810	-1.872261
H	-3.481472	-5.062952	-1.559470	H	-4.618284	-3.758383	-2.088277	H	-2.933631	-5.469813	-1.122062
H	-3.718020	-4.176116	-3.097497	H	-4.786487	-2.653523	-3.487852	H	-2.979340	-4.619345	-2.698425
H	-2.335849	-5.286182	-2.907431	H	-3.705530	-4.068920	-3.587118	H	-1.595500	-5.663460	-2.283917
C	-6.857647	-3.017934	0.553444	C	-7.093637	-1.323477	0.726383	C	-6.657492	-3.499117	0.460017
H	-7.945473	-3.200061	0.626606	H	-8.174733	-1.286007	0.953824	H	-7.737485	-3.722458	0.389719
H	-6.405928	-3.876882	0.027604	H	-6.914696	-2.198842	0.078238	H	-6.106231	-4.357502	0.039115
H	-6.440412	-2.988256	1.575165	H	-6.544972	-1.483335	1.671142	H	-6.389090	-3.412644	1.527350
C	-7.183020	-1.758831	-1.613324	C	-7.429719	0.189369	-1.269964	C	-6.721690	-2.339287	-1.786193
H	-6.738704	-2.581280	-2.200322	H	-7.260109	-0.643114	-1.974685	H	-6.172779	-3.167180	-2.267020
H	-8.273945	-1.929945	-1.563259	H	-8.514422	0.242321	-1.063651	H	-7.802529	-2.549910	-1.879281
H	-7.003672	-0.816404	-2.159931	H	-7.124821	1.125003	-1.770604	H	-6.498495	-1.413502	-2.344632
C	-7.274262	-0.546719	0.578495	C	-6.954452	1.164862	0.989566	C	-7.169740	-1.048770	0.316747
H	-6.896971	-0.465803	1.612978	H	-6.429500	1.061536	1.955412	H	-6.942662	-0.907892	1.387931
H	-7.125190	0.426985	0.079657	H	-6.667604	2.133011	0.542928	H	-6.995275	-0.090461	-0.202865
H	-8.360720	-0.737397	0.629388	H	-8.038764	1.196108	1.196076	H	-8.243546	-1.289423	0.228222
C	-2.408420	2.314884	3.606448	C	-1.353411	3.689289	3.199620	C	-2.559364	2.206425	3.704691
H	-3.444701	2.361487	3.980131	H	-2.311361	4.113917	3.543547	H	-3.582243	2.096010	4.100881
H	-2.040381	1.280876	3.692027	H	-1.194548	2.716991	3.689059	H	-2.029328	1.244670	3.800910
H	-1.773330	2.964592	4.233364	H	-0.539677	4.373225	3.497285	H	-2.023638	2.960260	4.307007
C	-2.922193	4.174463	1.970865	C	-1.676119	4.838200	0.971054	C	-3.341094	3.962300	2.050097
H	-3.928472	4.225548	2.419350	H	-2.640052	5.222683	1.344193	H	-4.338978	3.905350	2.516462
H	-2.272303	4.907284	2.477455	H	-0.891744	5.588554	1.162715	H	-2.772335	4.773700	2.534217
H	-2.990579	4.454163	0.910092	H	-1.757168	4.692259	-0.116841	H	-3.454015	4.211468	0.985357

Intermediate-4 from elimination^B pathway: In Ni catalyzed reaction energy profile

Int4B ² : $\nu_{\text{lowest}} = 12.8268 \text{ cm}^{-1}$				Int4B ⁴ : $\nu_{\text{lowest}} = 10.9964 \text{ cm}^{-1}$				Int4B ⁶ : $\nu_{\text{lowest}} = 11.3050 \text{ cm}^{-1}$			
109				109				109			
Ni	0.446648	0.747651	-0.807267	Ni	0.615380	-0.357835	0.801487	Ni	0.305965	-0.460766	-0.249442
C	0.309155	0.258515	2.893530	C	0.597629	1.109786	-2.784842	C	2.696201	-0.731146	-2.440609
C	-1.441320	-1.248317	2.136869	C	-1.648871	1.252226	-1.871680	C	0.805703	0.680796	-3.044311
C	-0.610828	1.029254	3.618571	C	0.185341	0.197545	-3.765181	C	2.322960	-1.702870	-3.380043
C	-2.366513	-0.479664	2.859671	C	-2.068419	0.332084	-2.845309	C	0.424879	-0.295357	-3.985078
H	-1.779635	-2.114801	1.560070	H	-2.366636	1.649778	-1.148199	H	0.206475	1.585920	-2.912489
C	-1.959152	0.652434	3.593036	C	-1.162326	-0.185790	-3.791520	C	1.176834	-1.473997	-4.154156
H	-0.260039	1.895813	4.189106	H	0.912376	-0.187018	-4.488662	H	2.917868	-2.616413	-3.478492
H	-3.424946	-0.758800	2.840920	H	-3.114986	0.011094	-2.865655	H	-0.470687	-0.133304	-4.594337
H	-2.705808	1.232780	4.145442	H	-1.523309	-0.885494	-4.553052	H	0.856492	-2.215794	-4.894211
N	1.628163	1.885822	-0.034697	N	2.057303	0.085530	-0.342219	N	1.676673	-1.719060	0.087442
C	3.119069	0.477785	-1.224497	C	3.284849	-0.940620	1.435319	C	1.088644	-1.509850	2.310030
C	2.008722	-1.272346	-2.297824	C	2.017552	-1.561116	3.293180	C	-0.854652	-0.226299	2.677086
C	4.404265	-0.001885	-1.590216	C	4.500528	-1.388266	2.028008	C	1.211400	-1.838360	3.689669
C	2.897677	1.629714	-0.388398	C	3.235792	-0.335218	0.104133	C	1.997296	-2.065504	1.328959
C	3.242226	-1.810023	-2.721565	C	3.171917	-2.009838	3.968270	C	-0.807583	-0.502199	4.037565
H	1.050271	-1.740084	-2.530348	H	1.023142	-1.626647	3.748283	H	-1.644653	0.390297	2.238219
C	4.437146	-1.190202	-2.370810	C	4.410117	-1.930996	3.338682	C	0.229287	-1.305906	4.576837
C	5.529819	0.741045	-1.116547	C	5.701131	-1.265601	1.262655	C	2.292904	-2.694221	4.061375
C	4.053265	2.323848	0.066708	C	4.475993	-0.237021	-0.604136	C	3.071651	-2.920790	1.752257
H	3.240160	-2.731811	-3.309424	H	3.077709	-2.422308	4.977183	H	-1.584462	-0.088166	4.688052
H	5.397629	-1.616132	-2.678968	H	5.315853	-2.284715	3.843572	H	0.276886	-1.527364	5.647297
C	5.332833	1.870675	-0.311549	C	5.664893	-0.705919	-0.021033	C	3.198148	-3.214775	3.106547
H	6.540429	0.413464	-1.379826	H	6.645941	-1.613517	1.692713	H	2.413330	-2.954732	5.118817
H	3.926324	3.188256	0.723401	H	4.463561	0.211144	-1.602396	H	3.761767	-3.307016	0.998315
H	6.210900	2.417762	0.049441	H	6.600154	-0.621855	-0.586016	H	4.014150	-3.862052	3.444419
N	1.953061	-0.155128	-1.560421	N	2.079164	-1.043772	2.060361	N	0.089418	-0.714074	1.808207
C	1.781187	0.429997	2.802236	C	1.952476	1.681912	-2.568906	C	3.802445	-0.786979	-1.455130
O	2.465449	1.279893	3.351307	O	2.966991	1.437190	-3.209839	O	4.637674	-1.673775	-1.325553
O	-0.730534	-0.621476	-1.361466	O	-1.088412	0.312515	1.298376	O	-0.626246	1.201538	-0.336587
C	-2.003706	-0.789120	-1.078399	C	-2.299119	-0.111402	1.025791	C	-1.914804	1.387972	-0.181915
C	-2.791752	0.212810	-0.422043	C	-2.548129	-1.236107	0.163836	C	-2.878011	0.351850	-0.462647
C	-2.662266	-2.028766	-1.420913	C	-3.439866	0.583630	1.568719	C	-2.400381	2.671390	0.256142
C	-4.151381	-0.008300	-0.093731	C	-3.870489	-1.625498	-0.165129	C	-4.265185	0.595698	-0.310469
C	-2.199007	1.472324	-0.047615	C	-1.454237	-1.971378	-0.434214	C	-2.454035	-0.955991	-0.914094
C	-3.998374	-2.193075	-1.054597	C	-4.714421	0.147573	1.206328	C	-3.779014	2.840841	0.391594
C	-4.776900	-1.213664	-0.384595	C	-4.973006	-0.945435	0.338170	C	-4.740037	1.830497	0.121031
H	-4.679106	0.800599	0.414073	H	-3.986538	-2.477704	-0.836979	H	-4.946431	-0.225571	-0.539270
N	-0.944236	1.826900	-0.192404	N	-0.174927	-1.840080	-0.181089	N	-1.220560	-1.392744	-1.036072
O	-2.990981	2.404328	0.517607	O	-1.751525	-2.898022	-1.375036	O	-3.405164	-1.858035	-1.247340
H	-4.481499	-3.142455	-1.299370	H	-5.574840	0.684272	1.614446	H	-4.146160	3.812510	0.730947
C	-0.744943	3.179146	0.354763	C	0.587320	-2.680218	-1.112980	C	-1.234773	-2.818433	-1.399170
C	-2.213696	3.659519	0.641041	C	-0.509822	-3.642007	-1.691562	C	-2.722032	-3.019140	-1.862824
H	-0.183268	3.078417	1.298992	H	0.951628	-2.019019	-1.921952	H	-0.561152	-2.974991	-2.257770

C	0.051923	4.080923	-0.563454	C	1.787821	-3.336937	-0.470884	C	-0.740416	-3.670083	-0.245444
C	0.041557	3.900607	-1.957740	C	1.724570	-3.865508	0.831320	C	-1.215557	-3.462578	1.062065
C	0.787714	5.147858	-0.019257	C	2.999217	-3.417694	-1.178736	C	0.242924	-4.648697	-0.468592
C	0.763816	4.764668	-2.791128	C	2.843737	-4.479634	1.405761	C	-0.705462	-4.212508	2.128457
H	-0.518558	3.062097	-2.384861	H	0.797925	-3.763884	1.404622	H	-1.959163	-2.683334	1.257153
C	1.503741	6.017756	-0.851140	C	4.123702	-4.025613	-0.604055	C	0.751131	-5.404424	0.596474
H	0.820334	5.278504	1.068492	H	3.067314	-2.972228	-2.177278	H	0.637429	-4.793018	-1.480832
C	1.496107	5.827095	-2.241529	C	4.046781	-4.562205	0.688386	C	0.281174	-5.183714	1.898378
H	0.757256	4.605453	-3.874895	H	2.782403	-4.881059	2.422528	H	-1.061989	-4.019254	3.144895
H	2.081078	6.839009	-0.412738	H	5.065559	-4.063615	-1.160548	H	1.532812	-6.148880	0.412806
H	2.063967	6.500252	-2.892618	H	4.926957	-5.029122	1.142844	H	0.696812	-5.751589	2.736768
C	-0.092970	-0.869361	2.154053	C	-0.304764	1.643601	-1.848924	C	1.950509	0.454559	-2.266402
C	1.448105	-2.944268	2.043634	C	-0.136353	4.114679	-1.224315	C	3.321940	2.590675	-1.762809
C	2.602256	-3.466771	1.202165	C	0.592470	5.038971	-0.264990	C	3.778955	3.397553	-0.559813
H	0.602484	-3.617642	2.238890	H	-1.223777	4.231465	-1.327365	H	2.817174	3.117127	-2.584064
O	2.111560	-2.589369	3.274293	O	0.526427	4.399121	-2.475058	O	4.551649	1.996451	-2.215525
C	3.144845	-1.772175	2.683458	C	1.876927	4.205940	-2.000250	C	4.956702	1.442243	-0.941832
C	3.710424	-2.700610	1.619674	C	1.905807	5.105813	-0.775161	C	4.844350	2.645769	-0.023367
C	2.716078	-4.394942	0.169519	C	0.243488	5.687325	0.917265	C	3.324991	4.555242	0.067572
H	3.822079	-1.375767	3.451533	H	2.604536	4.387069	-2.802782	H	5.924301	0.930167	-1.027164
C	4.953529	-2.837086	1.005876	C	2.899488	5.822891	-0.112585	C	5.478403	3.033799	1.154985
C	3.981506	-4.565553	-0.428961	C	1.238075	6.439073	1.576465	C	3.982315	4.969102	1.244298
H	1.856806	-4.984919	-0.165396	H	-0.771649	5.626891	1.323542	H	2.489268	5.134635	-0.337476
C	5.081825	-3.797587	-0.018509	C	2.544768	6.506070	1.069113	C	5.041546	4.219855	1.779460
H	5.810513	-2.226410	1.309384	H	3.924682	5.867652	-0.495999	H	6.296435	2.445838	1.584786
H	4.108223	-5.309354	-1.223208	H	0.987126	6.981356	2.494555	H	3.663586	5.888585	1.746860
H	6.055024	-3.949773	-0.498073	H	3.298413	7.100614	1.596942	H	5.537051	4.563518	2.693771
C	1.077564	-1.534261	1.464080	C	0.362789	2.653606	-0.940942	C	2.553685	1.337280	-1.189950
H	0.924294	-1.566144	0.375174	H	0.268538	2.378162	0.121020	H	1.810095	1.657624	-0.440842
C	2.314655	-0.700056	1.907899	C	1.831678	2.736413	-1.454852	C	3.744865	0.506736	-0.619768
H	2.905962	-0.271384	1.090114	H	2.601653	2.567069	-0.691086	H	3.677208	0.267968	0.452810
C	-1.898921	-3.144598	-2.156871	C	-3.237998	1.780825	2.517366	C	-1.408833	3.812483	0.552230
C	-6.235489	-1.520715	-0.010754	C	-6.424083	-1.317867	-0.006248	C	-6.234088	2.134133	0.314769
C	-0.719841	-3.633913	-1.279317	C	-2.488837	2.917891	1.778033	C	-0.618484	4.155546	-0.736698
H	-0.061961	-2.801491	-0.994942	H	-1.508160	2.572120	1.422036	H	-0.023804	3.292732	-1.071280
H	-1.101342	-4.102871	-0.354354	H	-3.077195	3.270684	0.911678	H	-1.307849	4.446796	-1.548967
H	-0.123039	-4.388491	-1.823857	H	-2.335280	3.774795	2.459272	H	0.062818	5.003930	-0.544735
C	-1.392169	-2.605242	-3.518884	C	-2.423404	1.334608	3.758252	C	-0.430287	3.395552	1.680326
H	-2.248098	-2.378803	-4.178524	H	-2.963553	0.543740	4.308784	H	-0.981172	3.196810	2.616321
H	-0.810403	-1.680730	-3.389109	H	-1.437515	0.947681	3.459911	H	0.129609	2.488647	1.410992
H	-0.762318	-3.362056	-4.022007	H	-2.277034	2.191105	4.441716	H	0.292027	4.209650	1.871813
C	-2.789254	-4.369659	-2.449824	C	-4.580433	2.351631	3.017976	C	-2.134261	5.094200	1.010388
H	-3.165018	-4.838030	-1.522979	H	-5.202522	2.731365	2.188132	H	-2.823276	5.478150	0.237233
H	-3.654536	-4.107295	-3.083534	H	-5.165557	1.598384	3.574772	H	-2.708452	4.931019	1.939473
H	-2.195334	-5.128072	-2.989757	H	-4.383582	3.196449	3.701024	H	-1.386551	5.880506	1.213504
C	-6.269779	-2.744656	0.937581	C	-7.105827	-0.114983	-0.704040	C	-6.640122	3.314616	-0.601936
H	-7.310804	-2.990864	1.215755	H	-8.155487	-0.355530	-0.953486	H	-7.710701	3.554352	-0.468602

H	-5.826207	-3.636905	0.462684	H	-7.108035	0.779329	-0.057056	H	-6.058966	4.224467	-0.372771
H	-5.703640	-2.536729	1.862862	H	-6.577159	0.143994	-1.638254	H	-6.470202	3.061037	-1.662909
C	-7.042816	-1.840020	-1.292693	C	-7.192440	-1.661380	1.293365	C	-6.488767	2.519196	1.793224
H	-6.622484	-2.707812	-1.829923	H	-7.200026	-0.810308	1.996166	H	-5.903050	3.407211	2.087316
H	-8.092862	-2.074980	-1.039891	H	-8.242419	-1.920222	1.064584	H	-7.557704	2.750739	1.951946
H	-7.035531	-0.977923	-1.982242	H	-6.726221	-2.520850	1.806120	H	-6.209087	1.689606	2.465832
C	-6.903920	-0.331067	0.704454	C	-6.494343	-2.533203	-0.950451	C	-7.116570	0.920055	-0.032910
H	-6.380110	-0.075686	1.642472	H	-5.981590	-2.333187	-1.907644	H	-6.988711	0.614133	-1.086023
H	-6.921963	0.568286	0.064475	H	-6.035898	-3.427937	-0.493995	H	-6.884940	0.052713	0.609683
H	-7.947515	-0.585990	0.959602	H	-7.548759	-2.771234	-1.175906	H	-8.179848	1.176691	0.117187
C	-2.386586	4.178014	2.062786	C	-0.412294	-3.792051	-3.203221	C	-2.833752	-2.838733	-3.378347
H	-3.445993	4.404031	2.270698	H	-1.260498	-4.378233	-3.594729	H	-3.892030	-2.783666	-3.682364
H	-2.027613	3.432720	2.788896	H	-0.402105	-2.804399	-3.687639	H	-2.322668	-1.912584	-3.691497
H	-1.800218	5.104644	2.187642	H	0.523580	-4.320254	-3.455209	H	-2.358603	-3.690607	-3.894974
C	-2.790389	4.615582	-0.402200	C	-0.630672	-4.991677	-0.985045	C	-3.415313	-4.278217	-1.364301
H	-3.861302	4.779511	-0.195550	H	-1.506459	-5.531481	-1.382220	H	-4.460652	-4.298175	-1.715523
H	-2.263208	5.582855	-0.370603	H	0.273216	-5.599786	-1.152372	H	-2.893942	-5.168980	-1.752460
H	-2.682601	4.201363	-1.417207	H	-0.764950	-4.860872	0.100300	H	-3.402247	-4.325909	-0.265379

Conformational analysis of stereo-selectivity with L7 ligand

Note: conformer 1 is for the major enantiomer and have been provided with the main free energy profile.

Intermediate-1: In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

Int1-conformer2 ² : $v_{\text{lowest}} = 14.4890 \text{ cm}^{-1}$				Int1-conformer3 ² : $v_{\text{lowest}} = 14.1745 \text{ cm}^{-1}$				Int1-conformer4 ² : $v_{\text{lowest}} = 10.6492 \text{ cm}^{-1}$			
109				109				109			
Ni	-0.585415	0.179928	0.269210	Ni	0.385253	-0.197759	0.026477	Ni	0.396525	-0.149152	0.081976
C	-1.004724	0.195168	3.012873	C	1.151142	-0.458336	2.663625	C	1.445315	-0.838502	2.551158
C	1.312025	0.718639	2.490741	C	-0.988916	-1.549608	2.291258	C	-0.798933	-1.734159	2.278985
C	-0.735229	0.268580	4.389905	C	1.076716	-0.720691	4.039169	C	1.527649	-1.370308	3.846857
C	1.577610	0.794402	3.871311	C	-1.050418	-1.834163	3.670017	C	-0.713624	-2.268398	3.578661
H	2.119452	0.896577	1.775358	H	-1.806685	-1.864919	1.637366	H	-1.709061	-1.882184	1.690028
C	0.563728	0.566554	4.818970	C	-0.031042	-1.415336	4.543131	C	0.441160	-2.088725	4.361254
H	-1.557398	0.089310	5.092262	H	1.899629	-0.387419	4.681517	H	2.447091	-1.210340	4.421175
H	2.593030	1.035245	4.207150	H	-1.913427	-2.383239	4.064253	H	-1.563242	-2.831004	3.982943
H	0.792273	0.626061	5.888567	H	-0.104305	-1.636426	5.613321	H	0.486587	-2.510253	5.371157
N	-2.308088	-0.083835	1.093901	N	2.123892	0.222509	0.651703	N	2.126401	0.362177	0.664045
C	-2.952426	-0.422972	-1.146040	C	2.389383	0.957706	-1.570228	C	2.140175	1.481184	-1.407324
C	-1.178618	-0.196136	-2.657589	C	0.455056	0.677860	-2.858824	C	0.243519	1.022510	-2.699811
C	-3.881745	-0.740013	-2.186052	C	3.114286	1.529407	-2.661770	C	2.689595	2.348747	-2.402137
C	-3.345087	-0.380553	0.235577	C	2.981144	0.778053	-0.276799	C	2.813098	1.225907	-0.165586
C	-2.026897	-0.500371	-3.747598	C	1.093405	1.236671	-3.991212	C	0.709302	1.865498	-3.735514
H	-0.110736	0.016910	-2.777459	H	-0.579649	0.320954	-2.883360	H	-0.705560	0.481187	-2.766344
C	-3.367803	-0.769797	-3.512756	C	2.411923	1.658537	-3.892884	C	1.921758	2.524090	-3.587124
C	-5.233335	-1.001047	-1.827501	C	4.465832	1.915555	-2.443446	C	3.944421	2.965450	-2.140040

C	-4.689866	-0.639786	0.547004	C	4.317472	1.168080	-0.101432	C	4.043893	1.863065	0.059521
H	-1.613264	-0.524585	-4.760027	H	0.539142	1.325537	-4.929905	H	0.105757	1.987709	-4.639501
H	-4.041699	-1.012593	-4.341710	H	2.924135	2.092852	-4.758444	H	2.298379	3.184230	-4.375998
C	-5.605964	-0.941978	-0.488875	C	5.033569	1.725397	-1.187697	C	4.586467	2.714312	-0.932330
H	-5.960111	-1.247763	-2.607711	H	5.041185	2.354301	-3.264511	H	4.385119	3.631304	-2.888212
H	-4.998977	-0.613912	1.592469	H	4.777533	1.046116	0.879083	H	4.564468	1.680042	0.999698
H	-6.647801	-1.143298	-0.214982	H	6.075589	2.021006	-1.022204	H	5.551831	3.191748	-0.731058
N	-1.637313	-0.152315	-1.410089	N	1.090119	0.545039	-1.698505	N	0.943409	0.840009	-1.582750
C	-2.365289	-0.105710	2.475183	C	2.321170	0.207663	2.024877	C	2.542319	-0.050813	1.923488
O	-3.369119	-0.341113	3.158247	O	3.293003	0.684818	2.617745	O	3.630712	0.213846	2.440992
O	1.025997	0.642626	-0.683278	O	-1.165585	-0.956033	-0.764521	O	-1.068673	-1.016290	-0.741636
C	2.211070	0.092743	-0.614422	C	-2.432680	-0.657870	-0.577102	C	-2.357268	-0.799324	-0.611259
C	2.428387	-1.257981	-0.170153	C	-2.872728	0.550546	0.063639	C	-2.909801	0.291496	0.146516
C	3.369997	0.863661	-1.001599	C	-3.442938	-1.574539	-1.046232	C	-3.284876	-1.695987	-1.260568
C	3.730281	-1.816751	-0.129465	C	-4.252013	0.832168	0.228265	C	-4.312052	0.469712	0.263504
C	1.320534	-2.068743	0.284890	C	-1.919106	1.506855	0.583797	C	-2.050476	1.245893	0.810390
C	4.621002	0.248986	-0.950796	C	-4.782747	-1.229593	-0.862850	C	-4.650559	-1.449620	-1.122386
C	4.844924	-1.086194	-0.523199	C	-5.230201	-0.040782	-0.231463	C	-5.206763	-0.383938	-0.367871
H	3.820789	-2.843914	0.228252	H	-4.512561	1.763920	0.733232	H	-4.657181	1.312288	0.865305
N	0.068408	-1.708103	0.384379	N	-0.617901	1.406504	0.565380	N	-0.745651	1.284867	0.774214
O	1.576124	-3.341653	0.677381	O	-2.386914	2.632802	1.170746	O	-2.619026	2.230484	1.545846
H	5.492867	0.838160	-1.247472	H	-5.542558	-1.928211	-1.222127	H	-5.343705	-2.131959	-1.620947
C	-0.730202	-2.829374	0.884261	C	-0.008033	2.578738	1.197243	C	-0.258047	2.452440	1.511598
C	0.375430	-3.818050	1.398566	C	-1.246852	3.255896	1.885709	C	-1.531082	2.861222	2.332689
H	-1.332705	-2.491743	1.743511	H	0.688785	2.244652	1.983819	H	0.538306	2.139181	2.206889
C	-1.677330	-3.339276	-0.186043	C	0.779373	3.381727	0.180597	C	0.310002	3.485605	0.556126
C	-1.253991	-3.471320	-1.521167	C	0.235203	3.676659	-1.083508	C	-0.358678	3.803309	-0.640890
C	-3.004316	-3.661085	0.145096	C	2.090366	3.790992	0.474488	C	1.525919	4.124565	0.849200
C	-2.140142	-3.929303	-2.504281	C	0.986198	4.380882	-2.031951	C	0.174128	4.753636	-1.520422
H	-0.230118	-3.193268	-1.791971	H	-0.773959	3.330784	-1.332001	H	-1.293013	3.290537	-0.891781
C	-3.893743	-4.116285	-0.837930	C	2.844636	4.494943	-0.475041	C	2.063140	5.073110	-0.032067
H	-3.349320	-3.525146	1.176032	H	2.536131	3.519833	1.438013	H	2.067904	3.857752	1.763158
C	-3.462202	-4.254126	-2.164269	C	2.293626	4.792351	-1.728373	C	1.386388	5.391937	-1.216861
H	-1.801252	-4.022004	-3.541488	H	0.556166	4.598237	-3.015214	H	-0.352754	4.988874	-2.450996
H	-4.930065	-4.344938	-0.569801	H	3.872633	4.789608	-0.242179	H	3.020751	5.549696	0.199869
H	-4.158947	-4.599958	-2.935281	H	2.887279	5.330165	-2.475037	H	1.810005	6.125780	-1.910577
C	0.015749	0.413891	2.063120	C	0.120900	-0.861237	1.790817	C	0.292443	-1.025800	1.765803
C	-1.248355	3.031152	-1.077588	C	3.663259	-3.297816	-1.493359	C	5.331651	-2.850786	-0.166667
C	-0.952660	4.472961	-0.649952	C	3.934670	-2.944737	-0.019931	C	3.966684	-3.262881	0.412563
H	-0.694382	2.625364	-1.931058	H	4.532838	-3.459100	-2.144526	H	6.230613	-3.207313	0.353706
O	-0.851009	2.359197	0.160678	O	2.896554	-4.515201	-1.321862	O	5.218764	-3.435115	-1.488426
C	-1.774482	3.085768	1.033427	C	1.878271	-3.923717	-0.474945	C	4.004996	-2.733150	-1.851467
C	-1.294111	4.509265	0.719211	C	2.768286	-3.369795	0.650008	C	3.091807	-3.180612	-0.691764
C	-0.454719	5.592574	-1.301267	C	4.988708	-2.359468	0.667455	C	3.520551	-3.675680	1.659610
H	-1.693759	2.727786	2.066520	H	1.105964	-4.654514	-0.201903	H	3.685423	-2.986138	-2.871494
C	-1.146264	5.668523	1.467852	C	2.638838	-3.242521	2.025273	C	1.747374	-3.503973	-0.568964
C	-0.301281	6.778318	-0.545705	C	4.869784	-2.234388	2.071115	C	2.159588	-4.038776	1.785780

H	-0.175148	5.563782	-2.359728	H	5.889341	-2.010638	0.150749	H	4.194728	-3.731445	2.520894
C	-0.640821	6.815345	0.811986	C	3.721698	-2.675878	2.736766	C	1.291363	-3.953882	0.693836
H	-1.398750	5.700073	2.532939	H	1.731707	-3.557954	2.550932	H	1.057947	-3.441031	-1.417285
H	0.096433	7.677510	-1.028030	H	5.682411	-1.777170	2.644589	H	1.776884	-4.378664	2.752943
H	-0.505509	7.743395	1.377436	H	3.649801	-2.560453	3.822785	H	0.241985	-4.233942	0.819401
C	-2.772597	2.832285	-1.022264	C	-3.042762	-2.901536	-1.721196	C	-2.767152	-2.912232	-2.051898
H	-3.426506	2.742837	-1.891426	C	-6.737095	0.221498	-0.078220	C	-6.733172	-0.227288	-0.278292
C	-3.096398	2.865614	0.280742	C	-7.375068	-0.920024	0.751198	C	-2.021874	-3.855655	-1.075863
H	-4.080290	2.802661	0.748024	H	-8.462158	-0.754853	0.863835	H	-1.209419	-3.316616	-0.569029
C	3.209969	2.333464	-1.436496	H	-7.231006	-1.901461	0.267023	H	-2.716990	-4.245604	-0.311374
C	6.275487	-1.648606	-0.499109	H	-6.924584	-0.968830	1.757973	H	-1.592041	-4.715311	-1.621784
C	7.150286	-0.789011	0.446408	C	-7.394754	0.268194	-1.479350	C	-1.811182	-2.462305	-3.185684
H	8.187212	-1.171669	0.469447	H	-7.250543	-0.680049	-2.025677	H	-2.326180	-1.767718	-3.874000
H	7.185931	0.264298	0.118259	H	-8.482149	0.445330	-1.390159	H	-0.923060	-1.960946	-2.774754
H	6.748628	-0.810394	1.474609	H	-6.959052	1.080082	-2.087618	H	-1.483008	-3.341011	-3.770309
C	6.868883	-1.604343	-1.928740	C	-7.014737	1.557865	0.636355	C	-3.915631	-3.710085	-2.702176
H	6.894861	-0.573799	-2.323484	H	-6.584886	1.570598	1.653244	H	-4.618648	-4.109852	-1.950343
H	7.903370	-1.994258	-1.931181	H	-6.597787	2.412045	0.074605	H	-4.487050	-3.097278	-3.422113
H	6.264549	-2.217220	-2.620280	H	-8.104026	1.713419	0.728334	H	-3.493090	-4.568929	-3.252246
C	6.308834	-3.106543	-0.002189	C	-2.231088	-3.767705	-0.724360	C	-7.343589	-1.503554	0.351570
H	5.917847	-3.192793	1.026723	H	-1.905376	-4.704476	-1.212088	H	-8.443530	-1.415069	0.415365
H	5.713799	-3.770205	-0.653712	H	-1.341249	-3.232073	-0.364547	H	-7.111096	-2.401199	-0.247238
H	7.348930	-3.477718	-0.000566	H	-2.854217	-4.033194	0.147999	H	-6.947839	-1.663055	1.369822
C	2.582648	3.156230	-0.281398	C	-2.206294	-2.621756	-2.995443	C	-7.313387	-0.028236	-1.700097
H	2.468619	4.212101	-0.588242	H	-2.790257	-2.018299	-3.713323	H	-7.079142	-0.884466	-2.356192
H	1.593470	2.767541	-0.000084	H	-1.280963	-2.080433	-2.752603	H	-8.413119	0.074685	-1.658001
H	3.239990	3.128920	0.606142	H	-1.934565	-3.573614	-3.486511	H	-6.896813	0.881334	-2.167213
C	2.310628	2.414506	-2.695487	C	-4.276030	-3.722695	-2.151150	C	-7.133467	0.983171	0.586599
H	2.777965	1.880583	-3.542293	H	-4.913423	-3.991503	-1.290323	H	-6.762200	0.882120	1.621462
H	1.329347	1.961423	-2.492561	H	-4.895532	-3.181015	-2.887803	H	-6.740403	1.926914	0.169558
H	2.163484	3.469875	-2.991118	H	-3.938388	-4.661784	-2.623100	H	-8.233794	1.064980	0.629143
C	4.564631	2.979795	-1.791352	C	-1.365974	4.762550	1.720525	C	-1.516175	2.165906	3.695771
H	5.253833	2.988419	-0.928436	H	-2.289652	5.124086	2.202708	H	-2.495665	2.271977	4.190642
H	5.063855	2.462480	-2.630146	H	-0.502350	5.258304	2.194095	H	-1.287473	1.092607	3.576323
H	4.397085	4.028032	-2.095402	H	-1.382112	5.042874	0.656487	H	-0.740759	2.616480	4.339130
C	0.179544	-5.284982	1.049327	C	-1.344134	2.794941	3.341438	C	-1.828036	4.349720	2.416613
H	1.034847	-5.878415	1.413849	H	-0.527988	3.244399	3.933143	H	-2.765370	4.517347	2.973046
H	-0.740989	-5.663115	1.524440	H	-2.310358	3.098324	3.777440	H	-1.007776	4.864618	2.943978
H	0.085777	-5.419766	-0.039052	H	-1.250642	1.696708	3.402190	H	-1.921789	4.789300	1.412048
C	0.634213	-3.576761	2.887575	C	1.446599	-2.721403	-1.341552	C	4.415092	-1.277204	-1.559447
H	-0.224863	-3.932880	3.482178	H	0.442329	-2.293647	-1.369340	H	4.022002	-0.393115	-2.063477
H	1.540668	-4.114260	3.212145	C	2.563962	-2.337351	-1.985287	C	5.236637	-1.349465	-0.499932
H	0.766725	-2.498361	3.082493	H	2.718295	-1.493775	-2.659443	H	5.665324	-0.541642	0.094594

Transition State (1-2): In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

TS1-conformer2²: $\nu_{\text{lowest}} = -238.3719 \text{ cm}^{-1}$

TS1-conformer3²: $\nu_{\text{lowest}} = -241.0712 \text{ cm}^{-1}$

TS1-conformer4²: $\nu_{\text{lowest}} = -350.4708 \text{ cm}^{-1}$

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Ni	-0.766501	0.209345	0.206567
C	-1.511050	-0.176658	2.889527
C	0.569298	1.107211	2.728079
C	-1.312335	-0.347606	4.266758
C	0.774143	0.898022	4.102882
H	1.284946	1.678636	2.129901
C	-0.167102	0.189301	4.873465
H	-2.057924	-0.920147	4.829708
H	1.677168	1.298100	4.577751
H	0.002621	0.049741	5.946340
N	-2.501435	-0.600223	0.811793
C	-2.696693	-1.010803	-1.498337
C	-0.797342	-0.412963	-2.733607
C	-3.358269	-1.529127	-2.657350
C	-3.302165	-1.084504	-0.192848
C	-1.372842	-0.914445	-3.924370
H	0.197632	0.039478	-2.702267
C	-2.646481	-1.460862	-3.887509
C	-4.657334	-2.088418	-2.504790
C	-4.585598	-1.646043	-0.088185
H	-0.803997	-0.860104	-4.857021
H	-3.113991	-1.852562	-4.797527
C	-5.242014	-2.129477	-1.243820
H	-5.175082	-2.488880	-3.381954
H	-5.040951	-1.722729	0.900242
H	-6.241377	-2.564496	-1.130927
N	-1.445214	-0.456638	-1.573889
C	-2.676112	-0.784011	2.161092
O	-3.604240	-1.389157	2.719093
O	0.922645	0.976843	-0.638867
C	2.162658	0.577799	-0.553978
C	2.550504	-0.620801	0.148716
C	3.238682	1.315328	-1.199538
C	3.911934	-0.980394	0.332373
C	1.559991	-1.561108	0.607666
C	4.551392	0.893301	-0.993461
C	4.938512	-0.226351	-0.213015
H	4.113977	-1.886720	0.905010
N	0.254387	-1.455425	0.570709
O	2.014223	-2.745896	1.088186
H	5.348360	1.472983	-1.465767
C	-0.343436	-2.729663	0.998731
C	0.865751	-3.446891	1.688525
H	-1.116724	-2.546647	1.759045
C	-0.981811	-3.459296	-0.167214
C	-0.342594	-3.522052	-1.419054

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Ni	0.484282	-0.472262	-0.294015
C	1.305775	-1.291610	2.250138
C	-1.018947	-1.946484	1.927904
C	1.207705	-1.621346	3.613120
C	-1.110653	-2.256761	3.293327
H	-1.898049	-2.072371	1.286773
C	0.008242	-2.116650	4.135119
H	2.089836	-1.439969	4.237413
H	-2.062637	-2.617661	3.698145
H	-0.069636	-2.371619	5.197292
N	2.310790	-0.195536	0.440669
C	2.537406	1.058790	-1.530850
C	0.578553	1.141905	-2.815530
C	3.241654	1.908515	-2.442742
C	3.148193	0.575537	-0.320817
C	1.198960	1.984840	-3.766118
H	-0.462249	0.811941	-2.898638
C	2.521187	2.361699	-3.582814
C	4.589072	2.251692	-2.142418
C	4.478202	0.947439	-0.059178
H	0.624129	2.330410	-4.630095
H	3.020591	3.016917	-4.304844
C	5.173927	1.769711	-0.975570
H	5.143597	2.900403	-2.827534
H	4.941204	0.602230	0.865835
H	6.209983	2.042974	-0.745471
N	1.236295	0.697447	-1.748596
C	2.525298	-0.586498	1.734394
O	3.516848	-0.333304	2.434630
O	-1.325560	-0.618445	-1.272012
C	-2.512426	-0.310369	-0.826973
C	-2.710601	0.570668	0.294333
C	-3.701666	-0.836501	-1.466976
C	-4.005620	0.843196	0.806222
C	-1.589260	1.240770	0.908416
C	-4.943882	-0.525818	-0.914941
C	-5.141133	0.293068	0.228554
H	-4.070873	1.505323	1.671079
N	-0.309819	1.053016	0.689972
O	-1.867898	2.205394	1.817561
H	-5.833817	-0.942877	-1.393496
C	0.464985	2.018812	1.483030
C	-0.604002	2.542699	2.502604
H	1.253364	1.492322	2.041825
C	1.121729	3.064271	0.601913
C	0.441538	3.616917	-0.498100

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Ni	-0.741607	0.582462	-0.338183
C	-3.008420	1.126367	1.262887
C	-1.083607	2.507052	1.888203
C	-3.659521	1.466995	2.455379
C	-1.720712	2.796397	3.105316
H	-0.081616	2.888938	1.674977
C	-3.011022	2.302744	3.378169
H	-4.651226	1.042573	2.647506
H	-1.207092	3.421374	3.844279
H	-3.502209	2.560343	4.322765
N	-2.580369	-0.198110	-0.614478
C	-1.422455	-1.409990	-2.277644
C	0.872213	-0.963641	-2.407245
C	-1.345078	-2.377870	-3.332866
C	-2.672157	-1.132654	-1.617562
C	1.038607	-1.915149	-3.440213
H	1.717598	-0.384410	-2.031157
C	-0.064266	-2.613617	-3.904206
C	-2.530901	-3.056418	-3.728410
C	-3.816051	-1.832710	-2.034078
H	2.036632	-2.077451	-3.857056
H	0.035216	-3.352042	-4.707535
C	-3.728335	-2.776705	-3.082157
H	-2.479699	-3.799199	-4.530805
H	-4.756750	-1.638950	-1.517773
H	-4.638183	-3.308367	-3.381580
N	-0.311148	-0.726496	-1.843828
C	-3.564217	0.130107	0.285504
O	-4.718653	-0.321675	0.343999
O	1.217286	1.154914	-0.084976
C	2.190395	0.302071	0.143378
C	2.012695	-0.882587	0.938711
C	3.534608	0.503638	-0.375919
C	3.050533	-1.817127	1.171818
C	0.729941	-1.184221	1.530904
C	4.502202	-0.479183	-0.154591
C	4.306143	-1.660004	0.600120
H	2.813276	-2.680793	1.795831
N	-0.447825	-0.791724	1.125598
O	0.725802	-2.029892	2.590074
H	5.493616	-0.316941	-0.584990
C	-1.459257	-1.566335	1.871932
C	-0.649452	-2.021800	3.127259
H	-2.282863	-0.913848	2.195105
C	-2.019922	-2.707330	1.044019
C	-1.206006	-3.427925	0.149898

C	-2.229913	-4.083355	-0.003848	C	2.428642	3.495469	0.886120	C	-3.360325	-3.094107	1.208804
C	-0.939383	-4.204702	-2.486294	C	1.056686	4.590754	-1.295264	C	-1.721738	-4.522827	-0.554798
H	0.619025	-3.017955	-1.560698	H	-0.567352	3.267025	-0.739915	H	-0.167055	-3.121349	-0.006751
C	-2.829782	-4.764790	-1.071984	C	3.046351	4.467959	0.088014	C	-3.876993	-4.189226	0.503113
H	-2.747692	-4.004292	0.958513	H	2.973574	3.042574	1.721575	H	-4.012740	-2.515119	1.869954
C	-2.184436	-4.828947	-2.314457	C	2.360184	5.019585	-1.002823	C	-3.057897	-4.909729	-0.376676
H	-0.435802	-4.241608	-3.458018	H	0.520325	5.009286	-2.153382	H	-1.080511	-5.067424	-1.255552
H	-3.811644	-5.229629	-0.937425	H	4.071571	4.781500	0.308868	H	-4.928102	-4.468849	0.630444
H	-2.656932	-5.352689	-3.152296	H	2.845228	5.772845	-1.632800	H	-3.463489	-5.758609	-0.937068
C	-0.581574	0.574903	2.128519	C	0.197596	-1.489768	1.391441	C	-1.740090	1.686278	0.954582
C	-0.898839	3.205514	-0.570586	C	2.247142	-2.933067	-1.744130	C	-2.213900	4.089356	-1.032052
C	-1.837469	4.409817	-0.414238	C	3.231111	-2.852302	-0.587936	C	-1.107687	4.669150	-0.182238
H	-0.291300	3.120859	-1.476037	H	2.659010	-2.883827	-2.759900	H	-3.207229	4.552090	-0.972542
O	-0.062889	3.375630	0.597470	O	1.662402	-4.254397	-1.483553	O	-1.635083	4.247088	-2.366430
C	-1.118164	3.431480	1.569963	C	1.248836	-3.944819	-0.112833	C	-0.404926	3.500446	-2.071582
C	-1.992400	4.550600	0.982815	C	2.583238	-3.516215	0.471416	C	0.069604	4.279468	-0.848769
C	-2.505866	5.247138	-1.299182	C	4.533553	-2.381926	-0.455257	C	-1.083475	5.476307	0.950167
H	-0.727518	3.548584	2.588105	H	0.741914	-4.800467	0.350449	H	0.255956	3.492433	-2.945772
C	-2.817760	5.528492	1.525300	C	3.219666	-3.731342	1.689874	C	1.307138	4.730377	-0.406982
C	-3.331788	6.257096	-0.755238	C	5.186810	-2.604894	0.773522	C	0.173722	5.911595	1.414942
H	-2.394998	5.141166	-2.383583	H	5.041987	-1.861242	-1.272348	H	-2.005466	5.767790	1.462823
C	-3.485175	6.395243	0.630624	C	4.543680	-3.270699	1.826391	C	1.348878	5.547389	0.741384
H	-2.944672	5.638179	2.607569	H	2.714762	-4.241673	2.515797	H	2.221713	4.485481	-0.944090
H	-3.858055	6.943471	-1.427070	H	6.214229	-2.251831	0.908536	H	0.232390	6.557916	2.297097
H	-4.129078	7.187739	1.026354	H	5.074479	-3.424240	2.770945	H	2.315364	5.916539	1.100601
C	-1.762393	1.998867	-0.161392	C	-3.595561	-1.708483	-2.734328	C	3.945531	1.820356	-1.056398
H	-2.595178	1.660425	-0.784875	C	-6.564100	0.537828	0.755719	C	5.447480	-2.676487	0.754687
C	-1.873608	2.144139	1.239421	C	-7.206615	-0.816683	1.143618	C	3.960733	2.886418	0.067943
H	-2.723720	1.789830	1.822632	H	-8.236693	-0.665425	1.515430	H	2.980695	2.945786	0.564942
C	2.972434	2.567395	-2.060396	H	-7.256123	-1.502325	0.279854	H	4.716905	2.610846	0.823718
C	6.428005	-0.558746	-0.034117	H	-6.619998	-1.312628	1.936811	H	4.224959	3.884261	-0.330737
C	7.140480	0.635087	0.647861	C	-7.415524	1.211870	-0.348192	C	2.974322	2.190792	-2.200637
H	8.218156	0.423265	0.775116	H	-7.473785	0.583900	-1.254164	H	3.055800	1.453256	-3.019966
H	7.045083	1.557287	0.048626	H	-8.446996	1.385545	0.009653	H	1.939552	2.195936	-1.834792
H	6.704478	0.831502	1.643030	H	-6.979115	2.184055	-0.636891	H	3.230555	3.181130	-2.620867
C	7.071030	-0.816062	-1.419055	C	-6.564298	1.450688	1.996794	C	5.361649	1.767545	-1.668041
H	6.979041	0.065088	-2.077569	H	-5.984141	1.007463	2.825115	H	6.143586	1.608802	-0.905391
H	8.146938	-1.046275	-1.310585	H	-6.137408	2.443246	1.769831	H	5.449728	0.971146	-2.428543
H	6.581906	-1.668270	-1.922616	H	-7.599417	1.600835	2.351165	H	5.574524	2.731711	-2.162952
C	6.631614	-1.811910	0.838630	C	-2.815146	-3.010019	-2.430680	C	6.669368	-1.990180	1.413165
H	6.202405	-1.676019	1.846790	H	-2.780579	-3.653869	-3.328521	H	7.504184	-2.706650	1.522390
H	6.165101	-2.702951	0.383198	H	-1.784513	-2.780025	-2.129583	H	7.030955	-1.140565	0.808246
H	7.710620	-2.017071	0.954504	H	-3.305636	-3.577904	-1.619950	H	6.407020	-1.606179	2.414432
C	2.580337	3.736192	-1.125728	C	-2.868609	-0.918261	-3.850851	C	5.848716	-3.206175	-0.644098
H	2.285860	4.625565	-1.714763	H	-3.420794	0.006538	-4.095393	H	6.181326	-2.386289	-1.304415
H	1.753687	3.463757	-0.456888	H	-1.851753	-0.648604	-3.529131	H	6.677242	-3.933636	-0.562322
H	3.444094	4.015713	-0.496456	H	-2.797051	-1.531380	-4.767864	H	4.992799	-3.707151	-1.129905

C	1.859301	2.296595	-3.100480	C	-4.982641	-2.111486	-3.276382	C	5.030278	-3.873625	1.630134
H	2.158976	1.480658	-3.783438	H	-5.547252	-2.723106	-2.550579	H	4.749354	-3.551717	2.648150
H	0.924173	2.004912	-2.604068	H	-5.594719	-1.230571	-3.538813	H	4.174275	-4.416493	1.192311
H	1.679542	3.201956	-3.708505	H	-4.852263	-2.715335	-4.191509	H	5.871169	-4.583880	1.719653
C	4.220275	3.004767	-2.859747	C	-0.607153	4.042014	2.759002	C	-0.702726	-0.945282	4.214630
H	5.046245	3.328386	-2.202999	H	-1.427341	4.303827	3.448408	H	0.046108	-1.154196	4.996427
H	4.592340	2.197833	-3.516168	H	0.349240	4.345903	3.215956	H	-0.505084	0.049538	3.780957
H	3.953463	3.866635	-3.496679	H	-0.733731	4.601299	1.819662	H	-1.705332	-0.925684	4.674978
C	1.023402	-4.930655	1.390818	C	-0.562603	1.711766	3.785380	C	-0.944598	-3.416790	3.656414
H	1.927509	-5.319945	1.888504	H	0.363183	1.927428	4.345929	H	-0.277072	-3.644097	4.504669
H	0.146870	-5.483458	1.767782	H	-1.430507	1.947995	4.423361	H	-1.989259	-3.474488	4.004735
H	1.104170	-5.108823	0.307891	H	-0.577167	0.635782	3.544866	H	-0.799677	-4.172683	2.869797
C	0.887582	-3.130628	3.184658	C	0.324594	-2.742874	-0.438663	C	-1.080507	2.136657	-1.730514
H	0.047712	-3.635547	3.692131	H	-0.757621	-2.846888	-0.383988	H	-1.175223	1.425315	-2.557087
H	1.834886	-3.473091	3.633470	C	0.966636	-2.096471	-1.513202	C	-2.213690	2.547793	-0.983286
H	0.786029	-2.044990	3.347157	H	0.419660	-1.691563	-2.367442	H	-3.159989	2.012105	-1.015380

Intermediate-2: In Ni catalyzed reaction energy profile for other 3 possible intermediates

Int2-conformer2 ² : $\nu_{\text{lowest}} = 11.9663 \text{ cm}^{-1}$				Int2-conformer3 ² : $\nu_{\text{lowest}} = 9.5400 \text{ cm}^{-1}$				Int2-conformer4 ² : $\nu_{\text{lowest}} = 13.1775 \text{ cm}^{-1}$			
109				109				109			
Ni	-0.588391	0.029666	0.227874	Ni	0.397004	-0.304296	-0.378778	Ni	-0.693704	0.312892	-0.122610
C	-1.556685	-0.371610	2.950564	C	1.414000	-1.607787	2.099950	C	-2.950542	0.623863	1.826384
C	-0.451860	1.747507	3.370502	C	-0.426728	-3.191197	2.082956	C	-2.019024	2.788777	2.367414
C	-0.860233	-0.942351	4.026987	C	1.235645	-1.487941	3.494985	C	-2.955402	0.287661	3.189394
C	0.293177	1.151736	4.397691	C	-0.627958	-3.019531	3.455374	C	-1.955172	2.418904	3.719063
H	-0.277111	2.795198	3.114244	H	-1.072101	-3.881349	1.527808	H	-1.659047	3.775063	2.075959
C	0.066041	-0.185210	4.754338	C	0.228213	-2.175131	4.175521	C	-2.451640	1.179197	4.142945
H	-1.046293	-1.994527	4.265868	H	1.918965	-0.817993	4.025511	H	-3.354012	-0.689084	3.483980
H	1.041107	1.744584	4.934717	H	-1.437946	-3.556184	3.960503	H	-1.533318	3.121081	4.446125
H	0.620774	-0.639001	5.582452	H	0.105347	-2.044771	5.255941	H	-2.438065	0.906502	5.203513
N	-2.127019	-1.048059	0.754096	N	2.132862	-0.064299	0.371960	N	-2.464734	-0.526403	-0.203485
C	-2.251527	-1.341529	-1.596472	C	2.333147	1.357974	-1.512236	C	-1.540180	-1.344414	-2.243593
C	-0.472981	-0.373689	-2.772688	C	0.460986	1.325278	-2.921937	C	0.693870	-0.741488	-2.610962
C	-2.844375	-1.854806	-2.794867	C	3.016856	2.302623	-2.343389	C	-1.599437	-2.083977	-3.470498
C	-2.833283	-1.586502	-0.303739	C	2.917197	0.852777	-0.297944	C	-2.666464	-1.276412	-1.350310
C	-0.975069	-0.863495	-4.001633	C	1.066594	2.251004	-3.803598	C	0.728884	-1.465923	-3.825548
H	0.445886	0.217861	-2.714454	H	-0.540473	0.919059	-3.096905	H	1.567171	-0.196205	-2.241809
C	-2.156443	-1.590108	-4.012051	C	2.332914	2.736939	-3.513659	C	-0.414274	-2.122441	-4.256023
C	-4.054864	-2.592960	-2.692490	C	4.307245	2.746312	-1.945819	C	-2.809812	-2.745746	-3.811389
C	-4.030408	-2.317802	-0.249848	C	4.189948	1.329124	0.061886	C	-3.836015	-1.958050	-1.723114
H	-0.429074	-0.653560	-4.925990	H	0.525199	2.575041	-4.697132	H	1.653594	-1.487863	-4.409339
H	-2.569904	-1.970439	-4.952525	H	2.817962	3.461583	-4.176591	H	-0.417357	-2.680675	-5.198721
C	-4.622504	-2.799083	-1.440536	C	4.859411	2.259147	-0.766445	C	-3.891339	-2.669540	-2.943919
H	-4.519775	-2.993133	-3.598891	H	4.842809	3.471266	-2.566590	H	-2.867719	-3.315921	-4.743865
H	-4.471361	-2.527925	0.724927	H	4.637526	0.963226	0.985082	H	-4.686178	-1.942406	-1.041798
H	-5.556155	-3.366888	-1.361599	H	5.851193	2.606464	-0.455881	H	-4.822822	-3.186932	-3.198153

N	-1.099737	-0.608789	-1.625107	N	1.084415	0.905791	-1.825427	N	-0.404039	-0.689221	-1.863388
C	-2.404719	-1.262289	2.080999	C	2.469904	-0.669024	1.555434	C	-3.373082	-0.413675	0.820493
O	-3.175233	-2.118589	2.537363	O	3.468284	-0.386478	2.232439	O	-4.396138	-1.097893	0.969166
O	0.819561	1.239781	-0.243333	O	-1.310146	-0.824472	-1.060976	O	1.046296	1.144419	-0.050807
C	2.117705	1.042245	-0.311719	C	-2.524373	-0.503567	-0.687081	C	2.186012	0.493091	0.085640
C	2.767987	-0.160831	0.130166	C	-2.811767	0.424928	0.368813	C	2.308520	-0.763842	0.771050
C	2.972688	2.078834	-0.859335	C	-3.648020	-1.112296	-1.364366	C	3.420950	1.049716	-0.432739
C	4.179161	-0.311267	0.080983	C	-4.146331	0.715727	0.754397	C	3.544155	-1.445551	0.900630
C	2.003334	-1.284120	0.610765	C	-1.741959	1.116509	1.044866	C	1.155692	-1.390510	1.367900
C	4.349110	1.860941	-0.888334	C	-4.933043	-0.778315	-0.940700	C	4.599609	0.312370	-0.306879
C	4.996999	0.689032	-0.420742	C	-5.227147	0.124311	0.115906	C	4.709380	-0.941574	0.341130
H	4.591200	-1.252029	0.448610	H	-4.285833	1.426618	1.570415	H	3.535479	-2.392296	1.443167
N	0.700085	-1.381492	0.713625	N	-0.452042	0.982951	0.842795	N	-0.101076	-1.130195	1.113433
O	2.690525	-2.395237	0.967461	O	-2.080812	2.033069	1.980632	O	1.375730	-2.390510	2.249596
H	4.977709	2.653681	-1.301168	H	-5.777083	-1.245597	-1.454377	H	5.510348	0.741204	-0.731427
C	0.365686	-2.774954	1.066235	C	0.252160	2.012425	1.624868	C	-0.915654	-2.177130	1.765072
C	1.733686	-3.321119	1.601848	C	-0.838320	2.442707	2.666313	C	0.068408	-2.721592	2.853080
H	-0.375249	-2.790762	1.879477	H	1.107439	1.563156	2.153767	H	-1.784502	-1.726658	2.262531
C	-0.208800	-3.516090	-0.125637	C	0.766327	3.125511	0.728738	C	-1.399791	-3.218757	0.775723
C	0.389358	-3.415051	-1.396140	C	0.009688	3.584763	-0.364810	C	-0.591275	-3.639933	-0.295439
C	-1.348648	-4.320809	0.030995	C	2.006286	3.727524	1.001354	C	-2.663100	-3.807920	0.951721
C	-0.140612	-4.112715	-2.487667	C	0.483244	4.632096	-1.165537	C	-1.040025	-4.633476	-1.174842
H	1.265729	-2.773325	-1.534448	H	-0.946551	3.107241	-0.600849	H	0.385119	-3.172305	-0.456814
C	-1.882485	-5.018287	-1.062036	C	2.482939	4.773633	0.199987	C	-3.110925	-4.803668	0.073912
H	-1.844720	-4.365360	1.006881	H	2.612520	3.355760	1.834476	H	-3.316201	-3.456566	1.756464
C	-1.279477	-4.916791	-2.322371	C	1.720458	5.230184	-0.884118	C	-2.300478	-5.219957	-0.991350
H	0.328784	-4.020267	-3.472532	H	-0.111784	4.975807	-2.018036	H	-0.407535	-4.940351	-2.014307
H	-2.785131	-5.623521	-0.931560	H	3.458706	5.221200	0.413846	H	-4.105475	-5.240595	0.211833
H	-1.703677	-5.451417	-3.178746	H	2.095577	6.041562	-1.516857	H	-2.656127	-5.986821	-1.687277
C	-1.416059	1.012040	2.654423	C	0.593294	-2.520194	1.371054	C	-2.547841	1.918319	1.395339
C	-1.555871	2.883555	-0.247474	C	2.431942	-2.403990	-1.748954	C	-2.991702	3.739892	-0.553589
C	-2.904170	3.543671	-0.502349	C	3.582769	-2.374082	-0.761286	C	-1.898997	4.668362	-0.077900
H	-0.769572	2.985629	-0.998871	H	2.646235	-2.058732	-2.769241	H	-4.024154	4.107091	-0.476122
O	-1.162228	3.521011	0.990292	O	2.135666	-3.839913	-1.755063	O	-2.612327	3.603049	-1.956349
C	-2.368761	3.224171	1.728769	C	1.980609	-3.976413	-0.318534	C	-1.239781	3.141437	-1.709712
C	-3.441634	3.746077	0.786432	C	3.273903	-3.376203	0.183059	C	-0.759365	4.262494	-0.801455
C	-3.639040	3.852133	-1.645845	C	4.783774	-1.673565	-0.689615	C	-1.875423	5.775487	0.767635
H	-2.326177	3.661966	2.735615	H	1.769131	-5.019958	-0.049180	H	-0.708709	3.029669	-2.663617
C	-4.719783	4.269646	0.961097	C	4.118722	-3.648203	1.255957	C	0.421514	4.992169	-0.710005
C	-4.922366	4.409934	-1.474435	C	5.658397	-1.968421	0.375323	C	-0.668915	6.494399	0.883893
H	-3.234210	3.679621	-2.649025	H	5.050003	-0.918566	-1.434772	H	-2.769462	6.089285	1.317356
C	-5.455004	4.615326	-0.192063	C	5.326644	-2.928968	1.340630	C	0.460923	6.108675	0.149091
H	-5.146138	4.419928	1.958982	H	3.866721	-4.409442	2.001486	H	1.290949	4.732585	-1.311929
H	-5.512186	4.690468	-2.353875	H	6.611177	-1.433869	0.452009	H	-0.622243	7.377756	1.529702
H	-6.453704	5.052430	-0.086316	H	6.018879	-3.127882	2.165131	H	1.382437	6.695917	0.224700
C	-1.946423	1.449382	0.183739	C	-3.422370	-2.115918	-2.511841	C	3.468295	2.462385	-1.034018
H	-2.752761	1.046520	-0.446071	C	-6.690447	0.401091	0.496335	C	6.065310	-1.660576	0.404828

C	-2.380920	1.667683	1.659547	C	-7.366923	-0.923175	0.928679	C	3.137869	3.443918	0.118425
H	-3.389943	1.260892	1.837390	H	-8.425085	-0.747867	1.196192	H	2.127607	3.263632	0.515444
C	2.386635	3.401157	-1.385446	H	-7.342716	-1.672729	0.118682	H	3.867659	3.307140	0.935900
C	6.527772	0.578334	-0.494137	H	-6.853227	-1.354694	1.805511	H	3.207086	4.491727	-0.224323
C	7.164233	1.722225	0.333179	C	-7.439012	0.984137	-0.727410	C	2.478170	2.580309	-2.216258
H	8.267250	1.667074	0.285013	H	-7.418387	0.287898	-1.583713	H	2.767434	1.878428	-3.019535
H	6.858298	2.713054	-0.045032	H	-8.497553	1.179903	-0.476170	H	1.455008	2.345186	-1.893723
H	6.858146	1.654215	1.391719	H	-6.977002	1.933390	-1.050636	H	2.504965	3.598411	-2.645825
C	6.982004	0.698232	-1.969680	C	-6.798507	1.406327	1.658796	C	4.865820	2.832952	-1.573434
H	6.669864	1.660320	-2.411724	H	-6.297677	1.029531	2.567753	H	5.632424	2.835109	-0.779038
H	8.083190	0.633990	-2.042075	H	-6.348841	2.379777	1.395715	H	5.195098	2.147055	-2.374375
H	6.545680	-0.112742	-2.578834	H	-7.860702	1.580179	1.905679	H	4.826121	3.851103	-1.998868
C	7.030469	-0.766632	0.064274	C	-2.663951	-3.354165	-1.972768	C	7.094167	-0.758297	1.129602
H	6.748583	-0.895324	1.123977	H	-2.473381	-4.073651	-2.789826	H	8.079472	-1.256996	1.176741
H	6.624058	-1.619859	-0.506613	H	-1.701066	-3.053262	-1.536256	H	7.227805	0.204469	0.606555
H	8.131980	-0.810702	-0.000474	H	-3.260952	-3.863012	-1.195181	H	6.764209	-0.541543	2.160560
C	1.720896	4.157124	-0.209887	C	-2.608155	-1.452909	-3.651611	C	6.557791	-1.947404	-1.034946
H	1.200338	5.061549	-0.574738	H	-3.142398	-0.568970	-4.044142	H	6.669862	-1.015526	-1.616043
H	0.994285	3.531546	0.323841	H	-1.618616	-1.138378	-3.289798	H	7.539762	-2.454515	-1.014681
H	2.495801	4.476065	0.509956	H	-2.469575	-2.168176	-4.482692	H	5.842295	-2.596963	-1.569185
C	1.378284	3.105867	-2.523899	C	-4.752631	-2.607826	-3.118597	C	5.966720	-2.997138	1.164690
H	1.902264	2.662881	-3.390167	H	-5.375694	-3.134967	-2.374695	H	5.637005	-2.846554	2.207528
H	0.603259	2.400915	-2.192554	H	-5.344550	-1.777006	-3.542218	H	5.259290	-3.689813	0.675971
H	0.890611	4.039410	-2.858607	H	-4.536716	-3.317922	-3.935916	H	6.955976	-3.487022	1.190573
C	3.466516	4.330226	-1.979344	C	-0.944092	3.934037	2.950017	C	-0.045278	-1.906571	4.143654
H	4.215118	4.629323	-1.224886	H	-1.773772	4.124786	3.651209	H	0.792245	-2.145610	4.819662
H	3.994754	3.863920	-2.830321	H	-0.007416	4.297015	3.404892	H	-0.033896	-0.826300	3.922436
H	2.981699	5.251167	-2.348221	H	-1.119019	4.499371	2.022195	H	-0.994070	-2.143357	4.655124
C	2.105857	-4.734793	1.176891	C	-0.734726	1.600119	3.938182	C	0.042327	-4.222813	3.096637
H	3.098828	-4.997876	1.578470	H	0.175131	1.874691	4.499534	H	0.809424	-4.495203	3.840927
H	1.364862	-5.450234	1.570760	H	-1.614239	1.770202	4.581140	H	-0.945920	-4.523513	3.482326
H	2.124671	-4.827579	0.080981	H	-0.675105	0.528640	3.686705	H	0.230940	-4.774746	2.163496
C	1.855455	-3.113124	3.112194	C	0.783565	-2.978839	-0.068906	C	-1.653349	1.798115	-1.041529
H	1.159713	-3.784634	3.644587	H	-0.135985	-3.520560	-0.338760	H	-2.103712	1.231141	-1.869433
H	2.884071	-3.332492	3.443349	C	1.063826	-1.940725	-1.182212	C	-2.786324	2.262476	-0.073686
H	1.606988	-2.072963	3.376944	H	0.329327	-2.029208	-1.996571	H	-3.704792	1.730460	-0.367302

Ligand efficacy analysis for stereo-determining step with L3, L5, L6, and L7 ligands

Note: The L7 is the selected as the best ligand and the both pathways have been provided with the above conformational analysis. (conformer 1: TSI, and conformer 2: TSI'). Coordinates for the free ligand structures for L3, L5, L6, and L7 have been provided together with all the optimized ligand structures which can be found in the separate folder "Optimized_str_coordinates."

