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SUPPLEMENTARY INFORMATION

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Design of catalysts for site-selective and enantioselective functionalization of non-activated primary C–H bonds

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Design of Catalysts for Site-Selective and Enantioselective Functionalization of Non-Activated Primary C–H Bonds

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1 - General Considerations

1.1 Equipment and Methods

^{1}H and ^{13}C NMR spectra were recorded at either 500 MHz (^{13}C at 126 MHz) or 600 MHz (^{13}C at 151 MHz) on INOVA-500 or Bruker-600 spectrometer, as indicated. NMR spectra were run in solutions of deuterated chloroform ($CDCl_3$) with residual chloroform taken as an internal standard (7.26 ppm for ^{1}H, and 77.16 ppm for ^{13}C), and were reported in parts per million (ppm).

Abbreviations for signal multiplicity are as follow: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, etc. Coupling constants (*J* values) were calculated directly from the spectra. IR spectra were collected on a Nicolet iS10 FT-IR spectrometer. Mass spectra were taken on a Thermo Finnigan LTQ-FTMS spectrometer with APCI, ESI or NSI. Thin layer chromatographic (TLC) analysis was performed with glass-backed silica gel plates, visualizing with UV light (254 nm) and/or staining with aqueous $KMnO_4$ stain.

1.2 Solvents for Reaction

The dichloromethane(CH_2Cl_2) used for the carbene transformations was dried at reflux over calcium hydride in a 250mL round-bottom flask for 12 hours under argon, then distilled and stored under argon atmosphere and then used directly.

1.3 Substrates and Reagents

The substrates and reagents were purchased from the following suppliers and used without further purification:

Acros: 2-Methylbutane (1 LT, 99+% purity).

Sigma-Aldrich: 3-Methylpentane (1 LT, ≥99% purity); 2,2-Dimethylbutane (100 mL, ≥99% purity); 3,3-Dimethylpentane (5 g, 99% purity); 2,2-Diethyl-1,3-propanediol (100 g, ≥99% purity); 1-Bromobutane (500 mL, 99% purity); (*S*)-(+)-1-Bromo-2-methylbutane (1g, >99% purity); (*S*)-(-)-2-Methylbutanol (10g, ≥99% purity); (*S*)-(+)-2-Pentanol (5g, 98% purity).

Alfa-Aesar: 2-Methylpentane (100 mL, 99+% purity); 3-Ethyl-3-hexanol (5g, 98% purity).

TCI: 3-Ethyl-3-methylpentane (5 mL, >99% purity); 2,2-Dimethylpentane (5 mL, 97% purity); 3,3-Dimethylhexane (1 mL, >99% purity); 3-Ethyl-3-pentanol (10 mL, ≥99% purity); 2-Methyl-2-propyl-1, 3-propanediol (25 g, >98% purity);

The following reagents were prepared according to reported procedures [1, 2, 3, 4]:

Methyl 2-(4-bromophenyl)-2-diazoacetate; 2,2,2-trichloroethyl 2-(4-bromophenyl)-2-diazoacetate; 2,2,2-trifluoroethyl 2-(4-bromophenyl)-2-diazoacetate; 2,2,2-tribromoethyl 2-(4-bromophenyl)-2-diazoacetate.

2 - C–H Functionalization Reactions

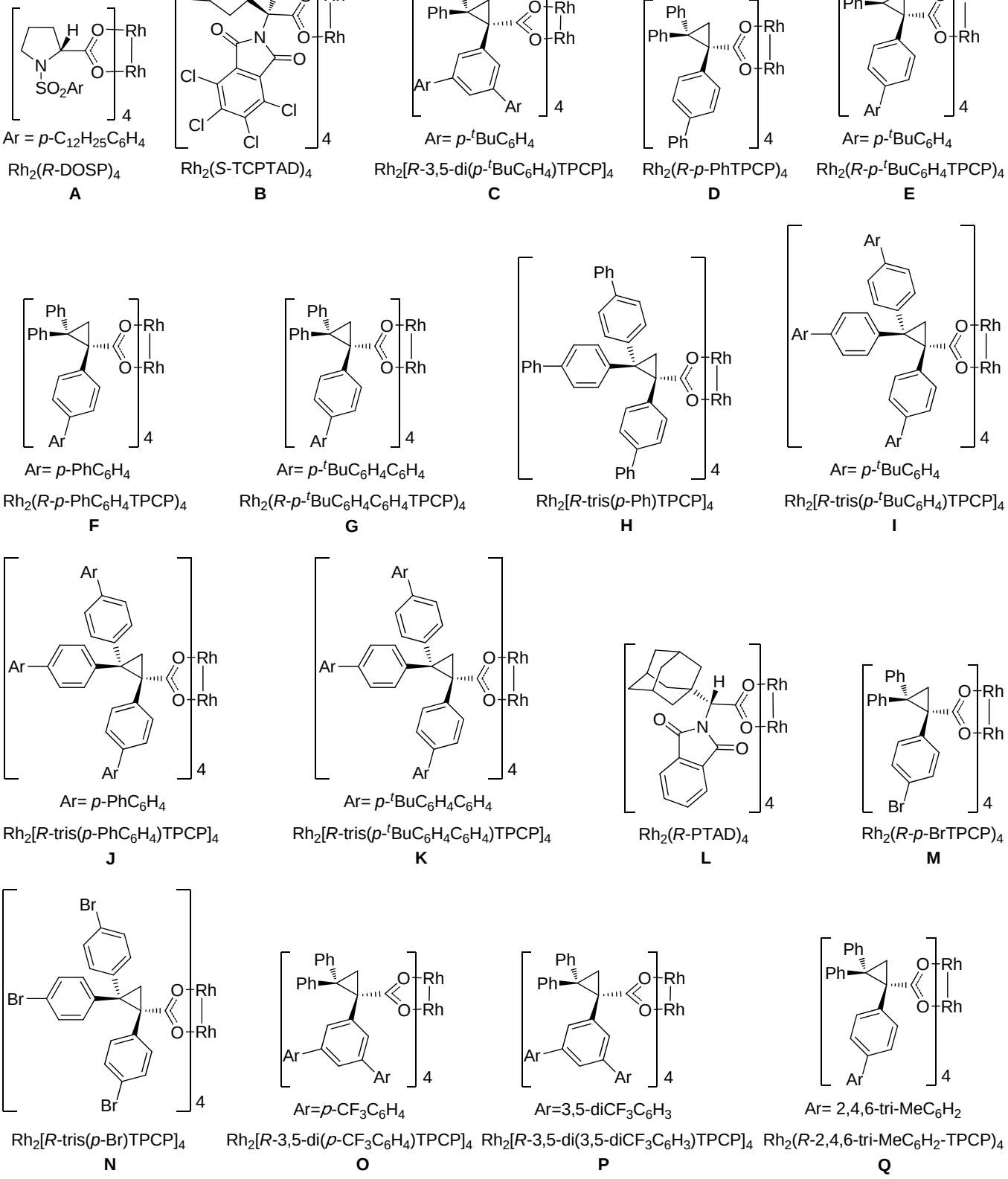
2.1 General Procedures A for C–H Functionalization Reactions

A 5-mL flask was equipped with a reflux condenser and an octagonal magnetic stir bar. The flask was charged with Rh_2L_4 (0.002 mmol, 1 mol%) and treated by vacuum/argon to replace the air in the flask to argon. Substrate (0.6 mmol, 3 *equiv.*) and distilled CH_2Cl_2 (0.5 mL) were added, then the catalyst/substrate solution was heated to reflux under argon for 5 minutes. Diazo (0.2 mmol, 1.0 *equiv.*) was dissolved in 3 mL of distilled CH_2Cl_2 and then the diazo solution was added dropwise to the catalyst solution over 6h with a syringe pump under reflux condition and argon atmosphere. After addition, 0.5 mL distilled CH_2Cl_2 was used to dilute the left over diazo in the syringe needle and then the diazo solution was added dropwise to the reaction solution. Then the rest of the diazo solution in the syringe needle was further pushed into the reaction solution. Then the reaction mixture was allowed to stir for another 1 min, then the reaction mixture was transferred into a 25-mL round-bottom flask with diethyl ether (5 mL x 3) and concentrated under vacuum, and crude ^1H NMR spectrum was obtained to analyze the reaction and measure the selectivity. Then the crude was purified by flash chromatography on silica gel to obtain the product.

2.2 General Procedures B for C–H Functionalization Reactions

A 5-mL flask was equipped with a reflux condenser and an octagonal magnetic stir bar. The flask was charged with Rh_2L_4 (0.002 mmol, 1 mol%) and treated by vacuum/argon to replace the air in the flask to argon. Substrate (0.2 mmol, 1 *equiv.*) and distilled CH_2Cl_2 (0.5 mL) were added, then the catalyst/substrate solution was heated to reflux under argon for 5 minutes. Diazo (0.2 mmol, 1.0 *equiv.*) was dissolved in 3 mL of distilled CH_2Cl_2 and then the diazo solution was added dropwise to the catalyst solution over 6h with a syringe pump under reflux condition and argon atmosphere. After addition, 0.5 mL distilled CH_2Cl_2 was used to dilute the left over diazo in the syringe needle and then the diazo solution was added dropwise to the reaction solution. Then the rest of the diazo solution in the syringe needle was further pushed into the reaction solution. Then the reaction mixture was allowed to stir for another 1 min, then the reaction mixture was transferred into a 25-mL round-bottom flask with diethyl ether (5 mL x 3) and concentrated under vacuum, and crude ^1H NMR spectrum was obtained to analyze the reaction and measure the selectivity. Then the crude was purified by flash chromatography on silica gel to obtain the product.

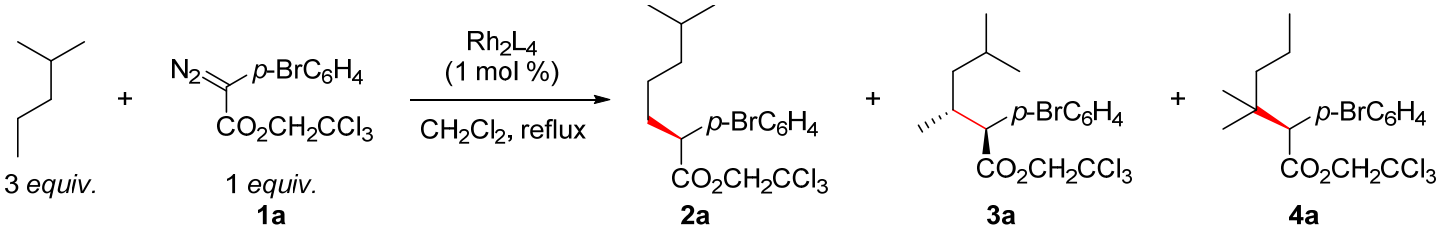
2.3 Catalysts Structures



Supplementary Figure 1. Catalyst Structures

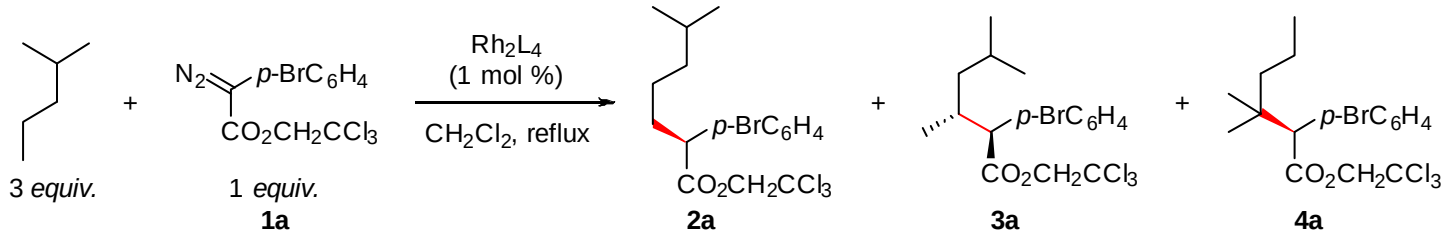
2.4 Result Summary of Catalysts and Diazo Screen

Supplementary Table 1. Catalyst Screen Data Summary

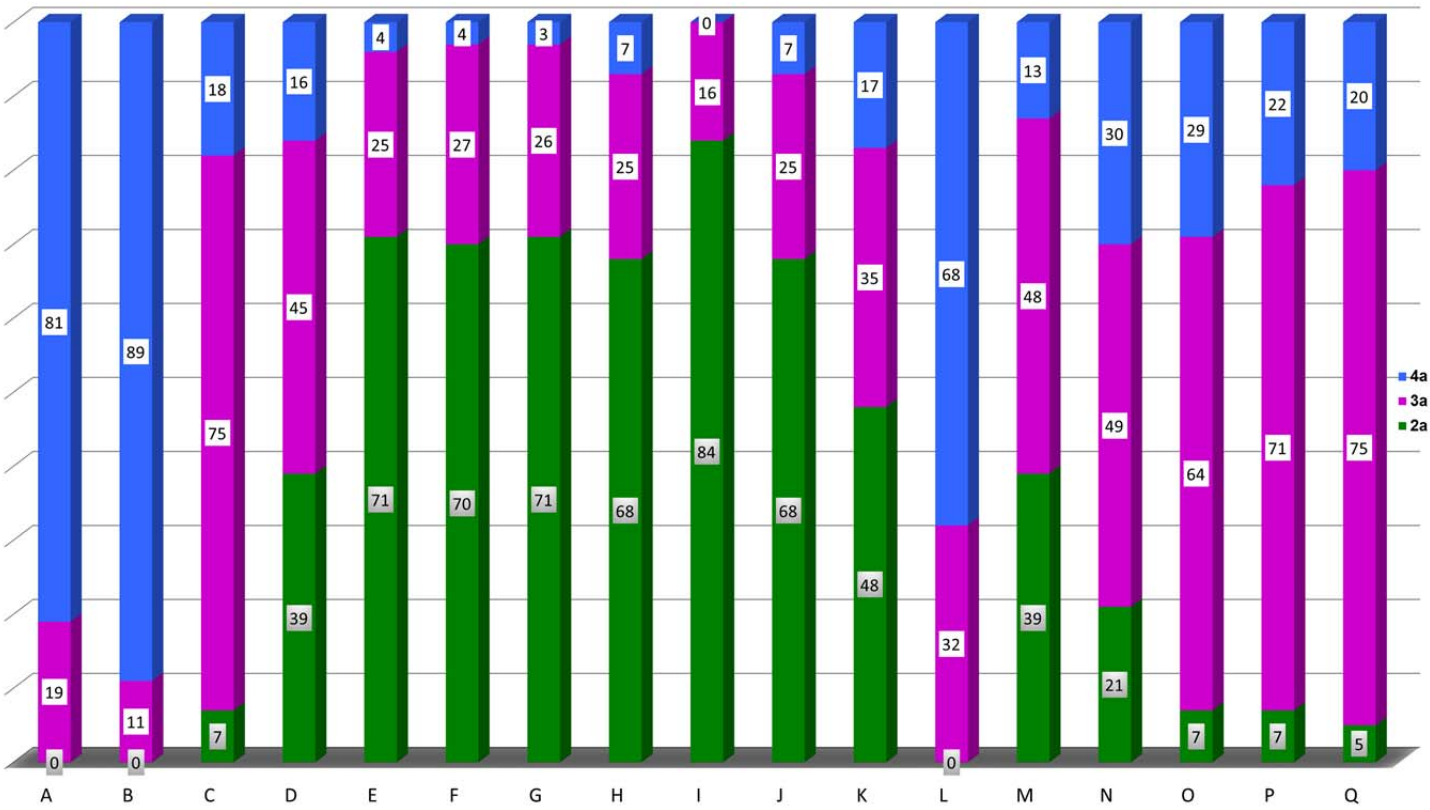


Catalyst	r.r. (**2a**: **3a**: **4a**)	e.e. (**2a**,%)	e.e. (**3a**,%)	d.r. (**3a**,%)	e.e. (**4a**,%)	yield (**2a+3a**,%)	yield (**4a**,%)
Rh_2(*R*-DOSP)$_4$ **(A)**	0: 19: 81	n.d.	69	2:1	29	16	72
Rh_2(*S*-TCPTAD)$_4$ **(B)** [5]	0: 11: 89	n.d.	-77	2:1	-84	10	74
Rh_2[*R*-3,5-di(*p*-^{t}BuC_6H_4)TPCP]$_4$ **(C)**	7: 75: 18	81	92	7:1	23	75	16
Rh_2(*R*-*p*-PhTPCP)$_4$ **(D)**	39: 45: 16	97	87	9:1	60	75	14
Rh_2(*R*-*p*-^{t}BuC_6H_4TPCP)$_4$ **(E)**	71: 25: 4	96	89	9:1	n.d.	86	4
Rh_2(*R*-*p*-PhC_6H_4TPCP)$_4$ **(F)**	70: 27: 4	98	94	11:1	n.d.	83	3
Rh_2(*R*-*p*-^{t}Bu$C_6H_4C_6H_4$TPCP)$_4$ **(G)**	71: 26: 3	97	96	15:1	n.d.	85	3
Rh_2[*R*-tris(*p*-Ph)TPCP]$_4$ **(H)**	68: 25: 7	90	83	5:1	40	71	5
Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$ **(I)**	84: 16: 0	98	92	2:1	n.d.	90	n.d.
Rh_2[*R*-tris(*p*-PhC_6H_4)TPCP]$_4$ **(J)**	68: 25: 7	92	82	5:1	35	78	5
Rh_2[*R*-tris(*p*-^{t}Bu$C_6H_4C_6H_4$)TPCP]$_4$ **(K)**	48: 35: 17	97	74	3:1	29	55	12

Supplementary Table 2. Data Summary for Extended Catalysts Screen (not presented in the paper)

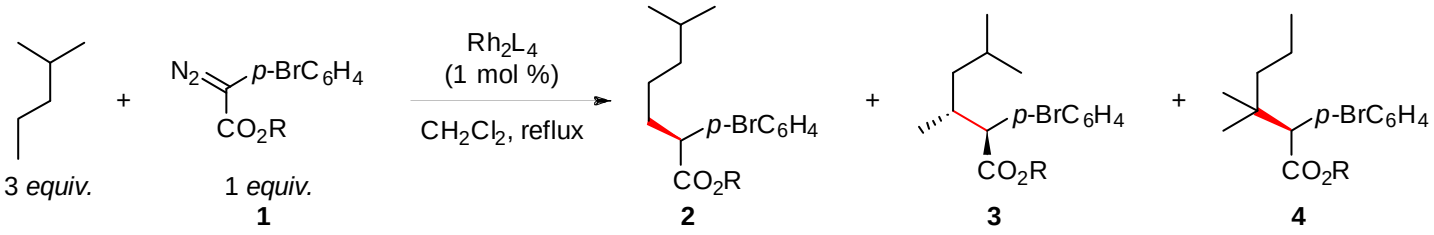


Catalyst	r.r. (**2a**: **3a**: **4a**)	e.e. (**2a**,%)	e.e. (**3a**,%)	d.r. (**3a**,%)	e.e. (**4a**,%)	yield (**2a+3a**,%)	yield (**4a**,%)
Rh_2(*R*-PTAD)$_4$ **(L)**	0: 32: 68	n.d.	-60	1:1	-22	28	59
Rh_2(*R*-*p*-BrTPCP)$_4$ **(M)**	39: 48: 13	97	87	3:1	35	75	11
Rh_2[*R*-tris(*p*-Br)TPCP]$_4$ **(N)**	21: 49: 30	91	62	2:1	14	62	27
Rh_2[*R*-3,5-di(*p*-$CF_3C_6H_4$)TPCP]$_4$ **(O)**	7: 64: 29	78	77	4:1	14	35	15
Rh_2[*R*-3,5-di(3,5-di$CF_3C_6H_3$)TPCP]$_4$ **(P)**	7: 71: 22	62	>99	4:1	8	70	19
Rh_2(*R*-2,4,6-tri-MeC_6H_2-TPCP)$_4$ **(Q)**	5: 75: 20	94	77	11:1	17	74	18



Supplementary Figure 2. Bar Graph for Catalyst Screen Data Summary

Supplementary Table 3. Diazo Screen Data Summary



Catalyst	R	r.r. (**2**: **3**: **4**)	e.e. (**2**, %)	e.e. (**3**, %)	d.r. (**3**, %)	e.e. (**4**, %)	yield (**2+3**, %)	yield (**4**, %)
Rh_2(*S*-TCPTAD)$_4$ (**B**) [5]	CH_2CF_3 (**1c**)	n.d.: 10: 90	n.d.	79	2:1	77	9	83
Rh_2(*S*-TCPTAD)$_4$ (**B**) [5]	CH_2CBr_3(**1d**)	n.d.: 13: 87	n.d.	79	2:1	77	11	77
Rh_2[*R*-3,5-di(*p*-^{t}BuC_6H_4)TPCP]$_4$ (**C**)	CH_2CF_3 (**1c**)	4: 71: 26	n.d.	93	6:1	67	57	20
Rh_2[*R*-3,5-di(*p*-^{t}BuC_6H_4)TPCP]$_4$ (**C**)	CH_2CBr_3(**1d**)	9: 82: 10	90	92	8:1	12	75	7
Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$ (**I**)	CH_3(**1b**)	51:35:15	n.d.	n.d.	3:1	n.d.	<5	n.d.
Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$ (**I**)	CH_2CF_3 (**1c**)	54: 36: 10	98	94	3:1	n.d.	78	5
Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$ (**I**)	CH_2CBr_3(**1d**)	87: 13: n.d.	>99	92	6:1	n.d.	84	n.d.
Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$ (**I**) (0.1mol%)	CH_2CBr_3(**1d**)	84: 14: 2	>99	n.d.	6:1	n.d.	77	n.d.

3 – General Procedure for Data Analysis

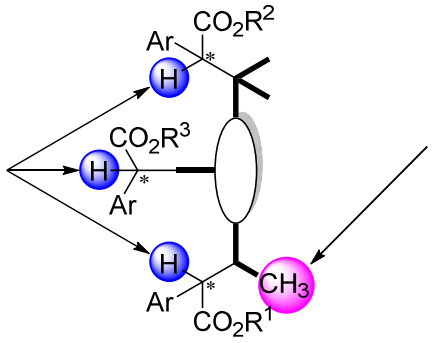
3.1 Regioisomeric Ratios (r.r.) and Diastereomeric Ratios (d.r.) Determination

To measure the regioisomeric ratios and diastereomeric ratios, the mixtures obtained as described in section 2.1 were analyzed by ^{1}H NMR using the following settings:

- Instrument: 600 MHz Bruker equipped with an prodigy probe with sensitivity over 1500:1
- Number of scans: 32
- Relaxation time: 5 seconds

The crude ^{1}H NMR spectra data was processed using MestReNova 11.0.2 (Mestrelab Research S.L.), applying an auto-phase correction as well as a Smooth Segment baseline correction. The baseline was manually inspected before integration. The ratios were measured by integrating the ^{1}H NMR peaks resulting from the indicated hydrogens below.

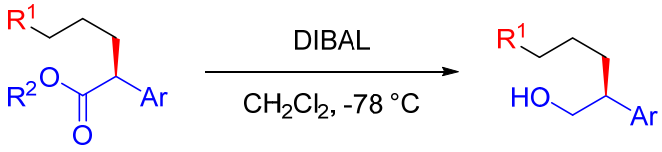
The regioisomeric ratios (*r.r.*) were measured by integrating the proton peaks of each regioisomers in the crude ^{1}H NMR spectra



The diastereoisomeric ratios (*d.r.*) were measured by integrating the proton peaks of each diastereomers in the crude ^{1}H NMR spectra

3.2 Enantiomeric Excess (e.e.) Determination

As most of the enantiomers of the C–H functionalization products were difficult to be separated on the HPLC, they were reduced to the corresponding alcohol derivatives, which will have better separation on the HPLC, without changing the *e.e.* of the products. Therefore, the *e.e.* of the products were determined from the corresponding alcohol derivatives. [4]



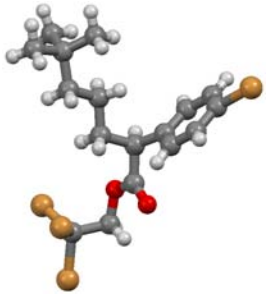
To a 25-mL round-bottom flask with a stirred solution of the ester (0.1 mmol, 1.0 *equiv.*) in CH_2Cl_2 (3 mL) was added 1 M diisobutylaluminum hydride (DIBAL) in CH_2Cl_2 (0.5 mL, 0.5 mmol, 5 *equiv.*) slowly at -78 °C. The mixture was stirred overnight and allowed to warm up to room temperature. Once the starting material was fully consumed and confirmed by TLC, the solution was cooled down to 0 °C, then methanol (0.5 mL) was added dropwise to quench the reaction and then stirred for 20 min. The reaction mixture was concentrated to dry solid mixture, then 10 mL of ethyl acetate (EA) was added into the flask to extract the organic compound. Then mixture in the flask was poured onto and filtered through a silica plug (3 *cm* height, 2 *cm* wide), and the solid residue was further extracted and washed by EA (10 mL x 4). Then the filtrate was concentrated and purified by

flash column chromatography to afford the corresponding alcohol derivatives as white solid or colorless oil. The sample was dissolved in hexanes/isopropanol (5~30 mg/mL) and the *e.e.* value of the corresponding alcohol derivatives were determined on the HPLC.

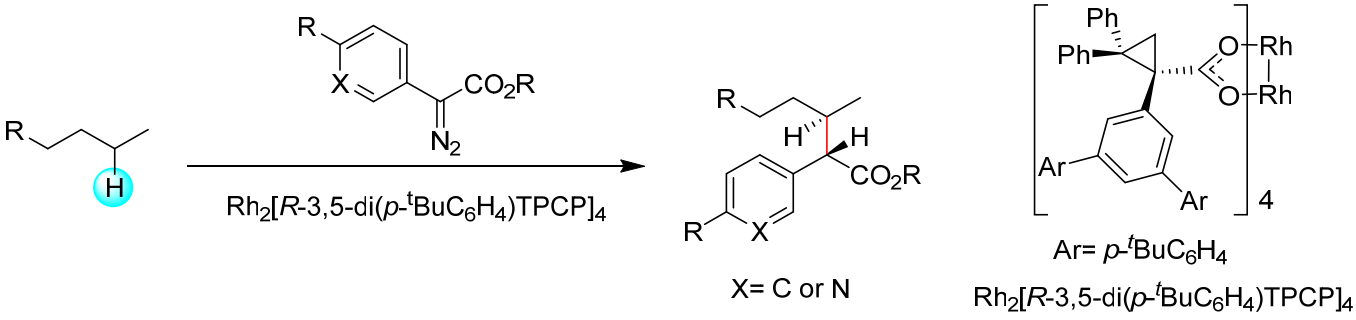
The *e.e.* of the C–H functionalization products were then obtained from the *e.e.* of the corresponding alcohol derivatives, in which the *e.e.* values were considered equal to each other.

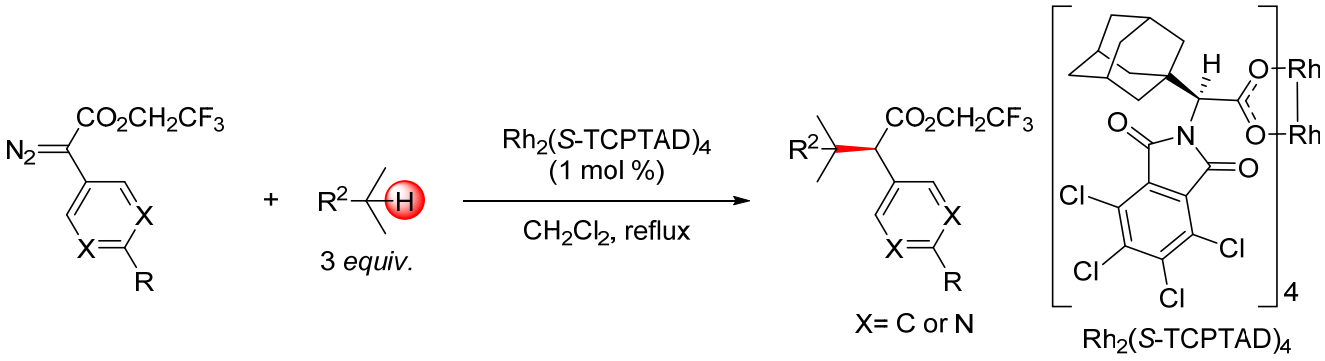
4 - Absolute Stereochemistry Determination

The absolute stereochemistry of Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$ catalyzed primary C–H insertion reaction of 2,2-dimethylpentane was determined by the X-Ray single crystal structure analysis of product **11** (see section 10 for detail), the absolute stereochemistry of the secondary C–H insertion products were tentatively assigned by analogy to the reported asymmetric induction of Rh_2[*R*-3,5-di(*p*-^{t}BuC_6H_4)TPCP]$_4$,[4] and the absolute stereochemistry of the tertiary C–H insertion products were tentatively assigned by analogy to the reported asymmetric induction of Rh_2(*S*-TCPTAD)$_4$.[5] Based on these data, the absolute stereochemistry of the rest of the reactions were tentatively assigned accordingly.

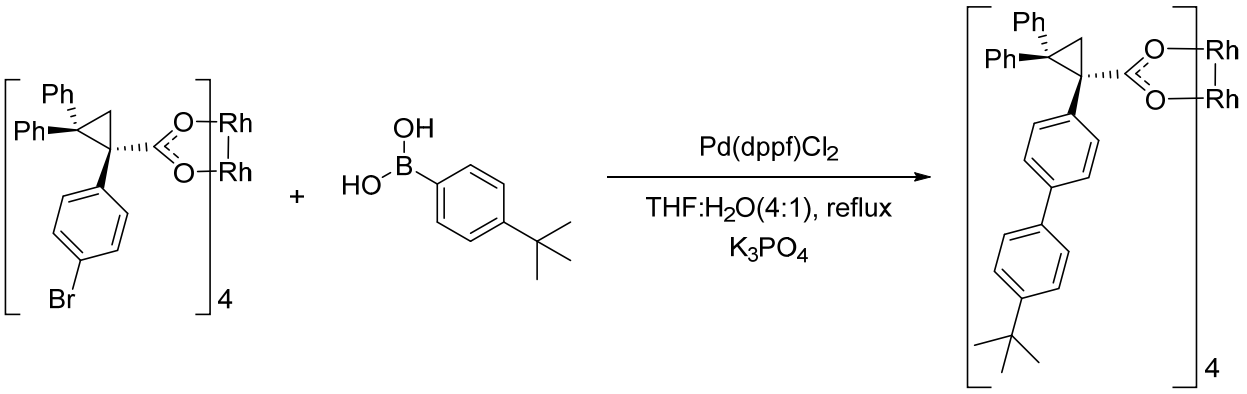


The single crystal X-ray structure of **11**



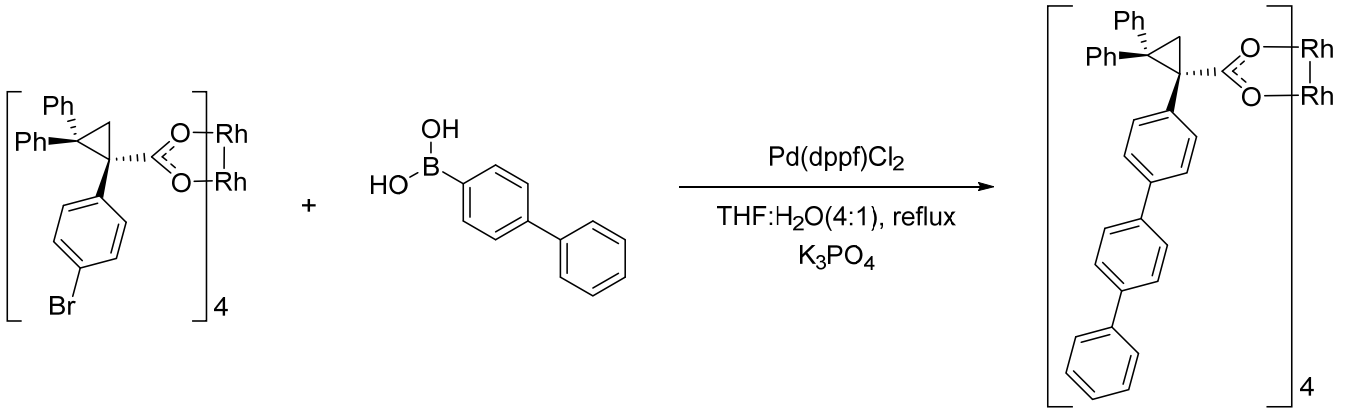


5 - Catalysts Preparation

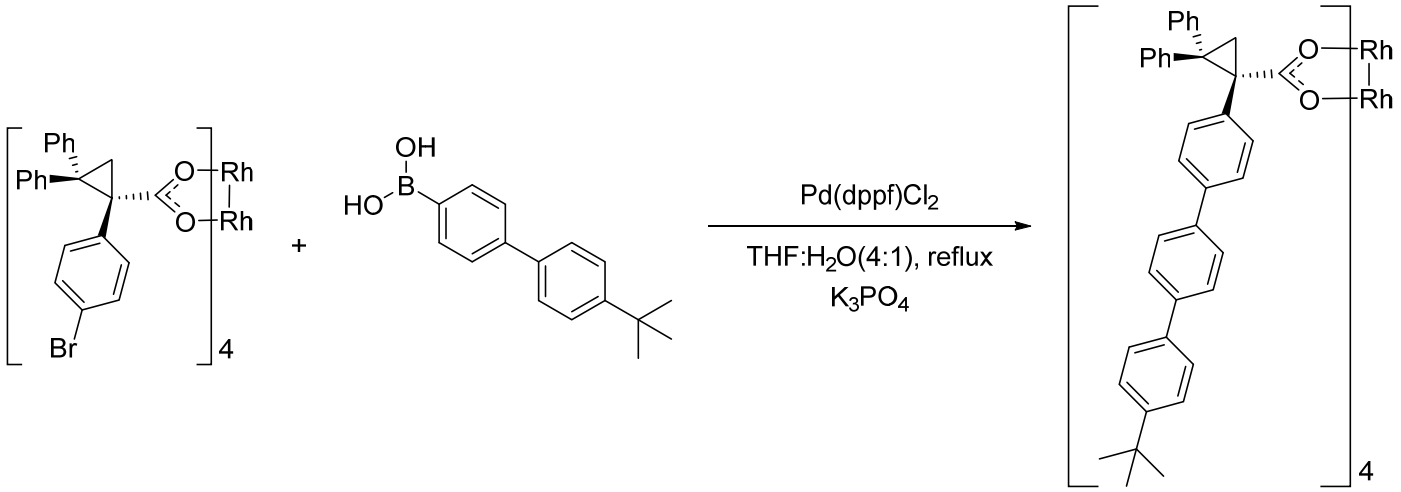


Dirhodium tetrakis [(R)-1-[4'-(tert-butyl)-(1,1'-biphenyl]-4-yl]-2,2-diphenylcyclopropane-1-carboxylate] (catalyst E). A 25-mL round-bottom flask was charged with Rh_2(*R*-*p*-BrTPCP)$_4$ (242 mg, 0.136 mmol, 1.00 equiv.), (4-(tert-butyl)phenyl)boronic acid (291 mg, 1.636 mmol, 12 equiv.). K_3PO_4 (521 mg, 2.454 mmol, 18 equiv.) and THF: H_2O (4:1) (15 mL). The flask was then degassed and Pd(dppf)Cl_2 (20 mg, 0.027 mmol, 0.2 equiv.) was added. The resulting red solution was then heated to reflux for 12 hours. After the allotted time had passed and the ester had disappeared on TLC, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM and washed with water (3x15ml), brine (3x15ml), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. The crude product was dissolved by ether (3X30 mL) and transferred to a silica plug (2x2 inch), then further flushed with ether (150 mL) and collect all green solution. The green solution was concentrated and further purified by column chromatography over silica gel to afford the cross-coupling product as green solid in 85% yield (230 mg).

TLC (diethyl ether: hexanes, 1:9 *v/v*); m.p. decomposed at 180 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 – 7.26 (m, 7H), 7.25 – 7.20 (m, 4H), 7.01 (d, J = 7.7 Hz, 2H), 6.92 (d, J = 7.8 Hz, 2H), 6.85 (t, J = 7.6 Hz, 2H), 6.78 (t, J = 7.3 Hz, 1H), 2.45 (d, J = 5.0 Hz, 1H), 1.96 (d, J = 4.8 Hz, 1H), 1.34 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.20, 149.98, 142.68, 141.22, 138.56, 137.85, 135.42, 131.51, 130.10, 129.30, 128.48, 128.22, 127.50, 126.58, 126.43, 125.89, 125.76, 125.68, 46.60, 43.03, 34.63, 31.57, 31.06; HRMS (ESI) calcd for $C_{128}H_{116}O_8Rh_2$ ($[M]^+$): 1986.6775 found 1986.6750; IR (neat): 3030, 2961, 1579, 1494, 1448, 1269, 1005, 823, 756, 748, 703, 693, 677.

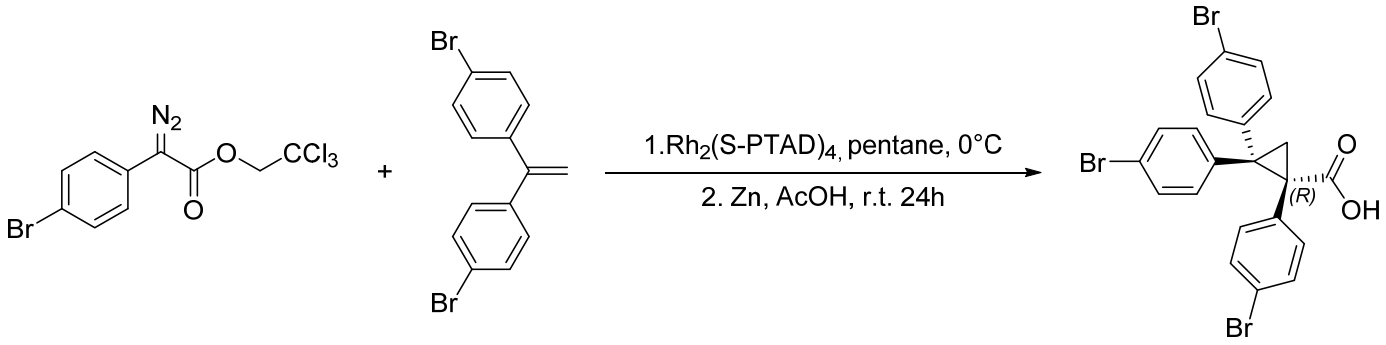


Dirhodium tetrakis [(R)-1-[(1,1':4',1''-terphenyl)-4-yl)-2,2-diphenylcyclopropane-1-carboxylate] (catalyst F). A 25-mL round-bottom flask was charged with Rh_2(*R*-*p*-BrTPCP)$_4$ (242 mg, 0.136 mmol, 1.00 equiv.), [1,1'-biphenyl]-4-ylboronic acid (324 mg, 1.636 mmol, 12 equiv.). K_3PO_4 (521 mg, 2.454 mmol, 18 equiv.) and THF: H_2O (4:1) (15 mL). The flask was then degassed and Pd(dppf)Cl_2 (20 mg, 0.027 mmol, 0.2 equiv.) was added. The resulting red solution was then heated to reflux for 12 hours. After the allotted time had passed and the ester had disappeared on TLC, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM and washed with water (3x15ml), brine (3x15ml), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. The crude product was dissolved by ether (3X30 mL) and transferred to a silica plug (2x2 inch), then further flushed with ether (150 mL) and collect all green solution. The green solution was concentrated and further purified by column chromatography over silica gel to afford the cross-coupling product as green solid in 44% yield (125 mg). TLC (diethyl ether: hexanes, 1:3 *v/v*); m.p. decomposed at 180 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 – 7.45 (m, 4H), 7.41 – 7.26 (m, 12H), 7.06 (s, 2H), 6.97 (d, J = 7.7 Hz, 2H), 6.91 (t, J = 7.7 Hz, 2H), 6.83 (t, J = 7.3 Hz, 1H), 2.51 (d, J = 5.2 Hz, 1H), 2.01 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.09, 142.66, 141.23, 140.50, 139.65, 139.49, 138.07, 135.87, 131.65, 130.07, 129.31, 128.91, 128.47, 128.28, 127.55, 127.42, 127.33, 127.18, 126.97, 126.52, 125.96, 125.74, 66.18, 46.73, 43.00; HRMS (ESI) calcd for $C_{136}H_{100}O_8Rh_2$ ([M]$^+$): 2066.5523 found 2066.5470; IR (neat): 3028, 2925, 2360, 1583, 1484, 1382, 761, 741, 694.

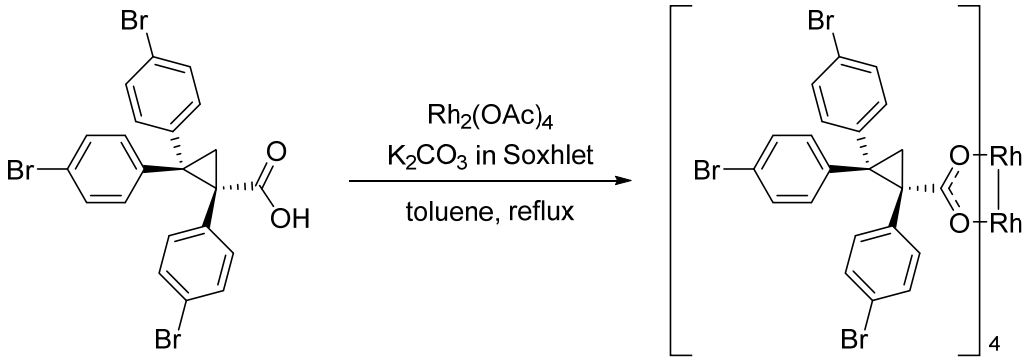


Dirhodium tetrakis [(R)-1-[4''-(tert-butyl)-(1,1':4',1''-terphenyl)-4-yl]-2,2-diphenylcyclopropane-1-carboxylate] (catalyst G). A 25 mL round-bottom flask was charged with Rh_2(*R*-*p*-BrTPCP)$_4$ (242 mg, 0.136 mmol, 1.00 equiv.), (4'-(tert-butyl)-[1,1'-biphenyl]-4-yl)boronic acid (415 mg, 1.636 mmol, 12 equiv.). K_3PO_4 (521 mg, 2.454 mmol, 18 equiv.) and THF: H_2O (4:1) (15 mL). The flask was then degassed and Pd(dppf)Cl_2 (20 mg, 0.027 mmol, 0.2 equiv.) was added. The resulting red solution was then heated to reflux for 12 hours. After the allotted time had passed and the ester had disappeared on TLC, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM and washed with water (3x15ml), brine (3x15ml), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. The crude product was dissolved by ether (3X30 mL) and transferred to a silica plug (2x2 inch), then further flushed with ether (150 mL) and collect all green solution. The green solution was concentrated and further purified by column chromatography over silica gel to afford the cross-coupling product as green solid in 50% yield (156 mg).

TLC (diethyl ether: hexanes, 1:9 *v/v*); m.p. decomposed at 200 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 (d, J = 8.1 Hz, 4H), 7.43 (d, J = 8.3 Hz, 2H), 7.39 – 7.27 (m, 9H), 7.05 (s, 2H), 6.96 (d, J = 7.6 Hz, 2H), 6.91 (t, J = 7.7 Hz, 2H), 6.83 (t, J = 7.3 Hz, 1H), 2.50 (d, J = 4.7 Hz, 1H), 1.99 (s, 1H), 1.38 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.10, 150.31, 142.68, 141.24, 139.56, 139.24, 138.21, 137.71, 135.73, 131.64, 130.09, 129.31, 128.48, 128.28, 127.54, 127.31, 127.17, 126.70, 126.51, 125.96, 125.81, 125.76, 46.66, 43.00, 34.68, 31.55, 29.85; HRMS (ESI) calcd for $C_{152}H_{132}O_8Rh_2$ ($[M]^+$): 2290.8027 found 2290.8047; IR (neat): 3028, 2961, 2956, 2360, 1583, 1491, 1381, 1005, 818, 703.

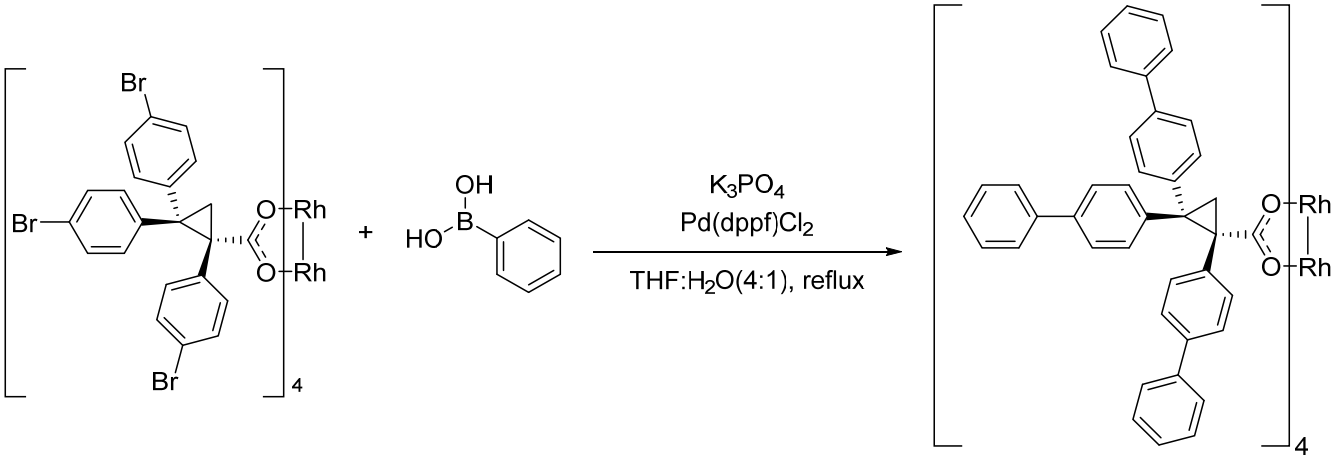


(R)-1,2,2-tris(4-bromophenyl)cyclopropane-1-carboxylic acid. To a flame-dried 500 mL round-bottom flask kept under a dry atmosphere of argon, was added Rh_2(*S*-PTAD)$_4$ (0.2 g, 0.125 mmol, 0.005 equiv.) 4,4'-(ethene-1,1-diyl)bis(bromobenzene) (10.1 g, 30.0 mmol, 1.2 equiv.), and pentane (100 mL). A solution of freshly prepared 2,2,2-trichloroethyl 2-(4-bromophenyl)-2-diazoacetate (9.3 g, 25 mmol, 1.0 equiv.) in CH_2Cl_2 (10 mL) and pentane (300 mL) was added to the former solution drop-wise over 3 hours at room temperature. The mixture was allowed to stir overnight, and then concentrated in vacuum. The crude material was dissolved in 30 mL of glacial acetic acid, and zinc powder (8.2 g, 125 mmol, 5.0 equiv.) was added. The solution was allowed to stir at room temperature for 24 h. The starting material has been fully consumed as indicated by TLC analysis. The solution was diluted with H_2O (10 mL) and extracted with EtOAc (2 x 15 mL). The organic extracts were washed with H_2O and brine, dried over $MgSO_4$ and concentrated to give the product as a white solid in 81% yield (20.2 g).
$[\alpha]^{20}_D$ -235.6° (c = 1.00, $CHCl_3$); TLC (ethyl acetate: hexanes, 1:4 *v/v*); m.p. decomposed at 200 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.3 Hz, 2H), 7.29 (dd, J = 8.3, 4.5 Hz, 4H), 7.13 (dd, J = 10.9, 8.5 Hz, 4H), 6.78 (d, J = 8.6 Hz, 2H), 2.56 (d, J = 5.7 Hz, 1H), 2.35 (d, J = 5.7 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.85, 139.99, 137.73, 133.45, 131.93, 131.50, 131.26, 131.19, 130.34, 121.98, 121.58, 121.13, 44.68, 42.21, 23.57; HRMS (ESI) calcd for $C_{22}H_{16}O_2Br_3$ ($[M+H]^+$): 548.8695 found 548.8704; IR (neat): 1694, 1489, 1395, 1239, 1074, 1007, 842, 753.



Dirhodium tetrakis[(R)-1,2,2-tris(4-bromophenyl)cyclopropane-1-carboxylate] (catalyst N). A 100 mL round-bottom flask, equipped with a Teflon-coated stirring bar and nitrogen inlet, was flushed with nitrogen and then charged with rhodium(II) acetate (0.625 mmol, 0.276 g, 1.0 *equiv.)*, (R)-1,2,2-tris(4-

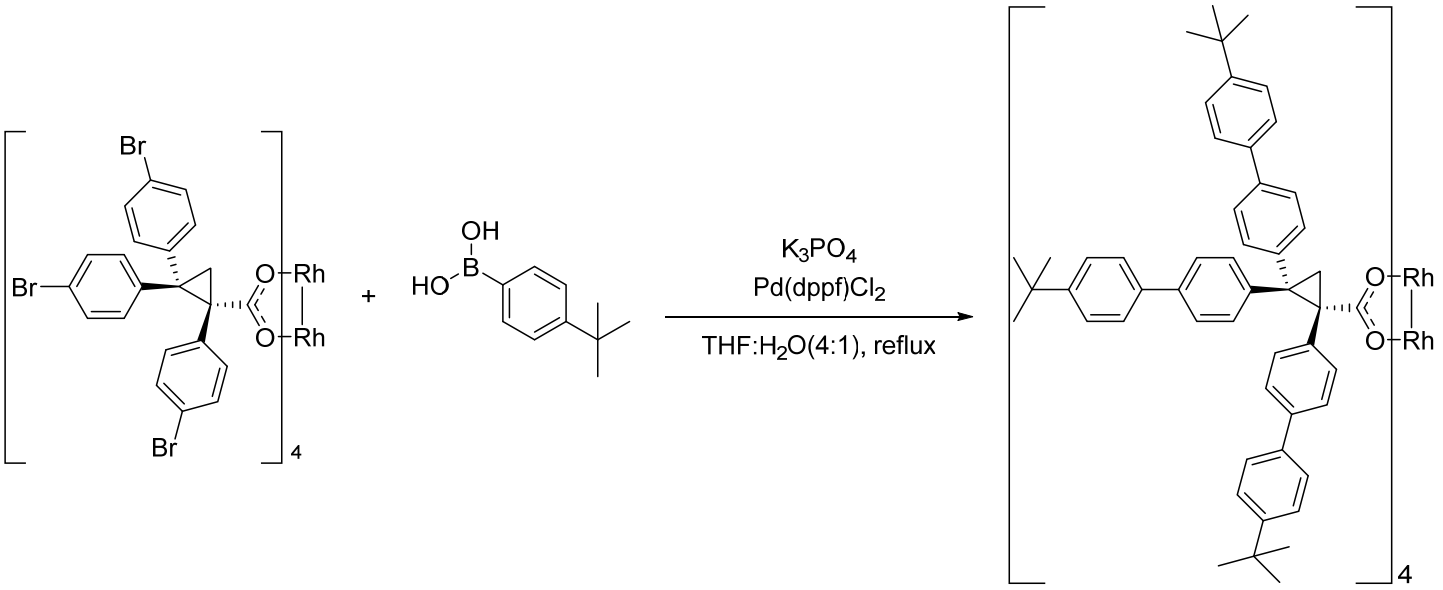
bromophenyl)cyclopropane-1-carboxylic acid (8 mmol, 2.76 g, 8.0 equiv.), and 75 mL of toluene. The flask was fitted with a Soxhlet extraction apparatus into which was placed a thimble containing 15 g of an oven-dried mixture of 2 parts sodium carbonate and 1 part of sand. The solution was heated at reflux and monitored by TLC and MS; removal of the solvent under reduced pressure using a rotary evaporator and then purified by flash column chromatography (hexanes/diethyl ether = 30/1) to give green solid in 55% overall yield (0.827 g). TLC (diethyl ether: hexanes, 1:4 *v/v*); m.p. decomposed at 215 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37 (d, J = 8.3 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 7.07 (d, J = 8.5 Hz, 2H), 6.97 (d, J = 8.3 Hz, 2H), 6.82 (d, J = 8.1 Hz, 2H), 6.67 (d, J = 8.5 Hz, 2H), 2.41 (d, J = 5.2 Hz, 1H), 1.84 (d, J = 5.0 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 188.86, 140.84, 139.18, 134.83, 132.44, 131.57, 131.38, 131.30, 131.01, 130.74, 128.48, 121.60, 120.90, 120.80, 45.55, 42.80, 29.85; HRMS (ESI) calcd for $C_{88}H_{56}O_8Rh_2Br_9{}^{81}Br_3([M]^+)$: 2399.2219 found 2399.2248; IR (neat): 2360, 2342, 1684, 1653, 1559, 1540, 1507, 1489, 1382, 1010.



Dirhodium tetrakis [(R)-1,2,2-tri[(1,1'-biphenyl)-4-yl]cyclopropane-1-carboxylate] (catalyst H). A 25 mL round-bottom flask was charged with **catalyst N** (241 mg, 0.10 mmol, 1.00 equiv.), phenylboronic acid (439 mg, 3.60 mmol, 36 equiv.). K_3PO_4 (1.146 g, 5.40 mmol, 54 equiv.) and THF: H_2O (4:1) (15 mL). The flask was then degassed and Pd(dppf)Cl_2 (44 mg, 0.06 mmol, 0.6 equiv.) was added. The resulting red solution was then heated to reflux for 12 hours. After the allotted time had passed and the ester had disappeared on TLC, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM and washed with water (3x15ml), brine (3x15ml), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. The crude product was dissolved by ether (3X30 mL) and transferred to a silica plug (2x2 inch), then further flushed with ether (150 mL) and collect all green solution. The green solution was concentrated and further purified by column chromatography over silica gel to afford the cross-coupling product as green solid in 50% yield (119 mg).

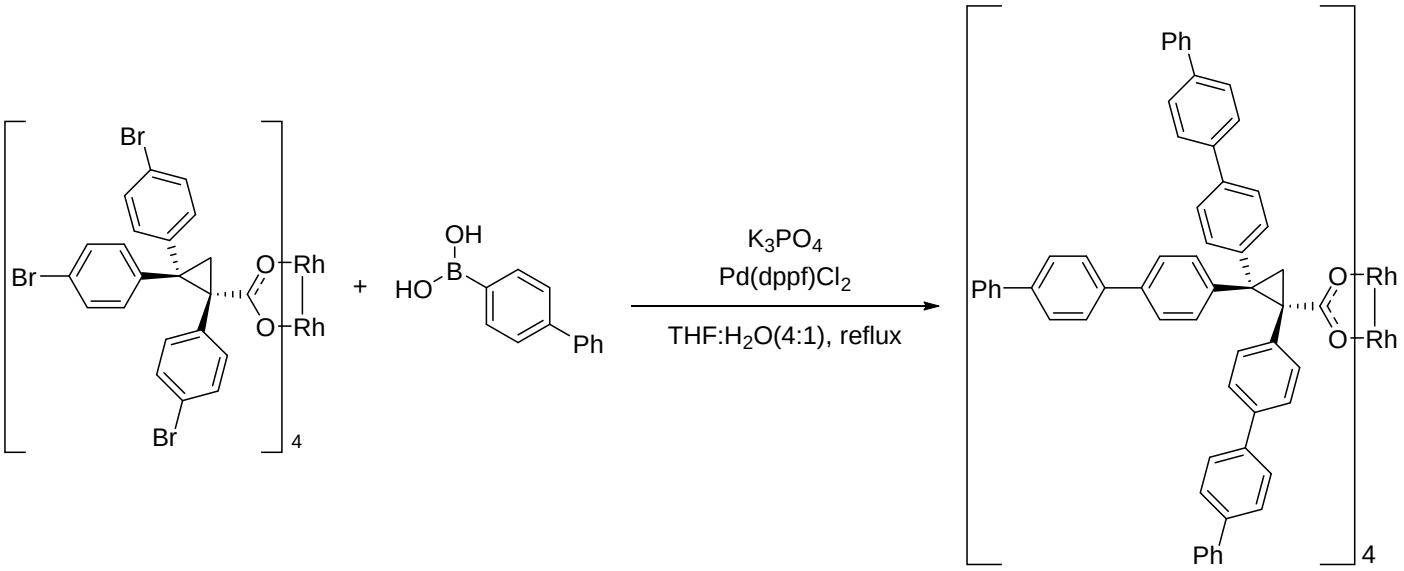
TLC (ethyl acetate: hexanes, 1:4 *v/v*); m.p. decomposed at 205 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, J = 7.4 Hz, 2H), 7.60 (d, J = 8.1 Hz, 2H), 7.56 (t, J = 7.6 Hz, 2H), 7.43 (t, J = 7.3 Hz, 1H), 7.40 – 7.36 (m, 2H), 7.32 (t, J = 8.1 Hz, 5H), 7.26 – 7.19 (m, 5H), 7.13 (d, J = 8.0 Hz, 2H), 7.09 (d, J = 8.4 Hz, 2H), 6.90 (d, J = 7.4 Hz,

2H), 6.87 (d, J = 8.3 Hz, 2H), 2.28 (d, J = 4.8 Hz, 1H), 2.03 (d, J = 4.1 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.43, 141.66, 141.43, 140.65, 140.02, 139.20, 138.82, 138.51, 135.64, 131.50, 130.57, 129.54, 129.01, 128.68, 128.64, 128.47, 127.54, 127.41, 127.16, 127.08, 126.97, 126.93, 126.91, 126.19, 125.98, 45.91, 43.35, 23.51; HRMS (ESI) calcd for $C_{160}H_{116}O_8Rh_2$ ($[M]^+$): 2370.6775 found 2370.6702; IR (neat): 3027, 2973, 2925, 2869, 1582, 1486, 1379, 1007, 845, 762, 742, 733, 695.

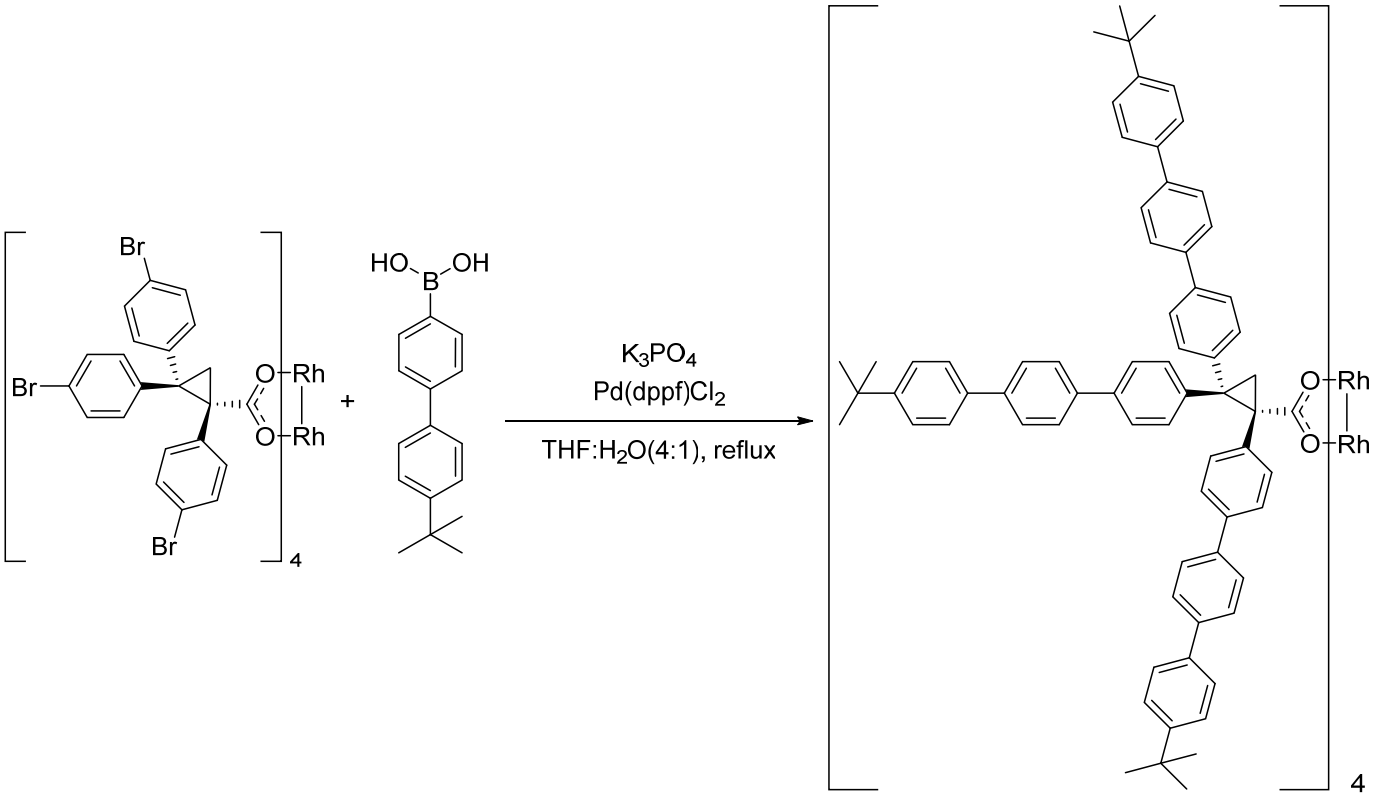


Dirhodium tetrakis [(R)-1,2,2-tris[4'-(tert-butyl)-(1,1'-biphenyl)-4-yl]cyclopropane-1-carboxylate] (catalyst I). A 100 mL round-bottom flask was charged with **catalyst N** (1.5 g, 0.623 mmol, 1.00 equiv.), (4-(tert-butyl)phenyl)boronic acid (4.0 g, 22.44 mmol, 36 equiv.). K_3PO_4 (7.15 g, 2.454 mmol, 18 equiv.) and THF: H_2O (4:1) (75 mL). The flask was then degassed and $Pd(dppf)Cl_2$ (274 mg, 0.374 mmol, 0.6 equiv.) was added. The resulting red solution was then heated to reflux for 12 hours. After the allotted time had passed and the ester had disappeared on TLC, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM and washed with water (3x15ml), brine (3x15ml), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. The crude product was dissolved by ether (3X30 mL) and transferred to a silica plug (2x2 inch), then further flushed with ether (150 mL) and collect all green solution. The green solution was concentrated and further purified by column chromatography over silica gel to afford the cross-coupling product as green solid in 53% yield (1.006 g). TLC (diethyl ether: hexanes, 1:9 *v/v*); m.p. decomposed at 200 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, J = 8.3 Hz, 2H), 7.58 (t, J = 7.0 Hz, 4H), 7.34 (d, J = 8.0 Hz, 4H), 7.32 (d, J = 8.5 Hz, 2H), 7.27 (d, J = 8.3 Hz, 2H), 7.22 (d, J = 8.3 Hz, 2H), 7.11 (d, J = 8.1 Hz, 2H), 7.06 (t, J = 7.1 Hz, 4H), 6.80 (d, J = 8.1 Hz, 4H), 2.24 (s, 1H), 1.99 (s, 1H), 1.40 (s, 9H), 1.29 (s, 18H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.40, 150.37, 149.93, 149.71, 141.30, 139.70, 139.09, 138.61, 138.10, 138.03, 137.79, 135.37, 131.55, 130.73, 129.39, 128.48, 127.25, 126.99, 126.71,

126.56, 126.52, 125.89, 125.86, 125.56, 125.53, 114.90, 34.75, 34.56, 31.69, 31.63, 31.54, 31.45; HRMS (ESI) calcd for $C_{208}H_{212}O_8Rh_2$ ($[M]^+$): 3043.4287 found 3043.4203; IR (neat): 3028, 2960, 2903, 2867, 2359, 1497, 1383, 1363, 1004, 828, 785.



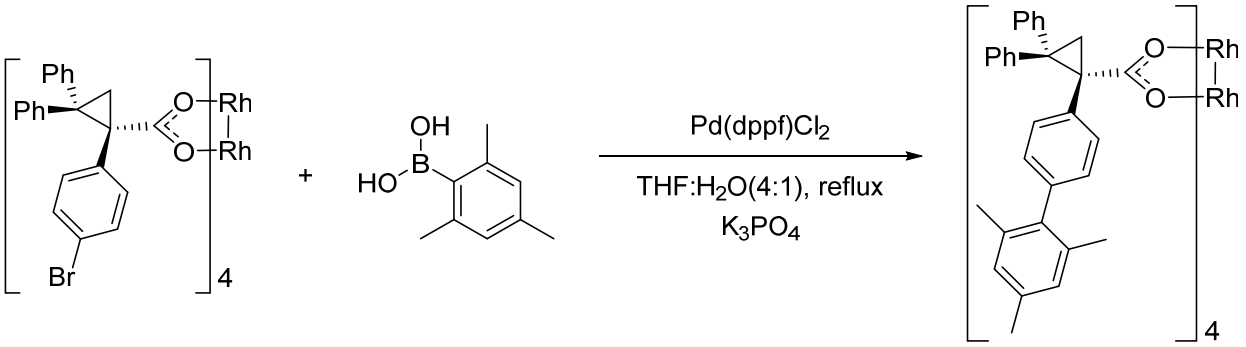
Dirhodium tetrakis [(R)-1,2,2-tri [(1,1':4',1''-terphenyl)-4-yl]cyclopropane-1-carboxylate] (catalyst J). A 25 mL round-bottom flask was charged with **catalyst N** (241 mg, 0.10 mmol, 1.00 equiv.), [1,1'-biphenyl]-4-ylboronic acid (713 mg, 3.60 mmol, 36 equiv.). K_3PO_4 (1.146 g, 5.40 mmol, 54 equiv.) and THF: H_2O (4:1) (15 mL). The flask was then degassed and $Pd(dppf)Cl_2$ (44 mg, 0.06 mmol, 0.6 equiv.) was added. The resulting red solution was then heated to reflux for 12 hours. After the allotted time had passed and the ester had disappeared on TLC, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM and washed with water (3x15ml), brine (3x15ml), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. The crude product was dissolved by ether (3X30 mL) and transferred to a silica plug (2x2 inch), then further flushed with ether (150 mL) and collect all green solution. The green solution was concentrated and further purified by column chromatography over silica gel to afford the cross-coupling product as green solid in 70% yield (230 mg). TLC (ethyl ether: hexanes, 1:3 *v/v*); m.p. decomposed at 200 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (d, J = 28.8 Hz, 4H), 7.78 – 7.68 (m, 4H), 7.45 (dddd, J = 58.5, 29.0, 23.7, 12.9 Hz, 27H), 7.19 (d, J = 37.8 Hz, 2H), 6.97 (d, J = 27.0 Hz, 2H), 2.35 (s, 1H), 2.13 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.44, 141.64, 140.76, 140.74, 140.45, 140.36, 140.29, 140.05, 139.90, 139.57, 139.46, 139.42, 138.74, 138.22, 137.90, 135.88, 131.68, 130.70, 129.62, 129.01, 128.87, 128.46, 127.98, 127.73, 127.38, 127.32, 127.22, 127.18, 127.07, 126.91, 126.07, 125.84, 45.93, 43.51, 29.85; HRMS (ESI) calcd for $C_{232}H_{164}O_8Rh_2$ ($[M]^+$): 3283.0531 found 3283.0432; IR (neat): 3027, 2923, 2852, 1581, 1484, 1380, 1005, 824, 760, 695.



Dirhodium tetrakis [(R)-1,2,2-tris[4''-(tert-butyl)-(1,1':4',1''-terphenyl]-4-yl]cyclopropane-1-carboxylate] (catalyst K). A 25 mL round-bottom flask was charged with **catalyst N** (170 mg, 0.71 mmol, 1.00 equiv.), (4'-(tert-butyl)-[1,1'-biphenyl]-4-yl)boronic acid (646 mg, 2.54 mmol, 36 equiv.). K_3PO_4 (810 mg, 3.82 mmol, 54 equiv.) and THF: H_2O (4:1) (15 mL). The flask was then degassed and $Pd(dppf)Cl_2$ (31 mg, 0.042 mmol, 0.6 equiv.) was added. The resulting red solution was then heated to reflux for 12 hours. After the allotted time had passed and the ester had disappeared on TLC, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM and washed with water (3x15ml), brine (3x15ml), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. The crude product was dissolved by ether (3X30 mL) and transferred to a silica plug (2x2 inch), then further flushed with ether (150 mL) and collect all green solution. The green solution was concentrated and further purified by column chromatography over silica gel to afford the cross-coupling product as green solid in 47% yield (131 mg).

TLC (diethyl ether: hexanes, 1:3 *v/v*); m.p. decomposed at 205 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 8.0 Hz, 2H), 7.80 (d, J = 7.9 Hz, 2H), 7.71 (d, J = 7.9 Hz, 2H), 7.64 (d, J = 7.9 Hz, 2H), 7.56 – 7.51 (m, 4H), 7.49 (d, J = 8.1 Hz, 4H), 7.42 (ddd, J = 28.9, 14.8, 7.3 Hz, 13H), 7.28 (d, J = 7.4 Hz, 1H), 7.22 – 7.15 (m, 3H), 6.96 (d, J = 29.0 Hz, 3H), 2.34 (s, 1H), 2.13 (s, 1H), 1.38 (s, 9H), 1.37 (s, 9H), 1.37 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.54, 150.53, 150.36, 150.21, 141.53, 140.11, 140.04, 139.99, 139.75, 139.48, 139.29, 139.17, 138.84, 138.38, 137.95, 137.90, 137.86, 137.74, 135.80, 131.69, 130.73, 129.58, 128.48, 127.93, 127.55,

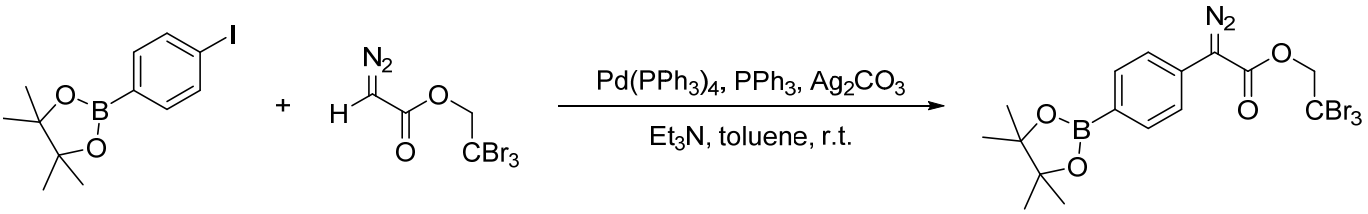
127.27, 127.22, 127.14, 127.06, 126.88, 126.72, 126.66, 126.07, 125.92, 125.84, 125.78, 45.97, 43.60, 34.70, 34.66, 34.66, 31.54, 31.50, 29.86; HRMS (ESI) calcd for $C_{279}{}^{13}CH_{262}O_8NRh_2$ ($[M+NH_2]^-$): 3972.8264 found 3972.8234; IR (neat): 3027, 2959, 2867, 2360, 1583, 1491, 1379, 1004, 816.



Dirhodium tetrakis [(R)-2,2-diphenyl-1-[2',4',6'-trimethyl-(1,1'-biphenyl)-4-yl]cyclopropane-1-carboxylate] (catalyst Q). A 25 mL round-bottom flask was charged with Rh_2(*R*-*p*-BrTPCP)$_4$ (242 mg, 0.136 mmol, 1.00 equiv.), mesitylboronic acid (268 mg, 1.636 mmol, 12 equiv.). K_3PO_4 (521 mg, 2.454 mmol, 18 equiv.) and THF: H_2O (4:1) (15 mL). The flask was then degassed and Pd(dppf)Cl_2 (20 mg, 0.027 mmol, 0.2 equiv.) was added. The resulting red solution was then heated to reflux for 12 hours. After the allotted time had passed and the ester had disappeared on TLC, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM and washed with water (3x15ml), brine (3x15ml), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. The crude product was dissolved by ether (3X30 mL) and transferred to a silica plug (2x2 inch), then further flushed with ether (150 mL) and collect all green solution. The green solution was concentrated and further purified by column chromatography over silica gel to afford the cross-coupling product as green solid in 78% yield (206 mg).

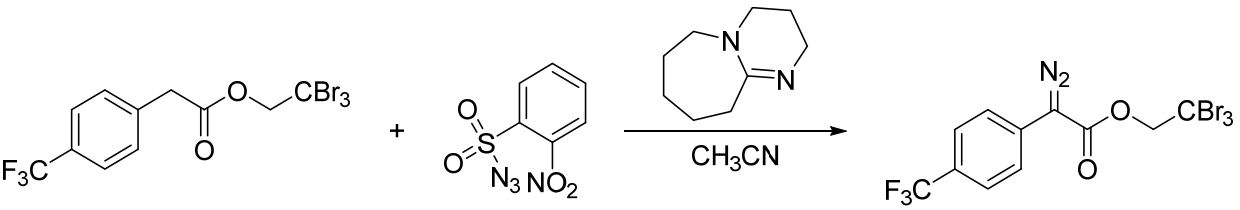
TLC (diethyl ether: hexanes, 1:9 *v/v*); m.p. decomposed at 200 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 (s, 1H), 7.27 (s, 2H), 7.21 (dq, J = 8.5, 5.0, 4.4 Hz, 1H), 7.13 (d, J = 7.9 Hz, 2H), 6.94 (d, J = 7.6 Hz, 2H), 6.90 – 6.86 (m, 5H), 6.82 (d, J = 8.0 Hz, 3H), 2.41 (d, J = 4.9 Hz, 1H), 2.30 (s, 3H), 2.09 (d, J = 6.8 Hz, 3H), 1.85 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.78, 142.42, 141.27, 138.91, 138.84, 136.46, 136.08, 135.32, 131.19, 130.12, 129.31, 128.44, 128.12, 128.08, 128.02, 127.54, 126.21, 125.72, 46.61, 43.31, 29.83, 24.74, 21.14, 20.94; HRMS (ESI) calcd for $C_{124}H_{108}O_8Rh_2$ ($[M]^+$): 1930.6149 found 1930.6121; IR (neat): 3023, 2921, 1583, 1494, 1448, 1382, 1005, 849, 783, 747, 701.

6 - Diazo Compounds Preparation



2,2,2-Tribromoethyl 2-diazo-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]acetate. 2-(4-Iodophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.0 g, 6.0 mmol, 1.0 *equiv.*), tetrakis(triphenylphosphine)palladium(0) [$Pd(PPh_3)_4$] (347 mg, 0.30 mmol, 0.05 *equiv.*), triphenylphosphine (PPh_3) (157 mg, 0.6 mmol, 0.1 *equiv.*), silver carbonate (Ag_2CO_3) (827 mg, 3.0 mmol, 0.5 *equiv.*) and triethylamine (Et_3N) (789 mg, 7.8 mmol, 1.3 *equiv.*) were suspended in toluene (20 mL) in a round-bottomed flask under nitrogen. Then 2,2,2-trichloroethyl 2-diazoacetate (2.74 g, 7.8 mmol, 1.3 *equiv.*) was added. After stirring at r.t. for 12 h, the mixture was filtered through a short silica plug (3 *cm* height, 2 *cm* wide), eluting with ethyl acetate. The solvents were removed under reduced pressure and the crude residue was purified by column chromatography on silica gel eluting with gradient diethyl ether/hexanes (1% to 5%) to give the diazo as a yellow solid in 20% yield (663 mg).

TLC (diethyl ether: hexanes, 1:9 *v/v*); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, J = 8.3 Hz, 2H), 7.52 (d, J = 8.3 Hz, 2H), 5.10 (s, 2H), 1.35 (s, 12H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.90, 135.43, 129.08, 127.74, 122.83, 84.47, 83.89, 35.81, 24.87; HRMS (NSI) calcd for $C_{16}H_{19}O_4BBr_3$ ([M-N_2+H]$^-$): 522.8932 found 522.8930; IR (neat): 2978, 2095, 1752, 1717, 1608, 1399, 1359, 1270, 1166, 1143, 1090, 857.



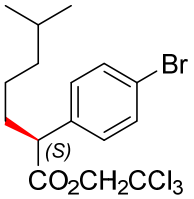
2,2,2-Tribromoethyl 2-diazo-2-[4-(trifluoromethyl)phenyl]acetate. A 100-mL three-necked flask is equipped with a 100-mL dropping funnel, a rubber septum fitted with argon inlet needle and an egg-shaped in magnetic stir bar. 1,8-Diazabicyclo(5.4.0)undec-7-ene (DBU) (457 mg, 3 mmol, 1.5 equiv.) in CH_3CN (60 mL) is added to the dropping funnel. The flask is charged with 2,2,2-tribromoethyl 2-(4-(trifluoromethyl)phenyl)acetate (938 mg, 2 mmol, 1.0 equiv.), 2-nitrobenzenesulfonyl azide (593 mg, 2.6 mmol, 1.3 equiv.) and CH_3CN (120 mL). The DBU solution is added dropwise into reaction mixture. The resulting mixture is stirred over 12 h, and reaction progress is monitored by TLC analysis. The reaction mixture is cooled with an ice bath, and saturated aqueous NH_4Cl (100 mL) is then added to quench the reaction. The mixture is extracted with ethyl ether (3 x

100 mL), and the combined organic layers are washed with saturated brine (150 mL), dried over sodium sulfate (10 g) and concentrated by rotary evaporation to afford the crude product. Column chromatography purification of the crude product over silica gel affords the diazo compounds as an orange solid in 85% yield (541 mg).

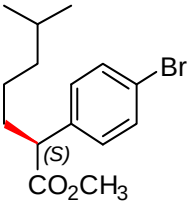
TLC (diethyl ether: hexanes, 1:9 *v/v*); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (s, 4H), 5.11 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.58, 130.66, 129.41, 128.21 (q, J = 32.8 Hz), 126.13 (q, J = 3.8 Hz), 124.11 (q, J = 271.8 Hz), 123.70, 35.69.; HRMS (NSI) calcd for $C_{11}H_6O_2N_2Br_3F_3$ ($[M]^-$): 491.7937 found 491.7941; IR (neat): 2095, 1712, 1616, 1372, 1322, 1234, 1113, 1071, 1015, 924, 839, 824, 737, 721.

7 - Experimental Data

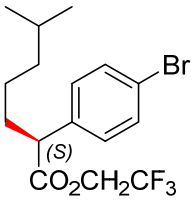
7.1 C–H Functionalization Products of 2-Methylpentane



2,2,2-Trichloroethyl (*S*)-2-(4-bromophenyl)-6-methylheptanoate (2a). $[\alpha]^{20}_{D}$ +5.9° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.4 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 4.74 (d, J = 12.0 Hz, 1H), 4.68 (d, J = 12.0 Hz, 1H), 3.65 (t, J = 7.7 Hz, 1H), 2.10 (dddd, J = 13.7, 9.9, 8.1, 5.6 Hz, 1H), 1.79 (dddd, J = 13.3, 10.1, 7.4, 5.4 Hz, 1H), 1.50 (tt, J = 13.2, 6.6 Hz, 1H), 1.36 – 1.25 (m, 2H), 1.22 – 1.13 (m, 2H), 0.84 (d, J = 6.5 Hz, 3H), 0.83 (d, J = 6.5 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.14, 137.32, 131.90, 129.98, 121.63, 94.95, 74.21, 51.17, 38.64, 33.47, 27.90, 25.35, 22.72, 22.62; HRMS (NSI) calcd for $C_{16}H_{19}BrCl_3O_2$ ($[M-H]^-$): 426.9629 found 426.9635; IR (neat): 2954, 2926, 2868, 1752, 1488, 1466, 1368, 1261, 1142, 1121, 1074, 1012, 823, 800, 758, 720.

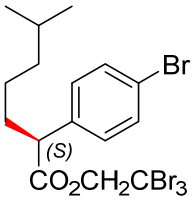


methyl (S)-2-(4-bromophenyl)-6-methylheptanoate (2b). TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.3 Hz, 2H), 3.65 (s, 3H), 3.50 (t, J = 7.7 Hz, 1H), 2.01 (dt, J = 13.9, 6.8 Hz, 1H), 1.71 (td, J = 13.9, 7.2 Hz, 1H), 1.49 (dp, J = 13.2, 6.6 Hz, 1H), 1.20 (m, 4H), 0.84 (d, J = 6.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.32, 138.38, 131.82, 129.82, 121.26, 77.37, 77.16, 76.95, 52.18, 51.21, 38.67, 33.80, 27.86, 25.38, 22.69, 22.66; HRMS (NSI) calcd for $C_{15}H_{22}BrO_2$ ($[M+H]^+$): 313.0798 found 313.0799; IR (neat): 2951, 2867, 1735, 1488, 1434, 1213, 1192, 1159, 1074, 1011, 820, 759.

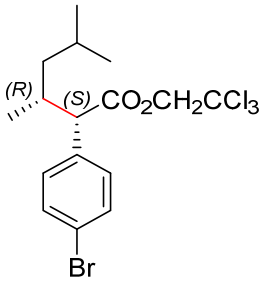


2,2,2-Trifluoroethyl (*S*)-2-(4-bromophenyl)-6-methylheptanoate (2c). $[\alpha]^{20}_{D}$ +29.6° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 7.2 Hz, 2H), 7.18 (d, J = 8.2 Hz, 2H), 4.53 (ddq, J = 16.9, 12.8, 8.4 Hz, 1H), 4.35 (ddq, J = 29.5, 12.8, 8.5 Hz, 1H), 3.61 (t, J = 7.7 Hz, 1H), 2.04

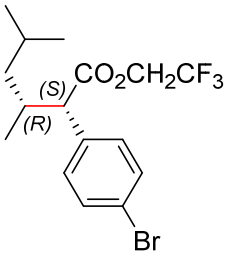
(ddt, J = 14.2, 8.3, 4.3 Hz, 1H), 1.80 – 1.70 (m, 1H), 1.49 (dq, J = 13.2, 6.6 Hz, 1H), 1.32 – 1.26 (m, 2H), 1.20 – 1.15 (m, 2H), 0.84 (d, J = 6.2 Hz, 3H), 0.84 (d, J = 6.2 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.30, 137.21, 131.99, 130.47, 129.78, 125.72, 123.88, 122.05, 120.21, 60.95, 60.71, 60.47, 60.23, 50.83, 38.58, 33.64, 27.87, 25.24, 22.66, 22.60; HRMS (NSI) calcd for $C_{16}H_{20}BrF_3O_2$ ([M]$^+$): 380.0593 found 380.0594; IR (neat): 2956, 2928, 2870, 1755, 1489, 1407, 1281, 1167, 1143, 1075, 1012, 978, 819.



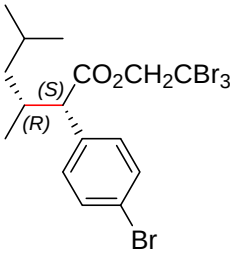
2,2,2-Tribromoethyl (*S*)-2-(4-bromophenyl)-6-methylheptanoate (2d). $[\alpha]^{20}_D$ +9.7° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.5 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 4.89 (d, *J* = 6.2 Hz, 2H), 3.67 (t, *J* = 7.7 Hz, 1H), 2.14 (dddd, *J* = 13.6, 10.0, 8.0, 5.5 Hz, 1H), 1.81 (dddd, *J* = 13.3, 10.2, 7.5, 5.4 Hz, 1H), 1.50 (dp, *J* = 13.2, 6.6 Hz, 1H), 1.37 – 1.25 (m, 3H), 1.21 (m, 2H), 0.84 (d, *J* = 6.7 Hz, 3H), 0.83 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.86, 137.35, 131.88, 130.10, 121.61, 77.10, 51.32, 38.66, 33.40, 27.91, 25.41, 22.75, 22.64; HRMS (NSI) calcd for $C_{16}H_{21}Br_4O_2$ ([M+H]$^+$): 560.8270 found 560.8278; IR (neat): 2952, 2867, 1747, 1488, 1466, 1366, 1140, 1117, 1073, 1011, 821, 727.



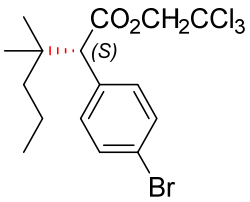
2,2,2-Trichloroethyl (2*S*,3*R*)-2-(4-bromophenyl)-3,5-dimethylhexanoate (3a). $[\alpha]^{20}_D$ +14° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.6 Hz, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 4.77 (d, *J* = 12.0 Hz, 1H), 4.63 (d, *J* = 12.0 Hz, 1H), 3.33 (d, *J* = 10.5 Hz, 1H), 2.29 (dddd, *J* = 16.8, 10.4, 6.5, 3.6 Hz, 1H), 1.03 (d, *J* = 6.5 Hz, 3H), 0.93 – 0.81 (m, 3H), 0.79 (d, *J* = 6.6 Hz, 3H), 0.74 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.97, 136.31, 131.83, 130.61, 121.70, 74.24, 58.79, 43.02, 34.25, 25.08, 24.18, 21.06, 18.04; HRMS (NSI) calcd for $C_{16}H_{21}BrCl_3O_2$ ([M+H]$^+$): 428.9785 found 428.9793; IR (neat): 2956, 2928, 2869, 1750, 1488, 1368, 1142, 1118, 1074, 1011, 825, 805, 759, 719.



2,2,2-Trifluoroethyl (*2S,3R*)-2-(4-bromophenyl)-3,5-dimethylhexanoate (**3c**).$[\alpha]^{20}_{D}$ +30.7° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, J = 8.5 Hz, 2H), 7.20 (d, J = 8.5 Hz, 2H), 4.55 (dd, J = 12.7, 8.5 Hz, 1H), 4.33 (dd, J = 12.7, 8.4 Hz, 1H), 3.30 (d, J = 10.4 Hz, 1H), 2.23 (ddtd, J = 16.7, 10.2, 6.5, 3.9 Hz, 1H), 0.99 (d, J = 6.5 Hz, 3H), 0.93 – 0.81 (m, 3H), 0.79 (d, J = 6.6 Hz, 3H), 0.73 (d, J = 6.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.11, 136.16, 131.89, 130.45, 121.77, 60.87, 60.58, 60.29, 60.00, 58.38, 43.00, 34.50, 25.07, 24.14, 21.02, 17.79; HRMS (NSI) calcd for $C_{16}H_{21}BrF_3O_2$ ($[M+H]^+$): 381.0672 found 381.0676; IR (neat): 2958, 2931, 2872, 1753, 1489, 1407, 1280, 1165, 1141, 1123, 1074, 1012, 979, 818, 758.

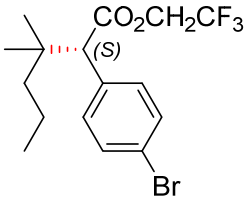


2,2,2-Tribromoethyl (2S,3R)-2-(4-bromophenyl)-3,5-dimethylhexanoate (**3d**).$[\alpha]^{20}_{D}$ +12.7° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.3 Hz, 3H), 4.92 (d, J = 12.3 Hz, 1H), 4.84 (d, J = 12.3 Hz, 1H), 3.35 (d, J = 10.6 Hz, 1H), 2.41 – 2.25 (m, 1H), 1.06 (d, J = 6.4 Hz, 3H), 0.94 – 0.82 (m, 3H), 0.79 (d, J = 6.6 Hz, 3H), 0.75 (d, J = 6.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.69, 136.37, 131.81, 130.72, 121.68, 58.98, 43.04, 34.17, 25.10, 24.20, 21.08, 18.19; HRMS (NSI) calcd for $C_{16}H_{21}Br_4O_2$ ($[M+H]^+$): 560.8270 found 560.8280; IR (neat): 2954, 2926, 2868, 1747, 1488, 1385, 1366, 1142, 1116, 1074, 1011, 821, 715.

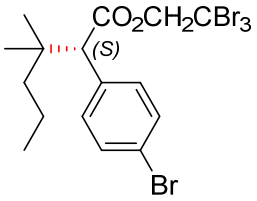


2,2,2-Trichloroethyl *(S)*-2-(4-bromophenyl)-3,3-dimethylhexanoate (**4a**).$[\alpha]^{20}_{D}$ +4.2° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, J = 8.6 Hz, 2H), 7.30 (d, J = 8.5

Hz, 2H), 4.84 (d, *J* = 12.0 Hz, 1H), 4.58 (d, *J* = 12.0 Hz, 1H), 3.63 (s, 1H), 1.35 (tdd, *J* = 11.5, 8.9, 5.2 Hz, 3H), 1.25 – 1.16 (m, 1H), 1.04 (s, 3H), 0.92 (s, 3H), 0.87 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.21, 134.32, 131.95, 131.16, 121.76, 94.89, 74.26, 59.78, 43.19, 37.53, 24.70, 24.37, 17.16, 14.92; HRMS (NSI) calcd for $C_{16}H_{19}BrCl_3O_2$ ([M-H]$^-$): 426.9629 found 426.9633; IR (neat): 2959, 2872, 1748, 1489, 1370, 1118, 1076, 1011, 826, 761, 716.

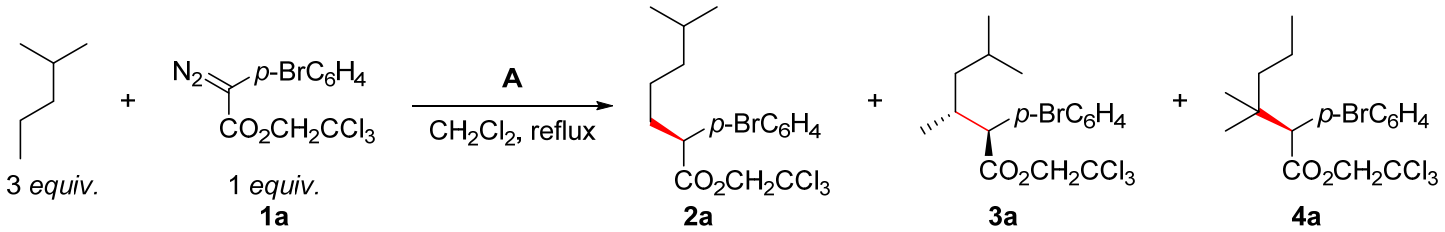


2,2,2-Trifluoroethyl *(S)*-2-(4-bromophenyl)-3,3-dimethylhexanoate (**4c**).$[\alpha]^{20}_D$ +13.9° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.6 Hz, 2H), 7.26 (d, *J* = 8.7 Hz, 2H), 4.62 (dq, *J* = 12.7, 8.5 Hz, 1H), 4.26 (dq, *J* = 12.7, 8.5 Hz, 1H), 3.59 (s, 1H), 1.37 – 1.26 (m, 3H), 1.21 – 1.11 (m, 1H), 1.00 (s, 3H), 0.89 (s, 3H), 0.87 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.26, 134.13, 131.83, 131.20, 121.82, 60.16 (q, *J* = 36.5 Hz), 59.31, 43.07, 37.55, 24.54, 24.24, 17.13, 14.81; HRMS (NSI) calcd for $C_{16}H_{21}BrF_3O_2$ ([M+H]$^+$): 381.0672 found 381.0673; IR (neat): 2963, 2935, 2874, 1752, 1489, 1414, 1278, 1164, 1122, 1076, 1012, 980, 825.



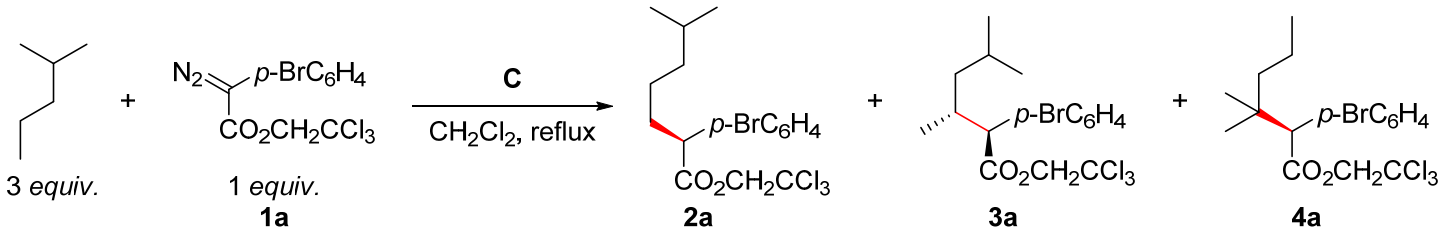
2,2,2-Tribromoethyl *(S)*-2-(4-bromophenyl)-3,3-dimethylhexanoate (**4d**).$[\alpha]^{20}_D$ +8.5° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:20 v/v); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.6 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 4.98 (d, *J* = 12.3 Hz, 1H), 4.81 (d, *J* = 12.3 Hz, 1H), 3.64 (s, 1H), 1.44 – 1.30 (m, 3H), 1.25 – 1.17 (m, 1H), 1.06 (s, 3H), 0.93 (s, 3H), 0.88 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.05, 134.41, 132.04, 131.16, 121.74, 60.04, 43.24, 37.54, 24.76, 24.46, 17.19, 14.97; HRMS (NSI) calcd for $C_{16}H_{21}Br_4O_2$ ([M+H]$^+$): 560.8270 found 560.8276; IR (neat): 2963, 2935, 2874, 1752, 1489, 1414, 1278, 1164, 1122, 1076, 1012, 980, 825.

7.2 Catalyst Screen of 2-Methylpentane



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst A** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **3a** as a colorless oil (14 mg, 16% combined yield) and **4a** as a colorless oil (62 mg, 72% yield).

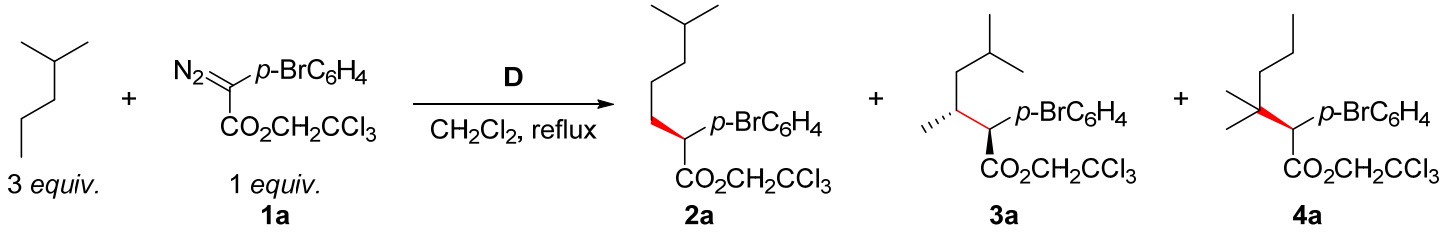
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a**: **3a: 4a**) of this reaction was *n.d.*: 19: 81 *r.r.* and the diastereoselectivity for **3a** was 2: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was not determined. The enantioselectivity of this reaction for compound **3a** was 69% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 101.4 min (minor) and 118.5 min (major). The enantioselectivity of this reaction for compound **4a** was 29% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 46.6 min (major) and 121.5 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst C** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled

CH_2Cl_2 were used. The crude residue was analyzed by ^1H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (65 mg, 75% combined yield) and **4a** as a colorless oil (14 mg, 16% yield).

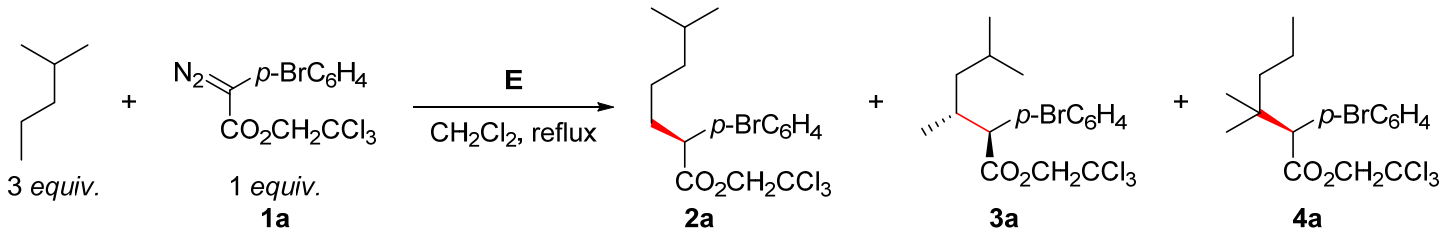
Analysis of the ^1H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 7: 75: 18 *r.r.* and the diastereoselectivity for **3a** was 7: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 81% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 62.3 min (major) and 102.7 min (minor). The enantioselectivity of this reaction for compound **3a** was 92% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 102.0 min (minor) and 113.2 min (major). The enantioselectivity of this reaction for compound **4a** was 23% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.8 min (major) and 123.4 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst D** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^1H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (65 mg, 75% combined yield) and **4a** as a colorless oil (12 mg, 14% yield).

Analysis of the ^1H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of

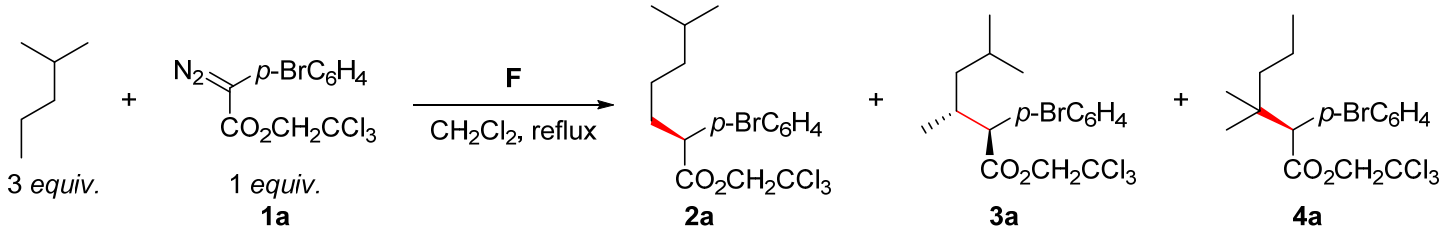
this reaction was 39: 45: 16 *r.r.* and the diastereoselectivity for **3a** was 9: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 97% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 60.3 min (major) and 105.2 min (minor). The enantioselectivity of this reaction for compound **3a** was 87% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 102.7 min (minor) and 115.3 min (major). The enantioselectivity of this reaction for compound **4a** was 60% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.0 min (major) and 122.9 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst E** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (74 mg, 86% combined yield) and **4a** as a colorless oil (3 mg, 4% yield).

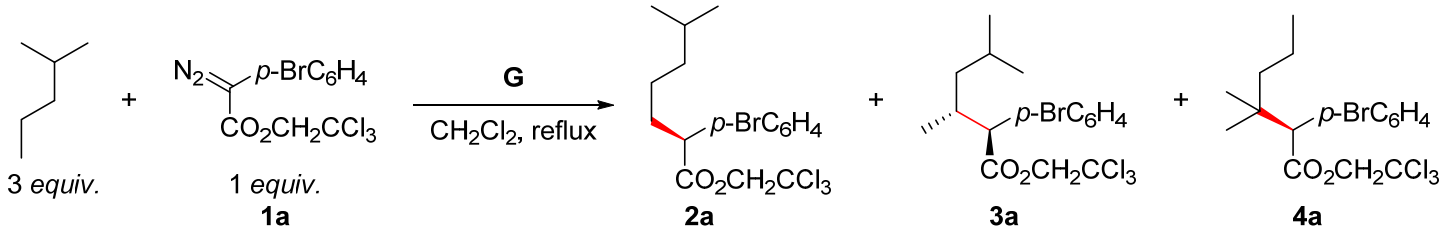
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 71: 25: 4 *r.r.* and the diastereoselectivity for **3a** was 9: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 96% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 58.1 min (major) and 106.3 min (minor). The enantioselectivity of this reaction for compound **3a** was 89% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-

bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 103.8 min (minor) and 114.9 min (major). The enantioselectivity of this reaction for compound **4a** was not determined.



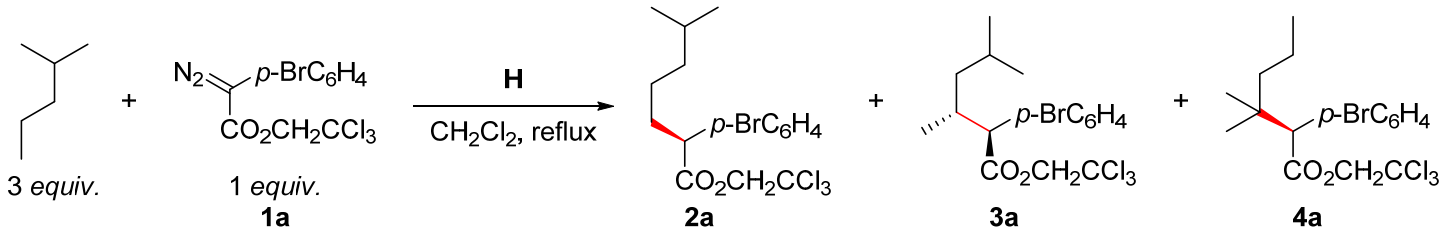
This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst F** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (71 mg, 83% combined yield) and **4a** as a colorless oil (3 mg, 3% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 70: 27: 4 *r.r.* and the diastereoselectivity for **3a** was 11: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 98% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 56.8 min (major) and 104.8 min (minor). The enantioselectivity of this reaction for compound **3a** was 94% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 102.4 min (minor) and 114.4 min (major). The enantioselectivity of this reaction for compound **4a** was not determined due to the low yielding.



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst G** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^1H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (73 mg, 85% combined yield) and **4a** as a colorless oil (3 mg, 3% yield).

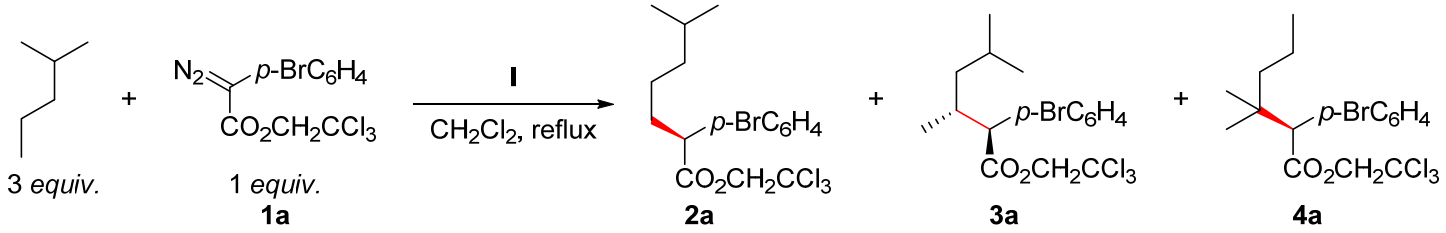
Analysis of the ^1H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 71: 26: 3 *r.r.* and the diastereoselectivity for **3a** was 15: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 97% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 56.0 min (major) and 104.2 min (minor). The enantioselectivity of this reaction for compound **3a** was 96% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 100.2 min (minor) and 112.7 min (major). The enantioselectivity of this reaction for compound **4a** was not determined due to the low yielding.



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst H** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled

CH_2Cl_2 were used. The crude residue was analyzed by ^1H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (61 mg, 71% combined yield) and **4a** as a colorless oil (4 mg, 5% yield).

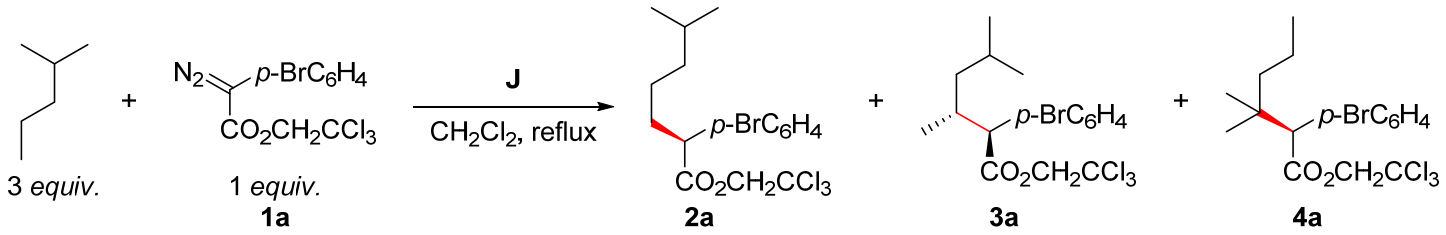
Analysis of the ^1H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 68: 25: 7 *r.r.* and the diastereoselectivity for **3a** was 5: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 90% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 56.3 min (major) and 93.4 min (minor). The enantioselectivity of this reaction for compound **3a** was 83% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 99.7 min (minor) and 115.5 min (major). The enantioselectivity of this reaction for compound **4a** was 40% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.0 min (major) and 123.0 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst I** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^1H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (77 mg, 90% combined yield).

Analysis of the ^1H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of

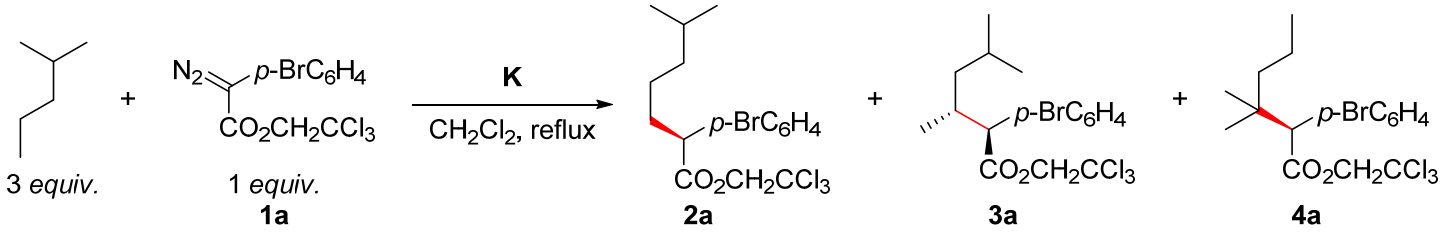
this reaction was 84: 16: *n.d. r.r.* and the diastereoselectivity for **3a** was 2: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 98% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 59.7 min (major) and 106.8 min (minor). The enantioselectivity of this reaction for compound **3a** was 92% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 105.4 min (minor) and 119.9 min (major). The enantioselectivity of this reaction for compound **4a** was not determined due to the low yielding.



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst J** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (67 mg, 78% combined yield) and **4a** as a colorless oil (4 mg, 5% yield).

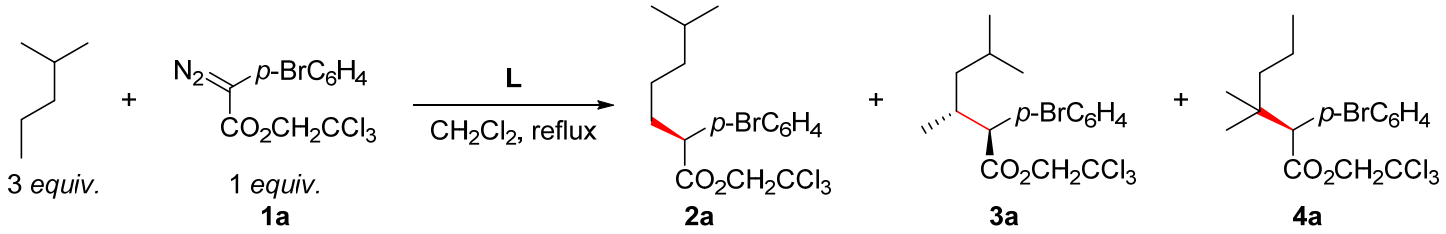
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 68: 25: 7 *r.r.* and the diastereoselectivity for **3a** was 5: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 92% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 56.0 min (major) and 95.2 min (minor). The enantioselectivity of this reaction for compound **3a** was 82% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 88.5 min

(major) and 100.2 min (minor). The enantioselectivity of this reaction for compound **4a** was 35% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 46.9 min (major) and 122.3 min (minor).



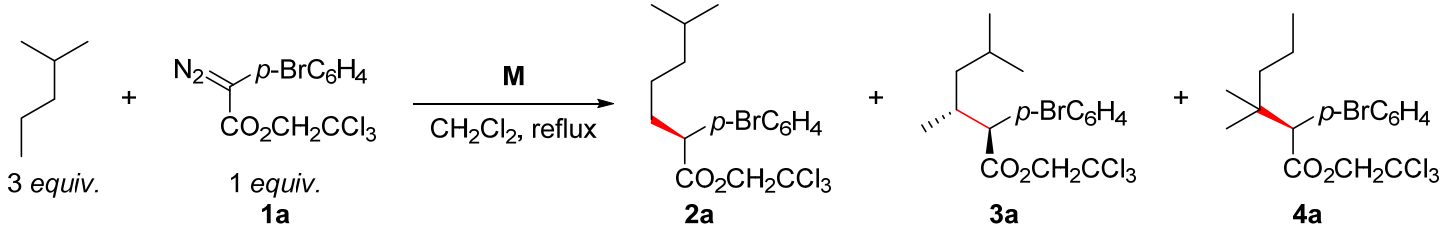
This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst K** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^1H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (47 mg, 55% combined yield) and **4a** as a colorless oil (10 mg, 12% yield).

Analysis of the ^1H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 48: 35: 17 *r.r.* and the diastereoselectivity for **3a** was 3: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 97% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 58.2 min (major) and 105.2 min (minor). The enantioselectivity of this reaction for compound **3a** was 74% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 98.9 min (minor) and 113.0 min (major). The enantioselectivity of this reaction for compound **4a** was 29% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.5 min (major) and 123.4 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst L** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **3a** as a colorless oil (24 mg, 28% combined yield) and **4a** as a colorless oil (50 mg, 59% yield).

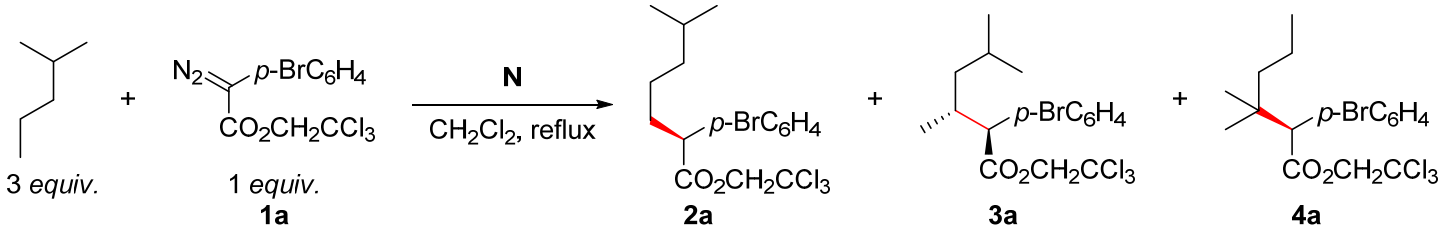
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was *n.d.:* 32: 68 *r.r.* and the diastereoselectivity for **3a** was 1: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was not determined. The enantioselectivity of this reaction for compound **3a** was 60% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 101.3 min (major) and 122.1 min (minor). The enantioselectivity of this reaction for compound **4a** was 22% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.0 min (major) and 119.8 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst M** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column

chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (65 mg, 75% combined yield) and **4a** as a colorless oil (9 mg, 11% yield).

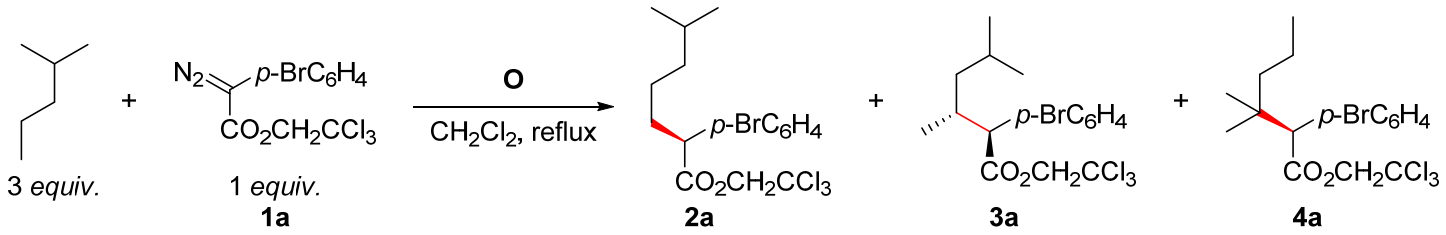
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 39: 48: 13 *r.r.* and the diastereoselectivity for **3a** was 3: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 97% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 61.9 min (major) and 100.8 min (minor). The enantioselectivity of this reaction for compound **3a** was 87% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 102.1 min (minor) and 121.1 min (major). The enantioselectivity of this reaction for compound **4a** was 35% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 59.6 min (major) and 124.5 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst N** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (53 mg, 62% combined yield) and **4a** as a colorless oil (23 mg, 27% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 21: 49: 30 *r.r.* and the diastereoselectivity for **3a** was 11: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 98% *e.e.*; the HPLC (in order to improve the separation, the product was

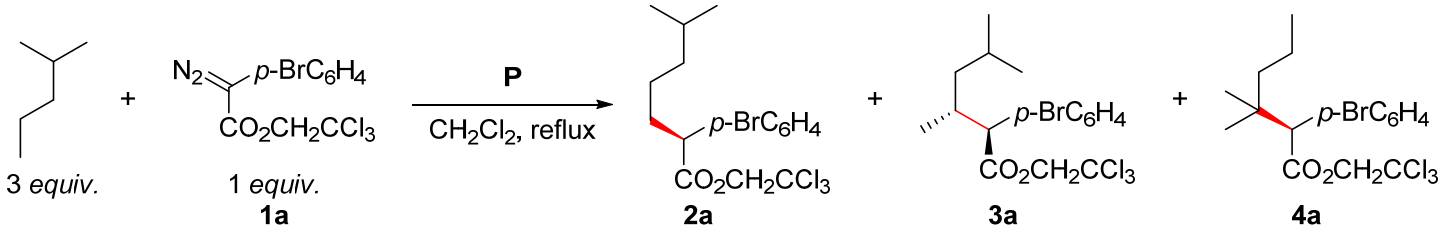
converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 59.4 min (major) and 104.0 min (minor). The enantioselectivity of this reaction for compound **3a** was 94% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 100.4 min (minor) and 116.1 min (major). The enantioselectivity of this reaction for compound **4a** was 14% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.9 min (major) and 124.2 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst O** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (30 mg, 35% combined yield) and **4a** as a colorless oil (13 mg, 15% yield).

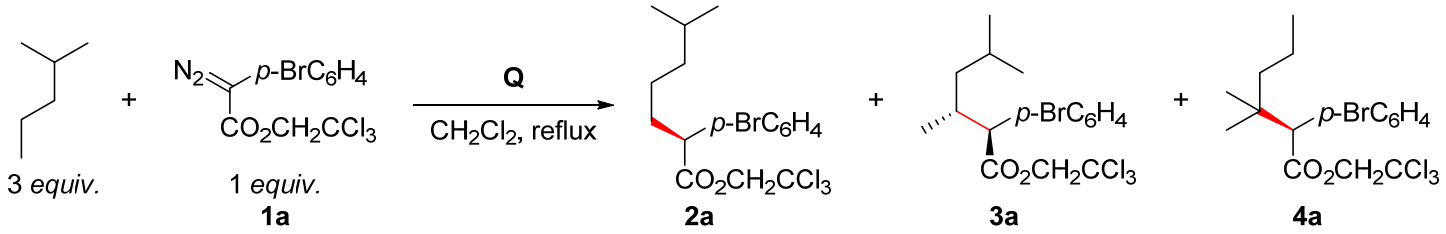
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 7: 64: 29 *r.r.* and the diastereoselectivity for **3a** was 4: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 78% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 62.3 min (major) and 103.3 min (minor). The enantioselectivity of this reaction for compound **3a** was 77% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 103.4 min

(major) and 121.2 min (minor). The enantioselectivity of this reaction for compound **4a** was 14% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.8 min (major) and 124.3 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst P** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (60 mg, 70% combined yield) and **4a** as a colorless oil (16 mg, 19% yield).

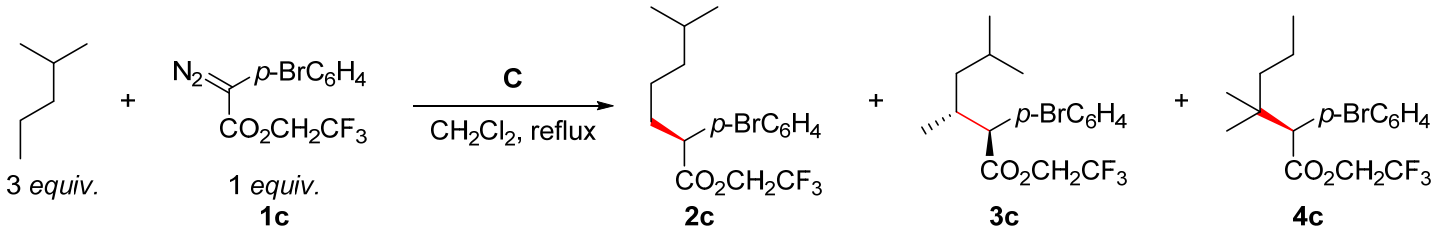
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 7: 71: 22 *r.r.* and the diastereoselectivity for **3a** was 4: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 62% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 61.4 min (major) and 102.9 min (minor). The enantioselectivity of this reaction for compound **3a** was >99% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 114.4 min (minor) and 132.0 min (major). The enantioselectivity of this reaction for compound **4a** was 8% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 46.7 min (major) and 119.8 min (minor).



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst Q** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2a** and **3a** as a colorless oil (64 mg, 74% combined yield) and **4a** as a colorless oil (16 mg, 18% yield).

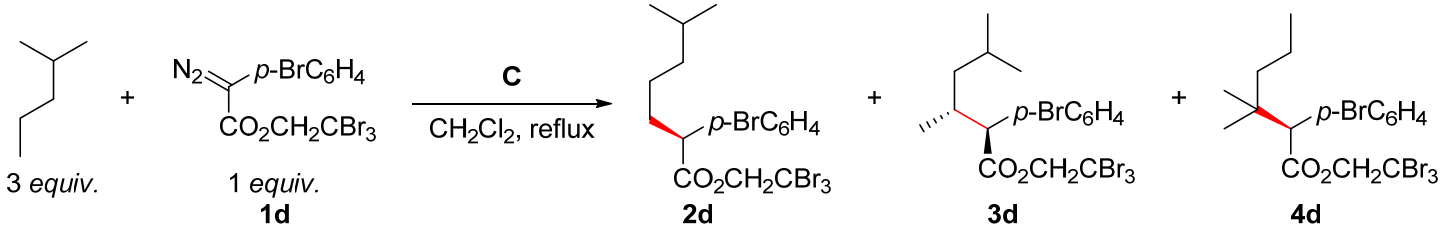
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2a**, **3a** and **4a** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2a** : **3a : 4a**) of this reaction was 5: 75: 20 *r.r.* and the diastereoselectivity for **3a** was 11: 1 *d.r.*. The enantioselectivity of this reaction for compound **2a** was 94% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 62.9 min (minor) and 103.6 min (major). The enantioselectivity of this reaction for compound **3a** was 77% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 101.2 min (minor) and 115.8 min (major). The enantioselectivity of this reaction for compound **4a** was 17% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 59.0 min (major) and 123.5 min (minor).

7.3 Diazo Screen of 2-Methylpentane



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trifluoroethyl 2-(4-bromophenyl)-2-diazoacetate **1c** (0.2 mmol, 65 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst C** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2c** and **3c** as a colorless oil (43 mg, 57% combined yield) and **4c** as a colorless oil (15 mg, 20% yield).

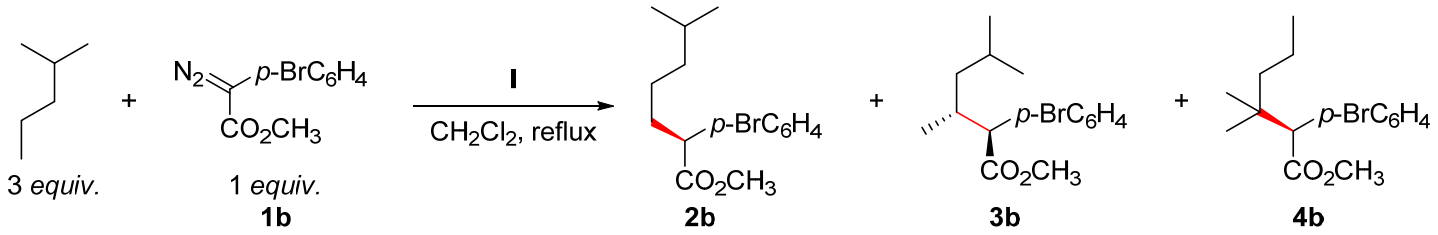
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2c**, **3c** and **4c** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2c** : **3c : 4c**) of this reaction was 4: 71: 26 *r.r.* and the diastereoselectivity for **3c** was 6: 1 *d.r.*. The enantioselectivity of this reaction for compound **2c** was not determined due to the low yielding. The enantioselectivity of this reaction for compound **3c** was 93% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 105.6 min (minor) and 119.1 min (major). The enantioselectivity of this reaction for compound **4c** was 67% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.2 min (major) and 123.0 min (minor).



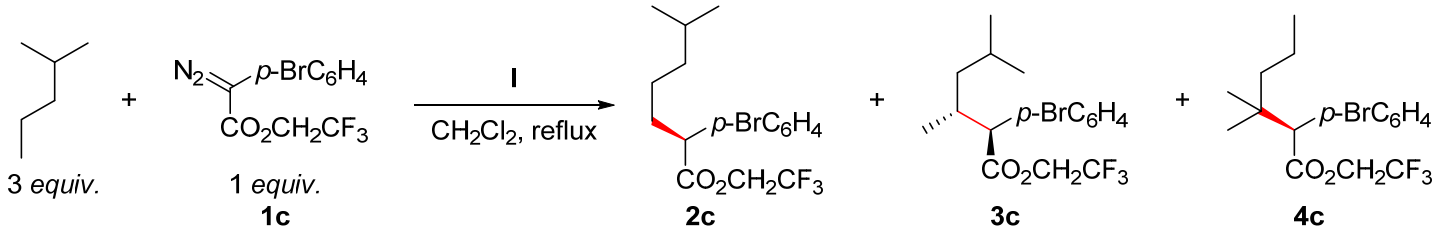
This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst C** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column

chromatography (hexanes/diethyl ether = 65/1) to afford compound **2d** and **3d** as a colorless oil (85 mg, 75% combined yield) and **4d** as a colorless oil (8 mg, 7% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2d**, **3d** and **4d** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2d** : **3d : 4d**) of this reaction was 9: 82: 9 *r.r.* and the diastereoselectivity for **3d** was 8: 1 *d.r.*. The enantioselectivity of this reaction for compound **2d** was 90% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 62.0 min (major) and 103.4 min (minor). The enantioselectivity of this reaction for compound **3d** was 92% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 104.1 min (minor) and 117.7 min (major). The enantioselectivity of this reaction for compound **4d** was 12% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "S, S-Whelk, 1% isopropanol in hexane, 1 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 47.1 min (major) and 122.3 min (minor).