Intermediate-0: In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

Int0 _{L3} ² : $\nu_{\text{lowest}} = 16.0063 \text{ cm}^{-1}$				Int0 _{L5} ² : $\nu_{\text{lowest}} = 13.0859 \text{ cm}^{-1}$				Int0 _{L6} ² : $\nu_{\text{lowest}} = 13.7555 \text{ cm}^{-1}$			
60				83				84			
Ni	0.465868	0.318629	-0.888547	Ni	-1.008624	0.154455	-0.687785	Ni	0.707421	0.601074	0.630960
C	0.756488	3.002364	-0.261808	C	-1.823471	2.732661	-1.293642	C	1.301936	3.240149	0.030958
C	2.927171	1.966336	-0.609573	C	0.599579	2.553178	-1.373213	C	-1.102721	2.911425	0.153293
C	1.362721	4.223116	0.073235	C	-1.758025	4.101497	-1.597160	C	1.126494	4.586454	-0.325018
C	3.533376	3.194009	-0.278912	C	0.662591	3.925818	-1.681647	C	-1.276596	4.264461	-0.197052
H	3.554804	1.108606	-0.868142	H	1.525694	1.977392	-1.285049	H	-1.981917	2.284060	0.326610
C	2.760158	4.315626	0.066609	C	-0.506199	4.698910	-1.790920	C	-0.171957	5.098723	-0.439947
H	0.721202	5.075672	0.323680	H	-2.694109	4.665474	-1.679287	H	2.015861	5.203447	-0.496627
H	4.626960	3.269402	-0.291266	H	1.641814	4.393810	-1.836034	H	-2.292656	4.667091	-0.282198
H	3.252118	5.259617	0.324303	H	-0.434886	5.765565	-2.029043	H	-0.329348	6.147164	-0.714819
N	-0.990599	1.524718	-0.751005	N	-2.827284	0.664105	-0.852446	N	2.468302	1.301798	0.630722
C	-2.235606	-0.415151	-1.231472	C	-3.182550	-1.607550	-0.331887	C	3.017756	-0.922120	1.176763
C	-0.882905	-2.301144	-1.532586	C	-1.184260	-2.810072	-0.126351	C	1.134594	-2.302130	1.337250
C	-3.437393	-1.159907	-1.441092	C	-3.981303	-2.755101	-0.032016	C	3.913860	-1.997354	1.466722
C	-2.251580	0.989841	-0.945540	C	-3.764462	-0.321990	-0.600214	C	3.485724	0.407785	0.913657
C	-2.019225	-3.118908	-1.733877	C	-1.894370	-3.997014	0.170585	C	1.946700	-3.426378	1.614530
H	0.139084	-2.692056	-1.574485	H	-0.091137	-2.775875	-0.176035	H	0.042723	-2.364385	1.286126
C	-3.285907	-2.551940	-1.690655	C	-3.281335	-3.968703	0.220984	C	3.325098	-3.274040	1.681861
C	-4.678230	-0.465607	-1.384033	C	-5.396100	-2.601876	-0.004811	C	5.308208	-1.717467	1.515170
C	-3.494319	1.640164	-0.903061	C	-5.163845	-0.212622	-0.563260	C	4.867390	0.645048	0.975672
H	-1.884118	-4.186907	-1.928174	H	-1.340008	-4.920748	0.359719	H	1.476501	-4.400270	1.778910
H	-4.177866	-3.168130	-1.848826	H	-3.849396	-4.875948	0.454395	H	3.970623	-4.131958	1.899974
C	-4.681236	0.900802	-1.127949	C	-5.949999	-1.353484	-0.267268	C	5.749630	-0.420404	1.279748
H	-5.611529	-1.014095	-1.544925	H	-6.028754	-3.465803	0.221357	H	6.013172	-2.524206	1.738749
H	-3.523376	2.707554	-0.683194	H	-5.620648	0.757227	-0.762027	H	5.238913	1.650116	0.774843
H	-5.636798	1.435442	-1.088576	H	-7.039153	-1.236904	-0.245718	H	6.823110	-0.204954	1.321078
N	-0.998428	-0.998453	-1.289674	N	-1.814783	-1.662560	-0.365238	N	1.661099	-1.098236	1.129059
C	-0.721104	2.819539	-0.322848	C	-3.109353	2.006224	-1.091667	C	2.643124	2.616298	0.212039
O	-1.567372	3.671393	-0.040244	O	-4.234985	2.505938	-1.131253	O	3.728865	3.169472	0.021501
O	1.823575	-0.779659	-1.616531	O	0.680438	-0.561489	-1.118814	O	-0.964836	-0.010750	1.263549
C	2.835431	-1.335133	-1.000248	C	1.830919	-0.431754	-0.502546	C	-2.084057	-0.220156	0.613763
C	2.975238	-1.436359	0.431622	C	1.955846	0.087771	0.831263	C	-2.155998	-0.329548	-0.817988
C	3.879866	-1.898825	-1.793693	C	3.035775	-0.835879	-1.185161	C	-3.309306	-0.364351	1.361646
C	4.112854	-2.068648	0.995367	C	3.222924	0.184480	1.461108	C	-3.388162	-0.583117	-1.472585
C	1.960043	-0.895962	1.306324	C	0.794706	0.559758	1.554496	C	-0.969173	-0.164077	-1.626119
C	4.980329	-2.517457	-1.212843	C	4.247045	-0.724562	-0.503143	C	-4.484895	-0.618566	0.655826
C	5.110202	-2.607422	0.191913	C	4.384694	-0.222949	0.817807	C	-4.568697	-0.736247	-0.756801
H	4.183239	-2.121225	2.085586	H	3.247780	0.593290	2.472503	H	-3.371123	-0.651192	-2.561681
N	0.863696	-0.287582	0.945941	N	-0.451596	0.544517	1.164682	N	0.241998	0.087957	-1.209031
O	2.135059	-1.012970	2.645342	O	0.997624	1.107162	2.779396	O	-1.094581	-0.261657	-2.974079
H	5.761522	-2.935197	-1.858250	H	5.156171	-1.035835	-1.023950	H	-5.409732	-0.726860	1.228239
C	0.116059	0.157447	2.131550	C	-1.305058	1.188126	2.174383	C	1.150780	0.260406	-2.351979
C	0.987891	-0.400435	3.295578	C	-0.275311	1.628016	3.248295	C	0.222236	-0.068554	-3.557237
H	0.100258	1.261981	2.140586	H	-1.783914	2.068584	1.708076	H	1.480381	1.314826	-2.378646

C	-1.310283	-0.356883	2.100362	C	-0.651794	1.957583	-1.185125	C	2.368568	-0.633597	-2.220137
C	-1.557445	-1.731063	1.919124	C	2.968397	-1.357855	-2.633270	C	2.205452	-2.018726	-2.026983
C	-2.394122	0.526385	2.214964	C	5.778846	-0.144576	1.460747	C	3.662615	-0.092791	-2.248509
C	-2.869260	-2.213033	1.857002	C	2.382272	-0.257663	-3.554891	C	3.320278	-2.848707	-1.868671
H	-0.715373	-2.422647	1.800816	H	1.370643	0.031310	-3.234261	H	1.196477	-2.443833	-1.975324
C	-3.709853	0.044029	2.155862	H	3.025815	0.639959	-3.540172	C	4.781506	-0.924013	-2.091692
H	-2.209302	1.601744	2.314275	H	2.331611	-0.626086	-4.595819	H	3.796366	0.989074	-2.358226
C	-3.949756	-1.323940	1.976174	C	2.085646	-2.629865	-2.702422	C	4.613113	-2.301128	-1.901266
H	-3.050964	-3.281739	1.702977	H	2.493049	-3.420005	-2.045939	H	3.181965	-3.922709	-1.706605
H	-4.547756	0.744221	2.227744	H	1.053820	-2.407317	-2.393632	H	5.785375	-0.488468	-2.096948
H	-4.977259	-1.696872	1.914876	H	2.067447	-3.019318	-3.736689	H	5.486713	-2.946539	-1.764258
C	1.531676	1.874865	-0.599693	C	4.365269	-1.728471	-3.172377	C	0.194576	2.401842	0.270255
H	0.469989	-1.181029	3.875936	H	5.046352	-0.859161	-3.184044	C	-3.300839	-0.222931	2.895720
H	1.361307	0.382005	3.973978	H	4.836899	-2.532190	-2.579184	C	-5.928604	-1.012465	-1.418166
H	5.982822	-3.091741	0.639894	H	4.268300	-2.091022	-4.210562	C	-2.801397	1.192044	3.285334
H	3.776272	-1.817361	-2.879718	C	6.688445	0.770706	0.604532	H	-1.784576	1.372443	2.906937
				H	7.700326	0.830974	1.045247	H	-3.473017	1.965177	2.871428
				H	6.791239	0.389525	-0.426244	H	-2.793406	1.298443	4.385525
				H	6.272010	1.791662	0.548882	C	-2.379725	-1.299917	3.523500
				C	6.393703	-1.564335	1.525485	H	-2.729980	-2.312881	3.254386
				H	6.487107	-2.010936	0.520385	H	-1.342907	-1.178414	3.177108
				H	7.402931	-1.528292	1.974857	H	-2.396116	-1.212972	4.625290
				H	5.764390	-2.234087	2.137380	C	-4.710501	-0.405685	3.494364
				C	5.718825	0.426910	2.890181	H	-5.420378	0.350643	3.115084
				H	5.308369	1.451785	2.900256	H	-5.122911	-1.408045	3.281153
				H	5.096466	-0.200849	3.551739	H	-4.655694	-0.292255	4.591081
				H	6.735218	0.466117	3.319896	C	-6.910056	0.134010	-1.070869
				H	-0.465647	1.198502	4.245059	H	-7.898683	-0.051656	-1.529023
				H	-0.177847	2.721981	3.335387	H	-7.055000	0.226350	0.019462
				C	-2.422789	0.240496	2.667008	H	-6.528958	1.100044	-1.445577
				H	-2.998231	-0.018946	1.762514	C	-6.494930	-2.352161	-0.886680
				C	-3.371366	0.972966	3.626324	H	-6.627869	-2.329083	0.208854
				H	-3.787629	1.882236	3.157465	H	-7.479485	-2.563441	-1.342504
				H	-4.215519	0.320795	3.908963	H	-5.813679	-3.186715	-1.128426
				H	-2.857024	1.272111	4.559263	C	-5.810803	-1.106341	-2.951399
				C	-1.873120	-1.061478	3.263641	H	-5.432410	-0.165266	-3.387451
				H	-1.329236	-0.884789	4.210325	H	-5.135207	-1.924595	-3.256614
				H	-2.698098	-1.761183	3.482403	H	-6.803721	-1.306621	-3.390951
				H	-1.184346	-1.556856	2.558894	H	0.508363	-1.002316	-4.068390
								H	0.151760	0.749487	-4.290301

Intermediate-1: In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

Int1 _{L3} ² : $\nu_{\text{lowest}} = 16.4355 \text{ cm}^{-1}$				Int1 _{L5} ² : $\nu_{\text{lowest}} = 14.0827 \text{ cm}^{-1}$				Int1 _{L6} ² : $\nu_{\text{lowest}} = 14.3068 \text{ cm}^{-1}$			
79				102				103			
Ni	0.162366	0.460161	-0.127283	Ni	-0.337265	-0.440570	0.241002	Ni	-0.287183	-0.172775	0.397322
C	-0.625922	0.758859	2.517143	C	-0.912005	-0.855394	2.923662	C	-0.797780	-0.141910	3.125849

C	-0.602298	2.909478	1.381474	C	1.030443	0.585276	2.679779	C	1.255871	1.059531	2.629133
C	-1.025096	1.370618	3.715607	C	-0.808545	-0.799030	4.322573	C	-0.633279	0.096178	4.499625
C	-1.007214	3.519827	2.584229	C	1.131177	0.640853	4.083657	C	1.416798	1.299362	4.007797
H	-0.442165	3.524867	0.490715	H	1.755422	1.128615	2.066890	H	2.002175	1.440852	1.926397
C	-1.218610	2.757529	3.746806	C	0.220236	-0.047145	4.903706	C	0.481217	0.820471	4.940981
H	-1.182995	0.737664	4.596183	H	-1.544471	-1.346442	4.922635	H	-1.390583	-0.291715	5.190562
H	-1.157314	4.605561	2.609166	H	1.935364	1.231373	4.537978	H	2.288260	1.868356	4.352282
H	-1.533952	3.250315	4.672780	H	0.316390	0.008133	5.993367	H	0.625333	1.016319	6.008952
N	-0.088860	-1.000749	1.076595	N	-1.822359	-1.465575	0.858581	N	-1.847532	-0.931965	1.192488
C	0.542826	-2.247167	-0.815509	C	-2.208299	-1.683790	-1.455087	C	-2.325210	-1.468329	-1.048920
C	1.146942	-0.897413	-2.632008	C	-0.621072	-0.554462	-2.756988	C	-0.648977	-0.775459	-2.530914
C	0.830843	-3.452735	-1.528850	C	-2.908052	-2.161107	-2.607976	C	-3.111087	-2.033986	-2.101403
C	0.082522	-2.257845	0.544789	C	-2.625604	-2.013188	-0.121217	C	-2.746186	-1.514806	0.321179
C	1.487832	-2.036010	-3.399890	C	-1.253193	-0.976366	-3.949917	C	-1.352604	-1.319570	-3.629716
H	1.224338	0.123847	-3.019706	H	0.276928	0.072080	-2.754120	H	0.314737	-0.267242	-2.640295
C	1.323727	-3.302218	-2.855479	C	-2.388327	-1.772491	-3.874959	C	-2.576054	-1.940619	-3.415869
C	0.606492	-4.694039	-0.871722	C	-4.051028	-2.984836	-2.408595	C	-4.352198	-2.641132	-1.763215
C	-0.136841	-3.505181	1.154973	C	-3.751671	-2.834948	0.032529	C	-3.975874	-2.120971	0.614086
H	1.866141	-1.902924	-4.417655	H	-0.837093	-0.672529	-4.914852	H	-0.924541	-1.241976	-4.633410
H	1.570971	-4.195857	-3.439112	H	-2.891930	-2.112247	-4.786782	H	-3.138973	-2.366143	-4.253972
C	0.122241	-4.694300	0.433008	C	-4.441923	-3.301777	-1.112171	C	-4.755577	-2.667181	-0.432989
H	0.815101	-5.629933	-1.399247	H	-4.604348	-3.359818	-3.275224	H	-4.971454	-3.078589	-2.552478
H	-0.485946	-3.528682	2.187656	H	-4.080016	-3.091940	1.039804	H	-4.309328	-2.158396	1.651206
H	-0.056156	-5.651606	0.935612	H	-5.321241	-3.937565	-0.960273	H	-5.714076	-3.131166	-0.174674
N	0.690151	-1.012583	-1.388397	N	-1.093704	-0.896500	-1.561168	N	-1.131403	-0.846420	-1.293095
C	-0.433045	-0.714026	2.386760	C	-1.990351	-1.612485	2.223996	C	-1.967060	-0.882293	2.568884
O	-0.537261	-1.537506	3.299576	O	-2.889559	-2.253842	2.778200	O	-2.890557	-1.366268	3.233473
O	0.136068	1.803820	-1.498737	O	0.907882	0.833185	-0.437718	O	1.075740	0.840434	-0.484670
C	0.899757	2.859887	-1.622637	C	2.221150	0.820130	-0.393768	C	2.380597	0.695272	-0.446651
C	2.128389	3.080943	-0.903104	C	2.991163	-0.352848	-0.085098	C	3.032725	-0.497627	0.020566
C	0.501911	3.873662	-2.546349	C	2.946328	2.038612	-0.670123	C	3.224290	1.775420	-0.904720
C	2.877692	4.265832	-1.116261	C	4.407953	-0.313127	-0.052479	C	4.446228	-0.605830	0.038991
C	2.614208	2.098899	0.040923	C	2.344733	-1.609251	0.231151	C	2.262420	-1.625780	0.496543
C	1.260916	5.021748	-2.741467	C	4.340517	2.004663	-0.635003	C	4.607708	1.599857	-0.868542
C	2.459142	5.232538	-2.023061	C	5.109714	0.853254	-0.329703	C	5.259724	0.429983	-0.402160
H	3.801071	4.398076	-0.545329	H	4.926006	-1.239430	0.200140	H	4.869675	-1.538290	0.415491
N	2.050642	0.964872	0.348985	N	1.067247	-1.871484	0.251120	N	0.965941	-1.716837	0.595298
O	3.778590	2.360628	0.686672	O	3.146480	-2.655834	0.561747	O	2.945049	-2.731867	0.894106
H	0.917689	5.775213	-3.459810	H	4.878830	2.931951	-0.847117	H	5.235240	2.424516	-1.216082
C	2.849181	0.270200	1.370461	C	0.856738	-3.277505	0.633682	C	0.591862	-3.036695	1.124637
C	4.044180	1.247385	1.581412	C	2.284737	-3.727659	1.028402	C	1.979583	-3.674721	1.428485
H	2.243989	0.182146	2.289550	H	0.181127	-3.305361	1.505885	H	0.011357	-2.897682	2.052046
C	3.244261	-1.118629	0.906055	C	0.001159	-0.165641	2.100760	C	-0.251077	-3.808629	0.125866
C	3.835357	-1.295009	-0.359154	C	-3.532974	1.298453	1.013640	C	0.164049	-3.914702	-1.214379
C	3.002815	-2.240376	1.713691	C	-4.349302	2.581967	0.768930	C	-1.454648	-4.412765	0.521666
C	4.180543	-2.574576	-0.808239	H	-3.768759	0.690972	1.896284	C	-0.612036	-4.618376	-2.142841
H	4.001184	-0.425344	-1.005154	O	-3.832854	0.587471	-0.209653	H	1.089993	-3.424236	-1.535068

C	3.351720	-3.522884	1.266341	C	-3.375226	1.617660	-1.110469	C	-2.231629	-5.120586	-0.406450
H	2.502086	-2.113887	2.679958	C	-4.245175	2.793264	-0.624028	H	-1.799008	-4.303194	1.555818
C	3.938933	-3.692728	0.005979	C	-5.059156	3.457319	1.578797	C	-1.812055	-5.224467	-1.738957
H	4.627534	-2.702529	-1.799650	H	-3.469869	1.304105	-2.158602	H	-0.286004	-4.685814	-3.186004
H	3.140635	-4.392792	1.895976	C	-4.847538	3.884002	-1.235201	H	-3.177061	-5.572342	-0.090774
H	4.196032	-4.696329	-0.348420	C	-5.686334	4.565819	0.961935	H	-2.426192	-5.765417	-2.466535
C	-0.419577	1.522414	1.351464	H	-5.143724	3.299143	2.659280	C	0.140672	0.337195	2.189595
C	-3.459024	0.704839	0.584157	C	-5.582623	4.775303	-0.417964	C	-3.220068	2.023206	0.927423
C	-4.807307	0.324586	-0.058958	H	-4.770219	4.053852	-2.314684	C	-3.878608	3.341783	0.477797
H	-3.454524	1.431530	1.406111	H	-6.264188	5.267366	1.573106	H	-3.494029	1.610342	1.906310
O	-3.028407	-0.598463	1.030295	H	-6.080459	5.638424	-0.872763	O	-3.653940	1.160283	-0.148133
C	-3.100554	-1.245954	-0.257613	C	-2.062071	1.695565	0.775048	C	-3.107441	1.953205	-1.222056
C	-4.572803	-0.955285	-0.609706	H	-1.343330	1.943402	1.556639	C	-3.803709	3.297669	-0.932357
C	-6.041441	0.947223	-0.183732	C	-1.964960	1.891126	-0.557448	C	-4.440828	4.426974	1.135249
H	-2.775895	-2.292384	-0.198157	H	-1.120054	2.284541	-1.121546	H	-3.281169	1.480098	-2.197571
C	-5.567639	-1.638210	-1.295517	C	2.189035	3.343030	-0.984133	C	-4.288312	4.337557	-1.713289
C	-7.064773	0.252736	-0.871497	C	6.644151	0.942571	-0.309880	C	-4.948290	5.486347	0.345987
H	-6.229864	1.939099	0.241136	C	1.290523	3.721649	0.220332	H	-4.501796	4.467453	2.228077
C	-6.832432	-1.015282	-1.416646	H	0.597137	2.905702	0.465832	C	-4.873534	5.442734	-1.050884
H	-5.392521	-2.631013	-1.724056	H	1.912581	3.929519	1.108841	H	-4.232703	4.309764	-2.807010
H	-8.053632	0.712358	-0.974326	H	0.703942	4.629897	-0.009067	H	-5.409376	6.350711	0.835777
H	-7.641880	-1.534996	-1.940473	C	1.336092	3.155221	-2.263554	H	-5.277044	6.273161	-1.640148
C	-2.499783	0.948168	-0.595330	H	1.986740	2.955855	-3.133540	C	-1.721943	2.181207	0.598874
H	-2.202746	1.916059	-0.998767	H	0.644168	2.308064	-2.148104	H	-0.950438	2.471180	1.312583
C	-2.274957	-0.275622	-1.127323	H	0.750666	4.069190	-2.472724	C	-1.653843	2.133265	-0.749489
H	-1.792149	-0.519493	-2.074240	C	3.146574	4.525293	-1.238352	H	-0.790053	2.317242	-1.387275
H	5.011462	0.804397	1.295022	H	3.776503	4.741025	-0.357441	C	2.602216	3.089899	-1.413297
H	4.104680	1.643866	2.607086	H	3.808242	4.342863	-2.103637	C	6.795287	0.360951	-0.399285
H	3.048037	6.141584	-2.176930	H	2.553346	5.430972	-1.455047	C	1.768066	3.740782	-0.281461
H	-0.429622	3.706779	-3.096050	C	7.083681	1.989597	0.743062	H	0.995880	3.050620	0.084233
				H	8.185447	2.076028	0.765909	H	2.422423	4.012858	0.565552
				H	6.671189	2.988318	0.517467	H	1.277612	4.661281	-0.647061
				H	6.736688	1.698625	1.749960	C	1.714226	2.799603	-2.649118
				C	7.151076	1.375653	-1.707461	H	2.328265	2.409264	-3.480080
				H	6.738642	2.356635	-2.000874	H	0.944579	2.051804	-2.407978
				H	8.253442	1.457236	-1.710905	H	1.218043	3.725887	-2.992006
				H	6.854493	0.639476	-2.474956	C	3.673403	4.111925	-1.846190
				C	7.291260	-0.409271	0.047087	H	4.336414	4.392544	-1.008885
				H	6.980584	-0.755470	1.048349	H	4.298514	3.730656	-2.673039
				H	7.026540	-1.191386	-0.685848	H	3.174018	5.031001	-2.199769
				H	8.390835	-0.307955	0.050870	C	7.357879	1.495437	0.492102
				H	2.612612	-4.658328	0.539779	H	8.462925	1.469440	0.499596
				H	2.421444	-3.818030	2.119019	H	7.045870	2.489377	0.127101
				C	0.201390	-4.085650	-0.511760	H	7.000376	1.387897	1.531108
				H	-0.755365	-3.577853	-0.715983	C	7.319692	0.536162	-1.845706
				C	-0.125068	-5.512676	-0.049547	H	7.005104	1.503057	-2.275437
				H	-0.759832	-5.501470	0.854206	H	8.424376	0.501315	-1.863567

H	-0.669014	-6.059685	-0.838791	H	6.935866	-0.266671	-2.499265
H	0.791103	-6.088611	0.181179	C	7.306265	-0.986444	0.145658
C	1.031569	-4.058465	-1.801830	H	6.978380	-1.153009	1.186640
H	2.000844	-4.577028	-1.680926	H	6.950791	-1.832854	-0.467721
H	0.486595	-4.561421	-2.619408	H	8.410330	-1.000351	0.132951
H	1.234208	-3.020792	-2.116712	H	2.130783	-4.640453	0.922297
				H	2.173044	-3.782433	2.508380

Intermediate-1': In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

Int1'L3': $\nu_{\text{lowest}} = 15.9421 \text{ cm}^{-1}$				Int1'L5': $\nu_{\text{lowest}} = 15.7537 \text{ cm}^{-1}$				Int1'L6': $\nu_{\text{lowest}} = 11.4680 \text{ cm}^{-1}$			
79				102				103			
Ni	0.049416	0.203328	0.021108	Ni	-0.681485	-0.369384	0.198906	Ni	-0.557360	-0.067488	0.308527
C	-0.239804	0.442849	2.769316	C	-1.281603	-0.485644	2.907239	C	-0.996714	0.105823	3.045979
C	-1.565514	2.128436	1.620401	C	0.935047	0.449159	2.553185	C	1.344800	0.499091	2.523987
C	-0.621615	0.958358	4.019173	C	-1.138665	-0.357603	4.299108	C	-0.740885	0.259619	4.418777
C	-1.948212	2.639702	2.875070	C	1.073936	0.577678	3.948306	C	1.596858	0.657181	3.900245
H	-1.964404	2.576814	0.707644	H	1.749726	0.770881	1.898626	H	2.168133	0.598612	1.811595
C	-1.476984	2.065430	4.069547	C	0.046861	0.174686	4.819929	C	0.563856	0.534374	4.845975
H	-0.241964	0.469894	4.923910	H	-1.969194	-0.675263	4.940016	H	-1.579101	0.166668	5.118954
H	-2.627812	3.498980	2.915167	H	1.999488	1.001107	4.355654	H	2.617195	0.880253	4.233456
H	-1.786004	2.481258	5.034621	H	0.175496	0.281745	5.902432	H	0.781480	0.658301	5.912336
N	0.756627	-1.056015	1.279231	N	-2.371501	-0.969382	0.897657	N	-2.295789	-0.180215	1.126414
C	1.569544	-2.068882	-0.684065	C	-2.856890	-1.209687	-1.395490	C	-2.969295	-0.430614	-1.114584
C	1.079679	-0.831933	-2.611769	C	-1.055664	-0.637260	-2.779720	C	-1.168062	-0.502126	-2.609261
C	2.282819	-3.064255	-1.422582	C	-3.686629	-1.554206	-2.509529	C	-3.929287	-0.601883	-2.161410
C	1.438853	-2.129704	0.744251	C	-3.313975	-1.335545	-0.037329	C	-3.359984	-0.315981	0.262526
C	1.786865	-1.755257	-3.417499	C	-1.805178	-0.952400	-3.938209	C	-2.044263	-0.698506	-3.702718
H	0.571151	0.048810	-3.018806	H	-0.021807	-0.277135	-2.820691	H	-0.080078	-0.444481	-2.723418
C	2.377671	-2.864754	-2.828389	C	-3.110188	-1.404919	-3.803523	C	-3.413759	-0.740312	-3.480595
C	2.840312	-4.161364	-0.709065	C	-5.005518	-2.020518	-2.249990	C	-5.308889	-0.622435	-1.815362
C	2.000742	-3.230261	1.411277	C	-4.620620	-1.807033	0.174835	C	-4.731565	-0.341699	0.562418
H	1.852284	-1.586281	-4.496333	H	-1.344638	-0.837931	-4.923827	H	-1.630754	-0.808315	-4.709568
H	2.922686	-3.594811	-3.436878	H	-3.707410	-1.655962	-4.687169	H	-4.109695	-0.883762	-4.314622
C	2.681889	-4.226275	0.671258	C	-5.438874	-2.135738	-0.932524	C	-5.676800	-0.486244	-0.480602
H	3.386158	-4.937962	-1.253721	H	-5.658695	-2.287604	-3.086618	H	-6.060712	-0.748733	-2.600673
H	1.918095	-3.285018	2.497185	H	-4.977742	-1.912102	1.199874	H	-5.040701	-0.260927	1.605013
H	3.109874	-5.073542	1.218644	H	-6.453378	-2.499569	-0.734557	H	-6.740083	-0.502241	-0.215728
N	0.978632	-0.996093	-1.296160	N	-1.574678	-0.758870	-1.561282	N	-1.625904	-0.366625	-1.368334
C	0.622245	-0.766034	2.626123	C	-2.531881	-0.998859	2.271975	C	-2.368390	-0.131485	2.505739
O	1.126546	-1.406950	3.555535	O	-3.543778	-1.369183	2.877146	O	-3.396069	-0.251520	3.183568
O	-0.817921	1.206528	-1.350148	O	0.833641	0.463142	-0.632803	O	1.070272	0.311381	-0.641591
C	-0.793595	2.502026	-1.527612	C	2.105342	0.178172	-0.519386	C	2.244479	-0.253368	-0.536564
C	0.246385	3.372695	-1.041121	C	2.585355	-1.115076	-0.117580	C	2.429301	-1.593375	-0.049949
C	-1.851695	3.108864	-2.268133	C	3.084843	1.199186	-0.809079	C	3.421351	0.486006	-0.930145
C	0.196334	4.764412	-1.305117	C	3.974290	-1.386433	-0.034961	C	3.718997	-2.177560	0.019616
C	1.346994	2.833442	-0.275638	C	1.656507	-2.159871	0.256758	C	1.295164	-2.364462	0.407646

C	-1.872889	4.476505	-2.516593	C	4.435298	0.861784	-0.721904	C	4.659262	-0.150570	-0.845099
C	-0.846803	5.321050	-2.036216	C	4.921421	-0.416959	-0.342648	C	4.851755	-1.477997	-0.378738
H	1.003091	5.391459	-0.915051	H	4.270011	-2.387193	0.283916	H	3.787188	-3.197065	0.402963
N	1.510740	1.591272	0.088932	N	0.351953	-2.103164	0.285443	N	0.048054	-1.981983	0.473204
O	2.320686	3.687674	0.128073	O	2.185758	-3.348371	0.654607	O	1.530658	-3.630415	0.845049
H	-2.706823	4.904481	-3.084800	H	5.172189	1.637474	-0.946648	H	5.546211	0.413766	-1.145261
C	2.726418	1.469230	0.907453	C	-0.185571	-3.387369	0.761367	C	-0.770340	-3.048556	1.068133
C	3.307161	2.913587	0.860453	C	1.095834	-4.158022	1.166330	C	0.260961	-4.200232	1.252703
H	2.430188	1.198097	1.936299	H	-0.820766	-3.193728	1.643428	H	-1.148136	-2.695922	2.044490
C	3.654322	0.400564	0.363701	C	-0.247621	-0.086378	2.033949	C	-1.950935	-3.399311	0.183291
C	3.988398	0.389848	-1.003531	C	-1.917514	2.388004	-1.063961	C	-1.750256	-3.659872	-1.185265
C	4.169183	-0.597940	1.204556	C	-1.827341	3.841154	-0.584425	C	-3.252298	-3.442535	0.705963
C	4.827979	-0.603206	-1.520317	H	-1.332750	2.104224	-1.945732	C	-2.835150	-3.958752	-2.016909
H	3.565095	1.150708	-1.668972	O	-1.395031	1.735805	0.137054	H	-0.739056	-3.599761	-1.603346
C	5.013746	-1.591516	0.688474	C	-2.392682	2.284937	1.055980	C	-4.340370	-3.745706	-0.125338
H	3.876204	-0.620242	2.260088	C	-2.134775	3.774942	0.791369	H	-3.419319	-3.199450	1.761218
C	5.343966	-1.596692	-0.672756	C	-1.513306	5.045066	-1.198777	C	-4.134776	-4.002436	-1.486819
H	5.071623	-0.610285	-2.587867	H	-2.234785	1.906407	2.072599	H	-2.669747	-4.146111	-3.083060
H	5.394779	-2.376366	1.349256	C	-2.133911	4.913349	1.585119	H	-5.353243	-3.757137	0.289160
H	5.991481	-2.381764	-1.076972	C	-1.511280	6.210508	-0.397423	H	-4.986844	-4.223145	-2.138169
C	-0.704235	1.027416	1.572579	H	-1.259688	5.097664	-2.262832	C	0.042533	0.219767	2.097623
C	-3.260501	-0.579992	-1.264617	C	-1.815438	6.145524	0.967631	C	-1.212607	2.807698	-1.131292
C	-4.524524	-1.427722	-1.019810	H	-2.358745	4.866725	2.655810	C	-0.691665	4.211264	-0.801129
H	-3.120219	-0.112273	-2.245851	H	-1.259575	7.175632	-0.849670	H	-0.817401	2.312674	-2.025217
O	-3.427681	0.408542	-0.226977	H	-1.798696	7.060742	1.568802	O	-0.763369	2.125262	0.082669
C	-3.514283	-0.523115	0.871508	C	-3.394489	1.963566	-0.988351	C	-1.481630	2.989117	1.019816
C	-4.689173	-1.392670	0.383140	H	-4.050593	1.813467	-1.847495	C	-0.864127	4.328984	0.594760
C	-5.400625	-2.137161	-1.829634	C	-3.686532	1.900018	0.321112	C	-0.130491	5.235818	-1.549867
H	-3.610679	-0.003709	1.832920	H	-4.638104	1.674990	0.805292	H	-1.328597	2.653655	2.052278
C	-5.732104	-2.065904	1.003909	C	2.630492	2.625738	-1.174641	C	-0.475753	5.474967	1.274214
C	-6.474350	-2.816072	-1.205827	C	6.437145	-0.664960	-0.273092	C	0.266652	6.408223	-0.865507
H	-5.279467	-2.169470	-2.917987	C	7.071487	0.309900	0.749430	H	0.018671	5.141767	-2.630684
C	-6.636870	-2.781186	0.183824	H	8.164364	0.153524	0.806916	C	0.097789	6.524888	0.519332
H	-5.864174	-2.043179	2.091061	H	6.895140	1.362613	0.468156	H	-0.593717	5.566795	2.359001
H	-7.190186	-3.373060	-1.819913	H	6.644009	0.151383	1.754970	H	0.721002	7.232168	-1.425894
H	-7.478006	-3.311415	0.643206	C	7.061539	-0.422193	-1.669161	H	0.421749	7.439124	1.027799
C	-2.093573	-1.413603	-0.701844	H	6.881630	0.609455	-2.018171	C	-2.733756	2.809583	-0.900418
H	-1.417298	-2.034290	-1.290711	H	8.154777	-0.583561	-1.637926	H	-3.489656	2.780787	-1.687103
C	-2.248621	-1.371580	0.639239	H	6.629253	-1.112610	-2.414482	C	-2.898329	2.922263	0.427679
H	-1.713602	-1.934023	1.405004	C	6.762219	-2.106583	0.162360	H	-3.822122	3.000643	1.002954
H	4.260058	2.967423	0.308908	H	6.360231	-2.326948	1.166723	C	3.294223	1.948490	-1.399131
H	3.426617	3.368997	1.855561	H	6.347800	-2.846332	-0.544753	C	6.271412	-2.065213	-0.320453
H	-2.655232	2.455876	-2.619880	H	7.856784	-2.248827	0.197930	C	7.147857	-1.197845	0.616525
H	-0.875420	6.397178	-2.231337	C	1.801166	3.222195	-0.007987	H	8.177384	-1.597812	0.663864
				H	1.480412	4.249771	-0.258790	H	7.206760	-0.153698	0.263394
				H	0.904360	2.619757	0.195564	H	6.731467	-1.187047	1.639001
				H	2.414203	3.270409	0.909833	C	6.885889	-2.066846	-1.741806

C	1.778630	2.596736	-2.468323	H	6.937035	-1.047072	-2.161227
H	2.374745	2.219462	-3.318671	H	7.912795	-2.475602	-1.719081
H	0.903837	1.944468	-2.333555	H	6.280399	-2.685495	-2.427165
H	1.429828	3.616396	-2.715943	C	6.271962	-3.510755	0.212428
C	3.828822	3.563082	-1.427840	H	5.865561	-3.564988	1.237516
H	4.468099	3.662805	-0.532809	H	5.674531	-4.179924	-0.431259
H	4.457294	3.215320	-2.267247	H	7.305232	-3.899668	0.237757
H	3.453266	4.569416	-1.683778	C	2.681431	2.806652	-0.262317
H	1.178702	-5.158392	0.712822	H	2.598712	3.860138	-0.586149
H	1.221182	-4.240874	2.258883	H	1.678258	2.449627	0.010981
C	-1.058475	-4.072369	-0.317007	H	3.328906	2.773971	0.632272
H	-1.865288	-3.353743	-0.535757	C	2.397916	2.026668	-2.660622
C	-0.290856	-4.326568	-1.620836	H	2.848523	1.457830	-3.493892
H	0.156858	-3.392352	-1.999920	H	1.401989	1.612278	-2.447485
H	0.520048	-5.066216	-1.485103	H	2.286560	3.079112	-2.980813
H	-0.970399	-4.719030	-2.397273	C	4.664240	2.556224	-1.762602
C	-1.712551	-5.344213	0.240711	H	5.350050	2.570595	-0.897004
H	-2.293535	-5.123772	1.153863	H	5.155483	2.008177	-2.586555
H	-2.401201	-5.783604	-0.501553	H	4.520808	3.600353	-2.091912
H	-0.959544	-6.115400	0.490761	H	0.049307	-5.064682	0.601994
				H	0.357291	-4.536634	2.296735

Transition State (1-2): In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

TS1 _{L3} ² : $\nu_{\text{lowest}} = -217.2188 \text{ cm}^{-1}$				TS1 _{L5} ² : $\nu_{\text{lowest}} = -191.2097 \text{ cm}^{-1}$				TS1 _{L6} ² : $\nu_{\text{lowest}} = -188.8787 \text{ cm}^{-1}$			
79				102				103			
Ni	-0.166721	0.316670	-0.150267	Ni	-0.686210	-0.244361	0.057403	Ni	-0.567300	0.053162	0.182048
C	-0.716729	0.447005	2.586978	C	-1.465428	-0.621332	2.718057	C	-1.290605	0.187423	2.881204
C	-1.316979	2.570494	1.542479	C	0.724671	0.456506	2.650935	C	1.034422	0.887475	2.621911
C	-0.889075	1.024215	3.856104	C	-1.327845	-0.813992	4.103012	C	-1.131062	0.176001	4.277222
C	-1.464713	3.140806	2.816677	C	0.859337	0.238478	4.031076	C	1.186509	0.851775	4.017045
H	-1.488797	3.182287	0.650651	H	1.528933	0.950715	2.095590	H	1.883183	1.164920	1.987788
C	-1.268945	2.366762	3.974778	C	-0.170628	-0.381535	4.762238	C	0.102473	0.513130	4.847529
H	-0.685851	0.393169	4.728876	H	-2.139900	-1.333463	4.624418	H	-1.992264	-0.130753	4.881741
H	-1.742801	4.197320	2.901751	H	1.775198	0.562548	4.538030	H	2.159798	1.097600	4.456514
H	-1.399673	2.818267	4.963952	H	-0.059830	-0.535403	5.840872	H	0.229417	0.500820	5.935251
N	0.193274	-1.148105	1.137638	N	-2.368504	-1.138434	0.622498	N	-2.348082	-0.459493	0.897989
C	1.096883	-2.147072	-0.781546	C	-2.587709	-1.433353	-1.696488	C	-2.696071	-1.057544	-1.342411
C	1.121005	-0.721829	-2.644299	C	-0.710547	-0.716744	-2.906186	C	-0.764973	-0.883778	-2.660018
C	1.749273	-3.199028	-1.499605	C	-3.246578	-1.902217	-2.878637	C	-3.466255	-1.579129	-2.430356
C	0.737804	-2.284426	0.606798	C	-3.171590	-1.590109	-0.386738	C	-3.257891	-0.891381	-0.026648
C	1.799079	-1.694421	-3.415672	C	-1.283175	-1.165035	-4.120228	C	-1.442423	-1.424925	-3.777394
H	0.819847	0.254466	-3.039262	H	0.272337	-0.238151	-2.851080	H	0.284765	-0.575541	-2.691892
C	2.102919	-2.924731	-2.850371	C	-2.543948	-1.743320	-4.107485	C	-2.784470	-1.758845	-3.666349
C	2.000275	-4.424246	-0.821504	C	-4.528873	-2.503363	-2.743866	C	-4.836172	-1.886793	-2.201436
C	0.989222	-3.518389	1.232968	C	-4.440669	-2.193245	-0.301506	C	-4.619620	-1.194595	0.151457
H	2.065134	-1.465876	-4.451838	H	-0.723376	-1.044131	-5.052133	H	-0.899274	-1.562256	-4.716898

H	2.617254	-3.695281	-3.435233	H	-3.008432	-2.089959	-5.037299	H	-3.330671	-2.167329	-4.523756
C	1.608583	-4.562296	0.507039	C	-5.093608	-2.630583	-1.477206	C	-5.381028	-1.678534	-0.937629
H	2.499184	-5.240793	-1.352671	H	-5.050127	-2.866063	-3.635266	H	-5.441938	-2.286415	-3.020673
H	0.719243	-3.632283	2.283807	H	-4.887491	-2.321907	0.685375	H	-5.053492	-1.072264	1.144844
H	1.798030	-5.510542	1.022791	H	-6.080434	-3.096724	-1.378332	H	-6.438199	-1.912111	-0.767714
N	0.791588	-0.953910	-1.376918	N	-1.351816	-0.846134	-1.748371	N	-1.382137	-0.707914	-1.495264
C	-0.159478	-0.940176	2.446541	C	-2.626964	-1.208374	1.969956	C	-2.555544	-0.311735	2.245336
O	0.025028	-1.710235	3.397161	O	-3.602621	-1.737629	2.513429	O	-3.573507	-0.617256	2.878951
O	-0.522959	1.629843	-1.660432	O	0.916935	0.695694	-0.787363	O	1.139855	0.590461	-0.808141
C	-0.139661	2.870257	-1.744378	C	2.190442	0.484325	-0.600485	C	2.367517	0.197811	-0.612680
C	0.940966	3.440189	-0.976436	C	2.693918	-0.704923	0.036301	C	2.696287	-0.967296	0.167867
C	-0.810170	3.747257	-2.655603	C	3.166526	1.458657	-1.045692	C	3.472112	0.927565	-1.203108
C	1.289421	4.807599	-1.130417	C	4.080952	-0.882401	0.281071	C	4.044063	-1.342219	0.409317
C	1.684048	2.623300	-0.046810	C	1.797513	-1.764783	0.434831	C	1.654112	-1.807354	0.708521
C	-0.444786	5.080651	-2.788831	C	4.513750	1.215208	-0.783616	C	4.770693	0.501665	-0.929539
C	0.610925	5.628256	-2.022516	C	5.012922	0.067527	-0.112321	C	5.102296	-0.616197	-0.118264
H	2.110716	5.200411	-0.524373	H	4.385187	-1.799929	0.786924	H	4.214588	-2.227089	1.024502
N	1.463392	1.375696	0.278111	N	0.492580	-1.817675	0.334421	N	0.358239	-1.627858	0.665872
O	2.745091	3.197234	0.575932	O	2.363683	-2.873137	0.983095	O	2.045693	-2.947884	1.335307
H	-0.987960	5.717798	-3.496758	H	5.241669	1.961027	-1.113481	H	5.597017	1.067366	-1.367860
C	2.473128	0.933542	1.256041	C	0.018359	-3.123328	0.830487	C	-0.324939	-2.750885	1.330449
C	3.249397	2.247865	1.549416	C	1.285379	-3.695592	1.499266	C	0.864849	-3.581587	1.886456
H	1.959294	0.578288	2.163706	H	-0.770721	-2.951304	1.579793	H	-0.937940	-2.356124	2.156851
C	3.327316	-0.191474	0.701985	C	-0.446087	0.042303	1.996720	C	-1.224831	-3.502534	0.367705
C	3.874439	-0.096103	-0.590675	C	-2.213054	2.310272	1.784819	C	-0.748270	-3.878871	-0.901462
C	3.575617	-1.340171	1.470107	C	-2.656076	3.651110	1.176994	C	-2.543531	-3.821338	0.728742
C	4.657813	-1.135352	-1.106770	H	-2.078432	2.239622	2.870766	C	-1.580141	-4.561867	-1.796634
H	3.664533	0.787544	-1.203527	O	-3.270371	1.451975	1.328303	H	0.272559	-3.611949	-1.196867
C	4.362494	-2.380213	0.955588	C	-3.160068	1.756798	-0.076590	C	-3.376649	-4.508061	-0.165698
H	3.119006	-1.435491	2.461501	C	-3.285481	3.288736	-0.035604	H	-2.931465	-3.494429	1.699913
C	4.903570	-2.280544	-0.332990	C	-2.526473	4.982390	1.553227	C	-2.897853	-4.877721	-1.429467
H	5.068889	-1.056977	-2.118721	H	-3.886506	1.183047	-0.665143	H	-1.204039	-4.838791	-2.787121
H	4.532435	-3.279868	1.555236	C	-3.796560	4.251537	-0.897301	H	-4.409627	-4.732328	0.118093
H	5.505614	-3.099777	-0.739968	C	-3.063868	5.965457	0.691656	H	-3.554084	-5.400238	-2.133419
C	-0.963436	1.216654	1.424265	H	-2.034568	5.269239	2.488717	C	-0.210392	0.574311	2.054009
C	-3.359810	-0.284021	0.995151	C	-3.687247	5.606686	-0.510626	C	-1.607774	3.041287	1.525623
C	-4.520859	-0.804640	0.133094	H	-4.278585	3.978593	-1.842096	C	-1.854009	4.332571	0.728144
H	-3.588152	0.211776	1.946322	H	-2.994092	7.022554	0.969129	H	-1.445721	3.109885	2.607972
O	-2.620074	-1.498552	1.200028	H	-4.097805	6.387559	-1.159527	O	-2.804167	2.309041	1.217469
C	-2.472376	-1.860562	-0.188742	C	-1.047307	1.866744	0.885389	C	-2.698965	2.382157	-0.218719
C	-3.943596	-1.842486	-0.633478	H	-0.047466	2.292846	0.963128	C	-2.577567	3.903164	-0.407626
C	-5.857020	-0.453750	-0.017566	C	-1.659741	1.538990	-0.342117	C	-1.500057	5.665607	0.896855
H	-1.900094	-2.790107	-0.296873	H	-1.204375	1.756080	-1.311109	H	-3.528470	1.853886	-0.704545
C	-4.690994	-2.548058	-1.568695	C	2.723069	2.730665	-1.796515	C	-2.960357	4.798940	-1.398478
C	-6.628227	-1.182622	-0.950990	C	6.523409	-0.073701	0.135786	C	-1.905607	6.585467	-0.096597
H	-6.308698	0.352033	0.570794	C	1.809011	3.593722	-0.893195	H	-0.934190	6.002989	1.771718
C	-6.055899	-2.210342	-1.712116	H	0.897441	3.039113	-0.633293	C	-2.622411	6.160091	-1.222685

H	-4.248404	-3.348499	-2.171098	H	2.333855	3.874807	0.037252	H	-3.514176	4.472009	-2.284977
H	-7.689119	-0.942774	-1.078858	H	1.516643	4.521685	-1.417955	H	-1.658055	7.646215	0.016812
H	-6.675983	-2.762153	-2.426563	C	1.955574	2.341229	-3.084443	H	-2.927105	6.893290	-1.977002
C	-2.454819	0.458415	-0.003027	H	2.593374	1.729881	-3.747453	C	-0.561008	2.287857	0.688230
H	-2.682533	1.449909	-0.395984	H	1.052165	1.766264	-2.833193	H	0.495360	2.554962	0.687270
C	-1.904988	-0.569514	-0.803998	H	1.653247	3.249526	-3.637357	C	-1.262845	1.887397	-0.468431
H	-1.753240	-0.453757	-1.879807	C	3.924617	3.602862	-2.215401	H	-0.815834	1.884564	-1.465307
H	4.335781	2.152624	1.401425	H	4.499244	3.959916	-1.342527	C	3.212107	2.139514	-2.120354
H	3.039846	2.649192	2.554939	H	4.613711	3.060336	-2.886508	C	6.578166	-0.969795	0.126315
H	0.888585	6.681030	-2.130447	H	3.555974	4.490808	-2.758397	C	2.481920	3.257696	-1.337630
H	-1.628049	3.318406	-3.243460	C	7.015493	1.116466	0.995644	H	1.501870	2.902663	-0.992020
				H	8.103488	1.040762	1.176473	H	3.077025	3.573238	-0.462119
				H	6.822093	2.082302	0.497263	H	2.326264	4.140164	-1.984890
				H	6.500830	1.129893	1.972423	C	2.345760	1.705296	-3.329081
				C	7.271559	-0.070767	-1.220007	H	2.856618	0.916431	-3.909529
				H	7.087897	0.861821	-1.781340	H	1.374274	1.319760	-2.986143
				H	8.361901	-0.160667	-1.061206	H	2.167644	2.566307	-3.999193
				H	6.940720	-0.915816	-1.848799	C	4.522171	2.736022	-2.675133
				C	6.861223	-1.382013	0.875885	H	5.177687	3.112076	-1.869795
				H	6.366640	-1.428573	1.861908	H	5.090742	1.999910	-3.270490
				H	6.552900	-2.267973	0.293737	H	4.281400	3.588012	-3.334903
				H	7.951187	-1.448335	1.040653	C	7.282468	0.222586	0.819356
				H	1.504134	-4.741338	1.234483	H	8.350034	-0.005500	0.993829
				H	1.273362	-3.586136	2.597254	H	7.228351	1.137147	0.203490
				C	-0.577237	-3.980872	-0.311248	H	6.810013	0.441105	1.793101
				H	-1.384877	-3.367993	-0.742656	C	7.271825	-1.258512	-1.227726
				C	-1.219565	-5.255853	0.253150	H	7.221820	-0.386220	-1.902357
				H	-1.981497	-5.009972	1.013880	H	8.338278	-1.504541	-1.071976
				H	-1.713811	-5.829351	-0.550019	H	6.789394	-2.110310	-1.738285
				H	-0.468363	-5.920397	0.720533	C	6.726871	-2.212651	1.024460
				C	0.437057	-4.271260	-1.425459	H	6.264932	-2.054067	2.014648
				H	1.270673	-4.905350	-1.071039	H	6.261148	-3.102223	0.565451
				H	-0.051617	-4.802681	-2.260626	H	7.797034	-2.434839	1.182227
				H	0.863812	-3.334577	-1.822830	H	0.853638	-4.630420	1.552457
								H	0.937112	-3.538118	2.985825

Transition State (1'-2'): In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

TS1' _{L3} ² : $\nu_{\text{lowest}} = -248.7400 \text{ cm}^{-1}$				TS1' _{L5} ² : $\nu_{\text{lowest}} = -229.6788 \text{ cm}^{-1}$				TS1' _{L6} ² : $\nu_{\text{lowest}} = -229.3008 \text{ cm}^{-1}$			
79				102				103			
Ni	-0.151509	0.090208	-0.054871	Ni	-0.864782	-0.194321	0.110433	Ni	-0.720881	0.151179	0.264643
C	-0.281467	0.673697	2.676958	C	-1.402228	-0.803184	2.788326	C	-1.374878	0.050427	2.985993
C	-1.858686	2.076949	1.438650	C	0.600475	0.593977	2.594536	C	0.831037	1.062845	2.649030
C	-0.433696	1.484931	3.810068	C	-1.081060	-1.099215	4.120470	C	-1.117664	-0.080231	4.358098
C	-1.982164	2.896656	2.573285	C	0.924064	0.268799	3.923122	C	1.085424	0.902284	4.022012
H	-2.426679	2.294884	0.530043	H	1.239986	1.256875	2.005168	H	1.575464	1.511781	1.985392
C	-1.279580	2.602594	3.756006	C	0.088100	-0.567788	4.685609	C	0.116704	0.341142	4.874800

H	0.133817	1.224535	4.710705	H	-1.753640	-1.758086	4.681151	H	-1.893391	-0.527333	4.989985
H	-2.638666	3.773075	2.530646	H	1.840893	0.674335	4.365772	H	2.052408	1.219387	4.428781
H	-1.394851	3.247837	4.633450	H	0.353262	-0.803715	5.721723	H	0.330239	0.232339	5.943482
N	0.753544	-0.958251	1.363095	N	-2.520395	-1.106526	0.753641	N	-2.511799	-0.374842	0.985977
C	1.678135	-2.019352	-0.521073	C	-2.829254	-1.378506	-1.566605	C	-2.851461	-0.939949	-1.273399
C	1.067922	-1.012874	-2.549926	C	-1.046201	-0.572221	-2.859433	C	-0.938755	-0.702226	-2.606358
C	2.515303	-2.976680	-1.176410	C	-3.522994	-1.864235	-2.721727	C	-3.618018	-1.461337	-2.364024
C	1.555088	-1.979584	0.912915	C	-3.337562	-1.596021	-0.234037	C	-3.409600	-0.825756	0.049856
C	1.888743	-1.909170	-3.274603	C	-1.667643	-1.014865	-4.051782	C	-1.618871	-1.222324	-3.732268
H	0.464961	-0.229155	-3.021929	H	-0.074626	-0.069791	-2.846794	H	0.106830	-0.383615	-2.641262
C	2.600258	-2.886624	-2.594172	C	-2.899224	-1.647935	-3.983861	C	-2.950113	-1.591108	-3.613786
C	3.206855	-3.929099	-0.377039	C	-4.753436	-2.553795	-2.534317	C	-4.971807	-1.828885	-2.127367
C	2.255054	-2.938167	1.663493	C	-4.546739	-2.300219	-0.096069	C	-4.750306	-1.199939	0.238585
H	1.946092	-1.821896	-4.363533	H	-1.164536	-0.851602	-5.009183	H	-1.083598	-1.322148	-4.680893
H	3.236731	-3.593779	-3.137421	H	-3.398079	-2.000105	-4.893527	H	-3.498124	-1.992622	-4.473191
C	3.059911	-3.897932	1.005762	C	-5.233675	-2.758448	-1.244713	C	-5.508074	-1.685909	-0.852314
H	3.851737	-4.669418	-0.860704	H	-5.297480	-2.929003	-3.406774	H	-5.570730	-2.229103	-2.951340
H	2.182876	-2.903752	2.751541	H	-4.922829	-2.493453	0.909641	H	-5.173354	-1.134331	1.242067
H	3.596186	-4.632591	1.616843	H	-6.175001	-3.301445	-1.104605	H	-6.550504	-1.973135	-0.674741
N	0.974486	-1.078344	-1.225817	N	-1.617858	-0.743091	-1.671817	N	-1.542759	-0.562997	-1.430559
C	0.654465	-0.498683	2.653841	C	-2.595899	-1.394970	2.097169	C	-2.643919	-0.443275	2.351366
O	1.258866	-0.931694	3.646341	O	-3.466850	-2.068629	2.665578	O	-3.614895	-0.882881	2.985611
O	-0.930777	0.988371	-1.643921	O	0.751717	0.665726	-0.750587	O	1.020014	0.616668	-0.675528
C	-1.119475	2.271352	-1.761691	C	2.015482	0.371764	-0.605469	C	2.212177	0.106726	-0.529631
C	-0.256580	3.262046	-1.168808	C	2.460657	-0.797226	0.114733	C	2.472534	-1.040774	0.306552
C	-2.222503	2.754638	-2.530577	C	3.058587	1.201077	-1.186886	C	3.359982	0.653736	-1.237323
C	-0.506768	4.644337	-1.359529	C	3.831474	-1.027349	0.401892	C	3.790111	-1.506298	0.559577
C	0.881948	2.839172	-0.389982	C	1.528818	-1.833522	0.479155	C	1.386482	-1.827547	0.831008
C	-2.446946	4.115721	-2.699850	C	4.386570	0.902088	-0.882362	C	4.622698	0.134788	-0.954497
C	-1.590536	5.077423	-2.114397	C	4.818694	-0.174390	-0.065977	C	4.890934	-0.917782	-0.041716
H	0.173506	5.362451	-0.892568	H	4.076072	-1.915073	0.986941	H	3.897725	-2.358876	1.231702
N	1.169235	1.620823	-0.011374	N	0.231061	-1.862169	0.305515	N	0.100243	-1.602506	0.744561
O	1.758677	3.793716	0.011548	O	2.052544	-2.968505	1.018694	O	1.716761	-2.998466	1.441992
H	-3.309355	4.447459	-3.290051	H	5.158759	1.552727	-1.300362	H	5.477486	0.575933	-1.473080
C	2.397581	1.637582	0.799857	C	-0.267566	-3.202738	0.674668	C	-0.635749	-2.753541	1.298210
C	2.805550	3.139554	0.771370	C	0.935501	-3.793491	1.434130	C	0.497741	-3.580509	1.959360
H	2.147313	1.330389	1.829422	H	-1.129973	-3.105343	1.350356	H	-1.341042	-2.410208	2.069075
C	3.450622	0.694702	0.251647	C	-0.562490	0.049763	2.031193	C	-1.412184	-3.487654	0.219857
C	3.748189	0.689341	-1.123472	C	-1.135840	2.834447	-0.459923	C	-0.818029	-3.765889	-1.024338
C	4.133587	-0.184843	1.106571	C	-2.082112	4.009637	-0.178164	C	-2.735215	-3.896421	0.456548
C	4.717416	-0.181642	-1.635014	H	-0.585376	2.811707	-1.405317	C	-1.536833	-4.445505	-2.015757
H	3.196590	1.354763	-1.796879	O	-0.230243	2.957823	0.661212	H	0.205183	-3.428961	-1.222783
C	5.107194	-1.055196	0.595656	C	-1.223611	2.937012	1.699727	C	-3.455312	-4.577118	-0.535194
H	3.874320	-0.212452	2.170756	C	-2.150950	4.070022	1.231586	H	-3.211280	-3.650756	1.412204
C	5.400711	-1.055288	-0.774319	C	-2.816025	4.882921	-0.971455	C	-2.857410	-4.853422	-1.772407
H	4.933491	-0.187045	-2.708566	H	-0.770942	3.006151	2.696349	H	-1.068475	-4.649434	-2.984466
H	5.621220	-1.749355	1.267915	C	-2.954299	5.001766	1.878228	H	-4.491474	-4.875087	-0.346188

H	6.151839	-1.744590	-1.174370	C	-3.620832	5.846317	-0.321435	H	-3.423424	-5.375594	-2.551204
C	-1.002153	0.966010	1.489825	H	-2.771218	4.839827	-2.064885	C	-0.401500	0.632932	2.137921
C	-2.789115	-1.011962	-1.178976	C	-3.688972	5.904665	1.076750	C	-0.507112	3.068347	-0.762338
C	-3.877405	-2.044679	-0.852970	H	-3.014086	5.049554	2.970734	C	-1.268993	4.398644	-0.684556
H	-2.509183	-0.830540	-2.221207	H	-4.197813	6.559452	-0.919709	H	0.045043	2.826705	-1.675264
O	-3.370588	0.172950	-0.587814	H	-4.317917	6.662513	1.555653	O	0.392441	3.220303	0.360015
C	-3.573924	-0.366418	0.728853	C	-1.945383	1.586609	-0.064620	C	-0.604922	3.499147	1.355807
C	-4.382883	-1.631337	0.400242	H	-2.802662	1.253269	-0.656677	C	-1.345114	4.675286	0.698670
C	-4.355689	-3.190719	-1.476794	C	-1.974655	1.654018	1.344137	C	-1.853632	5.243867	-1.619643
H	-4.013866	0.373977	1.408305	H	-2.765237	1.231345	1.964753	H	-0.159639	3.645962	2.347323
C	-5.374508	-2.352355	1.055030	C	2.750591	2.424544	-2.077631	C	-2.006995	5.799880	1.177076
C	-5.378701	-3.918515	-0.827038	C	6.315365	-0.360762	0.227731	C	-2.512159	6.400162	-1.142535
H	-3.965127	-3.522190	-2.444919	C	6.855072	0.898730	0.949032	H	-1.802816	5.033962	-2.693327
C	-5.878882	-3.507248	0.415460	H	7.934960	0.792297	1.160929	C	-2.587648	6.673098	0.229616
H	-5.765328	-2.038373	2.028805	H	6.718357	1.805306	0.334165	H	-2.072356	6.016117	2.248709
H	-5.787886	-4.816110	-1.302865	H	6.326501	1.055771	1.905619	H	-2.968150	7.094401	-1.856336
H	-6.673514	-4.087270	0.896616	C	7.083975	-0.558807	-1.101891	H	-3.101288	7.577289	0.572940
C	-1.655983	-1.338754	-0.183352	H	6.957790	0.307120	-1.774784	C	-1.502434	2.026789	-0.220755
H	-1.070884	-2.259324	-0.273718	H	8.165653	-0.683015	-0.909843	H	-2.392403	1.740360	-0.788744
C	-2.170051	-0.885903	1.052826	H	6.719390	-1.456066	-1.631989	C	-1.537691	2.303760	1.161925
H	-1.891834	-1.298827	2.023469	C	6.571724	-1.585365	1.126681	H	-2.392669	2.101978	1.807522
H	3.762055	3.309454	0.250762	H	6.053734	-1.489555	2.097027	C	3.229643	1.813724	-2.246866
H	2.839443	3.598258	1.772083	H	6.231797	-2.519317	0.645937	C	6.339745	-1.363501	0.209710
H	-2.893731	2.008981	-2.965670	H	7.653282	-1.683066	1.327787	C	7.150811	-0.169868	0.771469
H	-1.780298	6.146369	-2.251079	C	2.313467	3.601433	-1.172842	H	8.201779	-0.463610	0.949184
				H	2.001380	4.468962	-1.785031	H	7.151376	0.682783	0.070282
				H	1.487733	3.319328	-0.506258	H	6.720286	0.177857	1.726862
				H	3.159967	3.919222	-0.538334	C	6.976052	-1.834299	-1.121166
				C	1.653274	2.106088	-3.120215	H	6.977782	-1.029043	-1.876217
				H	1.961769	1.261910	-3.763887	H	8.023650	-2.148631	-0.959996
				H	0.710918	1.835727	-2.626296	H	6.416530	-2.689634	-1.538766
				H	1.483898	2.985367	-3.767931	C	6.412347	-2.522627	1.221921
				C	3.990921	2.882332	-2.879940	H	5.983341	-2.234425	2.197595
				H	4.794948	3.267263	-2.229434	H	5.871195	-3.413327	0.857492
				H	4.403663	2.064509	-3.497254	H	7.465593	-2.811083	1.386797
				H	3.697889	3.706487	-3.554105	C	2.999624	3.128489	-1.464402
				H	1.171875	-4.836309	1.173353	H	2.807355	3.967848	-2.159522
				H	0.830485	-3.698054	2.528903	H	2.157352	3.045333	-0.765277
				C	-0.722646	-3.997741	-0.574459	H	3.900941	3.374326	-0.875023
				H	-1.494760	-3.373095	-1.053148	C	2.073497	1.560064	-3.243333
				C	0.407415	-4.204032	-1.592172	H	2.250610	0.629329	-3.812978
				H	0.844304	-3.237676	-1.896505	H	1.115827	1.463611	-2.714957
				H	1.219303	-4.834337	-1.185228	H	2.007231	2.394385	-3.965167
				H	0.021672	-4.703187	-2.498317	C	4.507314	1.991187	-3.098400
				C	-1.391973	-5.315125	-0.157217	H	5.376878	2.298476	-2.492149
				H	-2.230740	-5.129052	0.536791	H	4.770464	1.065993	-3.641698
				H	-1.790735	-5.844814	-1.039758	H	4.333248	2.787372	-3.843652

H	-0.677428	-5.996063	0.342482	H	0.482546	-4.645392	1.682930
				H	0.505888	-3.474542	3.057756

Intermediate-2: In Ni catalyzed reaction energy profile for other 3 possible intermediates

Int2 _{L3} ² : v _{lowest} = 16.6068 cm ⁻¹				Int2 _{L5} ² : v _{lowest} = 11.2122 cm ⁻¹				Int2 _{L6} ² : v _{lowest} = 6.7229 cm ⁻¹			
79				102				103			
Ni	-0.067533	0.247267	-0.344300	Ni	0.679426	-0.322173	0.134084	Ni	-0.551723	-0.050024	-0.015006
C	-0.764916	0.826288	2.335238	C	0.797615	-0.437733	-2.685241	C	-0.594725	0.178881	2.799449
C	-2.137823	2.562683	1.328676	C	-1.198354	0.944517	-2.544635	C	1.601618	1.169169	2.468998
C	-0.239032	1.797759	3.208244	C	0.100782	-1.296633	-3.555750	C	-0.025832	-0.678709	3.760165
C	-1.547154	3.531373	2.147201	C	-1.903759	0.039813	-3.345276	C	2.168859	0.254815	3.363148
H	-2.901410	2.863231	0.603154	H	-1.705911	1.836297	-2.161459	H	2.240742	1.909704	1.976214
C	-0.609275	3.143851	3.113985	C	-1.243003	-1.075590	-3.878442	C	1.345980	-0.659083	4.035957
H	0.497872	1.464874	3.946903	H	0.638405	-2.168217	-3.943844	H	-0.692480	-1.388810	4.261034
H	-1.831506	4.582661	2.036829	H	-2.962908	0.214744	-3.559512	H	3.248852	0.267710	3.541521
H	-0.161444	3.886683	3.782618	H	-1.775118	-1.775924	-4.531070	H	1.772105	-1.359914	4.761670
N	0.353551	-0.891054	1.131779	N	2.183815	-0.990765	-0.837230	N	-2.117555	-0.321782	1.047454
C	1.332512	-2.173145	-0.591545	C	3.015962	-1.294176	1.353348	C	-3.054423	-0.753062	-1.076285
C	1.161490	-1.183267	-2.708593	C	1.512935	-0.646046	3.031406	C	-1.509582	-0.621213	-2.832308
C	2.045612	-3.302228	-1.106237	C	4.006831	-1.693473	2.307458	C	-4.125643	-1.098677	-1.960720
C	1.013756	-2.052776	0.807721	C	3.238708	-1.415540	-0.066261	C	-3.258065	-0.628000	0.344095
C	1.877458	-2.251349	-3.299277	C	2.432341	-1.017095	4.042037	C	-2.503546	-0.974430	-3.775190
H	0.780216	-0.335551	-3.288168	H	0.525500	-0.231538	3.259998	H	-0.473145	-0.417868	-3.121325
C	2.314008	-3.301662	-2.504251	C	3.668085	-1.534960	3.682384	C	-3.800657	-1.209033	-3.342183
C	2.428441	-4.330057	-0.201108	C	5.237582	-2.218223	1.825941	C	-5.419735	-1.304620	-1.408514
C	1.390120	-3.101369	1.662958	C	4.471426	-1.935480	-0.497611	C	-4.556322	-0.818808	0.844975
H	2.072818	-2.237190	-4.375594	H	2.154919	-0.890768	5.092612	H	-2.236233	-1.053982	-4.832979
H	2.865553	-4.140669	-2.942543	H	4.394697	-1.827283	4.448420	H	-4.586646	-1.479470	-4.055804
C	2.089176	-4.215957	1.143578	C	5.442899	-2.325670	0.453307	C	-5.608947	-1.153278	-0.038307
H	2.979536	-5.198969	-0.574219	H	6.006084	-2.531599	2.539431	H	-6.250029	-1.575161	-2.068291
H	1.145086	-3.021831	2.722478	H	4.648058	-2.029221	-1.569600	H	-4.719164	-0.718894	1.918487
H	2.375244	-5.015242	1.836357	H	6.393381	-2.727734	0.085425	H	-6.609589	-1.302029	0.382641
N	0.912288	-1.158427	-1.402943	N	1.807448	-0.786003	1.741991	N	-1.789526	-0.520996	-1.536308
C	-0.058739	-0.514698	2.385172	C	2.136966	-0.966265	-2.210912	C	-2.019036	-0.162311	2.407153
O	0.250954	-1.060873	3.448103	O	2.962893	-1.468500	-2.976593	O	-2.889262	-0.438721	3.237847
O	-0.744114	1.363426	-1.744759	O	-0.802936	0.568127	0.956623	O	1.044059	0.465428	-0.942336
C	-0.677093	2.669282	-1.799386	C	-2.084764	0.356838	0.770577	C	2.270810	0.038684	-0.761218
C	0.264068	3.480394	-1.072391	C	-2.610439	-0.821507	0.141644	C	2.598064	-1.153374	-0.030121
C	-1.592103	3.354973	-2.655187	C	-3.034749	1.348435	1.222594	C	3.367574	0.787306	-1.333898
C	0.251250	4.891682	-1.207519	C	-4.000486	-0.980946	-0.086094	C	3.943638	-1.551446	0.173605
C	1.244323	2.856564	-0.215817	C	-1.728838	-1.894038	-0.254952	C	1.551201	-1.999019	0.491952
C	-1.587748	4.740305	-2.764988	C	-4.388799	1.129343	0.969875	C	4.667393	0.343207	-1.093817
C	-0.665374	5.526617	-2.036975	C	-4.912951	-0.011260	0.307474	C	5.000858	-0.810181	-0.336258
H	0.982936	5.469411	-0.635494	H	-4.322280	-1.896605	-0.584725	H	4.113386	-2.462839	0.749195
N	1.320790	1.587268	0.086767	N	-0.422358	-1.915618	-0.200959	N	0.264017	-1.769413	0.476131
O	2.194059	3.644671	0.343837	O	-2.299313	-3.031756	-0.727017	O	1.917269	-3.176840	1.057340

H	-2.314968	5.227835	-3.424647	H	-5.098785	1.892402	1.299008	H	5.490972	0.925362	-1.515098
C	2.460230	1.367229	0.993690	C	0.058587	-3.246315	-0.609206	C	-0.448912	-2.900115	1.093171
C	3.092421	2.784922	1.092477	C	-1.224565	-3.901596	-1.169200	C	0.709073	-3.874173	1.452873
H	2.070014	1.050631	1.975620	H	0.811756	-3.125881	-1.405301	H	-0.950135	-2.544408	2.008740
C	3.388594	0.286570	0.476563	C	0.156411	0.742479	-2.202380	C	-1.502278	-3.470887	0.164079
C	3.795633	0.282081	-0.869986	C	2.137884	2.425075	-2.159849	C	-1.202536	-3.715022	-1.188373
C	3.832068	-0.735619	1.331022	C	2.509914	3.703985	-1.426864	C	-2.796101	-3.739059	0.639570
C	4.634052	-0.729809	-1.353170	H	2.097005	2.441160	-3.256981	C	-2.182916	-4.220024	-2.051125
H	3.427036	1.060091	-1.547826	O	3.159147	1.520111	-1.702896	H	-0.203191	-3.479006	-1.570769
C	4.675218	-1.747204	0.850208	C	2.968500	1.734992	-0.287035	C	-3.777918	-4.248718	-0.221634
H	3.484884	-0.757095	2.369867	C	3.054427	3.255552	-0.204446	H	-3.043140	-3.514125	1.682905
C	5.076184	-1.746592	-0.492365	C	2.347539	5.061901	-1.688481	C	-3.473217	-4.488507	-1.568235
H	4.933382	-0.733112	-2.406457	H	3.692311	1.150436	0.295188	H	-1.944170	-4.393295	-3.105671
H	4.999143	-2.549145	1.520752	C	3.441493	4.156974	0.785416	H	-4.787915	-4.436181	0.155835
H	5.721675	-2.545432	-0.872341	C	2.770274	5.979529	-0.704397	H	-4.243970	-4.871768	-2.245218
C	-1.778437	1.199094	1.400250	H	1.914487	5.415689	-2.630471	C	0.221733	1.166354	2.170063
C	-3.300568	-0.899452	1.422956	C	3.308039	5.533672	0.513091	C	-1.444572	3.152259	1.949233
C	-4.297324	-1.589537	0.505972	H	3.848231	3.814636	1.743239	C	-1.608529	4.385351	1.075102
H	-3.634443	-0.590579	2.422421	H	2.680366	7.054742	-0.892795	H	-1.369312	3.285291	3.036581
O	-2.261252	-1.890178	1.518707	H	3.631607	6.266699	1.259970	O	-2.621125	2.396752	1.610094
C	-2.065949	-2.082526	0.099119	C	0.857377	1.865814	-1.436708	C	-2.436924	2.411906	0.177097
C	-3.493642	-2.365007	-0.357107	H	0.115574	2.666929	-1.297138	C	-2.258406	3.904490	-0.081738
C	-5.680016	-1.537571	0.350562	C	1.465282	1.444971	-0.074813	C	-1.203994	5.713920	1.174936
H	-1.308713	-2.854968	-0.086671	H	1.041145	1.965280	0.795823	H	-3.267827	1.901496	-0.326488
C	-4.056530	-3.099105	-1.399301	C	-2.558084	2.624427	1.944560	C	-2.510998	4.742054	-1.166592
C	-6.258286	-2.306267	-0.681034	C	-6.425966	-0.122847	0.060871	C	-1.488769	6.574314	0.094272
H	-6.308036	-0.930139	1.011405	C	-1.686893	3.470420	0.983706	H	-0.688466	6.090071	2.065337
C	-5.458867	-3.074022	-1.542136	H	-0.818415	2.891093	0.642135	C	-2.131492	6.095386	-1.058014
H	-3.436649	-3.690036	-2.082336	H	-2.275179	3.780640	0.101633	H	-2.998985	4.370563	-2.074277
H	-7.345924	-2.307420	-0.810455	H	-1.323553	4.381626	1.493106	H	-1.207178	7.631049	0.155085
H	-5.932615	-3.665293	-2.333245	C	-1.740225	2.249737	3.206178	H	-2.343980	6.784592	-1.882462
C	-2.603028	0.218597	0.561963	H	-2.358690	1.659414	3.905763	C	-0.302038	2.298586	1.284690
H	-3.351385	0.814989	0.017418	H	-0.854711	1.658829	2.930872	H	0.561097	2.937850	1.044435
C	-1.786826	-0.655613	-0.423444	H	-1.409276	3.166381	3.727906	C	-1.014218	1.838434	-0.012706
H	-2.046742	-0.507486	-1.481204	C	-3.739186	3.504723	2.402992	H	-0.531574	2.172486	-0.942370
H	4.087712	2.840283	0.621299	H	-4.343679	3.862501	1.550829	C	3.102525	2.052269	-2.174227
H	3.146658	3.165637	2.124015	H	-4.405606	2.968178	3.101438	C	6.476881	-1.181059	-0.121009
H	-0.671020	6.616985	-2.127215	H	-3.345686	4.392984	2.927571	C	2.432224	3.133962	-1.292157
H	-2.304865	2.739899	-3.213069	C	-6.889838	1.068945	-0.812473	H	1.484595	2.760622	-0.881068
				H	-7.978669	1.015159	-0.995781	H	3.096005	3.415406	-0.455120
				H	-6.676226	2.035328	-0.323647	H	2.224153	4.042056	-1.886960
				H	-6.372407	1.060942	-1.788012	C	2.185744	1.709612	-3.375857
				C	-7.174758	-0.088790	1.415721	H	2.663829	0.951492	-4.021730
				H	-6.971014	0.845522	1.967008	H	1.219188	1.318675	-3.026189
				H	-8.266574	-0.156345	1.256474	H	2.005200	2.615267	-3.983440
				H	-6.863233	-0.934048	2.053962	C	4.405492	2.652655	-2.741513
				C	-6.791578	-1.431038	-0.666135	H	5.095434	2.973894	-1.941215

H	-6.299047	-1.497416	-1.652147	H	4.938158	1.938548	-3.394324
H	-6.501179	-2.317577	-0.075727	H	4.159806	3.543216	-3.346092
H	-7.882750	-1.476196	-0.829702	C	7.190204	-0.024663	0.622096
H	-1.426428	-4.910082	-0.775772	H	8.258028	-0.264146	0.778398
H	-1.243181	-3.924805	-2.271574	H	7.134818	0.917893	0.050260
C	0.731390	-3.982611	0.574321	H	6.725132	0.149392	1.608414
H	1.559957	-3.324291	0.886897	C	7.158538	-1.407714	-1.492719
C	1.343769	-5.310895	0.108422	H	7.106525	-0.504208	-2.124654
H	2.047950	-5.151533	-0.727409	H	8.225115	-1.664605	-1.357177
H	1.897899	-5.793226	0.932133	H	6.668769	-2.232541	-2.039242
H	0.566603	-6.022707	-0.228297	C	6.627462	-2.465121	0.716830
C	-0.209900	-4.153947	1.773845	H	6.175425	-2.350772	1.717709
H	-1.067240	-4.809964	1.534251	H	6.153191	-3.330269	0.221351
H	0.328175	-4.608968	2.623598	H	7.697865	-2.699160	0.854250
H	-0.606239	-3.178793	2.104346	H	0.661745	-4.820290	0.889259
				H	0.775962	-4.085712	2.531578

Intermediate-2': In Ni catalyzed reaction energy profile for other 3 possible intermediates

Int2', L3': $\nu_{\text{lowest}} = 18.8162 \text{ cm}^{-1}$				Int2', L5': $\nu_{\text{lowest}} = 5.0839 \text{ cm}^{-1}$				Int2', L6': $\nu_{\text{lowest}} = 11.0199 \text{ cm}^{-1}$			
79				102				103			
Ni	-0.085575	0.148879	-0.185680	Ni	0.700882	-0.309870	-0.054157	Ni	-0.582351	-0.010936	0.260897
C	-0.554874	0.780381	2.533719	C	1.165878	-0.804718	-2.815199	C	-1.364696	-0.017182	3.006509
C	-2.363028	1.987270	1.445792	C	-0.386022	1.062358	-2.896587	C	0.169139	1.865120	3.010691
C	-0.152839	1.967972	3.164195	C	0.295533	-1.560209	-3.614920	C	-0.618188	-0.623631	4.028749
C	-1.903752	3.182831	2.015805	C	-1.287571	0.272644	-3.623720	C	0.952188	1.217888	3.976417
H	-3.214542	2.008361	0.761403	H	-0.664574	2.077972	-2.605487	H	0.490759	2.828647	2.608395
C	-0.820469	3.172553	2.905289	C	-0.935493	-1.026543	-4.017924	C	0.544805	-0.012338	4.513118
H	0.716947	1.932886	3.829206	H	0.582874	-2.584595	-3.875245	H	-0.949707	-1.595341	4.410668
H	-2.402767	4.123990	1.764449	H	-2.266529	0.682154	-3.892762	H	1.879355	1.687419	4.321114
H	-0.482562	4.102106	3.375445	H	-1.628636	-1.628728	-4.614850	H	1.140568	-0.499531	5.292380
N	0.642466	-0.841037	1.320886	N	2.233853	-1.281112	-0.776136	N	-2.222813	-0.803247	0.961624
C	1.657193	-2.047328	-0.446257	C	2.726189	-1.475033	1.535465	C	-2.467390	-1.403011	-1.318207
C	1.157764	-1.207211	-2.576881	C	1.110802	-0.525462	2.942432	C	-0.647438	-0.804282	-2.663978
C	2.493063	-3.078458	-0.982008	C	3.518801	-1.915110	2.644850	C	-3.149903	-2.023195	-2.413619
C	1.456572	-1.899057	0.972443	C	3.108398	-1.762146	0.175137	C	-3.024132	-1.399551	0.009235
C	1.969419	-2.190531	-3.190566	C	1.834185	-0.916962	4.094697	C	-1.242936	-1.406753	-3.797136
H	0.607946	-0.450889	-3.147741	H	0.161991	0.015747	3.005338	H	0.327963	-0.310928	-2.712494
C	2.630535	-3.117826	-2.398216	C	3.030210	-1.602425	3.945788	C	-2.487330	-2.005961	-3.672847
C	3.126465	-3.975892	-0.078741	C	4.711723	-2.643481	2.382534	C	-4.419389	-2.617494	-2.174955
C	2.094985	-2.811630	1.827032	C	4.287724	-2.496251	-0.035877	C	-4.282788	-1.991539	0.198340
H	2.064003	-2.206696	-4.280308	H	1.437804	-0.674126	5.084855	H	-0.714967	-1.386856	-4.754939
H	3.264483	-3.887768	-2.851516	H	3.607434	-1.916509	4.822331	H	-2.970873	-2.474576	-4.536912
C	2.914364	-3.831366	1.287776	C	5.067578	-2.918029	1.066687	C	-4.958787	-2.583048	-0.894377
H	3.773096	-4.767225	-0.470735	H	5.327865	-2.986872	3.219423	H	-4.952309	-3.097811	-3.001490
H	1.960212	-2.699783	2.903510	H	4.572668	-2.738225	-1.060314	H	-4.706103	-2.009181	1.203098
H	3.401529	-4.525363	1.981744	H	5.982735	-3.485952	0.866164	H	-5.937970	-3.039551	-0.712195

N	1.021395	-1.150541	-1.256354	N	1.553172	-0.796156	1.718605	N	-1.249123	-0.807218	-1.479238
C	0.379321	-0.406451	2.596017	C	2.315764	-1.503111	-2.131413	C	-2.440254	-0.819544	2.317054
O	0.901598	-0.818462	3.639380	O	3.123842	-2.238606	-2.709979	O	-3.306985	-1.470036	2.915720
O	-0.953388	1.034289	-1.626624	O	-0.743422	0.795179	0.567055	O	0.960350	0.929023	-0.387289
C	-1.172187	2.324581	-1.688834	C	-2.038812	0.580845	0.507518	C	2.228868	0.587710	-0.356826
C	-0.332359	3.322919	-1.083385	C	-2.622612	-0.579850	-0.110228	C	2.728664	-0.571790	0.332675
C	-2.299183	2.787889	-2.429677	C	-2.961185	1.537130	1.089412	C	3.210025	1.402949	-1.048511
C	-0.624059	4.700526	-1.240744	C	-4.025309	-0.716293	-0.275191	C	4.117042	-0.861882	0.404459
C	0.822512	2.917354	-0.318034	C	-1.802977	-1.703931	-0.486009	C	1.825003	-1.528268	0.917625
C	-2.569997	4.145128	-2.560243	C	-4.328761	1.332290	0.904508	C	4.555382	1.051505	-0.949134
C	-1.733405	5.118336	-1.967038	C	-4.904762	0.241061	0.206478	C	5.056519	-0.058742	-0.222422
H	0.042195	5.426808	-0.766235	H	-4.382258	-1.615841	-0.778688	H	4.411539	-1.752579	0.961280
N	1.122944	1.699233	0.048901	N	-0.504874	-1.825775	-0.374339	N	0.516258	-1.499932	0.916694
O	1.692971	3.875523	0.081109	O	-2.440975	-2.813945	-0.940488	O	2.371014	-2.635762	1.486500
H	-3.453698	4.462274	-3.126000	H	-5.011120	2.073320	1.327510	H	5.281501	1.681098	-1.468949
C	2.374663	1.715172	0.824167	C	-0.133397	-3.227625	-0.648571	C	0.013677	-2.794634	1.419979
C	2.780246	3.216839	0.781432	C	-1.420448	-3.781471	-1.293570	C	1.284307	-3.397838	2.065887
H	2.150562	1.407565	1.859301	H	0.701690	-3.256045	-1.365539	H	-0.758737	-2.629336	2.184272
C	3.404491	0.758786	0.256426	C	0.868581	0.551470	-2.507104	C	-0.586200	-3.623091	0.297487
C	3.674745	0.738652	-1.123909	C	1.426338	2.624236	0.192230	C	0.078432	-3.751679	-0.935891
C	4.084404	-0.132064	1.102504	C	2.690029	3.468208	0.083557	C	-1.822077	-4.265047	0.481459
C	4.613184	-0.158257	-1.648441	H	0.835619	2.674251	1.112471	C	-0.485927	-4.511226	-1.968174
H	3.123859	1.410213	-1.791906	O	0.662426	3.123539	-0.930106	H	1.031848	-3.237109	-1.096948
C	5.027737	-1.027828	0.579667	C	1.683672	2.939771	-1.935865	C	-2.387287	-5.026862	-0.550756
H	3.847268	-0.145142	2.172034	C	2.865398	3.658175	-1.303981	H	-2.358527	-4.136667	1.427996
C	5.292688	-1.042769	-0.796115	C	3.627941	3.942429	0.999123	C	-1.720712	-5.150358	-1.777272
H	4.806925	-0.176337	-2.726007	H	1.333238	3.298400	-2.913592	H	0.034179	-4.596442	-2.928022
H	5.538952	-1.729346	1.246156	C	3.974763	4.333736	-1.805269	H	-3.359851	-5.506403	-0.402212
H	6.018429	-1.752325	-1.207287	C	4.738145	4.652421	0.498545	H	-2.167969	-5.734265	-2.588672
C	-1.721953	0.760366	1.714696	H	3.506630	3.782805	2.076051	C	-1.017021	1.276367	2.528688
C	-2.685731	-1.019048	-1.101494	C	4.909583	4.845222	-0.881210	C	-1.173823	2.871274	-0.525938
C	-3.549615	-2.236872	-0.796562	H	4.120774	4.475796	-2.881611	C	-2.423660	3.718837	-0.727335
H	-2.370260	-0.830915	-2.133254	H	5.476621	5.063088	1.195617	H	-0.466295	2.771472	-1.353969
O	-3.531018	0.053507	-0.623706	H	5.779686	5.402720	-1.244081	O	-0.555637	3.550354	0.591848
C	-3.756413	-0.481162	0.699948	C	1.891600	1.228819	-0.278885	C	-1.705210	3.530574	1.467424
C	-4.234654	-1.889909	0.387339	H	2.854901	0.940577	0.166017	C	-2.778506	4.132396	0.574483
C	-3.689314	-3.502940	-1.363029	C	1.941757	1.408079	-1.821056	C	-3.221899	4.034734	-1.825519
H	-4.435252	0.167194	1.271031	H	2.927120	1.128639	-2.227545	H	-1.482424	4.046692	2.411575
C	-5.080147	-2.794313	1.024253	C	-2.476638	2.787385	1.851663	C	-3.931388	4.877768	0.805872
C	-4.566976	-4.412604	-0.738829	C	-6.430075	0.154888	0.042400	C	-4.374860	4.814054	-1.600601
H	-3.146232	-3.785884	-2.271380	C	-6.930958	1.399812	-0.730436	H	-2.961547	3.701312	-2.835969
C	-5.251927	-4.064661	0.435941	H	-8.029315	1.365323	-0.851069	C	-4.724813	5.229056	-0.306158
H	-5.606190	-2.533194	1.949047	H	-6.677735	2.333562	-0.198959	H	-4.216658	5.193288	1.815388
H	-4.719840	-5.404570	-1.177725	H	-6.471927	1.446100	-1.733525	H	-5.005883	5.103372	-2.447977
H	-5.930009	-4.788949	0.899902	C	-7.099092	0.113856	1.438264	H	-5.624583	5.835960	-0.158920
C	-1.571061	-1.099727	-0.032464	H	-6.855241	1.012912	2.030379	C	-1.730077	1.570213	0.097522
H	-1.142886	-2.107679	0.066949	H	-8.198890	0.062390	1.339037	H	-2.639024	1.225729	-0.416576

C	-2.295826	-0.586012	1.240056	H	-6.759358	-0.769410	2.006975	C	-1.974043	1.999910	1.571444
H	-2.216230	-1.308974	2.068376	C	-6.849638	-1.105702	-0.737550	H	-3.009372	1.788095	1.883849
H	3.707164	3.390889	0.210632	H	-6.409517	-1.119692	-1.750077	C	2.797669	2.651508	-1.850592
H	2.867186	3.671883	1.780288	H	-6.540433	-2.027617	-0.214608	C	6.569257	-0.324123	-0.176074
H	-2.953262	2.030065	-2.869002	H	-7.948364	-1.131023	-0.845651	C	7.284059	0.896821	0.453432
H	-1.957370	6.183921	-2.074832	C	-1.904853	3.796760	0.828125	H	8.376622	0.731611	0.485181
				H	-1.463937	4.668958	1.346354	H	7.097785	1.817312	-0.126586
				H	-1.136610	3.342645	0.189008	H	6.927839	1.067940	1.484300
				H	-2.715330	4.163187	0.173077	C	7.097866	-0.542442	-1.615135
				C	-1.411577	2.415778	2.911313	H	6.908259	0.337815	-2.253610
				H	-1.830375	1.705706	3.647917	H	8.188342	-0.723299	-1.603549
				H	-0.535435	1.951776	2.439569	H	6.605983	-1.413345	-2.082758
				H	-1.089052	3.322151	3.454939	C	6.904539	-1.572418	0.662145
				C	-3.625485	3.486905	2.612215	H	6.562581	-1.462406	1.706160
				H	-4.391813	3.895005	1.930684	H	6.439032	-2.480574	0.240710
				H	-4.120994	2.805945	3.327319	H	7.997419	-1.729778	0.678957
				H	-3.211033	4.336973	3.182151	C	2.257980	3.715268	-0.864755
				H	-1.737602	-4.760959	-0.903689	H	1.862878	4.589741	-1.414305
				H	-1.359880	-3.823830	-2.394104	H	1.459105	3.316094	-0.226878
				C	0.324980	-3.946674	0.644149	H	3.076969	4.064827	-0.210989
				H	1.179948	-3.357335	1.014807	C	1.735878	2.279325	-2.914429
				C	-0.751970	-3.946467	1.737355	H	2.160657	1.569538	-3.647575
				H	-1.072927	-2.917773	1.973808	H	0.858046	1.812648	-2.447274
				H	-1.645461	-4.524178	1.437007	H	1.411185	3.182953	-3.461516
				H	-0.358755	-4.400645	2.663543	C	3.984941	3.280008	-2.611133
				C	0.841695	-5.356066	0.322142	H	4.771736	3.642360	-1.926686
				H	1.646039	-5.319690	-0.433883	H	4.441902	2.571539	-3.325248
				H	1.248684	-5.836371	1.228717	H	3.621027	4.150574	-3.184608
				H	0.036286	-6.008668	-0.064320	H	1.444792	-4.459280	1.827174
								H	1.305518	-3.244560	3.158922

Insertion step by benzamide coordinated complex in two conformations

N-(quinolin-8-yl)benzamide: In Ni catalyzed reaction energy profile

Benzamide¹: $\nu_{\text{lowest}} = 25.7957 \text{ cm}^{-1}$

31

O	1.465115	2.256916	-0.074075
C	1.432210	1.025908	-0.041262
N	0.258276	0.301499	-0.032144
C	-1.052091	0.766450	-0.011886
C	-1.447312	2.104122	0.009827
C	-2.827379	2.429274	0.034283
C	-3.813813	1.454692	0.036069
C	-3.443307	0.080092	0.013515
C	-4.373024	-0.997414	0.013055

C	-3.912273	-2.303529	-0.009597
C	-2.511934	-2.537126	-0.031538
N	-1.612911	-1.562806	-0.031543
C	-2.052236	-0.272558	-0.010290
H	-2.124904	-3.564803	-0.049595
H	-4.605698	-3.150267	-0.010657
H	-5.446620	-0.778771	0.030533
H	-4.874827	1.724515	0.053962
H	-3.110921	3.487036	0.051013
H	-0.681199	2.879923	0.004937
H	0.281638	-0.724367	-0.070487
C	2.690169	0.200167	-0.018097
C	3.895677	0.875480	-0.290979
C	5.112242	0.185697	-0.286220
C	5.140286	-1.187806	0.002394
C	3.946297	-1.865819	0.289518
C	2.726388	-1.177297	0.279990
H	1.810840	-1.724729	0.530670
H	3.964753	-2.934431	0.527915
H	6.092400	-1.729078	0.008968
H	6.043219	0.718901	-0.506101
H	3.842595	1.947543	-0.502934

Intermediate-0: In Ni catalyzed reaction energy profile for other 3 possible intermediates

Int0-conf-2²: $\nu_{\text{lowest}} = 15.6090 \text{ cm}^{-1}$

60

Ni	-0.049420	0.062320	0.000960
C	-0.438576	2.147087	1.781719
C	1.892581	2.038704	1.105024
C	-0.178584	3.272844	2.579350
C	2.151639	3.163747	1.909727
H	2.711904	1.577327	0.544786
C	1.122525	3.785324	2.637904
H	-1.008027	3.716685	3.141515
H	3.172933	3.558481	1.963488
H	1.342870	4.663268	3.254545
N	-1.702094	0.399694	0.870753
C	-2.381302	-1.460898	-0.407506
C	-0.678485	-2.305490	-1.780287
C	-3.312263	-2.457269	-0.843634
C	-2.739028	-0.453141	0.552711
C	-1.527583	-3.332718	-2.253830
H	0.354475	-2.196933	-2.127699
C	-2.833802	-3.406114	-1.791136
C	-4.631149	-2.426818	-0.311690
C	-4.055875	-0.451931	1.044655

H	-1.143208	-4.051132	-2.983402
H	-3.509196	-4.190089	-2.150827
C	-4.972502	-1.436381	0.604017
H	-5.359702	-3.177970	-0.631984
H	-4.345260	0.316647	1.762140
H	-5.990596	-1.410529	1.008028
N	-1.098644	-1.407321	-0.890594
C	-1.783954	1.511483	1.701991
O	-2.800735	1.896812	2.282464
C	0.587009	1.541304	1.029068
N	0.926222	-1.318599	1.103988
C	2.099579	-1.675992	0.504056
C	0.532888	-1.887972	2.237337
C	2.950219	-2.678698	1.073988
C	2.450097	-0.981756	-0.709015
C	1.308577	-2.892340	2.863828
H	-0.416817	-1.537903	2.656073
C	2.506007	-3.283999	2.283973
C	4.169714	-2.990329	0.412386
N	1.517015	-0.045566	-1.125608
C	3.672954	-1.311838	-1.317496
H	0.954877	-3.341547	3.796217
H	3.125928	-4.056217	2.752452
C	4.504578	-2.308125	-0.751244
H	4.830547	-3.755339	0.831837
C	1.795599	0.962141	-2.030118
H	3.965854	-0.779595	-2.222346
H	5.448009	-2.541410	-1.256972
C	0.700782	1.993686	-2.069873
O	2.842956	1.084132	-2.673436
C	-0.664758	1.636257	-2.034447
C	-1.652966	2.624516	-1.899087
H	-0.959112	0.592807	-2.181565
C	0.072547	4.332938	-1.870352
C	-1.283488	3.970755	-1.794043
H	-2.708557	2.336270	-1.867773
H	0.360578	5.386904	-1.796134
H	-2.050171	4.741196	-1.662420
C	1.058906	3.351623	-2.020830
H	2.119848	3.615524	-2.061712

Intermediate-1: In Ni catalyzed reaction energy profile for other 3 possible intermediates

Int1-conf-1²: $\nu_{\text{lowest}} = 15.8930 \text{ cm}^{-1}$

79

Ni	-0.538739	-0.355588	-0.245020
C	0.282300	-0.466955	2.410267

C	-0.288936	-2.686921	1.621730
C	0.590076	-0.969813	3.682364
C	0.028902	-3.194062	2.896229
H	-0.633927	-3.380405	0.848965
C	0.463265	-2.342843	3.925993
H	0.933117	-0.267111	4.449850
H	-0.073148	-4.269414	3.083003
H	0.698813	-2.754187	4.913261
N	0.173928	1.115756	0.698890
C	-0.150641	2.171225	-1.376373
C	-1.089473	0.759787	-2.991575
C	-0.132195	3.287477	-2.272416
C	0.285388	2.285001	-0.014193
C	-1.114463	1.808283	-3.939106
H	-1.468220	-0.238624	-3.231390
C	-0.633101	3.061306	-3.584153
C	0.360342	4.530864	-1.789377
C	0.768132	3.530352	0.423818
H	-1.515833	1.617270	-4.938442
H	-0.643189	3.886861	-4.304270
C	0.799729	4.623680	-0.471900
H	0.384202	5.397439	-2.457330
H	1.089949	3.629357	1.460346
H	1.174987	5.583771	-0.100817
N	-0.610859	0.936664	-1.759427
C	0.458703	0.964763	2.052413
O	0.802824	1.866414	2.814261
C	-0.158066	-1.314462	1.375762
C	3.310882	-1.177192	0.964100
C	4.748772	-1.103791	0.415674
H	3.126145	-1.741839	1.886605
O	3.049274	0.230037	1.146118
C	3.320834	0.621797	-0.215313
C	4.754985	0.077469	-0.359230
C	5.880748	-1.899362	0.525956
H	3.153906	1.695978	-0.363951
C	5.893740	0.487556	-1.038548
C	7.049158	-1.482663	-0.155066
H	5.883174	-2.815299	1.126787
C	7.055546	-0.312078	-0.922332
H	5.906329	1.403830	-1.638821
H	7.962691	-2.081632	-0.075311
H	7.973999	-0.007065	-1.435258
C	2.419466	-1.489920	-0.253445
H	1.993565	-2.470318	-0.468641
C	2.419291	-0.363207	-0.992337
H	2.008723	-0.178969	-1.987501

N	-0.953170	-1.957749	-1.292669
C	-2.182559	-2.484306	-0.997968
C	-0.153800	-2.565974	-2.173297
C	-2.612149	-3.738578	-1.552887
C	-3.008475	-1.724952	-0.095419
C	-0.520439	-3.777699	-2.800512
H	0.807383	-2.088982	-2.382858
C	-1.732624	-4.368728	-2.477112
C	-3.865817	-4.266424	-1.149430
N	-2.535621	-0.470759	0.206161
C	-4.226252	-2.313871	0.303539
H	0.166146	-4.238580	-3.516243
H	-2.026574	-5.322670	-2.928326
C	-4.632165	-3.555916	-0.228917
H	-4.206921	-5.222314	-1.558335
C	-3.061043	0.276055	1.254407
H	-4.849078	-1.790586	1.028886
H	-5.592851	-3.968630	0.098750
C	-2.797127	1.750911	1.167256
O	-3.741333	-0.186335	2.174979
C	-2.522198	2.484462	2.335448
C	-2.348391	3.871106	2.268850
H	-2.425878	1.950934	3.285325
C	-2.812348	3.822578	-0.115312
C	-2.502851	4.543828	1.045854
H	-2.094023	4.431062	3.174711
H	-2.939118	4.344710	-1.069512
H	-2.374722	5.630508	0.997542
C	-2.940269	2.428283	-0.058590
H	-3.170290	1.850649	-0.959148

Intermediate-1: In Ni catalyzed reaction energy profile for other 3 possible intermediates

Int1-conf-2²: $\nu_{\text{lowest}} = 17.9409 \text{ cm}^{-1}$

79

Ni	-1.115477	0.009757	0.025233
C	-0.181696	-0.811964	2.498007
C	-1.529032	-2.568573	1.500633
C	0.023066	-1.587680	3.648152
C	-1.311182	-3.350952	2.651468
H	-2.148922	-2.974448	0.695633
C	-0.539964	-2.867847	3.721371
H	0.624698	-1.164403	4.460578
H	-1.759056	-4.349802	2.708372
H	-0.386739	-3.489403	4.610123
N	0.076581	1.034335	1.079880
C	-0.223072	2.575425	-0.676981

C	-1.625891	1.770550	-2.373952
C	-0.034746	3.829406	-1.343254
C	0.378482	2.292361	0.594321
C	-1.498224	2.978965	-3.096736
H	-2.238187	0.935804	-2.732922
C	-0.704000	3.997646	-2.587581
C	0.790376	4.804621	-0.718315
C	1.180562	3.284024	1.181106
H	-2.026376	3.092907	-4.047619
H	-0.588923	4.940239	-3.133933
C	1.373467	4.515668	0.511722
H	0.955653	5.767538	-1.211413
H	1.654025	3.074491	2.138978
H	2.012572	5.266284	0.989209
N	-0.998469	1.579739	-1.213871
C	0.387040	0.557137	2.350306
O	1.007545	1.172269	3.217619
C	-0.946298	-1.297587	1.417796
C	4.141282	0.201649	1.818165
C	5.262677	-0.093676	0.803820
H	4.428195	0.579212	2.808066
O	3.402990	1.197353	1.069615
C	3.166650	0.366050	-0.091297
C	4.623767	0.020495	-0.451242
C	6.609799	-0.414075	0.899996
H	2.563020	0.892155	-0.840795
C	5.326559	-0.169621	-1.633215
C	7.332249	-0.610729	-0.301181
H	7.110654	-0.503505	1.870365
C	6.703191	-0.487337	-1.544886
H	4.844971	-0.065617	-2.611489
H	8.399562	-0.853200	-0.256242
H	7.284177	-0.631638	-2.462327
C	3.170239	-0.992575	1.755866
H	3.066499	-1.768859	2.515903
C	2.559347	-0.890679	0.565108
H	1.831545	-1.559436	0.105467
N	-2.892195	0.654011	0.701611
C	-3.915255	-0.000044	0.079859
C	-3.123871	1.583118	1.622237
C	-5.282114	0.292698	0.398548
C	-3.553349	-1.005577	-0.882533
C	-4.443409	1.940280	1.987372
H	-2.246252	2.052139	2.079458
C	-5.511842	1.299223	1.378836
C	-6.304595	-0.438162	-0.264909
N	-2.186428	-1.140195	-1.112664

C	-4.599656	-1.714965	-1.495764
H	-4.599631	2.711585	2.746784
H	-6.542379	1.553485	1.649669
C	-5.948156	-1.416282	-1.184721
H	-7.354009	-0.228169	-0.035946
C	-1.655734	-2.288968	-1.664660
H	-4.356976	-2.505430	-2.204644
H	-6.732776	-1.988894	-1.691244
C	-0.166067	-2.270457	-1.874449
O	-2.303354	-3.298510	-1.968217
C	0.496038	-1.169849	-2.452948
C	1.859560	-1.252596	-2.771522
H	-0.067873	-0.267416	-2.696817
C	1.927567	-3.515020	-1.894723
C	2.580762	-2.419031	-2.483873
H	2.356795	-0.401155	-3.248130
H	2.490174	-4.425634	-1.664241
H	3.649652	-2.475533	-2.711206
C	0.559876	-3.449135	-1.610430
H	0.028975	-4.306209	-1.186081

Transition State (1-2): In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

TS1-conf-1 ² : $\nu_{\text{lowest}} = -210.3720 \text{ cm}^{-1}$				TS1-conf-1 ⁴ : $\nu_{\text{lowest}} = -200.8462 \text{ cm}^{-1}$			
79				79			
Ni	-0.093881	0.329732	-0.252991	Ni	-0.101476	0.349550	-0.305876
C	-0.146474	0.232726	2.553075	C	-0.195291	0.345804	2.539841
C	-1.041910	2.375890	1.813133	C	-1.142011	2.456133	1.805126
C	-0.135413	0.693029	3.878237	C	-0.083179	0.847478	3.848412
C	-1.009770	2.831880	3.139924	C	-0.994704	2.967200	3.102875
H	-1.403705	3.043263	1.023871	H	-1.581483	3.092682	1.025414
C	-0.571110	1.989144	4.175485	C	-0.482551	2.157004	4.132185
H	0.252568	0.014479	4.645957	H	0.350230	0.195279	4.614156
H	-1.334317	3.854430	3.362582	H	-1.289977	4.001187	3.316353
H	-0.552913	2.354492	5.207517	H	-0.382205	2.556948	5.146605
N	0.541230	-1.190447	0.828939	N	0.483984	-1.153059	0.831656
C	1.114173	-2.000312	-1.299370	C	1.038115	-2.146685	-1.236132
C	0.728324	-0.471073	-3.033088	C	0.747054	-0.773789	-3.099584
C	1.664923	-2.970117	-2.200804	C	1.496349	-3.236709	-2.042101
C	1.054667	-2.237678	0.120587	C	0.964653	-2.260889	0.205693
C	1.274463	-1.361025	-3.986532	C	1.188842	-1.791659	-3.974327
H	0.354310	0.517781	-3.315745	H	0.451819	0.213350	-3.473718
C	1.728055	-2.605791	-3.574304	C	1.557851	-3.022187	-3.446463
C	2.133823	-4.200645	-1.666656	C	1.889540	-4.445626	-1.398862
C	1.534018	-3.468776	0.604938	C	1.378841	-3.475680	0.796271
H	1.328613	-1.054951	-5.035271	H	1.239856	-1.597129	-5.049808
H	2.148666	-3.313783	-4.296936	H	1.905730	-3.830719	-4.098735

C	2.056258	-4.424020	-0.294434	C	1.824808	-4.541809	-0.011626
H	2.559435	-4.951358	-2.339824	H	2.250117	-5.282273	-2.006054
H	1.506414	-3.645505	1.680487	H	1.344018	-3.554764	1.882798
H	2.426596	-5.371202	0.113376	H	2.136394	-5.471516	0.476621
N	0.646441	-0.791080	-1.742725	N	0.672777	-0.950730	-1.780969
C	0.433400	-1.099382	2.197303	C	0.360542	-1.000166	2.215107
O	0.807154	-1.939178	3.021879	O	0.726937	-1.818282	3.062548
C	-0.620969	1.070353	1.518415	C	-0.743144	1.143679	1.504536
C	-3.005361	-0.586448	1.468996	C	-2.953524	-0.528964	1.395644
C	-4.269697	-1.156162	0.805166	C	-4.300288	-0.968529	0.815972
H	-3.080452	-0.148530	2.471462	H	-2.929959	-0.131334	2.416947
O	-2.160001	-1.745811	1.461484	O	-2.206203	-1.754662	1.295487
C	-2.248691	-2.031185	0.053705	C	-2.430137	-1.984370	-0.113193
C	-3.774554	-2.109277	-0.114595	C	-3.961957	-1.936992	-0.158351
C	-5.631432	-0.903063	0.919663	C	-5.619680	-0.592484	1.034088
H	-1.641589	-2.904272	-0.214333	H	-1.923359	-2.901340	-0.443863
C	-4.632550	-2.827114	-0.938968	C	-4.943672	-2.546339	-0.933412
C	-6.510643	-1.645732	0.099134	C	-6.623289	-1.222859	0.263012
H	-6.020382	-0.164141	1.628333	H	-5.883835	0.159357	1.785809
C	-6.020420	-2.589781	-0.812750	C	-6.289402	-2.181672	-0.702989
H	-4.256136	-3.563975	-1.656585	H	-4.692455	-3.294887	-1.692922
H	-7.590763	-1.484543	0.181024	H	-7.674651	-0.963223	0.426756
H	-6.723109	-3.155728	-1.433527	H	-7.084929	-2.661305	-1.283763
C	-2.365801	0.269025	0.361770	C	-2.288685	0.319574	0.279469
H	-2.735744	1.265551	0.116808	H	-2.696255	1.309618	0.051721
C	-1.895381	-0.668879	-0.581067	C	-2.007044	-0.643302	-0.733547
H	-1.966661	-0.546358	-1.665056	H	-2.150672	-0.468489	-1.803532
N	-0.683744	1.981078	-1.440794	N	-0.518837	2.027692	-1.494775
C	0.117901	3.059953	-1.187684	C	0.342284	3.061479	-1.255013
C	-1.748615	2.122994	-2.232789	C	-1.580644	2.236049	-2.280045
C	-0.185402	4.366751	-1.712851	C	0.126982	4.373094	-1.795817
C	1.273601	2.831366	-0.356300	C	1.483532	2.784547	-0.407531
C	-2.103617	3.358516	-2.820139	C	-1.856400	3.484635	-2.879899
H	-2.361461	1.231958	-2.408633	H	-2.249870	1.384334	-2.438825
C	-1.330155	4.476106	-2.550020	C	-1.008401	4.553018	-2.633683
C	0.649160	5.460213	-1.368400	C	1.034214	5.416776	-1.462526
N	1.549914	1.522069	-0.053580	N	1.656945	1.487550	-0.049930
C	2.047548	3.961430	-0.015208	C	2.336573	3.868482	-0.083453
H	-2.985166	3.414924	-3.465369	H	-2.737555	3.590653	-3.519398
H	-1.589843	5.452730	-2.973256	H	-1.202562	5.538595	-3.070474
C	1.734645	5.237095	-0.525269	C	2.107618	5.150023	-0.613493
H	0.422687	6.457619	-1.757399	H	0.869382	6.419932	-1.867924
C	2.485489	1.216436	0.943938	C	2.546108	1.139867	0.977232
H	2.897082	3.835113	0.656228	H	3.175394	3.693851	0.592289
H	2.374356	6.079541	-0.239182	H	2.796020	5.959164	-0.346506
C	3.263452	-0.044875	0.729758	C	3.304812	-0.129009	0.748411
O	2.714118	1.934318	1.919804	O	2.683733	1.798155	2.009918

C	3.740918	-0.759702	1.844417	C	3.764924	-0.861662	1.858920
C	4.526267	-1.901733	1.660662	C	4.490749	-2.041121	1.666601
H	3.465122	-0.417588	2.845451	H	3.518423	-0.501336	2.861378
C	4.438468	-1.584786	-0.747041	C	4.365244	-1.734650	-0.742445
C	4.882117	-2.312815	0.365076	C	4.793635	-2.478770	0.366255
H	4.865112	-2.475157	2.529899	H	4.820212	-2.625711	2.531983
H	4.719286	-1.899130	-1.757735	H	4.606054	-2.070793	-1.756472
H	5.501228	-3.205272	0.223633	H	5.361691	-3.403433	0.217852
C	3.620153	-0.461436	-0.566528	C	3.616211	-0.566272	-0.552587
H	3.259240	0.114537	-1.423765	H	3.263069	0.018172	-1.407085

Transition State (1-2): In Ni catalyzed reaction energy profile for other 3 possible intermediate conformations

TS1-conf-2 ² : $\nu_{\text{lowest}} = -133.9145 \text{ cm}^{-1}$				TS1-conf-2 ⁴ : $\nu_{\text{lowest}} = -204.5301 \text{ cm}^{-1}$				TS1-conf-2 ⁶ : $\nu_{\text{lowest}} = -228.6372 \text{ cm}^{-1}$			
79				79				79			
Ni	-0.623717	0.139398	0.049418	Ni	-0.554116	0.106247	0.007707	Ni	-0.570141	0.129884	0.008102
C	-0.956465	0.568833	2.798838	C	-0.933005	0.519072	2.817203	C	-0.947092	0.804550	2.776617
C	-1.018117	-1.827358	2.304813	C	-0.862099	-1.880799	2.426889	C	-0.948512	-1.621050	2.605584
C	-1.332983	0.310435	4.126714	C	-1.447741	0.302146	4.108418	C	-1.483629	0.719395	4.077288
C	-1.410834	-2.067538	3.632814	C	-1.413769	-2.090215	3.699914	C	-1.519932	-1.698770	3.883920
H	-0.875627	-2.667144	1.612813	H	-0.622139	-2.742190	1.789958	H	-0.724653	-2.542841	2.052813
C	-1.556706	-1.007181	4.545392	C	-1.689362	-1.002878	4.550988	C	-1.770222	-0.530534	4.631552
H	-1.463935	1.168452	4.795772	H	-1.670995	1.176535	4.729670	H	-1.692269	1.652330	4.612287
H	-1.595113	-3.098591	3.955010	H	-1.620114	-3.112952	4.036525	H	-1.761014	-2.680315	4.308461
H	-1.854781	-1.213101	5.578984	H	-2.099024	-1.178977	5.551444	H	-2.198108	-0.603186	5.637084
N	-0.697614	1.923037	0.910096	N	-0.665720	1.886344	0.900476	N	-0.589864	1.981470	0.743134
C	-0.595641	2.610179	-1.331319	C	-0.574228	2.705254	-1.313170	C	-0.465557	2.585288	-1.523788
C	-0.804179	0.840293	-2.854711	C	-0.743038	1.077399	-2.972032	C	-0.806312	0.845884	-3.047907
C	-0.566236	3.587062	-2.378877	C	-0.468591	3.757284	-2.277721	C	-0.324404	3.545787	-2.574503
C	-0.585509	2.987835	0.059501	C	-0.589593	2.990789	0.107844	C	-0.422817	2.997363	-0.137278
C	-0.808687	1.738464	-3.947529	C	-0.645616	2.046247	-3.996295	C	-0.682550	1.712588	-4.137745
H	-0.910266	-0.242514	-2.972082	H	-0.878575	0.014598	-3.196216	H	-1.041775	-0.214383	-3.180996
C	-0.667786	3.098273	-3.712754	C	-0.496541	3.382288	-3.650880	C	-0.424007	3.073995	-3.912874
C	-0.464641	4.959642	-2.019452	C	-0.365234	5.101246	-1.816009	C	-0.100585	4.908117	-2.213705
C	-0.492744	4.358056	0.369002	C	-0.506033	4.343911	0.514241	C	-0.199257	4.378561	0.172346
H	-0.916773	1.345587	-4.962660	H	-0.695829	1.733006	-5.043483	H	-0.798248	1.322206	-5.153494
H	-0.651736	3.809900	-4.545623	H	-0.415005	4.156823	-4.421195	H	-0.320565	3.775620	-4.746632
C	-0.424353	5.311972	-0.672711	C	-0.385294	5.366773	-0.448100	C	-0.036556	5.299857	-0.863241
H	-0.433398	5.720975	-2.805043	H	-0.282983	5.913261	-2.545784	H	0.022490	5.650954	-3.009328
H	-0.491768	4.653273	1.419283	H	-0.531928	4.561812	1.582243	H	-0.162133	4.671379	1.221638
H	-0.350398	6.370947	-0.400884	H	-0.309302	6.403292	-0.101975	H	0.142744	6.352009	-0.619072
N	-0.672559	1.268318	-1.602021	N	-0.688904	1.396970	-1.680331	N	-0.669391	1.261277	-1.767807
C	-0.818741	1.967803	2.282139	C	-0.806877	1.908876	2.293211	C	-0.784256	2.131800	2.136426
O	-0.884203	2.983318	2.980757	O	-0.915571	2.923256	2.985990	O	-0.902721	3.213203	2.715031
C	-0.779014	-0.506139	1.900457	C	-0.617131	-0.573026	1.971673	C	-0.649914	-0.369683	2.038356
C	2.121738	0.034575	2.204184	C	2.075906	0.122076	2.171751	C	2.048838	0.295884	2.199456
C	3.583024	-0.116069	1.743620	C	3.540637	-0.125207	1.801369	C	3.511169	-0.016601	1.875342

H	1.855081	-0.233144	3.233395	H	1.756302	-0.067001	3.203314	H	1.717837	0.234586	3.243000
O	1.901976	1.428158	1.944135	O	1.934015	1.510727	1.827461	O	1.937003	1.640237	1.695275
C	2.295815	1.419684	0.559704	C	2.414253	1.405872	0.467593	C	2.425062	1.368587	0.359504
C	3.698741	0.797591	0.671422	C	3.769884	0.729595	0.698184	C	3.764785	0.699691	0.682330
C	4.641808	-0.937937	2.109766	C	4.519816	-1.000619	2.254346	C	4.471023	-0.848829	2.437980
H	2.192784	2.414283	0.109301	H	2.392602	2.385626	-0.028760	H	2.427601	2.285229	-0.246147
C	4.875674	0.905833	-0.057932	C	4.989205	0.722063	0.028151	C	4.989156	0.593142	0.029942
C	5.851085	-0.813561	1.388464	C	5.768719	-0.995915	1.591682	C	5.724688	-0.943248	1.791540
H	4.553855	-1.655354	2.932488	H	4.340121	-1.672260	3.100871	H	4.272599	-1.413143	3.355671
C	5.965214	0.090627	0.324468	C	5.997013	-0.149104	0.498137	C	5.976643	-0.234936	0.608331
H	4.966569	1.598318	-0.901267	H	5.171422	1.368510	-0.837102	H	5.189927	1.131170	-0.902773
H	6.710805	-1.432853	1.665656	H	6.567933	-1.659671	1.938593	H	6.508974	-1.575383	2.221522
H	6.912570	0.166464	-0.219841	H	6.973643	-0.161453	0.001730	H	6.956607	-0.322515	0.126314
C	1.344260	-0.631559	1.059292	C	1.282029	-0.565223	1.030127	C	1.247409	-0.500958	1.138617
H	1.248164	-1.714126	0.992984	H	1.310333	-1.656324	0.983456	H	1.259453	-1.591683	1.211870
C	1.468601	0.255029	-0.018878	C	1.562247	0.263247	-0.104978	C	1.552029	0.187217	-0.085079
H	1.587713	-0.053484	-1.058583	H	1.800848	-0.137730	-1.090583	H	1.803211	-0.335415	-1.008112
N	-2.623378	-0.073555	-0.043258	N	-2.662392	-0.065524	-0.099913	N	-2.642517	-0.020722	-0.081139
C	-3.050892	-1.293238	-0.480903	C	-3.090108	-1.288421	-0.510106	C	-3.093817	-1.255823	-0.416101
C	-3.489918	0.859039	0.341481	C	-3.542916	0.852950	0.290767	C	-3.537688	0.945068	0.241221
C	-4.451914	-1.616640	-0.510250	C	-4.482434	-1.633798	-0.530519	C	-4.487988	-1.582540	-0.442069
C	-2.046505	-2.238766	-0.884491	C	-2.075917	-2.237834	-0.905460	C	-2.098293	-2.253313	-0.716543
C	-4.885089	0.634588	0.307788	C	-4.934532	0.605005	0.303050	C	-4.914229	0.713840	0.247702
H	-3.063231	1.801385	0.696320	H	-3.131975	1.817448	0.605990	H	-3.119112	1.924468	0.490812
C	-5.360246	-0.598330	-0.107210	C	-5.402047	-0.634309	-0.106133	C	-5.407252	-0.555598	-0.099210
C	-4.849922	-2.914917	-0.922630	C	-4.865576	-2.937017	-0.950907	C	-4.863251	-2.916576	-0.780440
N	-0.735068	-1.788168	-0.963392	N	-0.770850	-1.806473	-0.913522	N	-0.798160	-1.845566	-0.709427
C	-2.497518	-3.520393	-1.253983	C	-2.514595	-3.522034	-1.303692	C	-2.530510	-3.584484	-1.037208
H	-5.562852	1.432212	0.624569	H	-5.619611	1.391814	0.631998	H	-5.594569	1.526470	0.518834
H	-6.435462	-0.807797	-0.124005	H	-6.474214	-0.859103	-0.106044	H	-6.481710	-0.764157	-0.100582
C	-3.872032	-3.837959	-1.275748	C	-3.882963	-3.850234	-1.326051	C	-3.888477	-3.890897	-1.071205
H	-5.913431	-3.171617	-0.947723	H	-5.925811	-3.208639	-0.965419	H	-5.926437	-3.179068	-0.796286
C	0.268637	-2.739439	-0.857677	C	0.236660	-2.775365	-0.852712	C	0.212988	-2.829215	-0.605976
H	-1.765957	-4.281925	-1.529204	H	-1.775268	-4.272901	-1.588379	H	-1.782972	-4.351277	-1.249667
H	-4.167868	-4.846918	-1.583797	H	-4.174821	-4.856536	-1.645282	H	-4.203672	-4.908006	-1.325237
C	1.568530	-2.430394	-1.552567	C	1.492661	-2.477297	-1.614101	C	1.411793	-2.660259	-1.468769
O	0.182666	-3.792072	-0.201026	O	0.159654	-3.803965	-0.167570	O	0.141178	-3.734438	0.235318
C	1.621707	-1.723137	-2.767083	C	1.468848	-1.797965	-2.845107	C	1.344184	-2.021145	-2.722101
C	2.855139	-1.425129	-3.363798	C	2.665011	-1.498655	-3.510319	C	2.505313	-1.836984	-3.481931
H	0.688383	-1.410245	-3.239428	H	0.506125	-1.503729	-3.269677	H	0.379737	-1.662768	-3.087488
C	4.001955	-2.559249	-1.546861	C	3.922153	-2.561296	-1.719575	C	3.812571	-2.936658	-1.747998
C	4.047919	-1.823573	-2.742707	C	3.893475	-1.860550	-2.936622	C	3.742580	-2.280088	-2.988908
H	2.885084	-0.875266	-4.310785	H	2.640595	-0.970857	-4.469779	H	2.447469	-1.336725	-4.454306
H	4.931123	-2.872982	-1.060873	H	4.879865	-2.837778	-1.267914	H	4.778810	-3.274635	-1.360245
H	5.013464	-1.569056	-3.192660	H	4.830846	-1.599675	-3.439457	H	4.654639	-2.115572	-3.572479
C	2.769533	-2.880416	-0.970052	C	2.726146	-2.890971	-1.075094	C	2.650842	-3.143843	-1.000071
H	2.711633	-3.462831	-0.045129	H	2.725943	-3.439385	-0.128282	H	2.681150	-3.646808	-0.029033