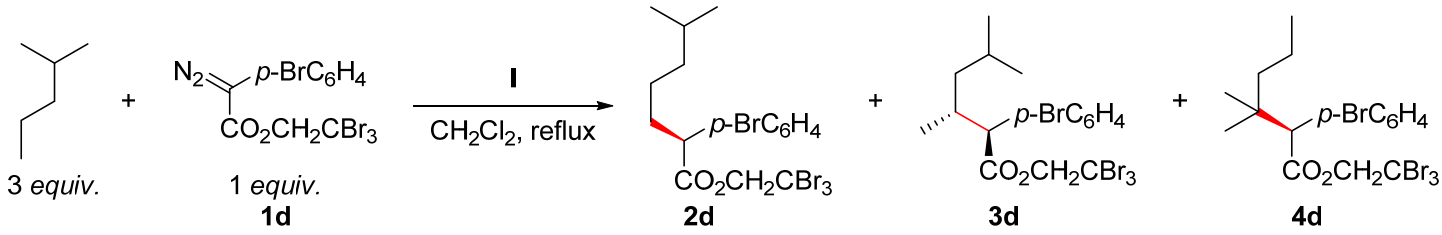


This reaction was conducted according to the general procedure A for C–H functionalization reactions. Methyl 2-(4-bromophenyl)-2-diazoacetate **1b** (0.2 mmol, 51 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst I** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and only trace amount of C–H functionalization product was observed (<5%), the regioselectivity (**2b** : **3b : 4b**) of this reaction was 51: 35: 15 *r.r.* and the diastereoselectivity for **3b** was 3: 1 *d.r.*.



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Trifluoroethyl 2-(4-bromophenyl)-2-diazoacetate **1c** (0.2 mmol, 65 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst I** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2c** and **3c** as a colorless oil (59 mg, 78% combined yield) and **4c** as a colorless oil (4 mg, 5% yield).

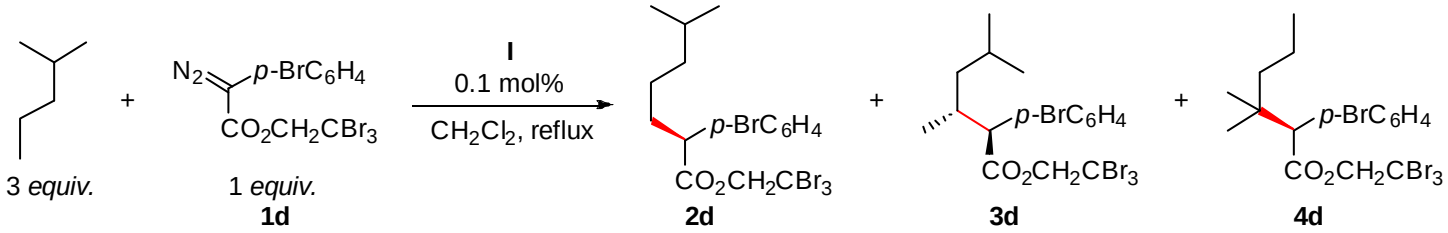
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2c**, **3c** and **4c** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2c** : **3c : 4c**) of this reaction was 54: 36: 10 *r.r.* and the diastereoselectivity for **3c** was 3: 1 *d.r.*. The enantioselectivity of this reaction for compound **2c** was 98% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 64.1 min (major) and 105.7 min (minor). The enantioselectivity of this reaction for compound **3c** was 94% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 100.9 min (minor) and 116.7 min (major). The enantioselectivity of this reaction for compound **4c** was not determined due to the low yielding.



This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst I** (0.002 mmol, 4 mg, 1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column

chromatography (hexanes/diethyl ether = 65/1) to afford compound **2d** and **3d** as a colorless oil (95 mg, 84% combined yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2d** and **3d** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2d** : **3d : 4d**) of this reaction was 87: 13: *n.d. r.r.* and the diastereoselectivity for **3d** was 7: 1 *d.r.*. The enantioselectivity of this reaction for compound **2d** was >99% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 58.0 min (major) and 105.5 min (minor). The enantioselectivity of this reaction for compound **3d** was 92% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,5-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C) condition was "ASH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 150 min, UV 230 nm, with the retention times at 103.5 min (minor) and 120.5 min (major). The enantioselectivity of this reaction for compound **4d** was not determined due to the low yielding.

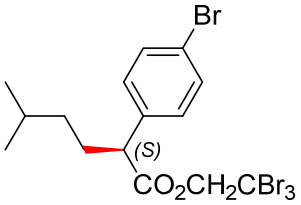


This reaction was conducted according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 equiv.) in 3 mL distilled CH_2Cl_2, **catalyst I** (0.0002 mmol, 0.4 mg, 0.1 mol%) and 2-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **2d** and **3d** as a colorless oil (87 mg, 77% combined yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **2d**, **3d** and **4d** were observed and no evident signal of other regioisomer was detected. The regioselectivity (**2d** : **3d : 4d**) of this reaction was 84: 14: 2. *r.r.* and the diastereoselectivity for **3d** was 7: 1 *d.r.*. The enantioselectivity of this reaction for compound **2d** was >99% *e.e.*; the HPLC (in order to improve the separation, the product was converted to 2-(4-bromophenyl)-3,3-dimethylhexan-1-ol prepared by using DIBAL in DCM at -78 °C)

condition was “OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm, with the retention times at 61.4 min (major) and 105.9 min (minor). The enantioselectivity of this reaction for compound **3d** and **4d** were not determined.

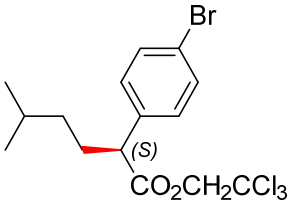
7.4 C–H Functionalization Products **5-29**



2,2,2-Tribromoethyl (*S*)-2-(4-bromophenyl)-5-methylhexanoate (**5**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 2-methylbutane (0.6 mmol, 43 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **5** as a colorless oil (44 mg, 40% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **5** and the tertiary C–H insertion product, 2,2,2-tribromoethyl (*S*)-2-(4-bromophenyl)-3,3-dimethylpentanoate, were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 90: 10 *r.r.*

$[\alpha]^{20}_D$ +6.3° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.3 Hz, 2H), 7.25 (d, J = 6.3 Hz, 2H), 4.89 (d, J = 2.3 Hz, 2H), 3.62 (t, J = 7.7 Hz, 1H), 2.16 (tdd, J = 13.4, 7.9, 5.2 Hz, 1H), 1.84 (tdd, J = 13.2, 7.6, 5.1 Hz, 1H), 1.61 – 1.55 (m, 1H), 1.24 – 1.19 (m, 1H), 1.18 – 1.10 (m, 1H), 0.87 (d, J = 4.8 Hz, 3H), 0.86 (d, J = 5.2 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.86, 137.36, 131.89, 130.12, 121.62, 77.10, 51.54, 36.67, 35.48, 31.09, 28.01, 22.65, 22.52; HRMS (NSI) calcd for $C_{15}H_{19}Br_4O_2$ ($[M+H]^+$): 546.8113 found 546.8121; IR (neat): 2953, 2923, 2853, 1750, 1488, 1458, 1122, 1074, 1012, 825, 727; HPLC (to improve the separation, the product was converted to (*S*)-2-(4-bromophenyl)-5-methylhexan-1-ol prepared using DIBAL in DCM at -78 °C), (OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm) retention times of 80.0 min (minor) and 122.2 min (major), >99% *e.e.*.

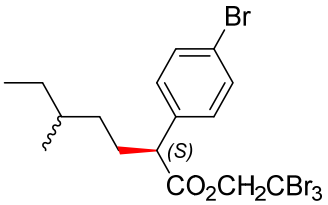


2,2,2-Trichloroethyl (*S*)-2-(4-bromophenyl)-5-methylhexanoate (**6**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-

diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC$_6$H$_4$)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 2-methylbutane (0.6 mmol, 43 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **6** as a colorless oil (68 mg, 82% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **6** and the tertiary C–H insertion product, 2,2,2-trichloroethyl (*S*)-2-(4-bromophenyl)-3,3-dimethylpentanoate, were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 89: 11 *r.r.*

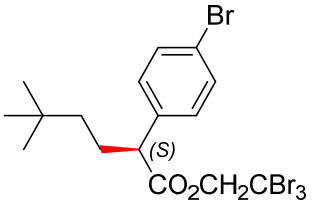
$[\alpha]^{20}_D$ +14° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 1H NMR (600 MHz, Chloroform-d) δ 7.45 (d, J = 8.5 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 4.73 (d, J = 12.0 Hz, 1H), 4.69 (d, J = 12.0 Hz, 1H), 3.61 (t, J = 7.7 Hz, 1H), 2.18 – 2.07 (m, 1H), 1.81 (dddd, J = 13.5, 11.2, 7.5, 5.1 Hz, 1H), 1.56 (dq, J = 13.3, 6.7 Hz, 1H), 1.20 (dddd, J = 13.3, 11.5, 6.7, 5.1 Hz, 1H), 1.13 (dddd, J = 13.2, 11.0, 6.9, 5.1 Hz, 1H), 0.87 (d, J = 5.3 Hz, 3H), 0.86 (d, J = 5.3 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.10, 137.31, 131.90, 129.98, 121.63, 94.94, 74.20, 51.39, 36.62, 31.15, 27.98, 22.61, 22.51; HRMS (NSI) calcd for $C_{15}H_{17}BrCl_3O_2$ ([M-H]$^-$): 412.9472 found 412.9481; IR (neat): 2955, 2928, 2870, 1753, 1489, 1144, 1075, 1012, 827, 720; HPLC (to improve the separation, the product was converted to (*S*)-2-(4-bromophenyl)-5-methylhexan-1-ol prepared using DIBAL in DCM at -78 °C), (OBH, 0.1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 140 min, UV 230 nm) retention times of 73.3 min (minor) and 109.6 min (major), 90% *e.e.*.



2,2,2-Tribromoethyl (2*S*)-2-(4-bromophenyl)-5-methylheptanoate (**7**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC$_6$H$_4$)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 3-methylpentane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **7** as a colorless oil (94 mg, 83% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **7** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 *r.r.* The diastereoselectivity of this reaction is 1:1.

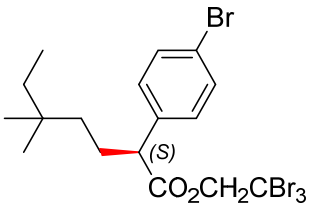
$[\alpha]^{20}_{D}$ +8.7° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.3 Hz, 2H), 7.26 (dd, J = 8.4, 1.6 Hz, 2H), 4.96 – 4.84 (m, 2H), 3.62 (td, J = 7.7, 2.3 Hz, 1H), 2.19 (dddd, J = 13.3, 11.1, 8.1, 5.0 Hz, 0.5H), 2.12 (dddd, J = 12.4, 11.0, 7.7, 4.9 Hz, 0.5H), 1.87 (tdd, J = 12.6, 9.3, 4.8 Hz, 0.5H), 1.84 – 1.75 (m, 0.5H), 1.40 – 1.23 (m, 4H), 1.22 – 1.03 (m, 2H), 0.86 (d, J = 6.5 Hz, 1.5H), 0.85 (d, J = 6.6 Hz, 1.5H), 0.83 (t, *J* = 7.3 Hz, 1.5H), 0.83 (t, *J* = 7.4 Hz, 1.5H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.89, 171.85, 137.43, 137.33, 131.88, 130.13, 130.09, 121.61, 77.11, 77.10, 51.64, 51.59, 35.51, 35.49, 34.41, 34.36, 34.34, 34.31, 30.84, 30.75, 29.43, 29.29, 19.21, 19.17, 11.49, 11.42; HRMS (NSI) calcd for $C_{16}H_{20}Br_4O_2$ ($[M+H]^+$): 560.8270 found 560.8281; IR (neat): 2956, 2925, 2871, 1747, 1488, 1458, 1367, 1139, 1120, 1073, 1011, 823, 728; HPLC (to improve the separation, the product was converted to (2S)-2-(4-bromophenyl)-5-methylheptan-1-ol prepared using DIBAL in DCM at -78 °C), (OBH, 0% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 160 min, UV 230 nm) retention times of one diastereomer is 65.9 min (major) and 144.7 min (minor), >99% *e.e.*, and retention times of another diastereomer is 74.3 min (major) and 100.3 min (minor), 95% *e.e.*.



2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-5,5-dimethylhexanoate (**8**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 2,2-dimethylbutane (0.6 mmol, 52 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **8** as a colorless oil (79 mg, 70% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **8** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 *r.r.*

$[\alpha]^{20}_D$ +4.4° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.5 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.89 (s, 2H), 3.58 (t, J = 7.7 Hz, 1H), 2.14 (tdd, J = 12.5, 7.8, 4.4 Hz, 1H), 1.81 (tdd, J = 13.0, 7.6, 4.3 Hz, 1H), 1.24 (td, J = 13.0, 4.5 Hz, 1H), 1.12 (td, J = 12.9, 4.3 Hz, 1H), 0.87 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.87, 137.38, 131.90, 130.13, 121.64, 52.03, 41.81, 35.47, 30.43, 29.39, 28.46.; HRMS (NSI) calcd for $C_{16}H_{21}Br_4O_2$ ($[M+H]^+$): 560.8270 found 560.8271; IR (neat): 2954, 2931, 2868, 2110, 1748, 1488, 1364, 1130, 1074, 1011, 824, 731; HPLC (to improve the separation, the product was converted to (S)-2-(4-bromophenyl)-5,5-dimethylhexan-1-ol prepared using DIBAL in DCM at -78 °C), (OJH, 0.3% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 30 min, UV 230 nm) retention times of 12.1 min (minor) and 18.3 min (major), 98 % *e.e.*.

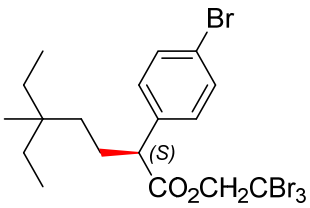


2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-5,5-dimethylheptanoate (**9**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 3,3-dimethylpentane (0.6 mmol, 60 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **9** as a colorless oil (89 mg, 77% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **9** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 *r.r.*

$[\alpha]^{20}_D$ +9.9° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.91 (d, J = 12.3 Hz, 1H), 4.88 (d, J = 12.3 Hz, 1H), 3.58 (t, J = 7.7 Hz, 1H), 2.10 (tdd, J = 12.7, 7.9, 4.4 Hz, 1H), 1.77 (tdd, J = 13.1, 7.5, 4.2 Hz, 1H), 1.21 (m, 3H), 1.10 (td, J = 13.0, 4.2 Hz, 1H), 0.81 (s, 6H), 0.76 (t, J = 7.5 Hz, 3H).; ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.90, 137.40, 131.88, 130.12, 121.63, 77.09, 52.07, 39.17, 35.49, 34.01, 32.82, 27.99, 26.76, 26.71, 8.49; HRMS (NSI) calcd for $C_{17}H_{23}Br_4O_2$ ($[M+H]^+$): 574.8426 found 574.8440; IR (neat): 2958, 1747, 1488, 1364, 1126, 1073, 1011, 821,

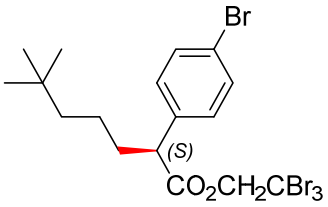
727; HPLC (to improve the separation, the product was converted to (*S*)-2-(4-bromophenyl)-5,5-dimethylheptan-1-ol prepared using DIBAL in DCM at -78 °C), (OJH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 140 min, UV 230 nm) retention times of 95.1 min (minor) and 97.6 min (major), >99% *e.e.*.



2,2,2-Tribromoethyl (*S*)-2-(4-bromophenyl)-5-ethyl-5-methylheptanoate (**10**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 3-ethyl-3-methylpentane (0.6 mmol, 69 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **10** as a colorless oil (89 mg, 75% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **10** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 *r.r.*

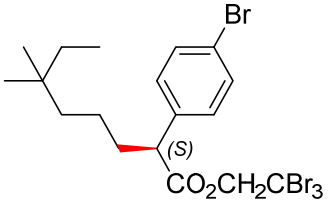
$[\alpha]^{20}_D$ +11.3° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.3 Hz, 2H), 7.26 (d, J = 8.3 Hz, 2H), 4.92 (d, J = 12.3 Hz, 1H), 4.87 (d, J = 12.3 Hz, 1H), 3.57 (t, J = 7.6 Hz, 1H), 2.07 (tdd, J = 12.6, 7.9, 4.4 Hz, 1H), 1.73 (tdd, J = 12.9, 7.4, 4.2 Hz, 1H), 1.19 (q, J = 7.6 Hz, 5H), 1.09 (td, J = 13.1, 4.2 Hz, 1H), 0.76 (s, 3H), 0.72 (t, J = 7.5 Hz, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.93, 137.43, 131.87, 130.11, 121.63, 77.07, 52.09, 36.22, 35.51, 35.09, 30.99, 30.97, 27.57, 24.03, 8.03; HRMS (NSI) calcd for $C_{18}H_{25}Br_4O_2$ ($[M+H]^+$): 588.8583 found 588.8596; IR (neat): 2960, 2876, 1747, 1488, 1462, 1371, 1258, 1126, 1073, 1011, 822, 730; HPLC (to improve the separation, the product was converted to (*S*)-2-(4-bromophenyl)-5-ethyl-5-methylheptan-1-ol prepared using DIBAL in DCM at -78 °C), (OJH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 140 min, UV 230 nm) retention times of 90.6 min (minor) and 96.3 min (major), >99% *e.e.*.



2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6,6-dimethylheptanoate (**11**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 2,2-dimethylpentane (0.6 mmol, 60 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **11** as a colorless oil (102 mg, 88% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **11** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 *r.r.*

$[\alpha]^{20}_D$ +7.9° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.89 (d, J = 2.7 Hz, 2H), 3.69 (t, J = 7.7 Hz, 1H), 2.13 (ddt, J = 14.0, 8.9, 4.2 Hz, 1H), 1.85 – 1.75 (m, 1H), 1.24 (dtdt, J = 41.8, 24.4, 12.6, 6.0 Hz, 4H), 0.83 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.86, 137.38, 131.88, 130.08, 121.61, 77.12, 51.33, 43.90, 35.50, 34.08, 30.47, 29.50, 22.73; HRMS (NSI) calcd for $C_{17}H_{23}Br_4O_2$ ($[M+H]^+$): 586.8426 found 586.8442; IR (neat): 2950, 2864, 1748, 1488, 1364, 1126, 1074, 1011, 823, 728; HPLC (to improve the separation, the product was converted to (S)-2-(4-bromophenyl)-6,6-dimethylheptan-1-ol prepared using DIBAL in DCM at -78 °C), (OJH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 140 min, UV 230 nm) retention times of 100 min (minor) and 112.7 min (major), 98% *e.e.*.

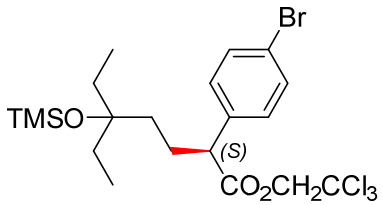


2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6,6-dimethyloctanoate (**12**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-

tris(*p*-^{t}BuC$_6$H$_4$)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 3,3-dimethylhexane (0.6 mmol, 69 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **12** as a colorless oil (95 mg, 80% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **12**, another primary C–H functionalization product, 2,2,2-tribromoethyl (S)-2-(4-bromophenyl)-5,5-dimethyloctanoate, and the secondary C–H functionalization product, 2,2,2-tribromoethyl (2*S*,3*R*)-2-(4-bromophenyl)-3,5,5-trimethylheptanoate, were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 84:13:3 *r.r.*

$[\alpha]^{20}_D$ +9.0° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.93 – 4.85 (m, 2H), 3.69 (t, J = 7.7 Hz, 1H), 2.12 (dqd, J = 17.2, 8.3, 2.8 Hz, 1H), 1.80 (dddd, J = 17.0, 13.6, 6.1, 3.3 Hz, 1H), 1.32 – 1.17 (m, 4H), 1.16 (q, J = 7.5 Hz, 2H), 0.77 (s, 6H), 0.76 (4, J = 7.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.85, 137.37, 131.87, 130.09, 121.61, 77.12, 51.33, 41.24, 35.50, 34.16, 34.11, 32.84, 26.77, 22.17, 8.53; HRMS (NSI) calcd for $C_{18}H_{25}Br_4O_2$ ([M+H]$^+$): 588.8583 found 588.8586; IR (neat): 2956, 2866, 1748, 1488, 1458, 1364, 1125, 1074, 1011, 822, 727; HPLC (to improve the separation, compound **12** was converted to (S)-2-(4-bromophenyl)-6,6-dimethyloctan-1-ol prepared using DIBAL in DCM at -78 °C), (OJH, 0.2% isopropanol in hexane, 0.2 mL/min, 10 mg/mL, 140 min, UV 230 nm) retention times of 82.2 min (minor) and 92.8 min (major), 98% *e.e.*. HPLC (to improve the separation, another primary C–H functionalization product, 2,2,2-tribromoethyl (S)-2-(4-bromophenyl)-5,5-dimethyloctanoate was converted to (*S*)-2-(4-bromophenyl)-5,5-dimethyloctan-1-ol prepared using DIBAL in DCM at -78 °C), (OJH, 0.2% isopropanol in hexane, 0.2 mL/min, 10 mg/mL, 140 min, UV 230 nm) retention times of 102.4 min (minor) and 111.6 min (major), 95% *e.e.*.

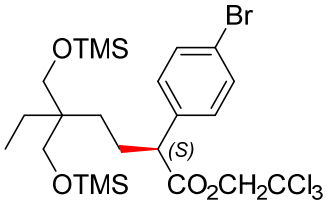


2,2,2-Trichloroethyl (S)-2-(4-bromophenyl)-5-ethyl-5-[(trimethylsilyl)oxy]heptanoate (**13**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh$_2$[*R*-tris(*p*-^{t}BuC$_6$H$_4$)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and ((3-ethylpentan-3-yl)oxy)trimethylsilane (0.6 mmol,

113 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **13** as a colorless oil (46 mg, 43% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **13** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 *r.r.*

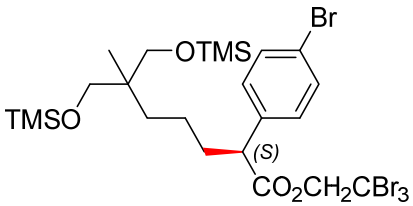
$[\alpha]^{20}_D$ +17.1° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.5 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 4.76 (d, J = 12.0 Hz, 1H), 4.67 (d, J = 12.0 Hz, 1H), 3.59 (t, J = 7.7 Hz, 1H), 2.12 (dddd, J = 13.4, 12.3, 7.7, 4.6 Hz, 1H), 1.81 (dddd, J = 13.2, 12.2, 7.7, 4.3 Hz, 1H), 1.50 – 1.40 (m, 5H), 1.30 (ddd, J = 13.5, 12.3, 4.3 Hz, 1H), 0.78 (t, J = 7.5 Hz, 3H), 0.77 (t, J = 7.5 Hz, 3H), 0.07 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.99, 137.15, 131.77, 129.86, 121.54, 94.80, 78.49, 74.05, 51.42, 35.94, 31.46, 31.35, 29.71, 27.47, 8.23, 8.20, 2.70; HRMS (NSI) calcd for $C_{16}H_{18}BrNCl_3O_2$ ($[M\text{-}C_4H_{16}O+NH_4]^+$): 439.9582 found 439.9581; IR (neat): 2963, 2880, 1752, 1488, 1456, 1373, 1249, 1141, 1126, 1061, 1012, 880, 836; HPLC (R, R-Whelk, 0.5% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 30 min, UV 230 nm) retention times of 18.3 min (minor) and 20.3 min (major), 97% *e.e.*.



2,2,2-Trichloroethyl (S)-2-(4-bromophenyl)-5,5-bis{[(trimethylsilyl)oxy]methyl}heptanoate (**14**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 5,5-diethyl-2,2,8,8-tetramethyl-3,7-dioxa-2,8-disilanonane (0.6 mmol, 166 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **14** as a colorless oil (65 mg, 52% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **14** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 *r.r.*

$[\alpha]^{20}_D$ +10.1° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.4 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 4.74 (d, J = 12.0 Hz, 1H), 4.67 (d, J = 12.0 Hz, 1H), 3.56 (t, J = 7.7 Hz, 1H), 3.28 – 3.20 (m, 4H), 2.04 (tdd, J = 12.6, 7.2, 4.5 Hz, 1H), 1.79 (tdd, J = 12.7, 8.1, 4.4 Hz, 1H), 1.18 (q, J = 7.5 Hz, 2H), 1.13 (td, J = 13.1, 4.5 Hz, 1H), 1.05 (td, J = 13.2, 4.4 Hz, 1H), 0.71 (t, J = 7.5 Hz, 3H), 0.06 (s, 9H), 0.04 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.21, 137.23, 131.84, 130.07, 121.61, 94.97, 74.17, 63.66, 63.58, 51.90, 41.92, 29.86, 27.80, 26.64, 22.48, 7.30, -0.43, -0.44; HRMS (NSI) calcd for $C_{23}H_{39}BrCl_3Si_2O_4$ ($[M+H]^+$): 619.0630 found 619.0619; IR (neat): 2956, 2925, 2868, 1754, 1488, 1250, 1128, 1086, 1012, 873, 839, 721; HPLC (R, R-Whelk, 0.5% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 30 min, UV 230 nm)-retention times of 14.8 min (minor) and 17.4 min (major), 96% *e.e.*.

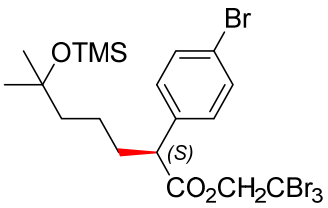


2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6-methyl-7-[(trimethylsilyl)oxy]-6-{[(trimethylsilyl)oxy]methyl}heptanoate (**15**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 2,2,5,8,8-pentamethyl-5-propyl-3,7-dioxa-2,8-disilanonane (0.6 mmol, 166 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **15** as a colorless oil (137 mg, 91% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **15** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 *r.r.*

$[\alpha]^{20}_D$ +9.1° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.25 (d, J = 8.4 Hz, 2H), 4.89 (s, 2H), 3.68 (t, J = 7.7 Hz, 1H), 3.23 (d, J = 5.8 Hz, 4H), 2.16 – 2.07 (m, 1H), 1.81 (dddd, J = 14.0, 11.5, 5.8, 2.8 Hz, 1H), 1.30 – 1.16 (m, 5H), 0.69 (s, 2H), 0.05 (s, 9H), 0.04 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.84, 137.32, 131.87, 130.14, 121.61, 77.09, 66.30, 66.21, 51.28, 39.62, 35.52, 34.12, 33.63, 21.40, 18.63, -0.39, -0.42; HRMS (NSI) calcd for $C_{23}H_{39}Br_4Si_2O_4$ ($[M+H]^+$):

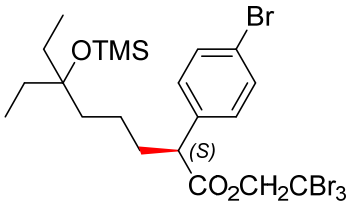
750.9115 found 750.9117; IR (neat): 2924, 2854, 1745, 1488, 1260, 1123, 1073, 1027, 1011, 819, 797, 728; HPLC (OD, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 30 min, UV 230 nm) retention times of 22.2 min (minor) and 24.6 min (major), 99% *e.e.*.



2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6-methyl-6-[(trimethylsilyl)oxy]heptanoate (**16**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and trimethyl((2-methylpentan-2-yl)oxy)silane (0.6 mmol, 105 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **16** as a colorless oil (117 mg, 90% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **16** and the secondary C–H functionalization product, 2,2,2-tribromoethyl (2*S*,3*R*)-2-(4-bromophenyl)-3,5-dimethyl-5-((trimethylsilyl)oxy)hexanoate, were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 94:6 *r.r.*

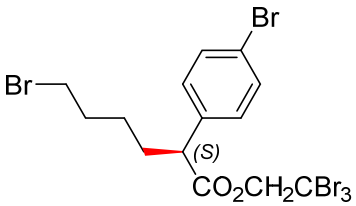
$[\alpha]^{20}_D$ +9.5° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.91 (d, J = 12.3 Hz, 1H), 4.88 (d, J = 12.3 Hz, 1H), 3.68 (t, J = 7.7 Hz, 1H), 2.15 (dddd, J = 13.5, 9.9, 8.0, 5.6 Hz, 1H), 1.82 (dddd, J = 13.3, 9.2, 7.5, 5.7 Hz, 1H), 1.49 – 1.29 (m, 4H), 1.16 (s, 3H), 1.16 (s, 3H), 0.06 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.82, 137.32, 131.87, 130.11, 121.61, 77.09, 73.83, 51.33, 44.49, 35.51, 33.64, 30.04, 29.92, 22.43, 2.73; HRMS (NSI) calcd for $C_{19}H_{29}Br_4SiO_3$ ($[M+H]^+$): 648.8614 found 648.8609; IR (neat): 2966, 2943, 2868, 1745, 1366, 1247, 1184, 1142, 1123, 1073, 1043, 1011, 905, 823, 728; HPLC (R, R-Whelk, 0.5% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 40 min, UV 230 nm) retention times of 24.6 min (minor) and 27.4 min (major), 98% *e.e.*.



2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6-ethyl-6-[(trimethylsilyl)oxy]octanoate (**17**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and trimethyl((2-methylpentan-2-yl)oxy)silane (0.6 mmol, 105 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **17** as a colorless oil (127 mg, 93% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **17**, another primary C–H functionalization product, 2,2,2-tribromoethyl (2S)-2-(4-bromophenyl)-5-ethyl-5-((trimethylsilyl)oxy)octanoate, and the secondary C–H functionalization product, 2,2,2-tribromoethyl (2S,3R)-2-(4-bromophenyl)-5-ethyl-3-methyl-5-((trimethylsilyl)oxy)heptanoate, were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 93: 4: 3 *r.r.*

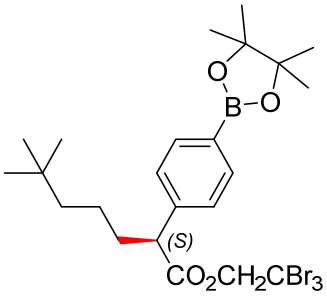
$[\alpha]^{20}_D$ +9.0° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.89 (d, J = 1.2 Hz, 2H), 3.68 (t, J = 7.7 Hz, 1H), 2.14 (dddd, J = 13.6, 9.9, 7.9, 5.9 Hz, 1H), 1.82 (dddd, J = 13.4, 9.6, 7.6, 5.7 Hz, 1H), 1.48 – 1.35 (m, 6H), 1.35 – 1.21 (m, 2H), 0.78 (t, J = 7.5 Hz, 3H), 0.77 (t, J = 7.5 Hz, 3H), 0.04 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.75, 137.24, 131.87, 130.11, 121.63, 78.73, 77.08, 51.34, 38.27, 35.50, 33.73, 31.52, 31.32, 21.74, 8.41, 8.36, 2.83; HRMS (NSI) calcd for $C_{18}H_{23}Br_4O_3$ ([M-C_3H_9]$^-$): 586.8426 found 586.8417; IR (neat): 2961, 2943, 2877, 1749, 1488, 1458, 1367, 1248, 1140, 1123, 1072, 1011, 835, 751, 728; HPLC (OD, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 40 min, UV 230 nm) retention times of 25.2 min (minor) and 29.2 min (major), 97% *e.e.*.



2,2,2-Tribromoethyl (S)-6-bromo-2-(4-bromophenyl)hexanoate (**18**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 1-bromobutane (0.6 mmol, 82 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **18** as a colorless oil (65 mg, 53% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **18**, and the secondary C–H functionalization product, 2,2,2-tribromoethyl (2S,3R)-5-bromo-2-(4-bromophenyl)-3-methylpentanoate, were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 84: 16 r.r.

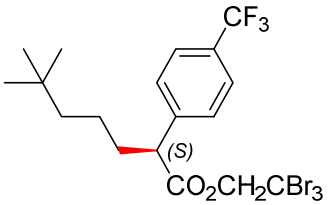
$[\alpha]^{20}_D$ +14.3° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.47 (d, J = 8.4 Hz, 2H), 7.25 (d, J = 8.9 Hz, 2H), 4.91 (d, J = 12.2 Hz, 1H), 4.88 (d, J = 12.3 Hz, 1H), 3.68 (t, J = 7.7 Hz, 1H), 3.38 (tq, J = 6.8, 3.2 Hz, 2H), 2.19 (dtt, J = 10.5, 7.9, 5.4 Hz, 1H), 1.94 – 1.82 (m, 3H), 1.54 – 1.48 (m, 1H), 1.47 – 1.39 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.53, 136.90, 132.01, 130.06, 121.83, 77.12, 51.10, 35.38, 33.32, 32.45, 32.22, 26.20; HRMS (NSI) calcd for $C_{14}H_{16}Br_4{}^{81}BrO_2$ ([M+H]$^+$): 612.7041 found 612.7036; IR (neat): 2924, 2854, 1746, 1488, 1260, 1123, 1073, 1011, 804, 728; HPLC (OJH, 0.25% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 40 min, UV 230 nm) retention times of 26.9 min (minor) and 29.3 min (major), 93% *e.e.*.



2,2,2-Tribromoethyl (S)-6,6-dimethyl-2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]heptanoate (**19**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-tribromoethyl 2-diazo-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)acetate (0.2 mmol, 111 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 2,2-dimethylpentane (0.6 mmol, 60 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 50/1) to afford compound **19** as a colorless oil (110 mg, 88% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **19** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 r.r.

$[\alpha]^{20}_{D}$ +6.8° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:5 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, J = 8.1 Hz, 2H), 7.39 (d, J = 8.1 Hz, 2H), 4.91 (d, J = 12.3 Hz, 1H), 4.86 (d, J = 12.3 Hz, 1H), 3.74 (t, J = 7.7 Hz, 1H), 2.15 (ddt, J = 14.0, 8.6, 4.3 Hz, 1H), 1.88 – 1.78 (m, 1H), 1.34 (s, 12H), 1.32 – 1.14 (m, 4H), 0.82 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.09, 141.50, 135.22, 127.74, 83.95, 77.11, 52.08, 43.94, 35.65, 34.14, 30.47, 29.85, 29.51, 25.03, 22.77; HRMS (NSI) calcd for $C_{23}H_{35}BBr_3O_4$ ($[M+H]^+$): 623.0179 found 623.0191; IR (neat): 2950, 2866, 1750, 1610, 1359, 1141, 1121, 1090, 1021, 858, 724; HPLC (S, S-Whelk, 0.1% isopropanol in hexane, 0.1 mL/min, 10 mg/mL, 120 min, UV 230 nm) retention times of 58.9 min (minor) and 91.2 min (major), >99% *e.e.*.

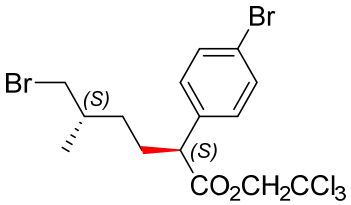


2,2,2-Tribromoethyl (S)-6,6-dimethyl-2-[4-(trifluoromethyl)phenyl]heptanoate (**20**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-tribromoethyl 2-diazo-2-(4-(trifluoromethyl)phenyl)acetate (0.2 mmol, 99 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and 2,2-dimethylpentane (0.6 mmol, 60 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 50/1) to afford compound **20** as a colorless oil (93 mg, 82% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **20** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98:2 r.r.

$[\alpha]^{20}_{D}$ +10.7° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:5 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, J = 8.1 Hz, 2H), 7.51 (d, J = 8.2 Hz, 2H), 4.92 (d, J = 12.3 Hz, 1H), 4.89 (d, J = 12.3 Hz, 1H), 3.80 (t, J = 7.7 Hz, 1H), 2.24 – 2.14 (m, 1H), 1.90 – 1.79 (m, 1H), 1.38 – 1.17 (m, 4H), 0.83 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$)

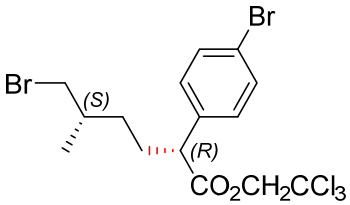
δ 171.59, 142.34, 129.96 (q, J = 32.5 Hz), 128.77, 125.72 (q, J = 3.7 Hz), 124.20 (q, J = 272.0 Hz), 51.73, 43.88, 35.35, 34.15, 30.47, 29.49, 22.76; HRMS (NSI) calcd for $C_{18}H_{21}Br_3F_3O_2$ ([M-H]$^-$): 562.9049 found 562.9061; IR (neat): 2950, 2867, 1750, 1618, 1364, 1324, 1165, 1125, 1068, 1019, 842, 720; HPLC (OJH, 0.15% isopropanol in hexane, 0.25 mL/min, 10 mg/mL, 40 min, UV 230 nm) retention times of 19.7 min (minor) and 25.8 min (major), >99% *e.e.*.



2,2,2-Trichloroethyl (2S,5S)-6-bromo-2-(4-bromophenyl)-5-methylhexanoate (**24**). This compound was prepared according to the general procedure for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, catalyst **I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol %.) and (S)-1-bromo-2-methylbutane (0.6 mmol, 91 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **24** as a colorless oil (68 mg, 69 % yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **24** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98: 2 *r.r.*

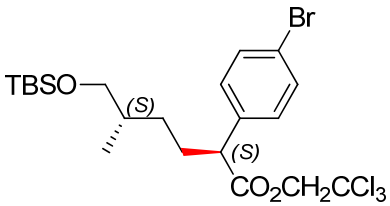
$[\alpha]^{20}_D$ +20.5° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, J = 8.5 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 4.74 (d, J = 12.0 Hz, 1H), 4.70 (d, J = 12.0 Hz, 1H), 3.63 (t, J = 7.7 Hz, 1H), 3.38 – 3.29 (m, 2H), 2.16 (dddd, J = 13.1, 11.4, 8.1, 4.8 Hz, 1H), 1.85 – 1.77 (m, 2H), 1.48 – 1.39 (m, 1H), 1.34 – 1.23 (m, 2H), 1.02 (d, J = 6.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.77, 136.90, 132.00, 129.89, 121.82, 94.86, 74.22, 51.17, 40.83, 35.02, 32.64, 30.50, 18.83; HRMS (NSI) calcd for $C_{15}H_{18}Br_2Cl_3O_2$ ([M+H]$^+$): 492.8724 found 492.8748; IR (neat): 2956, 2927, 2854, 1750, 1488, 1131, 1074, 1011, 826, 767, 718; HPLC (ODH, 0.3 % isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 40 min, UV 230 nm) retention times of 20.8 min (minor) and 26.1 min (major), >100:1 d.*r.*.



2,2,2-Trichloroethyl (2R,5S)-6-bromo-2-(4-bromophenyl)-5-methylhexanoate (**27**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*S*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and (S)-1-bromo-2-methylbutane (0.6 mmol, 91 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **27** as a colorless oil (68 mg, 69% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **27** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98: 2 r.r.

$[\alpha]^{20}_D$ -25.2° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.47 (d, J = 8.5 Hz, 2H), 7.22 (d, J = 8.4 Hz, 2H), 4.75 (d, J = 12.0 Hz, 1H), 4.69 (d, J = 12.0 Hz, 1H), 3.62 (t, J = 7.7 Hz, 1H), 3.32 (dd, J = 5.6, 1.1 Hz, 2H), 2.11 (tdd, J = 12.8, 7.0, 3.8 Hz, 1H), 1.91 – 1.77 (m, 2H), 1.50 (ddt, J = 13.4, 11.0, 5.3 Hz, 1H), 1.23 – 1.12 (m, 1H), 1.00 (d, J = 6.7 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.80, 136.83, 132.01, 129.94, 121.83, 94.87, 74.22, 51.13, 40.75, 35.11, 32.54, 30.44, 18.76; HRMS (NSI) calcd for $C_{15}H_{18}Br_2Cl_3O_2$ ($[M+H]^+$): 492.8724 found 492.8748; IR (neat): 2955, 2927, 2854, 1751, 1488, 1131, 1074, 1012, 827, 766, 719; HPLC (ODH, 0.3% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 40 min, UV 230 nm) retention times of 20.3 min (minor) and 25.6 min (major), >100:1 d.*r.*.

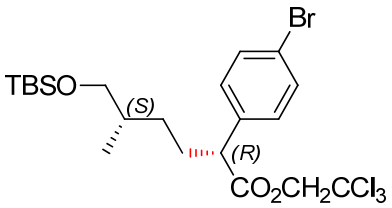


(2S,5S)-2,2,2-Trichloroethyl 2-(4-bromophenyl)-6-[(tert-butyldimethylsilyl)oxy]-5-methylhexanoate (**25**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and (S)-trimethyl(2-

methylbutoxy)silane (0.6 mmol, 96 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **25** as a colorless oil (93 mg, 92% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **25** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98: 2 r.r.

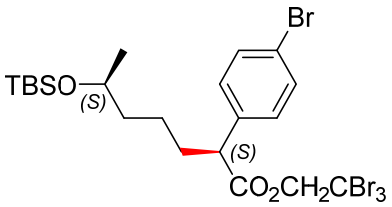
$[\alpha]^{20}_D$ +11.7° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 4.73 (d, J = 12.0 Hz, 1H), 4.69 (d, J = 12.0 Hz, 1H), 3.62 (t, J = 7.7 Hz, 1H), 3.37 (dd, J = 6.0, 3.7 Hz, 2H), 2.19 (tdd, J = 12.9, 7.3, 3.9 Hz, 1H), 1.79 (dddd, J = 12.9, 11.5, 7.6, 5.0 Hz, 1H), 1.59 (h, J = 6.3 Hz, 1H), 1.39 (ddt, J = 13.2, 10.9, 5.2 Hz, 1H), 1.13 – 1.04 (m, 1H), 0.87 (d, J = 6.8 Hz, 3H), 0.86 (s, 9H), 0.00 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.03, 137.25, 131.90, 129.97, 121.65, 94.93, 74.20, 68.02, 51.48, 35.77, 31.13, 30.91, 26.04, 18.42, 16.75, -5.25; HRMS (NSI) calcd for $C_{21}H_{33}BrCl_3SiO_3$ ($[M+H]^+$): 545.0442 found 545.0437; IR (neat): 2954, 2928, 2856, 1752, 1488, 1471, 1462, 1250, 1139, 1094, 1075, 1012, 834, 773, 719; HPLC (R, R-Whelk, 0.5% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 30 min, UV 230 nm) retention times of 17.5 min (minor) and 19.8 min (major), >100:1 d.*r.*.



(2R,5S)-2,2,2-Trichloroethyl 2-(4-bromophenyl)-6-[(tert-butyldimethylsilyl)oxy]-5-methylhexanoate (**28**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Trichloroethyl 2-(4-bromophenyl)-2-diazoacetate **1a** (0.2 mmol, 74 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*S*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and (S)-trimethyl(2-methylbutoxy)silane (0.6 mmol, 96 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **28** as a colorless oil (90 mg, 89% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **28** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >98: 2 r.r.

$[\alpha]^{20}_D$ -19..9° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.22 (d, J = 8.5 Hz, 2H), 4.73 (d, J = 12.0 Hz, 1H), 4.69 (d, J = 12.0 Hz, 1H), 3.61 (t, J = 7.7 Hz, 1H), 3.37 (dd, J = 6.1, 3.2 Hz, 2H), 2.18 (tdd, J = 12.9, 7.3, 3.9 Hz, 1H), 1.79 (dddd, J = 12.8, 11.5, 7.6, 5.0 Hz, 1H), 1.64 – 1.52 (m, 1H), 1.39 (ddt, J = 13.3, 10.7, 5.2 Hz, 1H), 1.08 (dddd, J = 13.0, 11.7, 7.9, 4.9 Hz, 1H), 0.86 (d, J = 6.8 Hz, 3H), 0.85 (s, 9H), 0.00 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.06, 137.26, 131.91, 129.98, 121.66, 94.94, 74.21, 68.03, 51.50, 35.78, 31.14, 30.92, 26.04, 18.43, 16.75, -5.26; HRMS (NSI) calcd for $C_{21}H_{33}BrCl_3SiO_3$ ($[M+H]^+$): 545.0442 found 545.0437; IR (neat): 2954, 2928, 2856, 1752, 1488, 1471, 1462, 1251, 1138, 1094, 1075, 1011, 834, 773, 719; HPLC (R, R-Whelk, 0.5% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 30 min, UV 230 nm) retention times of 18.0 min (minor) and 19.0 min (major), >100:1 d.*r.*.

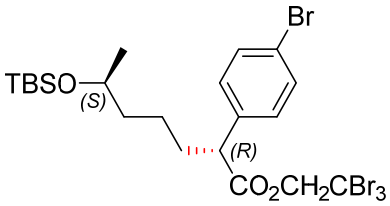


2,2,2-Tribromoethyl (2S,6S)-2-(4-bromophenyl)-6-[(tert-butyldimethylsilyl)oxy]heptanoate (**26**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and (S)-tert-butyldimethyl(pentan-2-yloxy)silane (0.6 mmol, 121 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **26** as a colorless oil (102 mg, 75% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **26,** and the secondary C–H insertion product, (5S)-2,2,2-tribromoethyl 2-(4-bromophenyl)-5-((tert-butyldimethylsilyl)oxy)-3-methylhexanoate , were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 96: 4 *r.r.*

$[\alpha]^{20}_D$ +15.1° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.25 (d, J = 8.4 Hz, 2H), 4.89 (s, 2H), 3.77 – 3.69 (m, 1H), 3.66 (t, J = 7.7 Hz, 1H), 2.14 (dtt, J = 10.0, 7.8, 5.0 Hz, 1H), 1.84 (dddd, J = 13.3, 9.6, 6.1, 3.8 Hz, 1H), 1.50 – 1.44 (m, 0H), 1.44 – 1.35 (m, 2H), 1.08 (d, J = 6.1 Hz, 3H), 0.85 (s, 9H), 0.01 (s, 3H), -0.02 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.76, 137.22, 131.89, 130.11, 121.64, 77.11, 68.37, 51.30, 39.34, 35.47, 33.25, 29.86, 26.02, 23.95, 23.78, 18.25, -

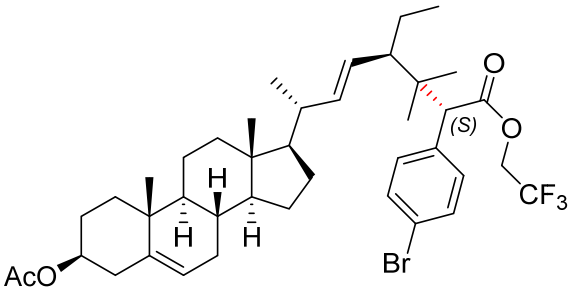
4.20, -4.60; HRMS (NSI) calcd for $C_{17}H_{23}Br_4SiO_3$ ([M-C_4H_9]$^-$): 618.8144 found 618.8138; IR (neat): 2951, 2926, 2855, 1749, 1488, 1461, 1371, 1254, 1133, 1094, 1074, 1042, 1011, 833, 773, 727; HPLC (R, R-Whelk, 0.5% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 40 min, UV 230 nm) retention times of 25.2 min (minor) and 27.7 min (major), >100:1 d.*r.*.



2,2,2-Tribromoethyl (2R,6S)-2-(4-bromophenyl)-6-](tert-butyldimethylsilyl)oxy]heptanoate (**29**). This compound was prepared according to the general procedure A for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*S*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and (S)-tert-butyldimethyl(pentan-2-yloxy)silane (0.6 mmol, 121 mg, 3.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 65/1) to afford compound **29** as a colorless oil (110 mg, 81% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **29,** and the secondary C–H insertion product, (5S)-2,2,2-tribromoethyl 2-(4-bromophenyl)-5-((tert-butyldimethylsilyl)oxy)-3-methylhexanoate , were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 94: 6 *r.r.*

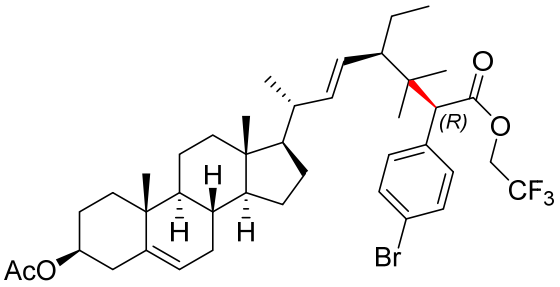
$[\alpha]^{20}_D$ -6.2° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.25 (d, J = 8.4 Hz, 2H), 4.90 (d, J = 12.3 Hz, 1H), 4.87 (d, J = 12.3 Hz, 1H), 3.73 (h, J = 6.1 Hz, 1H), 3.66 (t, J = 7.7 Hz, 1H), 2.15 (dddd, J = 13.1, 9.8, 7.5, 5.5 Hz, 1H), 1.83 (dtt, J = 10.3, 8.1, 5.0 Hz, 1H), 1.44 – 1.38 (m, 2H), 1.38 – 1.31 (m, 1H), 1.31 – 1.21 (m, 1H), 1.07 (d, J = 6.1 Hz, 3H), 0.83 (s, 9H), 0.01 (s, 3H), -0.02 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.77, 137.16, 131.89, 130.12, 121.64, 77.08, 68.44, 51.31, 39.46, 35.51, 33.26, 26.00, 23.99, 23.92, 18.23, -4.19, -4.63; HRMS (NSI) calcd for $C_{17}H_{23}Br_4SiO_3$ ([M-C_4H_9]$^-$): 618.8144 found 618.8138; IR (neat): 2952, 2927, 2855, 1749, 1488, 1461, 1371, 1254, 1133, 1094, 1074, 1042, 1011, 833, 773, 728; HPLC (R, R-Whelk, 0.5% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 30 min, UV 230 nm) retention times of 25.0 min (minor) and 26.8 min (major), 20:1 d.*r.*.



2,2,2-Trifluoroethyl (2S,4R,7R,E)-7-[(3S,8S,9S,10R,13R,14S,17R)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-(4-bromophenyl)-4-ethyl-3,3-dimethyloct-5-enoate (**31**). This compound was prepared according to the general procedure B for C–H functionalization reactions. 2,2,2-Trifluoroethyl 2-(4-bromophenyl)-2-diazoacetate **1c** (0.2 mmol, 65 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, Rh_2(*R*-TCPTAD)$_4$, (0.002 mmol, 4 mg, 1 mol%) and Stigmasteryl acetate (0.2 mmol, 91 mg, 1.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 30/1) to recover Stigmasteryl acetate (40 mg, 56% conversion) and afford compound **31** as a colorless oil (68 mg, 82% yield).

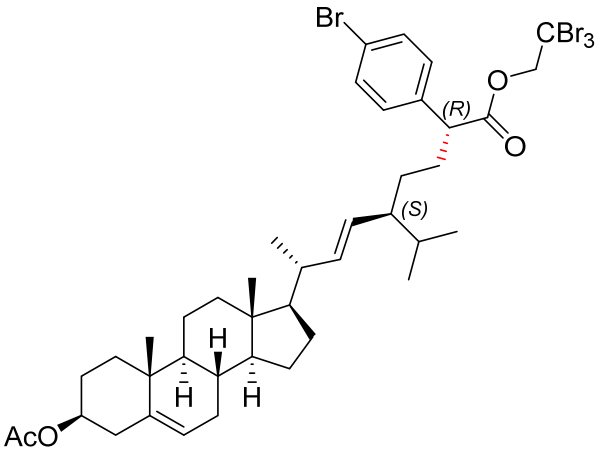
Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **31** was observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as >95: 5 *r.r.*

$[\alpha]^{20}_D$ 9.1° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (d, J = 8.5 Hz, 2H), 7.28 (d, J = 8.5 Hz, 2H), 5.38 (s, 1H), 5.25 (dd, J = 15.2, 8.7 Hz, 1H), 5.03 (dd, J = 15.2, 9.6 Hz, 1H), 4.64 – 4.53 (m, 2H), 4.27 – 4.19 (m, 1H), 3.88 (s, 1H), 2.30 (dd, J = 24.0, 5.7 Hz, 3H), 2.15 – 2.05 (m, 1H), 2.03 (s, 3H), 2.02 – 1.94 (m, 3H), 1.86 (dd, J = 14.2, 2.9 Hz, 2H), 1.75 (ddt, J = 15.4, 9.6, 5.0 Hz, 1H), 1.65 – 1.56 (m, 4H), 1.53 – 1.44 (m, 4H), 1.32 – 1.17 (m, 5H), 1.05 (d, J = 6.6 Hz, 3H), 1.02 (s, 3H), 0.97 (s, 3H), 0.81 (s, 3H), 0.76 (t, J = 7.2 Hz, 3H), 0.72 (s, 3H), 0.73 – 0.68 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.36, 170.71, 141.08, 139.77, 134.32, 132.27, 131.16, 127.65, 123.99, 122.77, 121.81, 74.12, 60.24 (q, J = 36.4 Hz), 56.85, 56.79, 56.01, 52.45, 50.17, 42.47, 40.91, 40.35, 39.77, 38.26, 37.14, 36.75, 32.01, 31.99, 29.86, 29.26, 27.92, 24.53, 22.15, 21.86, 21.61, 21.32, 21.21, 21.16, 19.47, 12.80, 12.21; HRMS (NSI) calcd for $C_{41}H_{57}BrF_3O_4$ ($[M+H]^+$): 749.3419 found 749.3412; IR (neat): 2936, 2870, 2360, 2342, 1752, 1732, 1372, 1278, 1245, 1168, 1139, 1114, 1076, 1033, 1012, 980, 759; HPLC (ADH, 0.5% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 30 min, UV 230 nm) retention times of 14.7 min (minor) and 20.2 min (major), 14:1 d.*r.*.



2,2,2-Trifluoroethyl (2R,4R,7R,E)-7-[(3S,8S,9S,10R,13R,14S,17R)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-(4-bromophenyl)-4-ethyl-3,3-dimethyloct-5-enoate. This compound was prepared according to the general procedure B for C–H functionalization reactions. 2,2,2-Trifluoroethyl 2-(4-bromophenyl)-2-diazoacetate **1c** (0.2 mmol, 65 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, Rh_2(*S*-TCPTAD)$_4$, (0.002 mmol, 4 mg, 1 mol%) and Stigmasteryl acetate (0.2 mmol, 91 mg, 1.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 30/1) to recover Stigmasteryl acetate (61 mg, 33% conversion) and afford mixture of the desired product and compound **31** as a colorless oil (36 mg).

Mismatched reaction occurred when *S*-catalyst is used, please see the crude ^{1}H NMR spectra in Section 8.3. The mixture was used to determine the diastereoselectivity of the reaction generated compound **31**.

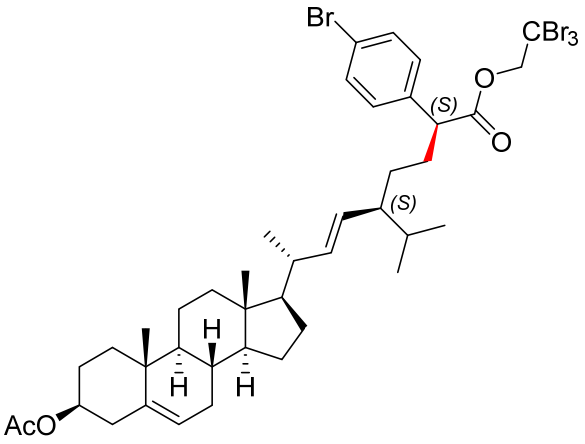


2,2,2-Tribromoethyl (2R,5S,8R,E)-8-[(3S,8S,9S,10R,13R,14S,17R)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-(4-bromophenyl)-5-isopropylnon-6-enoate (**32**). This compound was prepared according to the general procedure B for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d**

(0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*S*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and Stigmasteryl acetate (0.2 mmol, 91 mg, 1.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 30/1) to recover Stigmasteryl acetate (45 mg, 50% conversion) and afford compound **31** as a white solid (82 mg, 88% yield).

Analysis of the ^{1}H NMR spectrum of the crude reaction mixture revealed that only compound **31** and the tertiary C–H insertion product, 2,2,2-tribromoethyl (2R,4R,7R,E)-7-((3S,8S,9S,10R,13R,14S,17R)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl)-2-(4-bromophenyl)-4-ethyl-3,3-dimethyloct-5-enoate, were observed and no evident signal of other regioisomer was detected, so the regioselectivity of this reaction was recoded as 94:6 *r.r.*

$[\alpha]^{20}_D$ -21.3° (c = 1.00, $CHCl_3$); TLC (diethyl ether: hexanes, 1:10 v/v); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 8.4 Hz, 2H), 7.23 (d, J = 8.4 Hz, 2H), 5.37 (d, J = 4.9 Hz, 1H), 5.18 (dd, J = 15.2, 8.7 Hz, 1H), 4.97 (dd, J = 15.2, 9.3 Hz, 1H), 4.88 (d, J = 4.0 Hz, 2H), 4.65 – 4.56 (m, 1H), 3.64 (t, J = 7.7 Hz, 1H), 2.31 (dd, J = 8.4, 3.7 Hz, 2H), 2.03 (s, 3H), 1.99 (ddt, J = 27.0, 13.6, 4.5 Hz, 4H), 1.89 – 1.82 (m, 2H), 1.67 (ddt, J = 12.9, 9.6, 5.8 Hz, 2H), 1.55 (dddt, J = 29.4, 18.0, 9.5, 3.6 Hz, 3H), 1.48 – 1.43 (m, 2H), 1.40 (ddd, J = 13.7, 6.4, 3.8 Hz, 1H), 1.25 – 1.17 (m, 3H), 1.17 – 1.09 (m, 3H), 1.02 (s, 3H), 1.01 (d, J = 6.6 Hz, 3H), 1.09 – 0.91 (m, 3H), 0.86 (dt, J = 21.3, 5.8 Hz, 2H), 0.79 (d, J = 6.7 Hz, 3H), 0.76 (d, J = 6.8 Hz, 3H), 0.68 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.91, 170.70, 139.79, 139.13, 137.19, 131.83, 130.18, 128.83, 122.75, 121.56, 77.06, 74.12, 56.90, 55.95, 51.23, 50.16, 49.19, 42.38, 40.60, 39.76, 38.26, 37.13, 36.74, 35.57, 32.36, 32.02, 31.99, 31.18, 30.28, 29.86, 29.08, 27.91, 24.50, 21.61, 21.40, 21.15, 21.08, 19.47, 19.20, 12.20; HRMS (NSI) calcd for $C_{39}H_{53}Br_4O_2$ ([M-$C_2H_3O_2$]$^+$): 869.0774 found 869.0789; IR (neat): 2936, 2870, 2360, 2342, 1752, 1732, 1489, 1465, 1372, 1278, 1245, 1168, 1139, 1114, 1076, 1033, 1012, 980, 759; HPLC (ADH, 1% isopropanol in hexane, 0.5 mL/min, 10 mg/mL, 30 min, UV 230 nm) retention times of 16.2 min (minor) and 19.8 min (major), >100:1 d*.r.*.