Intermediate-2: In Ni catalyzed reaction energy profile for other 3 possible intermediates

Int2-conf-1²: $\nu_{\text{lowest}} = 17.5266 \text{ cm}^{-1}$

79

Ni	-0.073544	-0.243160	0.500559
C	-0.706004	-0.779608	-2.234632
C	-2.961172	-1.373740	-1.540651
C	-0.652150	-1.985446	-2.961680
C	-2.873923	-2.590026	-2.224159
H	-3.880419	-1.122257	-0.999016
C	-1.715463	-2.891351	-2.952195
H	0.267501	-2.213200	-3.505735
H	-3.708630	-3.297493	-2.187998
H	-1.628771	-3.838808	-3.493061
N	0.979517	0.355349	-0.956246
C	2.177084	1.387373	0.798393
C	1.331321	0.929825	2.934297
C	3.222397	2.214697	1.325304
C	2.042429	1.155615	-0.616201
C	2.344379	1.708375	3.541163
H	0.572008	0.409956	3.528839
C	3.276892	2.352564	2.740250
C	4.134153	2.815932	0.416711
C	2.964697	1.770820	-1.478465
H	2.375540	1.795141	4.631177
H	4.065785	2.967293	3.187335
C	3.987598	2.588444	-0.948112
H	4.943617	3.443244	0.802772
H	2.869455	1.592815	-2.549528
H	4.693026	3.051743	-1.646517
N	1.257714	0.784940	1.612956
C	0.579745	0.020731	-2.229817
O	1.236446	0.212271	-3.254978
C	-1.900122	-0.443097	-1.529772
C	-2.122683	2.109013	-1.884236
C	-2.731653	3.303475	-1.168982
H	-2.455585	1.881483	-2.905202
O	-0.723086	2.440239	-1.866693
C	-0.614310	2.683289	-0.449531
C	-1.747222	3.680493	-0.231056
C	-3.961310	3.954530	-1.224112
H	0.399948	3.007998	-0.187713
C	-1.973862	4.713785	0.676322
C	-4.183561	5.023270	-0.330675
H	-4.733028	3.660852	-1.944008
C	-3.205536	5.396495	0.604504

H	-1.217563	5.003086	1.414382
H	-5.129697	5.573686	-0.370185
H	-3.400214	6.234417	1.282666
C	-2.181373	0.903802	-0.870169
H	-3.184523	0.835813	-0.418936
C	-1.146185	1.371557	0.185858
H	-1.584964	1.576281	1.173517
N	-1.457805	-1.005483	1.689256
C	-1.636905	-2.339892	1.413425
C	-2.298154	-0.383235	2.519509
C	-2.769618	-3.063733	1.917563
C	-0.630518	-2.970101	0.601777
C	-3.408926	-1.034521	3.097913
H	-2.104785	0.675464	2.719743
C	-3.656667	-2.360850	2.777756
C	-2.933824	-4.422376	1.538419
N	0.463097	-2.171493	0.326283
C	-0.842484	-4.317833	0.249920
H	-4.065472	-0.476572	3.771395
H	-4.529001	-2.881692	3.187474
C	-1.979683	-5.012525	0.715969
H	-3.802129	-4.981972	1.899589
C	1.499811	-2.624628	-0.475878
H	-0.117679	-4.805414	-0.400709
H	-2.104150	-6.059147	0.416308
C	2.806349	-1.912067	-0.292731
O	1.417883	-3.560663	-1.282516
C	3.647811	-1.722894	-1.404927
C	4.888072	-1.096744	-1.247846
H	3.299305	-2.047652	-2.389195
C	4.502698	-0.918807	1.143939
C	5.319047	-0.693190	0.027015
H	5.523662	-0.918816	-2.121791
H	4.840356	-0.617887	2.141567
H	6.291199	-0.203639	0.148206
C	3.245866	-1.517923	0.983406
H	2.594562	-1.691200	1.845223

Intermediate-2: In Ni catalyzed reaction energy profile for other 3 possible intermediates

Int2-conf-2²: $\nu_{\text{lowest}} = 17.8617 \text{ cm}^{-1}$

79

Ni	0.524715	0.328346	0.340323
C	1.474219	-0.132095	-2.305530
C	1.318334	-2.514096	-1.853119
C	2.809625	-0.327892	-2.713227
C	2.659718	-2.684784	-2.207093

H	0.740558	-3.373154	-1.499108
C	3.410950	-1.587325	-2.651739
H	3.370452	0.547266	-3.055803
H	3.116823	-3.676609	-2.132847
H	4.459988	-1.711483	-2.939764
N	0.546659	1.664346	-1.038102
C	-0.321437	3.009870	0.693535
C	-0.435716	1.943197	2.767946
C	-0.834774	4.237147	1.230039
C	0.059075	2.899532	-0.690355
C	-0.934580	3.114103	3.385175
H	-0.260143	1.031483	3.342106
C	-1.145410	4.249607	2.618894
C	-0.986219	5.350718	0.359462
C	-0.103634	4.026408	-1.516021
H	-1.150478	3.102794	4.457442
H	-1.541598	5.165441	3.070932
C	-0.626011	5.224752	-0.978628
H	-1.377057	6.293231	0.755295
H	0.188257	3.946684	-2.563279
H	-0.744248	6.083711	-1.648311
N	-0.157278	1.891445	1.467368
C	1.024145	1.309149	-2.278325
O	1.226860	2.080671	-3.218052
C	0.695050	-1.247125	-1.882125
C	-1.712361	-0.700630	-2.707616
C	-3.137555	-1.020636	-2.283926
H	-1.387945	-0.983162	-3.717609
O	-1.668776	0.728412	-2.540299
C	-2.147460	0.763497	-1.180067
C	-3.425354	-0.062318	-1.289272
C	-4.046563	-2.028136	-2.597030
H	-2.240156	1.797179	-0.824565
C	-4.625079	-0.094330	-0.581637
C	-5.279157	-2.042377	-1.911116
H	-3.823631	-2.784801	-3.357138
C	-5.563459	-1.090069	-0.919822
H	-4.840217	0.628916	0.212038
H	-6.025807	-2.805350	-2.156495
H	-6.528041	-1.122680	-0.401651
C	-0.791705	-1.198883	-1.532252
H	-1.079191	-2.219808	-1.237502
C	-1.189798	-0.187941	-0.422193
H	-1.691929	-0.637603	0.440833
N	2.473497	0.567197	0.687244
C	3.079823	-0.632819	0.928969
C	3.197571	1.657477	0.443785

C	4.508121	-0.762211	0.906933
C	2.211364	-1.748797	1.183179
C	4.609550	1.622341	0.420916
H	2.642339	2.577972	0.237245
C	5.258208	0.416758	0.643017
C	5.081224	-2.041625	1.135706
N	0.843534	-1.456772	1.234006
C	2.830777	-2.990745	1.410908
H	5.167307	2.540686	0.217068
H	6.351781	0.357102	0.615094
C	4.239131	-3.116636	1.387296
H	6.168736	-2.161227	1.107389
C	-0.057827	-2.512688	1.308894
H	2.212208	-3.870849	1.578886
H	4.669846	-4.108168	1.565616
C	-1.399210	-2.210199	1.912686
O	0.168506	-3.671263	0.928522
C	-1.530151	-1.333719	3.002845
C	-2.789692	-1.078470	3.560838
H	-0.625031	-0.877646	3.412534
C	-3.800585	-2.600069	1.956096
C	-3.929212	-1.697373	3.025009
H	-2.884609	-0.398369	4.414558
H	-4.687909	-3.086338	1.538948
H	-4.917480	-1.485795	3.447341
C	-2.539652	-2.872299	1.416718
H	-2.418149	-3.578796	0.590210

Effect of the Oxa-Bridge of the Alkene on the Insertion Step

CH₂ bridged alkene: In Ni catalyzed reaction energy profile for migratory insertion step

Int1 ² : $\nu_{\text{lowest}} = 10.8067 \text{ cm}^{-1}$				TS1 ² : $\nu_{\text{lowest}} = -210.9064 \text{ cm}^{-1}$				Int1 ² : $\nu_{\text{lowest}} = 10.1123 \text{ cm}^{-1}$			
111				111				111			
Ni	-0.471022	-0.129242	0.319212	Ni	-0.656647	0.258778	0.161096	Ni	-0.564000	0.040285	0.087213
C	-0.908800	-0.459495	3.039458	C	-1.209433	0.071480	2.902756	C	-1.355927	0.040330	2.902756
C	0.864006	1.157329	2.644100	C	1.134218	0.673843	2.613147	C	0.288734	1.757411	3.372137
C	-0.733688	-0.347066	4.428437	C	-0.975356	-0.175637	4.266611	C	-0.911500	-0.645518	4.051627
C	1.035162	1.269588	4.037203	C	1.362978	0.393696	3.968861	C	0.762476	1.038527	4.473934
H	1.496420	1.745248	1.972413	H	1.965540	1.006384	1.982260	H	0.752505	2.717097	3.118405
C	0.244215	0.521814	4.927702	C	0.305202	-0.006897	4.805537	C	0.142820	-0.166452	4.832822
H	-1.371170	-0.949842	5.085259	H	-1.819842	-0.535638	4.864978	H	-1.419525	-1.581759	4.303881

H	1.800041	1.950652	4.428202	H	2.375034	0.501095	4.374768	H	1.601358	1.429204	5.059514
H	0.395543	0.621074	6.007877	H	0.489437	-0.205534	5.866530	H	0.482522	-0.730287	5.708006
N	-1.826846	-1.264612	1.045977	N	-2.438026	-0.207656	0.928512	N	-2.194489	-0.683236	0.771985
C	-2.151047	-1.777395	-1.230786	C	-2.952944	-0.499215	-1.344072	C	-2.566197	-1.070102	-1.531896
C	-0.707000	-0.602071	-2.649221	C	-1.111355	-0.216425	-2.765175	C	-0.779152	-0.409602	-2.893413
C	-2.755195	-2.478233	-2.321238	C	-3.818008	-0.834394	-2.433814	C	-3.332408	-1.525678	-2.651198
C	-2.540801	-2.013484	0.130891	C	-3.421016	-0.496236	0.018545	C	-3.066937	-1.159770	-0.186126
C	-1.242547	-1.252821	-3.784687	C	-1.892049	-0.548752	-3.896356	C	-1.457265	-0.852990	-4.053409
H	0.094480	0.140591	-2.719978	H	-0.048363	0.038726	-2.827684	H	0.216461	0.043839	-2.936375
C	-2.259939	-2.182202	-3.621796	C	-3.236109	-0.849828	-3.732097	C	-2.725048	-1.403427	-3.932583
C	-3.789356	-3.411435	-2.033113	C	-5.178697	-1.137848	-2.148792	C	-4.627772	-2.061721	-2.412153
C	-3.570653	-2.936992	0.372896	C	-4.773035	-0.797980	0.253785	C	-4.354030	-1.686618	0.003827
H	-0.845541	-1.015169	-4.775812	H	-1.423671	-0.561963	-4.884724	H	-0.974904	-0.749319	-5.029767
H	-2.687999	-2.698983	-4.487628	H	-3.860451	-1.107686	-4.594594	H	-3.271190	-1.747004	-4.817876
C	-4.175463	-3.614381	-0.713009	C	-5.625760	-1.107050	-0.832029	C	-5.110306	-2.122636	-1.109919
H	-4.265745	-3.957672	-2.853038	H	-5.854049	-1.398348	-2.969719	H	-5.226798	-2.418994	-3.255633
H	-3.878199	-3.120720	1.402624	H	-5.131571	-0.810209	1.284130	H	-4.739139	-1.770638	1.020184
H	-4.974888	-4.330934	-0.493782	H	-6.674611	-1.341878	-0.618307	H	-6.110398	-2.531329	-0.927747
N	-1.157636	-0.855785	-1.423863	N	-1.635391	-0.191959	-1.543458	N	-1.325190	-0.523385	-1.686824
C	-1.910951	-1.375836	2.423962	C	-2.535200	-0.282350	2.291835	C	-2.422416	-0.689723	2.119486
O	-2.673217	-2.126716	3.041955	O	-3.525470	-0.631140	2.953513	O	-3.341171	-1.295291	2.693391
O	0.686975	1.171596	-0.482739	O	1.059672	0.727028	-0.862380	O	0.987565	1.016181	-0.434345
C	1.999921	1.232449	-0.493047	C	2.252076	0.216715	-0.731582	C	2.257022	0.697662	-0.442292
C	2.849853	0.148076	-0.078986	C	2.483537	-1.055565	-0.098923	C	2.761190	-0.571131	-0.001239
C	2.647833	2.442861	-0.947175	C	3.411408	0.917460	-1.246785	C	3.213522	1.673405	-0.914950
C	4.262079	0.274717	-0.080243	C	3.794573	-1.568852	0.077938	C	4.150205	-0.860738	-0.028546
C	2.292920	-1.114157	0.354925	C	1.374631	-1.865478	0.347718	C	1.857061	-1.585341	0.484691
C	4.042096	2.493523	-0.938191	C	4.670462	0.354974	-1.041844	C	4.562249	1.323235	-0.920760
C	4.886533	1.439422	-0.505862	C	4.909006	-0.875557	-0.373507	C	5.072583	0.069895	-0.486932
H	4.837645	-0.585972	0.264296	H	3.889421	-2.531899	0.582281	H	4.461965	-1.844580	0.326106
N	1.029857	-1.436003	0.424461	N	0.103570	-1.548142	0.393527	N	0.552475	-1.502840	0.592807
O	3.147666	-2.096823	0.729298	O	1.654183	-3.123280	0.766720	O	2.389416	-2.768869	0.870908
H	4.519561	3.414998	-1.280638	H	5.540426	0.898366	-1.419952	H	5.281020	2.063894	-1.280978
C	0.896852	-2.828392	0.860620	C	-0.673360	-2.702755	0.863547	C	0.029115	-2.810347	1.020249
C	2.336659	-3.137146	1.402091	C	0.442949	-3.647260	1.428944	C	1.319382	-3.536953	1.538302
H	0.182122	-2.884586	1.697533	H	-1.321982	-2.392212	1.697040	H	-0.669519	-2.672164	1.860802
C	0.379027	-3.699123	-0.269205	C	-1.552470	-3.263893	-0.237016	C	-0.715604	-3.490490	-0.112617
C	0.852843	-3.533184	-1.583597	C	-1.070656	-3.395433	-1.552059	C	-0.188633	-3.504839	-1.417762
C	-0.602460	-4.671456	-0.014159	C	-2.872943	-3.648779	0.049597	C	-1.955147	-4.104220	0.129723
C	0.360687	-4.334513	-2.621481	C	-1.894478	-3.909891	-2.560968	C	-0.886669	-4.128700	-2.458546
H	1.597196	-2.758748	-1.795729	H	-0.051298	-3.072212	-1.787724	H	0.764079	-3.005331	-1.622644
C	-1.098671	-5.472067	-1.052171	C	-3.699721	-4.162164	-0.959199	C	-2.657222	-4.727753	-0.911364
H	-1.000198	-4.781058	1.000755	H	-3.264112	-3.513003	1.064001	H	-2.390145	-4.057622	1.134327
C	-0.615761	-5.306940	-2.357538	C	-3.211228	-4.295267	-2.266084	C	-2.124117	-4.741744	-2.206961
H	0.732530	-4.192148	-3.641573	H	-1.511545	-4.000180	-3.582901	H	-0.470947	-4.125597	-3.471473
H	-1.876923	-6.212767	-0.842919	H	-4.733061	-4.438657	-0.727141	H	-3.633085	-5.182140	-0.713278
H	-1.009913	-5.925130	-3.171110	H	-3.859978	-4.685298	-3.057567	H	-2.678398	-5.216218	-3.023531

C	-0.115748	0.289684	2.147275	C	-0.158388	0.543523	2.075798	C	-0.779990	1.302539	2.567324
C	-3.524031	2.119391	1.362580	C	-1.215106	3.275439	1.860508	C	-2.653301	2.985175	1.812327
C	-4.212696	3.358821	0.764551	C	-1.148140	4.608860	1.098849	C	-2.714874	4.145439	0.832671
H	-3.581834	2.003819	2.453690	H	-0.932486	3.292079	2.921534	H	-2.804019	3.228360	2.874324
C	-3.745937	1.708032	-0.859346	C	-2.432955	2.985875	-0.043610	C	-2.970582	2.064687	-0.244707
C	-4.352256	3.102157	-0.620732	C	-1.911128	4.432541	-0.083230	C	-2.916012	3.575917	-0.448781
C	-4.643878	4.560842	1.316324	C	-0.478272	5.803020	1.347651	C	-2.533910	5.519961	0.982861
H	-4.011039	1.215767	-1.805955	H	-3.265096	2.740713	-0.717730	H	-3.420928	1.486257	-1.063990
C	-4.924221	4.044014	-1.469719	C	-2.009085	5.448639	-1.029451	C	-2.927027	4.375136	-1.593260
C	-5.229595	5.518418	0.458193	C	-0.591122	6.841889	0.397584	C	-2.574926	6.331737	-0.169009
H	-4.539694	4.764083	2.387866	H	0.117691	5.941550	2.256224	H	-2.369443	5.965100	1.970606
C	-5.367617	5.264324	-0.912321	C	-1.344056	6.667478	-0.771332	C	-2.767935	5.766514	-1.439416
H	-5.036054	3.849520	-2.542274	H	-2.590097	5.315175	-1.948471	H	-3.064716	3.936769	-2.588062
H	-5.580295	6.470943	0.870232	H	-0.081483	7.794880	0.575616	H	-2.454653	7.416337	-0.072571
H	-5.825137	6.020259	-1.559899	H	-1.415971	7.486210	-1.495378	H	-2.796945	6.416286	-2.321040
C	-2.116163	2.131397	0.751941	C	-0.373076	2.370556	0.949983	C	-1.264424	2.295009	1.502878
H	-1.225714	2.474080	1.279326	H	0.711060	2.480984	0.922229	H	-0.491375	3.078638	1.479471
C	-2.248131	1.884223	-0.574185	C	-1.121504	2.218618	-0.251587	C	-1.480447	1.767146	0.063191
H	-1.472874	1.981557	-1.334832	H	-0.630634	2.237495	-1.228151	H	-0.818421	2.246641	-0.670846
C	1.816750	3.650684	-1.422756	C	3.251032	2.246781	-2.012041	C	2.740651	3.062783	-1.386152
C	6.412222	1.624583	-0.524978	C	6.350574	-1.377470	-0.191721	C	6.586055	-0.194381	-0.538582
C	0.933258	4.162358	-0.258970	C	2.616548	3.322673	-1.097446	C	2.044909	3.801021	-0.214234
H	0.268893	3.366680	0.101627	H	1.610631	3.014506	-0.783626	H	1.191136	3.217198	0.157339
H	1.565149	4.503518	0.580196	H	3.236715	3.484522	-0.197730	H	2.754999	3.957424	0.617306
H	0.312337	5.013354	-0.592987	H	2.533555	4.284571	-1.635668	H	1.678303	4.788758	-0.548346
C	0.934349	3.239249	-2.627280	C	2.350695	2.028519	-3.253755	C	1.758286	2.918416	-2.576539
H	1.564734	2.919754	-3.476290	H	2.796382	1.277099	-3.929692	H	2.251819	2.409744	-3.424346
H	0.268833	2.407984	-2.353355	H	1.352748	1.681542	-2.947430	H	0.871005	2.339020	-2.283073
H	0.315116	4.092874	-2.957457	H	2.238259	2.974688	-3.814301	H	1.428857	3.916609	-2.918147
C	2.706261	4.823808	-1.883599	C	4.605049	2.794502	-2.508484	C	3.917279	3.940702	-1.859512
H	3.344442	5.203169	-1.066141	H	5.290574	3.018851	-1.672139	H	4.648463	4.120319	-1.051549
H	3.356079	4.542473	-2.731274	H	5.110007	2.088989	-3.191815	H	4.449389	3.490307	-2.716372
H	2.061298	5.655656	-2.216675	H	4.434418	3.734709	-3.061763	H	3.529287	4.922219	-2.183594
C	6.795106	2.820162	0.381636	C	7.155525	-0.339364	0.628287	C	7.320158	0.847709	0.340743
H	7.889264	2.977214	0.373364	H	8.200322	-0.675409	0.761564	H	8.412467	0.680875	0.308047
H	6.316951	3.755094	0.041467	H	7.177816	0.643051	0.125314	H	7.125140	1.877732	-0.004782
H	6.477989	2.636393	1.423079	H	6.705449	-0.198747	1.626721	H	6.988127	0.773877	1.391087
C	6.877391	1.909489	-1.974204	C	7.012975	-1.559585	-1.579514	C	7.079849	-0.070699	-2.001083
H	6.401393	2.818912	-2.380226	H	7.032849	-0.612030	-2.145449	H	6.877358	0.933282	-2.412754
H	7.972396	2.057174	-2.007232	H	8.055903	-1.909243	-1.468706	H	8.169818	-0.246253	-2.057736
H	6.620098	1.066222	-2.638825	H	6.459132	-2.301907	-2.180507	H	6.574560	-0.810335	-2.646591
C	7.146341	0.370140	-0.014072	C	6.396438	-2.726579	0.550818	C	6.938753	-1.602475	-0.022407
H	6.865388	0.132495	1.026875	H	5.952904	-2.648760	1.558955	H	6.626910	-1.738571	1.027942
H	6.925930	-0.511806	-0.640638	H	5.854920	-3.512733	-0.003834	H	6.457333	-2.388937	-0.629650
H	8.237363	0.538671	-0.039616	H	7.444425	-3.055112	0.666651	H	8.030983	-1.757102	-0.073409
C	2.402122	-2.841631	2.902232	C	0.622428	-3.408208	2.928706	C	1.492442	-3.317562	3.042310
H	3.448236	-2.854396	3.250451	H	1.529105	-3.919294	3.293223	H	2.488543	-3.662015	3.366384

H	1.963663	-1.851695	3.117431	H	0.711483	-2.328650	3.136060	H	1.383178	-2.248743	3.289383
H	1.830089	-3.602217	3.461205	H	-0.252080	-3.794529	3.480097	H	0.722700	-3.881696	3.597171
C	2.919560	-4.490035	1.025896	C	0.321658	-5.119789	1.067023	C	1.476955	-4.995479	1.133191
H	3.947881	-4.580151	1.414343	H	1.179649	-5.679862	1.475388	H	2.433849	-5.390637	1.513600
H	2.305703	-5.295788	1.461767	H	-0.606819	-5.534736	1.493194	H	0.653550	-5.592763	1.558980
H	2.934435	-4.620669	-0.066911	H	0.290075	-5.255446	-0.024644	H	1.451348	-5.106034	0.038826
C	-4.191791	1.032206	0.470911	C	-2.661384	2.862926	1.485268	C	-3.664297	2.024383	1.140714
H	-5.288217	1.001295	0.585239	H	-3.396683	3.598938	1.848045	H	-4.675536	2.463356	1.103472
H	-3.756053	0.035823	0.616673	H	-2.947645	1.860691	1.816024	H	-3.728724	1.033111	1.605134

Alkene without any bridge: In Ni catalyzed reaction energy profile for migratory insertion step

Int1 ² : $\nu_{\text{lowest}} = 14.4354 \text{ cm}^{-1}$				TS1 ² : $\nu_{\text{lowest}} = -298.2797 \text{ cm}^{-1}$				Int1 ² : $\nu_{\text{lowest}} = 9.5132 \text{ cm}^{-1}$			
110				110				110			
Ni	0.323451	-0.508882	0.242226	Ni	-0.605406	0.234329	0.061776	Ni	-0.527896	0.115616	0.045693
C	0.849518	-0.509587	2.965468	C	-1.127256	0.193484	2.821915	C	-1.148824	0.251136	2.850286
C	-1.398608	-1.325241	2.529521	C	0.987408	1.344633	2.426215	C	0.387107	2.129241	2.893652
C	0.643121	-0.609767	4.351012	C	-0.813005	0.084562	4.185897	C	-0.485530	-0.288373	3.965916
C	-1.601546	-1.427711	3.919139	C	1.307348	1.196643	3.784753	C	1.089144	1.547692	3.956372
H	-2.204689	-1.603947	1.844749	H	1.687705	1.850693	1.753587	H	0.711224	3.096621	2.494915
C	-0.590366	-1.069301	4.828336	C	0.400590	0.588573	4.671857	C	0.632816	0.346806	4.517945
H	1.460270	-0.321181	5.021999	H	-1.531655	-0.432113	4.831801	H	-0.861297	-1.231135	4.376611
H	-2.565853	-1.791618	4.292612	H	2.267125	1.574917	4.153674	H	1.973579	2.048548	4.363700
H	-0.770052	-1.152000	5.905605	H	0.650917	0.496216	5.733878	H	1.150595	-0.095990	5.375434
N	2.016920	-0.039629	0.996991	N	-2.257617	-0.515799	0.899135	N	-2.079789	-0.674654	0.872470
C	2.502893	0.455004	-1.253623	C	-2.622368	-1.199973	-1.322317	C	-2.457740	-1.368710	-1.358349
C	0.704988	0.029831	-2.693462	C	-0.892719	-0.607751	-2.792147	C	-0.810053	-0.652123	-2.860805
C	3.326616	0.934065	-2.320620	C	-3.357587	-1.855788	-2.360367	C	-3.200065	-2.025565	-2.390148
C	2.961462	0.430279	0.105808	C	-3.106213	-1.160816	0.036298	C	-2.906450	-1.366923	0.009980
C	1.450576	0.479827	-3.807240	C	-1.550537	-1.238673	-3.872990	C	-1.474013	-1.281065	-3.939929
H	-0.324891	-0.331552	-2.779517	H	0.071926	-0.099923	-2.896214	H	0.124592	-0.097062	-2.992414
C	2.751711	0.927259	-3.621283	C	-2.773968	-1.856096	-3.658122	C	-2.659949	-1.961642	-3.705245
C	4.638086	1.385637	-2.007158	C	-4.600326	-2.464352	-2.029733	C	-4.408092	-2.688801	-2.039384
C	4.257782	0.893239	0.374751	C	-4.341414	-1.769790	0.315187	C	-4.107653	-2.028127	0.310742
H	0.990184	0.473377	-4.799394	H	-1.084090	-1.231466	-4.862289	H	-1.044350	-1.220242	-4.944073
H	3.344602	1.285720	-4.469885	H	-3.301064	-2.352149	-4.480398	H	-3.192294	-2.454827	-4.525814
C	5.070285	1.356549	-0.686462	C	-5.064870	-2.406816	-0.720126	C	-4.834990	-2.674342	-0.716625
H	5.286332	1.754930	-2.807843	H	-5.172416	-2.974536	-2.810903	H	-4.985035	-3.201836	-2.815122
H	4.615245	0.882532	1.403768	H	-4.709020	-1.750085	1.342321	H	-4.450909	-2.040463	1.345549
H	6.081828	1.702924	-0.447502	H	-6.023207	-2.876548	-0.471766	H	-5.767616	-3.183263	-0.449046
N	1.225318	0.013723	-1.469329	N	-1.420258	-0.596464	-1.571520	N	-1.295366	-0.704272	-1.624208
C	2.131868	-0.027067	2.373812	C	-2.351037	-0.478385	2.265449	C	-2.231588	-0.598634	2.231222
O	3.124621	0.334629	3.017039	O	-3.246294	-0.970014	2.969667	O	-3.065423	-1.212716	2.911731
O	-1.254940	-1.201701	-0.596182	O	0.987466	1.021597	-0.918641	O	0.933267	1.143905	-0.622308
C	-2.491691	-0.763138	-0.541947	C	2.258681	0.784942	-0.746924	C	2.227592	0.954493	-0.565847
C	-2.854471	0.538342	-0.049268	C	2.747852	-0.366602	-0.036771	C	2.836854	-0.225563	-0.025202
C	-3.562247	-1.618250	-1.002384	C	3.247600	1.694842	-1.288261	C	3.102186	1.986871	-1.075380

C	-4.208480	0.954696	0.005519	C	4.136755	-0.578213	0.164579	C	4.247461	-0.379687	0.001965
C	-1.846709	1.465396	0.416615	C	1.833653	-1.360942	0.474235	C	2.021444	-1.292091	0.504720
C	-4.871166	-1.140430	-0.934889	C	4.595762	1.424385	-1.059919	C	4.477905	1.771425	-1.022552
C	-5.239496	0.134122	-0.433354	C	5.083646	0.306963	-0.331469	C	5.091609	0.604531	-0.493499
H	-4.405492	1.950294	0.406510	H	4.429169	-1.467536	0.725138	H	4.640127	-1.303256	0.430370
N	-0.556807	1.270639	0.458844	N	0.523438	-1.329530	0.490562	N	0.714863	-1.322009	0.613683
O	-2.250496	2.679609	0.863121	O	2.375366	-2.486257	1.000439	O	2.660297	-2.403412	0.941692
H	-5.671985	-1.797166	-1.284286	H	5.332902	2.123144	-1.464400	H	5.133270	2.555419	-1.410841
C	0.109704	2.478228	0.953547	C	0.013840	-2.590642	1.047469	C	0.314715	-2.649148	1.111438
C	-1.091779	3.287311	1.556726	C	1.297302	-3.205975	1.705828	C	1.669739	-3.238734	1.645896
H	0.801840	2.207915	1.767312	H	-0.719266	-2.372592	1.839441	H	-0.387736	-2.531868	1.952154
C	0.908520	3.144868	-0.151046	C	-0.664473	-3.436978	-0.012539	C	-0.364001	-3.467527	0.029909
C	0.388433	3.252378	-1.453900	C	-0.116697	-3.558857	-1.302343	C	0.154290	-3.508423	-1.277656
C	2.193724	3.645815	0.115475	C	-1.854399	-4.119031	0.292463	C	-1.514291	-4.214450	0.332013
C	1.137757	3.860834	-2.468674	C	-0.745325	-4.356197	-2.267181	C	-0.461105	-4.292490	-2.260950
H	-0.600841	2.839179	-1.676278	H	0.797293	-3.011005	-1.554160	H	1.036272	-2.910032	-1.528847
C	2.946469	4.252029	-0.899587	C	-2.486217	-4.915602	-0.672374	C	-2.134292	-4.997766	-0.651631
H	2.617416	3.533117	1.119406	H	-2.301752	-4.000861	1.285528	H	-1.942060	-4.157796	1.339065
C	2.418537	4.363300	-2.193116	C	-1.931014	-5.037882	-1.953526	C	-1.606523	-5.041027	-1.948901
H	0.725353	3.932980	-3.480547	H	-0.313378	-4.438538	-3.270088	H	-0.051830	-4.312232	-3.276296
H	3.954127	4.620356	-0.682845	H	-3.422666	-5.426599	-0.427286	H	-3.041127	-5.559929	-0.407512
H	3.009859	4.827583	-2.989504	H	-2.428562	-5.652428	-2.711333	H	-2.095303	-5.644993	-2.720656
C	-0.165410	-0.864536	2.053425	C	-0.239459	0.861555	1.939331	C	-0.746901	1.513313	2.326810
C	3.648319	-2.738842	0.704197	C	-3.054773	3.819841	0.961363	C	-3.763412	3.429659	0.866631
C	3.741764	-2.606379	-0.697765	C	-3.506689	3.397653	-0.309457	C	-3.710315	3.025388	-0.487247
C	4.764807	-2.420439	1.498319	C	-3.454713	5.065997	1.463671	C	-4.436847	4.610537	1.212582
C	4.954662	-2.182910	-1.271379	C	-4.350962	4.228496	-1.058749	C	-4.324511	3.812197	-1.472779
C	5.969637	-2.007902	0.918570	C	-4.305588	5.891530	0.711884	C	-5.062557	5.386189	0.224272
H	4.677823	-2.482592	2.588481	H	-3.099618	5.392360	2.447880	H	-4.470624	4.925685	2.262107
C	6.068291	-1.896240	-0.475976	C	-4.753709	5.472791	-0.548473	C	-5.004331	4.987906	-1.118978
H	5.017007	-2.066377	-2.359645	H	-4.694774	3.901609	-2.046870	H	-4.274061	3.499970	-2.522528
H	6.826050	-1.761719	1.555238	H	-4.612411	6.864967	1.109049	H	-5.588952	6.305570	0.502662
H	7.002261	-1.562708	-0.940341	H	-5.411933	6.117984	-1.140128	H	-5.485413	5.595191	-1.893483
C	1.156837	-3.100631	0.480974	C	-1.073317	2.357483	0.772933	C	-1.584001	2.315893	1.322976
H	0.179147	-3.241584	0.952875	H	-0.125216	2.902107	0.783747	H	-1.098774	3.307357	1.273626
C	1.241262	-2.950397	-0.860305	C	-1.536298	1.946134	-0.516749	C	-1.595684	1.763673	-0.119612
H	0.323934	-2.932269	-1.457016	H	-0.872300	2.154329	-1.362400	H	-0.891849	2.321728	-0.752593
C	-3.257649	-3.027259	-1.546810	C	2.809514	2.937568	-2.087689	C	2.515366	3.293737	-1.643095
C	-6.721297	0.540670	-0.393324	C	6.597218	0.129144	-0.130267	C	6.624276	0.486458	-0.486887
C	-2.585075	-3.875963	-0.439338	C	1.971946	3.871726	-1.180217	C	1.721929	4.028851	-0.532699
H	-1.667968	-3.388944	-0.080651	H	1.084868	3.342881	-0.804416	H	0.921133	3.386922	-0.138629
H	-3.272055	-4.003512	0.415929	H	2.572360	4.213576	-0.318360	H	2.393570	4.304898	0.299654
H	-2.327101	-4.878348	-0.827083	H	1.639832	4.762284	-1.744627	H	1.270643	4.954542	-0.934296
C	-2.330237	-2.921888	-2.783093	C	1.971031	2.508358	-3.317738	C	1.587430	2.986367	-2.846095
H	-2.828638	-2.357790	-3.591518	H	2.565722	1.855715	-3.981600	H	2.153818	2.479959	-3.648372
H	-1.394211	-2.406236	-2.523249	H	1.070943	1.961854	-2.999851	H	0.752108	2.339816	-2.540629
H	-2.085999	-3.929811	-3.165412	H	1.660799	3.397799	-3.896400	H	1.176425	3.926729	-3.256914

C	-4.535720	-3.768177	-1.990524	C	4.014827	3.747897	-2.607217	C	3.616918	4.251837	-2.141086
H	-5.240302	-3.912295	-1.152536	H	4.641743	4.129720	-1.782136	H	4.303538	4.548505	-1.328577
H	-5.062777	-3.233697	-2.800700	H	4.653633	3.149125	-3.280391	H	4.214357	3.804775	-2.955480
H	-4.260533	-4.767332	-2.371409	H	3.647672	4.618779	-3.178220	H	3.147569	5.170527	-2.534475
C	-7.503720	-0.459499	0.493029	C	7.161198	1.353854	0.631365	C	7.226022	1.647968	0.341908
H	-8.575314	-0.190272	0.527265	H	8.252272	1.251536	0.777495	H	8.329732	1.586191	0.350531
H	-7.426489	-1.490007	0.104950	H	6.980706	2.291901	0.078106	H	6.945954	2.630554	-0.075862
H	-7.110875	-0.455291	1.524820	H	6.684896	1.448325	1.623029	H	6.867137	1.608400	1.385274
C	-7.300172	0.515656	-1.829326	C	7.291970	0.018874	-1.509745	C	7.152187	0.566200	-1.940473
H	-7.215009	-0.487541	-2.281966	H	7.116204	0.918932	-2.124195	H	6.867631	1.517643	-2.422389
H	-8.370170	0.793144	-1.820372	H	8.384312	-0.097707	-1.385515	H	8.255288	0.495479	-1.956214
H	-6.761738	1.227798	-2.478912	H	6.910443	-0.853306	-2.068975	H	6.742173	-0.258450	-2.549471
C	-6.910083	1.956197	0.184761	C	6.920585	-1.140214	0.680722	C	7.092590	-0.845616	0.129370
H	-6.532838	2.024432	1.220127	H	6.465607	-1.104994	1.686136	H	6.761352	-0.945317	1.177878
H	-6.387387	2.715127	-0.423346	H	6.558304	-2.049802	0.170499	H	6.707906	-1.711470	-0.437468
H	-7.983591	2.214655	0.198481	H	8.013517	-1.235724	0.807254	H	8.195659	-0.896432	0.117154
C	-1.247396	2.955783	3.042561	C	1.384524	-2.798631	3.176869	C	1.837939	-2.957989	3.139431
H	-2.202823	3.350670	3.426009	H	2.371728	-3.064616	3.590114	H	2.857999	-3.222446	3.464269
H	-1.222346	1.862944	3.195859	H	1.232842	-1.711831	3.282661	H	1.659778	-1.891582	3.349789
H	-0.418749	3.404457	3.617200	H	0.602124	-3.314835	3.759490	H	1.113511	-3.554665	3.720750
C	-1.110676	4.779081	1.264019	C	1.517689	-4.694991	1.484665	C	1.957737	-4.691509	1.291763
H	-2.019186	5.236909	1.690064	H	2.468382	-5.006913	1.948821	H	2.947550	-4.982259	1.681912
H	-0.227448	5.259973	1.716450	H	0.695319	-5.267980	1.944325	H	1.193635	-5.345712	1.743547
H	-1.087310	4.966102	0.179613	H	1.546132	-4.934033	0.410866	H	1.941245	-4.845545	0.202704
C	2.368247	-3.214506	1.360648	C	-2.154813	2.860629	1.720483	C	-3.023496	2.562610	1.853896
H	2.479613	-4.280064	1.658181	H	-1.715953	3.316182	2.621167	H	-2.981734	3.028681	2.852418
H	2.201347	-2.671216	2.308215	H	-2.772600	2.007424	2.054210	H	-3.541364	1.591789	1.971979
C	2.553146	-2.903673	-1.590509	C	-3.025947	2.036138	-0.789068	C	-2.976117	1.732518	-0.775370
H	2.511327	-2.169320	-2.416698	H	-3.571194	1.257197	-0.226989	H	-3.584428	0.904898	-0.368826
H	2.700802	-3.885432	-2.092172	H	-3.245657	1.882298	-1.856720	H	-2.886150	1.566438	-1.860791

Rotational Barrier of the Quinoline Group

Lactam product: Rotational barrier along the C–N bond for the lactam product

Product: $v_{\text{lowest}} = 20.8763 \text{ cm}^{-1}$				TS: $v_{\text{lowest}} = -23.8719 \text{ cm}^{-1}$			
48				48			
C	0.525900	0.599461	2.187092	C	0.289454	0.719671	0.914066
C	2.074488	2.376664	1.623524	C	1.386667	2.090894	-0.761061
C	1.457941	0.089752	3.111928	C	1.457495	-0.053486	1.048683
C	3.003255	1.863933	2.535965	C	2.537187	1.299164	-0.649878
H	2.317376	3.273508	1.041281	H	1.371088	2.940168	-1.454036
C	2.690522	0.720689	3.291695	C	2.578322	0.232060	0.263881
H	1.182354	-0.813984	3.663231	H	1.452178	-0.887410	1.757367
H	3.973418	2.356968	2.660439	H	3.410762	1.520176	-1.272421
H	3.413859	0.321360	4.010212	H	3.482877	-0.378202	0.354870

N	-1.514636	0.199843	0.892233	N	-2.148482	0.619362	0.802380
C	-2.793244	-1.047413	-0.822641	C	-2.592351	-1.651599	-0.072797
C	-2.020565	-1.095839	-3.001901	C	-2.832942	-3.395723	1.421985
C	-3.930422	-1.868923	-1.158006	C	-2.795946	-2.524120	-1.203471
C	-2.630619	-0.616510	0.538528	C	-2.356689	-0.242861	-0.303206
C	-3.104664	-1.903402	-3.439705	C	-3.009018	-4.349746	0.384058
H	-1.251453	-0.779773	-3.720747	H	-2.865126	-3.715518	2.473388
C	-4.057961	-2.284610	-2.513234	C	-2.998499	-3.905799	-0.925881
C	-4.854052	-2.250655	-0.145636	C	-2.804193	-1.997671	-2.525517
C	-3.555683	-1.011877	1.500052	C	-2.369015	0.223849	-1.621665
H	-3.172354	-2.209268	-4.488410	H	-3.161997	-5.406430	0.626725
H	-4.911141	-2.908925	-2.801847	H	-3.146826	-4.599974	-1.760967
C	-4.661002	-1.829764	1.159079	C	-2.605343	-0.642340	-2.717135
H	-5.707138	-2.883324	-0.413790	H	-2.966404	-2.672929	-3.372370
H	-3.411613	-0.692982	2.533775	H	-2.169973	1.277404	-1.829788
H	-5.366326	-2.123586	1.943130	H	-2.604388	-0.223042	-3.728975
N	-1.863933	-0.681182	-1.754730	N	-2.636503	-2.105526	1.207379
C	-0.723062	-0.187483	1.970669	C	-0.950583	0.311764	1.629741
O	-0.977048	-1.187102	2.643269	O	-0.997164	-0.252873	2.693323
C	0.822088	1.758133	1.448301	C	0.252462	1.817754	0.022377
C	-0.905994	3.619267	1.278303	C	-0.730842	3.803942	1.232564
C	-1.607143	4.419533	0.195999	C	-1.810563	4.858394	1.076774
H	-0.263471	4.151652	1.991775	H	0.304823	4.135323	1.383699
O	-2.001814	2.982125	1.951438	O	-1.194594	3.053494	2.367304
C	-2.618859	2.426303	0.772355	C	-2.536365	2.818637	1.884239
C	-2.723202	3.629103	-0.142491	C	-2.988453	4.215993	1.507027
C	-1.322311	5.598543	-0.489549	C	-1.837502	6.159213	0.577802
H	-3.541137	1.887493	1.026208	H	-3.120871	2.245670	2.614509
C	-3.579905	3.995201	-1.178617	C	-4.223619	4.858439	1.448168
C	-2.205466	5.992675	-1.515304	C	-3.079412	6.824993	0.544386
H	-0.449665	6.211723	-0.239450	H	-0.926570	6.660731	0.233481
C	-3.315287	5.202971	-1.855442	C	-4.253249	6.184977	0.972828
H	-4.439328	3.375699	-1.456753	H	-5.143954	4.360066	1.770649
H	-2.025610	6.929532	-2.053410	H	-3.129603	7.858189	0.184584
H	-3.986415	5.533082	-2.655551	H	-5.204471	6.726812	0.941473
C	-0.209699	2.384682	0.554478	C	-0.924118	2.753669	0.060651
H	0.269355	2.726242	-0.376741	H	-1.046585	3.272713	-0.903355
C	-1.459166	1.512266	0.227065	C	-2.258093	2.051304	0.547042
H	-1.544700	1.327731	-0.852423	H	-3.078544	2.199955	-0.169233

Chemodivergent step in nickel catalysis (optimized at PBE0-D3(BJ)/def2-SVP level of theory)

Intermediate-2: In Ni catalyzed reaction energy profile

Int2 ² : $\nu_{\text{lowest}} = 10.0461 \text{ cm}^{-1}$				Int2 ⁴ : $\nu_{\text{lowest}} = 11.6712 \text{ cm}^{-1}$				Int2 ⁶ : $\nu_{\text{lowest}} = 8.1629 \text{ cm}^{-1}$			
109				109				109			
Ni	-0.538427	0.049545	0.063617	Ni	-0.340772	-0.243761	-0.048055	Ni	-0.320145	-0.227690	-0.176783
C	-1.333408	0.158504	2.862568	C	-1.480156	0.098067	2.652198	C	-1.261551	0.201726	2.636099
C	0.298917	1.903693	3.203178	C	-0.208993	2.123987	2.977284	C	0.075517	2.204498	2.772823
C	-0.841987	-0.475466	4.010069	C	-0.796472	-0.460365	3.739057	C	-0.506204	-0.328219	3.690097
C	0.818109	1.233938	4.305663	C	0.512076	1.534306	4.009786	C	0.869143	1.636566	3.763278
H	0.738525	2.856511	2.896857	H	0.007895	3.157284	2.693755	H	0.291037	3.220279	2.431985
C	0.227150	0.045517	4.729276	C	0.197577	0.238967	4.414004	C	0.557138	0.369862	4.249909
H	-1.326158	-1.405445	4.316687	H	-1.065788	-1.475886	4.039896	H	-0.771134	-1.324233	4.052682
H	1.671491	1.652481	4.844123	H	1.301774	2.097049	4.512730	H	1.713841	2.196338	4.170791
H	0.603023	-0.477733	5.611709	H	0.726050	-0.225420	5.250068	H	1.141686	-0.074152	5.059119
N	-2.131587	-0.719736	0.792372	N	-2.055140	-0.989477	0.623406	N	-2.021894	-0.936966	0.679703
C	-2.474205	-1.269271	-1.478463	C	-2.172098	-1.775415	-1.601404	C	-2.324542	-1.670579	-1.524723
C	-0.762997	-0.581601	-2.890186	C	-0.409676	-1.093320	-2.957016	C	-0.633837	-1.126648	-3.062272
C	-3.210759	-1.844120	-2.549490	C	-2.787928	-2.488402	-2.666713	C	-3.079459	-2.335173	-2.535506
C	-2.962843	-1.299008	-0.128649	C	-2.761130	-1.725362	-0.290584	C	-2.815656	-1.605323	-0.173718
C	-1.409923	-1.140440	-4.009834	C	-0.942764	-1.775487	-4.066241	C	-1.294153	-1.754127	-4.085768
H	0.197429	-0.064643	-2.974562	H	0.523709	-0.526324	-3.024298	H	0.329189	-0.630724	-3.205293
C	-2.625737	-1.764194	-3.836229	C	-2.124255	-2.468550	-3.915969	C	-2.544828	-2.375043	-3.838708
C	-4.461983	-2.442882	-2.271922	C	-4.009614	-3.160461	-2.423737	C	-4.322101	-2.907681	-2.158086
C	-4.209812	-1.880050	0.094673	C	-3.973542	-2.387993	-0.104554	C	-4.101728	-2.192889	0.150839
H	-0.945331	-1.066339	-4.994415	H	-0.419284	-1.744476	-5.023110	H	-0.853821	-1.766375	-5.084375
H	-3.154350	-2.201042	-4.687731	H	-2.563798	-3.008682	-4.759000	H	-3.092506	-2.877704	-4.637905
C	-4.934424	-2.439804	-0.975820	C	-4.574070	-3.092297	-1.166970	C	-4.815470	-2.825750	-0.828934
H	-5.036807	-2.891522	-3.084682	H	-4.489895	-3.714184	-3.233186	H	-4.912709	-3.417800	-2.923425
H	-4.594973	-1.900501	1.111919	H	-4.431125	-2.355212	0.882277	H	-4.453756	-2.113410	1.176936
H	-5.906543	-2.890657	-0.759813	H	-5.522466	-3.602169	-0.978007	H	-5.784651	-3.271135	-0.594154
N	-1.286501	-0.653997	-1.686140	N	-1.006809	-1.104189	-1.783163	N	-1.139904	-1.079266	-1.790974
C	-2.394054	-0.620254	2.120544	C	-2.411719	-0.850874	1.928857	C	-2.243519	-0.768133	2.026972
O	-3.283531	-1.197676	2.727468	O	-3.263415	-1.477155	2.538958	O	-3.004055	-1.419596	2.722373
O	0.964439	1.069607	-0.516885	O	0.952225	1.084360	-0.603752	O	1.013279	1.049860	-0.694622
C	2.235916	0.828340	-0.494382	C	2.242290	1.093413	-0.538082	C	2.303140	1.017583	-0.605687
C	2.800731	-0.387581	-0.011711	C	3.008935	0.019427	0.015249	C	3.020395	-0.080504	-0.036549
C	3.147553	1.831654	-0.978796	C	2.969169	2.231603	-1.036108	C	3.074844	2.129928	-1.090899
C	4.196232	-0.600954	-0.005879	C	4.420560	0.065716	0.042694	C	4.431548	-0.079147	0.020962
C	1.954700	-1.439128	0.491703	C	2.365100	-1.135369	0.590908	C	2.329909	-1.217935	0.524039
C	4.503771	1.556423	-0.952322	C	4.351246	2.210369	-0.980702	C	4.454309	2.066053	-1.003458
C	5.072379	0.354567	-0.473978	C	5.118038	1.145507	-0.454456	C	5.174042	0.978708	-0.458735
H	4.552812	-1.552942	0.384050	H	4.938079	-0.787318	0.478906	H	4.912573	-0.948589	0.466060
N	0.659089	-1.441787	0.574822	N	1.089750	-1.357034	0.703059	N	1.047298	-1.401514	0.621179
O	2.546079	-2.557319	0.922610	O	3.139045	-2.110142	1.078949	O	3.070840	-2.214631	1.015653
H	5.185307	2.322326	-1.323521	H	4.890376	3.076340	-1.366447	H	5.028981	2.913224	-1.379367
C	0.220161	-2.745742	1.049379	C	0.869827	-2.668062	1.289393	C	0.778551	-2.695158	1.223266

C	1.543673	-3.358640	1.600177	C	2.294450	-3.040595	1.806627	C	2.197979	-3.155080	1.692438
H	-0.491740	-2.618478	1.877984	H	0.192472	-2.569139	2.151243	H	0.145911	-2.552070	2.113391
C	-0.469492	-3.529248	-0.040320	C	0.211851	-3.599071	0.300208	C	0.023406	-3.599354	0.280709
C	0.060083	-3.584884	-1.334152	C	0.719795	-3.753470	-0.995152	C	0.411682	-3.738322	-1.055849
C	-1.656851	-4.209681	0.234022	C	-0.951617	-4.283546	0.654440	C	-1.112231	-4.276363	0.728910
C	-0.580641	-4.317073	-2.329419	C	0.085216	-4.588557	-1.909174	C	-0.314076	-4.549228	-1.922313
H	0.974950	-3.034823	-1.568825	H	1.609709	-3.194681	-1.297739	H	1.271223	-3.177017	-1.431494
C	-2.302531	-4.941630	-0.761223	C	-1.593653	-5.116861	-0.260760	C	-1.844061	-5.087723	-0.137043
H	-2.099056	-4.135602	1.231335	H	-1.385922	-4.129301	1.646150	H	-1.452560	-4.133178	1.758552
C	-1.764244	-4.998700	-2.044246	C	-1.075013	-5.273043	-1.543034	C	-1.444512	-5.226311	-1.463883
H	-0.159742	-4.347470	-3.337109	H	0.488557	-4.695081	-2.918852	H	-0.012286	-4.631610	-2.968508
H	-3.241811	-5.451390	-0.536452	H	-2.517197	-5.625007	0.024137	H	-2.743623	-5.592092	0.222404
H	-2.274670	-5.563262	-2.828081	H	-1.584142	-5.915279	-2.265287	H	-2.026123	-5.846241	-2.149997
C	-0.787293	1.403434	2.469922	C	-1.222451	1.440737	2.288923	C	-1.007316	1.523600	2.198394
C	-2.841881	2.740498	1.702737	C	-3.582391	2.289640	1.635247	C	-3.410834	2.345050	1.687282
C	-3.140222	3.900419	0.777487	C	-4.157646	3.437549	0.832638	C	-4.049441	3.497153	0.941956
H	-3.090184	2.847852	2.765090	H	-3.833437	2.223135	2.699991	H	-3.598587	2.255709	2.763365
O	-3.584492	1.693933	1.104383	O	-4.075886	1.168814	0.920945	O	-3.928062	1.227444	0.981552
C	-3.062421	1.821185	-0.211323	C	-3.613965	1.547546	-0.369948	C	-3.549403	1.640603	-0.329811
C	-3.285749	3.298579	-0.480121	C	-4.177516	2.956883	-0.486311	C	-4.138380	3.041993	-0.382531
C	-3.205096	5.274711	0.926450	C	-4.544350	4.732316	1.128019	C	-4.439763	4.778931	1.285858
H	-3.534422	1.109663	-0.897522	H	-3.898033	0.811348	-1.131917	H	-3.865470	0.917670	-1.090973
C	-3.492610	4.058569	-1.619008	C	-4.576773	3.764980	-1.538161	C	-4.610688	3.862217	-1.394036
C	-3.446113	6.047620	-0.218288	C	-4.978736	5.545782	0.071074	C	-4.946854	5.604367	0.271734
H	-3.082515	5.750250	1.902871	H	-4.524278	5.114352	2.151833	H	-4.367177	5.141583	2.314250
C	-3.586831	5.449053	-1.470332	C	-4.993155	5.069645	-1.239758	C	-5.029366	5.153357	-1.045706
H	-3.590437	3.595561	-2.604176	H	-4.582089	3.400552	-2.568436	H	-4.669540	3.516745	-2.429026
H	-3.527356	7.133598	-0.129056	H	-5.312972	6.565460	0.276900	H	-5.284303	6.614273	0.516548
H	-3.776452	6.073801	-2.346558	H	-5.339107	5.722408	-2.044926	H	-5.431115	5.815713	-1.816268
C	-1.366743	2.311173	1.400559	C	-2.046290	2.251245	1.302288	C	-1.897003	2.331416	1.266282
H	-0.720573	3.198178	1.355177	H	-1.638003	3.274868	1.326893	H	-1.498612	3.359204	1.281380
C	-1.543033	1.716557	-0.007556	C	-2.140669	1.767713	-0.121366	C	-2.068025	1.872444	-0.157329
H	-0.962895	2.221207	-0.788572	H	-1.415399	2.025690	-0.897324	H	-1.363382	2.080202	-0.966281
C	2.613967	3.170550	-1.499928	C	2.204751	3.432880	-1.602128	C	2.362120	3.349711	-1.684096
C	6.589690	0.173028	-0.492271	C	6.643459	1.239940	-0.451068	C	6.701265	1.024024	-0.419941
C	1.864634	3.898847	-0.372589	C	1.297987	4.024464	-0.509817	C	1.445938	3.977393	-0.620460
H	1.042518	3.281832	0.007725	H	0.600503	3.268673	-0.128993	H	0.714630	3.246135	-0.255881
H	2.548027	4.122833	0.461584	H	1.903216	4.394004	0.332964	H	2.039468	4.332463	0.236943
H	1.449246	4.851399	-0.739465	H	0.718213	4.871921	-0.910449	H	0.905357	4.840710	-1.041500
C	1.675092	2.934585	-2.694063	C	1.362778	2.996540	-2.812306	C	1.539208	2.928951	-2.912738
H	2.214826	2.439047	-3.516719	H	2.012054	2.607310	-3.612653	H	2.197639	2.518191	-3.694280
H	0.823663	2.306333	-2.406073	H	0.648552	2.212814	-2.531434	H	0.797710	2.164795	-2.649151
H	1.289187	3.895321	-3.071439	H	0.803550	3.855420	-3.217672	H	1.013929	3.800441	-3.336323
C	3.740177	4.090981	-1.976226	C	3.147473	4.542673	-2.072497	C	3.350054	4.427083	-2.136868
H	4.443222	4.338198	-1.165833	H	3.770018	4.931652	-1.251872	H	3.962571	4.803703	-1.302946
H	4.312009	3.649766	-2.807400	H	3.814005	4.204155	-2.881012	H	4.026634	4.062345	-2.925255
H	3.308212	5.036717	-2.337476	H	2.554269	5.383355	-2.463670	H	2.792893	5.281929	-2.549748

C	7.245378	1.269068	0.360343	C	7.078346	2.463275	0.369060	C	7.243668	1.151038	-1.850958
H	8.342113	1.161036	0.355616	H	8.176590	2.554637	0.378336	H	8.344914	1.193721	-1.847070
H	7.008318	2.275506	-0.016179	H	6.670010	3.397780	-0.044223	H	6.934840	0.290059	-2.463447
H	6.898538	1.212133	1.403550	H	6.731352	2.378598	1.410336	H	6.876517	2.062331	-2.346540
C	7.098843	0.276221	-1.937351	C	7.148068	1.386322	-1.894022	C	7.290030	-0.238846	0.208860
H	6.855723	1.250746	-2.386938	H	6.739473	2.285472	-2.379326	H	7.014391	-1.141683	-0.357253
H	8.193774	0.156263	-1.973041	H	8.247090	1.465574	-1.915653	H	8.388974	-0.174812	0.220164
H	6.646741	-0.505050	-2.567524	H	6.853997	0.516040	-2.500698	H	6.953111	-0.370632	1.248482
C	7.003668	-1.187183	0.069171	C	7.286933	-0.004203	0.161158	C	7.155836	2.234499	0.408528
H	6.683482	-1.309830	1.115135	H	6.979613	-0.147475	1.208373	H	6.787543	3.180755	-0.015521
H	6.579219	-2.015865	-0.517959	H	7.026219	-0.914831	-0.399587	H	6.782162	2.163141	1.441579
H	8.099703	-1.286390	0.042157	H	8.383273	0.094489	0.146059	H	8.255922	2.290587	0.443410
C	1.678956	-3.078669	3.087160	C	2.422296	-2.694853	3.280809	C	2.364331	-2.921527	3.183973
H	2.688760	-3.340461	3.434610	H	3.469212	-2.781349	3.605322	H	3.407814	-3.090607	3.486516
H	1.494591	-2.015483	3.298929	H	2.077767	-1.666595	3.464581	H	2.084761	-1.889732	3.441813
H	0.946193	-3.673158	3.653254	H	1.807851	-3.378656	3.885686	H	1.717756	-3.609390	3.749630
C	1.797014	-4.810696	1.265604	C	2.769402	-4.444043	1.506590	C	2.610511	-4.551931	1.284712
H	2.766245	-5.127111	1.677630	H	3.788518	-4.586875	1.894236	H	3.633121	-4.757360	1.633110
H	1.008591	-5.440666	1.701389	H	2.105148	-5.176089	1.987569	H	1.930639	-5.291652	1.730593
H	1.801097	-4.974560	0.180843	H	2.769184	-4.644901	0.428324	H	2.575790	-4.675687	0.195301