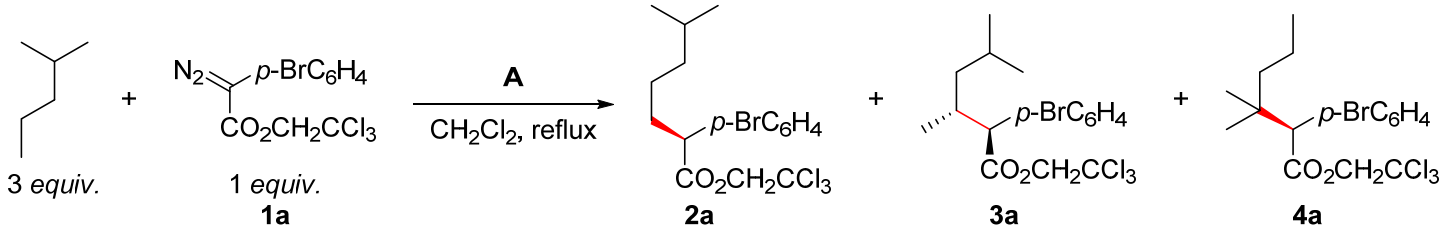


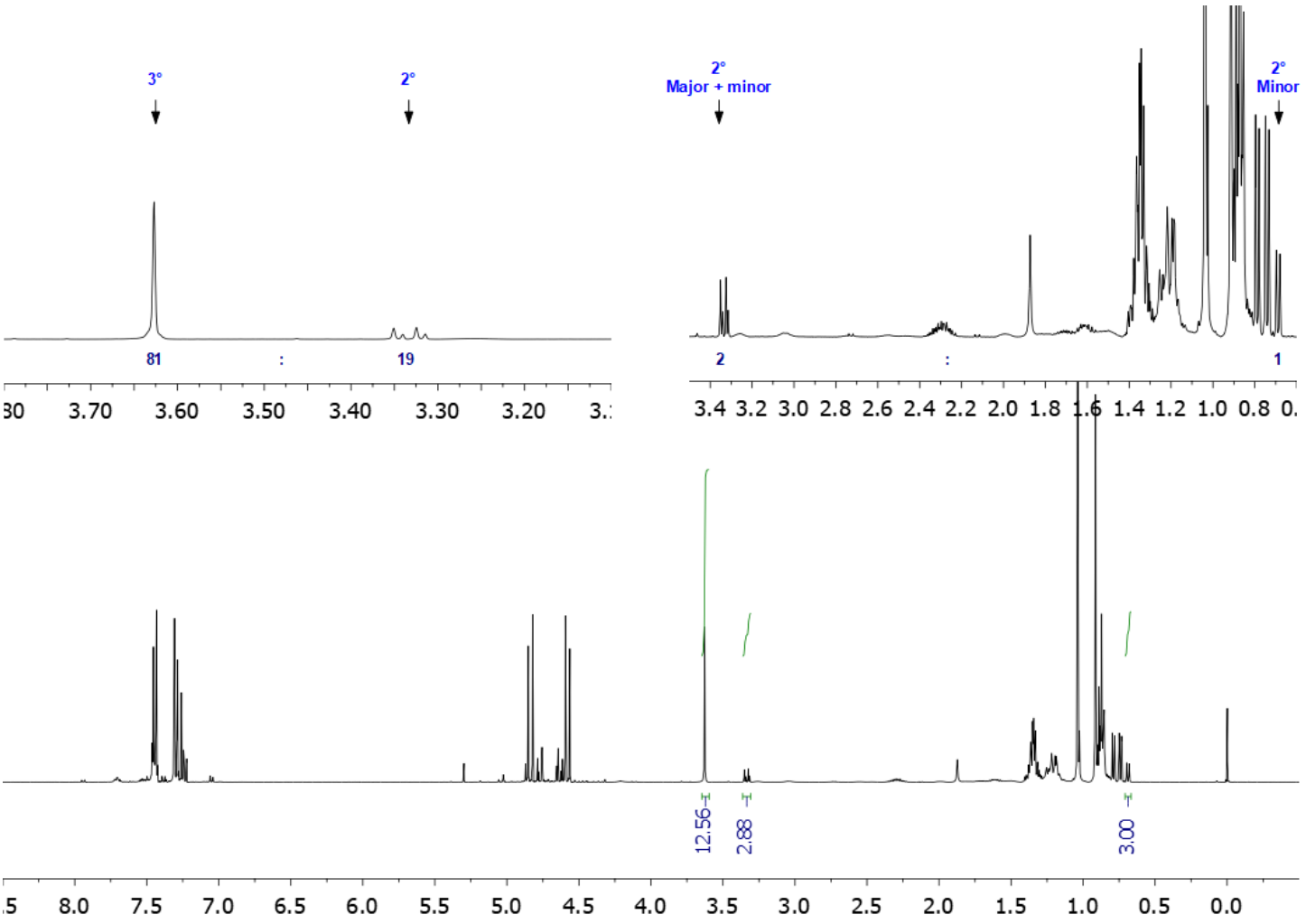
2,2,2-Tribromoethyl (2S,5S,8R,E)-8-[(3S,8S,9S,10R,13R,14S,17R)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-(4-bromophenyl)-5-isopropylnon-6-enoate. This compound was prepared according to the general procedure B for C–H functionalization reactions. 2,2,2-Tribromoethyl 2-(4-bromophenyl)-2-diazoacetate **1d** (0.2 mmol, 101 mg, 1.0 *equiv.*) in 3 mL distilled CH_2Cl_2, **catalyst I**, Rh_2[*R*-tris(*p*-^{t}BuC_6H_4)TPCP]$_4$, (0.002 mmol, 6 mg, 1 mol%) and Stigmasteryl acetate (0.2 mmol, 91 mg, 1.0 *equiv.*) in 0.5 mL distilled CH_2Cl_2 were used. The crude residue was analyzed by ^{1}H NMR and then purified by flash column chromatography (hexanes/diethyl ether = 30/1) to recover Stigmasteryl acetate (60 mg, 34% conversion) and afford mixture of the desired product and compound **32** as a colorless oil (50 mg).

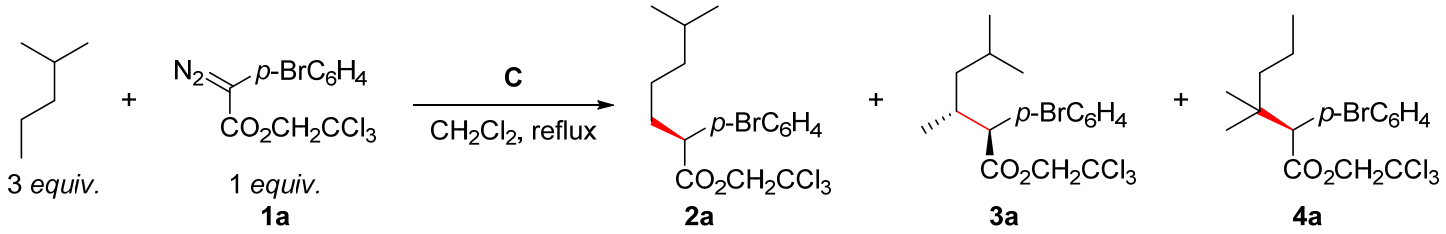
Mismatched reaction occurred when *S*-catalyst is used, please see the crude ^{1}H NMR spectra in Section 8.3. The mixture was used to determine the diastereoselectivity of the reaction generated compound **32**.

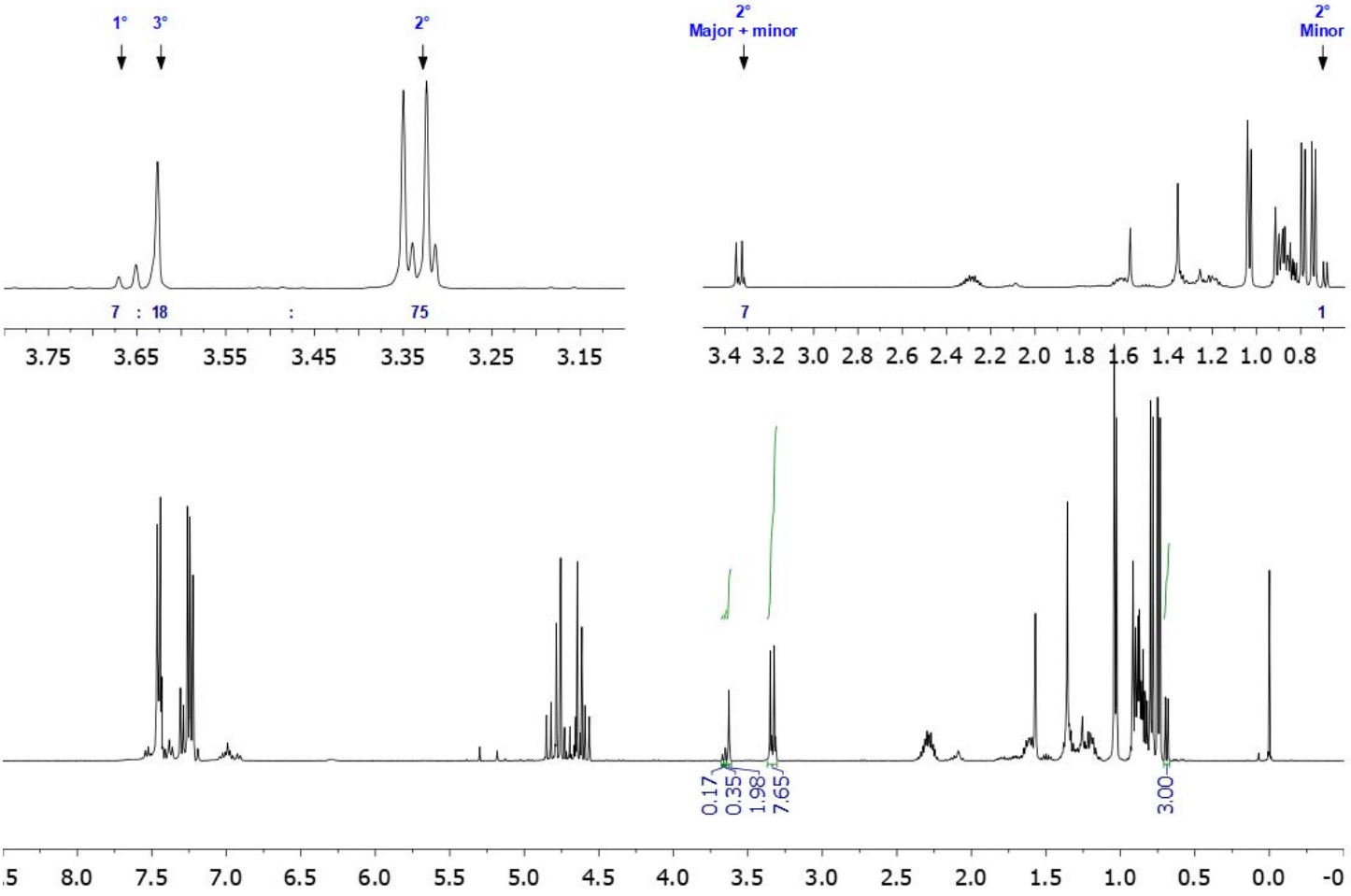
8 - Crude ^{1}H NMR Spectra for the Ratio Determination

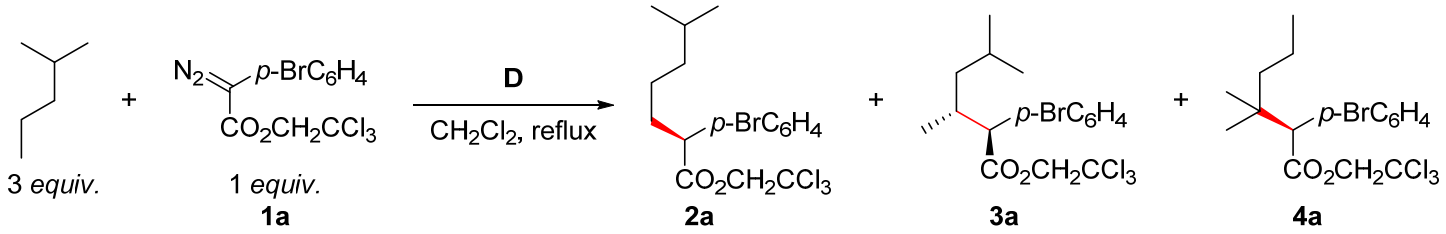
8.1 Crude ^{1}H NMR Spectra for Catalyst Screen of 2-Methylpentane

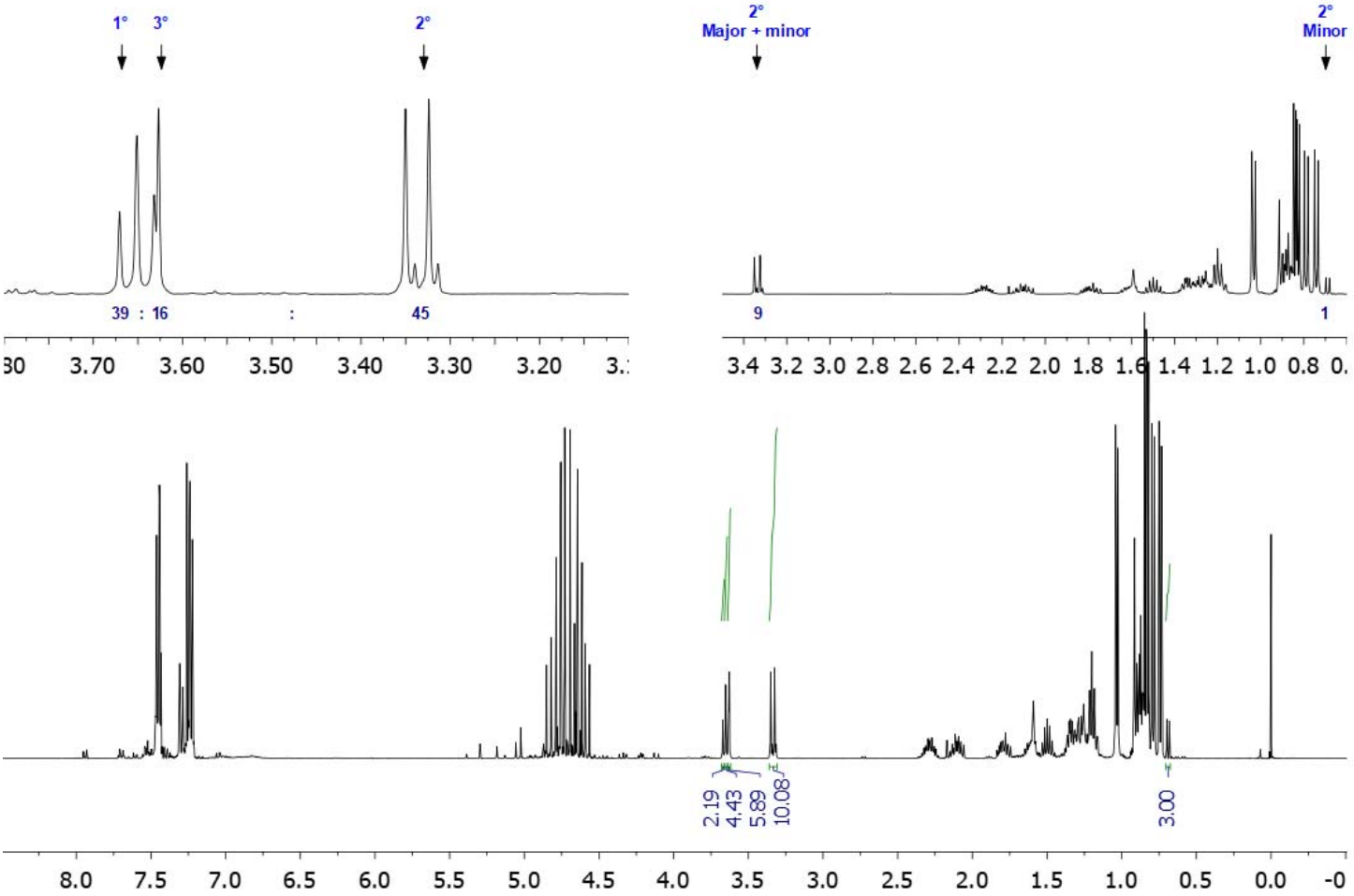


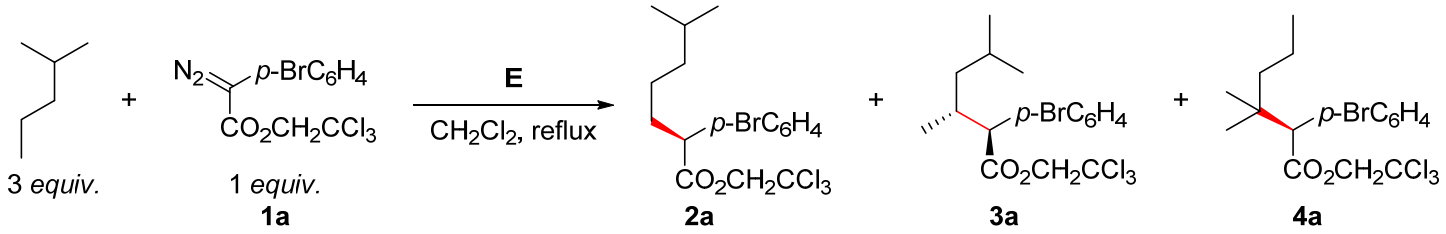


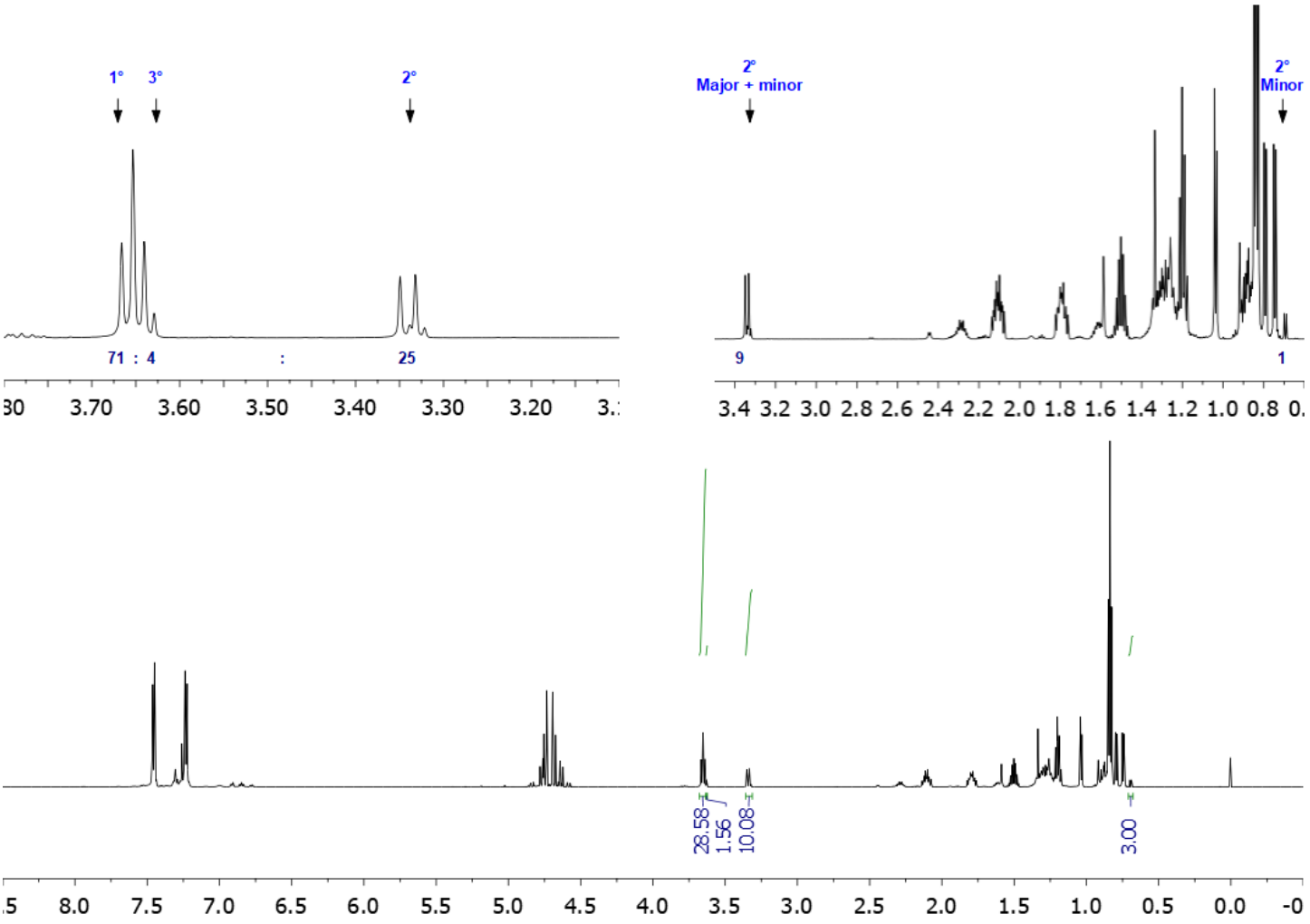

3 equiv.
1 equiv.
1a
C
CH2Cl2, reflux
2a
3a
4a

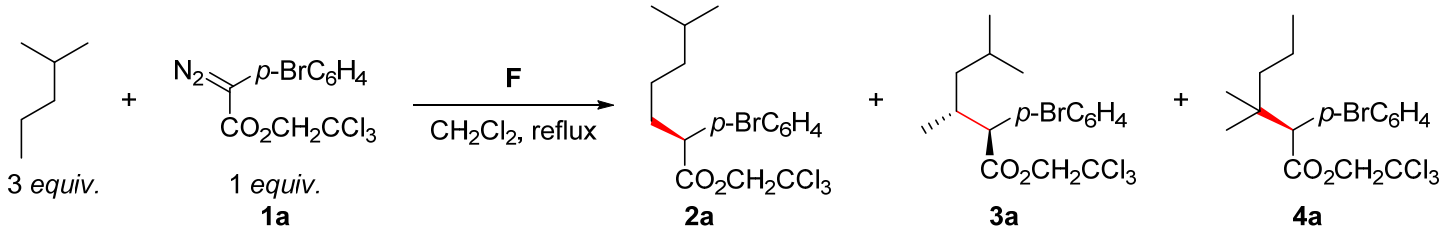

1°
3°
2°
7 : 18 : 75
2°
Major + minor
2°
Minor
7
1
0.17
0.35
1.98
7.65
3.00

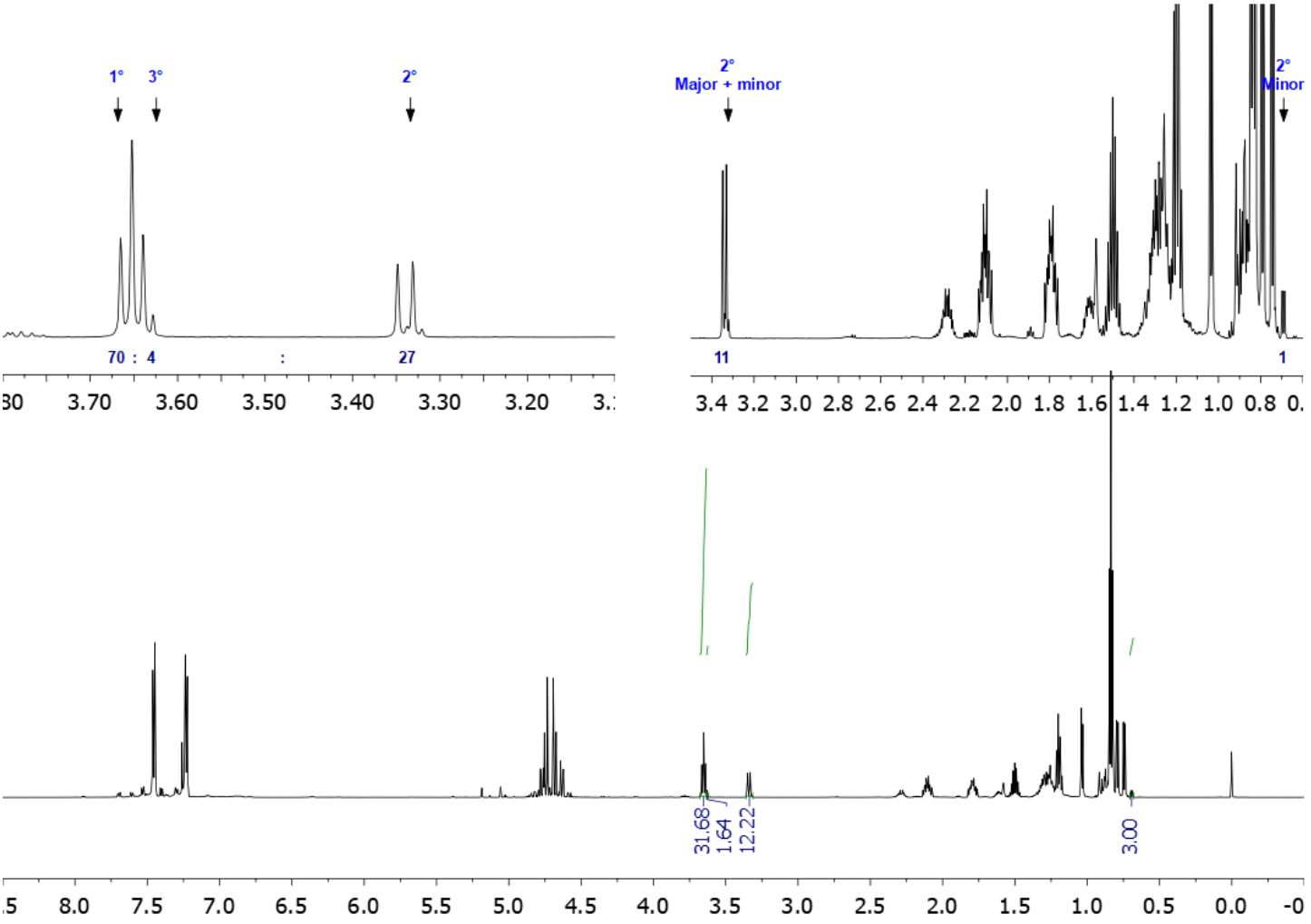

3 equiv.
1 equiv.
1a
D
CH2Cl2, reflux
2a
3a
4a

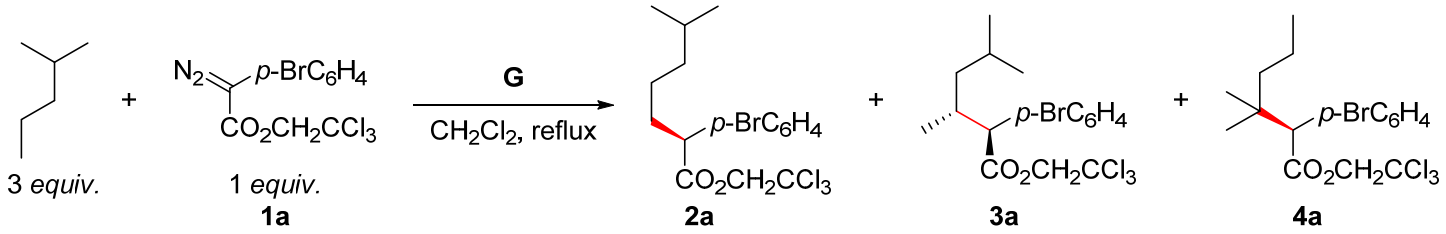

1°
3°
2°
39 : 16 : 45
2°
Major + minor
2°
Minor
9
1
2.19
4.43
5.89
10.08
3.00

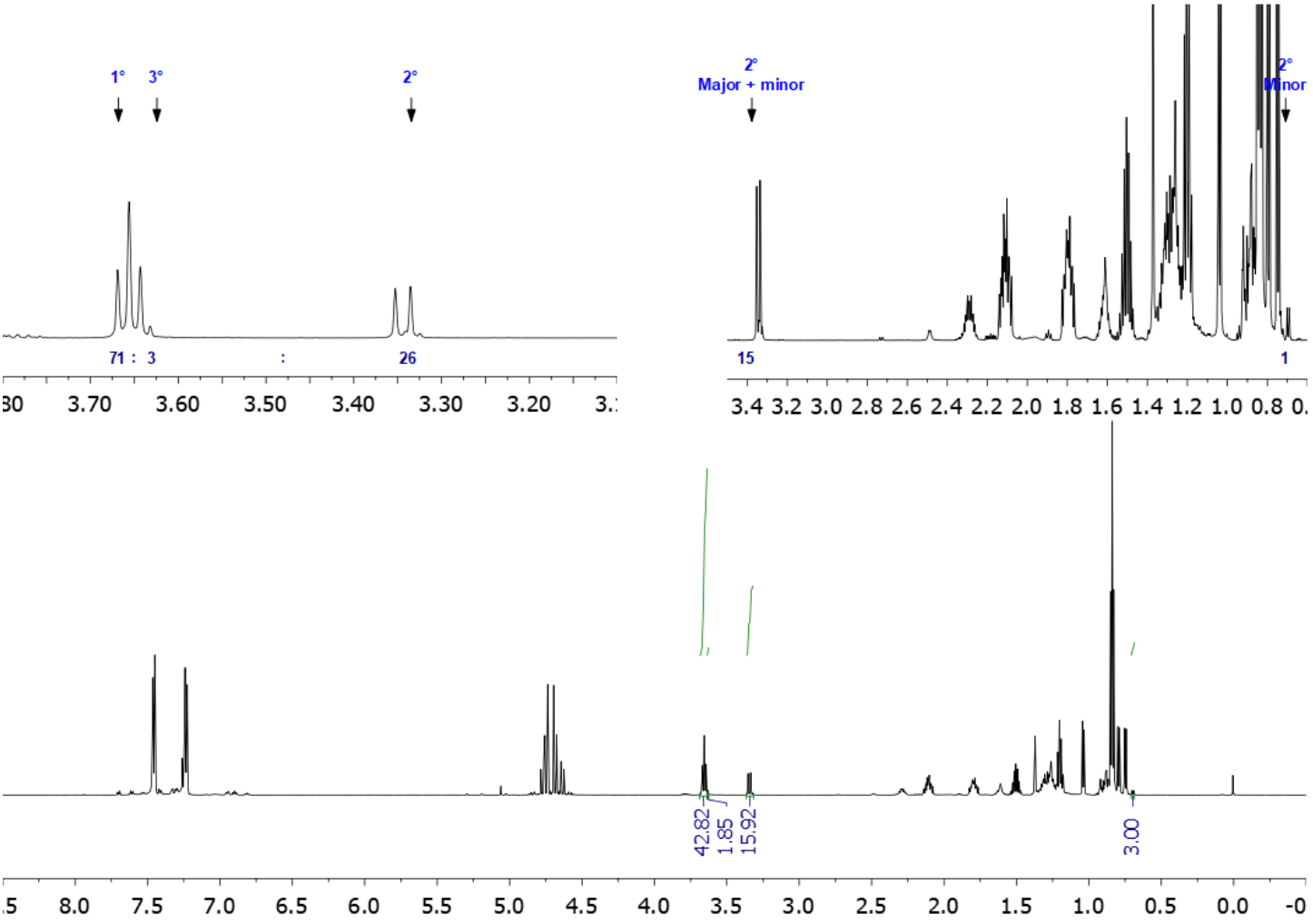

3 equiv.
1 equiv.
1a
E
CH2Cl2, reflux
2a
3a
4a

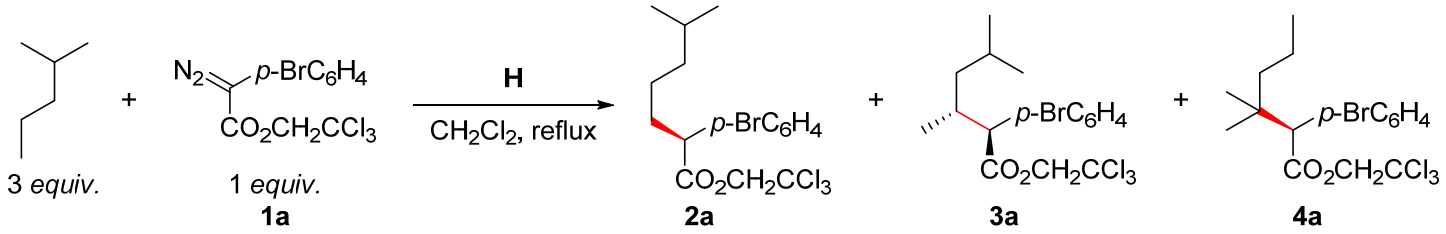

1°
3°
2°
71 : 4 : 25
2°
Major + minor
2°
Minor
9
1
28.58
1.56
10.08
3.00

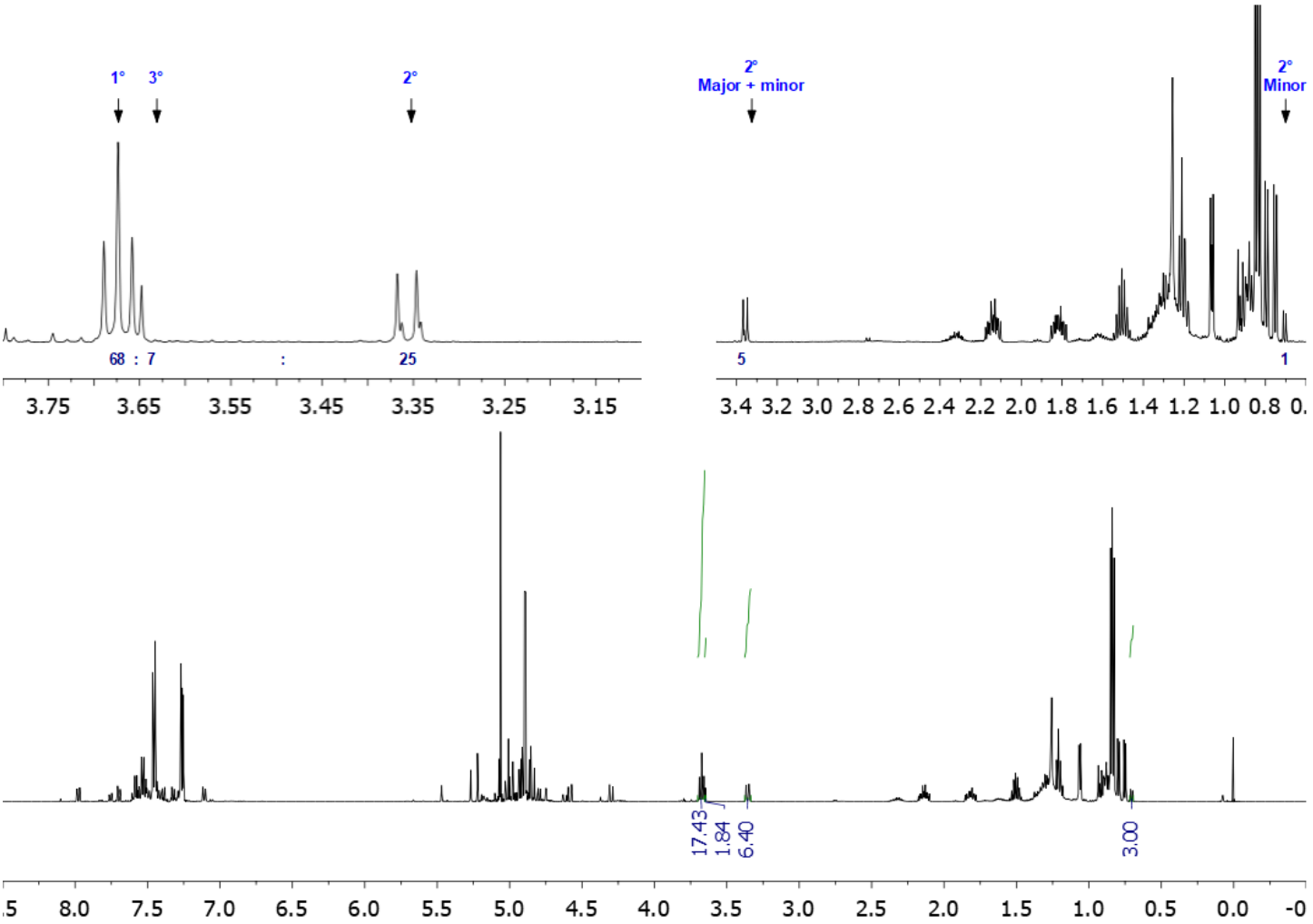

3 equiv.
1 equiv.
1a
F
CH2Cl2, reflux
2a
3a
4a

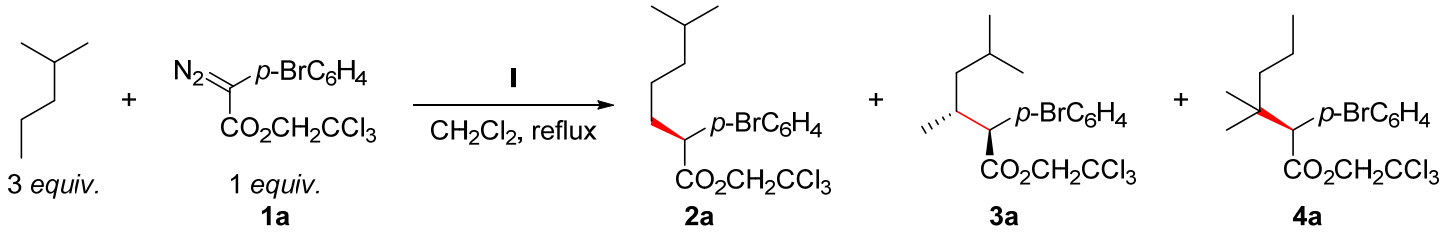

1°
3°
2°
70 : 4 : 27
2°
Major + minor
2°
Minor
11
1
31.68
1.64
12.22
3.00

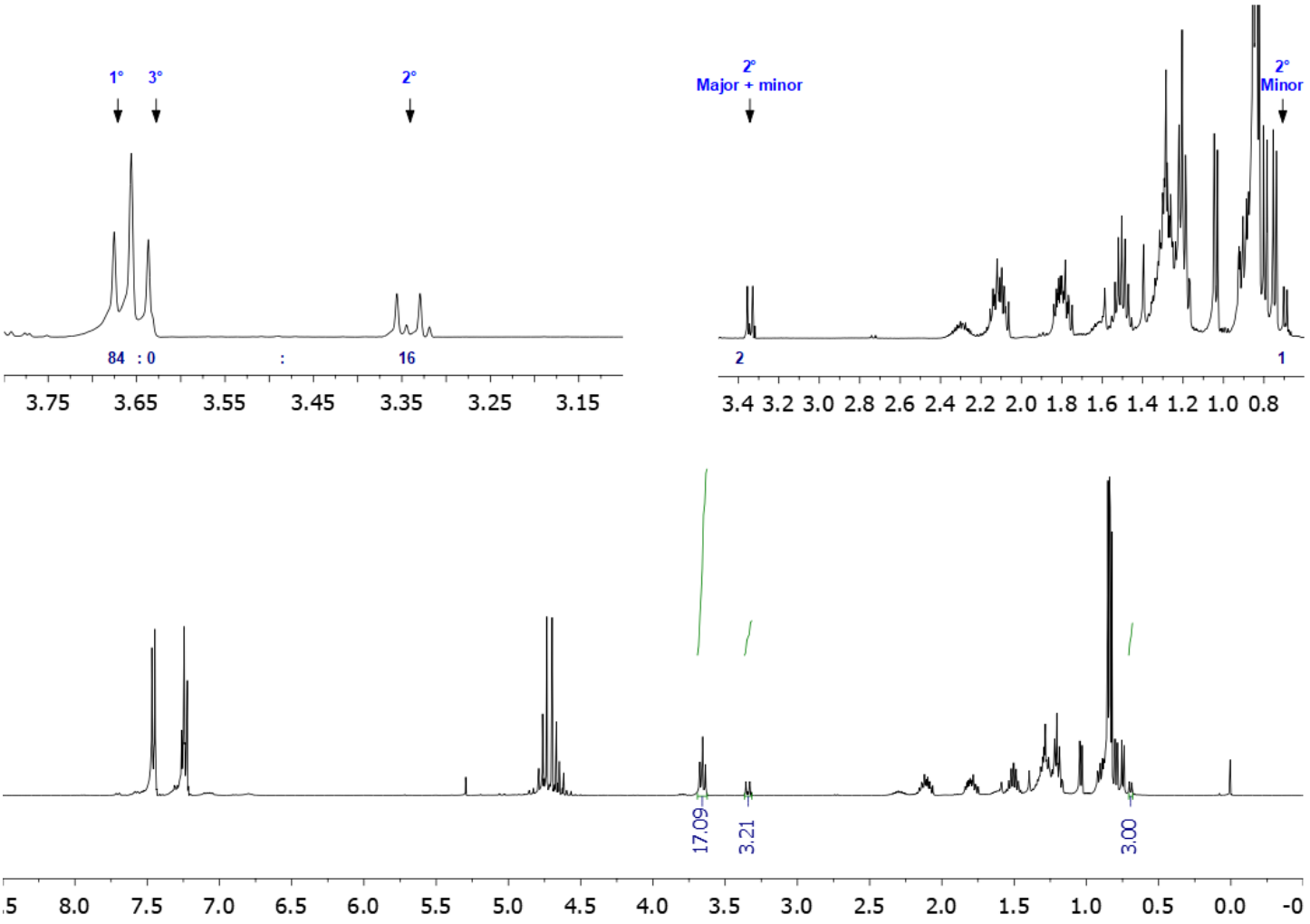

3 equiv.
1 equiv.
1a
G
CH2Cl2, reflux
2a
3a
4a

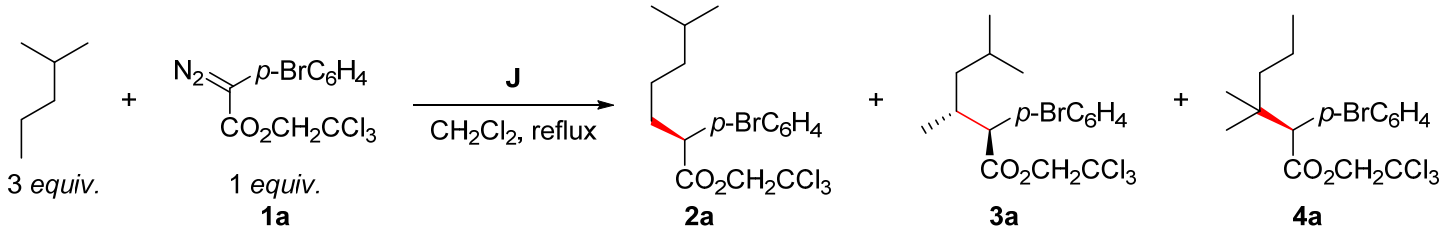

1°
3°
2°
71 : 3 : 26
2°
Major + minor
2°
Minor
15
1
42.82
1.85
15.92
3.00

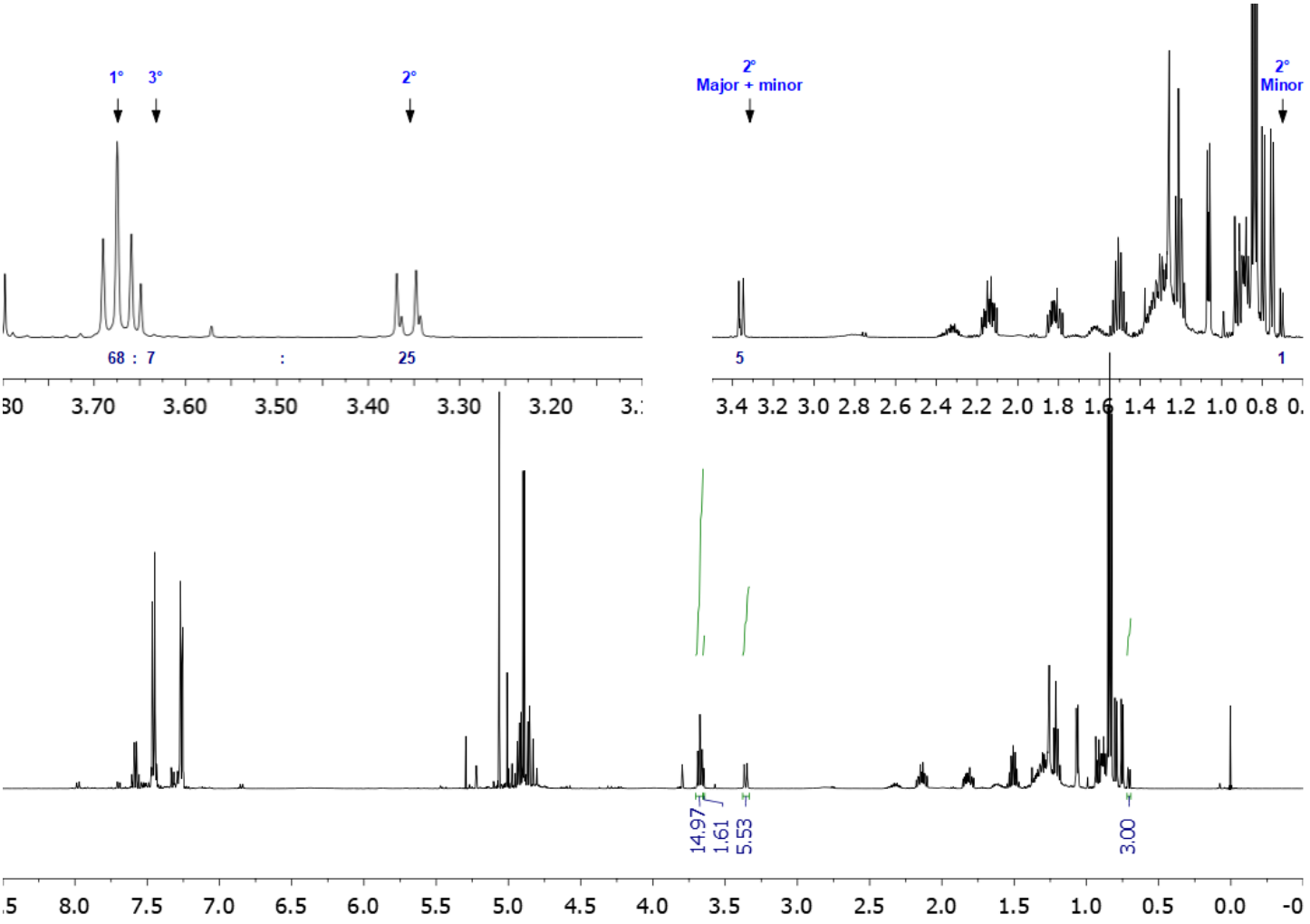

3 equiv.
1 equiv.
1a
H
CH2Cl2, reflux
2a
3a
4a

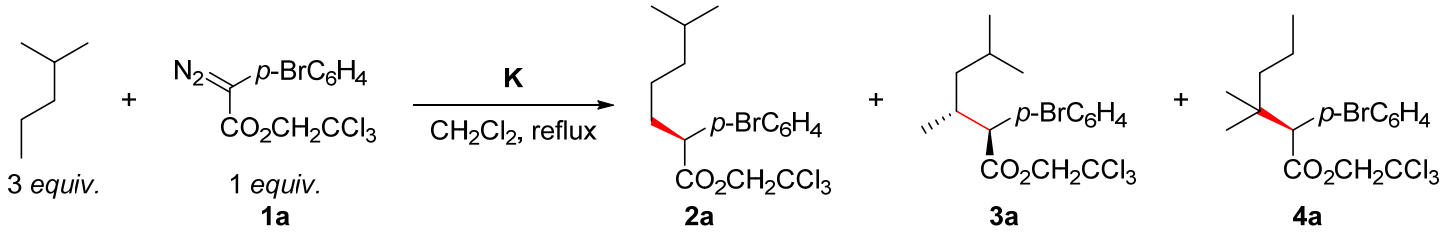

1°
3°
2°
68 : 7 : 25
2°
Major + minor
2°
Minor
5
1
17.43
1.84
6.40
3.00

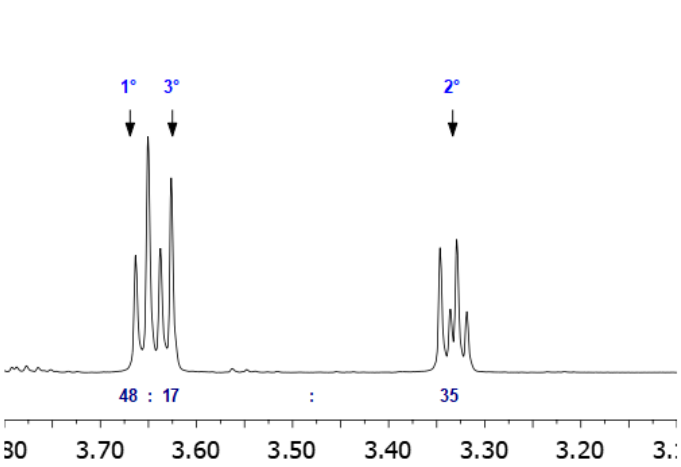

3 equiv.
1 equiv.
1a
I
CH2Cl2, reflux
2a
3a
4a

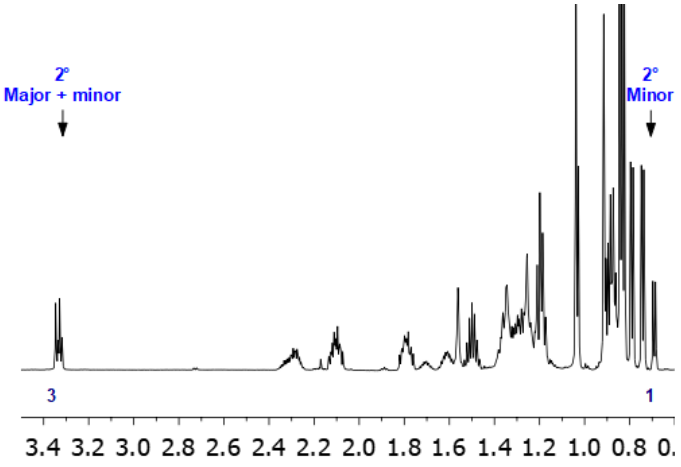

1°
3°
2°
84 : 0
:
16
2°
Major + minor
2°
Minor
2
1
17.09
3.21
3.00

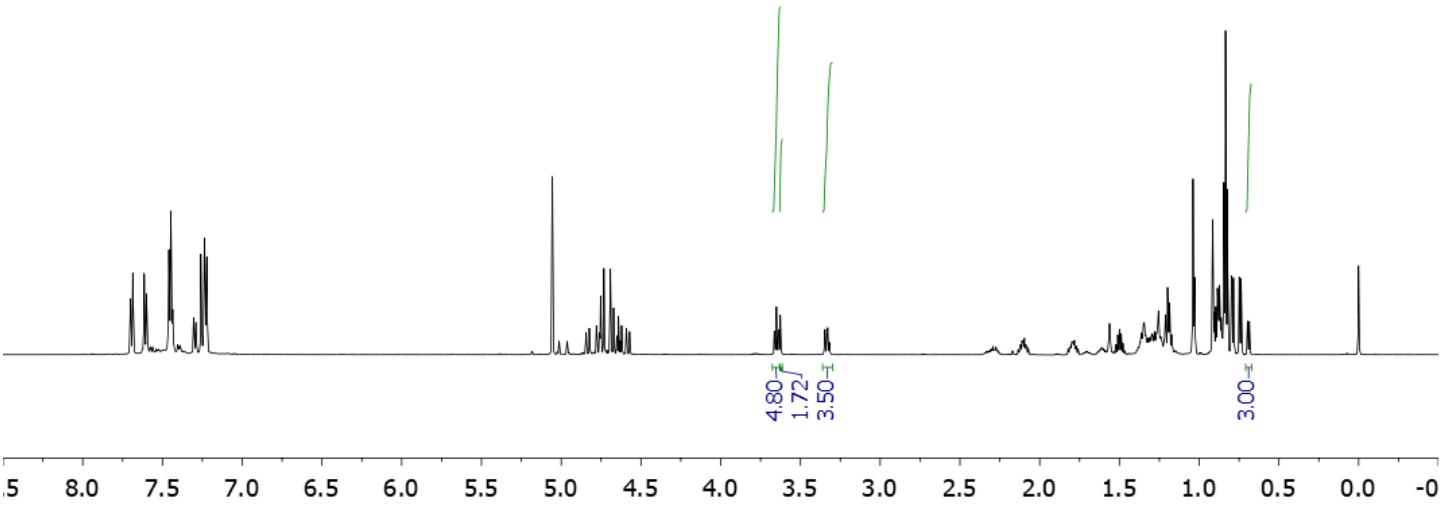

3 equiv.
1 equiv.
1a
J
CH2Cl2, reflux
2a
3a
4a

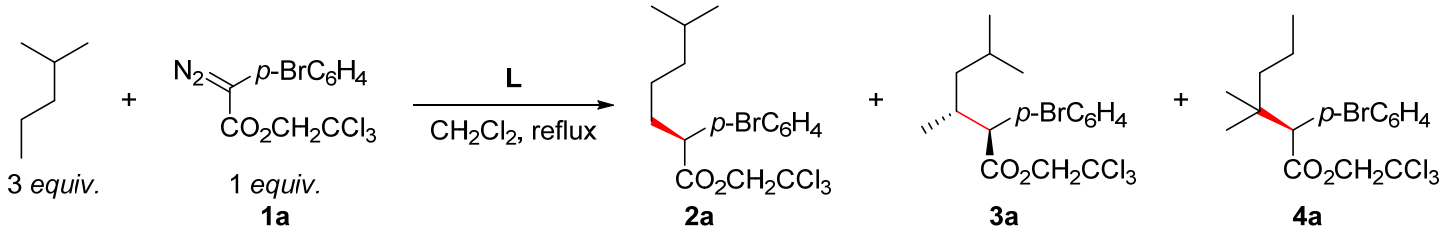

1°
3°
2°
68 : 7 : 25
2°
Major + minor
2°
Minor
5
1
14.97
1.61
5.53
3.00

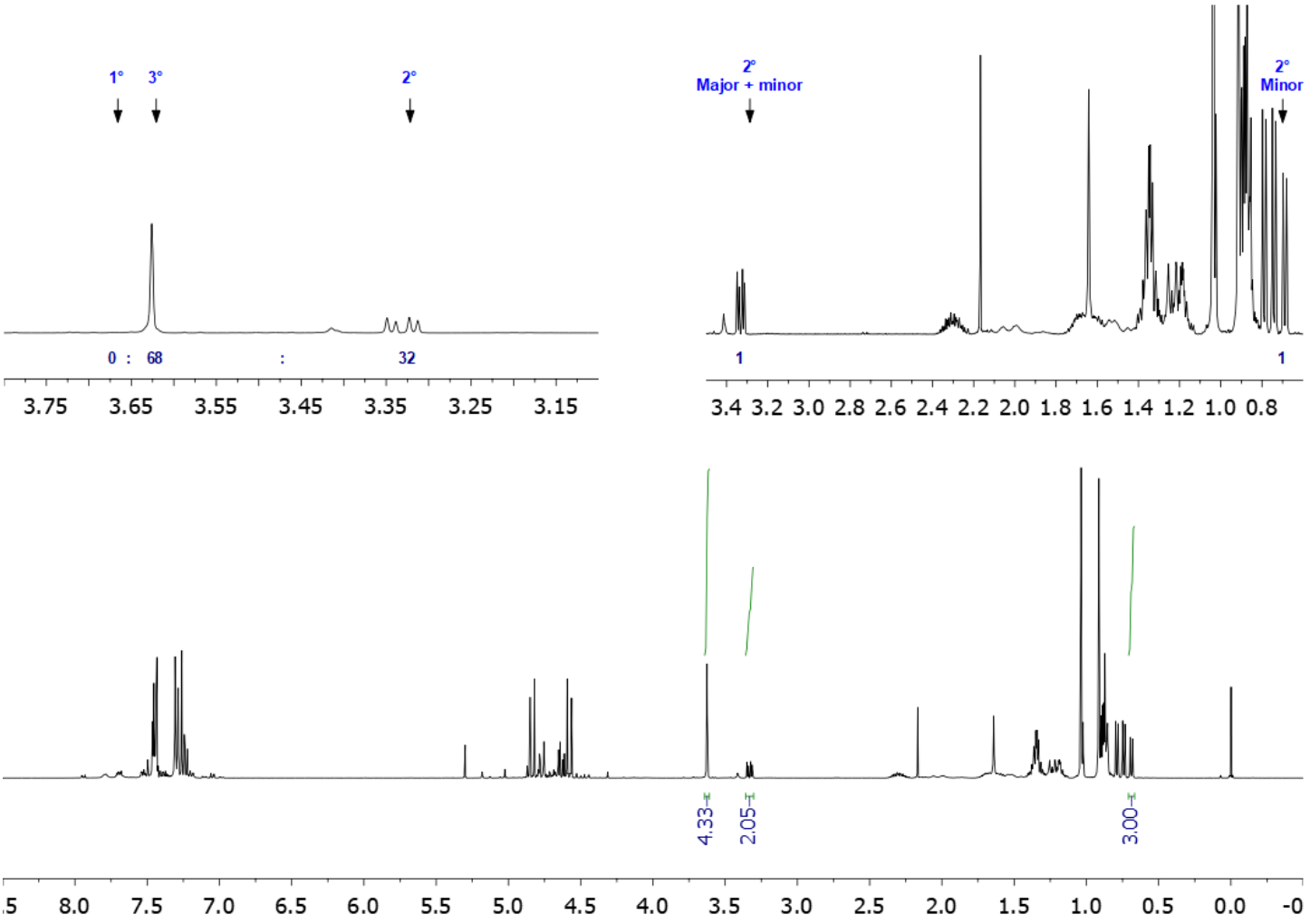

3 equiv.
1 equiv.
1a
K
CH2Cl2, reflux
2a
3a
4a

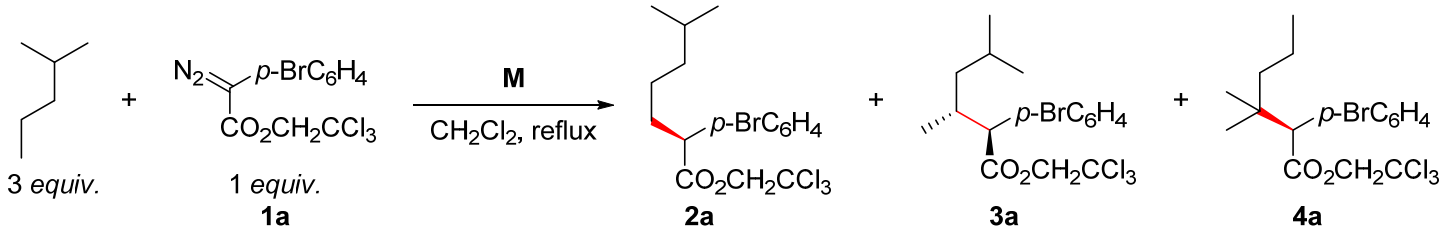

1°
3°
2°
48 : 17 : 35
3.70
3.60
3.50
3.40
3.30
3.20

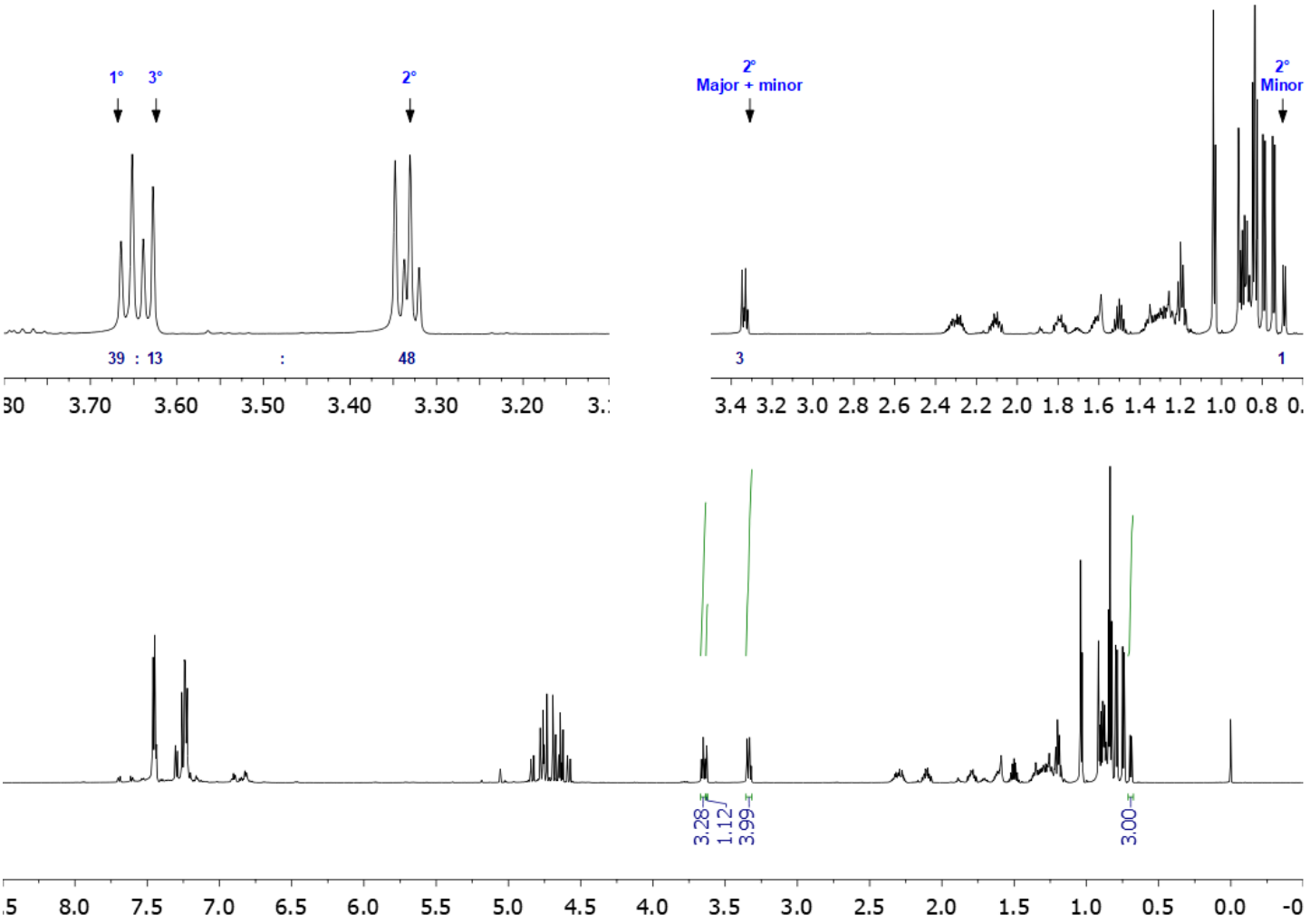

2°
Major + minor
2°
Minor
3
1
3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8

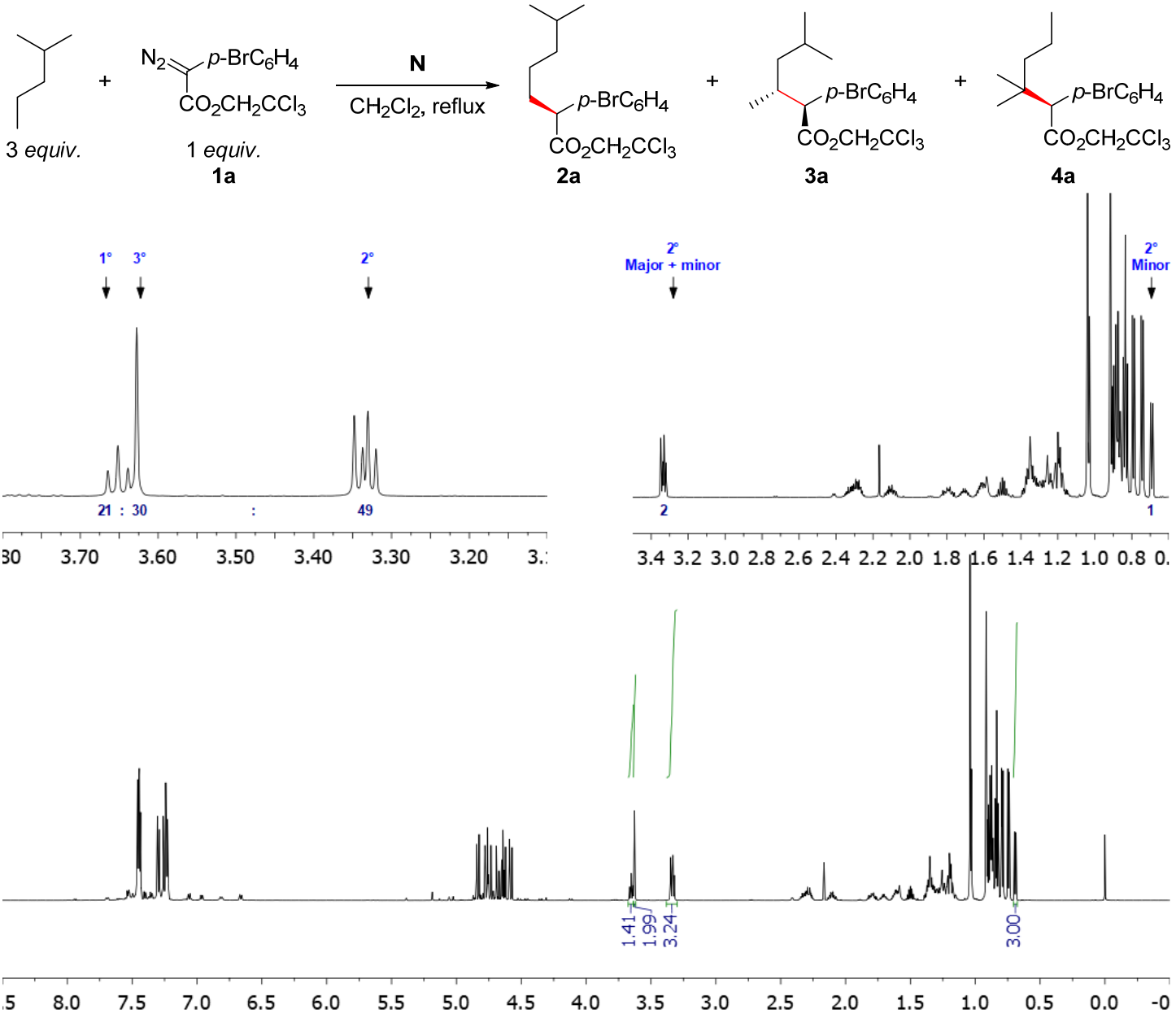

4.80
1.72
3.50
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

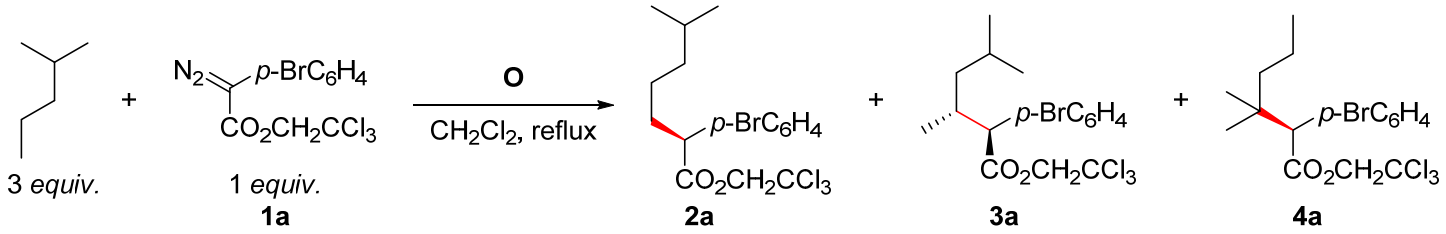

3 equiv.
1 equiv.
1a
L
CH2Cl2, reflux
2a
3a
4a

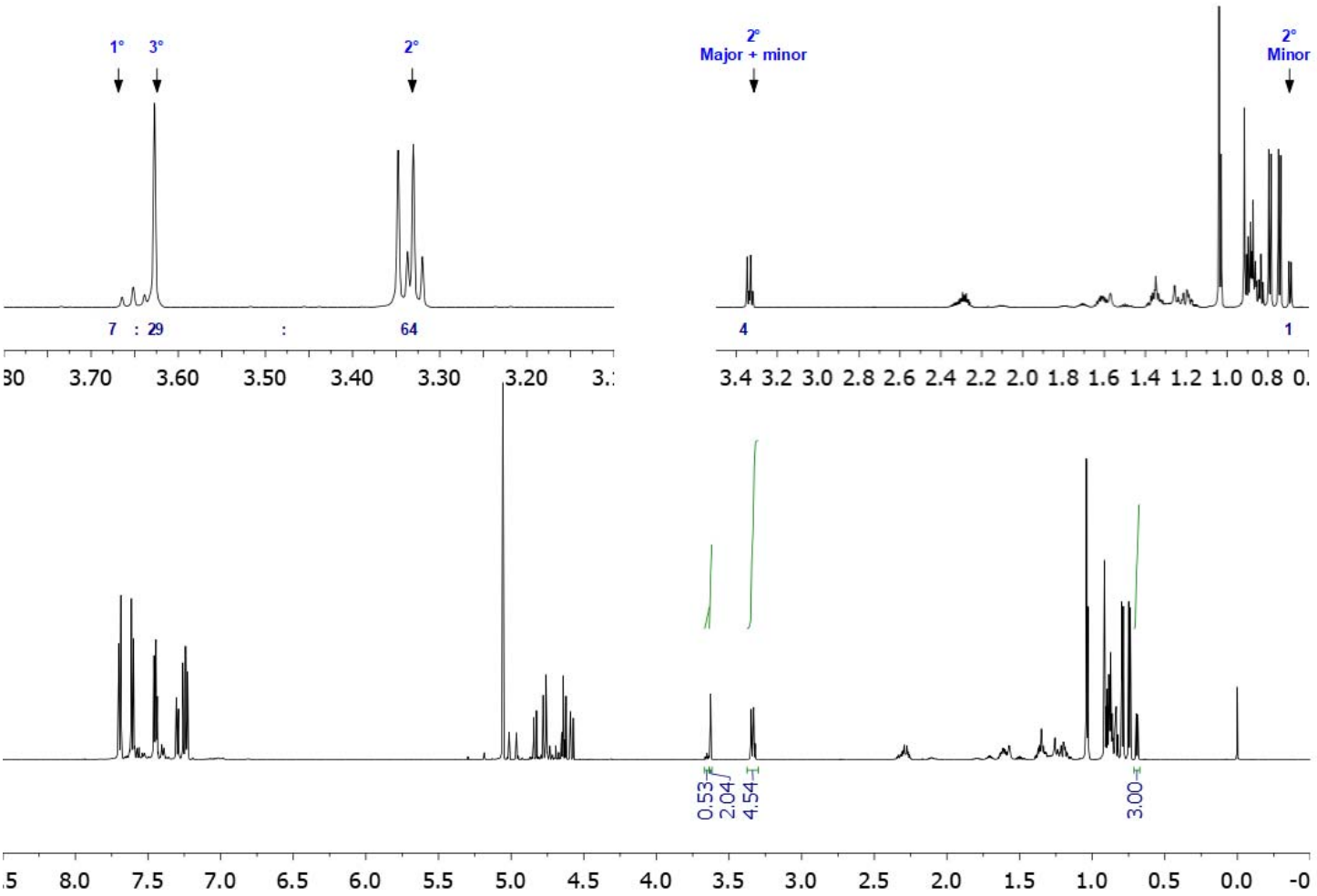

1°
3°
2°
0 : 68 : 32
2°
Major + minor
2°
Minor
1
1
4.33
2.05
3.00

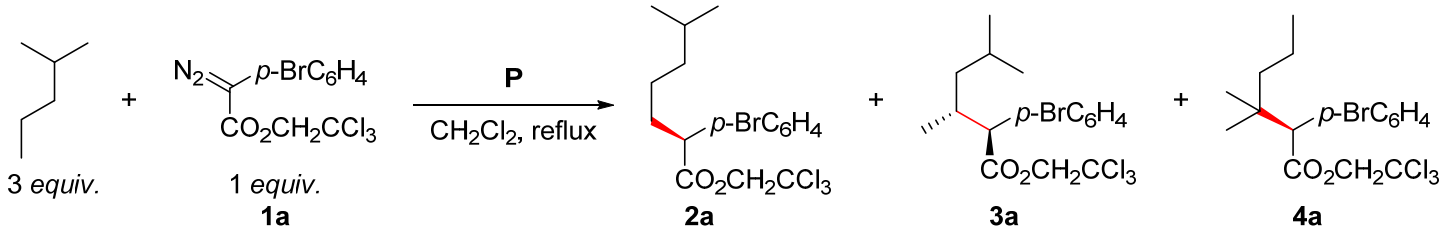

3 equiv.
1 equiv.
1a
M
CH2Cl2, reflux
2a
3a
4a

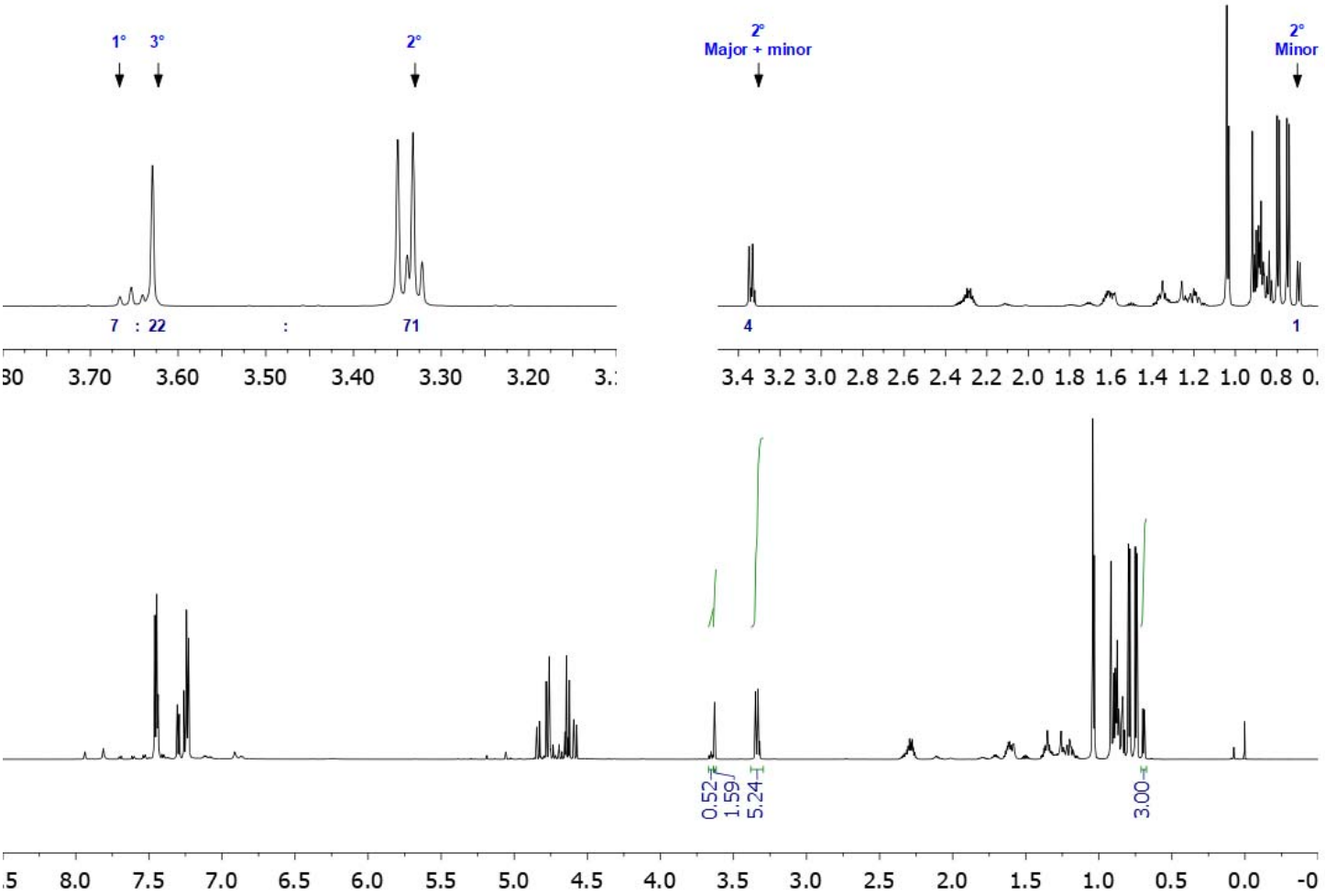

1°
3°
2°
39 : 13 : 48
2°
Major + minor
2°
Minor
3 1
3.28
1.12
3.99
3.00

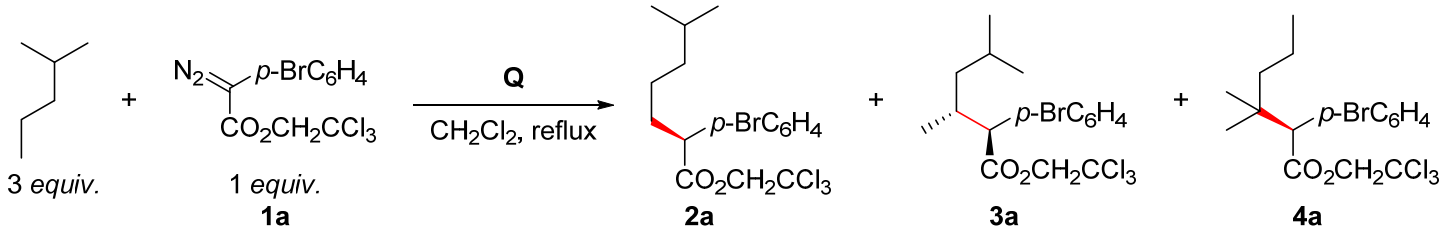

3 equiv.
1 equiv.
1a
N
CH2Cl2, reflux
2a
3a
4a
1° 3°
2°
21 : 30 : 49
2° Major + minor
2° Minor
2
1
1.41
1.99
3.24
3.00

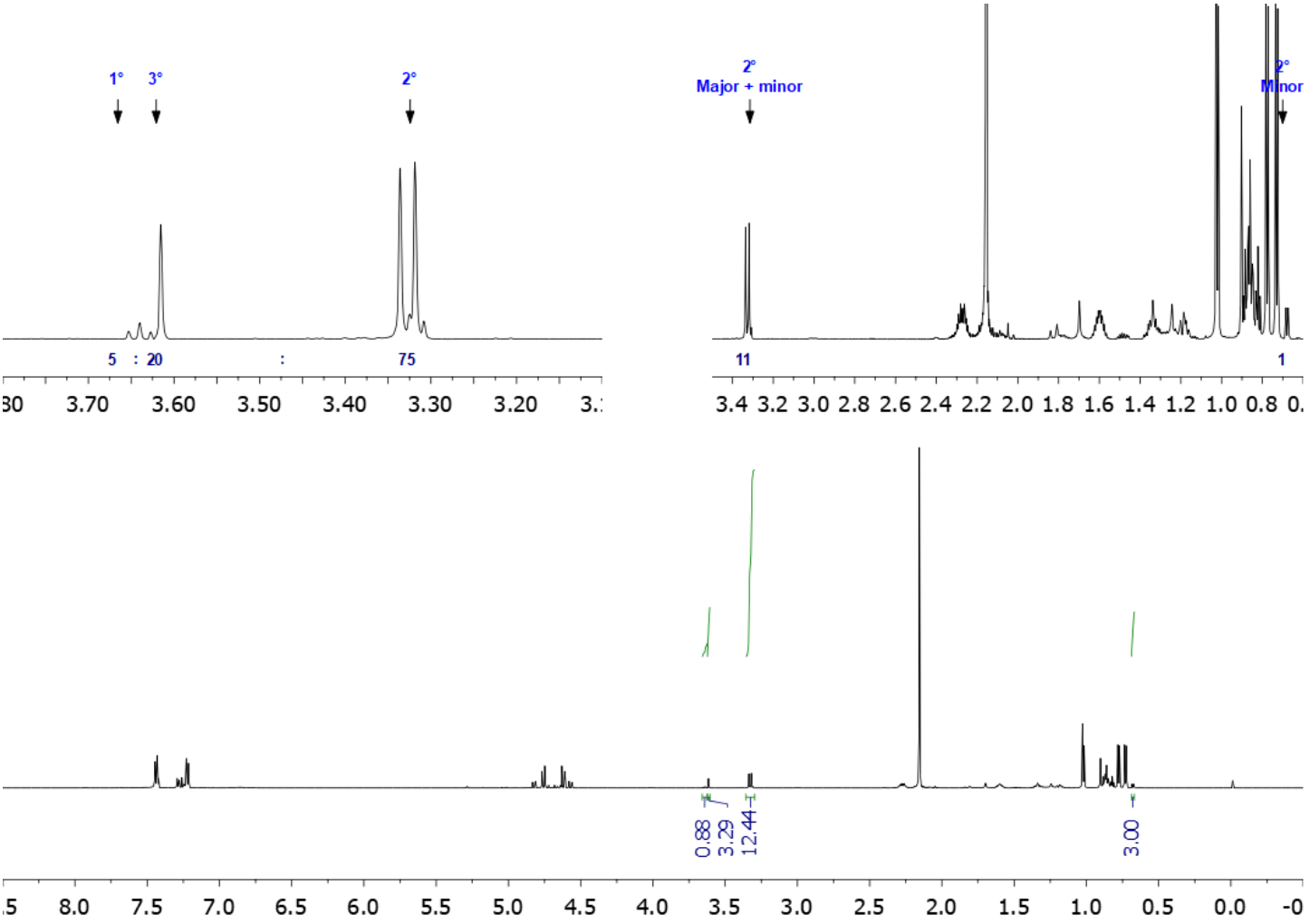

3 equiv.
1 equiv.
1a
O
CH2Cl2, reflux
2a
3a
4a


1°
3°
2°
7 : 29 : 64
2°
Major + minor
2°
Minor
4
1
0.53
2.04
4.54
3.00

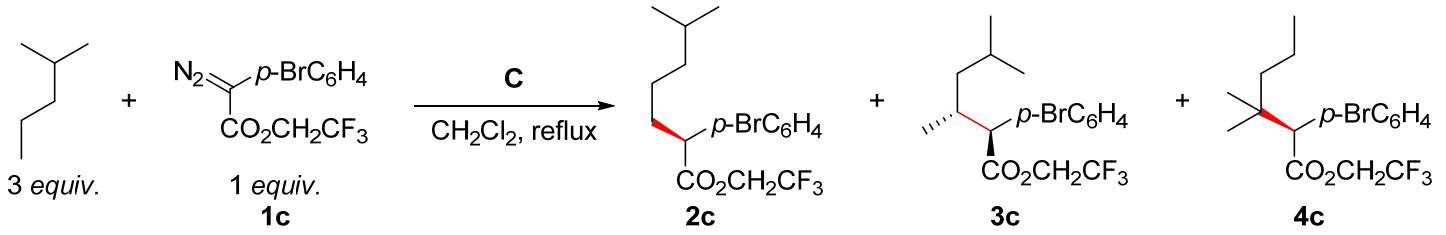

3 equiv.
1 equiv.
1a
P
CH2Cl2, reflux
2a
3a
4a

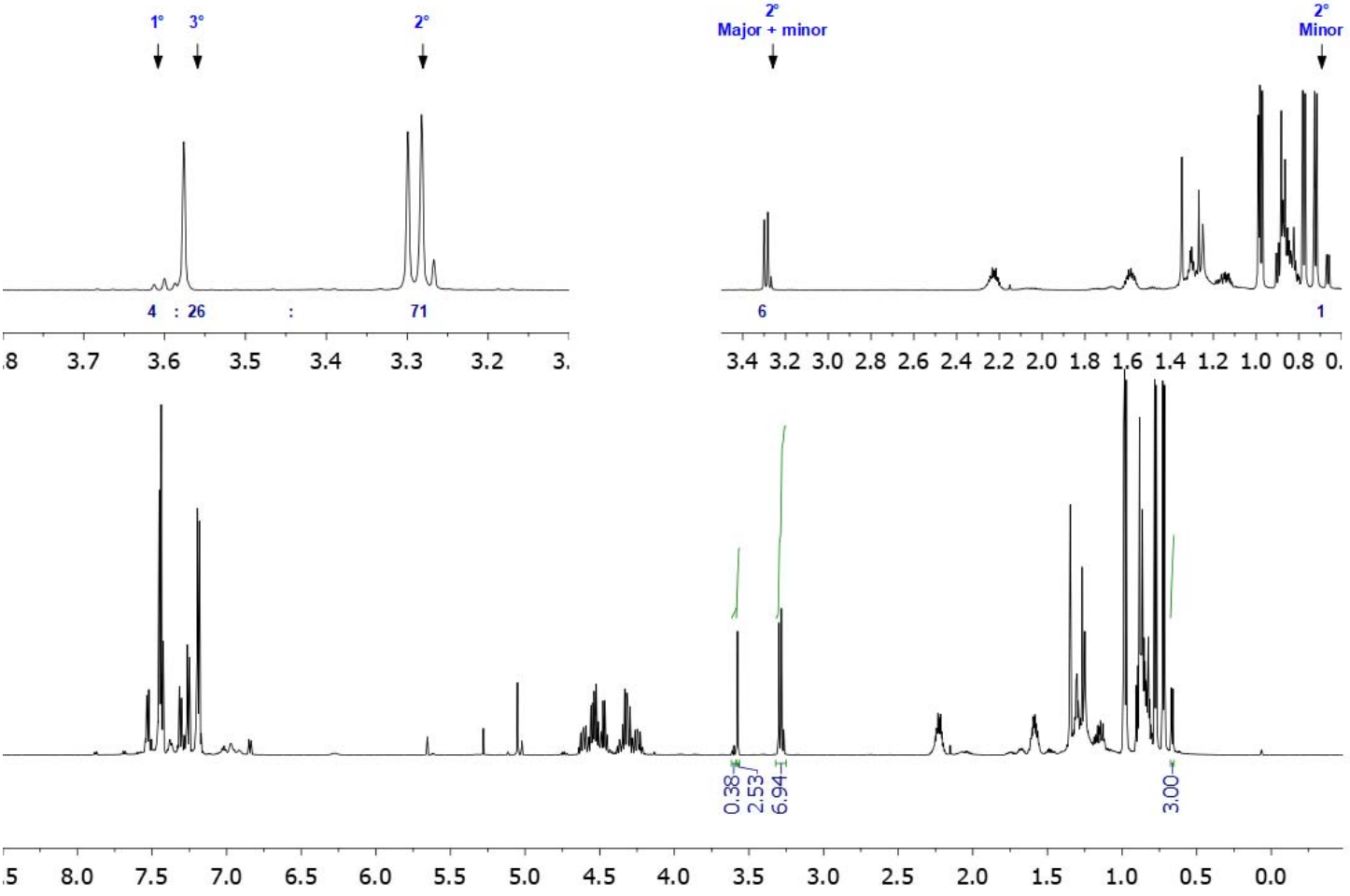

1°
3°
2°
7 : 22 : 71
2°
Major + minor
2°
Minor
4
1
0.52
1.59
5.24
3.00

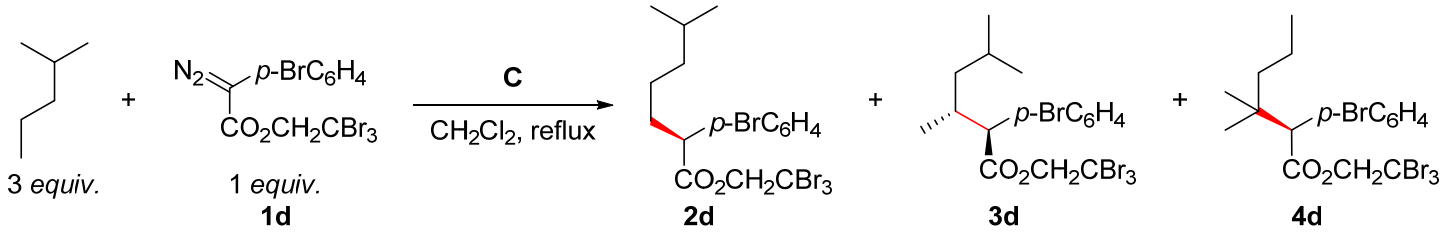

3 equiv.
1 equiv.
1a
Q
CH2Cl2, reflux
2a
3a
4a

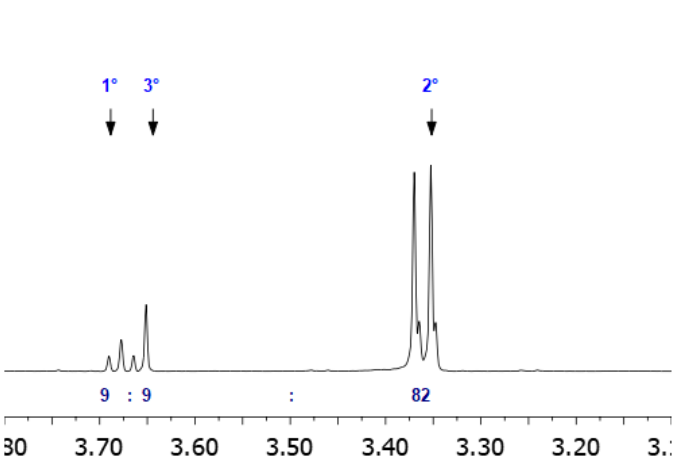

1°
3°
2°
5 : 20 : 75
2°
Major + minor
2°
Minor
11
1
0.88
3.29
12.44
3.00

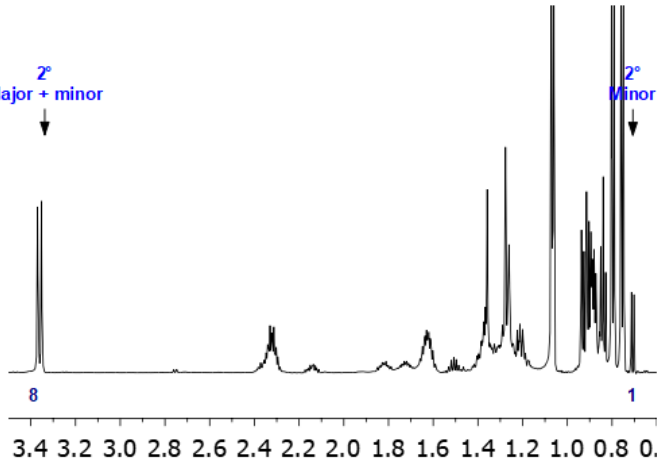
8.2 Crude ^{1}H NMR Spectra for Diazo Screen of 2-Methylpentane

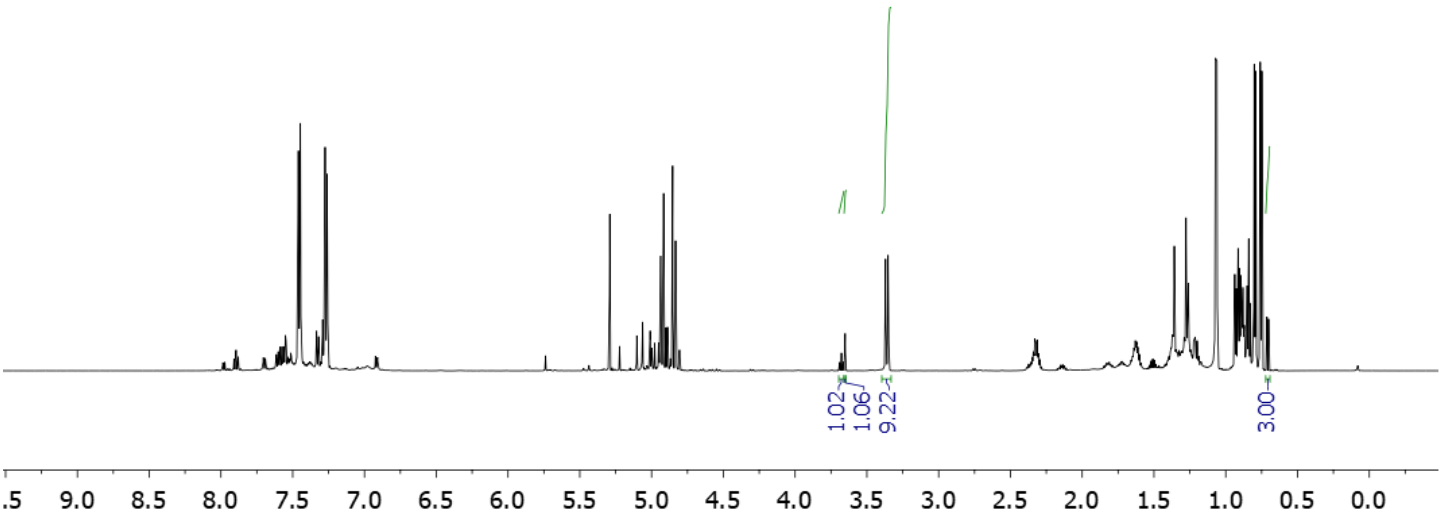


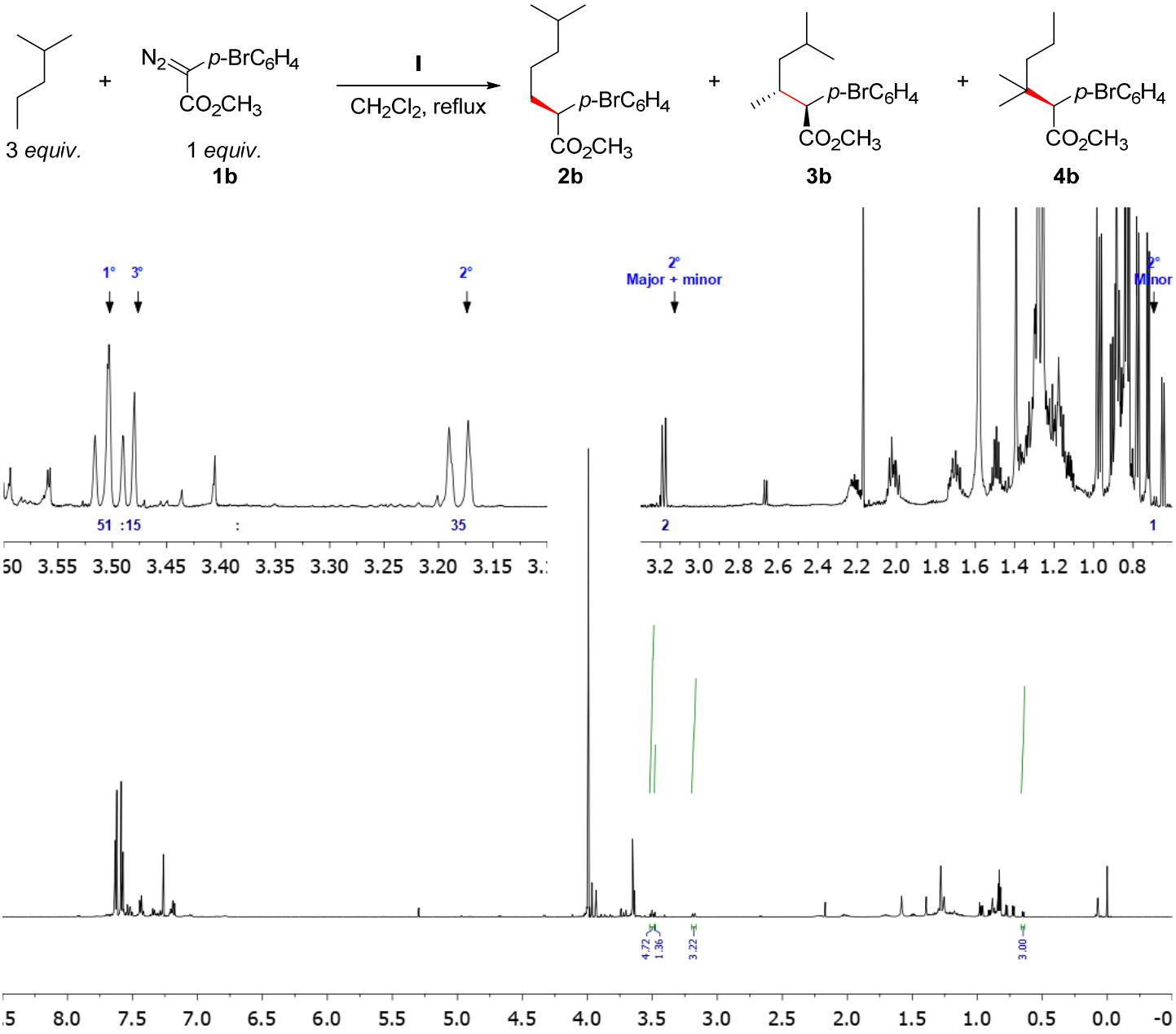


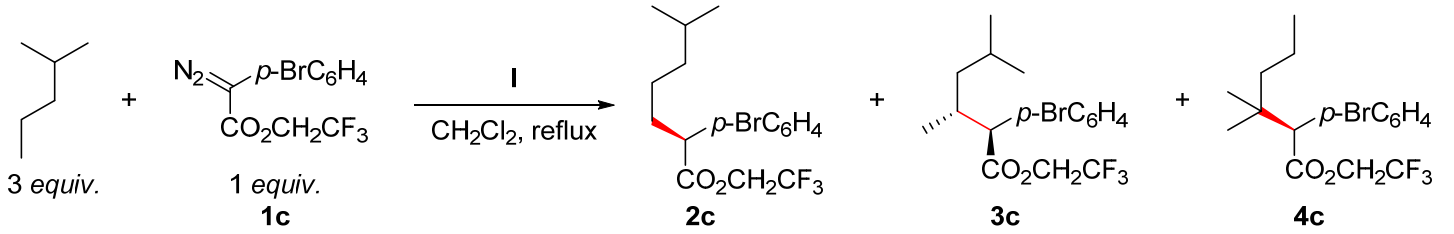

3 equiv.
1 equiv.
1d
C
CH2Cl2, reflux
2d
3d
4d

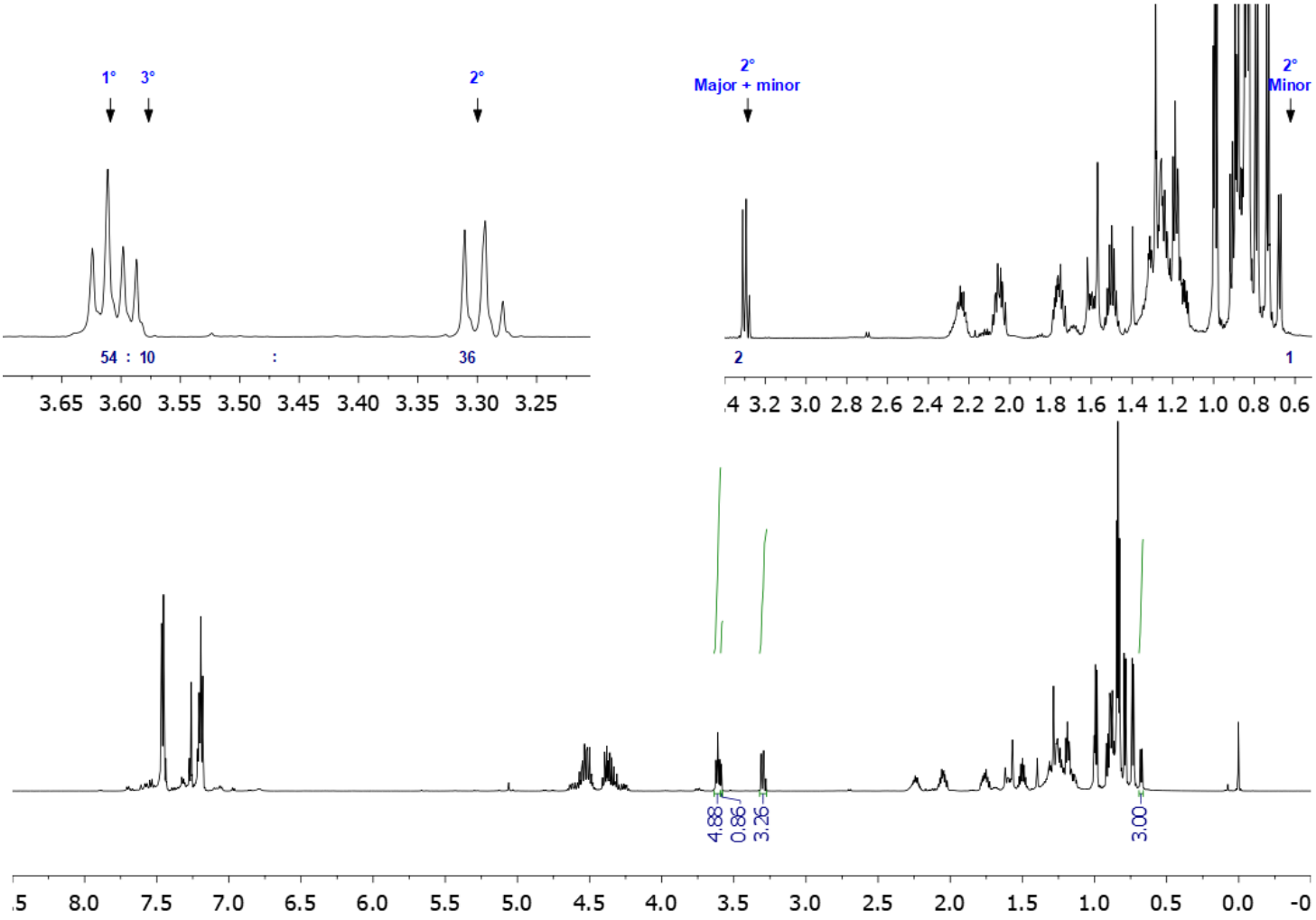

1°
3°
2°
9 : 9 : 82


2°
Major + minor
2°
Minor
8
1

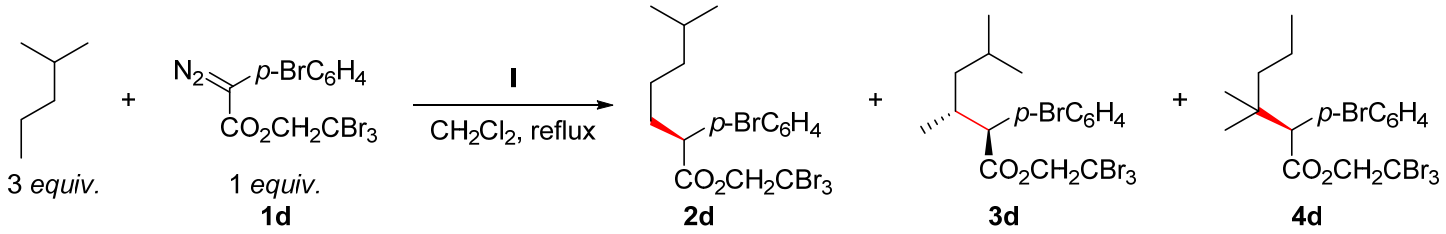

1.02
1.06
9.22
3.00

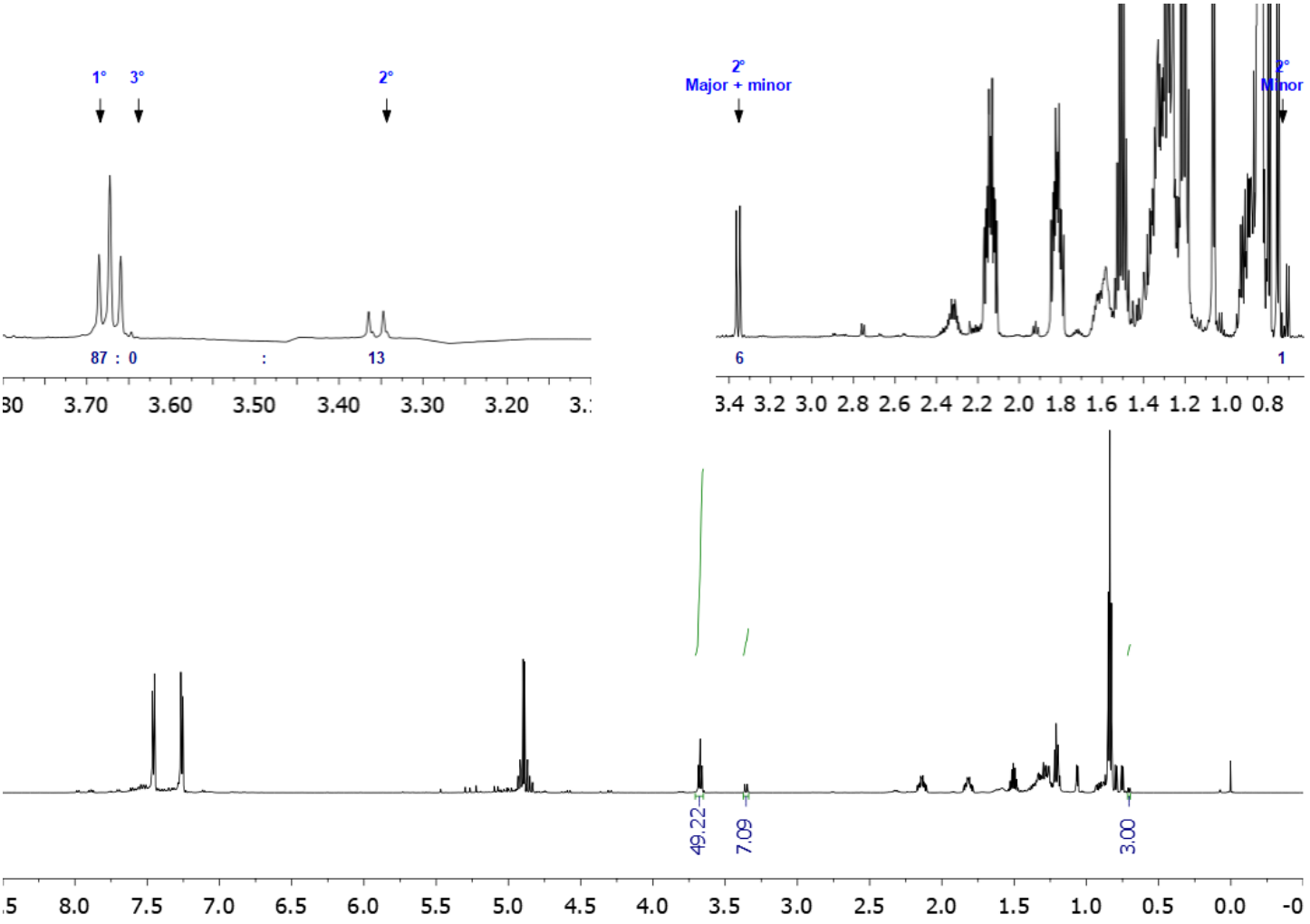

3 equiv.
1 equiv.
1b
I
CH2Cl2, reflux
2b
3b
4b
1° 3°
2°
51 :15
35
2°
Major + minor
2°
Minor
2
1
3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
4.72
1.36
3.22
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

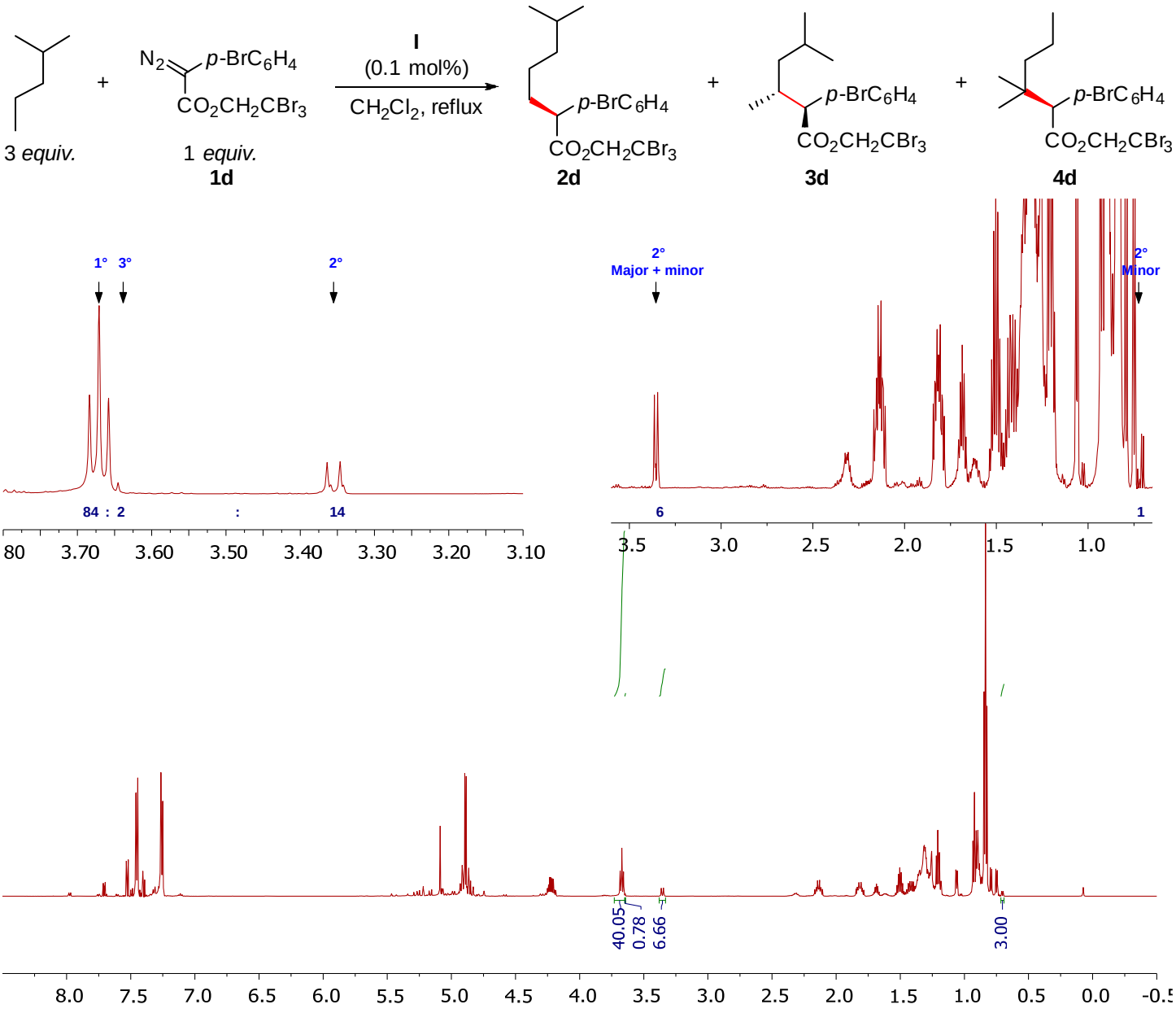

3 equiv.
1 equiv.
1c
I
CH2Cl2, reflux
2c
3c
4c


1°
3°
2°
54 : 10 : 36
2°
Major + minor
2°
Minor
2
1
3.65 3.60 3.55 3.50 3.45 3.40 3.35 3.30 3.25
4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6

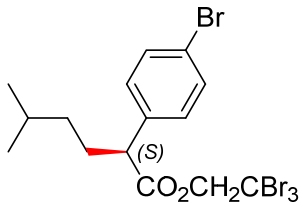
4.88
0.86
3.26
3.00
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

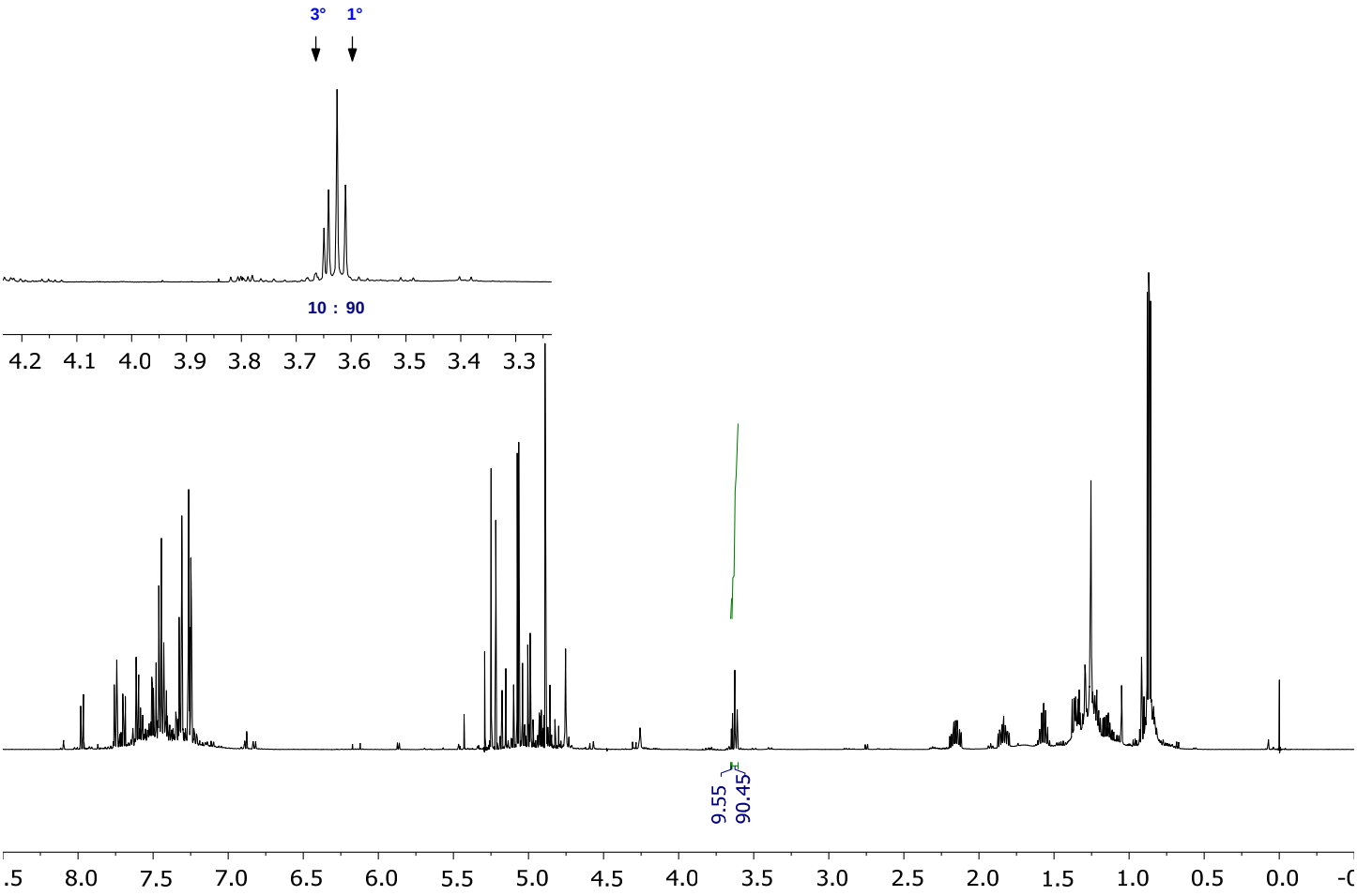

3 equiv.
1 equiv.
1d
I
CH2Cl2, reflux
2d
3d
4d

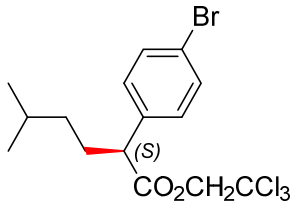

1°
3°
2°
87 : 0
:
13
2°
Major + minor
2°
Minor
6
1
49.22
7.09
3.00

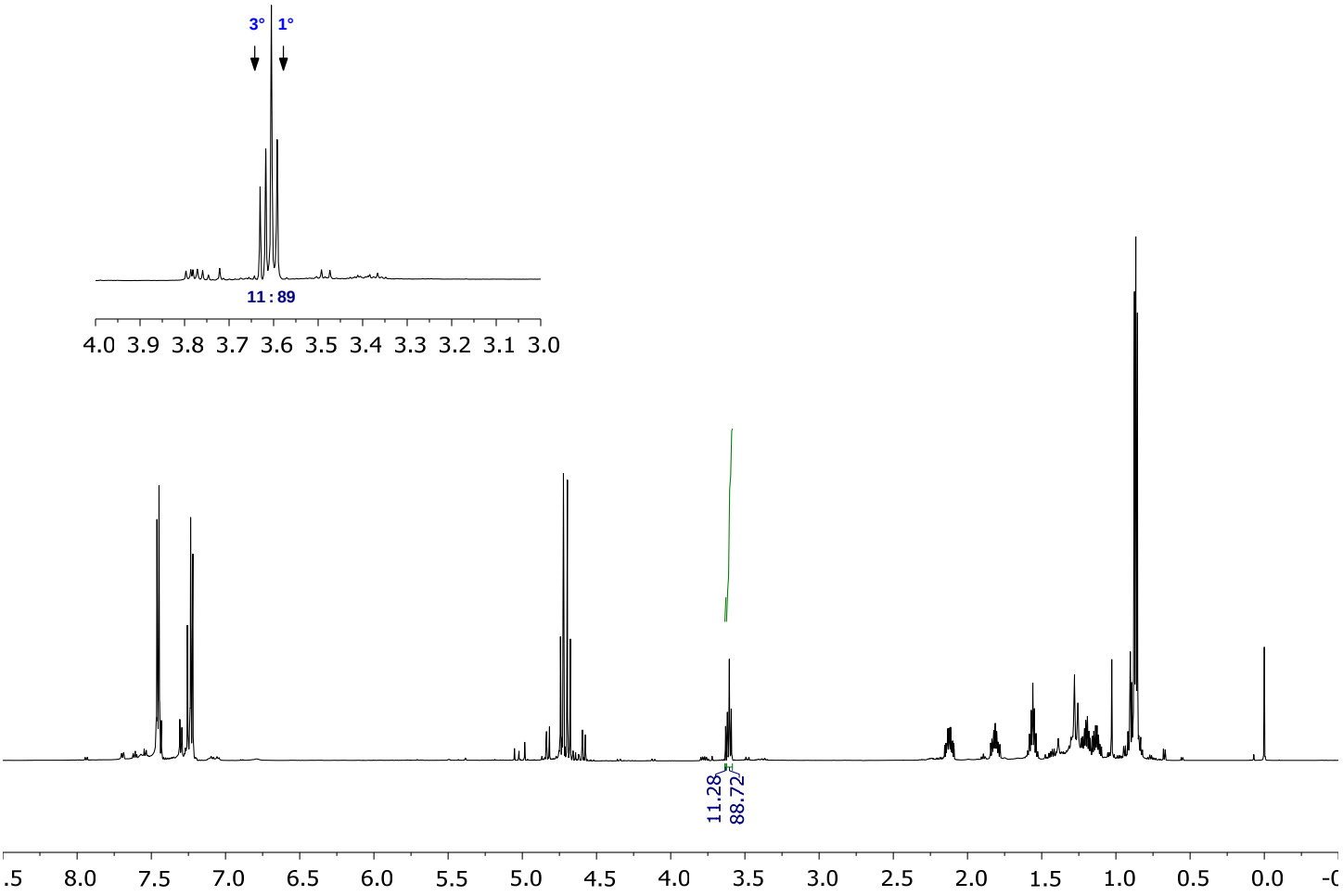

3 equiv.
1 equiv.
1d
I
(0.1 mol%)
CH2Cl2, reflux
2d
3d
4d
1° 3°
2°
84 : 2 : 14
2°
Major + minor
2°
Minor
6
1
40.05
0.78
6.66
3.00

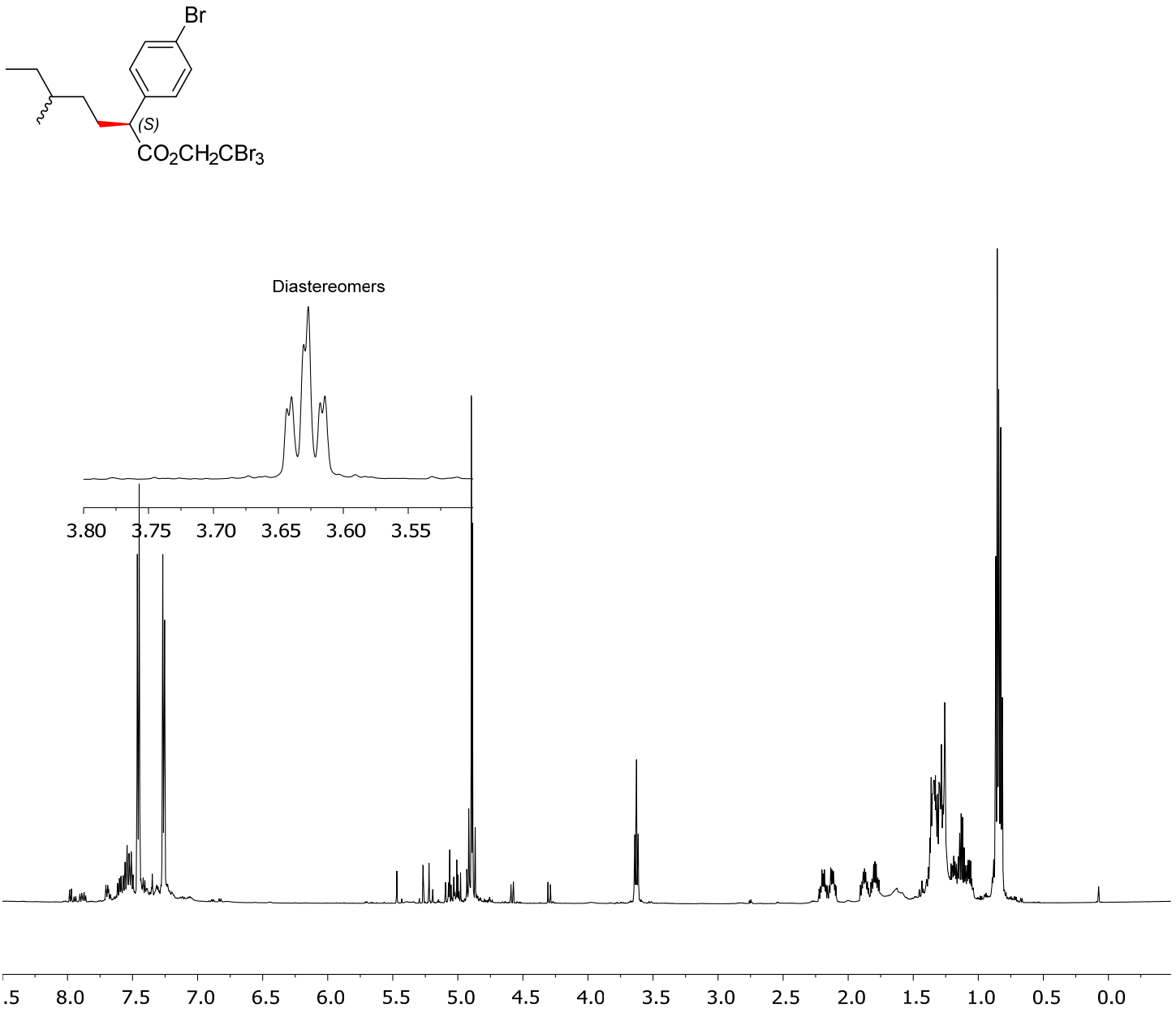
8.3 Crude ^{1}H NMR Spectra for C–H Functionalization Products **5-29**