Transition State (2-3) – reductive elimination^A pathway: In Ni catalyzed reaction energy profile

TS2A ² : $\nu_{\text{lowest}} = -622.9890 \text{ cm}^{-1}$				TS2A ⁴ : $\nu_{\text{lowest}} = -667.7055 \text{ cm}^{-1}$				TS2A ⁶ : $\nu_{\text{lowest}} = -864.7323 \text{ cm}^{-1}$			
109				109				109			
Ni	-0.428598	-0.121320	-0.117791	Ni	0.449846	-0.260131	0.553081	Ni	0.322717	-0.031597	0.161956
C	-1.336128	0.019759	2.758527	C	0.401110	0.428923	-2.397735	C	1.179691	0.162054	-2.554043
C	0.329776	1.738978	3.071676	C	-1.447045	1.917661	-1.958847	C	-0.390701	2.003868	-2.260437
C	-0.837553	-0.646175	3.882441	C	-0.410550	-0.283545	-3.287448	C	0.510654	-0.187201	-3.743758
C	0.853984	1.044823	4.157561	C	-2.269763	1.156326	-2.782760	C	-1.114301	1.568932	-3.361100
H	0.782345	2.682079	2.754481	H	-1.851703	2.792689	-1.445022	H	-0.720451	2.889328	-1.708676
C	0.250989	-0.139499	4.582924	C	-1.742225	0.066884	-3.476003	C	-0.624985	0.497506	-4.136232
H	-1.320894	-1.580595	4.175535	H	0.033087	-1.136043	-3.806626	H	0.889149	-1.043352	-4.307405
H	1.727934	1.437266	4.682483	H	-3.324060	1.420860	-2.889910	H	-2.042174	2.072306	-3.639884
H	0.640387	-0.674656	5.452035	H	-2.374405	-0.518001	-4.147820	H	-1.157671	0.195855	-5.041885
N	-2.281850	-0.460525	0.596966	N	2.057071	-0.062450	-0.721919	N	2.217966	-0.495696	-0.571910
C	-2.519951	-1.197922	-1.640280	C	3.100676	-0.968475	1.198044	C	2.340870	-1.394476	1.613933
C	-0.691445	-0.746549	-3.011786	C	1.758823	-1.066219	3.114357	C	0.612387	-0.810739	3.079882
C	-3.255002	-1.778641	-2.714248	C	4.236392	-1.468909	1.907431	C	3.040530	-2.092744	2.641900
C	-3.085003	-1.111413	-0.331423	C	3.197404	-0.635512	-0.189405	C	2.883633	-1.334204	0.279003
C	-1.341310	-1.297455	-4.123256	C	2.817385	-1.548733	3.881166	C	1.227184	-1.447383	4.127769
H	0.315877	-0.327311	-3.078850	H	0.766236	-0.896759	3.539394	H	-0.344397	-0.293486	3.175003
C	-2.616166	-1.812681	-3.980417	C	4.053293	-1.753662	3.283876	C	2.464586	-2.104272	3.921106
C	-4.547106	-2.284524	-2.452479	C	5.447467	-1.646914	1.205874	C	4.263630	-2.730696	2.291335
C	-4.374504	-1.609517	-0.116678	C	4.430050	-0.813343	-0.844894	C	4.120071	-2.038537	-0.037962
H	-0.833499	-1.310302	-5.089399	H	2.662052	-1.759724	4.940701	H	0.757384	-1.444905	5.112736
H	-3.142621	-2.249987	-4.832310	H	4.896376	-2.135778	3.864621	H	2.966380	-2.622032	4.740903

C	-5.079548	-2.196803	-1.175035	C	5.523947	-1.323230	-0.146387	C	4.779159	-2.694662	0.954475
H	-5.114008	-2.744661	-3.264836	H	6.317127	-2.039274	1.737352	H	4.811491	-3.271143	3.066713
H	-4.802938	-1.563960	0.882300	H	4.504432	-0.581662	-1.906020	H	4.463947	-2.012946	-1.070539
H	-6.078107	-2.595897	-0.980594	H	6.465462	-1.473556	-0.680677	H	5.714754	-3.214756	0.738058
N	-1.270012	-0.700541	-1.813765	N	1.905709	-0.784943	1.812947	N	1.169839	-0.783850	1.833266
C	-2.379959	-0.696721	1.962337	C	1.729471	-0.182119	-2.072603	C	2.155423	-0.738206	-1.971742
O	-3.109581	-1.530750	2.462299	O	2.335300	-0.865879	-2.871598	O	2.752504	-1.660798	-2.538556
O	1.020935	1.060221	-0.586922	O	-1.108633	0.575835	1.277777	O	-1.100528	0.986473	0.929608
C	2.295826	0.865505	-0.541034	C	-2.358432	0.355582	1.010291	C	-2.373758	0.895593	0.720895
C	2.895433	-0.332030	-0.031415	C	-2.808347	-0.755977	0.232274	C	-2.976077	-0.195216	0.018836
C	3.188128	1.890583	-1.021518	C	-3.359226	1.261105	1.504630	C	-3.249542	1.921488	1.220998
C	4.298628	-0.496750	-0.013809	C	-4.173159	-0.922751	-0.084796	C	-4.373599	-0.258749	-0.169958
C	2.095518	-1.412456	0.494640	C	-1.884538	-1.741344	-0.276346	C	-2.184451	-1.275929	-0.524842
C	4.551430	1.661925	-0.974244	C	-4.679556	1.044401	1.148047	C	-4.609715	1.797873	0.996161
C	5.150540	0.481531	-0.478955	C	-5.129040	-0.026912	0.344935	C	-5.214857	0.724703	0.305615
H	4.683540	-1.432410	0.388550	H	-4.441070	-1.785907	-0.691849	H	-4.763073	-1.117595	-0.713932
N	0.804584	-1.453983	0.628086	N	-0.591126	-1.755189	-0.149213	N	-0.890879	-1.377786	-0.559964
O	2.730997	-2.519503	0.899917	O	-2.379493	-2.765854	-0.973283	O	-2.834585	-2.308428	-1.064913
H	5.213513	2.445506	-1.344297	H	-5.427981	1.748061	1.513550	H	-5.262886	2.583860	1.376386
C	0.409105	-2.755986	1.136283	C	-0.045004	-2.857266	-0.922515	C	-0.506565	-2.634120	-1.176529
C	1.774166	-3.373828	1.576329	C	-1.307462	-3.714745	-1.238806	C	-1.872633	-3.189067	-1.702841
H	-0.219831	-2.623527	2.030382	H	0.329371	-2.451173	-1.877757	H	0.145842	-2.429590	-2.039260
C	-0.411758	-3.505165	0.114871	C	1.123249	-3.524765	-0.249411	C	0.271907	-3.504348	-0.221596
C	0.029119	-3.638289	-1.207249	C	1.110943	-3.815363	1.119103	C	-0.143796	-3.678383	1.103732
C	-1.655187	-4.031329	0.469159	C	2.271965	-3.808701	-0.992242	C	1.441627	-4.132662	-0.655991
C	-0.749577	-4.303367	-2.148352	C	2.216166	-4.402775	1.726090	C	0.583842	-4.486747	1.970593
H	0.981750	-3.193801	-1.508052	H	0.240785	-3.543030	1.720416	H	-1.032176	-3.153721	1.465105
C	-2.440693	-4.693680	-0.473971	C	3.381934	-4.393154	-0.385046	C	2.168581	-4.948371	0.211226
H	-2.035325	-3.881265	1.483177	H	2.315908	-3.517921	-2.044913	H	1.807694	-3.939136	-1.668079
C	-1.987741	-4.834140	-1.782363	C	3.354026	-4.695320	0.973699	C	1.739972	-5.130184	1.523158
H	-0.398464	-4.392299	-3.178812	H	2.199579	-4.610731	2.798109	H	0.256674	-4.604748	3.006115
H	-3.422171	-5.077345	-0.187748	H	4.282404	-4.584431	-0.972272	H	3.087799	-5.424240	-0.137622
H	-2.608278	-5.339668	-2.525827	H	4.230147	-5.135970	1.454898	H	2.314094	-5.760817	2.206284
C	-0.779789	1.252328	2.373511	C	-0.102886	1.580211	-1.765224	C	0.775188	1.339905	-1.838919
C	-2.679951	2.872057	1.984847	C	1.619658	3.415491	-2.044668	C	2.820818	2.845896	-1.901988
C	-3.076214	3.946677	1.001294	C	2.219579	4.539038	-1.234096	C	3.584164	3.811917	-1.020638
H	-2.560964	3.145945	3.039148	H	1.089392	3.664732	-2.970815	H	2.408539	3.217154	-2.846850
O	-3.707161	1.908765	1.813824	O	2.746216	2.592253	-2.300359	O	3.775434	1.823364	-2.122277
C	-3.619296	1.793058	0.401652	C	3.196860	2.472243	-0.955132	C	4.111492	1.588866	-0.763284
C	-3.683065	3.238788	-0.044184	C	3.246988	3.919085	-0.507341	C	4.430551	2.986593	-0.265691
C	-2.880784	5.314590	0.923486	C	1.908230	5.873001	-1.042123	C	3.535639	5.176499	-0.805367
H	-4.364200	1.097116	-0.001752	H	4.113222	1.874564	-0.877770	H	4.883061	0.815033	-0.660874
C	-4.109455	3.880856	-1.195328	C	3.985075	4.621551	0.433106	C	5.242876	3.506967	0.728758
C	-3.335787	5.974995	-0.226091	C	2.669830	6.596457	-0.112609	C	4.371222	5.714272	0.187149
H	-2.395941	5.870495	1.729768	H	1.102165	6.357685	-1.598747	H	2.875114	5.823750	-1.387593
C	-3.939572	5.269514	-1.267745	C	3.689634	5.979072	0.612820	C	5.208481	4.893095	0.940485
H	-4.571151	3.330725	-2.018904	H	4.779782	4.141895	1.009707	H	5.899907	2.868407	1.324482

H	-3.218085	7.058077	-0.307939	H	2.464249	7.657900	0.044459	H	4.366475	6.791257	0.370789
H	-4.287025	5.809587	-2.151665	H	4.270393	6.566144	1.328440	H	5.852042	5.337335	1.703694
C	-1.445097	2.129819	1.349075	C	0.801605	2.530146	-1.025878	C	1.774510	2.110998	-0.979200
H	-0.710089	2.847148	0.960427	H	0.188937	3.167467	-0.370793	H	1.226270	2.842395	-0.363990
C	-2.150313	1.398983	0.211285	C	1.962462	1.902603	-0.282644	C	2.748145	1.277715	-0.166467
H	-1.767703	1.574708	-0.800010	H	1.945246	1.839999	0.810615	H	2.661797	1.265596	0.925040
C	2.615786	3.201858	-1.571341	C	-2.957943	2.431222	2.409874	C	-2.669948	3.121231	1.979139
C	6.672893	0.346426	-0.478200	C	-6.612342	-0.144545	-0.002980	C	-6.731278	0.702714	0.116611
C	1.809610	3.913298	-0.472968	C	-2.012037	3.380573	1.659049	C	-1.699019	3.892746	1.070952
H	0.999144	3.265861	-0.117486	H	-1.112299	2.846924	1.331015	H	-0.874144	3.245317	0.749157
H	2.458455	4.166426	0.380474	H	-2.513503	3.809117	0.776476	H	-2.221181	4.268512	0.176800
H	1.371986	4.848033	-0.859547	H	-1.708190	4.214589	2.311887	H	-1.278364	4.758209	1.608098
C	1.713104	2.912530	-2.781637	C	-2.263359	1.890333	3.670239	C	-1.933338	2.638499	3.238923
H	2.289737	2.426122	-3.584369	H	-2.943468	1.231848	4.232929	H	-2.620870	2.091988	3.903655
H	0.881521	2.255216	-2.499916	H	-1.363162	1.320912	3.407433	H	-1.100574	1.976466	2.972617
H	1.299714	3.852317	-3.182646	H	-1.972582	2.723135	4.330840	H	-1.531879	3.498854	3.798690
C	3.715697	4.160683	-2.032633	C	-4.170699	3.247589	2.862452	C	-3.761000	4.097259	2.425577
H	4.391417	4.442012	-1.210037	H	-4.703095	3.704914	2.013929	H	-4.316666	4.515571	1.572024
H	4.321939	3.733375	-2.846450	H	-4.888782	2.638865	3.433449	H	-4.483128	3.625232	3.109735
H	3.256204	5.085565	-2.413710	H	-3.834514	4.064847	3.518565	H	-3.298585	4.939246	2.962998
C	7.285641	1.469487	0.371246	C	-7.046259	1.102720	-0.787043	C	-7.417522	0.701948	1.490341
H	8.385279	1.395563	0.379361	H	-8.116090	1.048022	-1.045770	H	-8.513801	0.695263	1.377429
H	7.021601	2.464740	-0.016898	H	-6.889764	2.023988	-0.205891	H	-7.126103	-0.186217	2.071807
H	6.929138	1.410963	1.411157	H	-6.471493	1.195170	-1.721763	H	-7.148865	1.590844	2.080773
C	7.195734	0.452129	-1.918250	C	-7.437623	-0.250927	1.287430	C	-7.188620	-0.537231	-0.651662
H	6.926931	1.414220	-2.379822	H	-7.300351	0.628504	1.934323	H	-6.922071	-1.464904	-0.122511
H	8.294323	0.366389	-1.940793	H	-8.512068	-0.329135	1.055564	H	-8.283096	-0.522950	-0.769442
H	6.775224	-0.348644	-2.545788	H	-7.145028	-1.140632	1.865815	H	-6.745478	-0.578233	-1.658415
C	7.122513	-0.995165	0.100418	C	-6.896993	-1.377291	-0.860886	C	-7.165030	1.947710	-0.670920
H	6.794099	-1.118347	1.143793	H	-6.349135	-1.344467	-1.815095	H	-6.889841	2.876598	-0.149020
H	6.730305	-1.841757	-0.483539	H	-6.621766	-2.307287	-0.340396	H	-6.688021	1.967763	-1.662851
H	8.221404	-1.060636	0.086494	H	-7.971227	-1.431415	-1.095087	H	-8.257794	1.956440	-0.813859
C	1.981261	-3.177991	3.068991	C	-1.373904	-4.109232	-2.697857	C	-1.991767	-2.972616	-3.200300
H	3.009097	-3.447126	3.352105	H	-2.303548	-4.653937	-2.917026	H	-3.007036	-3.217015	-3.544927
H	1.799945	-2.129333	3.346526	H	-1.327807	-3.218516	-3.339360	H	-1.770390	-1.926013	-3.453871
H	1.281940	-3.810999	3.635939	H	-0.522099	-4.761412	-2.942142	H	-1.273960	-3.615212	-3.732105
C	2.029775	-4.801466	1.148720	C	-1.529378	-4.899554	-0.318744	C	-2.209469	-4.608782	-1.303014
H	3.024912	-5.123367	1.488629	H	-2.497454	-5.366326	-0.551013	H	-3.200904	-4.881387	-1.692896
H	1.274940	-5.467319	1.590745	H	-0.732381	-5.644815	-0.447815	H	-1.465130	-5.304071	-1.716198
H	1.976669	-4.907640	0.058357	H	-1.540434	-4.589600	0.734674	H	-2.214022	-4.726868	-0.212262

Transition State (2-3) – nucleophilic addition^B pathway: In Ni catalyzed reaction energy profile

TS2B ² : $\nu_{\text{lowest}} = -394.4568 \text{ cm}^{-1}$				TS2B ⁴ : $\nu_{\text{lowest}} = -396.6049 \text{ cm}^{-1}$				TS2B ⁶ : $\nu_{\text{lowest}} = -442.5332 \text{ cm}^{-1}$			
109				109				109			
Ni	0.297120	0.335759	-0.114894	Ni	0.324409	0.308190	-0.134578	Ni	0.440389	0.388156	-0.490118
C	1.727768	-0.176581	2.334245	C	1.655303	-0.246993	2.370002	C	0.899889	-0.616127	2.257840

C	0.163366	-2.019289	2.451122	C	0.019902	-2.031254	2.419218	C	-1.116814	-1.873573	1.821187
C	1.162483	0.397087	3.469726	C	1.089294	0.325301	3.505708	C	0.249590	0.120739	3.244623
C	-0.435796	-1.421080	3.557403	C	-0.577576	-1.432952	3.526101	C	-1.787492	-1.094365	2.761089
H	-0.217134	-2.967866	2.063933	H	-0.388566	-2.956331	2.004745	H	-1.650533	-2.653466	1.273538
C	0.084883	-0.236395	4.086570	C	-0.022895	-0.279559	4.089029	C	-1.099771	-0.125401	3.495383
H	1.574272	1.331885	3.857949	H	1.526340	1.237044	3.920165	H	0.798302	0.883565	3.802062
H	-1.299565	-1.895525	4.028820	H	-1.467949	-1.883022	3.971103	H	-2.854256	-1.253614	2.931693
H	-0.360607	0.198034	4.985003	H	-0.469353	0.153305	4.987761	H	-1.626942	0.447899	4.261636
N	2.074239	1.037172	0.349798	N	2.084493	1.006657	0.424409	N	2.161744	0.473769	0.558523
C	1.819295	2.097573	-1.742095	C	1.947454	2.050685	-1.685672	C	2.822915	1.503118	-1.438680
C	-0.088659	1.476376	-2.913340	C	0.090539	1.448018	-2.946648	C	1.210352	1.608255	-3.148993
C	2.243076	2.970704	-2.778818	C	2.431568	2.914535	-2.703927	C	3.783959	2.160670	-2.258992
C	2.604287	1.908339	-0.544191	C	2.672269	1.856962	-0.450471	C	3.164334	1.074987	-0.108910
C	0.251084	2.313098	-3.991483	C	0.490269	2.279599	-4.007788	C	2.076360	2.249801	-3.994116
H	-0.996249	0.865400	-2.921734	H	-0.821945	0.846544	-2.997193	H	0.186805	1.360920	-3.440902
C	1.408988	3.057668	-3.917782	C	1.652879	3.009565	-3.880856	C	3.395782	2.542375	-3.562265
C	3.459145	3.680709	-2.621175	C	3.649862	3.606325	-2.492509	C	5.071922	2.383526	-1.712268
C	3.808095	2.617389	-0.446270	C	3.884268	2.544667	-0.301678	C	4.502303	1.312061	0.388879
H	-0.400269	2.360763	-4.865623	H	-0.118751	2.333974	-4.911556	H	1.744284	2.526179	-4.996552
H	1.697937	3.719633	-4.738713	H	1.988660	3.665760	-4.688478	H	4.107819	3.045651	-4.218537
C	4.207204	3.489390	-1.476631	C	4.343369	3.405816	-1.315071	C	5.413168	1.959282	-0.404378
H	3.791520	4.359765	-3.409121	H	4.027859	4.278097	-3.265965	H	5.817056	2.894939	-2.327189
H	4.409419	2.475341	0.450193	H	4.443562	2.393571	0.620107	H	4.740232	0.986400	1.398838
H	5.149253	4.031583	-1.358531	H	5.288316	3.932544	-1.156824	H	6.418771	2.156039	-0.026034
N	0.670871	1.387493	-1.840186	N	0.797874	1.351669	-1.838502	N	1.569944	1.231363	-1.880174
C	2.771273	0.535653	1.477759	C	2.741044	0.442212	1.546317	C	2.292014	-0.285111	1.756770
O	3.780085	1.073855	1.985909	O	3.763319	0.925538	2.084910	O	3.256780	-0.163644	2.555863
O	-0.897833	-1.046849	-0.711813	O	-0.917271	-1.018347	-0.758809	O	-1.071137	-0.529517	-1.235796
C	-2.177428	-1.167306	-0.580296	C	-2.198756	-1.106429	-0.613514	C	-2.327929	-0.431523	-0.943221
C	-2.990655	-0.209956	0.105708	C	-2.979029	-0.130633	0.084115	C	-2.854889	0.579322	-0.078864
C	-2.844742	-2.310356	-1.146928	C	-2.901260	-2.229934	-1.175981	C	-3.263837	-1.374940	-1.495587
C	-4.389379	-0.378451	0.210041	C	-4.379962	-0.264698	0.205228	C	-4.228065	0.624583	0.243728
C	-2.410580	0.951823	0.734780	C	-2.365123	1.020109	0.703020	C	-2.004060	1.590225	0.503806
C	-4.217577	-2.411635	-1.008319	C	-4.274496	-2.297851	-1.020132	C	-4.595917	-1.277634	-1.131099
C	-5.029907	-1.468157	-0.339135	C	-5.054369	-1.336993	-0.337949	C	-5.120382	-0.299064	-0.258044
H	-4.943985	0.388432	0.748472	H	-4.908747	0.514830	0.751333	H	-4.556013	1.419249	0.911833
N	-1.154098	1.274340	0.800429	N	-1.101134	1.312705	0.758543	N	-0.719667	1.721163	0.368779
O	-3.234829	1.819829	1.329528	O	-3.164839	1.910777	1.297037	O	-2.575382	2.514112	1.282160
H	-4.710906	-3.280711	-1.444775	H	-4.794663	-3.153086	-1.452649	H	-5.292809	-2.005230	-1.548139
C	-1.007574	2.547896	1.485378	C	-0.918718	2.585762	1.434229	C	-0.257901	2.825103	1.188249
C	-2.436095	2.774462	2.076873	C	-2.340744	2.859572	2.023856	C	-1.586259	3.526126	1.612422
H	-0.293580	2.424875	2.313963	H	-0.207296	2.448836	2.263079	H	0.208905	2.398696	2.092422
C	-0.451792	3.603036	0.560423	C	-0.338561	3.622835	0.504039	C	0.787734	3.672099	0.514388
C	-1.046549	3.868145	-0.678908	C	-0.906934	3.869489	-0.751102	C	0.689403	4.018566	-0.836673
C	0.703366	4.300978	0.915272	C	0.805616	4.330136	0.875482	C	1.902416	4.098016	1.240284
C	-0.510285	4.828307	-1.530567	C	-0.355347	4.820498	-1.603495	C	1.676672	4.787807	-1.443474
H	-1.928908	3.300971	-0.987946	H	-1.780678	3.295211	-1.071179	H	-0.149075	3.646500	-1.428781

C	1.251385	5.255717	0.059365	C	1.368325	5.276325	0.019837	C	2.896596	4.864712	0.635039
H	1.199734	4.071137	1.861910	H	1.280971	4.114652	1.836155	H	2.006920	3.799440	2.287319
C	0.642046	5.525092	-1.162628	C	0.785415	5.527028	-1.219074	C	2.783347	5.212848	-0.708735
H	-0.983962	5.023825	-2.495248	H	-0.808243	5.001454	-2.580919	H	1.596690	5.029442	-2.505159
H	2.168963	5.775579	0.342490	H	2.277011	5.804216	0.316550	H	3.771527	5.173614	1.211399
H	1.074393	6.266222	-1.838666	H	1.229627	6.261386	-1.894867	H	3.568671	5.798751	-1.191812
C	1.271343	-1.410251	1.856578	C	1.161671	-1.452792	1.858656	C	0.240382	-1.648930	1.586736
C	2.979010	-3.204291	1.517580	C	2.814308	-3.298364	1.510958	C	1.291141	-3.922417	1.489503
C	3.919729	-3.785745	0.485679	C	3.751151	-3.888499	0.480857	C	2.224883	-4.770890	0.655292
H	2.371802	-3.900176	2.108943	H	2.175250	-3.985595	2.078384	H	0.345377	-4.368289	1.819133
O	3.861780	-2.464105	2.341028	O	3.707285	-2.604082	2.362582	O	2.107996	-3.573083	2.592102
C	4.499454	-1.718934	1.313164	C	4.385195	-1.859420	1.360734	C	3.216707	-3.078532	1.856838
C	4.927489	-2.817844	0.357671	C	4.791419	-2.951424	0.388277	C	3.493258	-4.225236	0.899700
C	3.915495	-4.925577	-0.298540	C	3.721007	-5.010042	-0.328858	C	2.050544	-5.806690	-0.245077
H	5.241473	-1.019542	1.712907	H	5.142548	-1.192746	1.786570	H	4.019009	-2.723854	2.512314
C	5.949721	-2.966251	-0.565649	C	5.821542	-3.113103	-0.524070	C	4.617324	-4.697381	0.241747
C	4.966048	-5.096849	-1.211458	C	4.778572	-5.195696	-1.230705	C	3.189111	-6.311197	-0.889503
H	3.126316	-5.676652	-0.210522	H	2.906400	-5.736324	-0.268735	H	1.062477	-6.226786	-0.448957
C	5.966195	-4.133086	-1.341760	C	5.811396	-4.262650	-1.325580	C	4.450548	-5.765818	-0.649509
H	6.727835	-2.207894	-0.681861	H	6.625333	-2.378175	-0.612770	H	5.605598	-4.264739	0.415249
H	5.003629	-5.997903	-1.828348	H	4.795808	-6.083769	-1.867021	H	3.087960	-7.143613	-1.589849
H	6.775555	-4.292319	-2.058445	H	6.625488	-4.432709	-2.034374	H	5.321318	-6.179354	-1.163772
C	2.173769	-2.046387	0.828544	C	2.059066	-2.100594	0.833579	C	1.145860	-2.534587	0.770788
H	1.647192	-2.384766	-0.076241	H	1.537285	-2.403828	-0.086693	H	0.827887	-2.642267	-0.276619
C	3.328012	-1.077634	0.574439	C	3.246861	-1.163448	0.617614	C	2.580434	-2.035923	0.944738
H	3.534003	-0.733411	-0.441584	H	3.483057	-0.812161	-0.389589	H	3.165254	-1.715072	0.079004
C	-2.032104	-3.379990	-1.884543	C	-2.125666	-3.317920	-1.926803	C	-2.780419	-2.457478	-2.467374
C	-6.538843	-1.694108	-0.250983	C	-6.567204	-1.525681	-0.230673	C	-6.611018	-0.302404	0.078626
C	-1.011798	-4.006862	-0.920742	C	-1.114078	-3.977477	-0.975911	C	-1.771806	-3.377889	-1.763227
H	-0.347336	-3.237419	-0.510327	H	-0.425296	-3.228594	-0.567737	H	-0.918636	-2.796876	-1.394827
H	-1.526475	-4.507660	-0.085428	H	-1.634525	-4.468743	-0.138508	H	-2.245430	-3.893457	-0.912029
H	-0.400347	-4.759441	-1.444844	H	-0.527539	-4.743336	-1.509165	H	-1.399911	-4.146386	-2.460140
C	-1.305419	-2.750552	-3.084356	C	-1.393353	-2.703542	-3.130920	C	-2.123058	-1.799152	-3.691221
H	-2.032151	-2.319312	-3.791165	H	-2.114299	-2.246534	-3.827353	H	-2.847140	-1.158378	-4.218364
H	-0.621339	-1.958120	-2.757097	H	-0.682415	-1.934009	-2.806419	H	-1.264652	-1.184606	-3.393250
H	-0.724506	-3.517104	-3.622493	H	-0.841370	-3.483927	-3.679499	H	-1.775898	-2.570933	-4.397250
C	-2.918576	-4.507046	-2.418958	C	-3.048014	-4.417510	-2.457886	C	-3.930696	-3.331556	-2.972217
H	-3.453589	-5.031199	-1.611883	H	-3.588902	-4.931486	-1.648215	H	-4.431146	-3.873069	-2.154324
H	-3.661364	-4.140271	-3.144356	H	-3.787862	-4.026611	-3.173609	H	-4.689058	-2.743797	-3.512172
H	-2.291383	-5.249592	-2.935560	H	-2.446540	-5.173985	-2.984742	H	-3.535629	-4.083846	-3.671897
C	-6.815239	-3.016525	0.479155	C	-6.866672	-2.842511	0.500457	C	-6.976527	-1.633587	0.751459
H	-7.899130	-3.203508	0.548039	H	-7.953859	-3.002937	0.582993	H	-8.050473	-1.664057	0.996906
H	-6.362092	-3.872953	-0.042442	H	-6.441468	-3.708642	-0.028606	H	-6.758946	-2.492996	0.099530
H	-6.404885	-2.991865	1.500351	H	-6.442736	-2.830226	1.516320	H	-6.407334	-1.768843	1.684254
C	-7.128807	-1.759275	-1.667278	C	-7.176943	-1.573030	-1.639273	C	-7.428538	-0.139831	-1.211036
H	-6.684012	-2.574799	-2.257170	H	-6.760567	-2.398251	-2.236380	H	-7.229483	-0.952522	-1.925674
H	-8.216676	-1.931106	-1.627845	H	-8.268182	-1.717532	-1.585926	H	-8.508211	-0.147028	-0.990256

H	-6.948785	-0.817996	-2.209032	H	-6.980341	-0.635444	-2.181651	H	-7.185673	0.810868	-1.709949
C	-7.236882	-0.567640	0.510991	C	-7.227123	-0.383972	0.542487	C	-6.979379	0.836002	1.029977
H	-6.869931	-0.488286	1.545742	H	-6.845067	-0.316169	1.572580	H	-6.437887	0.759183	1.985322
H	-7.090850	0.406888	0.020435	H	-7.063093	0.587723	0.052019	H	-6.759065	1.820730	0.590317
H	-8.319935	-0.759739	0.555346	H	-8.313966	-0.549144	0.600417	H	-8.056731	0.804176	1.253888
C	-2.479182	2.341788	3.532264	C	-2.393066	2.460489	3.488056	C	-1.642627	3.779207	3.103515
H	-3.514853	2.341759	3.901269	H	-3.427606	2.496384	3.858558	H	-2.617781	4.194962	3.395667
H	-2.063525	1.330331	3.641279	H	-2.004306	1.441071	3.618508	H	-1.476650	2.846101	3.658951
H	-1.883945	3.029858	4.151309	H	-1.778421	3.145980	4.090821	H	-0.859820	4.499493	3.384985
C	-3.035574	4.149053	1.880837	C	-2.906136	4.244044	1.797036	C	-1.942459	4.766667	0.815407
H	-4.042741	4.183865	2.320854	H	-3.912492	4.312858	2.234904	H	-2.942824	5.114941	1.110527
H	-2.410187	4.905338	2.376207	H	-2.262847	4.995979	2.275765	H	-1.215002	5.569276	0.999608
H	-3.105605	4.412095	0.818721	H	-2.968899	4.484277	0.728963	H	-1.953591	4.557541	-0.262495

Intermediate-3 from reductive elimination^A pathway: In Ni catalyzed reaction energy profile

Int3A ² : $\nu_{\text{lowest}} = 14.3565 \text{ cm}^{-1}$				Int3A ⁴ : $\nu_{\text{lowest}} = 16.7324 \text{ cm}^{-1}$				Int3A ⁶ : $\nu_{\text{lowest}} = 14.4408 \text{ cm}^{-1}$			
109				109				109			
Ni	-0.586617	-0.363717	-0.676658	Ni	0.659730	-0.333421	0.745762	Ni	0.411878	-0.224048	0.523973
C	-0.204088	0.109009	2.503256	C	-0.393397	1.043697	-2.059521	C	0.155196	0.519076	-2.288845
C	1.807521	1.337887	2.002116	C	-1.808393	2.765220	-1.157389	C	-1.518069	2.119189	-1.597958
C	0.524372	-0.739540	3.341759	C	-1.460397	0.583662	-2.842232	C	-0.801152	-0.136783	-3.071951
C	2.539474	0.463644	2.800060	C	-2.874672	2.291112	-1.912668	C	-2.476788	1.434315	-2.336332
H	2.315199	2.144638	1.468145	H	-1.947900	3.625887	-0.500405	H	-1.799790	3.006039	-1.027010
C	1.894540	-0.562566	3.493095	C	-2.698621	1.203791	-2.770542	C	-2.113799	0.312122	-3.088628
H	-0.008105	-1.551959	3.840404	H	-1.296023	-0.282460	-3.484704	H	-0.494106	-1.025934	-3.625653
H	3.622364	0.582628	2.876348	H	-3.852416	2.770210	-1.828482	H	-3.515256	1.771466	-2.319406
H	2.467771	-1.237415	4.132517	H	-3.535004	0.831072	-3.365268	H	-2.867269	-0.227041	-3.666279
N	-2.085965	0.329518	0.989446	N	1.737930	0.494675	-0.978805	N	2.049158	0.228534	-0.828309
C	-3.350567	-0.314558	-0.978156	C	3.341483	-0.867374	0.226956	C	3.067367	-0.848235	1.058382
C	-2.227450	-0.268859	-3.026141	C	2.786788	-1.467011	2.443656	C	1.797769	-0.873471	3.054867
C	-4.571554	-0.681375	-1.610859	C	4.629792	-1.485776	0.346004	C	4.194986	-1.425998	1.723327
C	-3.324154	-0.118915	0.426742	C	2.987757	-0.239313	-0.978437	C	3.170563	-0.512816	-0.304247
C	-3.391514	-0.607086	-3.718016	C	4.020830	-2.040241	2.643022	C	2.856714	-1.390286	3.766297
H	-1.284825	-0.091111	-3.550201	H	2.019344	-1.473070	3.220925	H	0.831014	-0.663804	3.518494
C	-4.567903	-0.829349	-3.022618	C	4.962415	-2.065490	1.599661	C	4.068364	-1.685810	3.116031
C	-5.716749	-0.889623	-0.807438	C	5.471366	-1.488377	-0.785113	C	5.345501	-1.700449	0.956531
C	-4.463082	-0.327869	1.185644	C	3.842245	-0.266599	-2.094378	C	4.322439	-0.806668	-1.048794
H	-3.356223	-0.691620	-4.805920	H	4.246657	-2.495346	3.609048	H	2.737764	-1.581651	4.834760
H	-5.489678	-1.107417	-3.537733	H	5.938465	-2.536005	1.732165	H	4.910399	-2.116011	3.661438
C	-5.657706	-0.726057	0.560993	C	5.074433	-0.899529	-1.988559	C	5.398272	-1.412853	-0.408962
H	-6.649113	-1.190640	-1.291353	H	6.449204	-1.970049	-0.706199	H	6.204377	-2.158701	1.453300
H	-4.416480	-0.206876	2.267145	H	3.522368	0.182495	-3.034847	H	4.348145	-0.590774	-2.116845
H	-6.546282	-0.899898	1.171769	H	5.738555	-0.933288	-2.855150	H	6.294655	-1.661553	-0.981611
N	-2.184621	-0.142440	-1.688761	N	2.441345	-0.877930	1.257490	N	1.890931	-0.598474	1.717900
C	-1.588924	-0.286422	2.148826	C	0.857247	0.257608	-2.065219	C	1.461099	-0.145006	-2.069359
O	-2.173462	-1.197334	2.697500	O	1.065453	-0.638160	-2.852795	O	1.882846	-1.054666	-2.742731

O	1.011867	0.389525	-1.479730	O	-0.947584	0.419370	1.373741	O	-1.151868	0.456865	1.442368
C	2.237273	0.160449	-1.152406	C	-2.177473	0.174411	1.026924	C	-2.374896	0.339362	1.068583
C	2.652947	-0.978002	-0.385971	C	-2.526578	-0.832313	0.077596	C	-2.769758	-0.773795	0.155715
C	3.274982	1.071955	-1.570319	C	-3.248812	0.922061	1.621236	C	-3.371138	1.250071	1.547437
C	4.003730	-1.177884	-0.034275	C	-3.852924	-0.977778	-0.374716	C	-4.124601	-0.864336	-0.220792
C	1.695227	-1.947816	0.082715	C	-1.543846	-1.774445	-0.410192	C	-1.851471	-1.727135	-0.334830
C	4.576424	0.832003	-1.165422	C	-4.528772	0.739102	1.123099	C	-4.687007	1.099279	1.117571
C	4.985136	-0.276407	-0.389121	C	-4.868400	-0.175280	0.102730	C	-5.072712	0.051218	0.226786
H	4.238073	-2.065975	0.551231	H	-4.042867	-1.747729	-1.120711	H	-4.404136	-1.676166	-0.888145
N	0.404340	-1.830321	0.083263	N	-0.269378	-1.768894	-0.167740	N	-0.530944	-1.760713	-0.172249
O	2.147953	-3.097973	0.600455	O	-1.962479	-2.790231	-1.157328	O	-2.319059	-2.758028	-1.077246
H	5.345555	1.542303	-1.471261	H	-5.333203	1.335979	1.553745	H	-5.449828	1.787911	1.469770
C	-0.185296	-2.992110	0.721092	C	0.363460	-2.935597	-0.755822	C	-0.001232	-2.900334	-0.888884
C	1.015457	-3.980995	0.826261	C	-0.818865	-3.616636	-1.530996	C	-1.274873	-3.759017	-1.149328
H	-0.487045	-2.713900	1.744893	H	1.115976	-2.597372	-1.486480	H	0.377175	-2.569136	-1.873784
C	-1.434973	-3.434165	0.004685	C	1.071638	-3.762147	0.287981	C	1.152512	-3.559613	-0.182661
C	-1.507576	-3.420251	-1.393626	C	0.498140	-3.993855	1.542660	C	1.160997	-3.717444	1.207189
C	-2.571881	-3.785720	0.736173	C	2.331807	-4.294442	0.010740	C	2.256612	-3.992672	-0.921020
C	-2.685685	-3.771549	-2.044835	C	1.161842	-4.766833	2.490925	C	2.239724	-4.324179	1.841980
H	-0.639748	-3.098208	-1.973927	H	-0.469634	-3.545887	1.784839	H	0.328836	-3.328390	1.797335
C	-3.754445	-4.135234	0.085596	C	2.999803	-5.065607	0.960196	C	3.339228	-4.598447	-0.286508
H	-2.541309	-3.736147	1.826990	H	2.807612	-4.077079	-0.949470	H	2.282682	-3.812036	-1.998486
C	-3.812920	-4.131057	-1.305788	C	2.412817	-5.310271	2.198990	C	3.329549	-4.770608	1.095275
H	-2.731818	-3.743001	-3.135606	H	0.704249	-4.939146	3.468181	H	2.242321	-4.422253	2.929288
H	-4.640876	-4.388429	0.671550	H	3.993290	-5.459738	0.735554	H	4.205484	-4.912576	-0.872916
H	-4.743659	-4.388098	-1.817074	H	2.938914	-5.908357	2.946756	H	4.186234	-5.226496	1.597064
C	0.426643	1.181500	1.861759	C	-0.553774	2.152990	-1.225088	C	-0.192251	1.674959	-1.565796
C	-0.775346	3.357973	2.159342	C	1.166291	3.969692	-1.331940	C	1.520220	3.485987	-1.950958
C	-1.315948	4.497393	1.328770	C	2.113995	4.723228	-0.429527	C	2.336036	4.470932	-1.148286
H	-0.007212	3.581270	2.908272	H	0.395481	4.539115	-1.863854	H	0.817118	3.875450	-2.695955
O	-1.945287	2.830147	2.759831	O	2.044009	3.320678	-2.232477	O	2.514419	2.676255	-2.550321
C	-2.709715	2.694627	1.572430	C	2.896194	2.734447	-1.261365	C	3.241659	2.373914	-1.367768
C	-2.588131	4.060776	0.942519	C	3.248810	3.906908	-0.379224	C	3.460150	3.735344	-0.756432
C	-0.796253	5.694659	0.866080	C	2.028581	5.882388	0.323370	C	2.141917	5.772001	-0.715469
H	-3.715512	2.310081	1.776887	H	3.717854	2.174789	-1.718852	H	4.121346	1.754583	-1.572466
C	-3.375305	4.808163	0.082653	C	4.328518	4.221714	0.428609	C	4.419212	4.276959	0.082860
C	-1.599848	6.471002	0.020863	C	3.130229	6.224696	1.118675	C	3.124187	6.337476	0.108272
H	0.203105	6.033243	1.150203	H	1.140758	6.519122	0.297906	H	1.261243	6.348757	-1.008706
C	-2.868305	6.035345	-0.364310	C	4.260527	5.407811	1.171194	C	4.243021	5.602099	0.501864
H	-4.361829	4.462345	-0.235644	H	5.207971	3.575626	0.483515	H	5.288573	3.698536	0.404371
H	-1.228672	7.432165	-0.342521	H	3.105557	7.145666	1.705991	H	3.014183	7.370361	0.446988
H	-3.473867	6.660923	-1.024286	H	5.105123	5.699252	1.799935	H	4.993193	6.068184	1.144913
C	-0.389991	2.211476	1.153561	C	0.613838	2.749468	-0.505693	C	0.881979	2.486669	-0.913182
H	0.171302	2.612474	0.301949	H	0.303588	3.071879	0.496716	H	0.473694	3.037362	-0.055167
C	-1.806878	1.748308	0.725450	C	1.892015	1.867771	-0.442906	C	2.145860	1.672480	-0.516856
H	-1.963769	1.905022	-0.348842	H	2.253887	1.748381	0.589477	H	2.361314	1.739262	0.558559
C	2.925017	2.267016	-2.464457	C	-2.978700	1.848616	2.813205	C	-2.984352	2.338921	2.552121

C	6.452498	-0.423583	0.011308	C	-6.309353	-0.252817	-0.400089	C	-6.527938	-0.025631	-0.215297
C	1.902149	3.180152	-1.771352	C	-2.030253	2.992263	2.428085	C	-1.934118	3.285041	1.948774
H	0.974348	2.628933	-1.578159	H	-1.094149	2.595094	2.018551	H	-1.034195	2.734831	1.648592
H	2.301012	3.560402	-0.816656	H	-2.498656	3.649151	1.679259	H	-2.343469	3.809856	1.071131
H	1.669805	4.049332	-2.407679	H	-1.796638	3.605387	3.313237	H	-1.644764	4.047661	2.689104
C	2.337332	1.749501	-3.787446	C	-2.354643	1.020361	3.948895	C	-2.424340	1.681120	3.825389
H	3.075226	1.130700	-4.321458	H	-3.036784	0.213248	4.258161	H	-3.169453	1.002762	4.268986
H	1.442338	1.142791	-3.598995	H	-1.404578	0.571024	3.633085	H	-1.515137	1.106501	3.609693
H	2.062664	2.593753	-4.441028	H	-2.163935	1.660002	4.825679	H	-2.181575	2.454135	4.572079
C	4.153618	3.116315	-2.796997	C	-4.266159	2.477357	3.351171	C	-4.190120	3.189506	2.959541
H	4.615056	3.547288	-1.894512	H	-4.760687	3.115184	2.601967	H	-4.637742	3.709886	2.098989
H	4.922004	2.539739	-3.334698	H	-4.987778	1.717447	3.688339	H	-4.972591	2.587593	3.445515
H	3.853774	3.952849	-3.446747	H	-4.026122	3.113266	4.216838	H	-3.866925	3.956528	3.679442
C	6.871908	0.788793	0.855639	C	-6.707966	1.106437	-0.993387	C	-7.421314	-0.177519	1.026709
H	7.931432	0.713535	1.150006	H	-7.751452	1.086957	-1.346921	H	-8.478941	-0.231591	0.723907
H	6.744071	1.732450	0.304210	H	-6.620444	1.915541	-0.252571	H	-7.174350	-1.098955	1.575482
H	6.265718	0.853361	1.772967	H	-6.062770	1.362359	-1.848234	H	-7.311771	0.667683	1.720727
C	7.327013	-0.494518	-1.248909	C	-7.247097	-0.597333	0.765848	C	-6.798947	-1.201700	-1.153611
H	7.222222	0.408297	-1.869157	H	-7.202480	0.158247	1.564425	H	-6.576471	-2.166285	-0.673630
H	8.391349	-0.593018	-0.979965	H	-8.291655	-0.653989	0.419659	H	-7.861276	-1.208569	-1.440654
H	7.046864	-1.359834	-1.868915	H	-6.978545	-1.568654	1.208563	H	-6.204669	-1.133134	-2.077108
C	6.690695	-1.689178	0.834855	C	-6.474270	-1.318361	-1.483652	C	-6.883865	1.276920	-0.951459
H	6.104791	-1.683776	1.766892	H	-5.836288	-1.112355	-2.356905	H	-6.747997	2.161443	-0.313116
H	6.425314	-2.596444	0.271099	H	-6.225392	-2.322636	-1.108448	H	-6.254168	1.404877	-1.845734
H	7.754222	-1.764888	1.109280	H	-7.518334	-1.341662	-1.831527	H	-7.935796	1.250930	-1.277083
C	1.145498	-4.569990	2.214282	C	-0.630464	-3.490326	-3.030105	C	-1.284524	-4.359444	-2.537266
H	2.042637	-5.201306	2.291265	H	-1.546601	-3.789985	-3.559666	H	-2.222023	-4.903444	-2.723347
H	1.213244	-3.769311	2.963983	H	-0.360219	-2.461135	-3.304086	H	-1.177118	-3.573190	-3.297849
H	0.263851	-5.188400	2.440203	H	0.190492	-4.147738	-3.353800	H	-0.446406	-5.064232	-2.642634
C	1.059279	-5.046003	-0.252769	C	-1.143005	-5.036118	-1.115668	C	-1.563763	-4.795721	-0.078450
H	1.997299	-5.613975	-0.171728	H	-2.011158	-5.400680	-1.683783	H	-2.540463	-5.260851	-0.276301
H	0.211246	-5.737540	-0.149428	H	-0.286338	-5.694242	-1.317342	H	-0.790261	-5.576046	-0.066341
H	1.013332	-4.597044	-1.254107	H	-1.370395	-5.097879	-0.043907	H	-1.597766	-4.333202	0.917694

Intermediate-3 from nucleophilic addition^B pathway: In Ni catalyzed reaction energy profile

Int3B ² : $\nu_{\text{lowest}} = 12.6774 \text{ cm}^{-1}$				Int3B ⁴ : $\nu_{\text{lowest}} = 6.2164 \text{ cm}^{-1}$				Int3B ⁶ : $\nu_{\text{lowest}} = 10.2174 \text{ cm}^{-1}$			
109				109				109			
Ni	0.048956	0.150211	0.739050	Ni	0.312484	0.284596	-0.177817	Ni	0.381115	-0.488181	0.703775
C	-1.157917	-1.786223	-0.690811	C	1.689221	-0.296299	2.335609	C	0.667009	0.865375	-2.077311
C	-0.962783	-3.861999	0.538758	C	-0.011524	-2.012455	2.394722	C	-1.257204	2.217722	-1.578839
C	0.120281	-1.963403	-1.216182	C	1.161016	0.319045	3.461812	C	-0.049327	0.102394	-2.991793
C	0.344407	-4.005055	0.062326	C	-0.573492	-1.379067	3.502399	C	-2.003195	1.427113	-2.452181
H	-1.392838	-4.623578	1.195853	H	-0.461235	-2.922780	1.990633	H	-1.734891	3.031317	-1.029459
C	0.877299	-3.073381	-0.826393	C	0.028318	-0.242512	4.052611	C	-1.400244	0.394426	-3.175546
H	0.508186	-1.260558	-1.952178	H	1.638801	1.214192	3.866210	H	0.440588	-0.700311	-3.545420
H	0.942723	-4.865971	0.369807	H	-1.476723	-1.789770	3.959547	H	-3.071436	1.619859	-2.572264

H	1.888363	-3.205279	-1.219055	H	-0.396953	0.211938	4.950964	H	-1.996921	-0.195890	-3.874413
N	-1.683688	0.289749	0.290953	N	2.095508	0.919690	0.365378	N	1.992360	-0.365782	-0.480686
C	-1.521785	2.228829	1.575966	C	1.929537	2.063637	-1.684835	C	2.867722	-1.598038	1.307219
C	0.365251	2.246114	2.919192	C	0.069017	1.512249	-2.960039	C	1.425137	-1.985688	3.121285
C	-1.986290	3.466185	2.076413	C	2.423734	2.948537	-2.677024	C	3.925075	-2.299701	1.951472
C	-2.217202	1.509856	0.552058	C	2.660072	1.817582	-0.454738	C	3.068434	-0.993284	0.022276
C	-0.026715	3.467569	3.497016	C	0.477580	2.367291	-3.997737	C	2.392334	-2.674965	3.804719
H	1.290389	1.738546	3.205532	H	-0.849420	0.921558	-3.025925	H	0.425356	-1.831316	3.535057
C	-1.191427	4.076447	3.073583	C	1.647925	3.082519	-3.851517	C	3.676059	-2.851535	3.228578
C	-3.174550	4.004505	1.516987	C	3.651278	3.621288	-2.444909	C	5.166088	-2.383958	1.271630
C	-3.344999	2.104524	-0.017024	C	3.871634	2.512640	-0.276017	C	4.364731	-1.078104	-0.604208
H	0.602863	3.924118	4.262102	H	-0.129803	2.451565	-4.900324	H	2.164887	-3.080643	4.792312
H	-1.500787	5.036560	3.494542	H	1.990867	3.755598	-4.641982	H	4.465236	-3.390877	3.754918
C	-3.816422	3.329586	0.495508	C	4.340724	3.388084	-1.269652	C	5.374322	-1.773884	0.013827
H	-3.549573	4.964653	1.876735	H	4.034576	4.312900	-3.197967	H	5.985867	-2.925398	1.750882
H	-3.820586	1.618626	-0.868752	H	4.408831	2.356002	0.658165	H	4.514448	-0.614702	-1.580883
H	-4.711797	3.769074	0.048932	H	5.285363	3.910040	-1.094916	H	6.352682	-1.854538	-0.464758
N	-0.368878	1.657381	1.995101	N	0.777220	1.378698	-1.854998	N	1.644124	-1.444755	1.880046
C	-2.111468	-0.572583	-0.889919	C	2.818719	0.243821	1.435314	C	2.091643	0.606078	-1.555313
O	-2.129284	0.046942	-2.023640	O	3.804326	0.839171	2.031009	O	2.825277	0.255963	-2.620751
O	1.667511	-0.439512	1.441973	O	-0.946442	-1.015578	-0.802847	O	-1.143061	0.435580	1.378974
C	2.774518	-0.646978	0.792940	C	-2.225363	-1.101292	-0.634239	C	-2.389774	0.369845	1.032727
C	3.008515	-0.155973	-0.525902	C	-2.988714	-0.123640	0.078197	C	-2.890962	-0.595834	0.106254
C	3.821735	-1.406504	1.413861	C	-2.939944	-2.223094	-1.183473	C	-3.331172	1.307447	1.581297
C	4.203529	-0.448082	-1.216874	C	-4.388384	-0.250996	0.220354	C	-4.244404	-0.594058	-0.291717
C	2.042983	0.690640	-1.180196	C	-2.358161	1.018857	0.696021	C	-2.024112	-1.587559	-0.484959
C	4.968786	-1.658132	0.679517	C	-4.310918	-2.284921	-1.006484	C	-4.643211	1.260271	1.140973
C	5.198469	-1.207926	-0.639716	C	-5.075852	-1.319671	-0.313551	C	-5.139957	0.333814	0.197520
H	4.306389	-0.047337	-2.224214	H	-4.905157	0.529838	0.775925	H	-4.553236	-1.351709	-1.010059
N	0.863506	1.015097	-0.740850	N	-1.091094	1.301723	0.741608	N	-0.754343	-1.758081	-0.275542
O	2.346775	1.216382	-2.357871	O	-3.145869	1.909483	1.305671	O	-2.558043	-2.435731	-1.370436
H	5.751160	-2.253435	1.150674	H	-4.841286	-3.138700	-1.429381	H	-5.345382	1.986263	1.551994
C	0.233929	1.976778	-1.637777	C	-0.893339	2.563519	1.434970	C	-0.258818	-2.780756	-1.178714
C	1.157215	1.885204	-2.894228	C	-2.309941	2.844259	2.036135	C	-1.567741	-3.450230	-1.693522
H	-0.772163	1.593672	-1.899905	H	-0.179448	2.406719	2.257998	H	0.217244	-2.265753	-2.030219
C	0.128030	3.342431	-1.006194	C	-0.310592	3.613326	0.521147	C	0.789967	-3.674756	-0.577323
C	1.079072	3.808812	-0.092626	C	-0.885320	3.890375	-0.724684	C	0.679730	-4.165232	0.727122
C	-0.930479	4.181396	-1.365816	C	0.837380	4.309298	0.902478	C	1.922453	-4.001588	-1.327346
C	0.976990	5.090630	0.443638	C	-0.337407	4.861080	-1.557014	C	1.670670	-4.981703	1.261592
H	1.899831	3.154141	0.210520	H	-1.762597	3.325986	-1.052534	H	-0.171528	-3.869464	1.343455
C	-1.033197	5.464240	-0.832783	C	1.396349	5.275384	0.066708	C	2.919468	-4.816430	-0.794247
H	-1.689119	3.811688	-2.060470	H	1.317318	4.070641	1.855363	H	2.039320	-3.583944	-2.331364
C	-0.078048	5.923617	0.073016	C	0.806095	5.557282	-1.161984	C	2.792478	-5.311190	0.501275
H	1.726151	5.440589	1.158070	H	-0.796227	5.066845	-2.526741	H	1.581337	-5.337515	2.289778
H	-1.870058	6.105465	-1.119458	H	2.306935	5.795492	0.371301	H	3.807576	-5.046920	-1.386891
H	-0.158351	6.928890	0.493758	H	1.246236	6.308570	-1.821699	H	3.579479	-5.935646	0.930237
C	-1.713513	-2.757127	0.149783	C	1.149317	-1.481819	1.828571	C	0.099975	1.949577	-1.408805

C	-4.042838	-3.506854	-0.420716	C	2.771229	-3.345430	1.440723	C	1.412310	4.086809	-1.359370
C	-5.498052	-3.166695	-0.185442	C	3.751344	-3.886350	0.424888	C	2.496421	4.798399	-0.582441
H	-3.747124	-4.560197	-0.333269	H	2.104650	-4.060306	1.938806	H	0.521408	4.662119	-1.639530
O	-3.837914	-3.025513	-1.736096	O	3.626969	-2.705929	2.369922	O	2.112400	3.634262	-2.504836
C	-4.340964	-1.708499	-1.532452	C	4.355563	-1.914813	1.439628	C	3.183329	2.993812	-1.826389
C	-5.699078	-1.995998	-0.932595	C	4.803517	-2.959430	0.438670	C	3.663741	4.091671	-0.901113
C	-6.511569	-3.708563	0.586084	C	3.751604	-4.962049	-0.446240	C	2.515849	5.847568	0.320416
H	-4.251599	-1.100458	-2.439422	H	5.096266	-1.281826	1.938272	H	3.891476	2.551514	-2.534566
C	-6.920301	-1.343150	-0.919300	C	5.880345	-3.088608	-0.422573	C	4.878675	4.416258	-0.321934
C	-7.758439	-3.067047	0.579519	C	4.854165	-5.114426	-1.298462	C	3.748224	6.199859	0.887653
H	-6.357103	-4.615272	1.177027	H	2.926873	-5.679103	-0.468880	H	1.606340	6.394457	0.581514
C	-7.958960	-1.903141	-0.162157	C	5.901663	-4.193289	-1.285155	C	4.910201	5.496264	0.570868
H	-7.080168	-0.424188	-1.489214	H	6.695914	-2.361251	-0.428093	H	5.789727	3.859321	-0.554419
H	-8.585176	-3.486192	1.158349	H	4.896149	-5.967357	-1.980180	H	3.800854	7.038609	1.585846
H	-8.941486	-1.424466	-0.155926	H	6.751927	-4.336982	-1.956408	H	5.858776	5.793176	1.024622
C	-3.173684	-2.500026	0.403852	C	2.053368	-2.111226	0.801497	C	1.118969	2.732983	-0.635940
H	-3.444099	-2.490410	1.469932	H	1.563622	-2.362894	-0.151139	H	0.860414	2.874028	0.423029
C	-3.479101	-1.187117	-0.358728	C	3.251567	-1.131083	0.692643	C	2.458773	1.984625	-0.895943
H	-4.034216	-0.456620	0.241216	H	3.561031	-0.885783	-0.329650	H	3.046901	1.794882	0.010220
C	3.645855	-1.945661	2.837485	C	-2.179011	-3.315771	-1.942258	C	-2.876403	2.323466	2.634991
C	6.502098	-1.571104	-1.349280	C	-6.587858	-1.500901	-0.183751	C	-6.607061	0.394686	-0.225952
C	2.471483	-2.935835	2.873912	C	-1.151618	-3.972427	-1.006085	C	-1.805985	3.253738	2.044110
H	1.540330	-2.468869	2.530916	H	-0.451095	-3.224874	-0.615625	H	-0.953741	2.671896	1.673514
H	2.677485	-3.800435	2.224516	H	-1.658002	-4.456676	-0.156030	H	-2.222666	3.844673	1.212602
H	2.321712	-3.309283	3.899973	H	-0.578967	-4.744355	-1.545605	H	-1.446722	3.959034	2.810850
C	3.387494	-0.783396	3.809421	C	-1.467639	-2.707999	-3.162171	C	-2.307236	1.577984	3.853161
H	4.226228	-0.069499	3.794132	H	-2.200641	-2.255828	-3.849099	H	-3.076385	0.929974	4.301728
H	2.466249	-0.251707	3.542378	H	-0.751972	-1.935894	-2.854470	H	-1.449622	0.956054	3.568370
H	3.284339	-1.165565	4.837619	H	-0.924193	-3.491240	-3.715181	H	-1.980281	2.298295	4.620501
C	4.894706	-2.683981	3.325154	C	-3.112435	-4.416454	-2.451212	C	-4.032411	3.198627	3.124498
H	5.123014	-3.565424	2.706376	H	-3.640227	-4.924669	-1.629334	H	-4.474186	3.796162	2.311778
H	5.782043	-2.031934	3.340100	H	-3.863751	-4.028237	-3.156379	H	-4.833017	2.602848	3.589569
H	4.727514	-3.040216	4.352940	H	-2.521617	-5.177121	-2.984007	H	-3.659551	3.901895	3.884697
C	6.613047	-3.099269	-1.453055	C	-6.882974	-2.815784	0.552622	C	-6.892480	1.761741	-0.864904
H	7.549739	-3.386843	-1.957098	H	-7.969603	-2.970665	0.651358	H	-7.948063	1.835385	-1.172785
H	6.607757	-3.577206	-0.461846	H	-6.470058	-3.684386	0.017928	H	-6.689879	2.588094	-0.167063
H	5.771719	-3.514086	-2.029257	H	-6.444012	-2.805032	1.562097	H	-6.264187	1.914996	-1.756246
C	7.691209	-1.024009	-0.546480	C	-7.218443	-1.546076	-1.583206	C	-7.505967	0.207356	1.004748
H	7.721256	-1.437302	0.472926	H	-6.814910	-2.373637	-2.185866	H	-7.328729	0.985377	1.762343
H	8.642455	-1.282738	-1.038716	H	-8.309445	-1.685296	-1.513632	H	-8.569403	0.255660	0.719863
H	7.635105	0.072151	-0.462144	H	-7.025399	-0.609742	-2.129022	H	-7.320752	-0.768849	1.478459
C	6.560009	-0.985055	-2.759870	C	-7.230714	-0.355473	0.598238	C	-6.948804	-0.693891	-1.243268
H	5.740730	-1.361689	-3.391128	H	-6.833748	-0.289269	1.622782	H	-6.348449	-0.596354	-2.160822
H	6.505147	0.114238	-2.746711	H	-7.068633	0.615157	0.105011	H	-6.783421	-1.701340	-0.831941
H	7.508277	-1.265431	-3.243324	H	-8.317455	-0.514978	0.671729	H	-8.009214	-0.620416	-1.529463
C	0.534033	0.973369	-3.936052	C	-2.359239	2.433342	3.496974	C	-1.556813	-3.650383	-3.193033
H	1.294605	0.631505	-4.652904	H	-3.390892	2.481779	3.874039	H	-2.519788	-4.047841	-3.544811

H	0.024466	0.118824	-3.467526	H	-1.985506	1.407227	3.615908	H	-1.358472	-2.701475	-3.710229
H	-0.243695	1.526843	-4.482368	H	-1.730577	3.104025	4.101952	H	-0.766564	-4.367185	-3.462069
C	1.623376	3.199702	-3.476828	C	-2.865552	4.235523	1.825936	C	-1.974189	-4.712827	-0.957323
H	2.295233	3.012386	-4.327173	H	-3.867993	4.307882	2.272093	H	-2.965910	-5.034977	-1.306320
H	0.762346	3.781425	-3.833727	H	-2.212905	4.977877	2.306934	H	-1.250860	-5.519662	-1.138760
H	2.154871	3.800888	-2.727478	H	-2.934866	4.486693	0.760870	H	-2.029347	-4.540248	0.125911

Cobalt catalysis

Acetic acid: In Co catalyzed reaction energy profile

AcOH¹: $\nu_{\text{lowest}} = 70.4314 \text{ cm}^{-1}$

8

H	-4.874515	0.129130	4.247395
O	-5.817336	0.144358	4.517084
C	-5.806287	0.179817	5.879265
O	-4.776556	0.187623	6.521922
C	-7.209035	0.206726	6.440390
H	-7.764299	-0.685740	6.104491
H	-7.164020	0.234522	7.537401
H	-7.748522	1.090447	6.058835

Intermediate-0: In Co catalyzed reaction energy profile

Int0¹: $\nu_{\text{lowest}} = 12.4623 \text{ cm}^{-1}$

Int0³: $\nu_{\text{lowest}} = 14.0597 \text{ cm}^{-1}$

Int0⁵: $\nu_{\text{lowest}} = 10.6217 \text{ cm}^{-1}$

94				94				94			
C	0.977899	-1.893639	3.038166	C	0.721228	-2.148886	2.787683	C	1.115531	-2.160434	2.775500
C	-1.413072	-1.531927	2.844229	C	-1.627909	-2.048832	2.221225	C	-1.249882	-2.547598	2.423510
C	0.879505	-1.979518	4.435297	C	0.417577	-2.396994	4.136311	C	0.965841	-2.344851	4.161286
C	-1.514825	-1.620882	4.245517	C	-1.937079	-2.310392	3.568924	C	-1.409640	-2.723221	3.810534
H	-2.315589	-1.348920	2.251671	H	-2.448486	-1.921138	1.509122	H	-2.127000	-2.625513	1.770009
C	-0.376847	-1.840640	5.040918	C	-0.923413	-2.474943	4.529266	C	-0.305765	-2.625032	4.677520
H	1.789458	-2.161024	5.018365	H	1.241768	-2.533529	4.845619	H	1.849633	-2.271446	4.805353
H	-2.496773	-1.512591	4.721281	H	-2.988471	-2.386847	3.871012	H	-2.403757	-2.939221	4.220834
H	-0.474574	-1.903578	6.130124	H	-1.184537	-2.671868	5.574629	H	-0.442648	-2.773591	5.754424
N	2.030206	-1.987781	0.941137	N	2.085956	-1.940926	0.892325	N	2.324173	-1.682308	0.797391
C	2.478975	-1.901674	-1.369144	C	2.914568	-1.571009	-1.279195	C	2.937902	-1.527125	-1.463311
C	0.579410	-1.418503	-2.644951	C	1.252598	-0.868543	-2.766418	C	1.120420	-1.285658	-2.911042
C	3.321955	-1.950893	-2.522552	C	3.933571	-1.496587	-2.277220	C	3.879622	-1.460368	-2.536646
C	2.993940	-2.108171	-0.045221	C	3.201150	-1.959915	0.070685	C	3.364309	-1.670830	-0.093212
C	1.338773	-1.432264	-3.836840	C	2.195662	-0.759717	-3.813699	C	1.977965	-1.174904	-4.027346
H	-0.498036	-1.224244	-2.643105	H	0.192129	-0.634475	-2.905724	H	0.030957	-1.232737	-3.006528
C	2.700312	-1.697676	-3.776329	C	3.526982	-1.072817	-3.572353	C	3.352066	-1.273273	-3.842881
C	4.702460	-2.242814	-2.338363	C	5.264725	-1.839409	-1.906240	C	5.266993	-1.569991	-2.230548

C	4.358657	-2.404873	0.094107	C	4.524478	-2.291756	0.397298	C	4.743354	-1.786167	0.159982
H	0.842455	-1.236647	-4.791895	H	1.862415	-0.431517	-4.802586	H	1.548468	-1.027914	-5.022608
H	3.306912	-1.713982	-4.688454	H	4.272786	-0.994578	-4.370973	H	4.037256	-1.205673	-4.695139
C	5.184467	-2.470157	-1.054308	C	5.529728	-2.228431	-0.598403	C	5.667061	-1.738494	-0.909778
H	5.364976	-2.286651	-3.208413	H	6.061468	-1.793221	-2.655255	H	6.001240	-1.516023	-3.040720
H	4.761404	-2.569216	1.093834	H	4.759904	-2.577033	1.422706	H	5.074601	-1.883278	1.194522
H	6.246466	-2.700667	-0.914400	H	6.554704	-2.492501	-0.315669	H	6.735034	-1.819335	-0.679437
N	1.135308	-1.646813	-1.455241	N	1.605694	-1.263891	-1.543553	N	1.589523	-1.465151	-1.673228
C	2.271089	-2.056747	2.312349	C	2.117635	-2.110008	2.281946	C	2.453831	-1.874735	2.172811
O	3.373061	-2.228331	2.840994	O	3.141509	-2.208568	2.962070	O	3.510067	-1.810266	2.811106
O	-1.449010	-1.658779	-0.300792	O	-1.150508	-1.398186	-0.871796	O	-1.257565	-1.387923	-0.826517
C	-2.392123	-0.750357	-0.333335	C	-2.242581	-0.700676	-0.635597	C	-2.345571	-0.709949	-0.576119
C	-2.142375	0.617179	0.023185	C	-2.219903	0.533017	0.100449	C	-2.313185	0.524846	0.165664
C	-3.725667	-1.112212	-0.740942	C	-3.502089	-1.158950	-1.157402	C	-3.625753	-1.176739	-1.053008
C	-3.173626	1.590528	-0.023742	C	-3.401415	1.285173	0.294889	C	-3.495130	1.275779	0.390727
C	-0.823529	1.015387	0.435154	C	-0.977954	1.036380	0.651062	C	-1.068500	1.027485	0.692751
C	-4.691310	-0.106796	-0.772617	C	-4.633052	-0.373318	-0.923923	C	-4.748914	-0.395074	-0.788955
C	-4.459071	1.252194	-0.424811	C	-4.625166	0.850518	-0.207658	C	-4.726518	0.836487	-0.079148
H	-2.915902	2.610048	0.268985	H	-3.317593	2.214244	0.861288	H	-3.400409	2.207321	0.951178
N	0.243439	0.260206	0.562388	N	0.184811	0.455309	0.608246	N	0.125272	0.488514	0.602788
O	-0.604079	2.321124	0.728317	O	-0.999722	2.239549	1.284541	O	-1.104439	2.195285	1.386053
H	-5.703488	-0.383481	-1.078621	H	-5.591066	-0.726874	-1.313045	H	-5.717002	-0.751187	-1.150347
C	1.408464	1.073670	0.954025	C	1.172743	1.257945	1.332950	C	1.077201	1.283928	1.391867
C	0.704740	2.418120	1.361912	C	0.371790	2.592491	1.626037	C	0.268829	2.616698	1.621079
H	1.883732	0.626275	1.839491	H	1.385175	0.747260	2.290075	H	1.217776	0.775082	2.364420
C	2.418695	1.170959	-0.169036	C	2.465850	1.381716	0.557405	C	2.420294	1.432091	0.717236
H	0.527380	2.405040	2.452422	H	0.385463	2.811079	2.705326	H	0.332960	2.937153	2.671690
C	2.007949	1.477409	-1.478704	C	2.453323	1.764836	-0.797008	C	2.503133	1.627315	-0.672655
C	3.781783	0.965647	0.093141	C	3.690598	1.087045	1.175293	C	3.598899	1.402778	1.479679
C	2.948818	1.582067	-2.508953	C	3.648307	1.866320	-1.515052	C	3.747458	1.795445	-1.289884
H	0.944238	1.617968	-1.696197	H	1.499235	1.973136	-1.289676	H	1.585973	1.634133	-1.269032
C	4.725708	1.068300	-0.937831	C	4.889932	1.182107	0.454193	C	4.845094	1.575210	0.862050
H	4.101728	0.696586	1.105647	H	3.703667	0.741277	2.214829	H	3.544666	1.208026	2.555956
C	4.310940	1.378521	-2.239384	C	4.871584	1.575261	-0.889838	C	4.922063	1.774687	-0.523272
H	2.618353	1.815281	-3.526270	H	3.625739	2.162887	-2.568666	H	3.800754	1.935773	-2.374373
H	5.783960	0.887297	-0.725782	H	5.837057	0.927981	0.940386	H	5.758946	1.532629	1.463502
H	5.046875	1.449353	-3.047140	H	5.806981	1.640274	-1.455219	H	5.896364	1.894653	-1.008106
C	-0.161475	-1.677201	2.226784	C	-0.287396	-1.959939	1.813486	C	0.016705	-2.255292	1.890103
Co	0.280962	-1.564540	0.378943	Co	0.445719	-1.475629	0.089301	Co	0.459814	-1.390455	0.082493
C	-4.058060	-2.572755	-1.097325	C	-3.587597	-2.492669	-1.923670	C	-3.730758	-2.509667	-1.817173
C	-5.614577	2.263362	-0.497982	C	-5.937797	1.625409	-0.010238	C	-6.036482	1.609626	0.140514
C	-6.750885	1.814117	0.453447	C	-6.941176	0.738572	0.767946	C	-7.024297	0.725637	0.941446
H	-7.596467	2.524427	0.407459	H	-7.896690	1.274596	0.913288	H	-7.977737	1.261229	1.101540
H	-7.134184	0.814935	0.183061	H	-7.157830	-0.198484	0.226442	H	-7.250065	-0.214429	0.408893
H	-6.390962	1.768842	1.496120	H	-6.537380	0.472035	1.760230	H	-6.602041	0.464492	1.927427
C	-6.152380	2.323419	-1.948848	C	-6.533678	1.985059	-1.393651	C	-6.659043	1.962359	-1.232992
H	-6.516879	1.337800	-2.286651	H	-6.739300	1.081897	-1.993845	H	-6.873000	1.056260	-1.825894

H	-6.993114	3.037407	-2.019919	H	-7.485018	2.534145	-1.271813	H	-7.609671	2.509208	-1.096012
H	-5.359928	2.649192	-2.645251	H	-5.835993	2.621588	-1.965536	H	-5.973694	2.598522	-1.820017
C	-5.163315	3.677518	-0.085626	C	-5.720695	2.928833	0.782083	C	-5.806054	2.916918	0.922484
H	-4.791214	3.697712	0.953613	H	-5.319985	2.728781	1.791092	H	-5.384730	2.721785	1.924062
H	-4.363804	4.056623	-0.746154	H	-5.023243	3.608575	0.261880	H	-5.120236	3.595377	0.385399
H	-6.015675	4.376186	-0.152244	H	-6.682466	3.458003	0.900114	H	-6.766139	3.445170	1.057479
C	-3.804215	-3.474935	0.137640	C	-3.124565	-3.651895	-1.004511	C	-3.221930	-3.667087	-0.920643
H	-2.756174	-3.413079	0.466355	H	-2.090984	-3.499437	-0.660335	H	-2.173487	-3.508915	-0.627655
H	-4.453534	-3.169680	0.977302	H	-3.779989	-3.728727	-0.119007	H	-3.836230	-3.745600	-0.006154
H	-4.034905	-4.527145	-0.110044	H	-3.176331	-4.609812	-1.553372	H	-3.295421	-4.625879	-1.465543
C	-5.534600	-2.738587	-1.509983	C	-5.029193	-2.798837	-2.378688	C	-5.185573	-2.827330	-2.218787
H	-6.224093	-2.453746	-0.695700	H	-5.721415	-2.886969	-1.522697	H	-5.844849	-2.919274	-1.337564
H	-5.782918	-2.137303	-2.402770	H	-5.418990	-2.025064	-3.063891	H	-5.606335	-2.057274	-2.889674
H	-5.726135	-3.797821	-1.754770	H	-5.041599	-3.761523	-2.918669	H	-5.210800	-3.790682	-2.757269
C	-3.180079	-3.044004	-2.284307	C	-2.695746	-2.434312	-3.190061	C	-2.886801	-2.442077	-3.114747
H	-3.350966	-2.405514	-3.169906	H	-3.014460	-1.608250	-3.850970	H	-3.234259	-1.617769	-3.762911
H	-2.112541	-3.008888	-2.021815	H	-1.640844	-2.285522	-2.917769	H	-1.825245	-2.284046	-2.875585
H	-3.440703	-4.083158	-2.555731	H	-2.784574	-3.380062	-3.755077	H	-2.983403	-3.388271	-3.677684
C	1.407775	3.684982	0.955828	C	0.809201	3.808414	0.840793	C	0.634989	3.751022	0.690037
C	2.531078	4.104561	1.691087	C	2.003423	4.460245	1.199588	C	1.774377	4.526707	0.971676
C	1.004279	4.421181	-0.169695	C	0.082471	4.266130	-0.270139	C	-0.090353	3.995788	-0.487760
C	3.249481	5.239857	1.297333	C	2.474682	5.540523	0.445459	C	2.195580	5.517488	0.077817
H	2.848891	3.536553	2.573119	H	2.578792	4.106308	2.062133	H	2.347976	4.338075	1.885680
C	1.719757	5.562240	-0.557439	C	0.554064	5.351294	-1.023178	C	0.330583	4.991684	-1.380829
H	0.124824	4.096848	-0.732466	H	-0.854065	3.769671	-0.539786	H	-0.988617	3.409809	-0.703219
C	2.845390	5.971683	0.170530	C	1.752510	5.987171	-0.671940	C	1.476402	5.749884	-1.104516
H	4.125238	5.556128	1.873533	H	3.410394	6.033705	0.728631	H	3.089395	6.108369	0.303332
H	1.396167	6.132667	-1.434494	H	-0.019785	5.700528	-1.888291	H	-0.241669	5.174859	-2.296527
H	3.405482	6.861288	-0.136062	H	2.121683	6.831891	-1.263057	H	1.806066	6.524463	-1.804949

Intermediate-1: In Co catalyzed reaction energy profile

Int1 ¹ : $\nu_{\text{lowest}} = 9.3875 \text{ cm}^{-1}$				Int1 ³ : $\nu_{\text{lowest}} = 11.0464 \text{ cm}^{-1}$				Int1 ⁵ : $\nu_{\text{lowest}} = 11.3127 \text{ cm}^{-1}$			
113				113				113			
C	-0.908060	-1.189768	2.830193	C	0.904105	0.116696	3.105994	C	1.263911	0.457102	3.053686
C	-0.663306	1.229320	2.853511	C	-0.197121	-1.963539	2.540416	C	0.109155	-1.665940	3.013096
C	-0.734739	-1.238547	4.224291	C	0.790175	-0.162449	4.478090	C	1.256007	0.463752	4.461587
C	-0.484639	1.176672	4.246348	C	-0.303795	-2.251342	3.913838	C	0.081030	-1.661826	4.419502
H	-0.631360	2.194032	2.335092	H	-0.589164	-2.684672	1.816377	H	-0.347003	-2.506210	2.472622
C	-0.525930	-0.050612	4.934918	C	0.180181	-1.355161	4.883611	C	0.658152	-0.601838	5.144326
H	-0.758352	-2.217140	4.716757	H	1.189616	0.561790	5.197195	H	1.720779	1.303430	4.990854
H	-0.312197	2.106241	4.801375	H	-0.772712	-3.191131	4.229191	H	-0.393514	-2.491495	4.958161
H	-0.390217	-0.072709	6.021477	H	0.084000	-1.594673	5.948110	H	0.640485	-0.615232	6.239782
N	-1.045192	-2.068836	0.664479	N	1.580839	1.307149	1.201510	N	1.718728	1.386365	0.912255
C	-0.859514	-2.328476	-1.661758	C	1.894403	2.069615	-0.999992	C	2.028280	1.741221	-1.393351
C	-0.357816	-0.321946	-2.757429	C	0.742705	0.780809	-2.575168	C	0.854562	0.242046	-2.743220
C	-0.795346	-3.085216	-2.873631	C	2.405736	2.952818	-1.999731	C	2.565974	2.429833	-2.525855

C	-1.113617	-2.945348	-0.391731	C	2.189034	2.249439	0.390805	C	2.331084	2.152316	-0.045074
C	-0.248731	-0.995150	-3.996743	C	1.190371	1.611617	-3.627122	C	1.312395	0.877532	-3.918266
H	-0.212324	0.757712	-2.661261	H	0.093377	-0.084074	-2.746379	H	0.189804	-0.627672	-2.776137
C	-0.474534	-2.362601	-4.057201	C	2.021292	2.687860	-3.342606	C	2.175955	1.961267	-3.808687
C	-1.048258	-4.482748	-2.805252	C	3.248279	4.022850	-1.584659	C	3.437596	3.534337	-2.300099
C	-1.371063	-4.326973	-0.367288	C	3.017641	3.316561	0.760708	C	3.195282	3.247355	0.126921
H	0.006559	-0.423081	-4.893463	H	0.878515	1.393241	-4.652715	H	0.992028	0.502707	-4.894798
H	-0.404126	-2.898801	-5.009788	H	2.382632	3.341813	-4.143862	H	2.559022	2.464180	-4.703652
C	-1.340086	-5.063644	-1.574090	C	3.536370	4.179484	-0.234295	C	3.736164	3.913087	-0.997587
H	-1.008595	-5.083011	-3.719421	H	3.656111	4.708631	-2.333919	H	3.856092	4.072487	-3.156724
H	-1.566061	-4.806976	0.591616	H	3.245861	3.466782	1.815696	H	3.423576	3.573269	1.141485
H	-1.541922	-6.139671	-1.526986	H	4.186391	5.002729	0.081977	H	4.403656	4.764621	-0.826099
N	-0.660147	-0.975863	-1.638797	N	1.094470	1.002467	-1.309433	N	1.214130	0.658046	-1.527960
C	-1.050417	-2.419841	2.000286	C	1.570873	1.344932	2.596725	C	1.885617	1.576608	2.285373
O	-1.081142	-3.574957	2.441640	O	2.040992	2.250873	3.291752	O	2.452805	2.540933	2.813413
O	-0.807438	1.597866	-0.416294	O	-0.171966	-1.509472	-0.622012	O	-0.456037	-1.637653	-0.458649
C	0.172590	2.465782	-0.389945	C	-1.358002	-2.071448	-0.506447	C	-1.698575	-2.036359	-0.364126
C	1.488389	2.146200	0.081578	C	-2.481588	-1.393852	0.080244	C	-2.729328	-1.185174	0.166879
C	-0.056506	3.814554	-0.859827	C	-1.573012	-3.405885	-1.010089	C	-2.081200	-3.361191	-0.795775
C	2.513043	3.125907	0.148232	C	-3.747171	-2.018261	0.176870	C	-4.074571	-1.624271	0.251633
C	1.807942	0.797435	0.470840	C	-2.353852	-0.034233	0.563415	C	-2.414392	0.146009	0.629073
C	0.997557	4.724412	-0.781600	C	-2.847000	-3.964178	-0.885934	C	-3.421110	-3.729924	-0.686993
C	2.290918	4.428258	-0.275667	C	-3.956961	-3.309567	-0.297066	C	-4.447523	-2.893570	-0.173749
H	3.481533	2.811035	0.539998	H	-4.552912	-1.445909	0.639286	H	-4.805023	-0.926860	0.664627
N	1.029442	-0.255048	0.468445	N	-1.284255	0.702923	0.551521	N	-1.264814	0.771367	0.576566
O	3.083652	0.552115	0.871059	O	-3.467256	0.559577	1.074024	O	-3.425501	0.854977	1.198273
H	0.815351	5.744382	-1.129110	H	-2.998711	-4.978515	-1.263096	H	-3.703898	-4.733366	-1.015435
C	1.825650	-1.443388	0.830389	C	-1.574619	2.008901	1.146982	C	-1.396048	2.070297	1.255718
C	3.092866	-0.778476	1.460472	C	-3.142700	1.944971	1.372786	C	-2.960901	2.216642	1.396572
H	1.306546	-2.024633	1.604023	H	-1.070502	2.058596	2.128836	H	-0.949689	1.968032	2.262673
C	2.088041	-2.328505	-0.370891	C	-1.066616	3.143717	0.285185	C	-0.713057	3.202931	0.527046
H	2.915892	-0.645735	2.543652	H	-3.376236	2.106835	2.437158	H	-3.232983	2.506504	2.422764
C	2.486216	-1.777405	-1.601646	C	-1.321721	3.156228	-1.098362	C	-0.753684	3.279603	-0.875934
C	1.953114	-3.721100	-0.253537	C	-0.328952	4.191225	0.856570	C	-0.075583	4.221383	1.253336
C	2.748579	-2.607837	-2.697644	C	-0.860305	4.209242	-1.893861	C	-0.167556	4.361260	-1.542319
H	2.574609	-0.691480	-1.708082	H	-1.876265	2.328835	-1.550692	H	-1.238529	2.479130	-1.442431
C	2.212098	-4.553435	-1.350596	C	0.138332	5.246384	0.059524	C	0.509803	5.306025	0.586608
H	1.612985	-4.149932	0.695126	H	-0.086433	4.161439	1.924732	H	-0.006830	4.148884	2.343802
C	2.612484	-3.998630	-2.573668	C	-0.129706	5.259440	-1.315023	C	0.462302	5.380105	-0.812396
H	3.052081	-2.167917	-3.653318	H	-1.062924	4.207688	-2.969798	H	-0.196310	4.405361	-2.635902
H	2.084333	-5.636097	-1.253005	H	0.730826	6.047823	0.511998	H	1.020513	6.084954	1.162095
H	2.806947	-4.648353	-3.433585	H	0.243062	6.078752	-1.938692	H	0.931042	6.220468	-1.334804
C	-0.879878	0.041294	2.139513	C	0.408755	-0.768105	2.119904	C	0.698132	-0.600396	2.308950
C	-3.811710	-0.409317	1.675256	C	4.153118	-0.781419	0.988904	C	3.979647	-1.152692	0.926494
C	-5.176621	0.045365	1.127500	C	5.360714	-1.618167	0.523996	C	5.169850	-2.054544	0.548358
H	-3.674601	-0.476533	2.761030	H	4.152503	-0.391370	2.014430	H	3.985976	-0.662708	1.908021
O	-3.702680	-1.698097	1.050242	O	4.214344	0.286756	0.017036	O	4.061124	-0.187859	-0.148804

C	-3.887407	-1.256957	-0.307428	C	4.146341	-0.555983	-1.152351	C	3.973894	-1.143124	-1.226914
C	-5.230624	-0.517330	-0.168558	C	5.356358	-1.471585	-0.881194	C	5.166589	-2.050010	-0.864444
C	-6.209060	0.837509	1.613123	C	6.312515	-2.399977	1.163285	C	6.107823	-2.785608	1.263465
H	-3.820477	-2.097549	-1.009559	H	4.144711	0.039723	-2.074774	H	3.984906	-0.644170	-2.205350
C	-6.319438	-0.298764	-1.003190	C	6.302851	-2.103865	-1.675084	C	6.100347	-2.776313	-1.589988
C	-7.329993	1.045799	0.777144	C	7.288327	-3.039308	0.361955	C	7.070690	-3.520619	0.531304
H	-6.168987	1.282161	2.613249	H	6.321360	-2.517914	2.252196	H	6.115676	-2.793184	2.358738
C	-7.383995	0.487902	-0.506537	C	7.283704	-2.894270	-1.029922	C	7.067215	-3.516162	-0.868065
H	-6.365033	-0.725266	-2.011039	H	6.304998	-1.994388	-2.765112	H	6.103476	-2.777009	-2.685574
H	-8.168905	1.649535	1.139376	H	8.059975	-3.653078	0.838901	H	7.831425	-4.097486	1.068168
H	-8.264790	0.661604	-1.133954	H	8.051931	-3.395624	-1.628400	H	7.825358	-4.089253	-1.412661
C	-2.812468	0.435491	0.864817	C	2.908047	-1.553271	0.509365	C	2.716880	-1.939266	0.525941
H	-2.671805	1.493622	1.083735	H	2.315090	-2.223010	1.132373	H	2.106630	-2.526028	1.210921
C	-2.874951	-0.101495	-0.432248	C	2.903694	-1.408134	-0.834067	C	2.713798	-1.931573	-0.824385
H	-2.805768	0.497322	-1.342516	H	2.261753	-1.898945	-1.565403	H	2.056756	-2.475133	-1.503343
Co	-0.903400	-0.227526	0.211380	Co	0.613503	-0.067958	0.331079	Co	0.517886	-0.132075	0.305916
C	-1.429301	4.238681	-1.419310	C	-0.416131	-4.202706	-1.641628	C	-1.023631	-4.339198	-1.338162
C	3.361291	5.530176	-0.225422	C	-5.310475	-4.031842	-0.206287	C	-5.891585	-3.415006	-0.105404
C	2.859984	6.691352	0.668080	C	-5.144371	-5.324167	0.630866	C	-5.938867	-4.674440	0.794700
H	3.611543	7.500915	0.708434	H	-6.105957	-5.864588	0.701011	H	-6.969167	-5.070819	0.849268
H	1.919868	7.122080	0.281690	H	-4.404691	-6.007124	0.178246	H	-5.288537	-5.476190	0.403971
H	2.673584	6.338189	1.697341	H	-4.804438	-5.084699	1.653547	H	-5.603894	-4.434127	1.818768
C	3.622378	6.059725	-1.656970	C	-5.791976	-4.400401	-1.631204	C	-6.371007	-3.783409	-1.531155
H	2.704563	6.474237	-2.109080	H	-5.070146	-5.058599	-2.145121	H	-5.731341	-4.559648	-1.985814
H	4.382688	6.861898	-1.640015	H	-6.760633	-4.930731	-1.585690	H	-7.405324	-4.171898	-1.501761
H	3.987092	5.248986	-2.311773	H	-5.921398	-3.492536	-2.246047	H	-6.351089	-2.897832	-2.190234
C	4.690864	5.008459	0.352098	C	-6.385337	-3.152219	0.460602	C	-6.853796	-2.361976	0.476757
H	4.565964	4.635306	1.383592	H	-6.102379	-2.877512	1.491699	H	-6.571507	-2.079484	1.505925
H	5.106514	4.190614	-0.262276	H	-6.559211	-2.222329	-0.108722	H	-6.873737	-1.445969	-0.139361
H	5.434413	5.824457	0.375608	H	-7.341407	-3.702493	0.508081	H	-7.879249	-2.770109	0.507989
C	-2.503802	4.126241	-0.310521	C	0.691662	-4.412309	-0.580308	C	0.033968	-4.604823	-0.237749
H	-2.577056	3.091242	0.049796	H	1.031997	-3.449428	-0.177260	H	0.491766	-3.663378	0.095650
H	-2.251009	4.781151	0.541901	H	0.309485	-5.024201	0.255687	H	-0.435497	-5.093981	0.633876
H	-3.491898	4.430583	-0.701089	H	1.558235	-4.935464	-1.023802	H	0.829045	-5.270175	-0.620594
C	-1.423500	5.698900	-1.917554	C	-0.864939	-5.595092	-2.130386	C	-1.636532	-5.695888	-1.740123
H	-1.205242	6.412420	-1.103637	H	-1.242363	-6.220907	-1.302642	H	-2.110699	-6.203498	-0.881759
H	-0.686512	5.855645	-2.725045	H	-1.650965	-5.527984	-2.903367	H	-2.389795	-5.587550	-2.540610
H	-2.421261	5.947163	-2.319600	H	0.000006	-6.117429	-2.575371	H	-0.836980	-6.356394	-2.118806
C	-1.817697	3.340795	-2.620155	C	0.142683	-3.438998	-2.868340	C	-0.351360	-3.737824	-2.597251
H	-1.064087	3.420963	-3.424081	H	-0.635020	-3.338973	-3.646273	H	-1.096179	-3.586681	-3.398707
H	-1.891650	2.288556	-2.310270	H	0.476848	-2.431734	-2.580471	H	0.108838	-2.767688	-2.360268
H	-2.793707	3.656963	-3.030917	H	0.996365	-3.989995	-3.303351	H	0.430291	-4.421041	-2.976646
C	4.401573	-1.477715	1.220330	C	-3.966570	2.873752	0.510050	C	-3.608914	3.142099	0.390917
C	4.733399	-2.586812	2.019029	C	-3.995265	4.246517	0.817027	C	-3.585400	4.529588	0.621279
C	5.263159	-1.092879	0.180204	C	-4.652145	2.408157	-0.623431	C	-4.161498	2.652699	-0.804188
C	5.906781	-3.310140	1.772657	C	-4.680847	5.143066	-0.009964	C	-4.084025	5.416200	-0.339607
H	4.066467	-2.888074	2.835242	H	-3.460032	4.618629	1.697599	H	-3.152709	4.919023	1.549210

C	6.441470	-1.812522	-0.059475	C	-5.343497	3.306893	-1.448728	C	-4.666074	3.541688	-1.764090
H	5.005608	-0.224296	-0.431796	H	-4.641169	1.338980	-0.853981	H	-4.199052	1.573764	-0.981226
C	6.764091	-2.924323	0.731367	C	-5.354892	4.675766	-1.148799	C	-4.622531	4.924230	-1.538369
H	6.154614	-4.174467	2.397692	H	-4.687236	6.210683	0.233424	H	-4.050276	6.494693	-0.153389
H	7.109615	-1.503906	-0.870514	H	-5.874908	2.933660	-2.330821	H	-5.094583	3.150107	-2.692903
H	7.683693	-3.487358	0.540059	H	-5.890907	5.377364	-1.796699	H	-5.012215	5.617560	-2.291198

Transition State (1-2): In Co catalyzed reaction energy profile

TS1 ¹ : $\nu_{\text{lowest}} = -248.2525 \text{ cm}^{-1}$				TS1 ³ : $\nu_{\text{lowest}} = -245.8253 \text{ cm}^{-1}$				TS1 ⁵ : $\nu_{\text{lowest}} = -234.0396 \text{ cm}^{-1}$			
113				113				113			
C	-0.794291	-1.173633	2.778034	C	-1.208645	-0.384363	2.869126	C	1.247669	0.063808	2.851620
C	-0.886114	1.257926	2.676464	C	-0.100148	1.744432	2.470448	C	0.006195	-1.988908	2.468723
C	-0.417849	-1.108647	4.128719	C	-0.913025	-0.284476	4.239416	C	0.864808	0.052823	4.204844
C	-0.488256	1.315712	4.018464	C	0.216707	1.821147	3.834004	C	-0.423072	-1.968521	3.805278
H	-1.074807	2.185353	2.124804	H	0.208917	2.555330	1.802709	H	-0.317752	-2.807172	1.812587
C	-0.268504	0.135464	4.754352	C	-0.202104	0.817909	4.727793	C	0.024008	-0.961588	4.680616
H	-0.220092	-2.051308	4.651040	H	-1.229005	-1.107955	4.889691	H	1.217372	0.864963	4.850702
H	-0.354578	2.291801	4.498151	H	0.786493	2.681317	4.203646	H	-1.097583	-2.751419	4.171333
H	0.028105	0.193067	5.806964	H	0.036444	0.895738	5.793709	H	-0.291041	-0.969184	5.729665
N	-0.787837	-2.215288	0.683064	N	-1.698572	-1.624938	0.935671	N	1.893602	1.250565	0.904608
C	-0.520408	-2.583753	-1.610514	C	-1.778278	-2.384216	-1.278678	C	2.216448	2.065716	-1.290724
C	-0.298060	-0.583872	-2.808730	C	-0.635145	-0.990182	-2.768465	C	0.910064	0.999208	-2.904731
C	-0.336637	-3.385022	-2.779207	C	-2.100548	-3.323862	-2.305143	C	2.781740	2.960574	-2.254060
C	-0.701026	-3.160021	-0.311644	C	-2.166238	-2.599160	0.091262	C	2.564470	2.145941	0.106439
C	-0.091252	-1.300372	-4.010204	C	-0.881089	-1.881671	-3.838146	C	1.386408	1.863044	-3.918376
H	-0.304735	0.508093	-2.766075	H	-0.080713	-0.054210	-2.891049	H	0.182281	0.207437	-3.114234
C	-0.115496	-2.687413	-3.999962	C	-1.616384	-3.036727	-3.611587	C	2.326359	2.831545	-3.595043
C	-0.379166	-4.798989	-2.631088	C	-2.867462	-4.471119	-1.951733	C	3.746577	3.911807	-1.817451
C	-0.746601	-4.560366	-0.205639	C	-2.934211	-3.736158	0.394004	C	3.530034	3.094315	0.488654
H	0.082867	-0.744060	-4.935745	H	-0.495182	-1.642032	-4.833295	H	1.016811	1.749923	-4.941856
H	0.039231	-3.256203	-4.923132	H	-1.827624	-3.735402	-4.428454	H	2.724034	3.504236	-4.362995
C	-0.590473	-5.349087	-1.369573	C	-3.274855	-4.647202	-0.633457	C	4.109137	3.950349	-0.476053
H	-0.241448	-5.436449	-3.509856	H	-3.125990	-5.201992	-2.724488	H	4.191367	4.598917	-2.544462
H	-0.879156	-5.009896	0.778597	H	-3.234432	-3.902920	1.429082	H	3.800779	3.163993	1.542037
H	-0.626646	-6.439103	-1.263298	H	-3.869985	-5.528873	-0.371062	H	4.858242	4.677215	-0.143168
N	-0.508266	-1.215186	-1.654864	N	-1.074382	-1.240020	-1.536705	N	1.320936	1.100170	-1.643676
C	-0.772026	-2.469862	2.036813	C	-1.817628	-1.632335	2.318273	C	2.002387	1.226234	2.290444
O	-0.640114	-3.580169	2.565044	O	-2.272460	-2.551457	3.006223	O	2.557305	2.078716	2.993095
O	-0.987671	1.365711	-0.651043	O	-0.022859	1.417229	-1.001409	O	-0.367305	-1.411088	-0.922799
C	-0.175791	2.390340	-0.549926	C	1.063268	2.096485	-0.758629	C	-1.574193	-1.864273	-0.701768
C	1.136431	2.303271	0.023428	C	2.127428	1.564505	0.055069	C	-2.516381	-1.146553	0.117199
C	-0.600167	3.680079	-1.047240	C	1.260254	3.414378	-1.326068	C	-2.012475	-3.105474	-1.297209
C	1.964386	3.447033	0.158203	C	3.290060	2.320797	0.341862	C	-3.806640	-1.668712	0.381598
C	1.661481	1.028078	0.446641	C	2.043902	0.214370	0.559527	C	-2.179896	0.155053	0.644772
C	0.266754	4.762330	-0.892117	C	2.424986	4.107922	-0.998624	C	-3.293762	-3.563918	-0.993227
C	1.548689	4.694480	-0.286819	C	3.456226	3.605884	-0.160925	C	-4.214893	-2.885438	-0.151623

H	2.941538	3.304107	0.622411	H	4.048575	1.855600	0.973618	H	-4.466898	-1.076032	1.016831
N	1.061504	-0.131217	0.435336	N	1.047363	-0.621655	0.446485	N	-1.061160	0.812895	0.488789
O	2.946629	1.000016	0.893881	O	3.134025	-0.271665	1.212381	O	-3.130210	0.799148	1.375929
H	-0.065488	5.736914	-1.258161	H	2.559192	5.108821	-1.416831	H	-3.616209	-4.510729	-1.433633
C	2.013432	-1.174041	0.851737	C	1.388548	-1.888339	1.102900	C	-1.144219	2.083609	1.219582
C	3.165696	-0.313828	1.477360	C	2.898859	-1.669066	1.524136	C	-2.676152	2.163141	1.593136
H	1.567475	-1.797115	1.639621	H	0.773408	-1.979601	2.015375	H	-0.557454	1.980698	2.150503
C	2.411021	-2.060564	-0.311251	C	1.118530	-3.084632	0.217430	C	-0.583343	3.233744	0.414957
H	2.979085	-0.214303	2.562409	H	3.002693	-1.778304	2.615714	H	-2.799598	2.377561	2.665757
C	2.732534	-1.507389	-1.563147	C	1.524945	-3.082304	-1.128936	C	-0.890679	3.361591	-0.952080
C	2.469166	-3.453076	-0.140757	C	0.467341	-4.214368	0.735840	C	0.256889	4.179781	1.021636
C	3.111030	-2.334938	-2.626971	C	1.293560	-4.197552	-1.940378	C	-0.370086	4.423223	-1.698457
H	2.668503	-0.424440	-1.710250	H	2.014747	-2.194749	-1.540296	H	-1.528911	2.613009	-1.430387
C	2.844852	-4.283277	-1.205279	C	0.230855	-5.332240	-0.076995	C	0.782661	5.242784	0.273273
H	2.188407	-3.888508	0.824279	H	0.110799	-4.204020	1.772029	H	0.540598	4.057670	2.072758
C	3.168723	-3.725468	-2.449436	C	0.646381	-5.327270	-1.414813	C	0.469417	5.367708	-1.086460
H	3.353811	-1.894313	-3.599542	H	1.612460	-4.184046	-2.987723	H	-0.610399	4.508916	-2.763226
H	2.868051	-5.368665	-1.065989	H	-0.295857	-6.200186	0.332310	H	1.457136	5.960904	0.750429
H	3.454254	-4.374351	-3.284228	H	0.455041	-6.197221	-2.051962	H	0.890030	6.191312	-1.672911
C	-1.054418	0.011417	2.040023	C	-0.825971	0.645844	1.965485	C	0.839876	-0.969351	1.977123
C	-3.695314	-0.742104	1.853740	C	-3.553772	1.335498	1.668071	C	3.492857	-1.847973	1.519636
C	-5.083742	-0.447520	1.275962	C	-4.662721	2.124464	0.961632	C	4.512244	-2.803708	0.888682
H	-3.561604	-0.710130	2.941807	H	-3.418412	1.466177	2.748630	H	3.345982	-1.887745	2.605619
O	-3.459659	-2.059622	1.338106	O	-3.939933	-0.013254	1.349508	O	4.033305	-0.577671	1.111220
C	-3.699694	-1.756545	-0.054168	C	-4.010273	0.152877	-0.082198	C	4.081618	-0.858434	-0.307616
C	-5.096570	-1.128771	0.037772	C	-4.971514	1.345128	-0.176442	C	4.913334	-2.148981	-0.298759
C	-6.169198	0.313561	1.693998	C	-5.295257	3.339716	1.196746	C	5.012367	-4.053869	1.229354
H	-3.562688	-2.650435	-0.676309	H	-4.290049	-0.787865	-0.573196	H	4.466998	0.006444	-0.864295
C	-6.198521	-1.059572	-0.807708	C	-5.918289	1.767326	-1.102393	C	5.824699	-2.737476	-1.168805
C	-7.301412	0.366113	0.850988	C	-6.275158	3.763317	0.271089	C	5.952750	-4.649617	0.357341
H	-6.159292	0.850285	2.648763	H	-5.054739	3.951135	2.073096	H	4.700958	-4.565240	2.146754
C	-7.314965	-0.308689	-0.377419	C	-6.581094	2.991098	-0.857503	C	6.350263	-4.002285	-0.819882
H	-6.212926	-1.574906	-1.774120	H	-6.155726	1.173305	-1.991527	H	6.138317	-2.240434	-2.093340
H	-8.181114	0.939466	1.162147	H	-6.804998	4.706948	0.439446	H	6.378522	-5.627289	0.607316
H	-8.205943	-0.254735	-1.012245	H	-7.346629	3.340102	-1.558779	H	7.083592	-4.481692	-1.477547
C	-2.736210	0.115142	0.988399	C	-2.317142	1.524612	0.764998	C	2.233780	-1.942287	0.619944
H	-2.818157	1.202329	1.048178	H	-1.817707	2.493643	0.715410	H	1.594338	-2.827559	0.645907
C	-2.795222	-0.533878	-0.303469	C	-2.639301	0.777609	-0.413702	C	2.648489	-1.334413	-0.584963
H	-2.947952	0.055097	-1.213470	H	-2.441337	1.159637	-1.419783	H	2.293188	-1.620042	-1.578095
Co	-0.858775	-0.411523	0.093126	Co	-0.871101	-0.073329	0.092205	Co	0.725950	-0.104814	0.020953
C	-1.975281	3.858704	-1.723527	C	0.210181	4.027173	-2.273116	C	-1.085495	-3.892426	-2.243107
C	2.401102	5.967093	-0.158354	C	4.686616	4.476844	0.138248	C	-5.595651	-3.503358	0.119158
C	1.636914	7.012642	0.690656	C	4.231297	5.779803	0.840768	C	-5.411759	-4.883978	0.796470
H	2.228697	7.941431	0.786101	H	5.100635	6.427972	1.055410	H	-6.393904	-5.352067	0.991197
H	0.667592	7.275142	0.232234	H	3.528328	6.353433	0.212038	H	-4.828982	-5.572368	0.160138
H	1.438200	6.621417	1.703801	H	3.724393	5.551001	1.794595	H	-4.880083	-4.778290	1.758260
C	2.672838	6.549672	-1.567120	C	5.402183	4.832062	-1.188440	C	-6.350640	-3.684506	-1.220784

H	1.733350	6.801145	-2.089334	H	4.734840	5.382451	-1.874095	H	-5.796648	-4.341880	-1.913074
H	3.276634	7.472743	-1.494383	H	6.285036	5.467850	-0.992947	H	-7.343161	-4.138051	-1.045388
H	3.223008	5.822548	-2.189729	H	5.740286	3.916997	-1.705464	H	-6.496786	-2.710882	-1.720436
C	3.754205	5.681782	0.520817	C	5.690879	3.753035	1.055394	C	-6.449237	-2.614953	1.044273
H	3.619090	5.281991	1.541007	H	5.236890	3.492572	2.027456	H	-5.965341	-2.468914	2.025743
H	4.352820	4.955967	-0.057003	H	6.067717	2.824710	0.591541	H	-6.631337	-1.621511	0.598306
H	4.338370	6.615643	0.598324	H	6.557648	4.408392	1.251737	H	-7.429965	-3.091295	1.218607
C	-3.108506	3.533005	-0.720096	C	-1.138471	4.202831	-1.534348	C	0.186590	-4.341487	-1.484363
H	-3.044134	2.485650	-0.395486	H	-1.525533	3.229020	-1.205853	H	0.748006	-3.469438	-1.123053
H	-3.042315	4.186396	0.167934	H	-1.017257	4.854000	-0.650310	H	-0.079134	-4.976079	-0.620194
H	-4.095166	3.690774	-1.192430	H	-1.884824	4.667920	-2.203932	H	0.843347	-4.927430	-2.152681
C	-2.190199	5.304762	-2.217111	C	0.642323	5.412220	-2.796794	C	-1.771337	-5.155354	-2.803065
H	-2.174264	6.031761	-1.386081	H	0.760083	6.144273	-1.978300	H	-2.044264	-5.865571	-2.002618
H	-1.427523	5.605460	-2.957095	H	1.591978	5.362833	-3.358330	H	-2.682743	-4.909705	-3.376383
H	-3.178284	5.376848	-2.704266	H	-0.133232	5.798667	-3.481032	H	-1.074497	-5.673171	-3.484956
C	-2.090251	2.925132	-2.954307	C	0.011767	3.100743	-3.499224	C	-0.687681	-2.999086	-3.445379
H	-1.287873	3.140930	-3.682444	H	0.961116	2.976840	-4.050059	H	-1.584251	-2.686726	-4.009919
H	-2.018078	1.871079	-2.649585	H	-0.343587	2.110568	-3.178052	H	-0.156242	-2.100216	-3.099013
H	-3.062053	3.079523	-3.457642	H	-0.733267	3.538121	-4.188891	H	-0.026319	-3.559982	-4.130685
C	4.567270	-0.797534	1.225391	C	3.908757	-2.541115	0.813077	C	-3.494492	3.125934	0.761957
C	5.073586	-1.850908	2.007800	C	4.031161	-3.891736	1.187281	C	-3.427450	4.502314	1.045564
C	5.352451	-0.269488	0.187654	C	4.679707	-2.050075	-0.252773	C	-4.262571	2.684966	-0.328103
C	6.344403	-2.378213	1.747638	C	4.894510	-4.744359	0.490407	C	-4.100977	5.425811	0.238464
H	4.466550	-2.264090	2.821798	H	3.431754	-4.283194	2.016669	H	-2.826190	4.854430	1.890985
C	6.627425	-0.792793	-0.066335	C	5.549256	-2.903934	-0.946605	C	-4.940613	3.611139	-1.133928
H	4.958318	0.555953	-0.411362	H	4.594738	-0.996295	-0.533439	H	-4.330332	1.614245	-0.541693
C	7.124859	-1.850149	0.708317	C	5.654411	-4.253111	-0.582336	C	-4.857304	4.982527	-0.857397
H	6.727955	-3.201061	2.360037	H	4.973400	-5.796371	0.783998	H	-4.033285	6.495311	0.463495
H	7.234256	-0.373102	-0.875737	H	6.146275	-2.511281	-1.776780	H	-5.536633	3.257142	-1.981958
H	8.120031	-2.260010	0.506004	H	6.329831	-4.920250	-1.128322	H	-5.383860	5.704925	-1.490026

Intermediate-2: In Co catalyzed reaction energy profile

Int2 ¹ : $\nu_{\text{lowest}} = 12.4988 \text{ cm}^{-1}$				Int2 ³ : $\nu_{\text{lowest}} = 12.6895 \text{ cm}^{-1}$				Int2 ⁵ : $\nu_{\text{lowest}} = 10.0606 \text{ cm}^{-1}$			
113				113				113			
C	0.933629	-0.601081	-2.758586	C	-0.314064	-0.773981	-2.672048	C	-0.303340	-0.997826	-2.821626
C	0.879441	1.822652	-2.511781	C	1.782157	-1.922056	-2.225649	C	2.023222	-0.295588	-2.864864
C	-0.117368	-0.496152	-3.690014	C	0.369302	0.024485	-3.611213	C	-0.557951	-0.046835	-3.834551
C	-0.220427	1.901658	-3.367284	C	2.461531	-1.073780	-3.107074	C	1.733867	0.711022	-3.791438
H	1.287779	2.737663	-2.070242	H	2.337525	-2.700709	-1.691247	H	3.050200	-0.414761	-2.502096
C	-0.701533	0.737923	-3.989824	C	1.746749	-0.103204	-3.820930	C	0.434975	0.816500	-4.307298
H	-0.492441	-1.424401	-4.134150	H	-0.215928	0.767031	-4.163773	H	-1.579210	0.009571	-4.225916
H	-0.690042	2.870795	-3.562276	H	3.543536	-1.178048	-3.237460	H	2.525093	1.389713	-4.127007
H	-1.540460	0.793912	-4.691867	H	2.258512	0.554960	-4.530802	H	0.195808	1.566636	-5.068670
N	1.103647	-1.986480	-0.889373	N	-2.040370	-0.178318	-1.107181	N	-1.737321	-1.560787	-0.934200
C	1.063620	-2.640150	1.333381	C	-3.284532	0.343583	0.832437	C	-2.876867	-1.742450	1.136714
C	0.679883	-0.811224	2.759179	C	-2.024345	0.317632	2.801150	C	-1.720869	-0.812567	2.957998

C	1.108856	-3.565257	2.417953	C	-4.479209	0.714918	1.528397	C	-3.992224	-2.096801	1.961692
C	1.222102	-3.048407	-0.027367	C	-3.277118	0.151789	-0.594546	C	-2.857972	-2.027096	-0.278247
C	0.694766	-1.668317	3.882139	C	-3.150460	0.697328	3.568409	C	-2.784594	-1.109450	3.834580
H	0.528565	0.267611	2.835038	H	-1.043047	0.148884	3.258352	H	-0.802487	-0.317551	3.290542
C	0.908675	-3.030430	3.722300	C	-4.369461	0.893963	2.936603	C	-3.913657	-1.749255	3.337590
C	1.341313	-4.933812	2.104702	C	-5.677769	0.878351	0.780718	C	-5.098015	-2.764444	1.364451
C	1.468112	-4.402749	-0.299818	C	-4.485747	0.305742	-1.292518	C	-3.960507	-2.720386	-0.813497
H	0.537986	-1.233831	4.873604	H	-3.045388	0.828742	4.649502	H	-2.705167	-0.837512	4.891015
H	0.924220	-3.699996	4.588583	H	-5.256315	1.186270	3.509487	H	-4.752944	-1.993385	3.998146
C	1.522871	-5.318143	0.777449	C	-5.661109	0.665208	-0.593596	C	-5.056001	-3.070637	0.009424
H	1.373615	-5.670614	2.913119	H	-6.598833	1.166220	1.297468	H	-5.960935	-3.034267	1.981543
H	1.600179	-4.719056	-1.335296	H	-4.486217	0.157722	-2.372357	H	-3.955487	-2.955869	-1.877268
H	1.709012	-6.373914	0.551134	H	-6.588584	0.782416	-1.165110	H	-5.901316	-3.596002	-0.448709
N	0.859009	-1.293102	1.524105	N	-2.096480	0.151413	1.481946	N	-1.777199	-1.118488	1.659048
C	1.202946	-2.005485	-2.254424	C	-1.759665	-0.373174	-2.440839	C	-1.564940	-1.670210	-2.303850
O	1.285100	-2.998002	-2.980368	O	-2.506808	-0.094235	-3.383744	O	-2.407437	-2.083586	-3.106937
O	0.677373	1.419952	0.741404	O	0.876362	-0.770426	1.257913	O	0.946172	0.134891	1.520041
C	-0.261782	2.326734	0.626271	C	2.130136	-0.540184	0.935043	C	1.913738	0.915251	1.113218
C	-1.538748	2.078326	0.015784	C	2.511615	0.505925	0.025011	C	1.755185	1.807512	-0.010672
C	-0.017773	3.659239	1.134338	C	3.186232	-1.318133	1.536864	C	3.181313	0.952812	1.807390
C	-2.511779	3.102800	-0.111179	C	3.865750	0.719638	-0.329834	C	2.812909	2.631045	-0.463609
C	-1.875839	0.757832	-0.453845	C	1.515740	1.399126	-0.513178	C	0.456638	1.937584	-0.624851
C	-1.016432	4.619582	0.976395	C	4.497504	-1.069695	1.130468	C	4.194927	1.758418	1.288835
C	-2.272727	4.387502	0.356444	C	4.878176	-0.076202	0.190064	C	4.059637	2.597504	0.149723
H	-3.454493	2.838331	-0.593295	H	4.077574	1.524229	-1.035724	H	2.613845	3.280735	-1.318390
N	-1.098553	-0.292003	-0.495374	N	0.216009	1.294789	-0.398279	N	-0.529598	1.087821	-0.530596
O	-3.150701	0.545969	-0.881100	O	1.944562	2.490548	-1.197772	O	0.176828	3.059073	-1.335125
H	-0.818773	5.626908	1.351380	H	5.290616	-1.683598	1.564395	H	5.162760	1.752707	1.797022
C	-1.889240	-1.462535	-0.899813	C	-0.423443	2.402519	-1.121471	C	-1.715042	1.610260	-1.216795
C	-3.209929	-0.797147	-1.433007	C	0.795966	3.357089	-1.415998	C	-1.254613	3.069221	-1.611018
H	-1.388783	-1.983814	-1.729821	H	-0.800028	2.010120	-2.082150	H	-1.862859	1.031429	-2.141470
C	-2.049460	-2.434669	0.252635	C	-1.587630	2.993776	-0.362869	C	-2.958164	1.456166	-0.367452
H	-3.135133	-0.693954	-2.530531	H	0.808770	3.647563	-2.477690	H	-1.368908	3.218985	-2.696096
C	-2.317761	-1.973841	1.553458	C	-1.490833	3.255657	1.015374	C	-2.959194	1.826674	0.989442
C	-1.925440	-3.815132	0.027619	C	-2.787346	3.277693	-1.034419	C	-4.115418	0.887500	-0.923682
C	-2.464590	-2.880427	2.610234	C	-2.575307	3.804591	1.707681	C	-4.104444	1.642133	1.771609
H	-2.390216	-0.898039	1.743107	H	-0.564573	3.013320	1.544583	H	-2.049672	2.241112	1.435007
C	-2.069834	-4.724445	1.083797	C	-3.875478	3.827497	-0.342202	C	-5.263236	0.698575	-0.141209
H	-1.688681	-4.176640	-0.978830	H	-2.879266	3.032481	-2.098320	H	-4.103441	0.554046	-1.967506
C	-2.341612	-4.258259	2.377228	C	-3.769684	4.093895	1.029286	C	-5.259662	1.077560	1.207709
H	-2.666276	-2.509904	3.620621	H	-2.492503	3.999410	2.781800	H	-4.093322	1.929135	2.828179
H	-1.952889	-5.796752	0.898270	H	-4.812818	4.026054	-0.871220	H	-6.151180	0.233422	-0.580649
H	-2.445131	-4.966940	3.205732	H	-4.622657	4.512638	1.573799	H	-6.151062	0.920184	1.824090
C	1.499082	0.588016	-2.192468	C	0.396646	-1.803932	-1.986875	C	1.035485	-1.175010	-2.372864
C	4.001808	-0.138383	-2.070996	C	-1.338136	-3.718813	-1.845016	C	1.102155	-3.736178	-2.017417
C	5.257472	0.262635	-1.313321	C	-1.629614	-4.910376	-0.949112	C	1.922703	-4.739863	-1.228158
H	4.026855	-0.131401	-3.169252	H	-1.151006	-3.898612	-2.911988	H	1.054855	-3.838830	-3.109665

O	3.777845	-1.470023	-1.576834	O	-2.520466	-2.918997	-1.664201	O	-0.205085	-3.904861	-1.435758
C	3.811754	-1.144856	-0.165537	C	-2.490693	-2.884088	-0.218078	C	0.188267	-3.737153	-0.058879
C	5.139580	-0.401577	-0.072847	C	-2.385443	-4.367523	0.112142	C	1.326791	-4.742209	0.053081
C	6.321731	1.121736	-1.574229	C	-1.254635	-6.251523	-0.955682	C	3.066761	-5.487726	-1.492025
H	3.689369	-2.053471	0.438969	H	-3.356765	-2.334901	0.172469	H	-0.677717	-3.861960	0.606064
C	6.084601	-0.214143	0.933911	C	-2.777096	-5.156110	1.192731	C	1.872208	-5.487285	1.098441
C	7.298283	1.288571	-0.570293	C	-1.676937	-7.061241	0.118971	C	3.601072	-6.271689	-0.447860
H	6.411259	1.648042	-2.530936	H	-0.658306	-6.675159	-1.771287	H	3.538682	-5.481024	-2.480752
C	7.180429	0.631109	0.663972	C	-2.425793	-6.521204	1.176436	C	3.013008	-6.269113	0.827033
H	5.991744	-0.713208	1.904719	H	-3.350353	-4.737696	2.027306	H	1.426897	-5.479519	2.099310
H	8.161460	1.936585	-0.756683	H	-1.420477	-8.126112	0.128051	H	4.484291	-6.892228	-0.633778
H	7.953821	0.774004	1.426549	H	-2.745118	-7.171865	1.997856	H	3.445170	-6.888208	1.620812
C	2.821968	0.656275	-1.405705	C	-0.246093	-2.862789	-1.097613	C	1.512802	-2.309916	-1.480847
H	3.074345	1.723420	-1.312398	H	0.564354	-3.516171	-0.738418	H	2.611771	-2.235521	-1.429724
C	2.743923	-0.031794	-0.024525	C	-1.083554	-2.319288	0.090867	C	0.908935	-2.361913	-0.063092
H	2.936822	0.639358	0.825868	H	-0.713064	-2.636477	1.078748	H	1.649623	-2.246022	0.739892
Co	0.818611	-0.315584	-0.056710	Co	-0.625372	-0.405678	0.160745	Co	-0.364030	-0.731037	0.271054
C	1.324828	4.015114	1.804494	C	2.869637	-2.405382	2.581643	C	3.382715	0.143738	3.102953
C	-3.286291	5.536227	0.232371	C	6.355192	0.073405	-0.205868	C	5.262202	3.420048	-0.338772
C	-2.661750	6.682885	-0.600236	C	6.840886	-1.249127	-0.849256	C	6.415962	2.458039	-0.715540
H	-3.371408	7.525283	-0.693556	H	7.904754	-1.171315	-1.138635	H	7.297206	3.027792	-1.062880
H	-1.739817	7.067705	-0.130731	H	6.740214	-2.098816	-0.151945	H	6.727778	1.843805	0.146873
H	-2.404317	6.331427	-1.614876	H	6.251023	-1.481106	-1.753648	H	6.103800	1.773660	-1.523948
C	-3.643817	6.062752	1.644002	C	7.202856	0.375465	1.054052	C	5.732740	4.371032	0.789069
H	-2.749976	6.430570	2.177083	H	7.117067	-0.430055	1.803702	H	6.028545	3.811794	1.693502
H	-4.363996	6.898474	1.574461	H	8.270379	0.474838	0.785751	H	6.605540	4.962202	0.456695
H	-4.097598	5.262578	2.254548	H	6.874481	1.317018	1.527844	H	4.926016	5.070158	1.070662
C	-4.584282	5.080653	-0.461413	C	6.562138	1.214677	-1.219848	C	4.909716	4.267240	-1.576435
H	-4.390110	4.715841	-1.485285	H	5.996423	1.036748	-2.151256	H	4.584758	3.634047	-2.420822
H	-5.083604	4.273505	0.102622	H	6.245833	2.187780	-0.805288	H	4.104327	4.990006	-1.357683
H	-5.288109	5.928518	-0.532941	H	7.631515	1.291126	-1.483790	H	5.796160	4.838265	-1.904026
C	2.475681	3.850721	0.781351	C	2.033849	-3.531309	1.926307	C	3.155435	-1.368117	2.857613
H	2.515578	2.816165	0.413090	H	1.090525	-3.133571	1.527967	H	2.116063	-1.555577	2.553504
H	2.329961	4.530750	-0.077077	H	2.595741	-3.999510	1.098604	H	3.829227	-1.744843	2.068011
H	3.446049	4.093307	1.251604	H	1.797206	-4.315606	2.668036	H	3.361700	-1.935304	3.783680
C	1.349145	5.473134	2.308291	C	4.151447	-3.045424	3.153873	C	4.803761	0.317555	3.676395
H	1.225252	6.197581	1.484117	H	4.738547	-3.564067	2.375393	H	5.575992	-0.050883	2.977861
H	0.561840	5.662720	3.059384	H	4.802239	-2.298130	3.641474	H	5.026483	1.372090	3.916875
H	2.324491	5.674510	2.784721	H	3.871732	-3.795969	3.913531	H	4.891855	-0.264479	4.610431
C	1.580167	3.096911	3.025745	C	2.086317	-1.786336	3.767180	C	2.373799	0.652887	4.164433
H	0.754736	3.181329	3.755191	H	2.686390	-0.998276	4.256117	H	2.562944	1.714849	4.400884
H	1.670164	2.048338	2.708770	H	1.139804	-1.345887	3.421102	H	1.342646	0.555163	3.790958
H	2.517700	3.392564	3.530890	H	1.864522	-2.566046	4.518535	H	2.472604	0.067507	5.097145
C	-4.495630	-1.481806	-1.054675	C	0.888997	4.578585	-0.528931	C	-1.924369	4.186031	-0.843197
C	-4.921403	-2.597193	-1.797775	C	0.054993	5.680430	-0.792772	C	-3.248441	4.536595	-1.165070
C	-5.239857	-1.073956	0.064452	C	1.736621	4.609000	0.590515	C	-1.280883	4.832105	0.224809
C	-6.069849	-3.303769	-1.419406	C	0.053527	6.788410	0.061929	C	-3.925590	5.506909	-0.418066

H	-4.347268	-2.917726	-2.675066	H	-0.613137	5.661201	-1.660793	H	-3.758849	4.033007	-1.993575
C	-6.393121	-1.776938	0.437487	C	1.736666	5.721548	1.444411	C	-1.959749	5.807053	0.970252
H	-4.911248	-0.199335	0.632575	H	2.399112	3.761473	0.788898	H	-0.246410	4.570804	0.465543
C	-6.808692	-2.895192	-0.299119	C	0.892622	6.810262	1.186528	C	-3.283300	6.143325	0.655240
H	-6.390970	-4.173125	-2.002806	H	-0.606669	7.636260	-0.148485	H	-4.958715	5.765719	-0.672527
H	-6.968933	-1.449993	1.309857	H	2.400886	5.735734	2.315160	H	-1.449429	6.305597	1.801313
H	-7.708490	-3.445315	-0.004221	H	0.891147	7.676568	1.856464	H	-3.813050	6.902203	1.240700

Transition State (2-3) – reductive elimination^A pathway: In Co catalyzed reaction energy profile