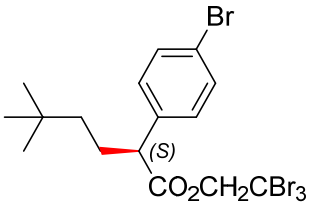


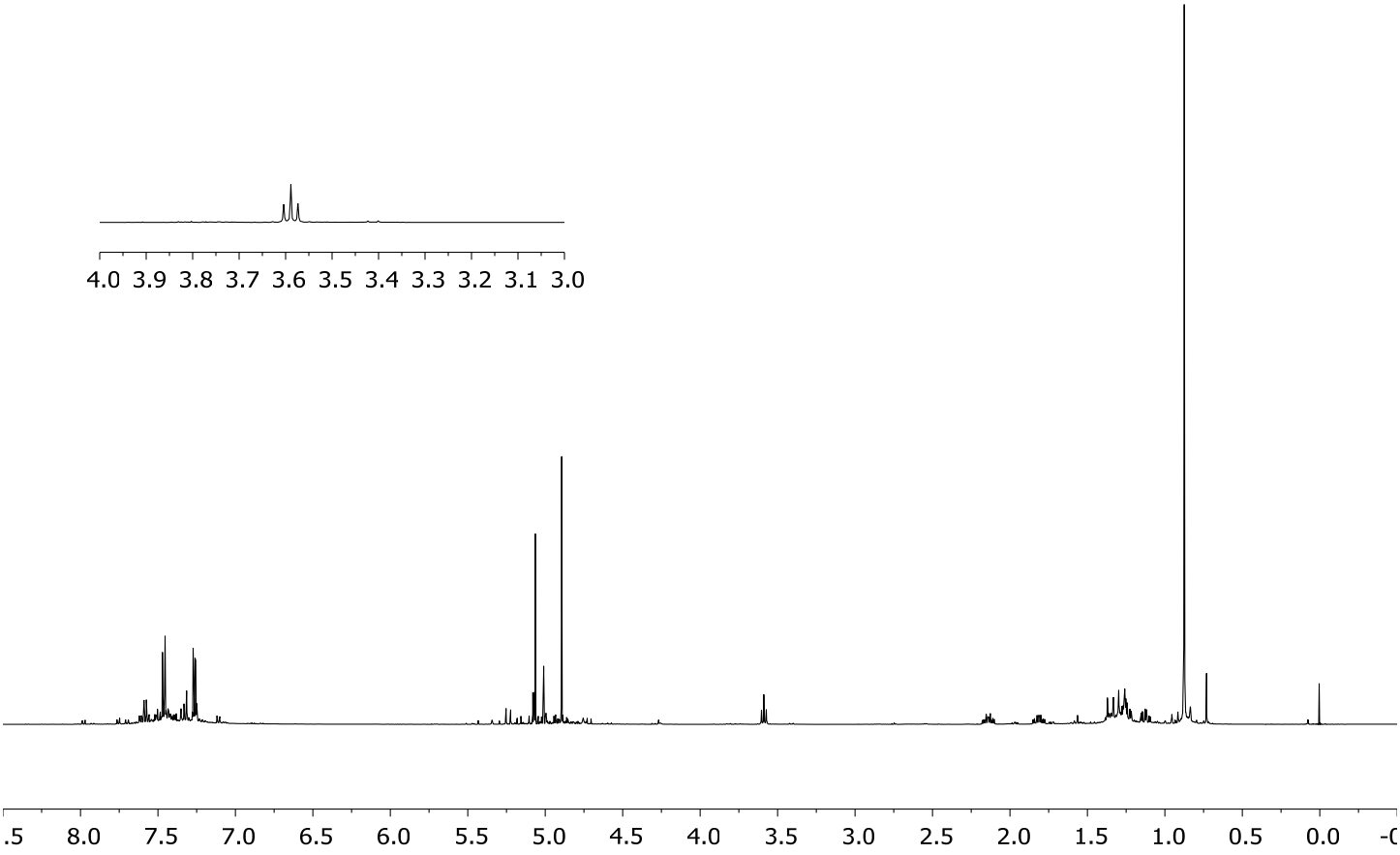


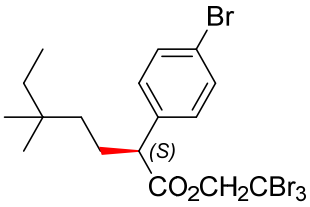

Br
(S)
CO2CH2CCl3

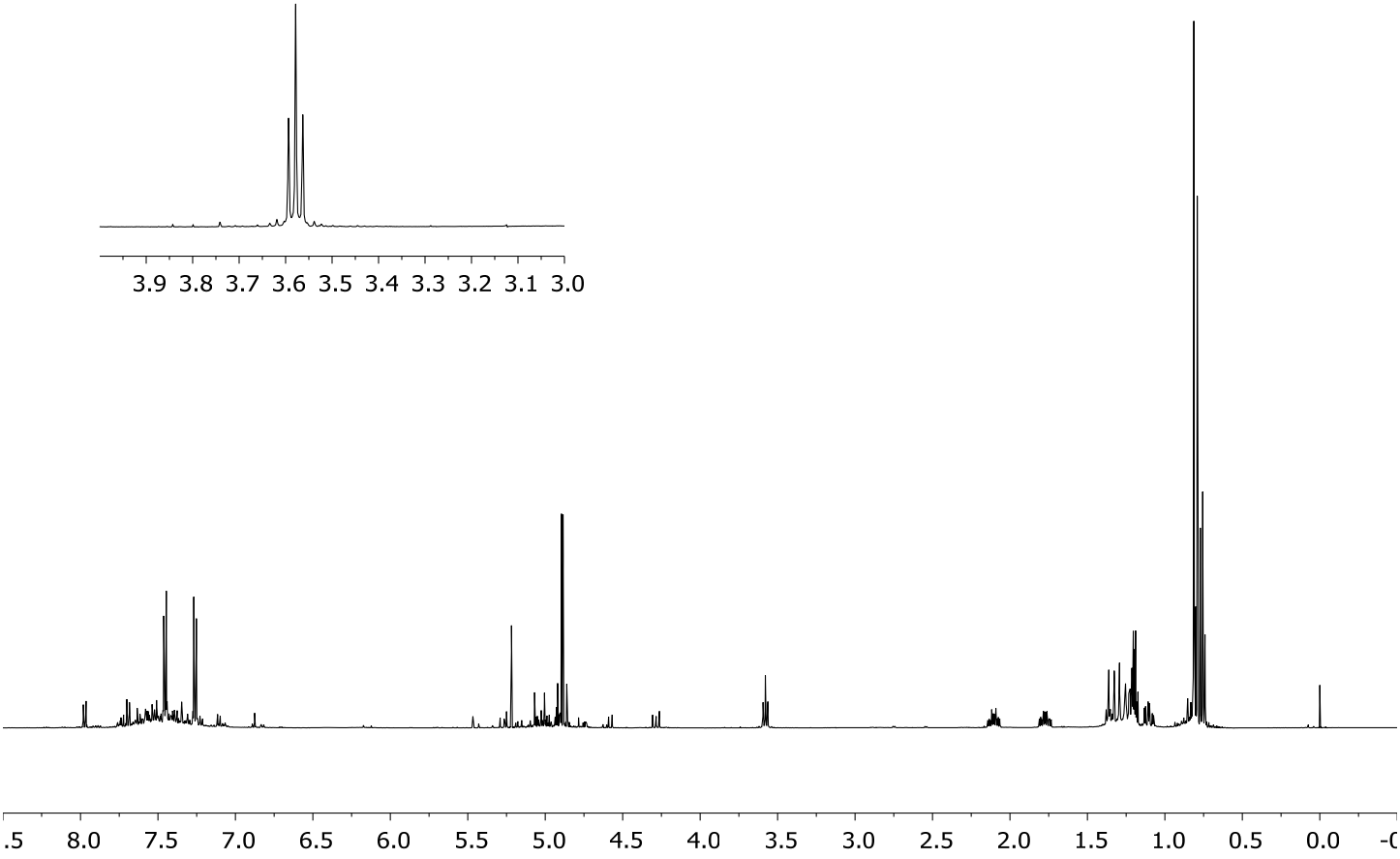

3°
1°
11 : 89
4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0
11.28
88.72
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

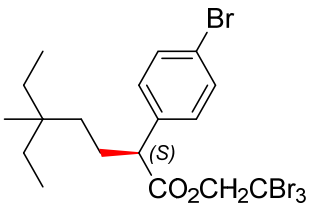

Br
(S)
CO2CH2CBr3
Diastereomers
3.80
3.75
3.70
3.65
3.60
3.55
.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

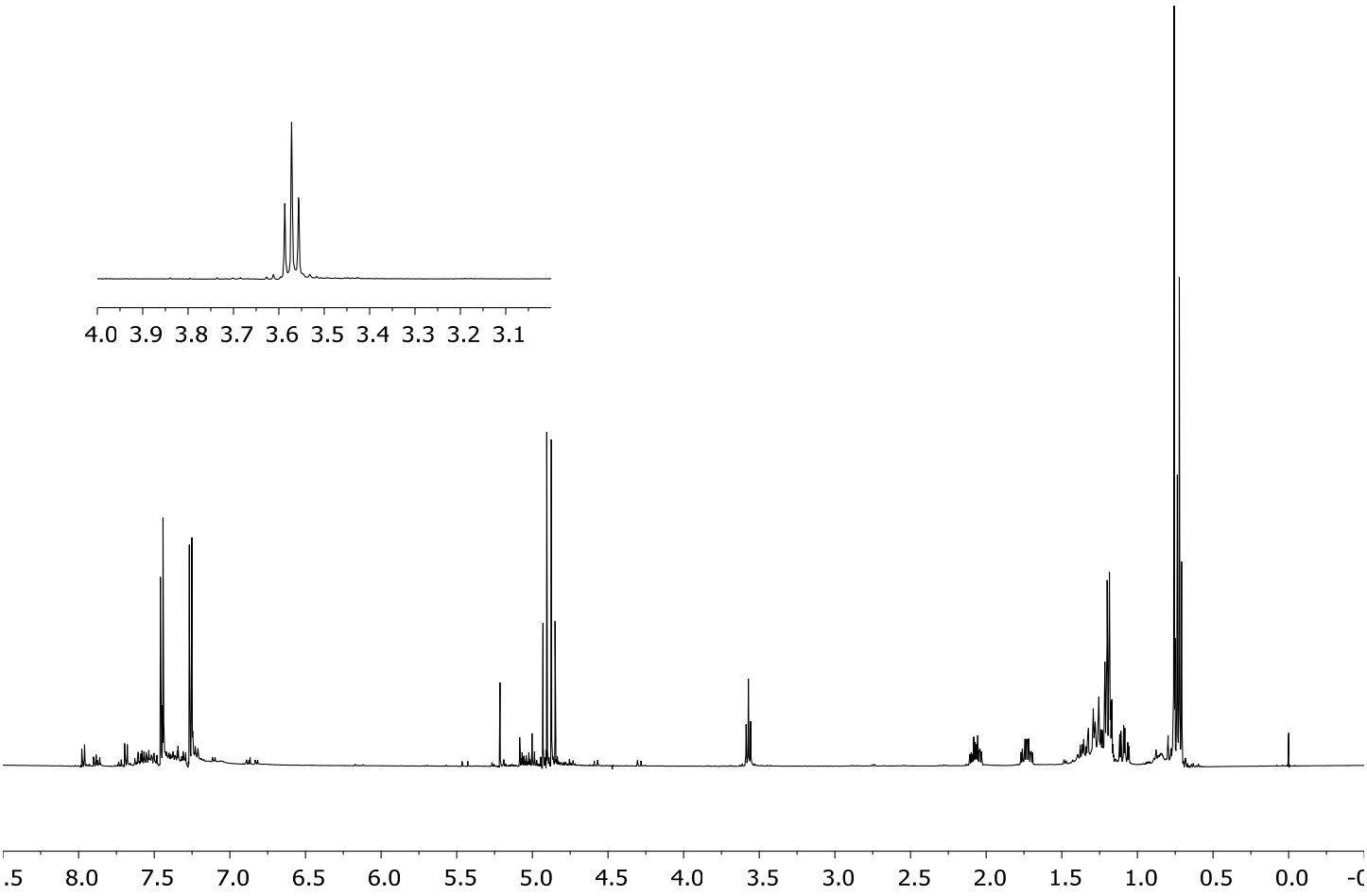

Br
(S)
CO2CH2CBr3

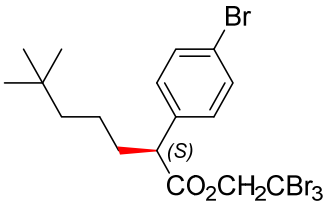

4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

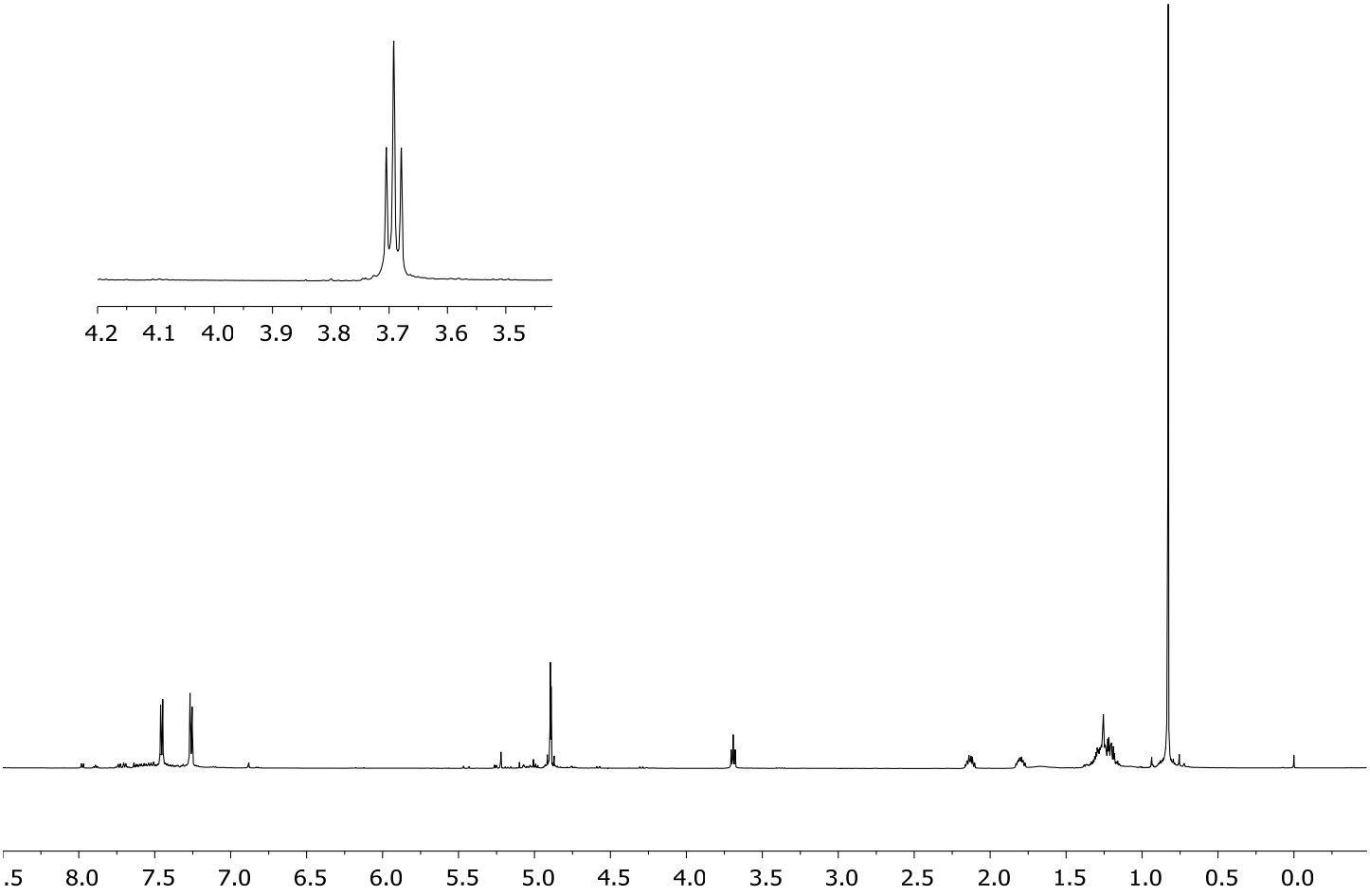

Br
(S)
CO2CH2CBr3

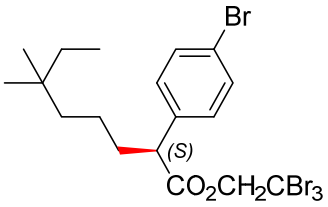

3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

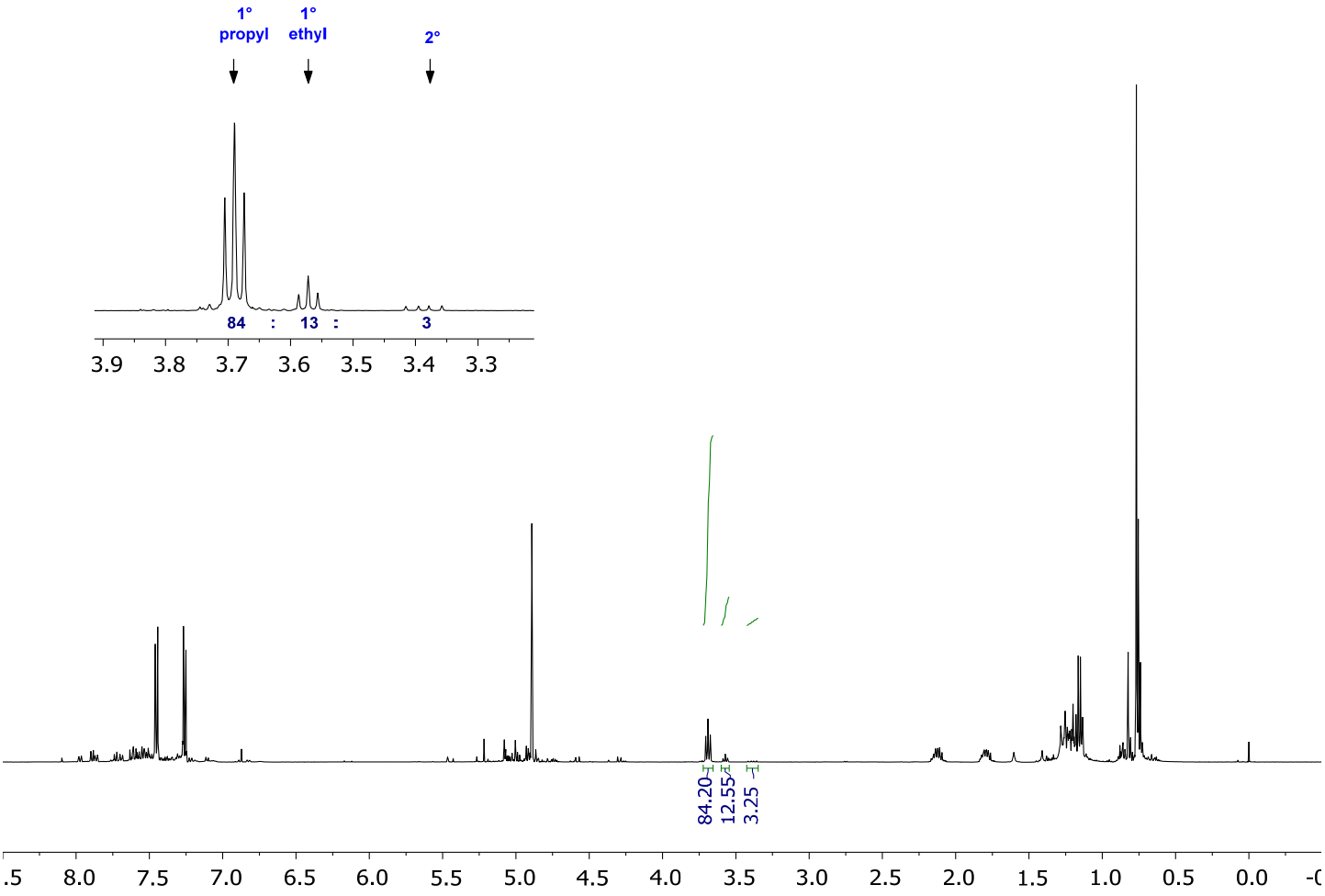

Br
(S)
CO2CH2CBr3

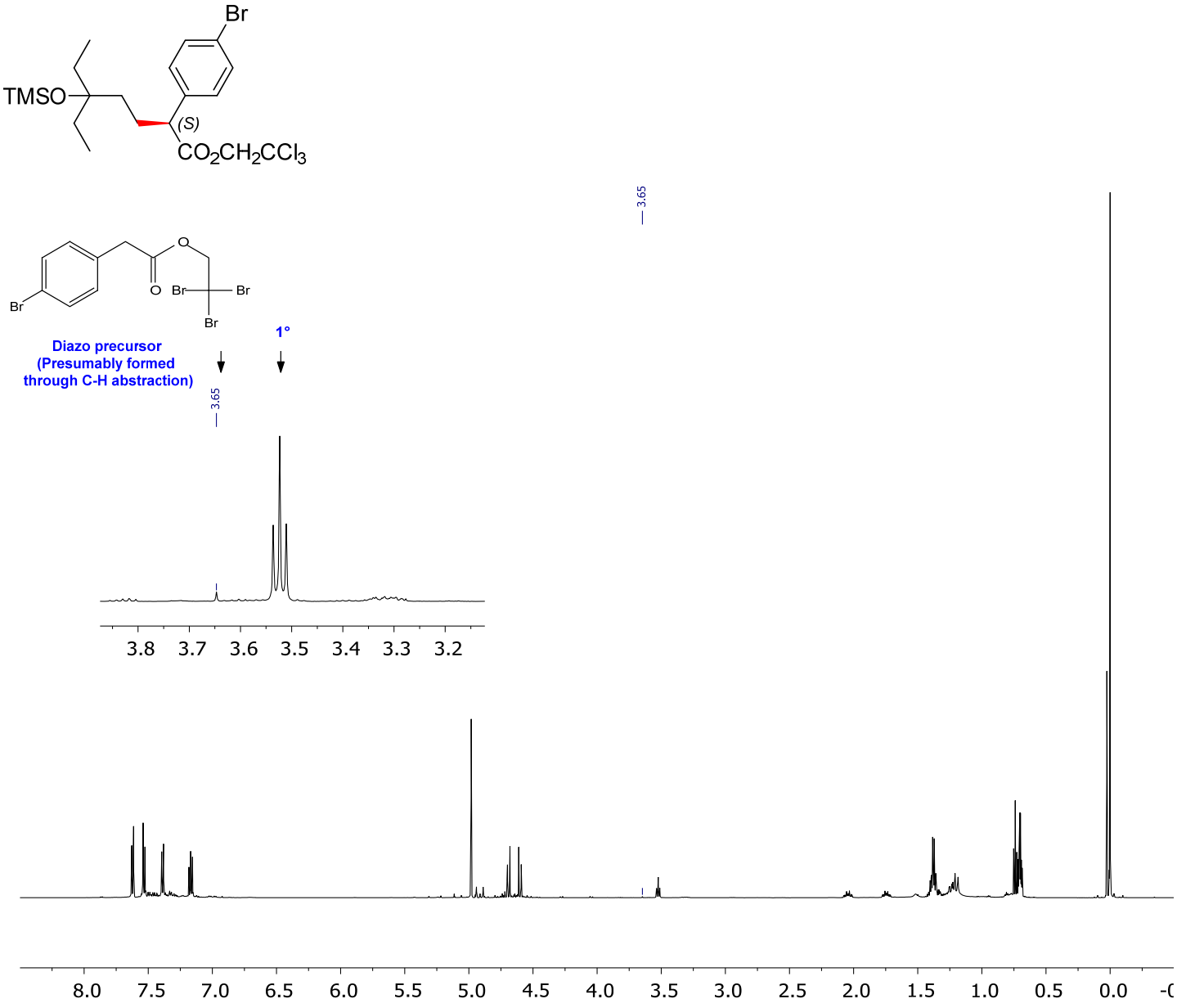

4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

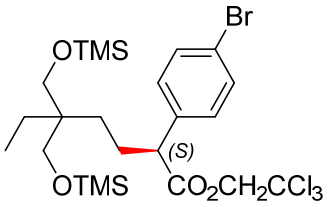

Br
(S)
CO2CH2CBr3

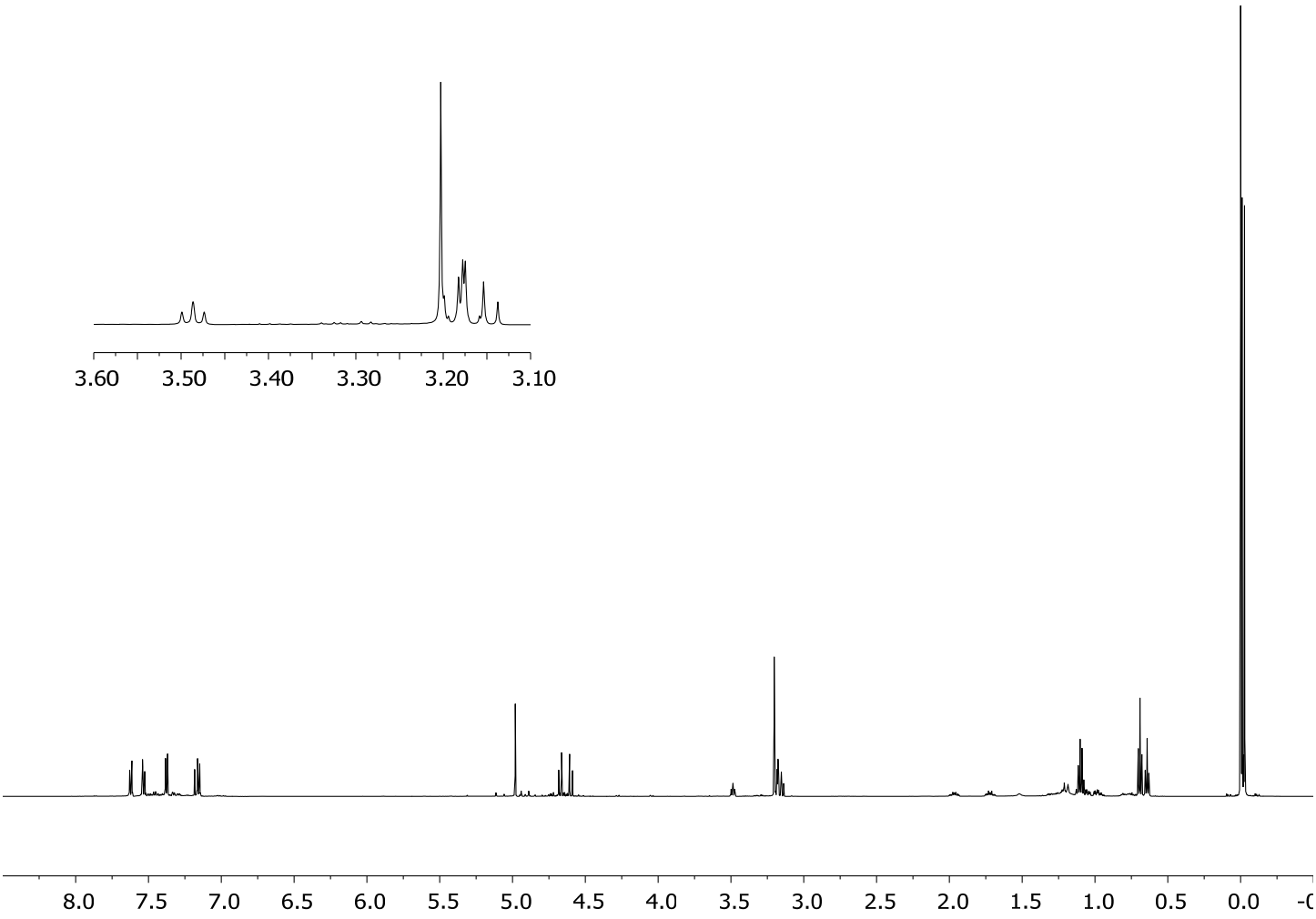

4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

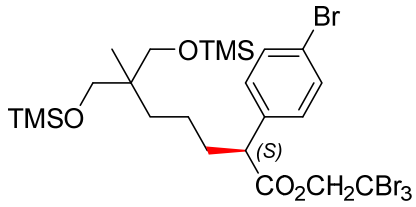

Br
(S)
CO2CH2CBr3

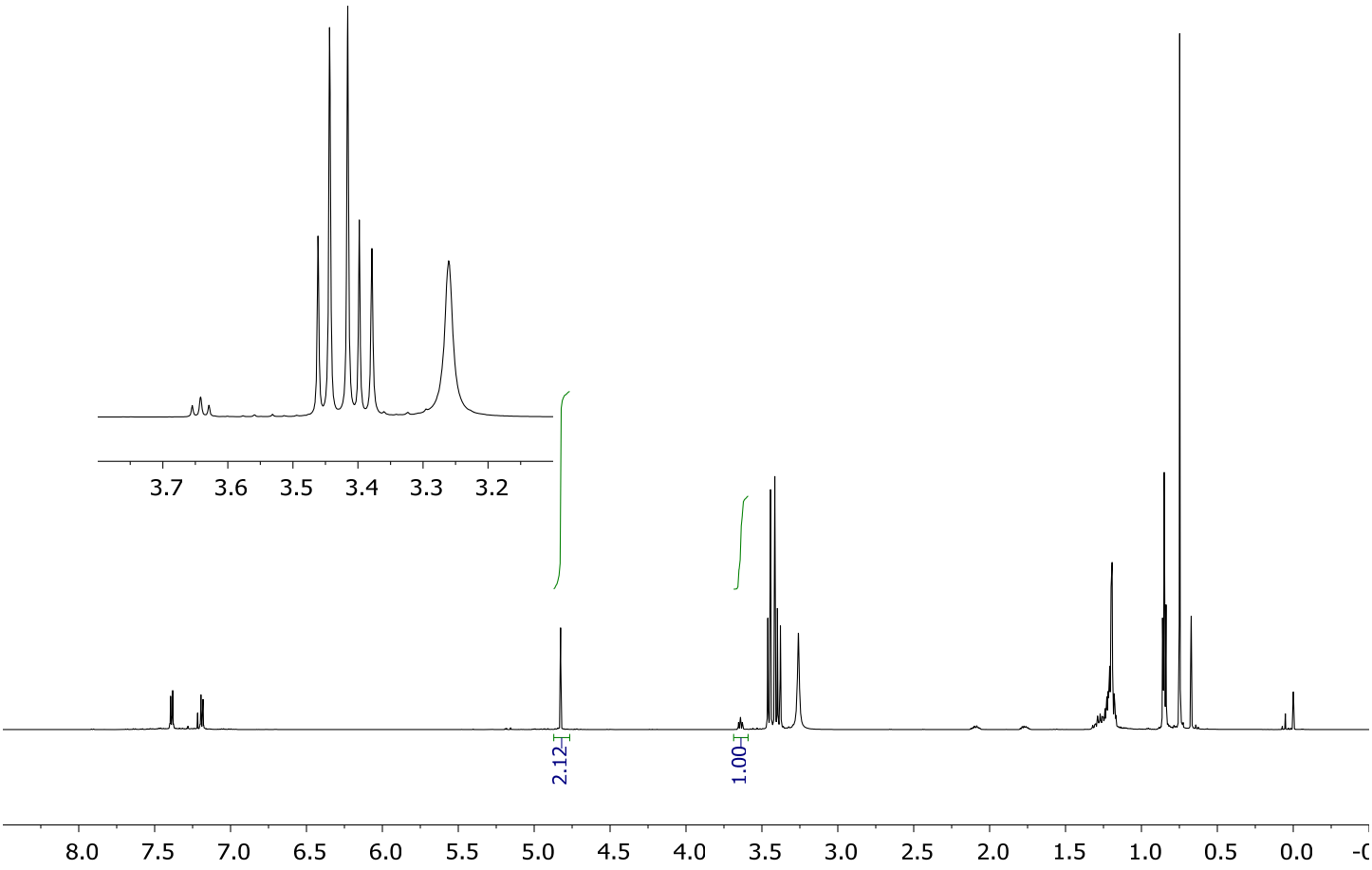

1°
propyl
1°
ethyl
2°
84 : 13 : 3
3.9 3.8 3.7 3.6 3.5 3.4 3.3
84.20
12.55
3.25
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

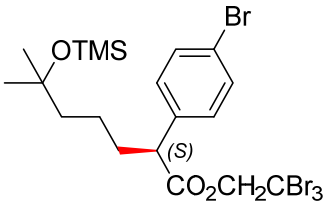

Br
TMSO
(S)
CO2CH2CCl3
3.65
O
O
Br
Br
Br
Br
Diazo precursor
(Presumably formed
through C-H abstraction)
1°
3.65
3.8
3.7
3.6
3.5
3.4
3.3
3.2
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

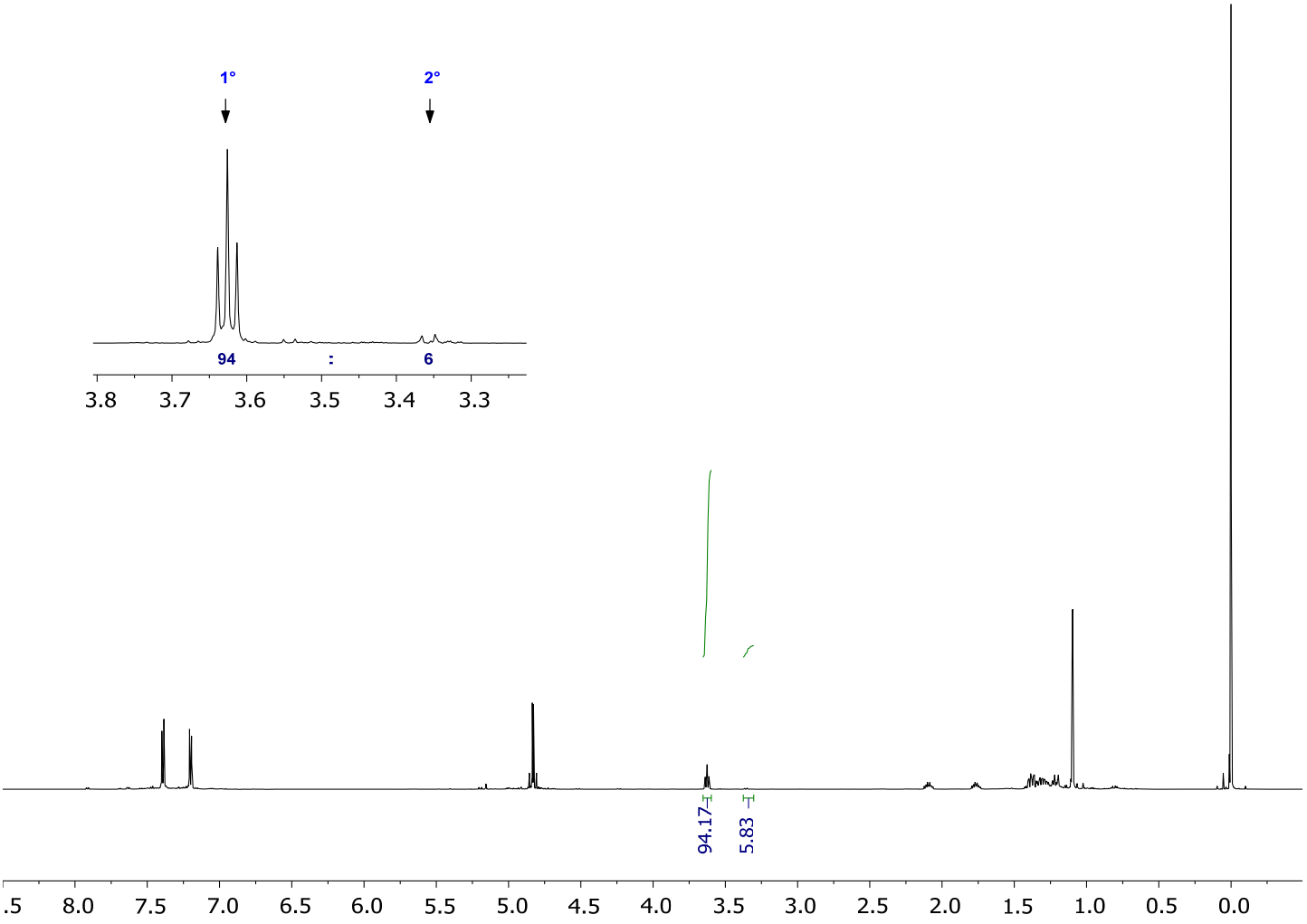

Br
OTMS
(S)
OTMS
CO2CH2CCl3

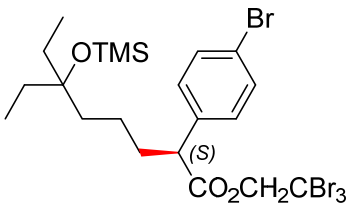

3.60
3.50
3.40
3.30
3.20
3.10
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

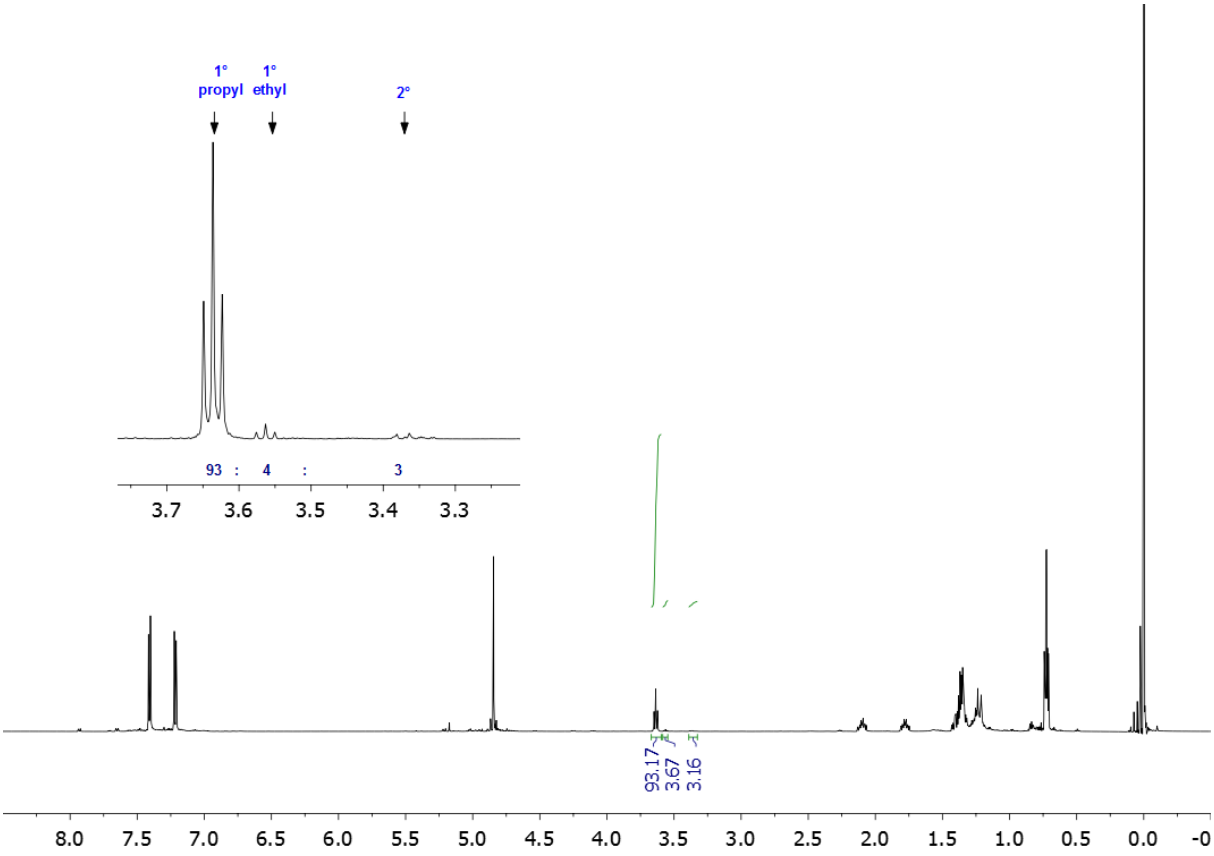

Br
OTMS
TMSO
(S)
CO2CH2CBr3

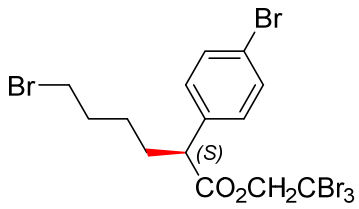

3.7
3.6
3.5
3.4
3.3
3.2
2.12
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

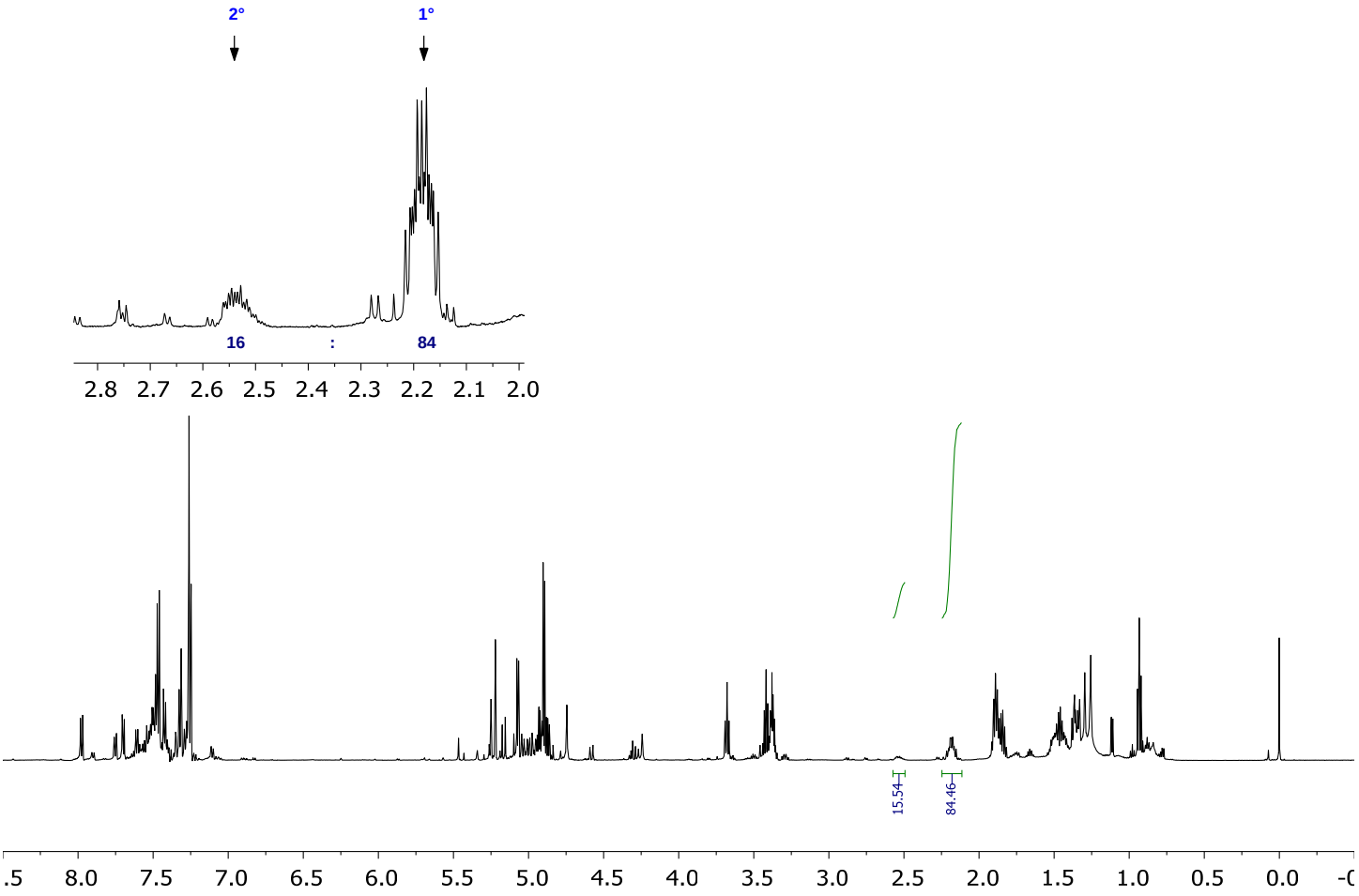

Br
OTMS
(S)
CO2CH2CBr3

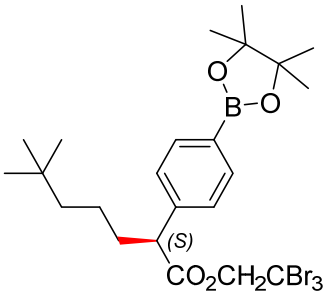

1°
2°
94 : 6
3.8 3.7 3.6 3.5 3.4 3.3
94.17
5.83
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

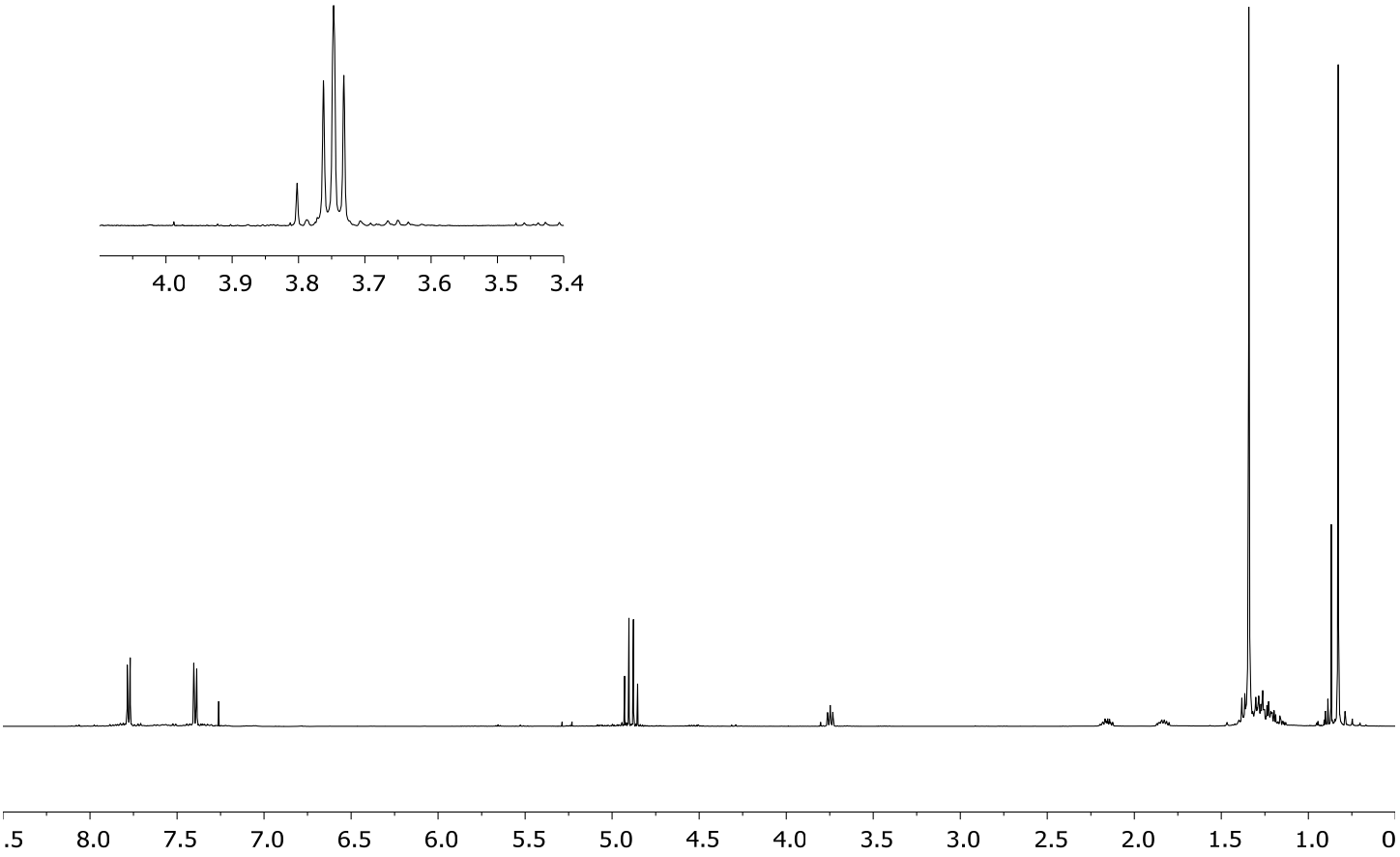

Br
OTMS
(S)
CO2CH2CBr3

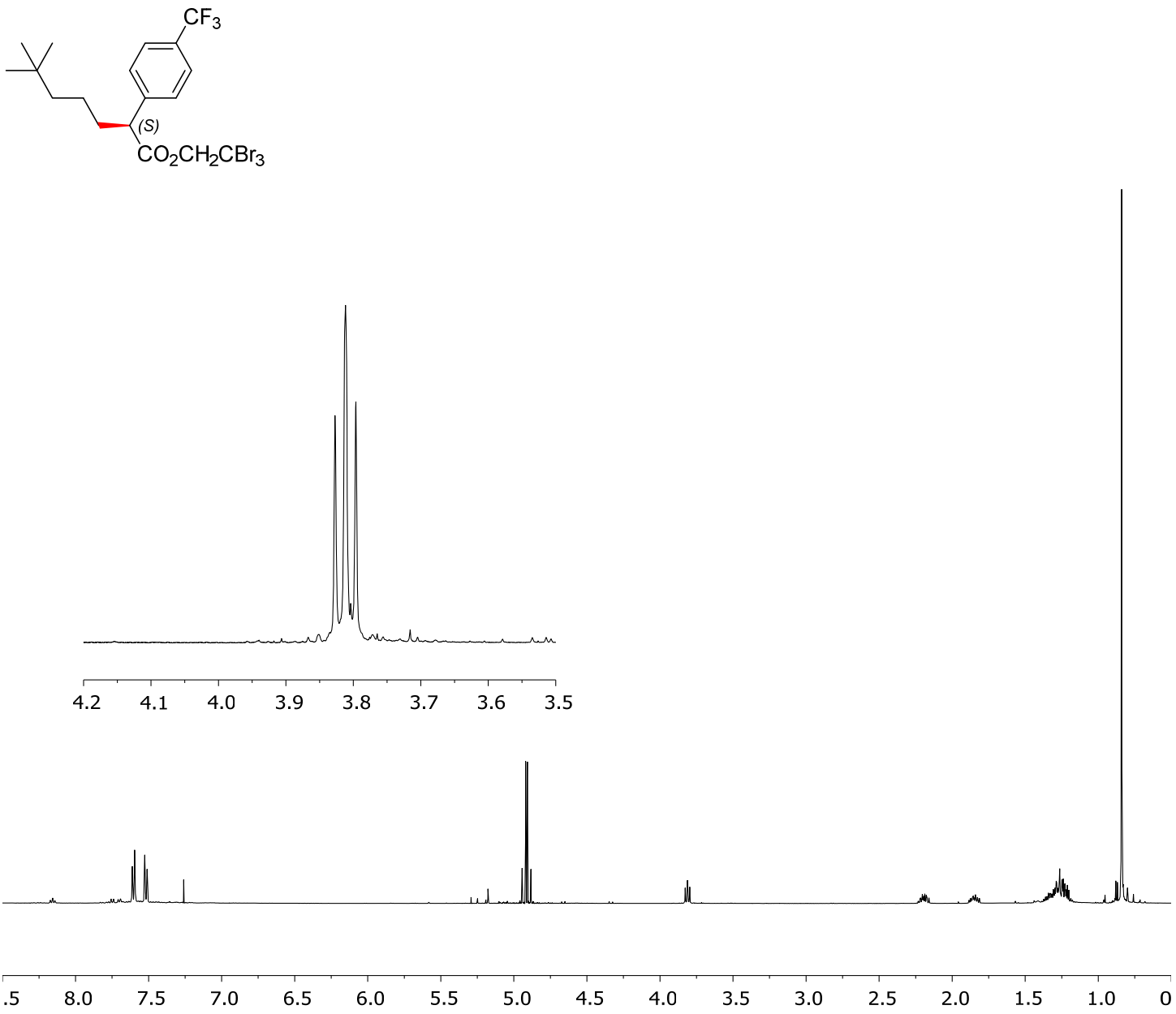

1°
propyl
1°
ethyl
2°
93 : 4 : 3
3.7
3.6
3.5
3.4
3.3
93.17
3.67
3.16
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0

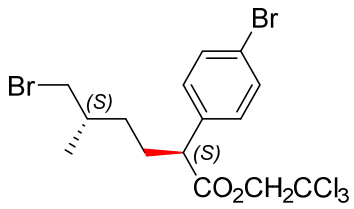

Br
Br
(S)
CO2CH2CBr3

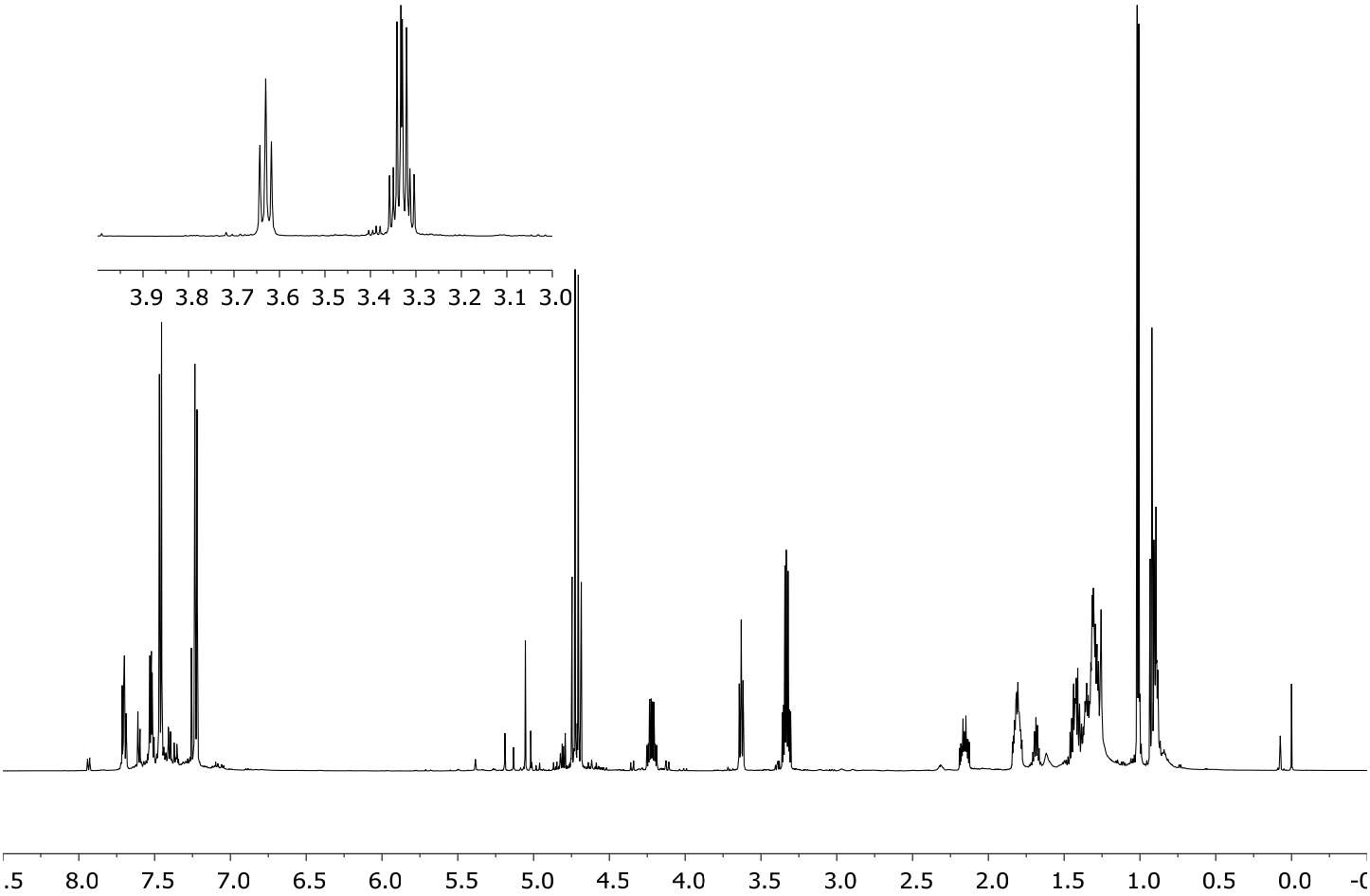

2°
1°
16 : 84
2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0
15.54
84.46
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

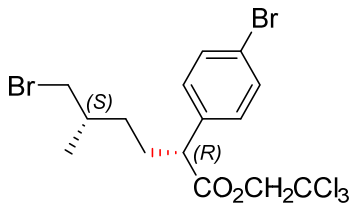

O
B–O
(S)
CO2CH2CBr3

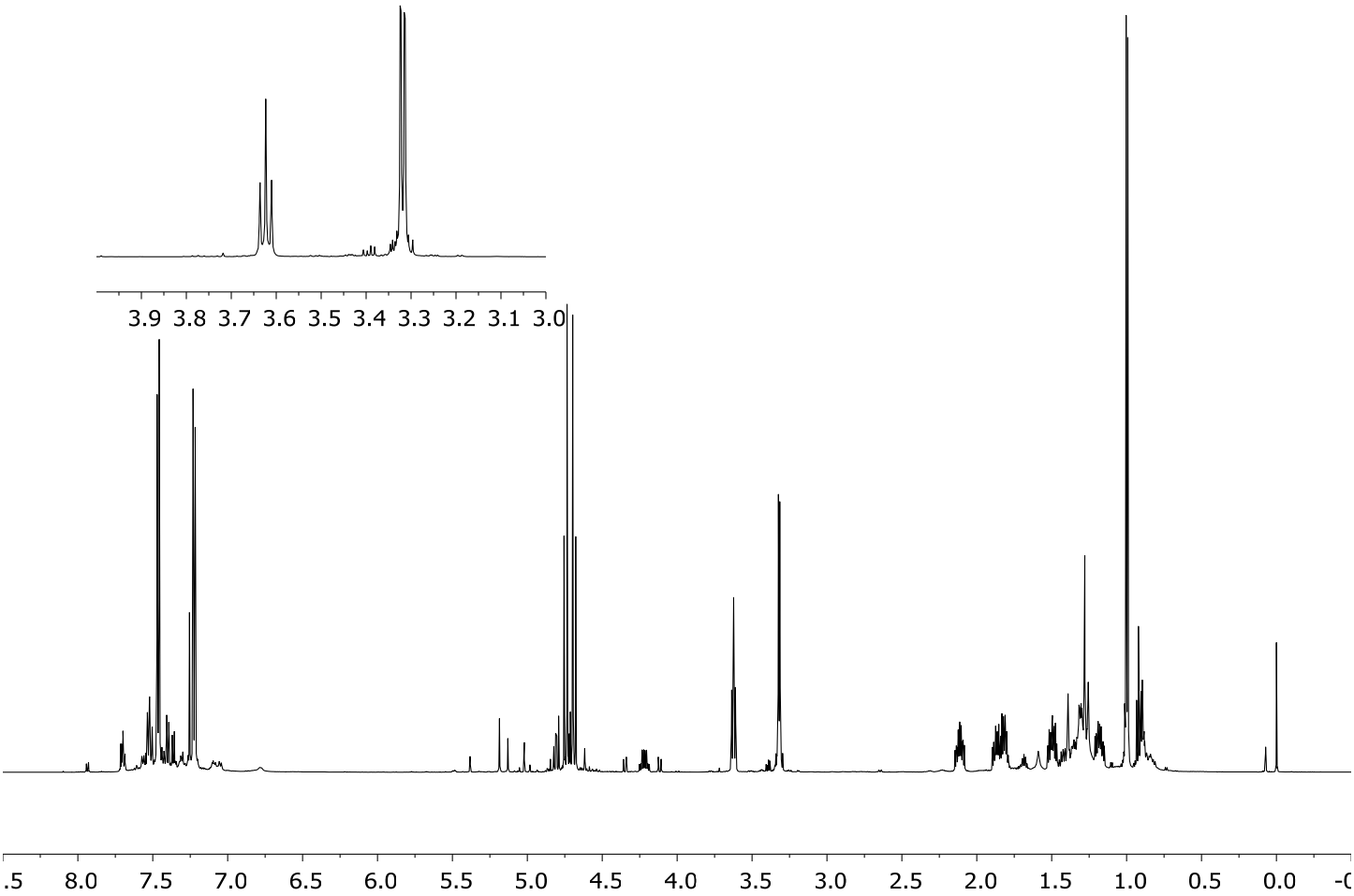

4.0
3.9
3.8
3.7
3.6
3.5
3.4
.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0