TS2A ¹ : $\nu_{\text{lowest}} = -462.0891 \text{ cm}^{-1}$				TS2A ³ : $\nu_{\text{lowest}} = -476.2876 \text{ cm}^{-1}$				TS2A ⁵ : $\nu_{\text{lowest}} = -420.3975 \text{ cm}^{-1}$			
113				113				113			
C	-0.540592	0.489254	2.880733	C	-0.170796	0.670233	2.695530	C	-0.726825	0.664631	2.418237
C	1.842576	0.933726	2.711196	C	2.181477	1.095721	2.255314	C	0.423215	2.734390	1.875351
C	-0.288879	-0.371139	3.966382	C	0.198668	-0.256752	3.688553	C	0.273471	0.384917	3.370575
C	2.092259	0.017396	3.741538	C	2.541632	0.128776	3.203370	C	1.449227	2.413215	2.771221
H	2.675120	1.453448	2.225164	H	2.956780	1.623952	1.690389	H	0.474059	3.664576	1.299759
C	1.021538	-0.614269	4.393327	C	1.547873	-0.534561	3.937452	C	1.363617	1.242912	3.540956
H	-1.144540	-0.867826	4.434624	H	-0.601012	-0.765612	4.235557	H	0.176047	-0.535793	3.954510
H	3.123542	-0.190902	4.045061	H	3.598881	-0.104554	3.364787	H	2.311525	3.079914	2.871305
H	1.209734	-1.305569	5.221297	H	1.823589	-1.278406	4.692007	H	2.150982	0.994991	4.259939
N	-2.028370	0.726456	0.937074	N	-1.905657	1.024308	1.010817	N	-2.095832	-0.533118	0.809259
C	-3.182077	0.653759	-1.132720	C	-3.378012	0.686360	-0.850905	C	-2.739055	-1.994127	-0.978184
C	-1.746627	0.335412	-2.968045	C	-2.334450	0.003760	-2.830976	C	-1.420610	-1.876851	-2.937077
C	-4.340037	0.652780	-1.968391	C	-4.670281	0.677040	-1.468621	C	-3.624324	-2.955687	-1.579715
C	-3.288738	0.775101	0.283511	C	-3.230636	1.037978	0.528882	C	-2.964398	-1.539963	0.364990
C	-2.844094	0.290853	-3.847169	C	-3.566063	-0.020290	-3.516890	C	-2.247226	-2.794061	-3.595451
H	-0.711841	0.247759	-3.309726	H	-1.396367	-0.262738	-3.329559	H	-0.543655	-1.433500	-3.419653
C	-4.139551	0.456167	-3.366168	C	-4.733914	0.311831	-2.844086	C	-3.344727	-3.340513	-2.924551
C	-5.609336	0.804710	-1.343660	C	-5.802535	1.017914	-0.679910	C	-4.702383	-3.460651	-0.808111
C	-4.550410	0.955872	0.863791	C	-4.367278	1.387746	1.269354	C	-4.061974	-2.057235	1.092712
H	-2.656433	0.143254	-4.915240	H	-3.583508	-0.305647	-4.573024	H	-2.021582	-3.075403	-4.628546
H	-5.002012	0.433743	-4.039744	H	-5.703987	0.293095	-3.351559	H	-3.998045	-4.067016	-3.419069
C	-5.696951	0.962019	0.035508	C	-5.640790	1.362248	0.657790	C	-4.902614	-3.013153	0.505047
H	-6.512690	0.779975	-1.962082	H	-6.795982	1.005416	-1.140059	H	-5.372587	-4.202952	-1.253953
H	-4.642574	1.039476	1.945424	H	-4.261515	1.646670	2.322533	H	-4.222041	-1.725049	2.119236
H	-6.679796	1.075716	0.505132	H	-6.517151	1.623966	1.260151	H	-5.734744	-3.418091	1.091231
N	-1.902699	0.507035	-1.638246	N	-2.235928	0.342776	-1.536330	N	-1.660614	-1.488169	-1.661298
C	-1.933197	0.497680	2.338865	C	-1.627308	0.754713	2.361152	C	-1.733501	-0.420065	2.166246
O	-2.901709	0.180596	3.025782	O	-2.496291	0.422079	3.170574	O	-2.033215	-1.241832	3.029194
O	0.866323	0.277300	-1.426075	O	1.142696	0.585481	-1.314869	O	0.472662	1.031585	-1.234375
C	2.096703	0.006587	-1.048023	C	2.262077	-0.001991	-0.980562	C	1.676326	1.454057	-0.920886
C	2.414032	-0.993360	-0.061100	C	2.310599	-1.182676	-0.153509	C	2.561216	0.751849	-0.022591
C	3.201998	0.709893	-1.654756	C	3.520482	0.534021	-1.449343	C	2.168064	2.674950	-1.515585
C	3.752909	-1.308385	0.274589	C	3.549640	-1.763356	0.222121	C	3.823250	1.294199	0.335045
C	1.336876	-1.709395	0.567806	C	1.102625	-1.781039	0.360517	C	2.193928	-0.515159	0.559169
C	4.496897	0.380483	-1.252427	C	4.701646	-0.072684	-1.024553	C	3.409509	3.159077	-1.106280

C	4.817536	-0.623283	-0.298743	C	4.759715	-1.213625	-0.179270	C	4.257372	2.512008	-0.168113
H	3.910682	-2.092134	1.018963	H	3.512447	-2.647909	0.860101	H	4.431581	0.719576	1.035484
N	0.104418	-1.280424	0.661207	N	-0.125586	-1.332954	0.264885	N	1.058458	-1.153420	0.423101
O	1.558910	-2.939494	1.103332	O	1.224386	-2.946074	1.066522	O	3.097547	-1.165557	1.344766
H	5.326645	0.932530	-1.701703	H	5.649521	0.351335	-1.366768	H	3.760538	4.098829	-1.540085
C	-0.744639	-2.322096	1.265932	C	-1.008359	-2.196246	1.066985	C	1.054905	-2.332958	1.302642
C	0.265043	-3.528193	1.417145	C	-0.112984	-3.468830	1.283782	C	2.588937	-2.519086	1.561990
H	-1.054271	-1.998552	2.272347	H	-1.145605	-1.719520	2.053191	H	0.585961	-2.033519	2.258039
C	-1.989161	-2.527588	0.425532	C	-2.372951	-2.374589	0.446488	C	0.225085	-3.447389	0.708870
H	0.306401	-3.853358	2.468819	H	-0.165084	-3.799337	2.332446	H	2.779737	-2.764566	2.617240
C	-1.891042	-2.668993	-0.973466	C	-2.517613	-2.749008	-0.902142	C	0.428179	-3.876584	-0.617189
C	-3.257432	-2.509664	1.024791	C	-3.522235	-2.139564	1.220073	C	-0.842352	-3.983127	1.449993
C	-3.044179	-2.791936	-1.753630	C	-3.790782	-2.899627	-1.460985	C	-0.416412	-4.836393	-1.183982
H	-0.906554	-2.663951	-1.450970	H	-1.625624	-2.908886	-1.514830	H	1.236183	-3.438970	-1.211137
C	-4.416499	-2.626326	0.240692	C	-4.799581	-2.288209	0.659888	C	-1.688923	-4.944919	0.880653
H	-3.342524	-2.354472	2.105418	H	-3.413410	-1.795900	2.254197	H	-1.044410	-3.604191	2.457059
C	-4.312079	-2.766490	-1.147791	C	-4.935547	-2.671467	-0.680476	C	-1.476860	-5.372025	-0.436083
H	-2.956779	-2.890279	-2.840228	H	-3.892064	-3.187555	-2.512414	H	-0.260016	-5.153550	-2.219802
H	-5.400881	-2.582457	0.717595	H	-5.686532	-2.083209	1.267818	H	-2.534405	-5.332793	1.456818
H	-5.215120	-2.841215	-1.762468	H	-5.931626	-2.778576	-1.123276	H	-2.151203	-6.105652	-0.889740
C	0.530341	1.191225	2.282433	C	0.830296	1.384419	2.000617	C	-0.679856	1.879349	1.692564
C	-0.090851	3.631058	2.193898	C	0.140676	3.856710	1.896398	C	-3.004844	2.939227	1.809100
C	-0.105460	4.795569	1.224161	C	0.177340	4.967685	0.865229	C	-3.921078	3.724028	0.890840
H	0.461928	3.730688	3.136348	H	0.688417	3.983104	2.838410	H	-2.656978	3.406378	2.739203
O	-1.491963	3.411077	2.441449	O	-1.272262	3.707329	2.141055	O	-3.783824	1.760265	2.087756
C	-1.906923	3.351779	1.064398	C	-1.677948	3.584006	0.766368	C	-4.071914	1.415033	0.711460
C	-1.289607	4.613431	0.482143	C	-0.998641	4.776257	0.112791	C	-4.604871	2.729485	0.157670
C	0.792887	5.813005	0.910810	C	1.113440	5.934763	0.506377	C	-4.097066	5.075892	0.612126
H	-2.992261	3.213366	0.976736	H	-2.767959	3.495068	0.676451	H	-4.708309	0.522581	0.643005
C	-1.602906	5.439377	-0.595905	C	-1.268276	5.545541	-1.017724	C	-5.478743	3.068660	-0.876780
C	0.464773	6.674050	-0.156045	C	0.830559	6.738995	-0.616098	C	-5.003686	5.426260	-0.411243
H	1.722784	5.950605	1.472854	H	2.038981	6.075766	1.074535	H	-3.559898	5.850430	1.170316
C	-0.713495	6.489986	-0.897382	C	-0.340743	6.547460	-1.366382	C	-5.680643	4.437166	-1.143485
H	-2.511327	5.287329	-1.188442	H	-2.172735	5.388431	-1.615115	H	-6.003003	2.302249	-1.457542
H	1.138262	7.498985	-0.411338	H	1.534689	7.525118	-0.908504	H	-5.183697	6.482713	-0.636721
H	-0.943881	7.173691	-1.721243	H	-0.535589	7.186581	-2.233990	H	-6.381498	4.735659	-1.930599
C	0.269514	2.335124	1.339879	C	0.471155	2.529412	1.093519	C	-1.854859	2.356831	0.871902
H	1.147900	2.504307	0.699773	H	1.295736	2.697871	0.387794	H	-1.503921	3.137833	0.179115
C	-1.005965	2.218136	0.496149	C	-0.846855	2.345461	0.315080	C	-2.662662	1.291800	0.146991
H	-0.861034	2.323985	-0.583066	H	-0.747685	2.339949	-0.801474	H	-2.525771	1.133962	-0.929743
Co	-0.637750	0.140986	-0.312461	Co	-0.585232	0.418886	-0.456408	Co	-0.494000	-0.419718	-0.451203
C	2.942095	1.797573	-2.715190	C	3.537717	1.730469	-2.422258	C	1.348066	3.398344	-2.603009
C	6.287848	-0.890974	0.060816	C	6.124429	-1.774983	0.251103	C	5.587913	3.166306	0.235920
C	6.915817	0.398497	0.644969	C	6.893426	-0.687479	1.041507	C	5.296452	4.541332	0.886291
H	7.977955	0.231648	0.902453	H	7.885151	-1.061798	1.355698	H	6.238504	5.040050	1.178693
H	6.869387	1.232940	-0.076129	H	7.050506	0.219328	0.431915	H	4.759305	5.210825	0.192271
H	6.381677	0.710930	1.559771	H	6.330861	-0.394222	1.945795	H	4.673696	4.419805	1.790349

C	7.063504	-1.307889	-1.212832	C	6.942724	-2.174938	-1.000890	C	6.471111	3.367805	-1.019712
H	7.020457	-0.522359	-1.987086	H	7.107954	-1.312199	-1.669260	H	5.973517	4.009741	-1.767080
H	8.127530	-1.492459	-0.976195	H	7.932747	-2.569727	-0.707280	H	7.428092	3.848082	-0.745680
H	6.637336	-2.231111	-1.642803	H	6.414580	-2.954314	-1.577531	H	6.693488	2.398351	-1.498809
C	6.425377	-2.015401	1.105007	C	5.974257	-3.015774	1.151906	C	6.365820	2.302946	1.247221
H	5.911267	-1.757699	2.047795	H	5.417274	-2.780125	2.075776	H	5.787770	2.146035	2.174830
H	6.006022	-2.966667	0.733424	H	5.445161	-3.832796	0.631051	H	6.617594	1.313641	0.826824
H	7.491911	-2.183248	1.337144	H	6.971356	-3.389936	1.444167	H	7.310920	2.805006	1.518973
C	2.023226	2.905292	-2.138889	C	2.863704	2.971886	-1.786398	C	-0.021437	3.858144	-2.047715
H	1.053229	2.486669	-1.835153	H	1.802049	2.771027	-1.584456	H	-0.609286	2.992780	-1.712341
H	2.494823	3.384671	-1.262232	H	3.364142	3.248528	-0.840691	H	0.115103	4.551087	-1.197913
H	1.847090	3.688590	-2.898337	H	2.931304	3.836704	-2.471359	H	-0.589769	4.390204	-2.832051
C	4.246824	2.474731	-3.181712	C	4.974277	2.131758	-2.814976	C	2.078539	4.647440	-3.137355
H	4.771755	2.972940	-2.347187	H	5.565861	2.454399	-1.939488	H	2.240306	5.400826	-2.345829
H	4.941564	1.754537	-3.648611	H	5.511975	1.304514	-3.310833	H	3.057151	4.394629	-3.582228
H	4.006951	3.244868	-3.935793	H	4.934671	2.978239	-3.522970	H	1.463288	5.117283	-3.924385
C	2.275235	1.150400	-3.954871	C	2.780824	1.342170	-3.718302	C	1.125785	2.434116	-3.797039
H	2.953310	0.409092	-4.413076	H	3.277250	0.488584	-4.213101	H	2.094338	2.122884	-4.227097
H	1.344094	0.640611	-3.666755	H	1.741582	1.062381	-3.487301	H	0.575788	1.536536	-3.475801
H	2.041279	1.921490	-4.712045	H	2.773541	2.193618	-4.423962	H	0.544463	2.941693	-4.588489
C	-0.004293	-4.706563	0.507862	C	-0.384257	-4.627118	0.349524	C	3.286932	-3.498876	0.646514
C	-1.083694	-5.561863	0.795515	C	-1.490844	-5.461060	0.593720	C	3.151098	-4.876989	0.895922
C	0.758714	-4.925535	-0.650291	C	0.407135	-4.849834	-0.789702	C	4.005745	-3.069965	-0.481937
C	-1.405999	-6.611192	-0.072467	C	-1.812251	-6.491861	-0.296712	C	3.712510	-5.813871	0.020795
H	-1.687921	-5.393334	1.693913	H	-2.116606	-5.287818	1.476278	H	2.584702	-5.217618	1.769742
C	0.436213	-5.979296	-1.517703	C	0.084068	-5.883152	-1.681313	C	4.567313	-4.010301	-1.358008
H	1.605652	-4.267914	-0.865363	H	1.278795	-4.214792	-0.972327	H	4.129631	-1.999762	-0.670814
C	-0.648039	-6.820898	-1.234820	C	-1.027179	-6.703146	-1.440541	C	4.419074	-5.382385	-1.112156
H	-2.253664	-7.265447	0.156836	H	-2.680363	-7.129647	-0.099744	H	3.594555	-6.883827	0.221234
H	1.036527	-6.141219	-2.419406	H	0.706509	-6.048128	-2.567376	H	5.124840	-3.666683	-2.235816
H	-0.901280	-7.640778	-1.915285	H	-1.278798	-7.508516	-2.138822	H	4.856817	-6.114810	-1.798581

Transition State (2-3) – nucleophilic addition^B pathway: In Co catalyzed reaction energy profile

TS2B ¹ : $\nu_{\text{lowest}} = -343.2527 \text{ cm}^{-1}$				TS2B ³ : $\nu_{\text{lowest}} = -423.2980 \text{ cm}^{-1}$				TS2B ⁵ : $\nu_{\text{lowest}} = -408.1587 \text{ cm}^{-1}$			
113				113				113			
C	1.315507	-1.163362	-2.486021	C	1.440034	-0.305895	-2.277884	C	1.254797	-0.750692	-2.364902
C	1.221967	1.245781	-2.917343	C	0.973291	2.053527	-1.862794	C	1.336533	1.673153	-2.154803
C	0.309845	-1.379916	-3.448180	C	0.484084	-0.330281	-3.298319	C	0.362762	-0.642036	-3.439497
C	0.191938	1.027463	-3.830895	C	-0.037030	2.005022	-2.830357	C	0.392417	1.780821	-3.185888
H	1.579082	2.260388	-2.712741	H	1.180598	2.988489	-1.333455	H	1.728461	2.574924	-1.672001
C	-0.247875	-0.287243	-4.114686	C	-0.258973	0.828685	-3.570232	C	-0.070976	0.629603	-3.845626
H	-0.019542	-2.404677	-3.650616	H	0.317792	-1.261681	-3.850066	H	0.013701	-1.550373	-3.942000
H	-0.270141	1.876357	-4.345759	H	-0.640962	2.896516	-3.026662	H	0.029694	2.768381	-3.489099
H	-1.031851	-0.442138	-4.865021	H	-1.022541	0.819131	-4.356012	H	-0.779463	0.726982	-4.675877
N	0.711593	-2.325388	-0.544654	N	1.430862	-1.711881	-0.409555	N	0.844509	-2.251092	-0.554640
C	0.479880	-2.390796	1.782200	C	1.114171	-2.508254	1.757670	C	-0.053836	-3.356882	1.353697

C	0.063805	-0.253993	2.678384	C	0.129325	-0.902603	3.150384	C	-0.971165	-1.946474	2.988263
C	0.344982	-3.030448	3.053858	C	1.137308	-3.492096	2.788335	C	-0.363021	-4.527783	2.118864
C	0.776645	-3.105027	0.579801	C	1.602945	-2.774882	0.435381	C	0.621978	-3.445195	0.069486
C	-0.137873	-0.819312	3.957454	C	0.091427	-1.824622	4.218018	C	-1.292342	-3.043958	3.814362
H	-0.004373	0.819805	2.494675	H	-0.241865	0.121820	3.242498	H	-1.201102	-0.916221	3.281322
C	0.004736	-2.187006	4.150016	C	0.593505	-3.109365	4.046398	C	-0.996967	-4.327595	3.376084
C	0.572373	-4.431014	3.106744	C	1.697587	-4.764984	2.477104	C	-0.021225	-5.804253	1.590809
C	1.057031	-4.480701	0.685188	C	2.178399	-4.034029	0.173071	C	0.953550	-4.738401	-0.398992
H	-0.392842	-0.155631	4.788621	H	-0.330404	-1.507896	5.176393	H	-1.774441	-2.870277	4.780812
H	-0.139692	-2.626275	5.142948	H	0.574828	-3.831751	4.869385	H	-1.247241	-5.198953	3.991343
C	0.943957	-5.111247	1.943260	C	2.210780	-5.002108	1.202250	C	0.621341	-5.881596	0.357837
H	0.469482	-4.958889	4.059644	H	1.720484	-5.543483	3.246084	H	-0.260356	-6.705195	2.164650
H	1.346616	-5.028174	-0.213508	H	2.568078	-4.231303	-0.826769	H	1.465413	-4.813912	-1.358886
H	1.147972	-6.186466	2.003504	H	2.647847	-5.981950	0.979568	H	0.888633	-6.865223	-0.044875
N	0.370591	-1.029131	1.631703	N	0.631010	-1.238353	1.954614	N	-0.379684	-2.106431	1.801873
C	1.812295	-2.283181	-1.533052	C	2.069630	-1.571009	-1.699135	C	1.638898	-2.098939	-1.746055
O	2.314742	-3.367044	-1.945796	O	2.477981	-2.537803	-2.383578	O	2.012345	-3.063897	-2.473798
O	0.858235	1.384753	0.272064	O	0.100499	1.402813	1.120856	O	0.432632	0.956515	1.248645
C	-0.031107	2.341618	0.306542	C	-0.882909	2.221580	0.820016	C	0.012563	2.156209	0.919812
C	-1.379318	2.160391	-0.163483	C	-1.982148	1.843848	-0.024731	C	-1.035659	2.391527	-0.043943
C	0.327099	3.645212	0.820430	C	-0.879162	3.560165	1.356950	C	0.587014	3.310766	1.570354
C	-2.317190	3.226311	-0.154327	C	-3.028202	2.753389	-0.321040	C	-1.425600	3.709605	-0.395970
C	-1.815166	0.872040	-0.628048	C	-2.047441	0.516130	-0.586132	C	-1.731246	1.296957	-0.677977
C	-0.647881	4.641170	0.817489	C	-1.935533	4.407417	1.020224	C	0.167868	4.577530	1.164987
C	-1.976013	4.477918	0.336929	C	-3.026746	4.046184	0.187187	C	-0.820586	4.820984	0.174823
H	-3.316419	3.018623	-0.541210	H	-3.829314	2.397855	-0.971666	H	-2.214163	3.813738	-1.143303
N	-1.137438	-0.255086	-0.640392	N	-1.125326	-0.408760	-0.532324	N	-1.477807	0.019580	-0.560626
O	-3.087800	0.745797	-1.080545	O	-3.183947	0.146085	-1.233359	O	-2.792179	1.581665	-1.483854
H	-0.372252	5.623854	1.208237	H	-1.922266	5.423892	1.421559	H	0.625078	5.446209	1.645238
C	-2.039359	-1.374587	-0.966682	C	-1.631305	-1.656960	-1.111485	C	-2.386339	-0.746995	-1.425173
C	-3.211329	-0.595713	-1.645446	C	-2.963948	-1.176521	-1.800885	C	-3.477811	0.328611	-1.775825
H	-1.541151	-2.036490	-1.688592	H	-0.926293	-2.009937	-1.880081	H	-1.830095	-0.983492	-2.348066
C	-2.402842	-2.174447	0.267674	C	-1.762578	-2.729153	-0.048291	C	-2.783710	-2.054700	-0.777320
H	-2.986230	-0.501075	-2.723646	H	-2.773321	-1.030182	-2.878766	H	-3.683796	0.323105	-2.857135
C	-2.805217	-1.538947	1.456001	C	-2.336451	-2.438467	1.202042	C	-3.373294	-2.096275	0.500802
C	-2.332504	-3.576326	0.232709	C	-1.294104	-4.028215	-0.300635	C	-2.468945	-3.263049	-1.421886
C	-3.132572	-2.294331	2.588359	C	-2.448416	-3.434333	2.179075	C	-3.657017	-3.323504	1.109114
H	-2.843388	-0.445832	1.505509	H	-2.678329	-1.421043	1.418183	H	-3.595328	-1.162765	1.025859
C	-2.657157	-4.334538	1.364777	C	-1.402979	-5.026999	0.676435	C	-2.743292	-4.494159	-0.809926
H	-1.989031	-4.072581	-0.680652	H	-0.816180	-4.250240	-1.260990	H	-1.972598	-3.237858	-2.398187
C	-3.057727	-3.694543	2.545322	C	-1.982739	-4.731909	1.917398	C	-3.341348	-4.525669	0.456279
H	-3.435799	-1.787896	3.510432	H	-2.891457	-3.195294	3.151316	H	-4.113126	-3.342877	2.104082
H	-2.576187	-5.425369	1.330144	H	-1.017190	-6.030924	0.473651	H	-2.468676	-5.426036	-1.313564
H	-3.298828	-4.285216	3.435266	H	-2.059294	-5.508226	2.685983	H	-3.545775	-5.485204	0.942317
C	1.800158	0.143139	-2.242320	C	1.730846	0.895689	-1.581239	C	1.782535	0.402942	-1.754621
C	4.378150	0.163948	-2.089491	C	4.156519	1.551616	-1.791886	C	4.289940	0.567509	-1.561768
C	5.443626	0.283507	-1.018335	C	5.481713	1.512198	-1.054226	C	5.443103	0.246947	-0.626833

H	4.441941	0.812739	-2.973935	H	3.845904	2.494318	-2.262516	H	4.264457	1.557095	-2.037821
O	4.464076	-1.217883	-2.458423	O	4.326494	0.520140	-2.777085	O	4.404813	-0.471089	-2.550767
C	4.383277	-1.775100	-1.136144	C	4.741857	-0.527021	-1.870192	C	4.444226	-1.585063	-1.635376
C	5.443959	-0.984024	-0.393446	C	5.873358	0.155439	-1.110277	C	5.554116	-1.160259	-0.679025
C	6.232978	1.326639	-0.540402	C	6.235354	2.453011	-0.358237	C	6.244959	1.002542	0.224054
H	4.402083	-2.871464	-1.174429	H	4.924691	-1.467160	-2.406855	H	4.509227	-2.540374	-2.170675
C	6.240690	-1.230760	0.725342	C	7.025244	-0.287616	-0.460279	C	6.466727	-1.840824	0.126650
C	7.065599	1.069942	0.568294	C	7.420553	2.016325	0.270280	C	7.195208	0.321940	1.013916
H	6.219573	2.316338	-1.010333	H	5.929241	3.503476	-0.302336	H	6.151434	2.092553	0.280487
C	7.068652	-0.189768	1.189841	C	7.807654	0.667742	0.219359	C	7.304193	-1.076907	0.964452
H	6.234672	-2.205044	1.225818	H	7.325974	-1.340478	-0.484571	H	6.544759	-2.933102	0.104987
H	7.721038	1.860931	0.948599	H	8.048553	2.738280	0.803237	H	7.858080	0.891642	1.674027
H	7.727876	-0.365006	2.047085	H	8.734527	0.354780	0.712247	H	8.052805	-1.581106	1.585171
C	2.997041	0.189685	-1.315586	C	3.066432	0.882929	-0.847000	C	2.953466	0.138881	-0.832252
H	2.945383	1.044487	-0.628463	H	3.033801	1.367811	0.142860	H	2.843850	0.613909	0.152840
C	3.025680	-1.188280	-0.625336	C	3.600597	-0.551886	-0.850406	C	3.181443	-1.377850	-0.787705
H	2.979186	-1.181951	0.476800	H	3.785282	-1.071914	0.095610	H	3.153536	-1.898540	0.174866
Co	0.645931	-0.476719	-0.153672	Co	0.579996	-0.214337	0.315512	Co	0.044577	-0.711329	0.390728
C	-4.591339	-1.151254	-1.432786	C	0.275811	4.040371	2.258529	C	1.608012	3.137923	2.713590
C	-5.003525	-2.253823	-2.202851	C	-4.128592	5.074581	-0.114848	C	-1.180292	6.266163	-0.204891
C	-5.448031	-0.640500	-0.443994	C	-3.503535	6.303075	-0.820670	C	0.083423	6.979445	-0.745563
C	-6.252282	-2.846064	-1.978583	H	-4.278756	7.060049	-1.039408	H	-0.148518	8.025701	-1.016254
H	-4.340660	-2.653988	-2.978936	H	-2.731911	6.781203	-0.192609	H	0.891397	6.995478	0.006307
C	-6.701220	-1.228788	-0.226978	H	-3.029749	6.005847	-1.772721	H	0.466424	6.464816	-1.644297
H	-5.128031	0.221815	0.146840	C	-4.789491	5.525206	1.211018	C	-1.698125	7.015766	1.047286
C	-7.104606	-2.334426	-0.988593	H	-4.053215	5.980688	1.895781	H	-0.940018	7.037087	1.849236
H	-6.562544	-3.706556	-2.580515	H	-5.578012	6.274640	1.015011	H	-1.951974	8.061320	0.794156
H	-7.364409	-0.822353	0.543898	H	-5.248385	4.665233	1.729488	H	-2.602643	6.525703	1.448088
H	-8.082547	-2.795280	-0.814443	C	-5.221092	4.489594	-1.030238	C	-2.271989	6.317345	-1.290735
C	-2.952671	5.663758	0.382416	H	-4.807883	4.173802	-2.004201	H	-1.946354	5.811202	-2.216443
C	-2.381124	6.831849	-0.458496	H	-5.714646	3.617706	-0.566331	H	-3.207592	5.841403	-0.948536
H	-3.065391	7.699305	-0.429524	H	-5.995277	5.252762	-1.223768	H	-2.500236	7.367887	-1.542532
H	-1.399689	7.163137	-0.077086	C	1.611420	3.980260	1.475387	C	2.869753	2.386695	2.223874
H	-2.250853	6.526793	-1.511492	H	1.812458	2.954475	1.133302	H	2.614722	1.361915	1.919721
C	-4.335710	5.286729	-0.181956	H	1.574934	4.648800	0.596558	H	3.330297	2.908699	1.366232
H	-4.270216	4.968563	-1.237130	H	2.447329	4.307623	2.120251	H	3.618758	2.333970	3.034627
H	-4.800743	4.469383	0.396742	C	0.072410	5.495286	2.728584	C	2.066618	4.496369	3.283096
H	-5.009859	6.159794	-0.133994	H	0.031354	6.201163	1.880322	H	2.579877	5.110345	2.521651
C	-3.130415	6.125729	1.849766	H	-0.852036	5.610270	3.321706	H	1.222155	5.080606	3.689312
H	-2.169776	6.436334	2.296018	H	0.921469	5.791397	3.369131	H	2.779723	4.320772	4.107348
H	-3.821572	6.986593	1.902363	C	0.374249	3.148646	3.521487	C	0.946446	2.340249	3.867113
H	-3.544073	5.309792	2.467993	H	-0.576851	3.165035	4.083044	H	0.067249	2.883216	4.257362
C	1.757879	3.930610	1.318299	H	0.606620	2.110391	3.244586	H	0.624655	1.347779	3.516287
C	1.886902	5.345905	1.918896	H	1.173750	3.522461	4.186880	H	1.665492	2.207006	4.696162
H	1.671135	6.133662	1.175898	C	-4.168991	-2.055679	-1.592380	C	-4.767755	0.243325	-0.991223
H	1.213395	5.487891	2.782770	C	-4.287989	-3.240495	-2.340929	C	-5.708540	-0.746615	-1.329714
H	2.922504	5.495938	2.270320	C	-5.139524	-1.751488	-0.624204	C	-5.019439	1.087480	0.103318

C	2.732270	3.836453	0.118210	C	-5.357255	-4.115778	-2.115338	C	-6.875887	-0.902992	-0.573654
H	2.663136	2.848166	-0.358038	H	-3.535459	-3.482970	-3.100328	H	-5.515711	-1.411890	-2.178721
H	2.491630	4.605664	-0.636561	C	-6.213301	-2.625022	-0.404447	C	-6.189919	0.929631	0.859876
H	3.774502	3.988418	0.452902	H	-5.048675	-0.823902	-0.052299	H	-4.298574	1.869867	0.357477
C	2.175823	2.921105	2.417174	C	-6.323220	-3.810272	-1.144771	C	-7.117694	-0.067325	0.527446
H	1.479440	2.972358	3.273836	H	-5.438245	-5.037798	-2.700596	H	-7.597531	-1.681468	-0.842344
H	2.186204	1.892374	2.030418	H	-6.967096	-2.378018	0.350739	H	-6.377222	1.591859	1.711912
H	3.187683	3.167890	2.785993	H	-7.160948	-4.493437	-0.969577	H	-8.030174	-0.189963	1.120419

Intermediate-3 from reductive elimination^A pathway: In Co catalyzed reaction energy profile

Int3A ¹ : $\nu_{\text{lowest}} = 8.1844 \text{ cm}^{-1}$				Int3A ³ : $\nu_{\text{lowest}} = 8.8788 \text{ cm}^{-1}$				Int3A ⁵ : $\nu_{\text{lowest}} = 14.9695 \text{ cm}^{-1}$			
113				113				113			
C	-0.772633	-0.460614	-2.640775	C	-0.481762	-0.809187	-2.413054	C	-0.460315	-0.943184	-2.350624
C	0.544414	-2.419838	-2.060809	C	0.961897	-2.650416	-1.778706	C	0.647766	-2.975031	-1.611892
C	0.147942	-0.140853	-3.652099	C	0.484703	-0.372125	-3.338817	C	0.599045	-0.705814	-3.255487
C	1.493447	-2.059658	-3.027006	C	1.938128	-2.191243	-2.670938	C	1.711552	-2.718612	-2.486007
H	0.701268	-3.311243	-1.444447	H	1.154181	-3.536990	-1.167151	H	0.667944	-3.864808	-0.974754
C	1.282247	-0.938542	-3.846492	C	1.695005	-1.058742	-3.465313	C	1.678562	-1.586809	-3.320925
H	-0.021633	0.765980	-4.241217	H	0.269357	0.524924	-3.926878	H	0.554988	0.193657	-3.876616
H	2.399676	-2.662474	-3.143523	H	2.896364	-2.715370	-2.739287	H	2.568592	-3.397957	-2.512180
H	2.013764	-0.674769	-4.616862	H	2.457945	-0.702708	-4.164472	H	2.507388	-1.387077	-4.007659
N	-2.186603	0.364946	-0.850054	N	-2.279400	-0.157394	-0.892846	N	-2.150384	0.049023	-0.882586
C	-2.721384	1.507525	1.178873	C	-3.195869	1.355044	0.781075	C	-2.966320	1.652804	0.767955
C	-1.362523	0.867710	2.987541	C	-1.929624	1.661711	2.733637	C	-1.835543	1.708682	2.858397
C	-3.497436	2.381274	1.999023	C	-4.245696	2.192824	1.284867	C	-3.949914	2.596215	1.233814
C	-3.011560	1.370469	-0.200325	C	-3.325822	0.763662	-0.501406	C	-3.073790	1.124544	-0.545322
C	-2.092169	1.699135	3.852110	C	-2.938363	2.445540	3.311582	C	-2.788792	2.567139	3.393333
H	-0.519150	0.261988	3.328084	H	-0.995106	1.458128	3.266117	H	-0.972276	1.361931	3.435051
C	-3.154794	2.468466	3.379062	C	-4.097859	2.732317	2.595469	C	-3.843972	3.036404	2.587221
C	-4.537756	3.124010	1.368061	C	-5.360718	2.455837	0.442748	C	-4.948411	3.027682	0.322095
C	-4.033226	2.100974	-0.796389	C	-4.423343	1.050187	-1.311585	C	-4.063136	1.588501	-1.437410
H	-1.806368	1.730930	4.908264	H	-2.786424	2.841102	4.320425	H	-2.693188	2.891177	4.434256
H	-3.719801	3.130576	4.041979	H	-4.885909	3.366001	3.013501	H	-4.585025	3.737983	2.983117
C	-4.787082	2.991840	0.008384	C	-5.436067	1.911688	-0.834441	C	-4.983791	2.547383	-0.996011
H	-5.128646	3.819284	1.973861	H	-6.158193	3.107128	0.816211	H	-5.691723	3.755748	0.664428
H	-4.223236	2.010996	-1.866576	H	-4.480189	0.625207	-2.315898	H	-4.088008	1.211771	-2.461709
H	-5.580115	3.584590	-0.459109	H	-6.290644	2.141492	-1.478875	H	-5.750178	2.913224	-1.687369
N	-1.641292	0.770760	1.663358	N	-2.026541	1.124108	1.491939	N	-1.908784	1.259634	1.566777
C	-1.751265	0.567753	-2.222708	C	-1.651671	0.062372	-2.155635	C	-1.467658	0.115581	-2.159865
O	-2.029796	1.580076	-2.850766	O	-1.955683	1.018285	-2.862792	O	-1.588204	1.098558	-2.886516
O	0.680584	-0.700013	1.403460	O	0.683747	-1.113397	1.197055	O	0.577572	-0.947538	1.269732
C	1.812443	-1.251793	1.012606	C	1.956712	-1.206291	0.897393	C	1.806197	-1.268811	0.929171
C	2.638542	-0.697396	-0.024786	C	2.628371	-0.263905	0.036787	C	2.596582	-0.506852	-0.006435
C	2.276125	-2.454209	1.658408	C	2.742377	-2.292809	1.434596	C	2.421076	-2.427832	1.530704
C	3.875871	-1.283168	-0.381682	C	3.979219	-0.466225	-0.349833	C	3.884576	-0.950604	-0.404494
C	2.188578	0.492122	-0.695237	C	1.952559	0.899456	-0.485238	C	2.113757	0.727525	-0.572979

C	3.487919	-3.005693	1.237433	C	4.060944	-2.439110	1.004084	C	3.683064	-2.815612	1.081945
C	4.319416	-2.451849	0.228021	C	4.708175	-1.561070	0.095183	C	4.435889	-2.120434	0.098698
H	4.452318	-0.794203	-1.170241	H	4.419341	0.271188	-1.022915	H	4.418194	-0.338674	-1.133527
N	0.951699	0.916117	-0.720310	N	0.715858	1.288147	-0.277814	N	0.927217	1.265393	-0.424405
O	3.081717	1.289605	-1.344202	O	2.667149	1.727764	-1.311588	O	2.953448	1.463522	-1.353186
H	3.822522	-3.928807	1.718069	H	4.639520	-3.280215	1.395256	H	4.129650	-3.711678	1.520316
C	0.882785	2.225411	-1.389635	C	0.446262	2.456152	-1.136086	C	0.824498	2.463595	-1.275802
C	2.407568	2.537922	-1.668022	C	1.896232	2.949843	-1.468986	C	2.337731	2.777998	-1.531150
H	0.355853	2.119237	-2.351120	H	-0.002131	2.088156	-2.075637	H	0.368122	2.157456	-2.234996
C	0.107430	3.193475	-0.518873	C	-0.530653	3.418340	-0.506210	C	-0.079419	3.492877	-0.638238
H	2.565146	2.721077	-2.742865	H	1.971714	3.246627	-2.526061	H	2.504726	3.067765	-2.579188
C	0.366395	3.260434	0.865647	C	-0.352854	3.876780	0.812206	C	0.087822	3.863998	0.709945
C	-0.899336	4.000628	-1.069439	C	-1.655543	3.841605	-1.235178	C	-1.167510	4.006471	-1.364494
C	-0.365220	4.130087	1.679039	C	-1.277776	4.755833	1.384024	C	-0.812282	4.746784	1.314861
H	1.135945	2.618249	1.303995	H	0.506181	3.526989	1.392317	H	0.914238	3.441570	1.289670
C	-1.639886	4.868080	-0.250501	C	-2.584648	4.720857	-0.660419	C	-2.067618	4.893765	-0.757990
H	-1.131677	3.918522	-2.135656	H	-1.820441	3.444089	-2.241315	H	-1.334244	3.668107	-2.391597
C	-1.372833	4.935420	1.121881	C	-2.395479	5.181874	0.649051	C	-1.890659	5.264699	0.581235
H	-0.162086	4.169272	2.753704	H	-1.133712	5.102381	2.412589	H	-0.684436	5.016642	2.367704
H	-2.438507	5.477053	-0.686395	H	-3.466577	5.028930	-1.231471	H	-2.925849	5.268192	-1.324277
H	-1.958398	5.602131	1.763694	H	-3.124744	5.860451	1.104471	H	-2.606725	5.938206	1.063320
C	-0.604219	-1.635162	-1.863144	C	-0.259565	-1.968412	-1.642785	C	-0.451097	-2.102254	-1.540366
C	-2.762296	-2.935875	-1.972931	C	-2.221351	-3.575340	-1.667122	C	-2.646836	-3.362778	-1.613535
C	-3.757094	-3.625154	-1.059416	C	-3.035068	-4.379398	-0.672246	C	-3.646369	-3.975143	-0.651522
H	-2.280974	-3.521580	-2.766312	H	-1.652173	-4.108520	-2.438881	H	-2.141064	-4.015534	-2.336337
O	-3.541647	-1.860904	-2.529566	O	-3.209975	-2.714521	-2.260375	O	-3.429421	-2.360953	-2.284856
C	-4.036174	-1.343897	-1.277476	C	-3.760183	-2.215775	-1.026921	C	-3.949701	-1.729431	-1.098370
C	-4.589227	-2.584080	-0.602618	C	-4.031940	-3.482690	-0.241632	C	-4.490893	-2.902316	-0.305908
C	-3.904076	-4.926783	-0.584241	C	-2.911482	-5.647068	-0.107414	C	-3.787773	-5.226358	-0.054773
H	-4.710117	-0.492544	-1.436848	H	-4.599676	-1.534445	-1.211086	H	-4.634729	-0.909871	-1.347313
C	-5.586368	-2.814985	0.342540	C	-4.931856	-3.828455	0.764529	C	-5.497336	-3.049702	0.646356
C	-4.932857	-5.174123	0.346940	C	-3.839356	-6.015573	0.887515	C	-4.825759	-5.391979	0.884277
H	-3.251870	-5.738493	-0.923708	H	-2.127450	-6.342866	-0.424538	H	-3.125286	-6.061247	-0.307235
C	-5.760244	-4.135680	0.803109	C	-4.832908	-5.121243	1.316923	C	-5.666169	-4.321455	1.229770
H	-6.222653	-2.004565	0.713649	H	-5.698433	-3.128350	1.113427	H	-6.143768	-2.212558	0.930130
H	-5.090593	-6.191616	0.719968	H	-3.785792	-7.014836	1.332420	H	-4.980960	-6.370554	1.350910
H	-6.552441	-4.356095	1.526347	H	-5.541357	-5.434161	2.091139	H	-6.465181	-4.478523	1.962008
C	-1.754286	-2.136849	-1.037699	C	-1.368172	-2.544462	-0.810810	C	-1.667655	-2.467427	-0.737848
H	-1.398080	-2.768585	-0.212265	H	-0.945024	-3.043086	0.070712	H	-1.369340	-3.008193	0.170140
C	-2.700719	-1.013101	-0.529128	C	-2.491036	-1.544107	-0.388190	C	-2.624837	-1.284657	-0.388471
H	-2.816849	-1.043184	0.561303	H	-2.585376	-1.467044	0.708179	H	-2.766400	-1.170777	0.697920
Co	-0.463335	0.277497	0.316948	Co	-0.603506	0.180371	0.613929	Co	-0.530749	0.381730	0.472432
C	1.445819	-3.099773	2.783946	C	2.139317	-3.238380	2.493261	C	1.713293	-3.182325	2.674551
C	5.630852	-3.157960	-0.152289	C	6.155350	-1.843263	-0.339588	C	5.804228	-2.664912	-0.340770
C	5.312097	-4.580615	-0.674692	C	6.211970	-3.218614	-1.049209	C	5.622513	-4.086414	-0.927401
H	6.241964	-5.113523	-0.946209	H	7.245827	-3.453655	-1.362503	H	6.597627	-4.506603	-1.234174
H	4.786699	-5.182079	0.087306	H	5.865492	-4.029685	-0.385424	H	5.173654	-4.774606	-0.190368

H	4.667061	-4.530121	-1.569952	H	5.569655	-3.218489	-1.947869	H	4.963753	-4.060761	-1.813372
C	6.544545	-3.261248	1.093441	C	7.077841	-1.869095	0.903603	C	6.751222	-2.731743	0.882548
H	6.057015	-3.826632	1.906418	H	6.765247	-2.644926	1.623804	H	6.345743	-3.386452	1.673294
H	7.488772	-3.777737	0.840552	H	8.121389	-2.082837	0.607785	H	7.738324	-3.130905	0.585933
H	6.790133	-2.256544	1.479557	H	7.056198	-0.895383	1.423509	H	6.898203	-1.727054	1.315840
C	6.392923	-2.395021	-1.252657	C	6.679971	-0.771031	-1.313580	C	6.455226	-1.773941	-1.415877
H	5.797119	-2.317881	-2.179247	H	6.068000	-0.723958	-2.231453	H	5.823545	-1.703191	-2.318831
H	6.657335	-1.373507	-0.928016	H	6.681697	0.231057	-0.850405	H	6.635739	-0.751405	-1.041038
H	7.329778	-2.926075	-1.497359	H	7.716992	-1.008719	-1.609794	H	7.428640	-2.199944	-1.716110
C	0.016114	-3.425671	2.280283	C	0.919158	-4.001555	1.924373	C	0.360699	-3.769356	2.204801
H	-0.496605	-2.511787	1.946358	H	0.141908	-3.288069	1.616428	H	-0.305376	-2.964956	1.862682
H	0.060251	-4.139658	1.437448	H	1.211983	-4.615428	1.053301	H	0.511935	-4.488445	1.379803
H	-0.574686	-3.891798	3.089931	H	0.498391	-4.677008	2.691561	H	-0.129312	-4.305544	3.037633
C	2.073111	-4.416008	3.286229	C	3.160045	-4.286752	2.980883	C	2.568226	-4.350254	3.207801
H	2.146379	-5.168856	2.481148	H	3.496339	-4.947225	2.161679	H	2.757986	-5.111342	2.429922
H	3.081822	-4.258550	3.706925	H	4.049923	-3.814988	3.433493	H	3.540675	-4.004073	3.599914
H	1.439866	-4.838810	4.086008	H	2.688310	-4.922542	3.750734	H	2.029915	-4.845057	4.034971
C	1.374396	-2.120922	3.982796	C	1.695734	-2.401541	3.720853	C	1.469502	-2.199353	3.849094
H	2.383386	-1.944762	4.395069	H	2.563029	-1.882001	4.165440	H	2.428812	-1.797136	4.220030
H	0.955368	-1.154980	3.664182	H	0.946516	-1.650553	3.426862	H	0.833882	-1.359432	3.529599
H	0.739202	-2.539334	4.785351	H	1.256106	-3.061136	4.491857	H	0.969723	-2.724358	4.683710
C	2.982769	3.670834	-0.847784	C	2.437849	4.039451	-0.570757	C	2.960241	3.782888	-0.588336
C	2.648203	4.996032	-1.181262	C	2.043132	5.371266	-0.794824	C	2.704395	5.151903	-0.789271
C	3.783489	3.424993	0.279063	C	3.272090	3.743753	0.520689	C	3.726993	3.380256	0.517914
C	3.093560	6.059548	-0.388294	C	2.462493	6.390522	0.067890	C	3.195619	6.103967	0.111198
H	2.018290	5.195186	-2.055445	H	1.385893	5.607131	-1.639204	H	2.099145	5.471435	-1.644766
C	4.231985	4.492078	1.070830	C	3.690863	4.765792	1.385018	C	4.217954	4.335801	1.419671
H	4.053023	2.395013	0.529430	H	3.596156	2.712665	0.689183	H	3.943664	2.318961	0.669690
C	3.884866	5.809817	0.743507	C	3.284952	6.089447	1.164260	C	3.951023	5.697501	1.221711
H	2.819427	7.086448	-0.652010	H	2.143050	7.422194	-0.113342	H	2.983995	7.165896	-0.051458
H	4.854740	4.290250	1.948973	H	4.339662	4.524763	2.233971	H	4.813256	4.012138	2.280107
H	4.231790	6.641649	1.365691	H	3.612178	6.885851	1.841172	H	4.333516	6.441680	1.928241

Intermediate-3 from nucleophilic addition^B pathway: In Co catalyzed reaction energy profile

Int3B ¹ : $\nu_{\text{lowest}} = 9.7802 \text{ cm}^{-1}$				Int3B ³ : $\nu_{\text{lowest}} = 9.6206 \text{ cm}^{-1}$				Int3B ⁵ : $\nu_{\text{lowest}} = 4.9182 \text{ cm}^{-1}$			
113				113				113			
C	1.685546	-0.603872	-2.071937	C	1.453667	0.032567	-2.188174	C	1.266209	-0.854139	-2.325924
C	1.097051	1.765634	-1.976241	C	0.723224	2.298172	-1.666885	C	1.422906	1.563184	-2.157057
C	0.825281	-0.811959	-3.153154	C	0.498168	-0.085481	-3.194516	C	0.358384	-0.761679	-3.381980
C	0.178049	1.542792	-3.005625	C	-0.288129	2.156790	-2.627978	C	0.467883	1.669055	-3.179900
H	1.226727	2.770082	-1.561362	H	0.822759	3.234496	-1.109189	H	1.845387	2.465330	-1.701754
C	0.065377	0.272441	-3.614705	C	-0.381571	0.988883	-3.409462	C	-0.042576	0.516976	-3.805104
H	0.782362	-1.805678	-3.612722	H	0.455232	-1.005639	-3.787579	H	-0.018261	-1.673005	-3.857287
H	-0.438079	2.372051	-3.368312	H	-0.997099	2.975315	-2.787949	H	0.130261	2.658531	-3.505203
H	-0.620800	0.143600	-4.460071	H	-1.150200	0.923944	-4.188063	H	-0.760909	0.620646	-4.626313
N	1.642668	-1.664913	-0.010472	N	1.636988	-1.380008	-0.301896	N	0.768679	-2.249314	-0.461517

C	0.716702	-2.388490	1.983811	C	1.396938	-2.348961	1.807079	C	-0.323080	-3.317200	1.359637
C	-0.774431	-0.780587	2.802378	C	0.103573	-1.019816	3.236400	C	-1.069559	-1.881623	3.055363
C	0.517773	-3.256019	3.089029	C	1.570893	-3.367101	2.786521	C	-0.756603	-4.476746	2.075663
C	1.614271	-2.680399	0.912698	C	1.959551	-2.440818	0.488385	C	0.353658	-3.423016	0.070818
C	-1.020006	-1.577141	3.943056	C	0.201171	-1.991660	4.254990	C	-1.508056	-2.970028	3.837419
H	-1.261150	0.185794	2.645813	H	-0.445928	-0.082673	3.363338	H	-1.183155	-0.845064	3.391017
C	-0.389392	-2.808799	4.088019	C	0.931620	-3.155540	4.039299	C	-1.359793	-4.260053	3.344913
C	1.257587	-4.477804	3.095012	C	2.360823	-4.499442	2.427851	C	-0.557812	-5.759677	1.489210
C	2.325775	-3.889660	0.945393	C	2.753181	-3.567844	0.177460	C	0.508361	-4.726677	-0.472000
H	-1.719684	-1.210837	4.699558	H	-0.297054	-1.809206	5.211561	H	-1.964763	-2.784426	4.813910
H	-0.585492	-3.434822	4.964999	H	1.018963	-3.912693	4.825895	H	-1.703840	-5.122340	3.926596
C	2.128985	-4.763809	2.045802	C	2.937388	-4.567192	1.158368	C	0.060687	-5.854619	0.243461
H	1.137633	-5.175150	3.929966	H	2.503563	-5.306202	3.153537	H	-0.898528	-6.652596	2.022752
H	2.990347	-4.125511	0.110863	H	3.175942	-3.634605	-0.827502	H	0.975213	-4.809361	-1.454456
H	2.686858	-5.706554	2.064178	H	3.545875	-5.441050	0.899891	H	0.202583	-6.843601	-0.206918
N	0.075900	-1.182054	1.852213	N	0.690744	-1.200226	2.047103	N	-0.501622	-2.059142	1.858949
C	2.534120	-1.650475	-1.301025	C	2.386166	-1.067604	-1.638082	C	1.725683	-2.152196	-1.610333
O	2.784469	-2.801609	-1.819395	O	2.708693	-2.079751	-2.366357	O	1.890095	-3.187229	-2.395962
O	0.166860	1.440421	0.905663	O	-0.221829	1.361049	1.286577	O	0.521903	0.971655	1.301258
C	-0.805493	2.282414	0.671189	C	-1.255734	2.083427	0.907487	C	0.172349	2.187842	0.947308
C	-1.959153	1.940208	-0.115307	C	-2.237624	1.596616	-0.019526	C	-0.861517	2.457264	-0.020911
C	-0.746132	3.614224	1.227821	C	-1.436221	3.404850	1.449612	C	0.816830	3.319865	1.568684
C	-2.996724	2.878114	-0.355144	C	-3.353922	2.386312	-0.387408	C	-1.182033	3.786816	-0.397625
C	-2.069155	0.619071	-0.670760	C	-2.101165	0.280972	-0.601064	C	-1.608484	1.387214	-0.640261
C	-1.798117	4.486487	0.954713	C	-2.550898	4.136784	1.036272	C	0.461278	4.599326	1.142518
C	-2.937575	4.162366	0.167631	C	-3.530771	3.666958	0.123738	C	-0.519531	4.875465	0.153586
H	-3.836779	2.550873	-0.970852	H	-4.059938	1.954029	-1.098843	H	-1.963897	3.918479	-1.147426
N	-1.184726	-0.343703	-0.590271	N	-1.074301	-0.519524	-0.500723	N	-1.428260	0.099903	-0.493881
O	-3.191092	0.290307	-1.356181	O	-3.135006	-0.214423	-1.325584	O	-2.636949	1.717395	-1.467644
H	-1.745175	5.494767	1.373599	H	-2.677798	5.144599	1.439433	H	0.967993	5.451328	1.602394
C	-1.684722	-1.566504	-1.243112	C	-1.357052	-1.801650	-1.151288	C	-2.367690	-0.633968	-1.352860
C	-3.020138	-1.049783	-1.901010	C	-2.731634	-1.506476	-1.867383	C	-3.374135	0.500088	-1.777877
H	-0.976181	-1.832241	-2.040405	H	-0.577313	-1.991143	-1.905620	H	-1.806979	-0.952822	-2.247221
C	-1.764620	-2.743322	-0.295435	C	-1.334231	-2.937733	-0.149416	C	-2.902582	-1.873308	-0.672420
H	-2.846410	-0.921344	-2.984114	H	-2.547626	-1.350308	-2.944383	H	-3.521249	0.486333	-2.868860
C	-2.612399	-2.736849	0.827185	C	-2.015776	-2.836518	1.076143	C	-3.488800	-1.814136	0.605921
C	-0.955718	-3.865923	-0.539911	C	-0.606983	-4.103878	-0.436686	C	-2.765219	-3.120976	-1.303287
C	-2.670359	-3.848177	1.674730	C	-1.980953	-3.892321	1.994289	C	-3.946337	-2.979970	1.228660
H	-3.231255	-1.858952	1.037362	H	-2.562593	-1.919318	1.318551	H	-3.576882	-0.850295	1.115782
C	-1.012064	-4.979928	0.310081	C	-0.571511	-5.162966	0.480751	C	-3.217196	-4.291891	-0.678422
H	-0.248104	-3.850570	-1.376920	H	-0.039326	-4.164759	-1.371694	H	-2.274691	-3.177673	-2.281228
C	-1.874899	-4.975735	1.413138	C	-1.260689	-5.059577	1.696405	C	-3.812653	-4.221732	0.587464
H	-3.337384	-3.835777	2.542955	H	-2.511552	-3.802566	2.947840	H	-4.400598	-2.921855	2.222959
H	-0.367880	-5.843109	0.116731	H	0.011869	-6.060509	0.253029	H	-3.084900	-5.259101	-1.172941
H	-1.918448	-5.844034	2.078997	H	-1.226165	-5.882237	2.418493	H	-4.158053	-5.135444	1.082331
C	1.875253	0.680587	-1.503062	C	1.614209	1.227364	-1.449422	C	1.835151	0.288291	-1.737576
C	4.271794	1.413552	-1.691660	C	3.961874	2.124446	-1.635687	C	4.346260	0.304217	-1.518379

C	5.605218	1.399387	-0.967059	C	5.331799	2.068628	-0.985108	C	5.471744	-0.151010	-0.607293
H	3.950597	2.353617	-2.162238	H	3.570555	3.105906	-1.938171	H	4.396824	1.319781	-1.935300
O	4.454424	0.386372	-2.681842	O	4.134628	1.271005	-2.778361	O	4.388104	-0.679723	-2.566745
C	4.899726	-0.652164	-1.770997	C	4.674474	0.131415	-2.065626	C	4.348727	-1.845355	-1.713801
C	6.027281	0.054057	-1.037959	C	5.806913	0.772730	-1.282222	C	5.489253	-1.555252	-0.750054
C	6.348523	2.356223	-0.280280	C	6.070126	2.945686	-0.194073	C	6.324499	0.496100	0.283813
H	5.094788	-1.589299	-2.308294	H	4.878367	-0.702005	-2.749496	H	4.344820	-2.767251	-2.307539
C	7.205872	-0.359841	-0.420349	C	7.031928	0.327321	-0.789064	C	6.364194	-2.341338	-0.002389
C	7.557772	1.947747	0.319892	C	7.325632	2.511052	0.279002	C	7.234617	-0.292510	1.017624
H	6.016484	3.398265	-0.212068	H	5.699837	3.947942	0.048730	H	6.301091	1.584104	0.410629
C	7.979176	0.610943	0.249411	C	7.798332	1.222490	-0.014847	C	7.254949	-1.688765	0.874505
H	7.533057	-1.404574	-0.457906	H	7.399423	-0.682372	-1.001732	H	6.372170	-3.432778	-0.095031
H	8.178255	2.682893	0.843881	H	7.942204	3.188334	0.879872	H	7.937306	0.189916	1.705687
H	8.924861	0.318909	0.719189	H	8.779042	0.910068	0.360299	H	7.974854	-2.279016	1.451985
C	3.201602	0.735788	-0.748739	C	2.973812	1.253369	-0.759140	C	2.983050	-0.064196	-0.819575
H	3.152473	1.218269	0.239110	H	2.963630	1.584736	0.292279	H	2.901186	0.368420	0.187375
C	3.725376	-0.737973	-0.758945	C	3.569806	-0.169303	-1.013557	C	3.060251	-1.622889	-0.868326
H	4.061478	-1.103782	0.222174	H	3.986335	-0.660821	-0.123094	H	3.140260	-2.105032	0.115704
Co	0.503500	-0.309428	0.222950	Co	0.550001	-0.111758	0.439498	Co	0.068811	-0.681714	0.472770
C	-4.258629	-1.879692	-1.670814	C	-0.411682	3.990511	2.441401	C	1.848323	3.112418	2.696262
C	-4.321329	-3.172956	-2.222063	C	-4.711653	4.572968	-0.260620	C	-0.807758	6.330413	-0.249025
C	-5.329563	-1.407906	-0.895226	C	-4.170455	5.864352	-0.922157	C	0.487627	6.970392	-0.806262
C	-5.433864	-3.988227	-1.986955	H	-5.003794	6.535298	-1.199652	H	0.306403	8.022019	-1.094068
H	-3.487376	-3.551050	-2.823866	H	-3.502427	6.418948	-0.240569	H	1.298654	6.959451	-0.057637
C	-6.445959	-2.225051	-0.664640	H	-3.599201	5.623812	-1.835946	H	0.840800	6.422252	-1.697317
H	-5.278892	-0.400502	-0.472807	C	-5.511979	4.943292	1.012178	C	-1.281189	7.124792	0.993134
C	-6.499801	-3.516836	-1.204967	H	-4.881445	5.472481	1.747544	H	-0.519105	7.120498	1.791572
H	-5.468062	-4.996335	-2.412961	H	-6.360060	5.604249	0.756273	H	-1.483081	8.177618	0.724085
H	-7.276829	-1.848429	-0.058462	H	-5.912397	4.036525	1.498369	H	-2.207385	6.687592	1.405419
H	-7.370108	-4.155334	-1.020523	C	-5.665217	3.879349	-1.252200	C	-1.900793	6.418907	-1.331154
C	-4.026464	5.221734	-0.066609	H	-5.150992	3.616164	-2.193115	H	-1.605458	5.882850	-2.250143
C	-3.405382	6.445222	-0.784482	H	-6.094570	2.956680	-0.824012	H	-2.857502	5.996127	-0.977646
H	-4.171015	7.224299	-0.953486	H	-6.500808	4.556122	-1.502869	H	-2.077250	7.475496	-1.598654
H	-2.592232	6.894159	-0.188144	C	0.983120	4.072837	1.771042	C	3.057981	2.288784	2.191096
H	-2.986326	6.151420	-1.762737	H	1.316303	3.079087	1.437168	H	2.743494	1.276566	1.901151
C	-5.175832	4.677241	-0.936077	H	0.952425	4.749965	0.898745	H	3.529017	2.777003	1.319378
H	-4.817714	4.365128	-1.932727	H	1.725030	4.471726	2.486597	H	3.818135	2.203176	2.988494
H	-5.669250	3.811678	-0.460022	C	-0.798952	5.413095	2.894434	C	2.388987	4.454241	3.232205
H	-5.938614	5.462051	-1.082350	H	-0.844602	6.117881	2.045473	H	2.918117	5.027156	2.449986
C	-4.611713	5.667958	1.295892	H	-1.774067	5.428975	3.412639	H	1.584810	5.088955	3.644497
H	-3.832807	6.095238	1.950951	H	-0.037732	5.788767	3.600231	H	3.108682	4.255117	4.045238
H	-5.389655	6.439166	1.148426	C	-0.330927	3.099658	3.706606	C	1.170913	2.370033	3.877025
H	-5.066929	4.811658	1.823752	H	-1.320726	3.023867	4.191027	H	0.329080	2.964367	4.274796
C	0.454457	4.039656	2.093923	H	0.016527	2.089208	3.447214	H	0.791129	1.389325	3.552146
C	0.309020	5.486752	2.606500	H	0.376069	3.539277	4.433583	H	1.899543	2.214764	4.693688
H	0.256977	6.214452	1.777329	C	-3.816126	-2.532567	-1.659447	C	-4.707425	0.500415	-1.064436
H	-0.589781	5.612044	3.236129	C	-3.725634	-3.763309	-2.334728	C	-5.682912	-0.441651	-1.439388

H	1.188615	5.743753	3.222119	C	-4.876172	-2.312829	-0.765467	C	-4.969899	1.376405	0.001913
C	1.756090	3.960906	1.257125	C	-4.676104	-4.765626	-2.108709	C	-6.896225	-0.519372	-0.746409
H	1.917961	2.937208	0.890665	H	-2.900467	-3.942337	-3.033583	H	-5.482499	-1.131869	-2.266408
H	1.701174	4.644865	0.391215	C	-5.831099	-3.315420	-0.545219	C	-6.186989	1.298312	0.694633
H	2.624325	4.256696	1.873882	H	-4.947827	-1.351289	-0.249461	H	-4.219993	2.121150	0.283761
C	0.568891	3.109533	3.328866	C	-5.731992	-4.544501	-1.211366	C	-7.150105	0.348658	0.326640
H	-0.351059	3.163563	3.938606	H	-4.592899	-5.722294	-2.634978	H	-7.644807	-1.261653	-1.042424
H	0.729790	2.066156	3.019348	H	-6.656005	-3.134174	0.152116	H	-6.382599	1.985419	1.524830
H	1.418395	3.425622	3.961391	H	-6.476459	-5.328059	-1.035348	H	-8.098936	0.287758	0.870033

Transition State (3B-4B) –elimination^B pathway: In Co catalyzed reaction energy profile

TS3B ¹ : $\nu_{\text{lowest}} = -173.2177 \text{ cm}^{-1}$				TS3B ³ : $\nu_{\text{lowest}} = -166.1560 \text{ cm}^{-1}$				TS3B ⁵ : $\nu_{\text{lowest}} = -271.0482 \text{ cm}^{-1}$			
113				113				113			
C	1.671754	-0.618053	-2.217686	C	-1.404668	-0.128206	-2.282590	C	1.655458	0.008532	-2.294029
C	1.127029	1.744947	-1.955382	C	-0.585566	-2.337039	-1.666681	C	0.833638	2.237880	-1.771366
C	0.737297	-0.754931	-3.246444	C	-0.412098	0.010938	-3.249705	C	0.691907	-0.154087	-3.289595
C	0.146581	1.597400	-2.945503	C	0.454637	-2.175548	-2.595957	C	-0.173380	2.059143	-2.733304
H	1.292661	2.720482	-1.488206	H	-0.659927	-3.259762	-1.082591	H	0.892776	3.173159	-1.205880
C	-0.030314	0.364754	-3.606393	C	0.526216	-1.024821	-3.402603	C	-0.231335	0.883192	-3.504633
H	0.636431	-1.722054	-3.751616	H	-0.386221	0.917587	-3.864866	H	0.679976	-1.078275	-3.877929
H	-0.472154	2.456452	-3.224330	H	1.205642	-2.964374	-2.705921	H	-0.911355	2.851599	-2.894410
H	-0.770558	0.288416	-4.411427	H	1.322524	-0.941547	-4.151070	H	-1.006024	0.780806	-4.273035
N	1.547629	-1.739392	-0.043507	N	-1.629539	1.295167	-0.298799	N	1.685642	-1.465526	-0.295840
C	0.624220	-2.506267	1.945143	C	-1.564253	2.282067	1.824786	C	1.263454	-2.665460	1.677650
C	-0.797957	-0.871218	2.828286	C	-0.217533	1.071448	3.308289	C	-0.178415	-1.565581	3.145599
C	0.409070	-3.401467	3.022402	C	-1.854950	3.290193	2.786045	C	1.424778	-3.778318	2.555228
C	1.503487	-2.772457	0.850786	C	-2.077575	2.311328	0.482408	C	1.943694	-2.590981	0.394326
C	-1.055679	-1.695566	3.946947	C	-0.426647	2.041545	4.312146	C	-0.082515	-2.622239	4.078022
H	-1.254191	0.115033	2.708125	H	0.400107	0.182388	3.465546	H	-0.798217	-0.682086	3.333897
C	-0.469884	-2.954183	4.047014	C	-1.241251	3.141186	4.060416	C	0.714943	-3.722827	3.785976
C	1.115887	-4.642485	2.974098	C	-2.721825	4.349618	2.384058	C	2.275604	-4.845216	2.139309
C	2.190464	-3.998899	0.840909	C	-2.958103	3.362732	0.133565	C	2.779359	-3.675861	0.030817
H	-1.731210	-1.327668	4.724445	H	0.052144	1.908341	5.286602	H	-0.636259	-2.560541	5.019553
H	-0.678726	-3.597940	4.908146	H	-1.413450	3.895088	4.836229	H	0.803411	-4.551562	4.497186
C	1.973370	-4.910107	1.906992	C	-3.256881	4.354119	1.093621	C	2.926863	-4.770889	0.906481
H	0.988888	-5.367217	3.784252	H	-2.958937	5.149157	3.092808	H	2.408339	-5.712561	2.793733
H	2.858432	-4.229930	0.007347	H	-3.359991	3.384541	-0.882549	H	3.272979	-3.636803	-0.943956
H	2.507642	-5.866544	1.888364	H	-3.928080	5.170478	0.803968	H	3.576404	-5.598707	0.600205
N	0.026340	-1.273209	1.854695	N	-0.775607	1.196601	2.098434	N	0.480169	-1.593148	1.985121
C	2.584214	-1.688951	-1.613545	C	-2.433608	0.907714	-1.831745	C	2.676490	-1.007930	-1.796684
O	2.747910	-2.823667	-2.112143	O	-2.723434	1.930279	-2.512894	O	2.993659	-2.031045	-2.462408
O	0.214103	1.380349	0.934014	O	0.323745	-1.324044	1.328164	O	-0.184957	1.346550	1.169200
C	-0.709225	2.275177	0.701635	C	1.379215	-2.008818	0.938128	C	-1.204566	2.111129	0.851894
C	-1.874889	2.000916	-0.094904	C	2.326673	-1.487935	-0.006241	C	-2.222710	1.688998	-0.072557
C	-0.578669	3.600237	1.262932	C	1.620027	-3.318434	1.484384	C	-1.325246	3.419763	1.441403
C	-2.855498	2.997118	-0.339996	C	3.472358	-2.231025	-0.381188	C	-3.303552	2.542307	-0.403152

C	-2.050374	0.691651	-0.659691	C	2.122799	-0.187497	-0.600821	C	-2.169010	0.380387	-0.689370
C	-1.576622	4.531686	0.984092	C	2.759521	-4.005314	1.062097	C	-2.411687	4.212150	1.069608
C	-2.726356	4.274674	0.186453	C	3.709137	-3.499150	0.136536	C	-3.417124	3.813349	0.150499
H	-3.707977	2.720364	-0.963414	H	4.150292	-1.774754	-1.104846	H	-4.039188	2.166497	-1.116233
N	-1.225366	-0.321744	-0.562609	N	1.059127	0.564975	-0.500143	N	-1.242390	-0.527991	-0.544796
O	-3.171371	0.432269	-1.375196	O	3.122915	0.350768	-1.338728	O	-3.191429	0.025268	-1.509989
H	-1.470129	5.534403	1.406140	H	2.933120	-5.005017	1.468062	H	-2.495864	5.207941	1.512064
C	-1.769543	-1.506219	-1.248797	C	1.270171	1.854043	-1.164902	C	-1.564797	-1.711607	-1.348989
C	-3.088661	-0.926665	-1.892533	C	2.663593	1.629964	-1.869896	C	-3.002298	-1.362768	-1.907929
H	-1.069669	-1.774258	-2.053590	H	0.482612	1.986399	-1.923004	H	-0.851359	-1.746237	-2.188070
C	-1.889796	-2.703441	-0.331559	C	1.168731	2.995122	-0.173253	C	-1.411616	-2.988631	-0.552232
H	-2.935074	-0.833322	-2.981622	H	2.498915	1.477453	-2.950121	H	-2.985466	-1.375923	-3.009582
C	-2.710867	-2.684353	0.810533	C	1.838624	2.944139	1.061876	C	-2.047255	-3.150323	0.692533
C	-1.145591	-3.858872	-0.622390	C	0.367204	4.107841	-0.474420	C	-0.604041	-4.024023	-1.048705
C	-2.805876	-3.812967	1.631391	C	1.714546	3.994884	1.978188	C	-1.896668	-4.338152	1.415081
H	-3.279012	-1.782178	1.057287	H	2.444991	2.068033	1.314635	H	-2.656708	-2.337405	1.098332
C	-1.236947	-4.989972	0.201431	C	0.243192	5.162357	0.440589	C	-0.448543	-5.214595	-0.324279
H	-0.465233	-3.858907	-1.481385	H	-0.191148	4.126284	-1.416825	H	-0.064331	-3.880424	-1.991352
C	-2.073231	-4.971183	1.324625	C	0.917197	5.107612	1.667948	C	-1.099220	-5.375547	0.905606
H	-3.451682	-3.789437	2.515232	H	2.235253	3.943250	2.940020	H	-2.396283	-4.453373	2.382359
H	-0.641697	-5.879054	-0.028261	H	-0.398564	6.016358	0.202543	H	0.198303	-6.007082	-0.713178
H	-2.144372	-5.852545	1.970596	H	0.811942	5.925263	2.388853	H	-0.972321	-6.301605	1.476082
C	1.907656	0.627401	-1.591480	C	-1.532644	-1.307602	-1.518574	C	1.762271	1.204143	-1.557350
C	4.324671	1.359945	-1.643053	C	-3.843478	-2.320132	-1.647488	C	4.093415	2.188029	-1.466110
C	5.620080	1.284680	-0.856642	C	-5.204157	-2.303901	-0.975633	C	5.374290	2.159824	-0.652817
H	4.022656	2.335911	-2.048245	H	-3.407793	-3.293602	-1.912748	H	3.698317	3.165411	-1.776383
O	4.561184	0.419459	-2.707018	O	-4.078516	-1.530308	-2.825201	O	4.445430	1.394437	-2.612598
C	4.963984	-0.690523	-1.866678	C	-4.663521	-0.388369	-2.154059	C	4.944494	0.248421	-1.882545
C	6.048131	-0.050584	-1.016372	C	-5.748725	-1.048251	-1.321086	C	5.940221	0.898649	-0.937466
C	6.323192	2.178763	-0.052719	C	-5.883859	-3.179173	-0.131782	C	5.966767	3.028959	0.260287
H	5.207377	-1.572727	-2.473079	H	-4.932156	0.395956	-2.873249	H	5.286580	-0.536240	-2.569796
C	7.192854	-0.517903	-0.373815	C	-6.986379	-0.642335	-0.825795	C	7.113387	0.481405	-0.311958
C	7.499542	1.718689	0.574485	C	-7.151364	-2.786138	0.345579	C	7.171371	2.624134	0.871625
H	5.984874	3.211791	0.085538	H	-5.459344	-4.149613	0.148711	H	5.522873	4.003048	0.494327
C	7.927425	0.391552	0.414901	C	-7.693457	-1.537642	0.003005	C	7.735432	1.370448	0.588715
H	7.523919	-1.556637	-0.480883	H	-7.408252	0.336907	-1.076805	H	7.550617	-0.502030	-0.515960
H	8.089441	2.405854	1.190776	H	-7.722607	-3.464801	0.988281	H	7.676035	3.297386	1.573049
H	8.847334	0.059084	0.908308	H	-8.682144	-1.257211	0.382515	H	8.674497	1.080624	1.072761
C	3.217372	0.606062	-0.811460	C	-2.890432	-1.362080	-0.827471	C	3.052095	1.241115	-0.750832
H	3.138171	0.992423	0.215976	H	-2.859596	-1.641174	0.238991	H	2.918624	1.513969	0.308952
C	3.729784	-0.867616	-0.928260	C	-3.549155	0.021002	-1.141908	C	3.719391	-0.152113	-1.000963
H	4.019879	-1.324029	0.028021	H	-3.981911	0.532289	-0.271006	H	4.044850	-0.673540	-0.090300
Co	0.458779	-0.387191	0.248969	Co	-0.509308	0.120545	0.489004	Co	0.482329	-0.235002	0.372622
C	-4.367422	-1.678273	-1.613668	C	0.629194	-3.940746	2.487729	C	-0.269650	3.917200	2.447581
C	-4.527897	-2.969106	-2.150573	C	4.923313	-4.356694	-0.254784	C	-4.562527	4.779717	-0.191090
C	-5.379119	-1.137731	-0.804147	C	4.430538	-5.674771	-0.901443	C	-3.972137	6.071717	-0.808196
C	-5.677095	-3.715044	-1.866766	H	5.288887	-6.311338	-1.183527	H	-4.779341	6.785516	-1.053871

H	-3.740940	-3.400520	-2.779171	H	3.794396	-6.252594	-0.208748	H	-3.277934	6.572698	-0.111509
C	-6.532717	-1.885112	-0.524897	H	3.839712	-5.465634	-1.810489	H	-3.417032	5.842675	-1.734702
H	-5.253561	-0.131765	-0.394000	C	5.752038	-4.683235	1.011824	C	-5.337992	5.134403	1.101610
C	-6.683045	-3.175487	-1.050171	H	5.152387	-5.233229	1.757675	H	-4.681447	5.609875	1.850660
H	-5.787036	-4.722266	-2.281925	H	6.624538	-5.309552	0.751074	H	-6.159934	5.838182	0.876831
H	-7.316769	-1.455004	0.107501	H	6.118821	-3.756779	1.487294	H	-5.772097	4.227252	1.557212
H	-7.582149	-3.759632	-0.827598	C	5.835698	-3.630304	-1.261536	C	-5.550677	4.163787	-1.199968
C	-3.750022	5.395788	-0.054102	H	5.300754	-3.396444	-2.198635	H	-5.053781	3.912721	-2.153365
C	-3.051520	6.584957	-0.758646	H	6.229754	-2.687018	-0.844479	H	-6.017788	3.245917	-0.802029
H	-3.769103	7.407671	-0.931696	H	6.696740	-4.272633	-1.516517	H	-6.357396	4.884727	-1.419964
H	-2.220482	6.983630	-0.151319	C	-0.767726	-4.079044	1.830661	C	1.120491	3.977073	1.764712
H	-2.639323	6.272295	-1.733997	H	-1.144090	-3.100348	1.498007	H	1.413560	2.986297	1.388610
C	-4.918773	4.922554	-0.939143	H	-0.718517	-4.756015	0.959128	H	1.104961	4.688159	0.919309
H	-4.567491	4.593863	-1.932889	H	-1.486097	-4.505794	2.554078	H	1.883010	4.321276	2.486971
H	-5.467299	4.085392	-0.472739	C	1.076055	-5.345984	2.939747	C	-0.597103	5.330474	2.971206
H	-5.632769	5.751040	-1.090669	H	1.140756	-6.050352	2.091674	H	-0.618333	6.077052	2.157622
C	-4.323641	5.868672	1.304363	H	2.056056	-5.322631	3.448371	H	-1.568323	5.360043	3.496236
H	-3.528500	6.246720	1.970085	H	0.337086	-5.749450	3.653778	H	0.181953	5.640788	3.689129
H	-5.053842	6.684465	1.152673	C	0.527203	-3.049988	3.751565	C	-0.216517	2.962552	3.667968
H	-4.833569	5.037672	1.822543	H	1.517312	-2.939634	4.228636	H	-1.200051	2.923457	4.169549
C	0.637401	3.953645	2.139841	H	0.144245	-2.052437	3.492119	H	0.064198	1.945404	3.356986
C	0.570029	5.404569	2.657701	H	-0.159295	-3.511690	4.484466	H	0.527660	3.327653	4.399148
H	0.566224	6.137249	1.831277	C	3.697783	2.702207	-1.637363	C	-4.140615	-2.214088	-1.393196
H	-0.325454	5.578288	3.280534	C	3.557008	3.936410	-2.297576	C	-4.270238	-3.535010	-1.860243
H	1.457656	5.608880	3.281499	C	4.758344	2.519354	-0.735791	C	-5.034566	-1.736956	-0.421207
C	1.939553	3.804741	1.313228	C	4.458242	4.978092	-2.049105	C	-5.267062	-4.372521	-1.347636
H	2.045667	2.775489	0.942064	H	2.731051	4.086787	-3.002164	H	-3.573173	-3.916844	-2.614364
H	1.931568	4.495746	0.451159	C	5.663936	3.561784	-0.492865	C	-6.035918	-2.576216	0.088798
H	2.818110	4.046668	1.938883	H	4.869914	1.555318	-0.231615	H	-4.941364	-0.706039	-0.067944
C	0.688868	3.013047	3.371084	C	5.514604	4.793767	-1.144025	C	-6.151714	-3.896055	-0.367838
H	-0.230994	3.117316	3.974385	H	4.336096	5.936827	-2.563865	H	-5.352094	-5.401712	-1.711670
H	0.791574	1.963694	3.057059	H	6.489719	3.409232	0.210271	H	-6.728263	-2.194763	0.846987
H	1.550467	3.276701	4.011279	H	6.220488	5.608265	-0.950418	H	-6.931342	-4.551670	0.034140

Intermediate-4 from elimination^B pathway: In Co catalyzed reaction energy profile

Int4B ¹ : $\nu_{\text{lowest}} = 8.0863 \text{ cm}^{-1}$				Int4B ³ : $\nu_{\text{lowest}} = 10.9447 \text{ cm}^{-1}$				Int4B ⁵ : $\nu_{\text{lowest}} = 6.1565 \text{ cm}^{-1}$			
113				113				113			
C	1.556659	-0.680485	-2.685836	C	1.287188	-0.006671	-2.856086	C	1.625439	-0.577541	-2.744214
C	1.316358	1.641276	-2.004257	C	0.567079	2.134477	-1.956921	C	1.266029	1.711768	-2.003323
C	0.503845	-0.561650	-3.602817	C	0.172547	-0.070709	-3.701368	C	0.567012	-0.489826	-3.657879
C	0.256296	1.764583	-2.914246	C	-0.554507	2.074381	-2.798812	C	0.201798	1.803213	-2.912945
H	1.622659	2.499522	-1.399687	H	0.705954	2.989563	-1.288851	H	1.526039	2.567822	-1.374104
C	-0.149568	0.673559	-3.709559	C	-0.754765	0.980098	-3.663217	C	-0.148286	0.712706	-3.734620
H	0.226861	-1.421210	-4.222731	H	0.051841	-0.926240	-4.374666	H	0.328662	-1.349218	-4.293574
H	-0.266231	2.722401	-3.003435	H	-1.288044	2.886627	-2.774542	H	-0.370397	2.734251	-2.977493
H	-0.969287	0.804657	-4.424710	H	-1.635834	0.962761	-4.314199	H	-0.977681	0.817093	-4.442843

N	1.067028	-2.181173	-0.023149	N	1.199857	-1.764750	-0.385254	N	1.033052	-2.177388	-0.140783
C	-0.004020	-2.824244	1.964595	C	1.339587	-2.694170	1.790291	C	0.184679	-2.963376	1.905834
C	-0.953243	-0.942404	2.981007	C	0.393857	-1.297625	3.414588	C	-0.675110	-1.272454	3.257932
C	-0.434227	-3.704720	2.985363	C	1.612981	-3.734075	2.722169	C	-0.127786	-3.985895	2.848426
C	0.770466	-3.212083	0.827081	C	1.632052	-2.786322	0.381422	C	0.824463	-3.247475	0.625642
C	-1.407093	-1.748940	4.049675	C	0.593127	-2.289821	4.399038	C	-1.010683	-2.209676	4.260470
H	-1.147262	0.133005	2.936185	H	-0.058640	-0.327705	3.641422	H	-0.881819	-0.202807	3.374165
C	-1.164493	-3.119838	4.057547	C	1.199169	-3.497408	4.063278	C	-0.741974	-3.559508	4.058454
C	-0.064638	-5.077898	2.838677	C	2.252966	-4.906306	2.221242	C	0.188552	-5.334039	2.501890
C	1.128619	-4.569723	0.733484	C	2.301026	-3.959131	-0.058592	C	1.119645	-4.606711	0.339421
H	-1.960607	-1.273802	4.864880	H	0.274170	-2.089681	5.426240	H	-1.482947	-1.862226	5.184423
H	-1.526685	-3.744650	4.881022	H	1.357473	-4.268830	4.825049	H	-1.000985	-4.299565	4.823962
C	0.694674	-5.474315	1.737541	C	2.592667	-4.983586	0.865021	C	0.792220	-5.611521	1.271622
H	-0.364395	-5.803612	3.601100	H	2.472714	-5.734925	2.901539	H	-0.044710	-6.139528	3.205384
H	1.723819	-4.914831	-0.117438	H	2.561709	-4.053794	-1.116820	H	1.589413	-4.851406	-0.617669
H	0.973972	-6.529802	1.643468	H	3.094456	-5.887316	0.500465	H	1.026547	-6.652850	1.022354
N	-0.264526	-1.471436	1.962186	N	0.757087	-1.505379	2.142261	N	-0.094230	-1.647337	2.115732
C	2.440565	-1.855804	-2.444328	C	2.409178	-0.976161	-2.732622	C	2.548826	-1.721296	-2.509848
O	2.375532	-2.944611	-2.993242	O	2.567351	-2.006769	-3.369753	O	2.545760	-2.797943	-3.085821
O	0.566443	1.133692	1.016617	O	0.088892	1.258901	1.281495	O	0.512109	1.212356	1.083776
C	-0.123356	2.223004	0.811161	C	-0.861277	2.115636	0.989151	C	-0.232368	2.267063	0.849854
C	-1.323071	2.243917	0.014949	C	-1.981056	1.773648	0.153235	C	-1.412708	2.214924	0.026854
C	0.316995	3.473509	1.387829	C	-0.800066	3.456698	1.515448	C	0.134967	3.539089	1.420609
C	-2.043652	3.446408	-0.206957	C	-3.010395	2.711958	-0.114288	C	-2.186425	3.379127	-0.210799
C	-1.781877	1.029937	-0.599050	C	-2.056469	0.475536	-0.469002	C	-1.833008	0.978616	-0.597973
C	-0.436312	4.617096	1.132324	C	-1.837427	4.334514	1.202690	C	-0.668638	4.645342	1.144635
C	-1.618150	4.648845	0.339856	C	-2.961278	4.001364	0.398992	C	-1.834317	4.607908	0.335204
H	-2.937323	3.388410	-0.831531	H	-3.830774	2.385007	-0.755862	H	-3.066392	3.273806	-0.847636
N	-1.227868	-0.154378	-0.502746	N	-1.143369	-0.463425	-0.452183	N	-1.241642	-0.183538	-0.541123
O	-2.893882	1.067188	-1.375355	O	-3.174162	0.153493	-1.163560	O	-2.969161	1.004155	-1.344970
H	-0.098187	5.559928	1.570174	H	-1.784083	5.351758	1.598974	H	-0.383571	5.607673	1.577470
C	-2.008185	-1.154637	-1.249216	C	-1.628098	-1.671107	-1.128470	C	-2.015952	-1.187110	-1.277790
C	-3.136947	-0.265362	-1.907265	C	-2.992942	-1.175106	-1.740566	C	-3.193514	-0.326094	-1.889684
H	-1.361956	-1.566440	-2.039955	H	-0.914259	-1.926153	-1.927464	H	-1.384993	-1.582335	-2.089794
C	-2.452913	-2.296857	-0.361491	C	-1.681361	-2.829817	-0.149748	C	-2.410702	-2.337534	-0.374384
H	-2.953101	-0.205609	-2.993253	H	-2.870504	-1.028519	-2.826905	H	-3.055287	-0.246156	-2.981333
C	-3.216504	-2.067912	0.797626	C	-2.172341	-2.648918	1.155526	C	-3.042824	-2.099418	0.859263
C	-2.088915	-3.611589	-0.691569	C	-1.178360	-4.086384	-0.520842	C	-2.139471	-3.659139	-0.759488
C	-3.626775	-3.138944	1.597889	C	-2.150256	-3.703776	2.075565	C	-3.410898	-3.166909	1.684564
H	-3.487231	-1.044764	1.076079	H	-2.546642	-1.666811	1.463034	H	-3.235357	-1.070641	1.179571
C	-2.494199	-4.687122	0.111708	C	-1.155265	-5.144895	0.396923	C	-2.502230	-4.731420	0.067623
H	-1.461866	-3.788447	-1.572281	H	-0.762608	-4.222558	-1.524954	H	-1.616941	-3.847035	-1.703918
C	-3.269496	-4.452702	1.254089	C	-1.637274	-4.954517	1.699171	C	-3.141798	-4.486832	1.289394
H	-4.222961	-2.949068	2.496244	H	-2.522494	-3.546234	3.093244	H	-3.899927	-2.969629	2.643912
H	-2.190602	-5.705898	-0.148513	H	-0.736335	-6.112058	0.101549	H	-2.267326	-5.756548	-0.235165
H	-3.583715	-5.290264	1.885592	H	-1.603300	-5.775359	2.423137	H	-3.417341	-5.322365	1.941243
C	1.967131	0.403645	-1.887833	C	1.488640	1.079567	-1.985234	C	1.978755	0.506129	-1.917535

C	4.464472	0.813339	-1.539421	C	3.867471	1.987270	-1.685230	C	4.475569	0.974927	-1.554896
C	5.605153	0.403010	-0.626096	C	5.096192	1.770003	-0.820564	C	5.598021	0.610787	-0.600231
H	4.329519	1.883373	-1.748788	H	3.504769	3.015132	-1.822767	H	4.317659	2.036391	-1.789881
O	4.773868	0.092759	-2.750561	O	4.278030	1.418850	-2.944489	O	4.834513	0.237961	-2.740064
C	4.923249	-1.209460	-2.139847	C	4.714695	0.143302	-2.422587	C	4.998517	-1.048415	-2.098919
C	5.910523	-0.915773	-1.021466	C	5.653897	0.568951	-1.305709	C	5.942166	-0.709433	-0.956761
C	6.259960	1.007134	0.444299	C	5.641456	2.428071	0.279294	C	6.205485	1.251152	0.477130
H	5.189248	-1.965758	-2.890500	H	5.105716	-0.495885	-3.225413	H	5.304613	-1.812288	-2.826122
C	6.881033	-1.659745	-0.354157	C	6.773640	0.000799	-0.702433	C	6.906169	-1.418684	-0.243733
C	7.263895	0.269044	1.104495	C	6.792826	1.873103	0.875192	C	7.202968	0.548314	1.183820
H	6.013746	2.025518	0.763735	H	5.200059	3.351619	0.669835	H	5.928094	2.270404	0.767132
C	7.569751	-1.042753	0.710581	C	7.350159	0.679538	0.390948	C	7.547971	-0.764763	0.828129
H	7.114193	-2.689309	-0.646611	H	7.203676	-0.939216	-1.064680	H	7.169266	-2.449036	-0.506190
H	7.814909	0.725827	1.933668	H	7.260779	2.381152	1.725302	H	7.717981	1.033803	2.019738
H	8.356789	-1.593881	1.236649	H	8.247186	0.270920	0.868677	H	8.328917	-1.287890	1.390475
C	3.180262	0.052970	-1.049339	C	2.786451	0.946840	-1.214903	C	3.198068	0.191762	-1.074458
H	3.001228	0.192215	0.028377	H	2.635640	0.991935	-0.122793	H	3.018498	0.344726	0.002470
C	3.530174	-1.411262	-1.452556	C	3.415392	-0.384903	-1.725572	C	3.585174	-1.267597	-1.463787
H	3.578864	-2.118738	-0.615029	H	3.643676	-1.122231	-0.944265	H	3.605660	-1.979350	-0.627356
Co	0.333953	-0.661727	0.387239	Co	0.464206	-0.429924	0.537849	Co	0.476025	-0.550154	0.366076
C	-4.563297	-0.686725	-1.647318	C	0.398878	3.898563	2.377362	C	1.392560	3.656816	2.303790
C	-5.038481	-1.875848	-2.230548	C	-4.041007	5.060319	0.124183	C	-2.638646	5.896388	0.098346
C	-5.409356	0.054043	-0.806926	C	-3.399290	6.269136	-0.600570	C	-1.730258	6.948669	-0.584116
C	-6.335558	-2.326554	-1.961809	H	-4.158092	7.047425	-0.800776	H	-2.287356	7.887968	-0.754271
H	-4.383446	-2.462139	-2.884698	H	-2.598135	6.726229	0.005708	H	-0.848908	7.186051	0.036509
C	-6.711191	-0.396045	-0.543033	H	-2.959470	5.957040	-1.564149	H	-1.368790	6.577761	-1.559266
H	-5.039282	0.981623	-0.361269	C	-4.652959	5.530891	1.466498	C	-3.134248	6.448985	1.457425
C	-7.176006	-1.588198	-1.114267	H	-3.886138	5.965831	2.130715	H	-2.292017	6.672712	2.134842
H	-6.691406	-3.258484	-2.413370	H	-5.424396	6.302418	1.289725	H	-3.706482	7.382884	1.308964
H	-7.363879	0.188935	0.113838	H	-5.122677	4.685111	1.998389	H	-3.789180	5.716249	1.960511
H	-8.191015	-1.941109	-0.903565	C	-5.173682	4.505846	-0.760823	C	-3.862876	5.649932	-0.803938
C	-2.353083	5.981760	0.126245	H	-4.796699	4.180024	-1.746153	H	-3.564973	5.275380	-1.798942
C	-1.399844	6.987339	-0.565448	H	-5.677835	3.647369	-0.283540	H	-4.557834	4.919240	-0.354326
H	-1.906142	7.957852	-0.718900	H	-5.931665	5.290010	-0.932955	H	-4.415057	6.594699	-0.950873
H	-0.495509	7.169964	0.040512	C	1.706732	3.776874	1.553399	C	2.648941	3.275744	1.479760
H	-1.077152	6.604302	-1.549461	H	1.862996	2.741507	1.217170	H	2.571267	2.244754	1.106467
C	-3.604243	5.810025	-0.756082	H	1.669321	4.437155	0.668140	H	2.769746	3.958644	0.619319
H	-3.344049	5.426325	-1.758154	H	2.573231	4.080281	2.169155	H	3.554276	3.354224	2.109134
H	-4.330541	5.115379	-0.298749	C	0.267719	5.365556	2.834720	C	1.594497	5.093248	2.827764
H	-4.106089	6.784689	-0.887895	H	0.227855	6.062308	1.978776	H	1.730610	5.817461	2.005051
C	-2.794091	6.551699	1.496942	H	-0.632610	5.523978	3.454352	H	0.744647	5.427872	3.448635
H	-1.929460	6.722008	2.161587	H	1.146991	5.635639	3.445259	H	2.501950	5.126151	3.455671
H	-3.314524	7.517842	1.364638	C	0.495775	3.015275	3.646998	C	1.264804	2.719669	3.532035
H	-3.481282	5.853519	2.006214	H	-0.429847	3.095554	4.244496	H	0.381769	2.996008	4.135738
C	1.586229	3.518917	2.259341	H	0.653209	1.961677	3.374437	H	1.164499	1.671141	3.215404
C	1.861103	4.935738	2.802318	H	1.341408	3.349541	4.275473	H	2.160976	2.813368	4.172337
H	2.023781	5.664788	1.988731	C	-4.192129	-2.043579	-1.456670	C	-4.593649	-0.796715	-1.576447

H	1.033545	5.301060	3.436014	C	-4.362779	-3.229990	-2.192470	C	-5.070904	-1.969964	-2.188938
H	2.774917	4.916394	3.421572	C	-5.102641	-1.728932	-0.435212	C	-5.407884	-0.122789	-0.652544
C	2.813970	3.087305	1.418395	C	-5.423178	-4.096608	-1.902110	C	-6.337896	-2.470586	-1.869052
H	2.676052	2.069059	1.028409	H	-3.655923	-3.481569	-2.991591	H	-4.440761	-2.504231	-2.908960
H	2.964823	3.778011	0.569013	C	-6.167905	-2.594270	-0.149901	C	-6.679591	-0.622419	-0.336989
H	3.727011	3.104857	2.041208	H	-4.973325	-0.800428	0.128080	H	-5.037255	0.793257	-0.184058
C	1.424814	2.568666	3.473612	C	-6.328943	-3.781017	-0.878137	C	-7.146193	-1.798477	-0.939305
H	0.559396	2.874514	4.088779	H	-5.543981	-5.020313	-2.477723	H	-6.695305	-3.389531	-2.345398
H	1.275771	1.531104	3.139904	H	-6.874622	-2.339417	0.647049	H	-7.307353	-0.089095	0.384936
H	2.328753	2.610978	4.108408	H	-7.159543	-4.457753	-0.651647	H	-8.137575	-2.190265	-0.688587

Intermediate-5 from elimination^B pathway: In Co catalyzed reaction energy profile

Int5B ¹ : $\nu_{\text{lowest}} = 11.2553 \text{ cm}^{-1}$				Int5B ³ : $\nu_{\text{lowest}} = 12.1031 \text{ cm}^{-1}$				Int5B ⁵ : $\nu_{\text{lowest}} = 12.2904 \text{ cm}^{-1}$			
121				121				121			
C	-0.731300	-0.045336	3.096308	C	-0.186422	2.997039	2.559072	C	-0.174097	2.888306	-2.710701
C	-1.145533	2.266276	2.482288	C	-1.537740	4.591831	1.324723	C	1.109414	4.561051	-1.505709
C	0.359027	0.317649	3.901402	C	0.790964	3.967234	2.833868	C	-1.210559	3.800731	-2.965229
C	-0.055528	2.638729	3.282803	C	-0.557583	5.563150	1.581376	C	0.071818	5.475210	-1.745296
H	-1.717955	3.024220	1.938827	H	-2.424000	4.843183	0.732239	H	1.990943	4.862187	-0.929816
C	0.693617	1.673955	3.990593	C	0.596888	5.259936	2.335354	C	-1.080286	5.103466	-2.471747
H	0.917134	-0.454470	4.440824	H	1.681302	3.694033	3.409908	H	-2.095306	3.476630	-3.523184
H	0.224172	3.695196	3.356438	H	-0.686773	6.576509	1.186134	H	0.151965	6.495808	-1.355752
H	1.535923	1.996192	4.612721	H	1.341146	6.041606	2.520031	H	-1.872400	5.840429	-2.640689
N	0.738816	-2.003243	0.677175	N	2.036578	-1.129277	1.810154	N	-2.035786	-1.335194	-1.857299
C	2.931187	-2.755631	0.206159	C	3.632603	-2.240560	0.477266	C	-3.624455	-2.300449	-0.412616
C	3.561862	-2.268416	-1.996845	C	2.819421	-2.944907	-1.586449	C	-2.731199	-3.102716	1.583693
C	4.180040	-3.380631	0.508681	C	4.943244	-2.741961	0.218252	C	-4.949542	-2.691724	-0.061050
C	1.830730	-2.709659	1.118925	C	3.305588	-1.578709	1.722404	C	-3.326498	-1.660876	-1.681113
C	4.828095	-2.861213	-1.783721	C	4.077552	-3.494174	-1.928383	C	-4.004602	-3.531302	2.018595
H	3.287267	-1.823092	-2.956906	H	1.960132	-2.995154	-2.264058	H	-1.832501	-3.239121	2.194838
C	5.142598	-3.397487	-0.542765	C	5.136317	-3.384642	-1.037363	C	-5.110161	-3.320302	1.203662
C	4.325828	-3.960861	1.797389	C	5.947971	-2.563742	1.213718	C	-6.002994	-2.439386	-0.990396
C	1.998459	-3.345801	2.364692	C	4.332368	-1.431848	2.679382	C	-4.407481	-1.445951	-2.570307
H	5.549564	-2.874356	-2.604821	H	4.203246	-3.992411	-2.894523	H	-4.105622	-4.019861	2.992126
H	6.123631	-3.852314	-0.367399	H	6.122610	-3.790584	-1.287747	H	-6.108565	-3.637349	1.524246
C	3.242330	-3.938727	2.679195	C	5.627675	-1.920142	2.408581	C	-5.714900	-1.832217	-2.212742
H	5.266990	-4.446847	2.071888	H	6.960242	-2.937807	1.031351	H	-7.025899	-2.734870	-0.737395
H	1.168043	-3.358514	3.075912	H	4.114150	-0.930195	3.627263	H	-4.213352	-0.966894	-3.535141
H	3.351054	-4.411895	3.661797	H	6.405356	-1.789124	3.169320	H	-6.529646	-1.647518	-2.921601
N	2.659831	-2.210631	-1.017940	N	2.618425	-2.330189	-0.424891	N	-2.560681	-2.501767	0.406682
C	-1.313370	-1.394278	2.893961	C	-0.150374	1.550111	2.872551	C	-0.126045	1.443634	-3.037241
O	-0.956257	-2.439446	3.420437	O	0.764889	0.967236	3.450353	O	-0.991286	0.812181	-3.638082
O	-0.744939	-0.814470	-1.659146	O	-0.350171	-2.081162	-0.865246	O	0.627598	-2.066997	0.922995
C	-1.272065	0.384154	-1.622318	C	-1.356958	-1.384123	-1.334430	C	1.574059	-1.301537	1.382159
C	-0.599365	1.506175	-1.040543	C	-1.361090	0.050697	-1.347283	C	1.467060	0.134402	1.367370
C	-2.586422	0.596334	-2.180553	C	-2.485189	-2.062010	-1.923969	C	2.771805	-1.877276	1.951941

C	-1.228703	2.772771	-0.933461	C	-2.431227	0.785248	-1.916572	C	2.503993	0.957704	1.875311
C	0.724965	1.337908	-0.515898	C	-0.210568	0.759687	-0.854753	C	0.261059	0.752107	0.880659
C	-3.150044	1.863972	-2.044063	C	-3.515325	-1.282717	-2.449679	C	3.756908	-1.013047	2.423398
C	-2.514607	2.971217	-1.415877	C	-3.529471	0.137982	-2.467286	C	3.665331	0.406241	2.400598
H	-0.664373	3.574656	-0.455376	H	-2.353190	1.874220	-1.911538	H	2.350744	2.038065	1.844148
N	1.477753	0.260332	-0.576899	N	0.786192	0.259045	-0.167874	N	-0.752935	0.167671	0.292428
O	1.296655	2.392870	0.114306	O	-0.119869	2.084865	-1.117325	O	0.148126	2.100091	1.033595
H	-4.156062	2.016813	-2.442045	H	-4.375085	-1.800150	-2.881979	H	4.664860	-1.452355	2.844389
C	2.748464	0.529523	0.120897	C	1.797976	1.303226	0.078477	C	-1.783256	1.173699	-0.006845
C	2.430301	1.871517	0.865306	C	1.142340	2.580583	-0.588063	C	-1.175181	2.506844	0.596547
H	2.921404	-0.254991	0.873724	H	1.878443	1.456509	1.165976	H	-1.870098	1.272187	-1.100753
C	3.932186	0.592042	-0.821977	C	3.168091	0.926586	-0.440438	C	-3.145650	0.803757	0.538048
H	2.049952	1.632823	1.871833	H	0.892802	3.317029	0.190579	H	-1.039486	3.251681	-0.201659
C	3.783006	1.001767	-2.157733	C	3.334359	0.386067	-1.726505	C	-3.283608	0.252053	1.822951
C	5.212762	0.274528	-0.339749	C	4.298275	1.137309	0.365111	C	-4.296804	1.068562	-0.220726
C	4.898137	1.082320	-3.002487	C	4.611520	0.064107	-2.198714	C	-4.554069	-0.016463	2.344915
H	2.784034	1.237108	-2.539701	H	2.455334	0.196281	-2.350208	H	-2.387204	0.024378	2.407827
C	6.328957	0.359423	-1.180974	C	5.578685	0.812415	-0.102563	C	-5.570426	0.797568	0.297656
H	5.332391	-0.053026	0.698631	H	4.169395	1.538858	1.376412	H	-4.191328	1.479931	-1.230812
C	6.174302	0.761161	-2.516029	C	5.736573	0.275885	-1.387264	C	-5.700931	0.259554	1.584947
H	4.770750	1.396585	-4.043970	H	4.729452	-0.364509	-3.199113	H	-4.650290	-0.446277	3.347275
H	7.321557	0.103280	-0.795884	H	6.449624	0.962151	0.543144	H	-6.459671	0.996670	-0.308801
H	7.046033	0.823462	-3.176015	H	6.734277	0.010965	-1.752736	H	-6.694581	0.043753	1.991839
C	-1.485686	0.909333	2.390965	C	-1.349154	3.294842	1.823533	C	0.981718	3.252915	-1.994763
C	-4.028999	0.577619	2.334959	C	-3.497537	2.079000	2.621996	C	3.182975	2.142460	-2.804424
C	-5.108284	-0.052534	1.470686	C	-4.310298	0.859782	2.222030	C	4.063951	0.976890	-2.391040
H	-4.176205	1.614839	2.666563	H	-4.015251	3.042822	2.725489	H	3.646168	3.131298	-2.927646
O	-3.997964	-0.317440	3.465710	O	-2.931840	1.667585	3.878367	O	2.631954	1.680025	-4.050402
C	-3.840453	-1.541973	2.706590	C	-2.376033	0.409493	3.414239	C	2.149524	0.401423	-3.561364
C	-4.986168	-1.435737	1.716635	C	-3.565959	-0.227801	2.719786	C	3.379478	-0.158103	-2.869021
C	-6.045399	0.438772	0.565043	C	-5.461313	0.661146	1.462463	C	5.225894	0.855474	-1.632473
H	-3.801887	-2.414004	3.372587	H	-1.888125	-0.138386	4.228547	H	1.686623	-0.183621	-4.365183
C	-5.802151	-2.358895	1.066999	C	-3.943145	-1.542017	2.453820	C	3.837971	-1.443723	-2.592718
C	-6.895054	-0.488928	-0.073275	C	-5.872220	-0.666328	1.226265	C	5.713894	-0.442205	-1.379574
H	-6.135235	1.510157	0.360255	H	-6.037864	1.503379	1.064028	H	5.752952	1.735302	-1.247291
C	-6.775972	-1.864872	0.175085	C	-5.121423	-1.749263	1.710233	C	5.029214	-1.572595	-1.851859
H	-5.698372	-3.434734	1.241398	H	-3.333095	-2.379681	2.798960	H	3.287786	-2.323788	-2.931764
H	-7.659303	-0.130928	-0.771360	H	-6.785697	-0.856596	0.652931	H	6.636576	-0.571364	-0.804186
H	-7.446957	-2.564588	-0.334301	H	-5.457095	-2.771271	1.503575	H	5.427348	-2.570295	-1.638532
C	-2.643687	0.276466	1.651251	C	-2.232917	2.081776	1.671194	C	1.929865	2.090081	-1.842707
H	-2.657025	0.542627	0.583573	H	-2.530270	1.912163	0.624948	H	2.246225	1.949351	-0.797978
C	-2.509308	-1.249763	1.939203	C	-1.414451	0.912994	2.294672	C	1.167265	0.873607	-2.447136
H	-2.376159	-1.894355	1.055702	H	-1.147319	0.089961	1.619643	H	0.934502	0.056960	-1.751658
C	-3.342806	-0.553391	-2.867514	C	-2.535455	-3.599819	-1.968313	C	2.927835	-3.405841	2.038788
C	-3.258369	4.310970	-1.300883	C	-4.705753	0.884994	-3.115962	C	4.808986	1.253259	2.981100
C	-4.559085	4.101404	-0.487132	C	-6.041234	0.418119	-2.489559	C	6.142589	0.885912	2.287048
H	-5.112078	5.052970	-0.388318	H	-6.890171	0.944072	-2.962895	H	6.973159	1.475979	2.715377

H	-5.226191	3.371446	-0.976659	H	-6.199475	-0.665486	-2.624777	H	6.387433	-0.182556	2.413593
H	-4.329844	3.726659	0.526230	H	-6.055553	0.628388	-1.407744	H	6.085920	1.093464	1.205803
C	-3.615732	4.826911	-2.716324	C	-4.716667	0.578456	-4.634348	C	4.926176	0.967320	4.499073
H	-4.252907	4.108199	-3.259844	H	-4.821935	-0.504206	-4.822482	H	5.130522	-0.100346	4.690907
H	-4.164100	5.784244	-2.651131	H	-5.560332	1.094355	-5.128588	H	5.749512	1.556917	4.942624
H	-2.701625	4.989582	-3.313466	H	-3.777232	0.914994	-5.106735	H	3.988676	1.231894	5.018697
C	-2.405974	5.380411	-0.591443	C	-4.588842	2.409151	-2.920516	C	4.560738	2.760937	2.781995
H	-2.141983	5.074438	0.436355	H	-4.564692	2.674882	-1.848595	H	4.464362	3.013921	1.711135
H	-1.470157	5.583659	-1.140470	H	-3.679427	2.814253	-3.397664	H	3.644756	3.095635	3.299407
H	-2.971453	6.326243	-0.525123	H	-5.459240	2.913052	-3.376235	H	5.408291	3.337601	3.192403
C	-3.665633	-1.644999	-1.819933	C	-2.410704	-4.181159	-0.537680	C	2.824474	-4.039612	0.628547
H	-2.753754	-2.054022	-1.365089	H	-1.417278	-3.967649	-0.120238	H	1.813551	-3.909055	0.219187
H	-4.303129	-1.230120	-1.023418	H	-3.179440	-3.747866	0.125589	H	3.554245	-3.576756	-0.058131
H	-4.219790	-2.473724	-2.297668	H	-2.552961	-5.277056	-0.568575	H	3.042464	-5.121746	0.691259
C	-4.676563	-0.072419	-3.474889	C	-3.857980	-4.110573	-2.574947	C	4.288999	-3.807319	2.641817
H	-5.369206	0.298758	-2.699460	H	-4.731739	-3.785574	-1.982182	H	5.131584	-3.445760	2.025470
H	-4.526750	0.723250	-4.226977	H	-3.997141	-3.769825	-3.616428	H	4.418584	-3.421497	3.668772
H	-5.169600	-0.922940	-3.976722	H	-3.849205	-5.214409	-2.583736	H	4.354562	-4.908377	2.687760
C	-2.485674	-1.147519	-4.014121	C	-1.368676	-4.125245	-2.842936	C	1.809972	-3.982123	2.945076
H	-3.053378	-1.949406	-4.520709	H	-1.454722	-3.744551	-3.876493	H	1.883498	-3.566774	3.966224
H	-2.245578	-0.373032	-4.765072	H	-0.402285	-3.807347	-2.423173	H	0.819331	-3.740483	2.530176
H	-1.547248	-1.571552	-3.627906	H	-1.390549	-5.229857	-2.878192	H	1.905702	-5.081450	3.010763
C	3.541727	2.876279	0.946392	C	1.944274	3.240705	-1.682525	C	-1.939025	3.116044	1.747726
C	4.386596	2.870523	2.069804	C	3.038355	4.050080	-1.327307	C	-3.084208	3.885858	1.475432
C	3.801326	3.766651	-0.109728	C	1.657542	3.025946	-3.039877	C	-1.568808	2.881511	3.081812
C	5.489931	3.732413	2.130630	C	3.848714	4.618167	-2.316864	C	-3.863249	4.391475	2.522495
H	4.178557	2.184430	2.899152	H	3.263191	4.225158	-0.269264	H	-3.373635	4.077660	0.436199
C	4.898931	4.633361	-0.044510	C	2.465264	3.602221	-4.030471	C	-2.344848	3.395526	4.130160
H	3.134983	3.776952	-0.976806	H	0.797030	2.408630	-3.313566	H	-0.667995	2.297878	3.292924
C	5.749029	4.614414	1.071729	C	3.565518	4.393335	-3.672780	C	-3.497135	4.144506	3.854492
H	6.144003	3.719986	3.008849	H	4.703879	5.239023	-2.029680	H	-4.758695	4.981055	2.299028
H	5.094374	5.325281	-0.870522	H	2.233620	3.429691	-5.086972	H	-2.047611	3.207507	5.167481
H	6.608869	5.290963	1.118811	H	4.198988	4.838255	-4.447387	H	-4.105924	4.540522	4.674192
Co	0.900636	-1.469778	-1.110830	Co	0.867616	-1.568228	0.460526	Co	-0.760551	-1.781523	-0.420814
O	0.350477	-3.119144	-1.835043	O	0.655033	-3.375228	1.244411	O	-0.376264	-3.804099	-1.088932
C	-0.692522	-3.773082	-1.392339	C	-0.297082	-3.131358	2.078259	C	0.428663	-3.357493	-1.961521
O	-1.290490	-3.566077	-0.324248	O	-0.797419	-1.983802	2.184859	O	0.644417	-2.100153	-2.056111
H	-0.157060	-2.528722	0.741473	H	1.742640	-0.588633	2.635560	H	-1.793921	-0.881671	-2.749115
C	-1.173221	-4.852280	-2.352732	C	-0.813031	-4.290516	2.909190	C	1.161854	-4.312667	-2.880769
H	-0.335488	-5.281704	-2.923941	H	-1.053538	-3.942619	3.926407	H	1.324418	-3.852330	-3.868084
H	-1.712637	-5.633493	-1.796157	H	-1.742718	-4.668223	2.447787	H	2.147723	-4.540725	-2.437494
H	-1.873313	-4.384821	-3.068901	H	-0.079984	-5.110211	2.944283	H	0.602306	-5.254976	-2.980143

Local nucleophilicity calculation

Tetracyanoethylene: As the reference scale for global nucleophilicity index (*N*)

TCE¹: $\nu_{\text{lowest}} = 72.6776 \text{ cm}^{-1}$

10

C	-0.179199	0.261930	-0.000011
C	1.208726	0.261912	-0.000001
C	-0.921615	1.484344	0.000006
N	-1.547017	2.473791	0.000019
C	1.951175	1.484301	0.000027
N	2.576606	2.473729	0.000050
C	1.951142	-0.960502	-0.000017
N	2.576544	-1.949948	-0.000030
C	-0.921648	-0.960459	-0.000039
N	-1.547079	-1.949887	-0.000062

NBO charge comparison with different alkenes (norbornadiene and cyclopentene) for Int2 in cobalt catalysis

Intermediate-2: In Co catalysis with norbornadiene.

Int2³ **norbornadiene:** $\nu_{\text{lowest}} = 15.5339 \text{ cm}^{-1}$

109

C	-0.041352	-1.267682	-2.583367
C	2.294900	-1.791389	-2.188276
C	0.376345	-0.362766	-3.581810
C	2.697463	-0.842121	-3.133098
H	3.056267	-2.361832	-1.644842
C	1.728316	-0.129187	-3.849767
H	-0.404515	0.166122	-4.137952
H	3.763912	-0.665701	-3.307395
H	2.021007	0.605698	-4.606880
N	-1.901397	-1.194528	-1.034220
C	-3.307267	-1.001263	0.855039
C	-2.160949	-0.545340	2.841934
C	-4.577912	-0.991236	1.514365
C	-3.197736	-1.233419	-0.560687
C	-3.370524	-0.511423	3.573763
H	-1.190299	-0.373476	3.320253
C	-4.570571	-0.732902	2.914298
C	-5.746705	-1.231774	0.740948
C	-4.376114	-1.471511	-1.286287
H	-3.343658	-0.310756	4.648906
H	-5.520773	-0.710886	3.459076
C	-5.625527	-1.470355	-0.623368
H	-6.726076	-1.225356	1.229825

H	-4.304459	-1.630924	-2.362134
H	-6.527200	-1.658186	-1.216929
N	-2.139079	-0.780650	1.531041
C	-1.542026	-1.268283	-2.353164
O	-2.326298	-1.222237	-3.314746
O	1.015815	-0.755803	1.396258
C	2.154602	-0.221992	1.013067
C	2.222869	0.808832	0.012318
C	3.392297	-0.628388	1.634349
C	3.462511	1.345497	-0.414294
C	1.012935	1.357958	-0.545680
C	4.579979	-0.076255	1.154158
C	4.661430	0.894541	0.120545
H	3.435458	2.112821	-1.189489
N	-0.205717	0.899511	-0.401214
O	1.112932	2.489960	-1.289792
H	5.517408	-0.414563	1.602702
C	-1.127909	1.740448	-1.179343
C	-0.234800	2.995834	-1.502681
H	-1.347638	1.222322	-2.129120
C	-2.433098	1.988668	-0.462821
H	-0.315115	3.262611	-2.567419
C	-2.453676	2.324156	0.902867
C	-3.645856	1.869723	-1.160217
C	-3.669913	2.546384	1.557124
H	-1.510464	2.396158	1.452318
C	-4.865803	2.092172	-0.506033
H	-3.633073	1.563389	-2.212078
C	-4.879052	2.432324	0.853175
H	-3.676120	2.801098	2.621883
H	-5.806148	1.976502	-1.054065
H	-5.831706	2.594550	1.368531
C	0.937538	-2.040376	-1.887804
C	0.101682	-4.513121	-1.525354
H	0.557770	-4.778480	-2.490684
C	-1.452627	-3.968062	0.022682
H	-2.426235	-3.753011	0.486243
C	0.677402	-3.174788	-0.894285
H	1.657614	-3.395938	-0.443554
C	-0.356144	-2.885580	0.217962
H	0.074256	-2.934438	1.234210
Co	-0.521709	-0.932057	0.290485
C	3.397610	-1.653453	2.784689
C	6.036127	1.390687	-0.353752
C	6.841326	0.189125	-0.907784
H	7.839668	0.516508	-1.251111
H	6.985436	-0.589781	-0.139034

H	6.313987	-0.271406	-1.761856
C	6.801886	2.019506	0.835770
H	6.949923	1.292316	1.652814
H	7.798459	2.370252	0.511136
H	6.246169	2.881393	1.244635
C	5.908511	2.447344	-1.467649
H	5.387512	2.041456	-2.352570
H	5.355561	3.337761	-1.120904
H	6.912608	2.776442	-1.788058
C	2.883252	-3.021477	2.275589
H	1.857777	-2.935753	1.889961
H	3.531416	-3.402815	1.466709
H	2.887273	-3.761122	3.096933
C	4.814249	-1.870019	3.356308
H	5.504990	-2.288917	2.603206
H	5.249203	-0.932050	3.744529
H	4.760226	-2.588238	4.192987
C	2.498365	-1.147526	3.941281
H	2.877215	-0.186163	4.331623
H	1.463706	-1.004801	3.596080
H	2.501838	-1.880393	4.768813
C	-0.480205	4.205575	-0.628309
C	-1.591650	5.027017	-0.891440
C	0.336110	4.485815	0.479923
C	-1.893966	6.101579	-0.047467
H	-2.236551	4.810325	-1.750146
C	0.033362	5.564491	1.323497
H	1.211844	3.860896	0.677605
C	-1.083562	6.371069	1.066033
H	-2.766726	6.728651	-0.257430
H	0.675673	5.774517	2.185417
H	-1.320344	7.211110	1.727554
C	0.213374	-5.534642	-0.401922
H	0.993185	-6.298185	-0.322561
C	-0.714123	-5.209976	0.526659
H	-0.835853	-5.644521	1.523994
C	-1.419916	-4.254324	-1.496160
H	-1.990471	-5.162681	-1.752023
H	-1.756789	-3.431366	-2.138956

Intermediate-2: In Co catalysis with cyclopentene.

Int2³_{cyclopentene}: $\nu_{\text{lowest}} = 12.8088 \text{ cm}^{-1}$

107

C	-0.153961	-1.507448	-2.590604
C	2.134870	-2.117587	-2.064277

C	0.337160	-0.582009	-3.529970
C	2.615545	-1.141238	-2.946337
H	2.845063	-2.737645	-1.506246
C	1.712464	-0.381034	-3.700411
H	-0.390790	-0.006316	-4.111568
H	3.694238	-0.984585	-3.048075
H	2.075105	0.369163	-4.410726
N	-1.957646	-1.365577	-1.035948
C	-3.265433	-1.054091	0.909564
C	-2.014882	-0.670957	2.845774
C	-4.505190	-0.948586	1.616059
C	-3.232530	-1.312738	-0.506956
C	-3.189649	-0.541529	3.622561
H	-1.016718	-0.570803	3.286385
C	-4.427122	-0.679054	3.011462
C	-5.718114	-1.114884	0.891019
C	-4.450916	-1.480230	-1.182392
H	-3.106565	-0.335916	4.693908
H	-5.351949	-0.583632	3.590784
C	-5.670819	-1.379529	-0.472184
H	-6.673962	-1.031975	1.418078
H	-4.430899	-1.663909	-2.256905
H	-6.606827	-1.510339	-1.026501
N	-2.058518	-0.915694	1.537777
C	-1.650509	-1.498836	-2.367740
O	-2.456958	-1.502925	-3.307906
O	1.075214	-1.041420	1.274535
C	2.205417	-0.470904	0.924658
C	2.264190	0.612029	-0.019656
C	3.448231	-0.897278	1.523852
C	3.497088	1.196010	-0.400956
C	1.051624	1.162770	-0.570896
C	4.628845	-0.291446	1.094279
C	4.699747	0.744504	0.125742
H	3.462864	2.005018	-1.132201
N	-0.166500	0.708219	-0.420060
O	1.154080	2.298921	-1.309487
H	5.568693	-0.639616	1.529957
C	-1.097526	1.572382	-1.158608
C	-0.188835	2.806046	-1.535070
H	-1.384547	1.052280	-2.089129
C	-2.354821	1.878600	-0.379775
H	-0.273732	3.031505	-2.609338
C	-2.292542	2.219404	0.982917
C	-3.603149	1.831995	-1.020405
C	-3.461316	2.522377	1.689348
H	-1.322537	2.235005	1.488363

C	-4.775897	2.133719	-0.313869
H	-3.657231	1.528783	-2.071890
C	-4.705748	2.482851	1.041238
H	-3.402873	2.783051	2.751026
H	-5.745410	2.076672	-0.818615
H	-5.621643	2.710122	1.597098
C	0.756030	-2.331506	-1.865445
C	0.320261	-3.514922	-0.993298
H	1.261647	-4.003968	-0.687991
C	-0.474521	-3.132326	0.281473
H	0.125438	-3.190568	1.203423
Co	-0.505988	-1.148561	0.215711
C	3.469697	-2.014518	2.584172
C	6.067442	1.304883	-0.294041
C	6.909296	0.164219	-0.917875
H	7.903499	0.538291	-1.223435
H	7.062679	-0.662151	-0.202383
H	6.404532	-0.248585	-1.809216
C	6.802164	1.867837	0.947044
H	6.958072	1.089754	1.714196
H	7.793664	2.263931	0.661407
H	6.220233	2.685955	1.406298
C	5.928061	2.433727	-1.333208
H	5.432568	2.078382	-2.253715
H	5.345476	3.282392	-0.934153
H	6.927605	2.810935	-1.612101
C	3.002325	-3.341939	1.939480
H	1.988974	-3.237376	1.526897
H	3.685397	-3.635690	1.122680
H	2.994792	-4.152469	2.691075
C	4.885030	-2.243585	3.154130
H	5.596103	-2.576630	2.377535
H	5.289255	-1.332019	3.628892
H	4.840716	-3.033585	3.924041
C	2.544211	-1.642494	3.770295
H	2.888748	-0.707921	4.247958
H	1.508482	-1.502806	3.428269
H	2.566307	-2.445143	4.529982
C	-0.418566	4.053143	-0.710224
C	-1.522069	4.875716	-1.001398
C	0.405076	4.367859	0.383035
C	-1.810378	5.984648	-0.198019
H	-2.172145	4.633675	-1.849370
C	0.117415	5.481706	1.185015
H	1.273983	3.740359	0.601621
C	-0.992694	6.288750	0.901205
H	-2.677671	6.612044	-0.428717

H	0.765491	5.718415	2.035651
H	-1.218545	7.155899	1.530790
C	-1.979571	-4.474446	-1.115041
H	-2.505317	-5.444310	-1.157535
H	-2.610832	-3.748796	-1.652793
C	-0.574077	-4.555129	-1.746487
H	-0.584298	-4.379137	-2.835212
H	-0.147368	-5.560869	-1.582560
C	-1.723784	-4.011460	0.330160
H	-1.501284	-4.891176	0.969362
H	-2.600273	-3.518618	0.784962

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