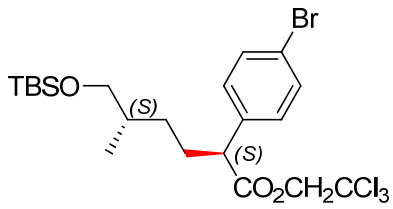

CF3
(S)
CO2CH2CBr3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0

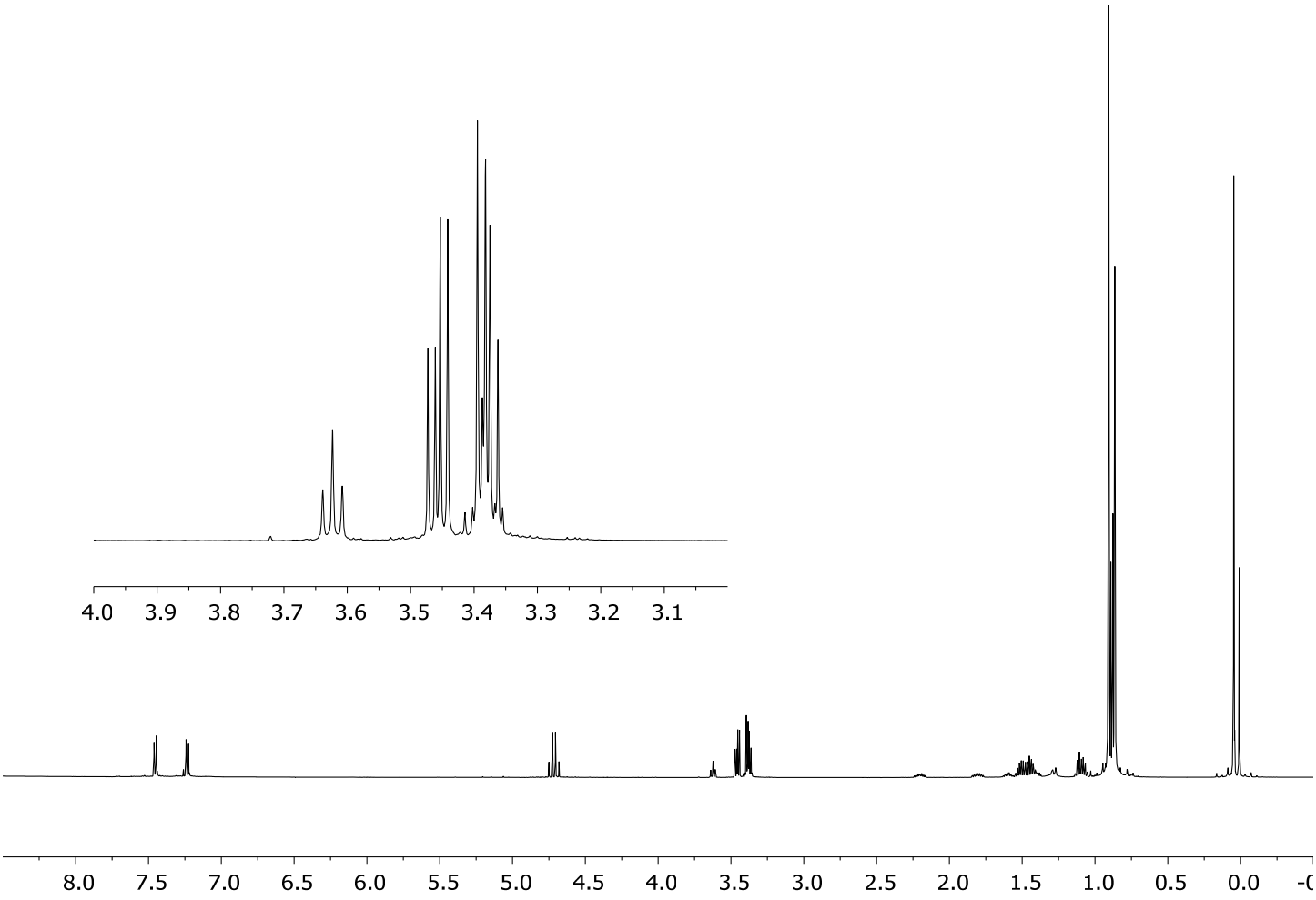

Br
Br
(S)
(S)
CO2CH2CCl3

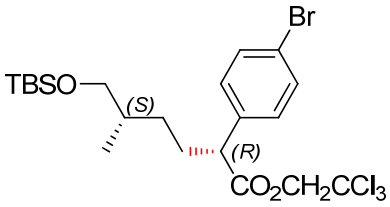

3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

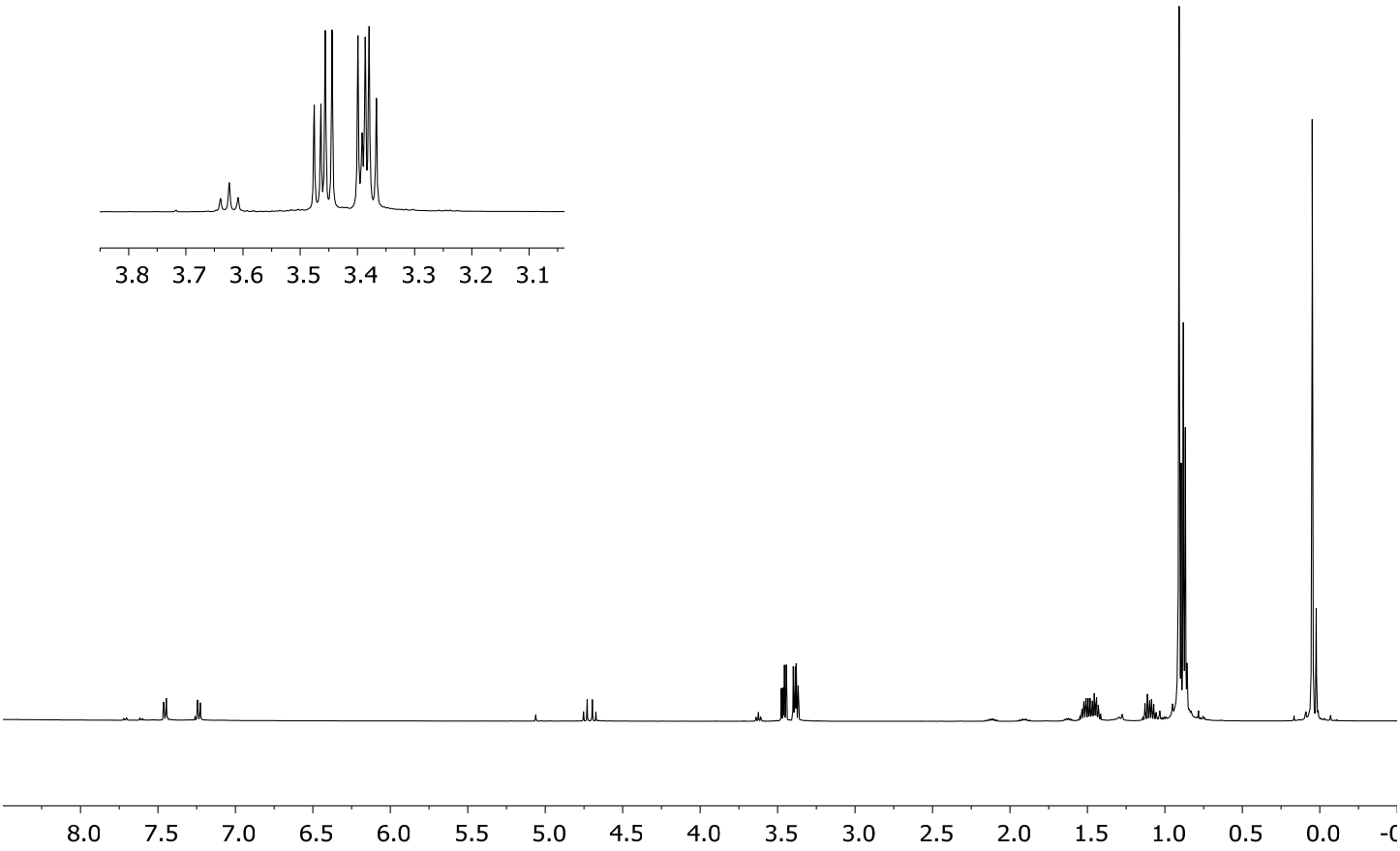

Br
Br
(S)
(R)
CO2CH2CCl3

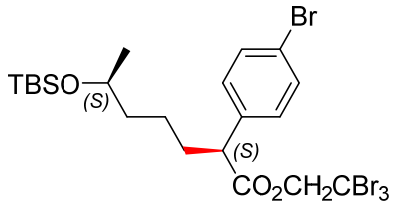

3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

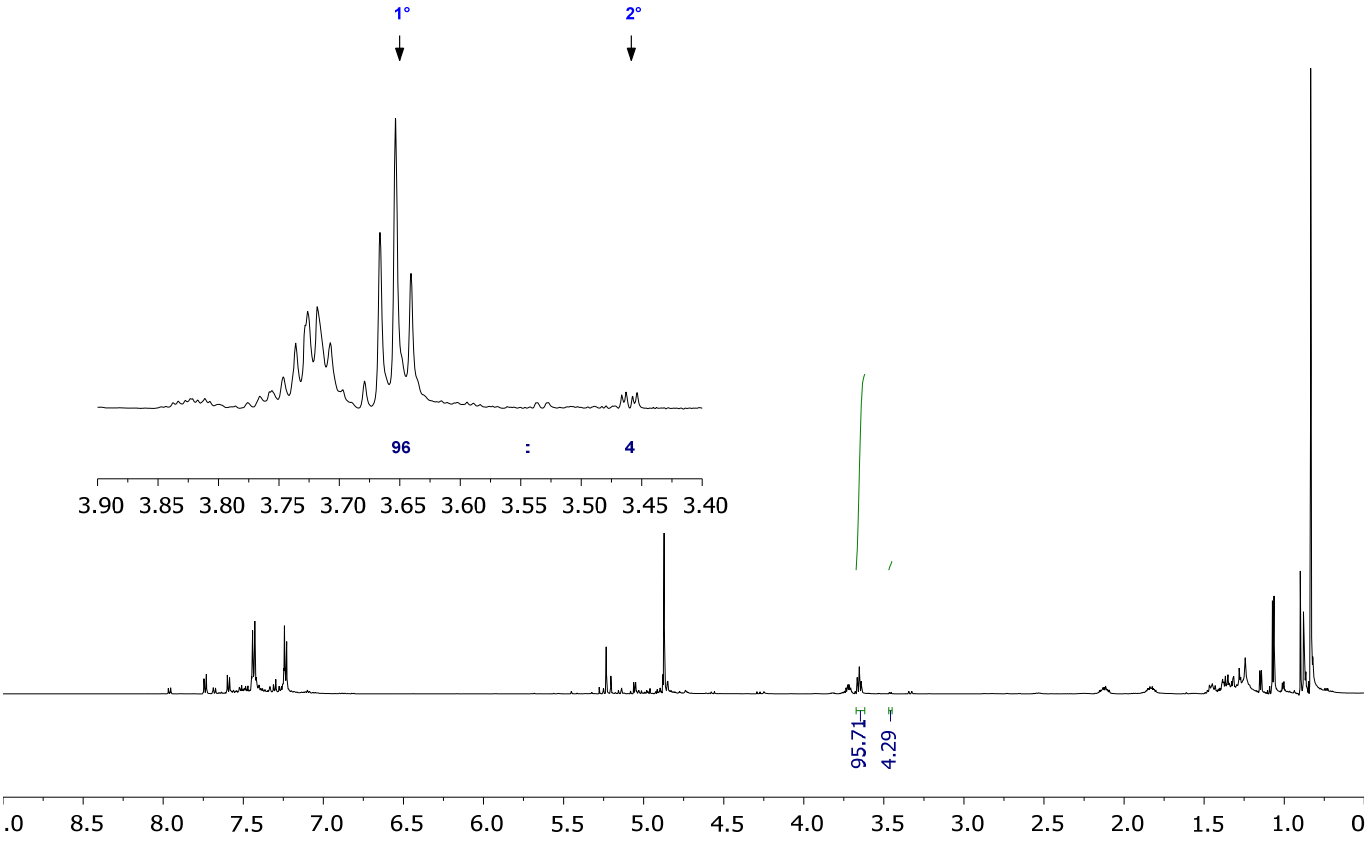

Br
TBSO
(S)
(S)
CO2CH2CCl3

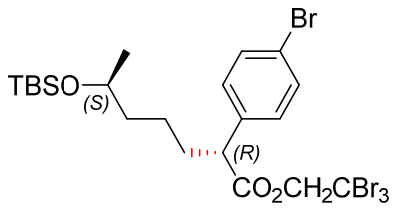

4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

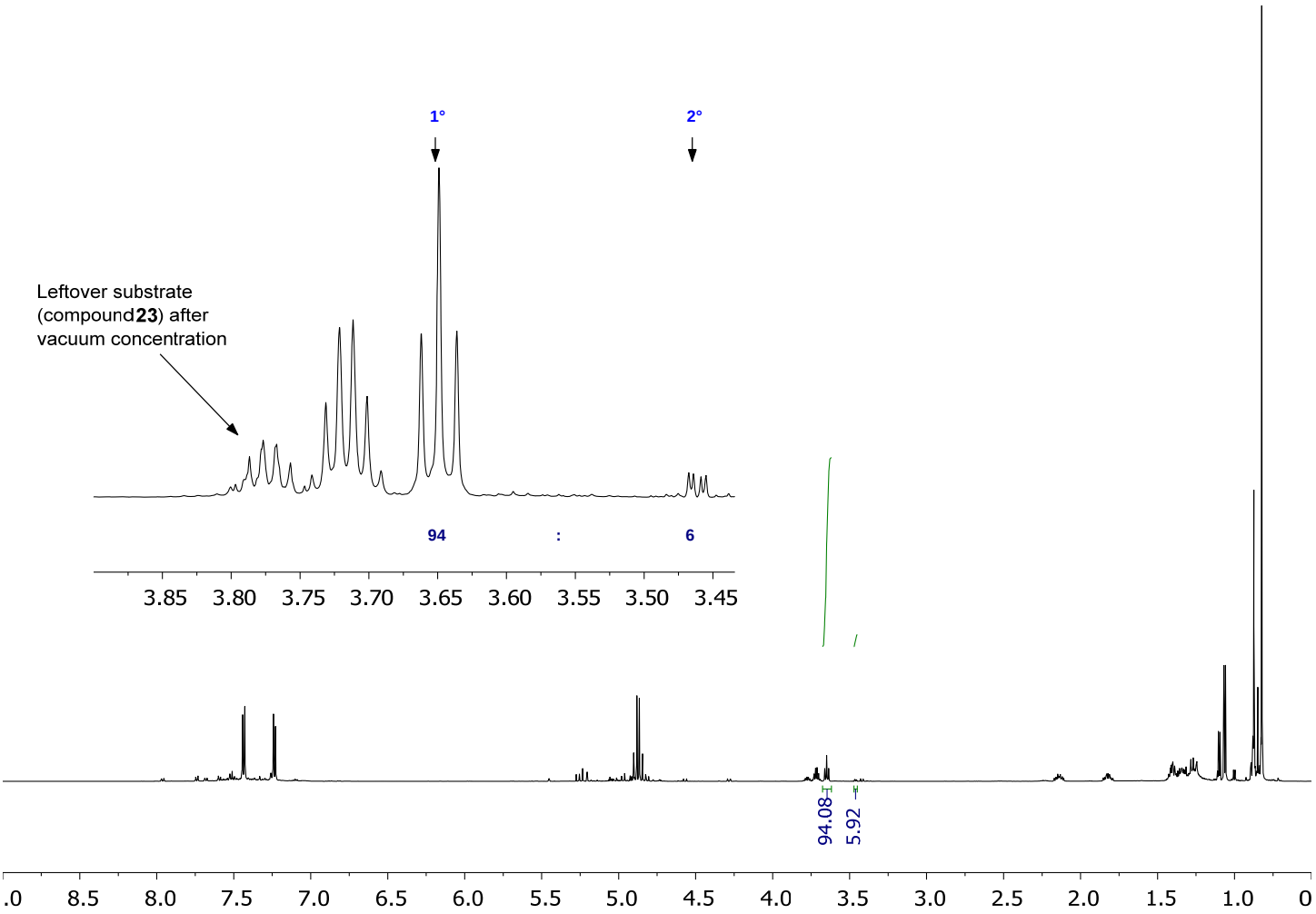

Br
TBSO
(S)
(R)
CO2CH2CCl3

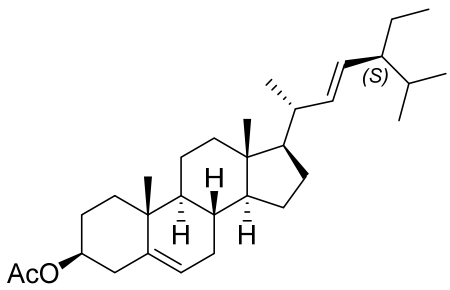

3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

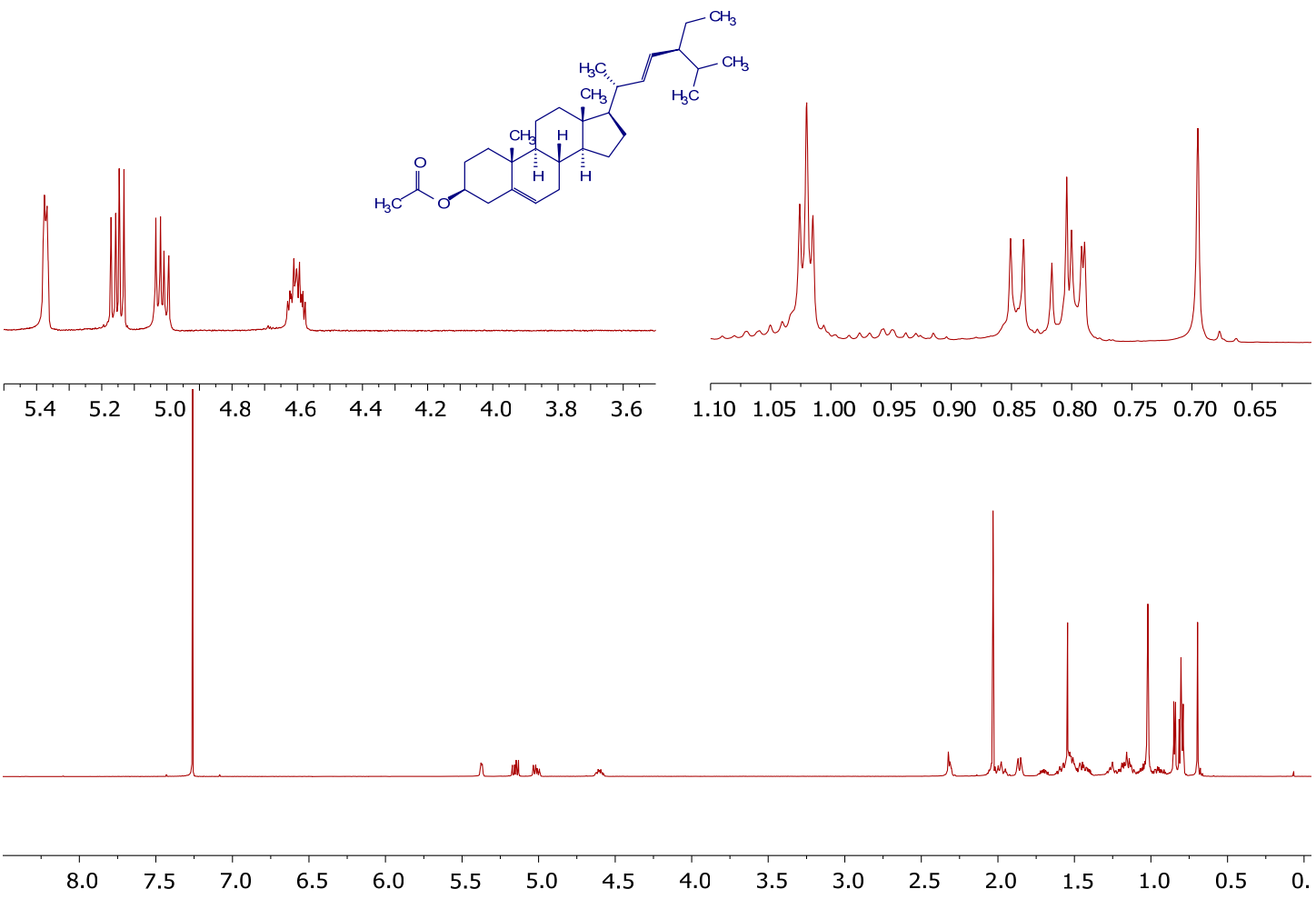

Br
TBSO
(S)
(S)
CO2CH2CBr3

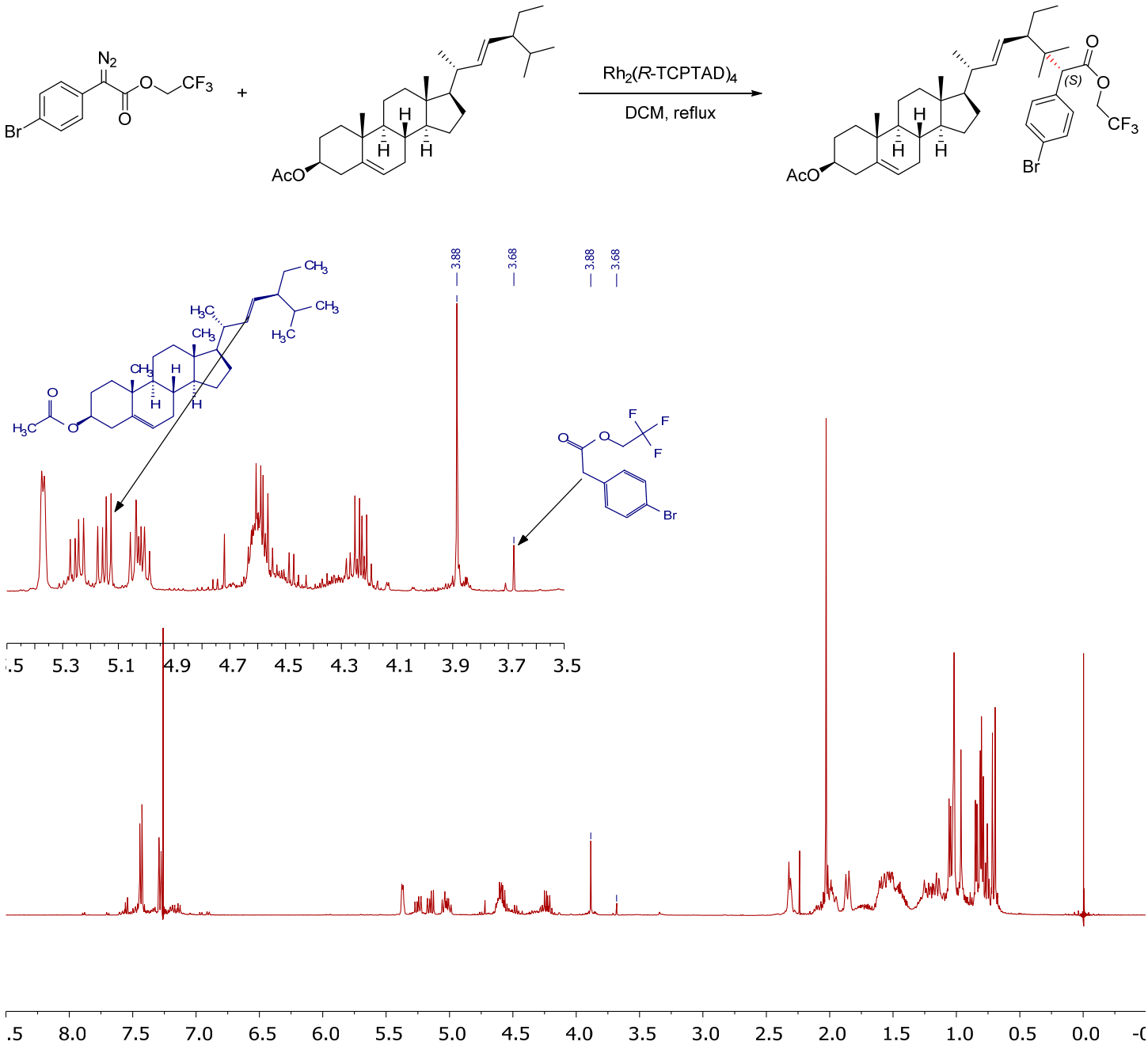

1°
2°
96 : 4
3.90 3.85 3.80 3.75 3.70 3.65 3.60 3.55 3.50 3.45 3.40
95.71
4.29
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0

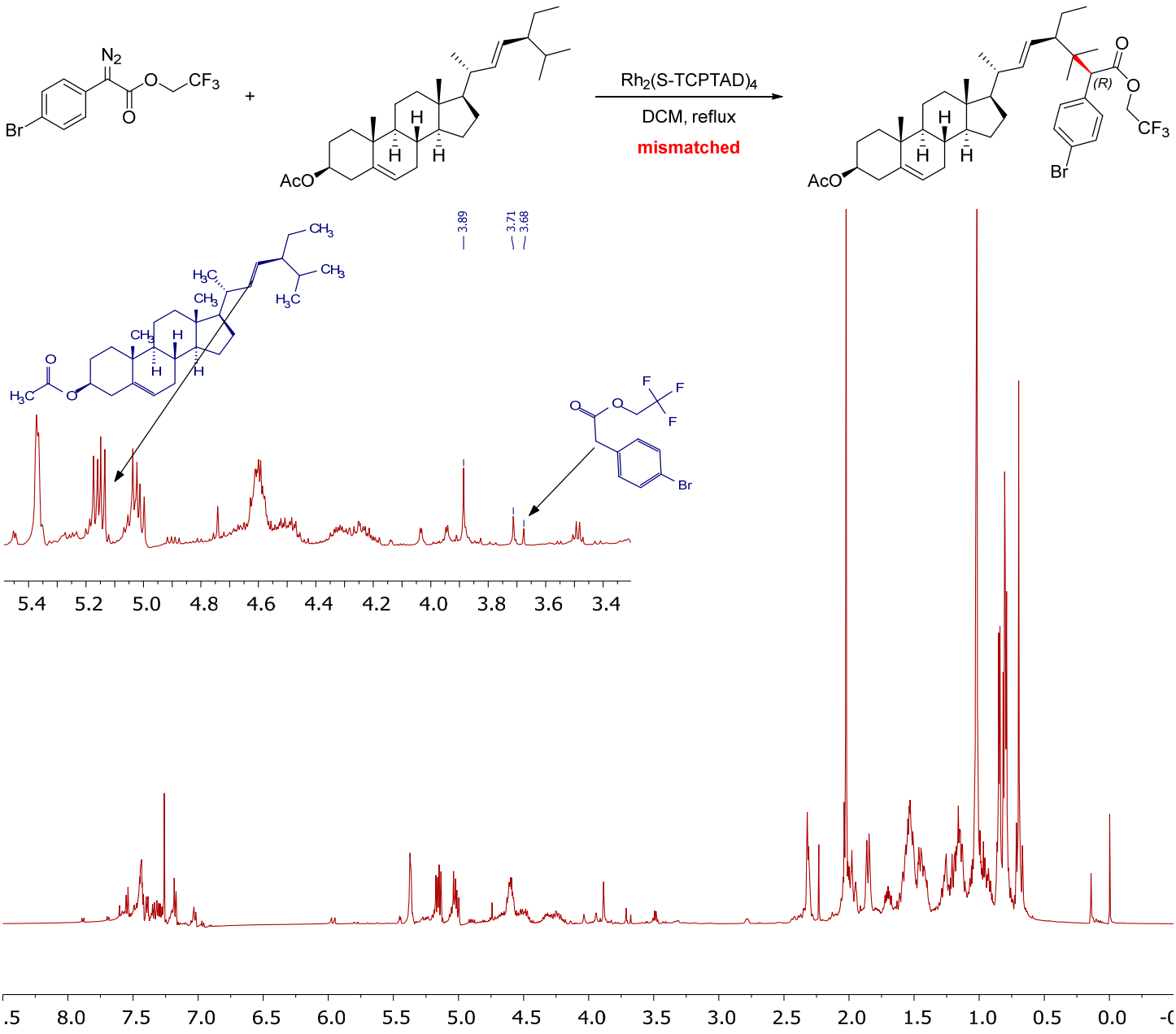

Br
TBSO
(S)
(R)
CO2CH2CBr3

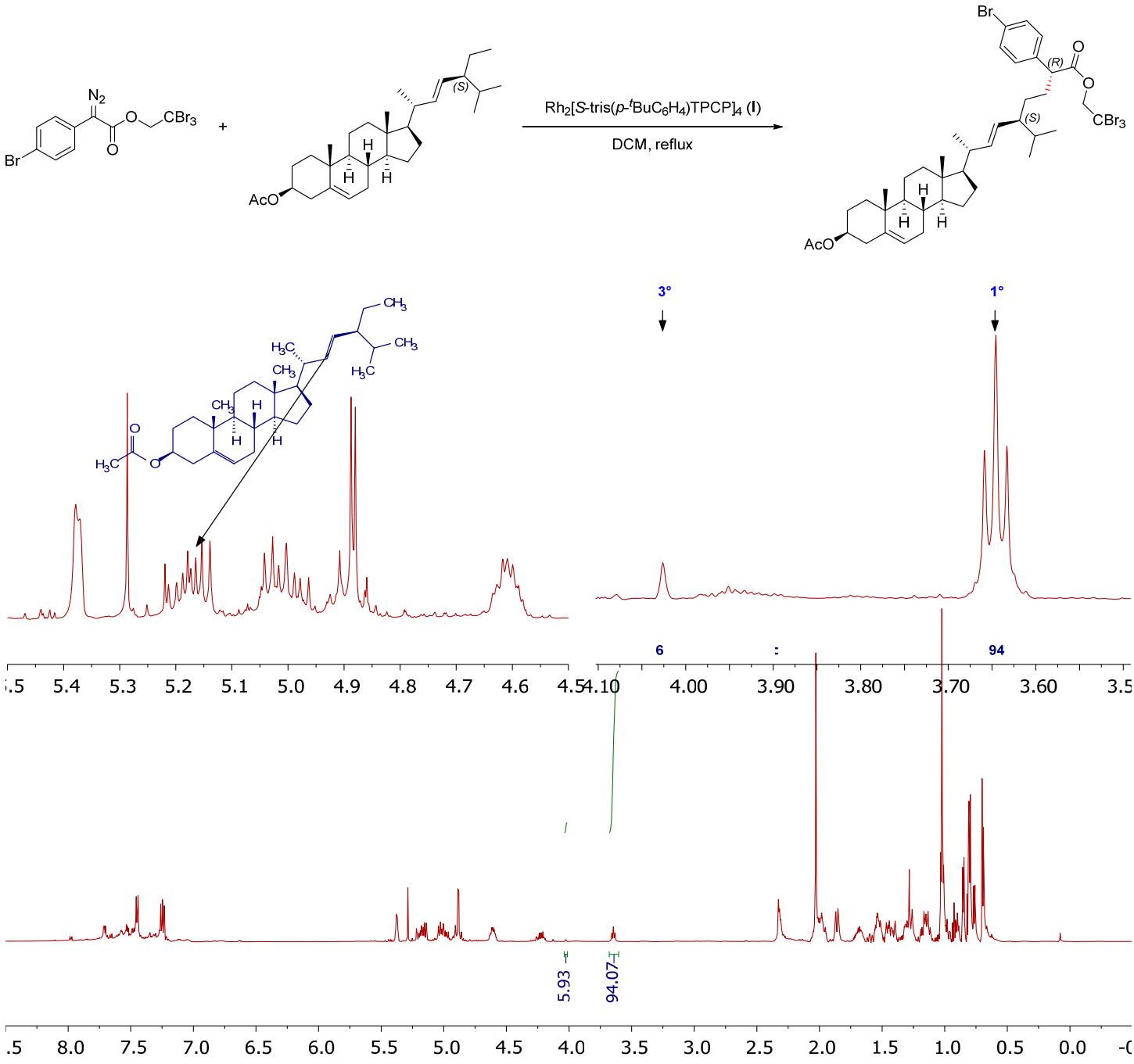

1°
2°
Leftover substrate
(compound 23) after
vacuum concentration
94 : 6
3.85 3.80 3.75 3.70 3.65 3.60 3.55 3.50 3.45
94.08
5.92
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0

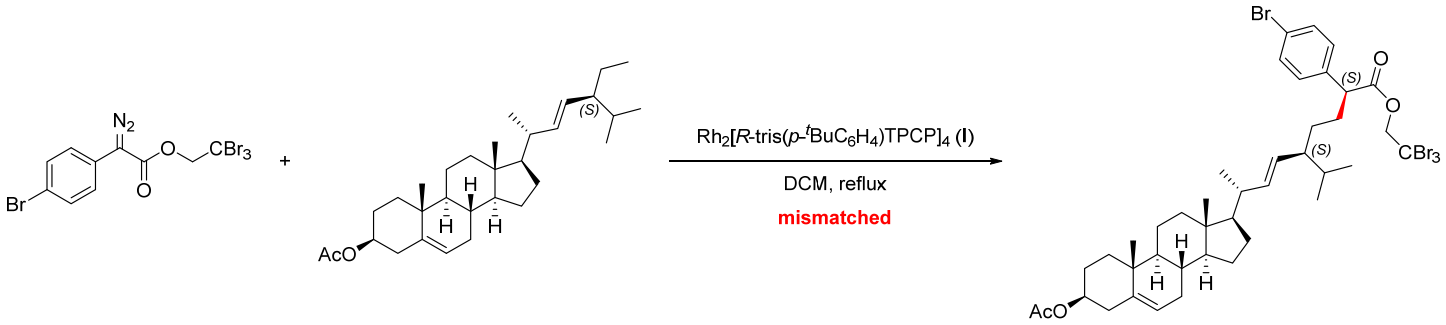

(S)
H
H
H
AcO

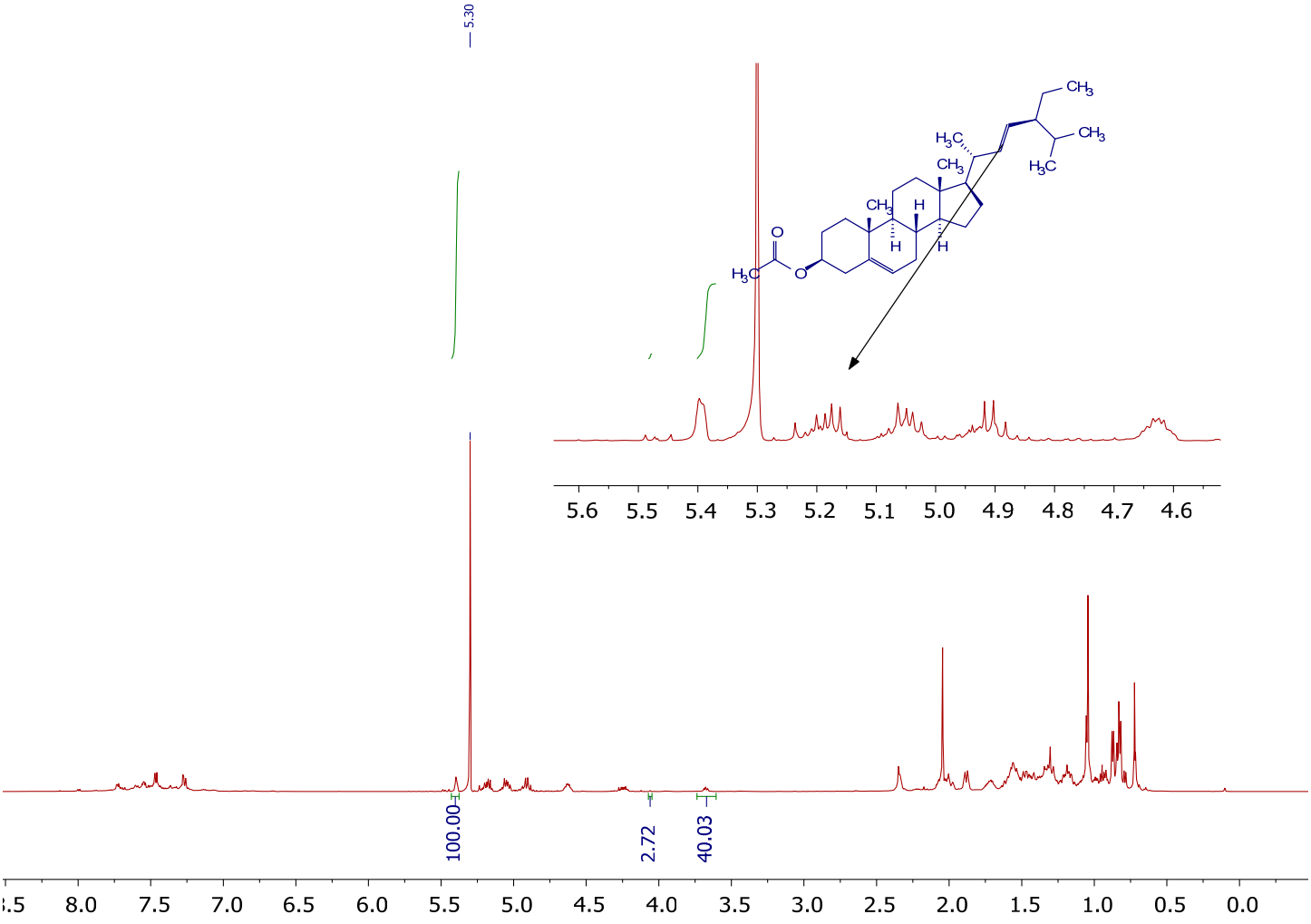

CH3
H3C
CH3
H3C
CH3
H
H
H
O
H3C
O
5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6
1.10 1.05 1.00 0.95 0.90 0.85 0.80 0.75 0.70 0.65
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.


Rh2(R-TCPTAD)4
DCM, reflux
3.88
3.68
3.88
3.68


Rh2(S-TCPTAD)4
DCM, reflux
mismatched
(R)
3.89
3.71
3.68

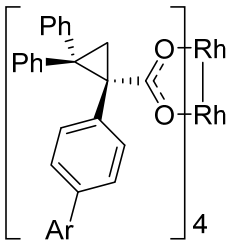

Rh2[S-tris(p-tBuC6H4)TPCP]4 (I)
DCM, reflux
3°
1°
6 : 94
5.93
94.07


Br
N2
O
CBr3
O
+
AcO
H
H
(S)
Rh2[R-tris(p-tBuC6H4)TPCP]4 (I)
DCM, reflux
mismatched
Br
(S)
O
O
CBr3
(S)
AcO
H
H


5.30
CH3
H3C
CH3
CH3
H3C
CH3
H
H
H
O
H3C
O
5.6
5.5
5.4
5.3
5.2
5.1
5.0
4.9
4.8
4.7
4.6
100.00
2.72
40.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

9 - NMR Spectra for Product Characterization

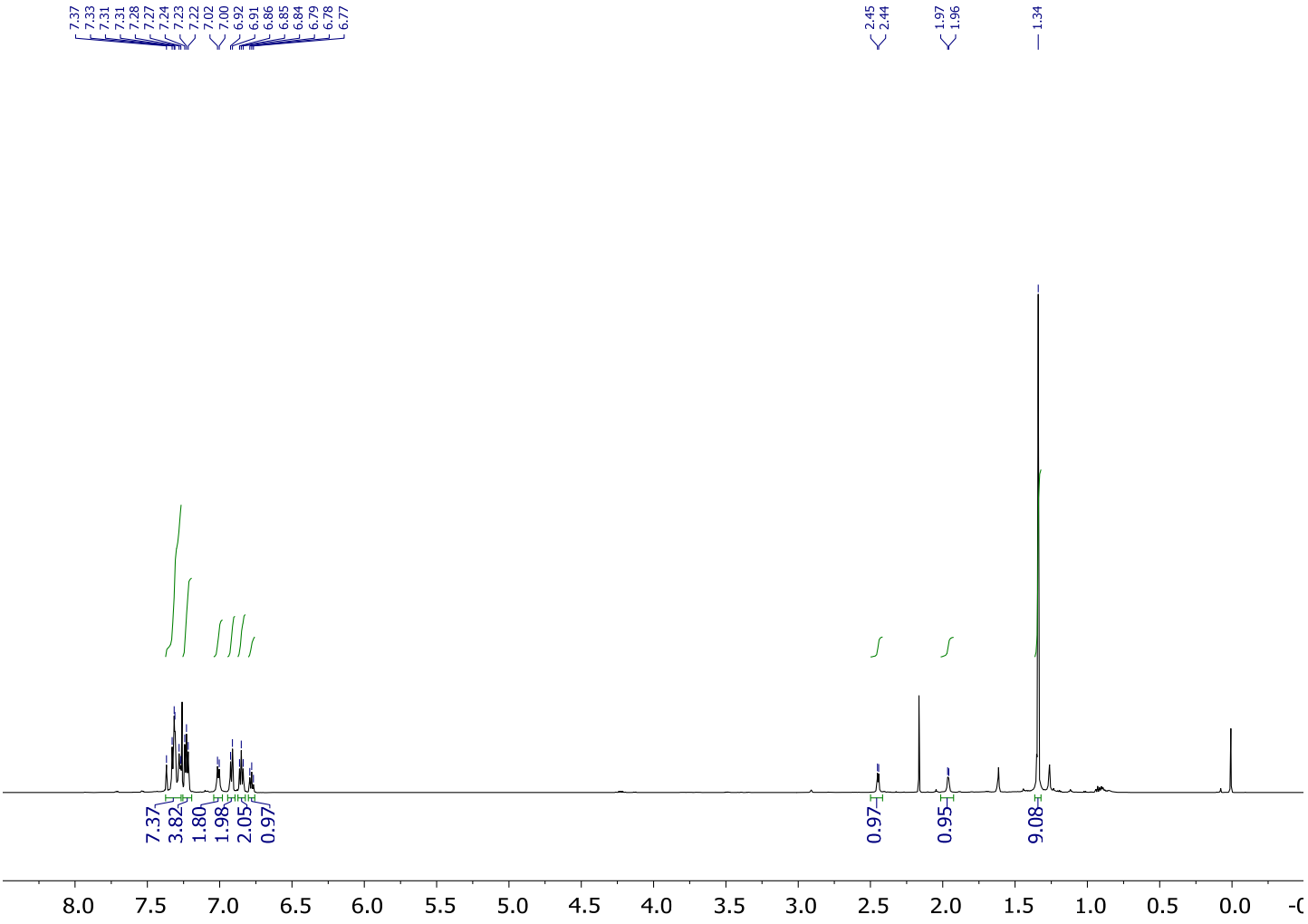
9.1 Catalysts Preparation

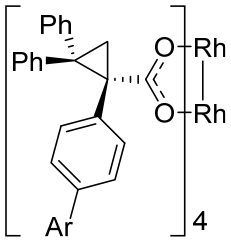


Ar= *p*-^{t}BuC$_6$H$_4$

Rh_2[*R*-*p*-^{t}BuC$_6$H$_4$TPCP]$_4$

E

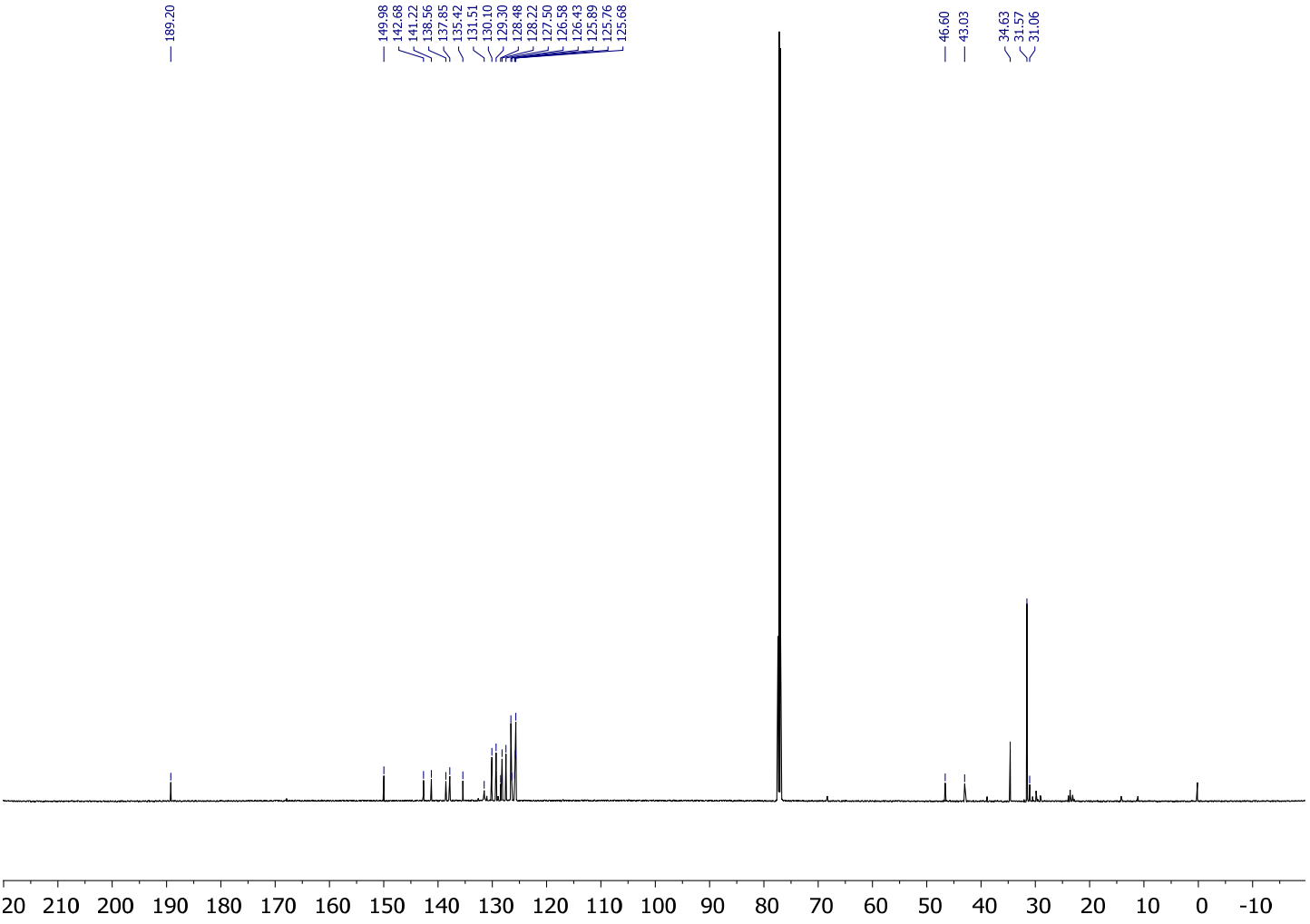


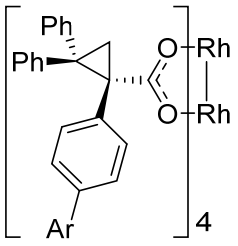


Ar= *p*-^{t}BuC$_6$H$_4$

Rh_2[*R*-*p*-^{t}BuC$_6$H$_4$TPCP]$_4$

E

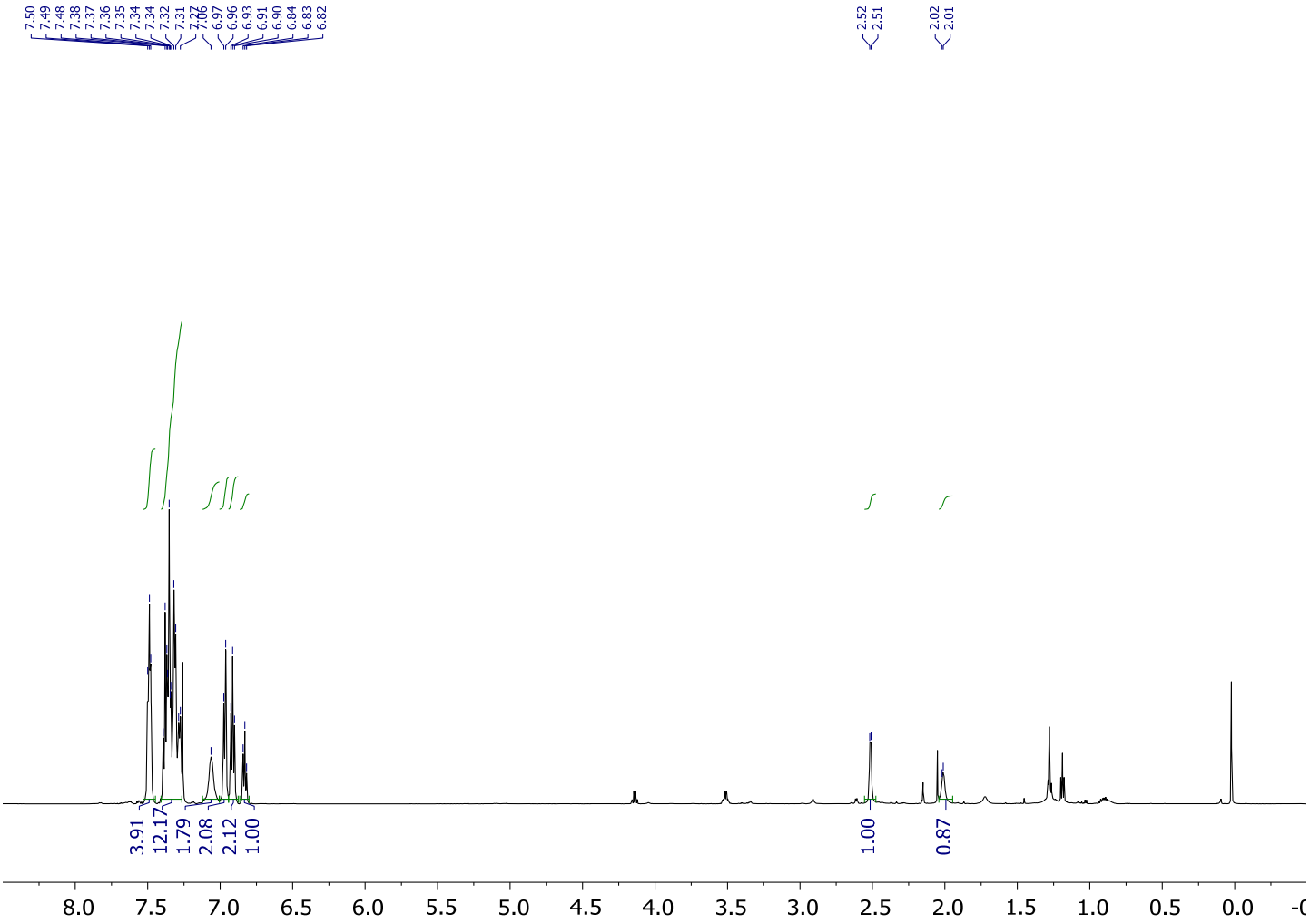


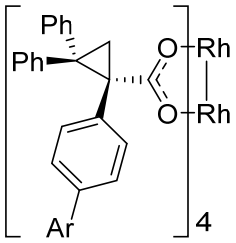


Ar= *p*-PhC_6H_4

Rh_2[*R*-*p*-PhC_6H_4TPCP]$_4$

F

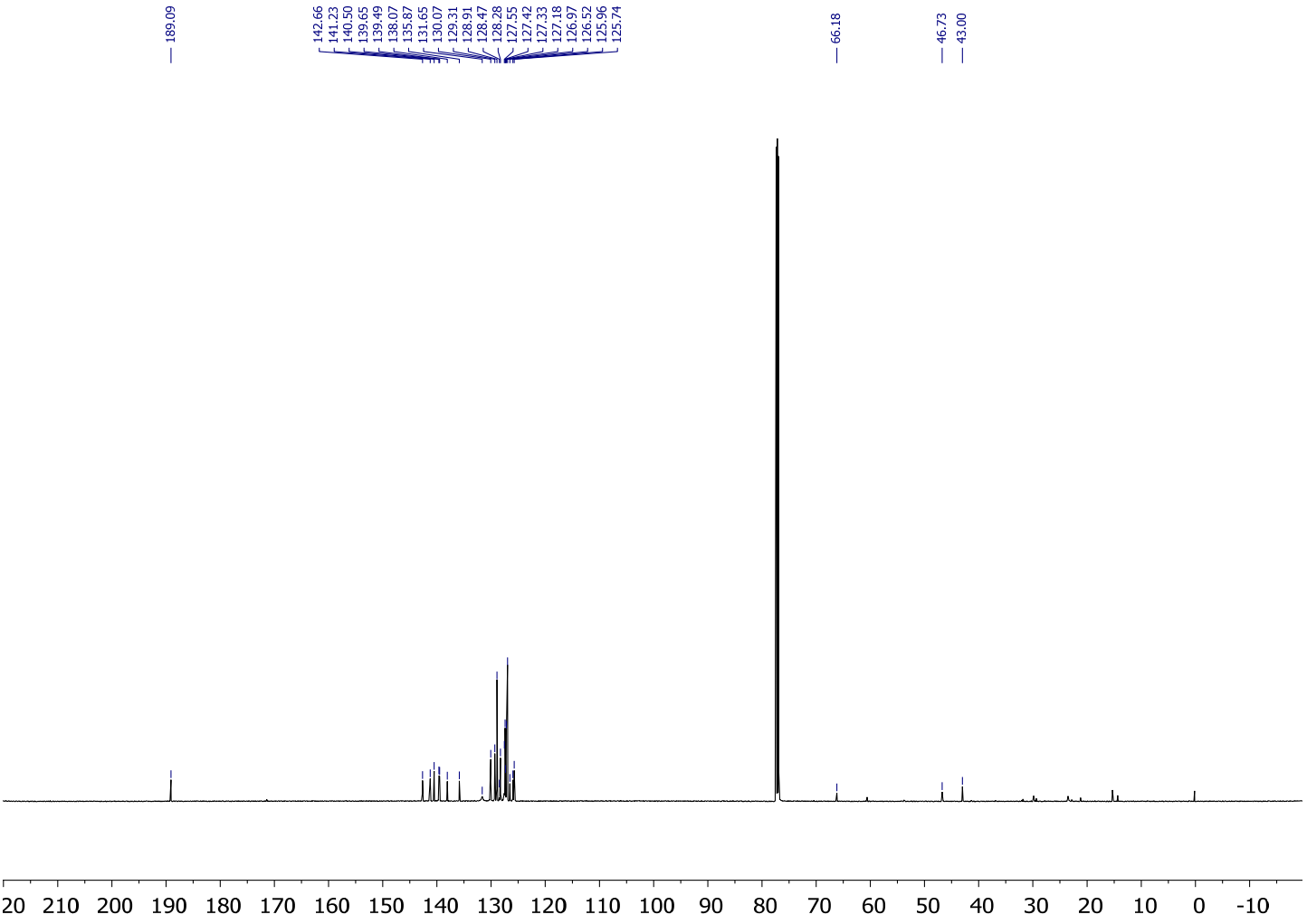


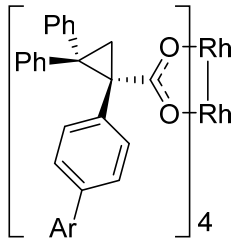


Ar= *p*-PhC$_6$H$_4$

Rh$_2$[*R*-*p*-PhC$_6$H$_4$TPCP]$_4$

F

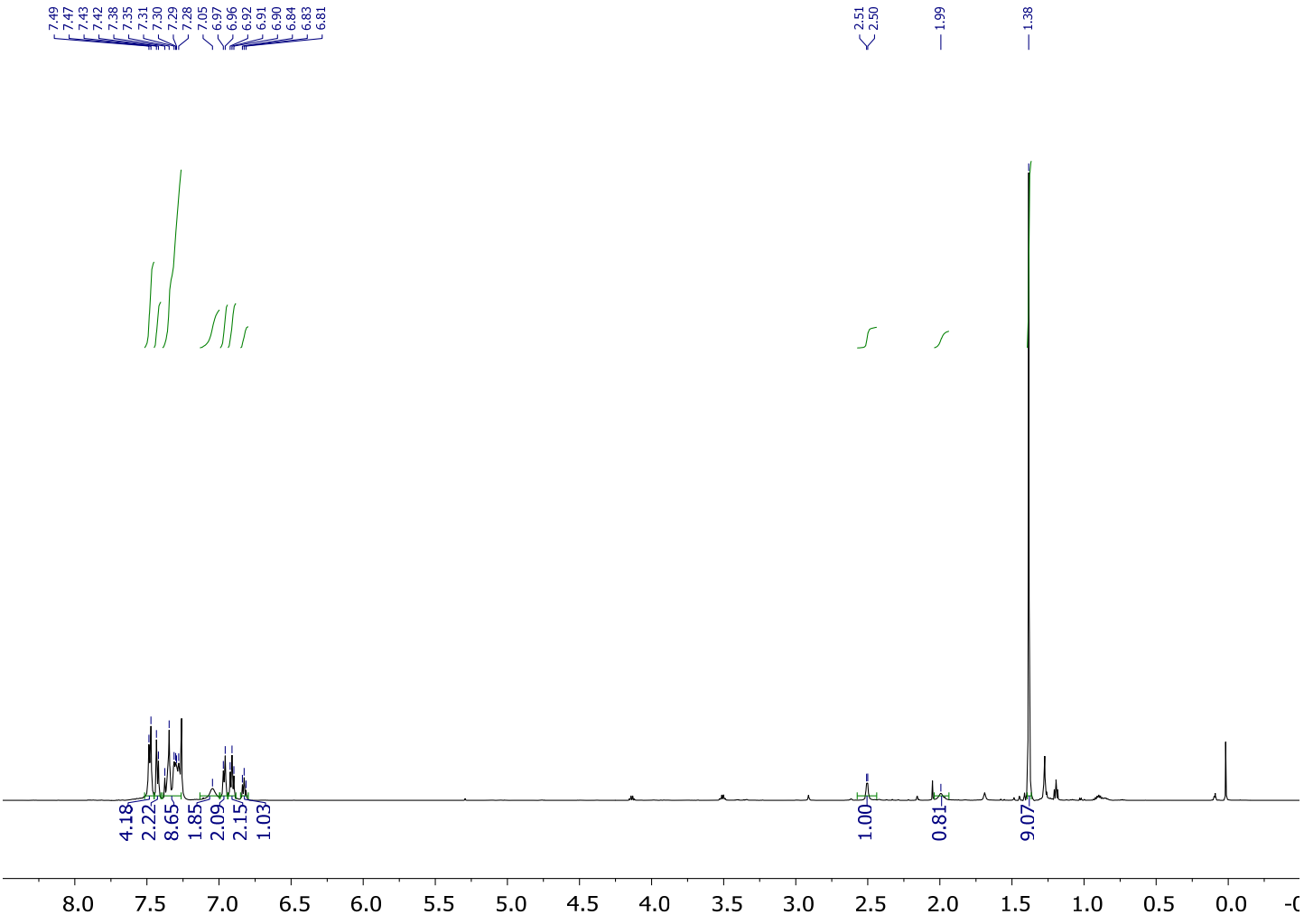


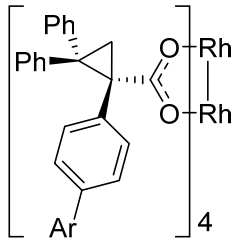


Ar= *p*-^{t}BuC$_6$H$_4$C$_6$H$_4$

Rh$_2$[*R*-*p*-^{t}BuC$_6$H$_4$C$_6$H$_4$TPCP]$_4$

G

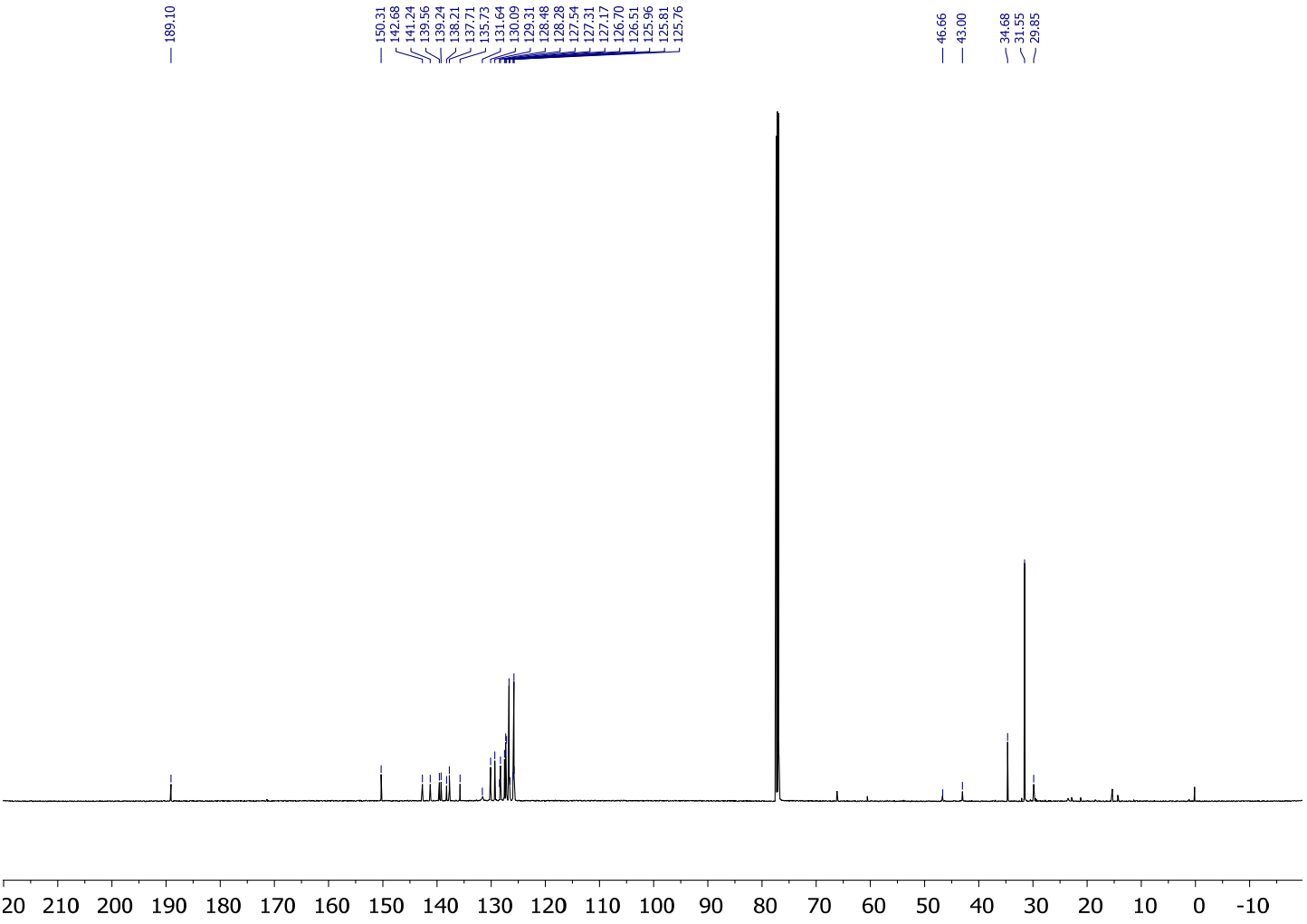


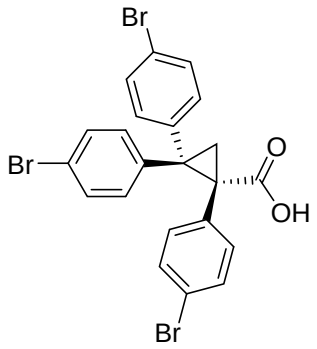


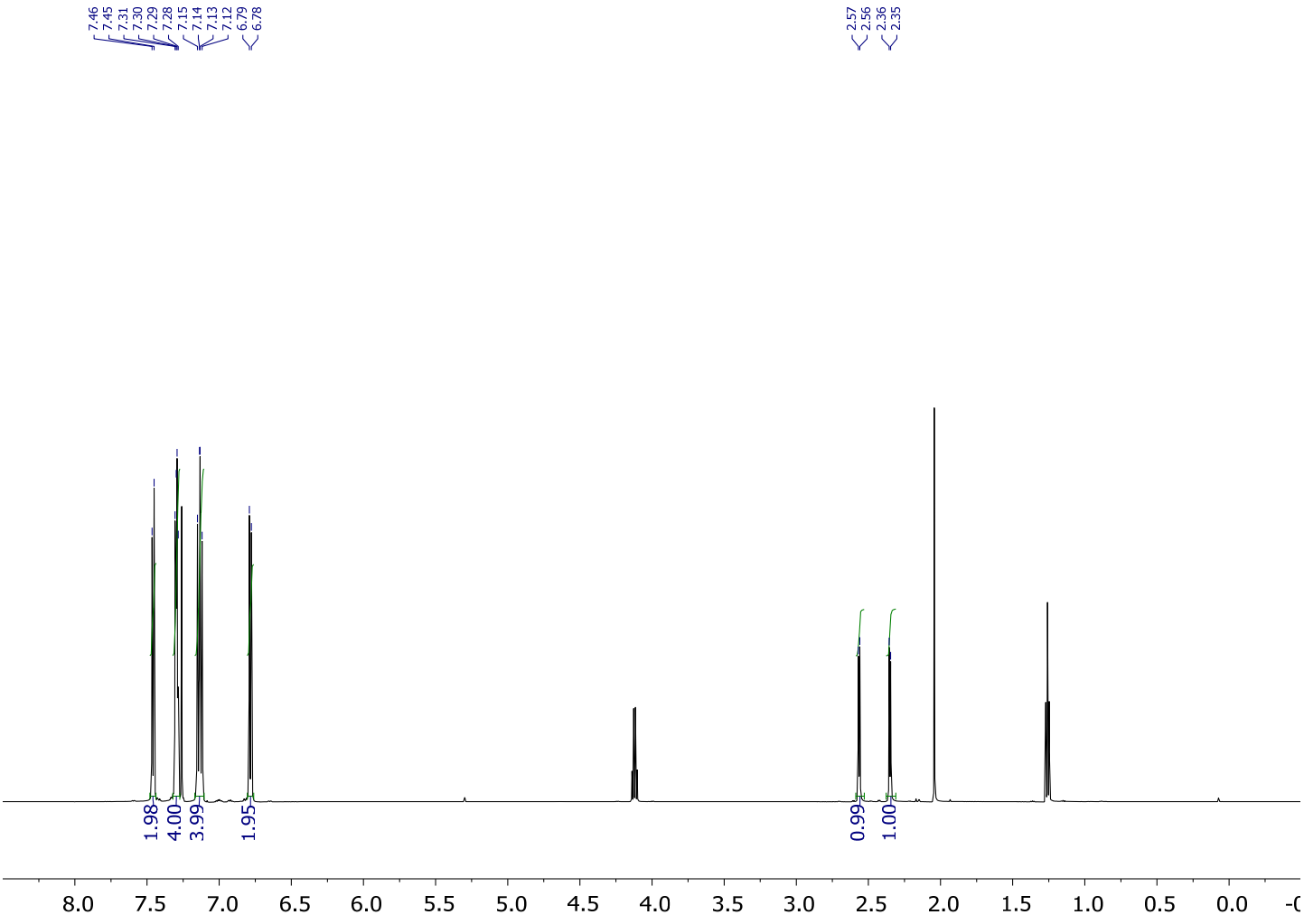
Ar= *p*-^{t}BuC$_6$H$_4$C$_6$H$_4$

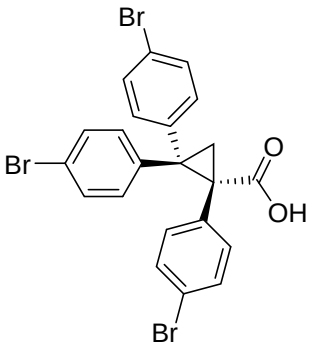
Rh$_2$[*R*-*p*-^{t}BuC$_6$H$_4$C$_6$H$_4$TPCP]$_4$

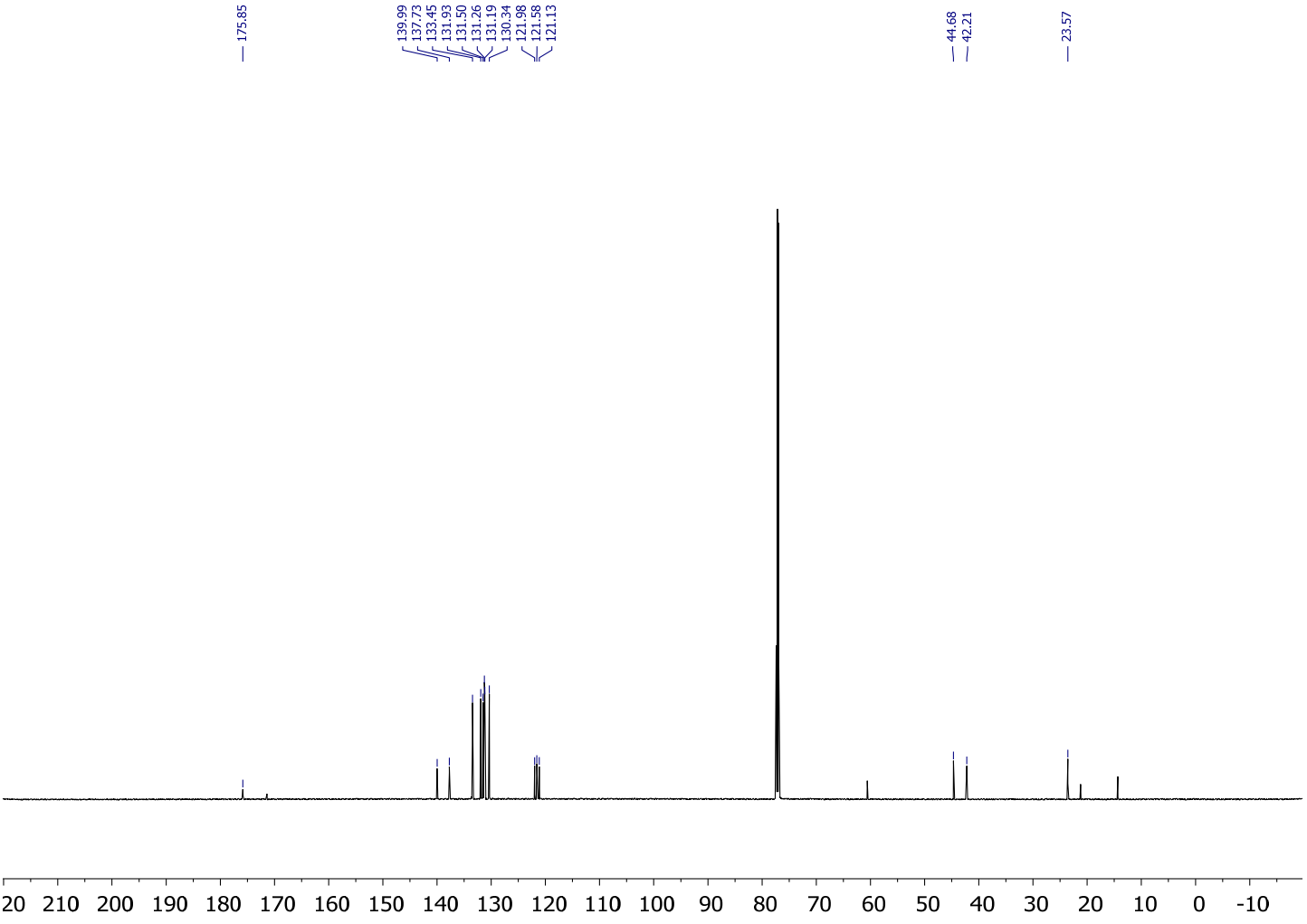
G

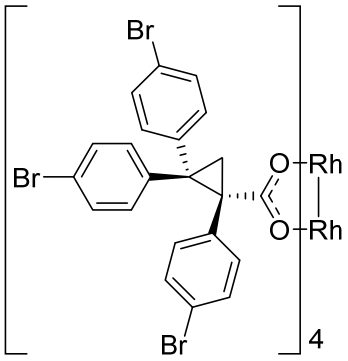



Br
Br
O
OH
Br


7.46
7.45
7.31
7.30
7.29
7.28
7.15
7.14
7.13
7.12
6.79
6.78
2.57
2.56
2.36
2.35
1.98
4.00
3.99
1.95
0.99
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

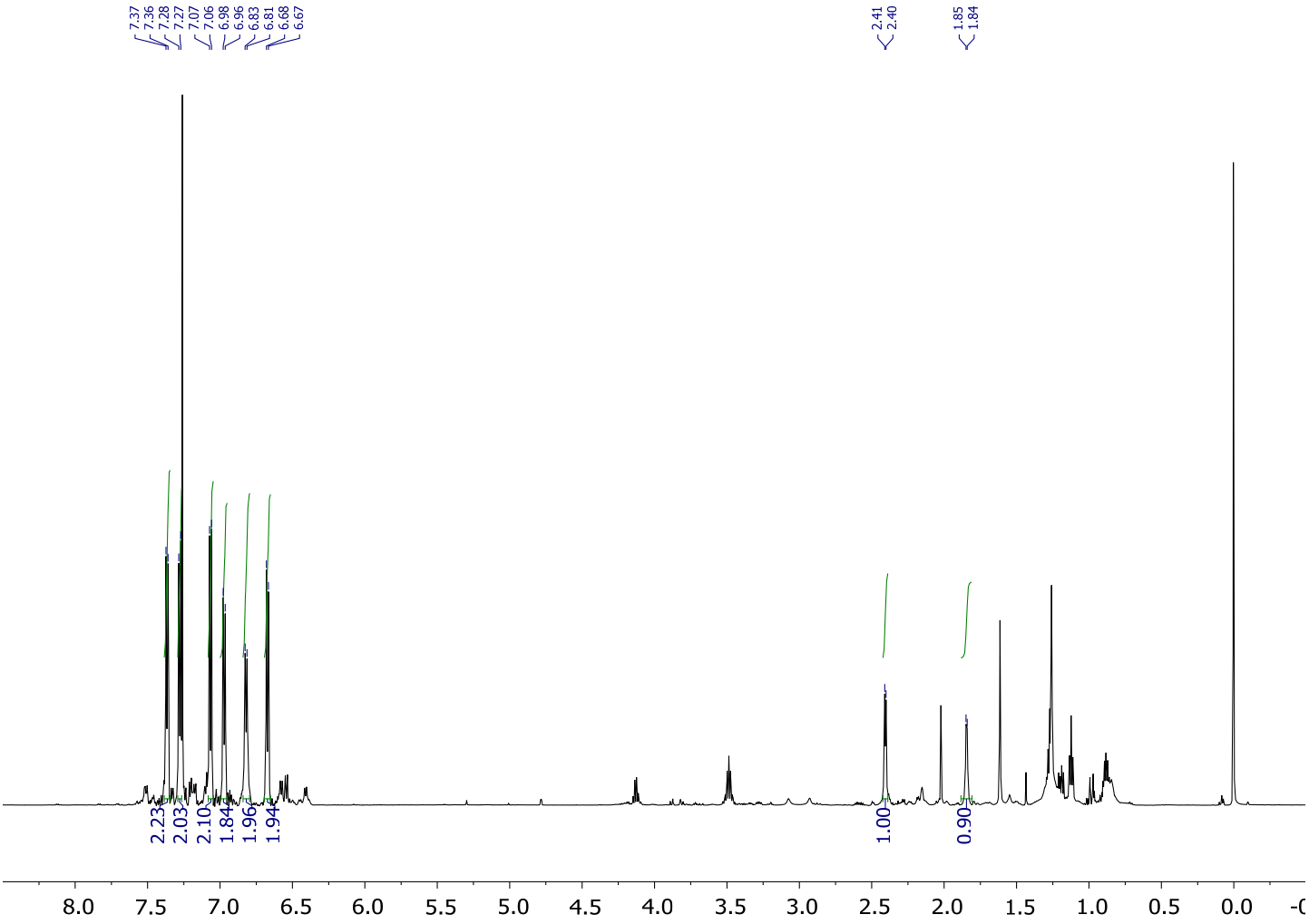

Br
Br
O
OH
Br

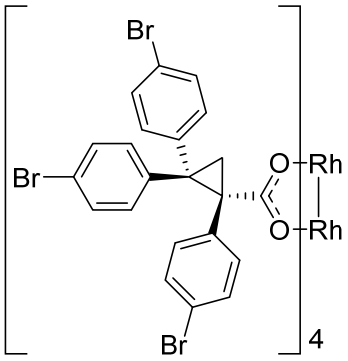

175.85
139.99
137.73
133.45
131.93
131.50
131.26
131.19
130.34
121.98
121.58
121.13
44.68
42.21
23.57
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10



Rh_2[*R*-tris(*p*-Br)TPCP]$_4$

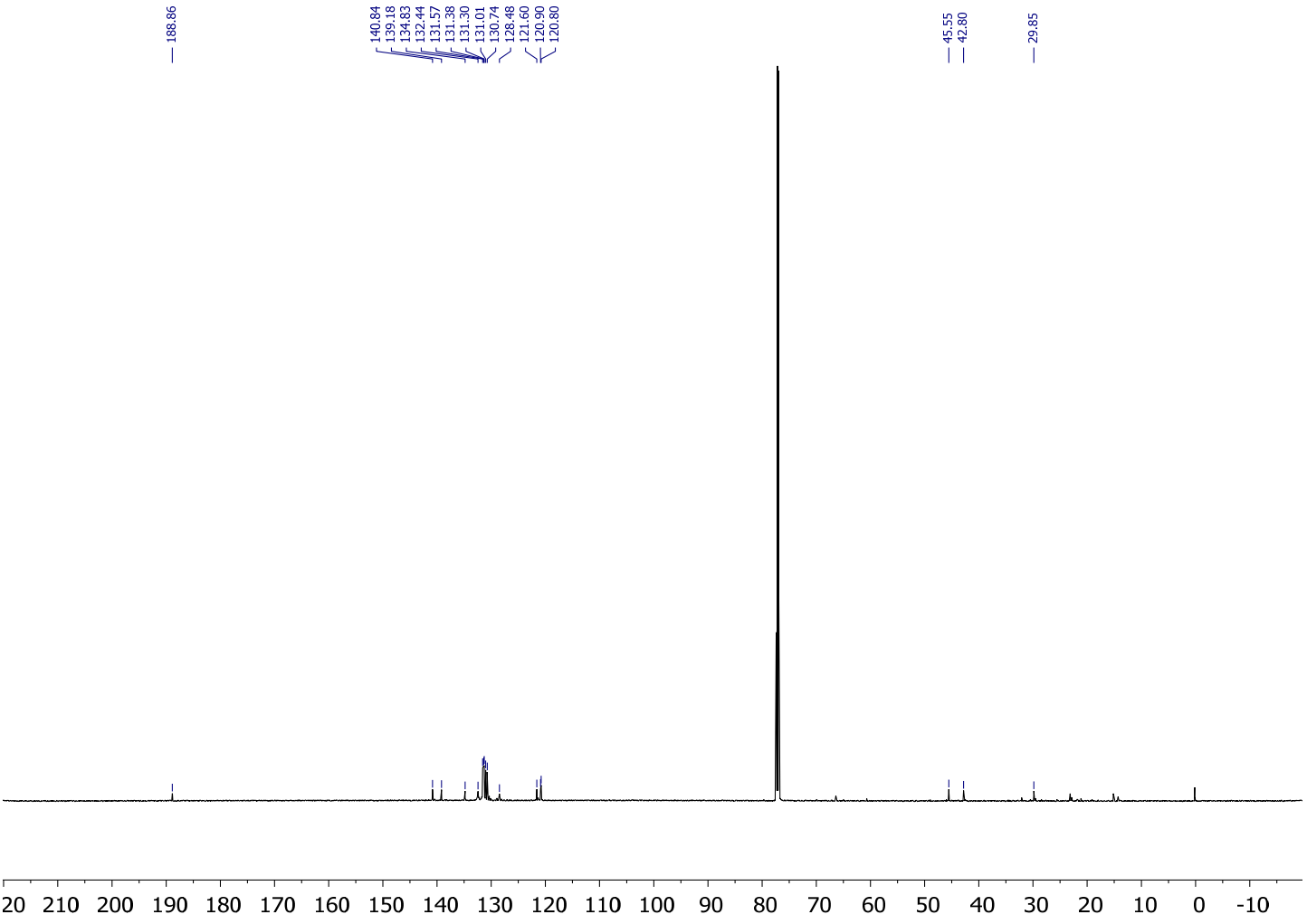
N

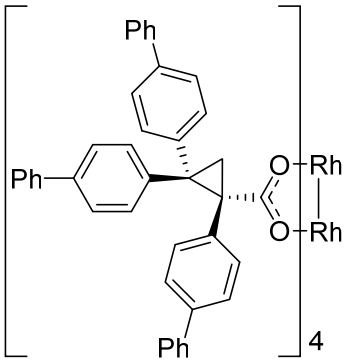




Rh_2[*R*-tris(*p*-Br)TPCP]$_4$

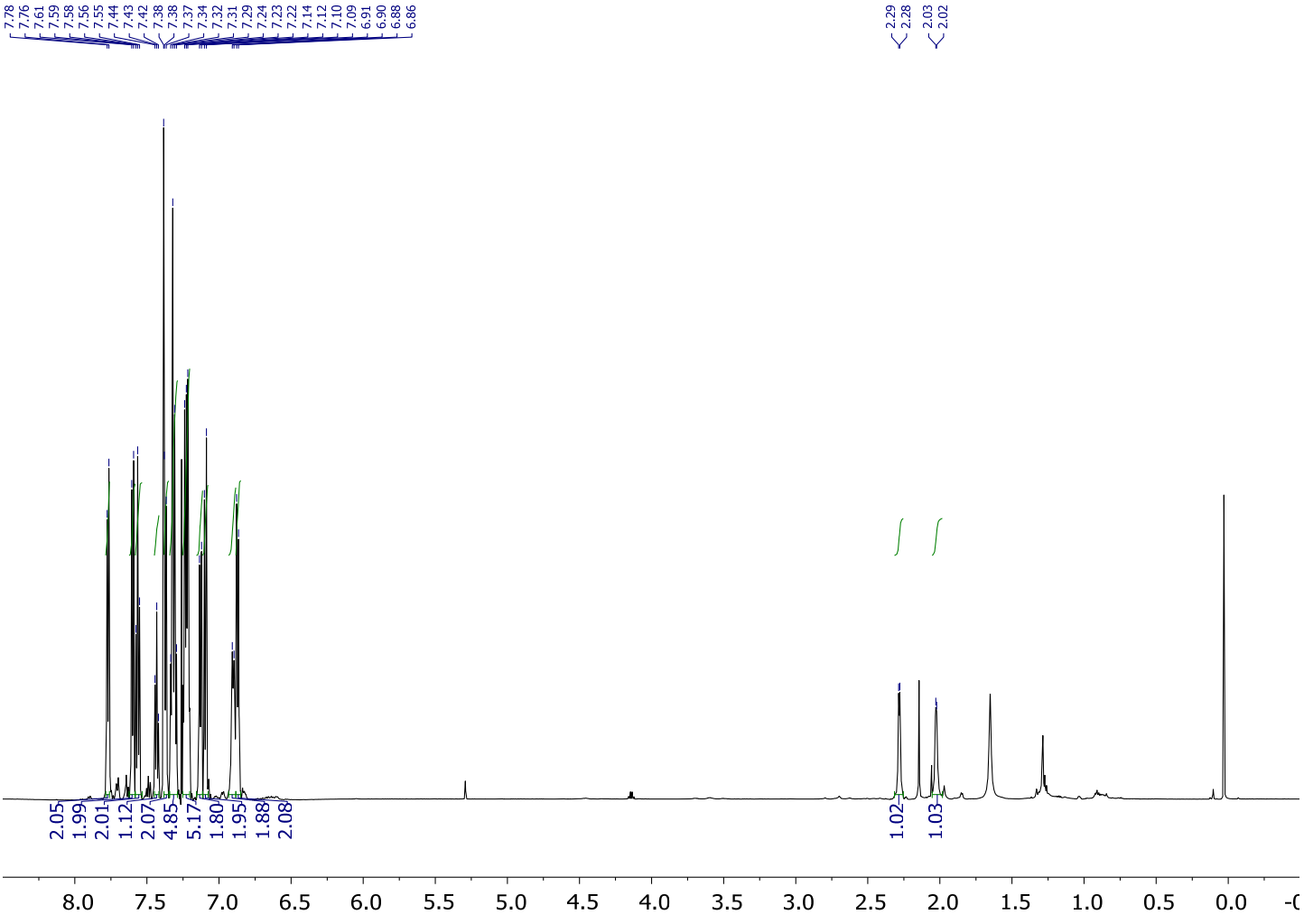
N

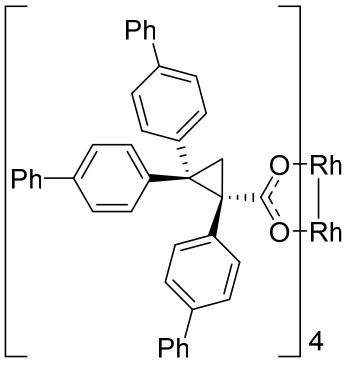




Rh_2[*R*-tris(*p*-Ph)TPCP]$_4$

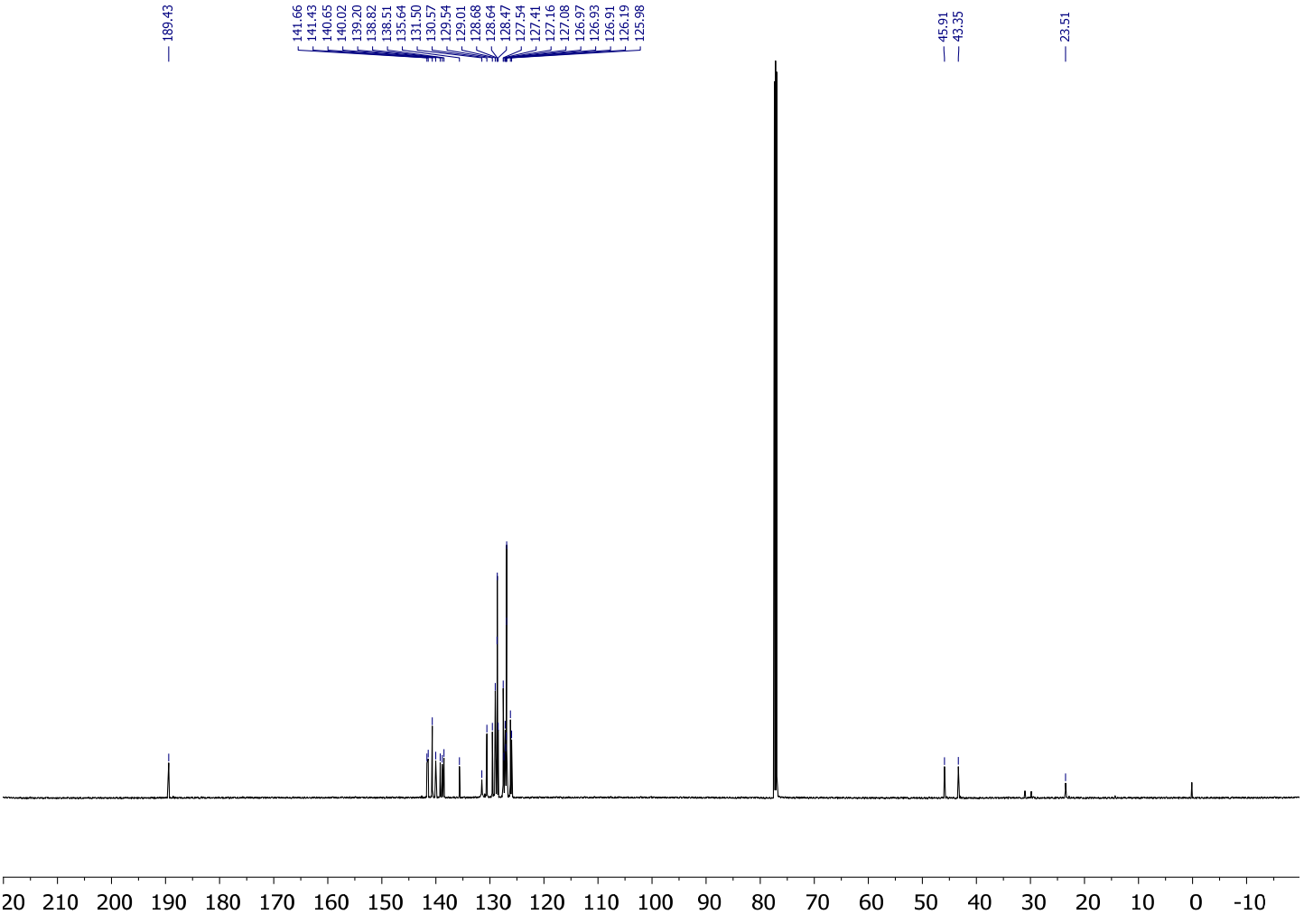
H

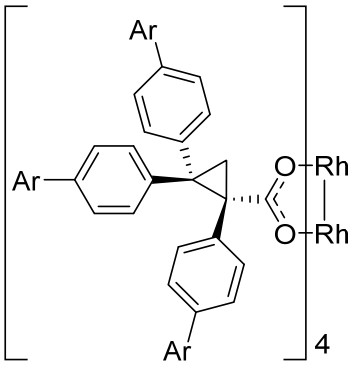




Rh_2[*R*-tris(*p*-Ph)TPCP]$_4$

H

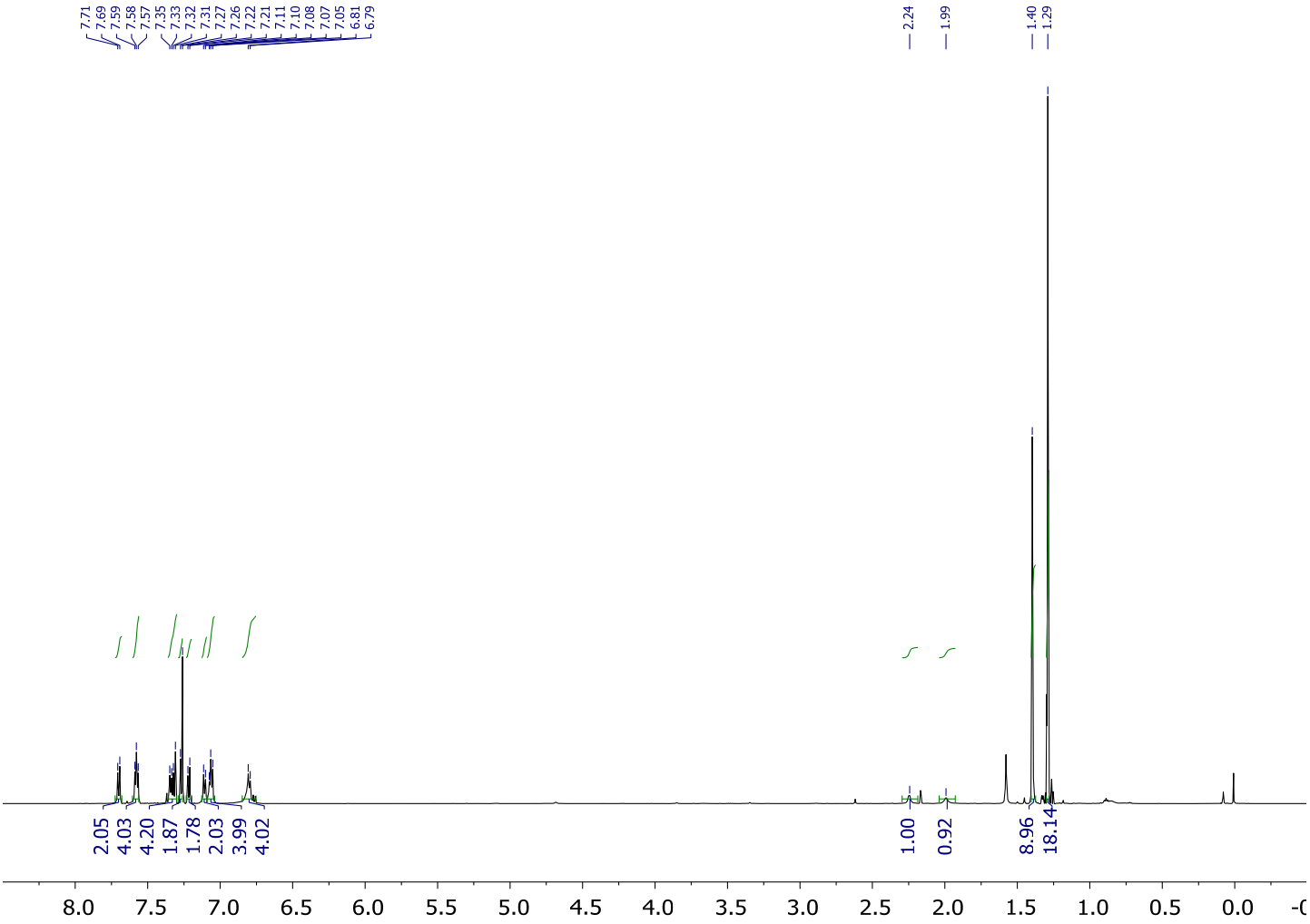


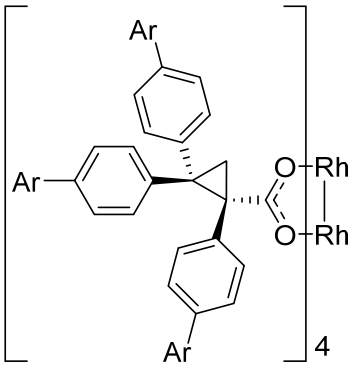


Ar= *p*-^{t}BuC$_6$H$_4$

Rh$_2$[*R*-tris(*p*-^{t}BuC$_6$H$_4$)TPCP]$_4$

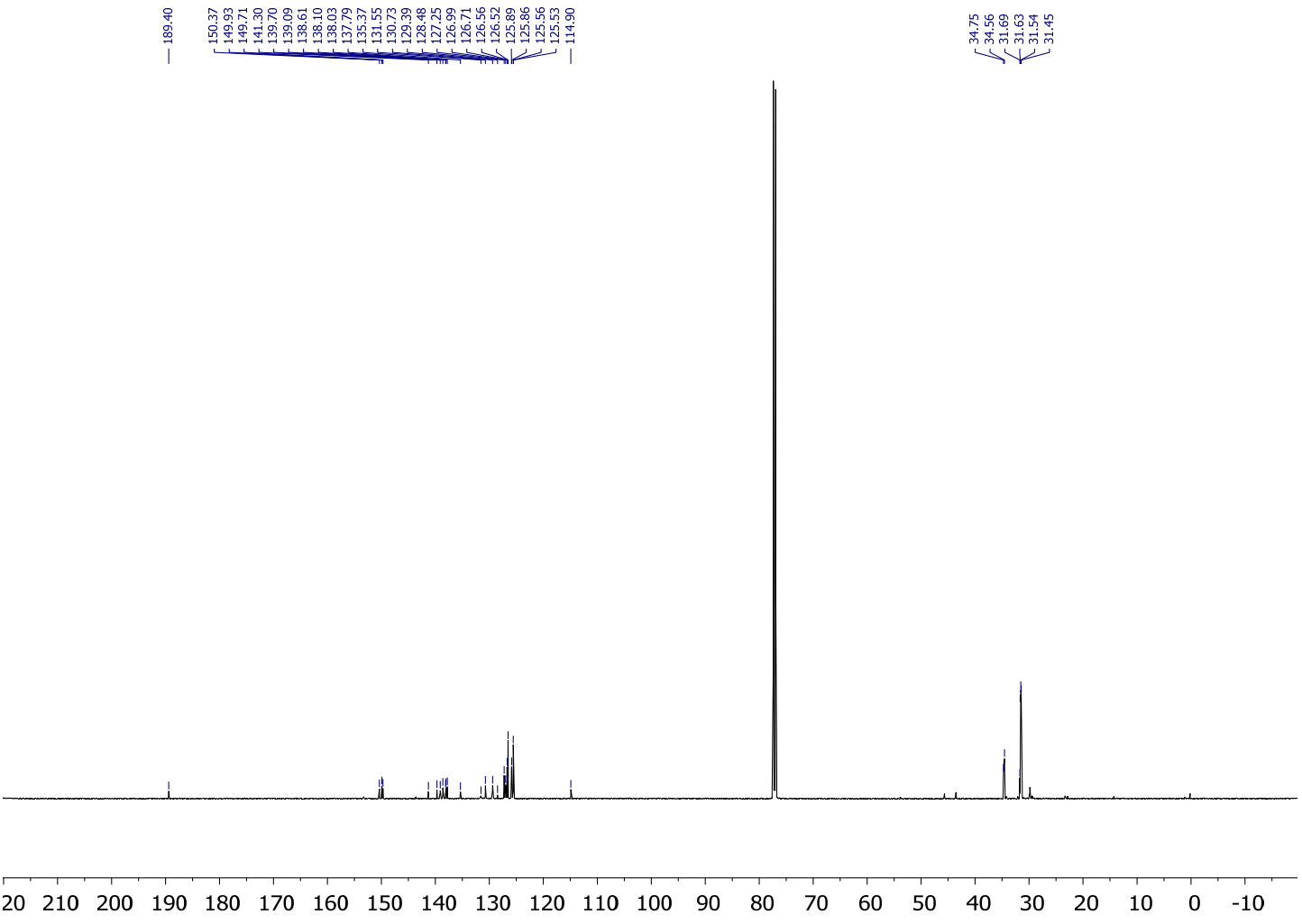
I

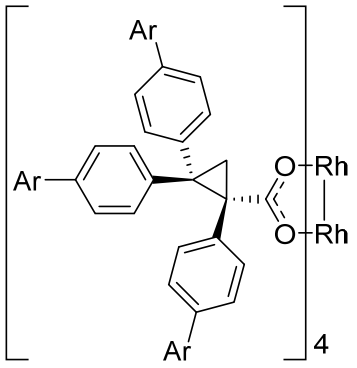




Ar= *p*-^{t}BuC$_6$H$_4$

Rh$_2$[*R*-tris(*p*-^{t}BuC$_6$H$_4$)TPCP]$_4$

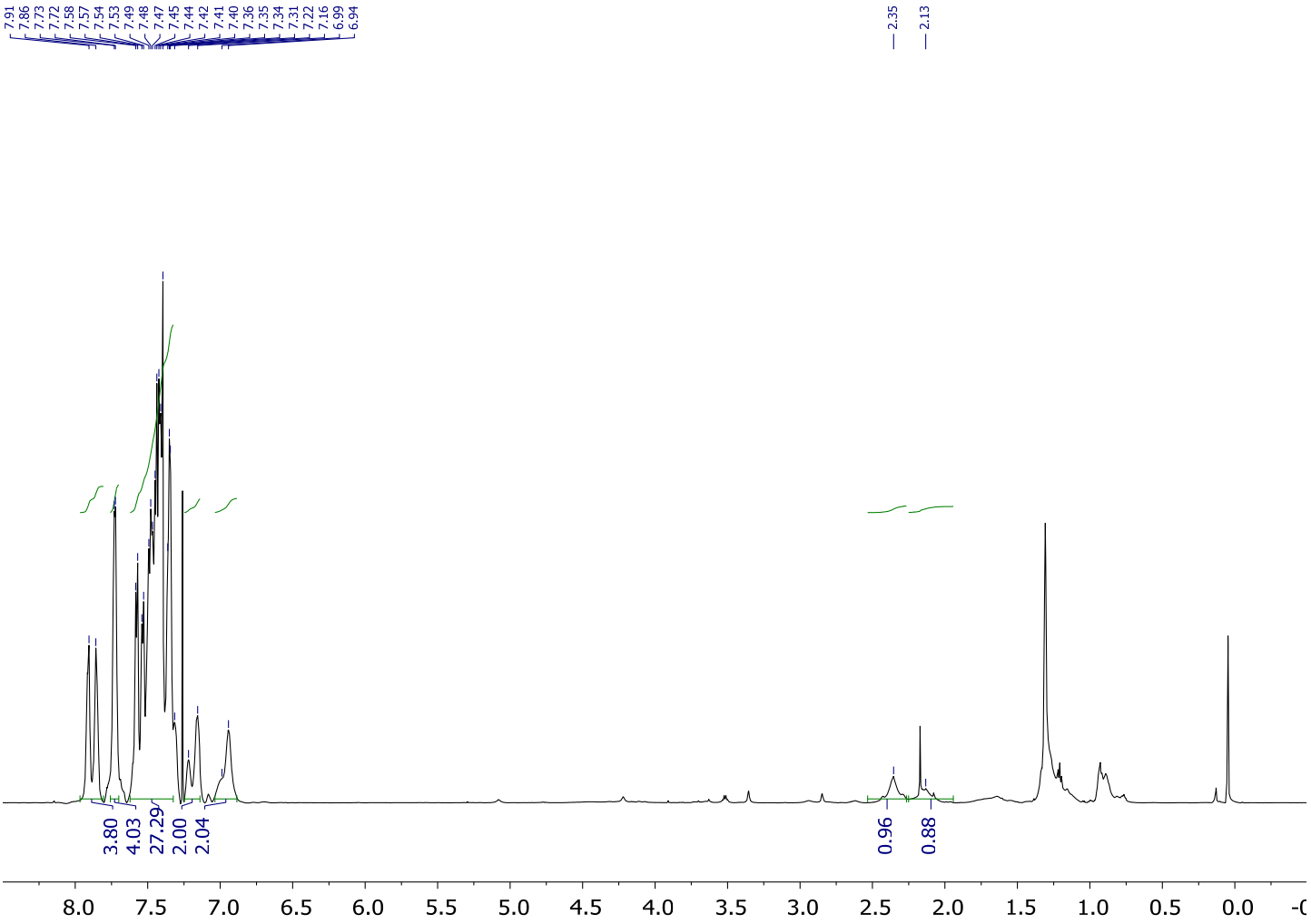


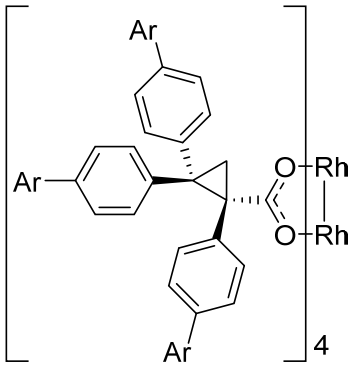


Ar= *p*-PhC$_6$H$_4$

Rh$_2$[*R*-tris(*p*-PhC$_6$H$_4$)TPCP]$_4$

J

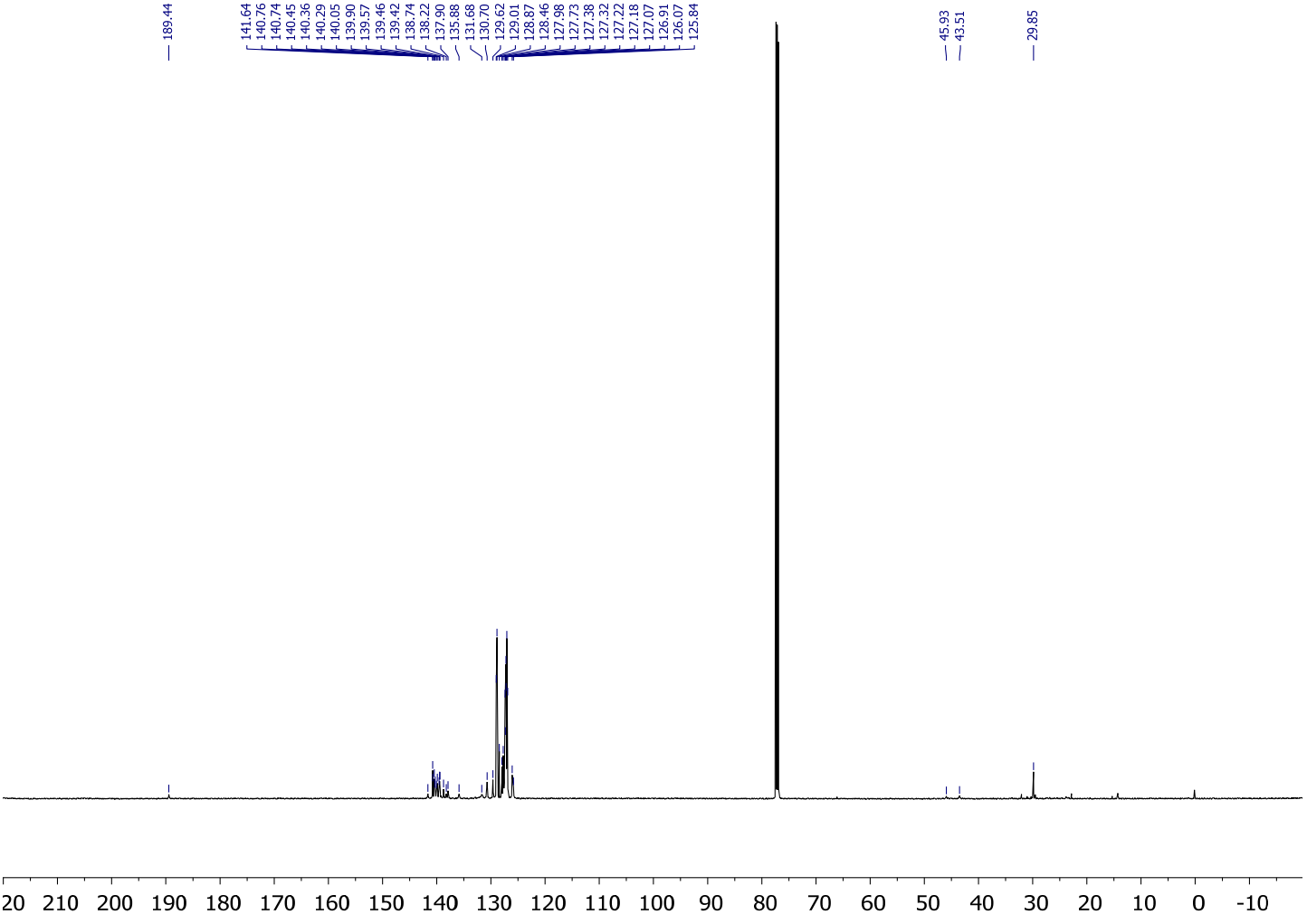


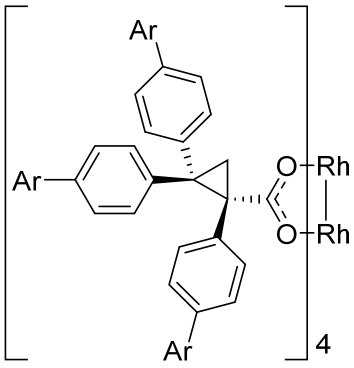


Ar= *p*-PhC_6H_4

Rh_2[*R*-tris(*p*-PhC_6H_4)TPCP]$_4$

J

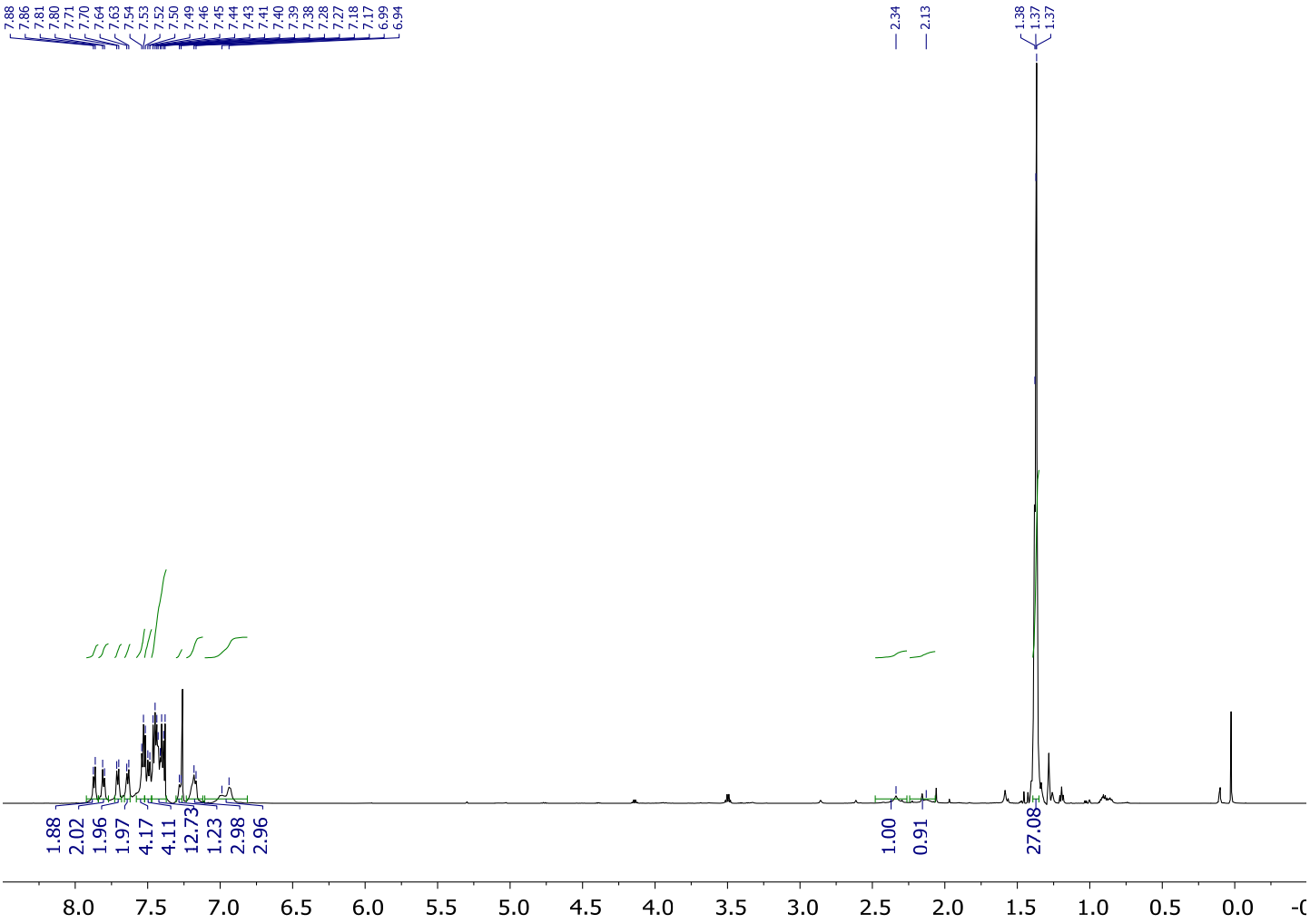


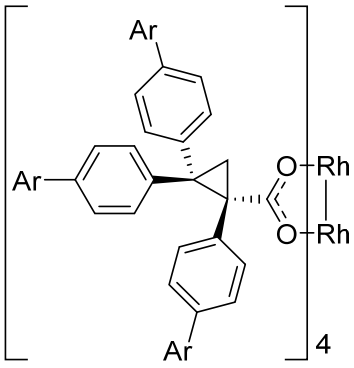


Ar= *p*-^{t}BuC$_6$H$_4$C$_6$H$_4$

Rh$_2$[*R*-tris(*p*-^{t}BuC$_6$H$_4$C$_6$H$_4$)TPCP]$_4$

K

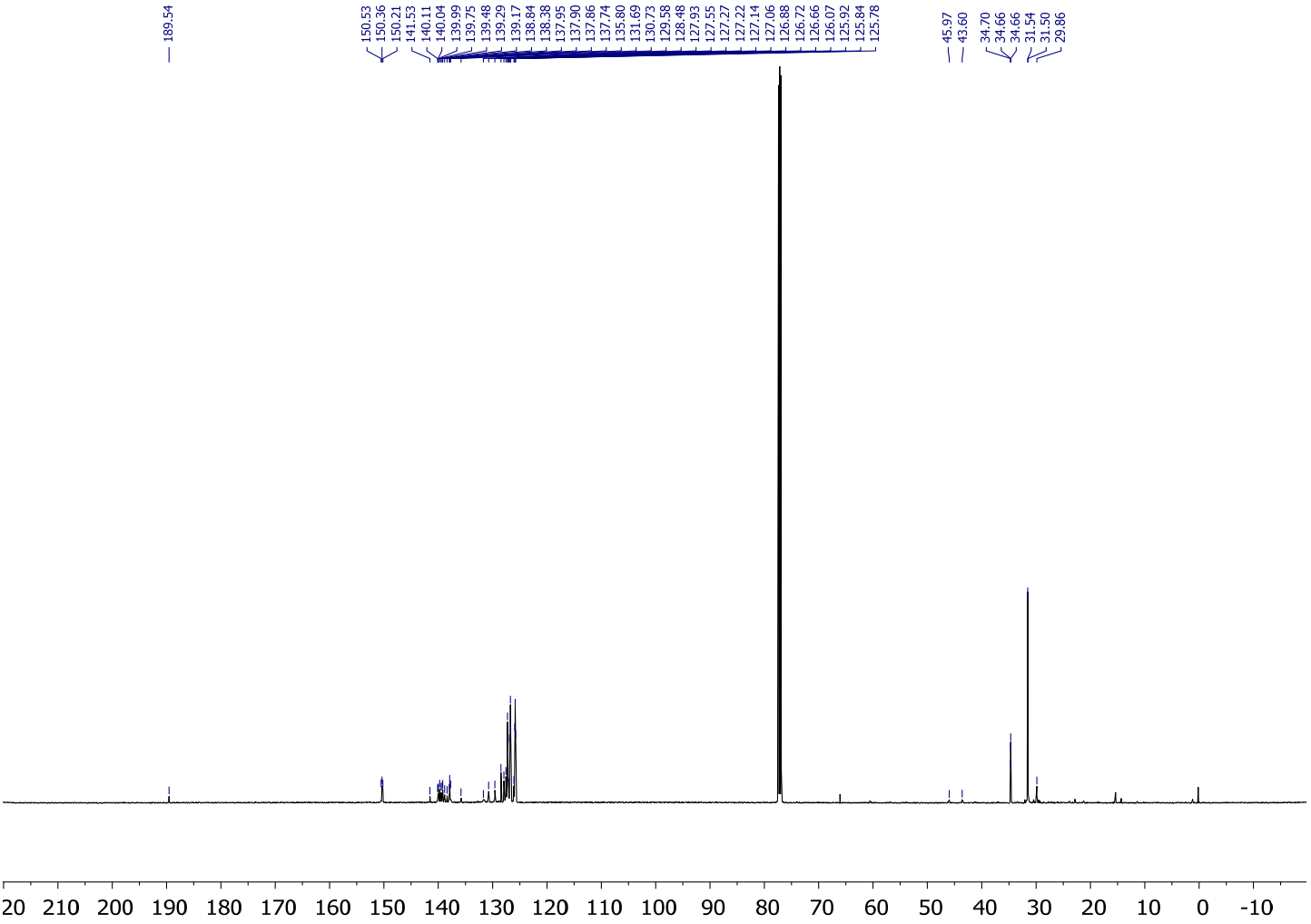


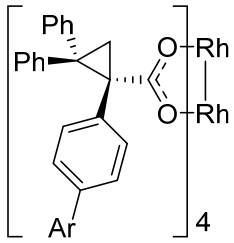


Ar= *p*-^{t}BuC$_6$H$_4$C$_6$H$_4$

Rh$_2$[*R*-tris(*p*-^{t}BuC$_6$H$_4$C$_6$H$_4$)TPCP]$_4$

K

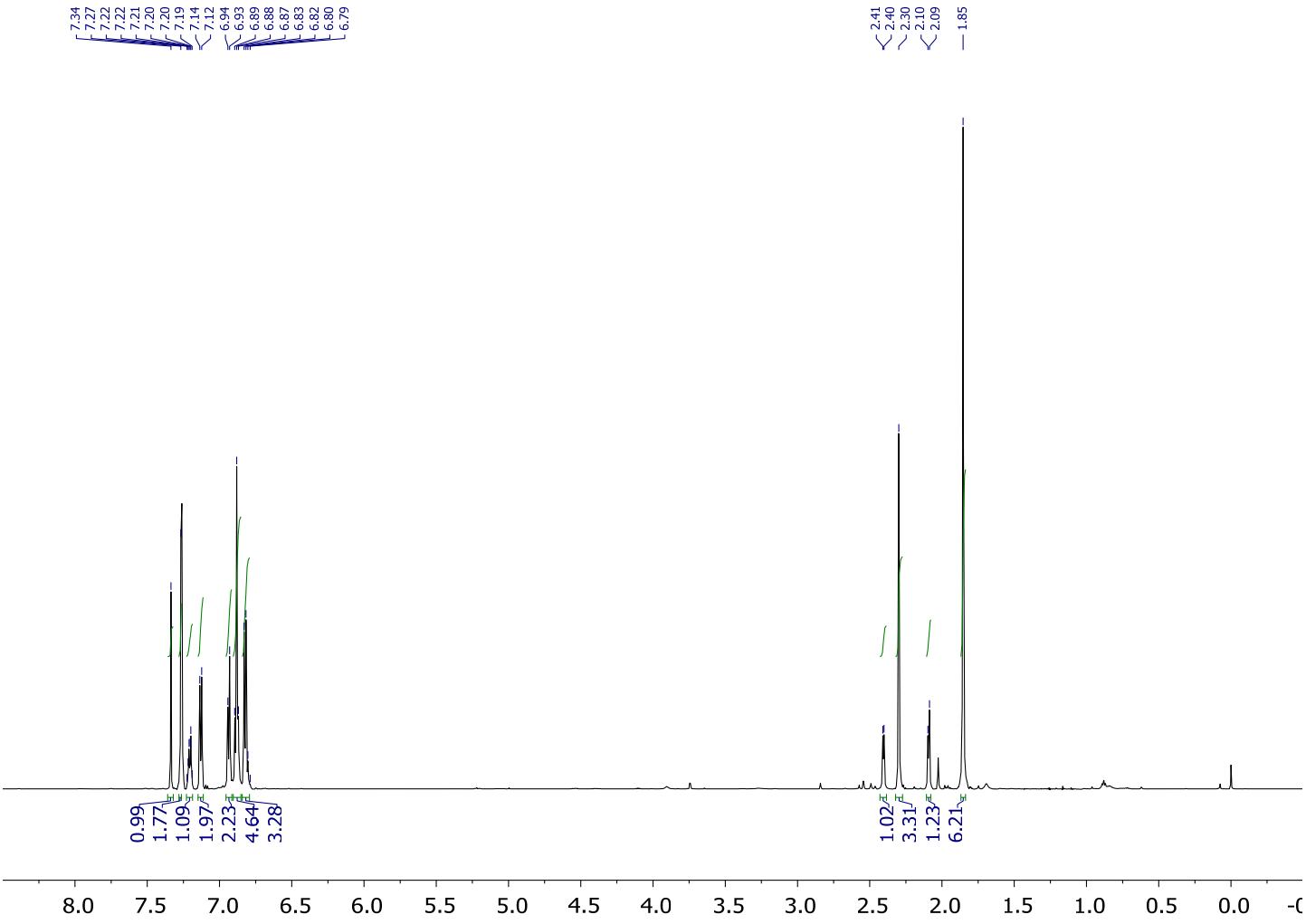


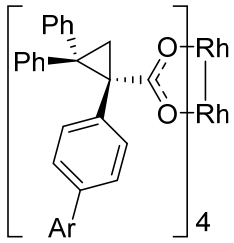


Ar= 2,4,6-tri-MeC_6H_2

Rh_2(*R*-2,4,6-tri-MeC_6H_2-TPCP)$_4$

Q

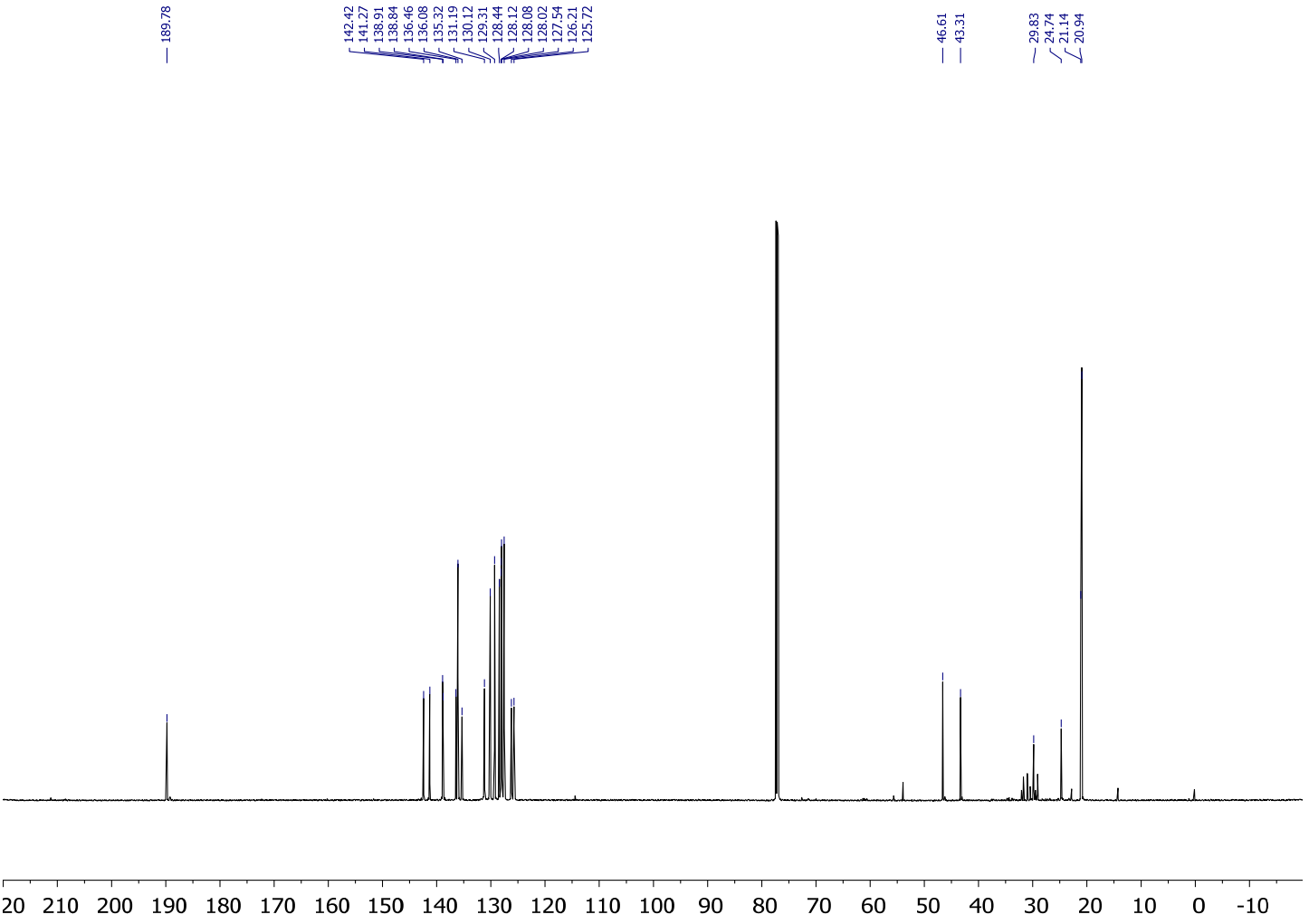




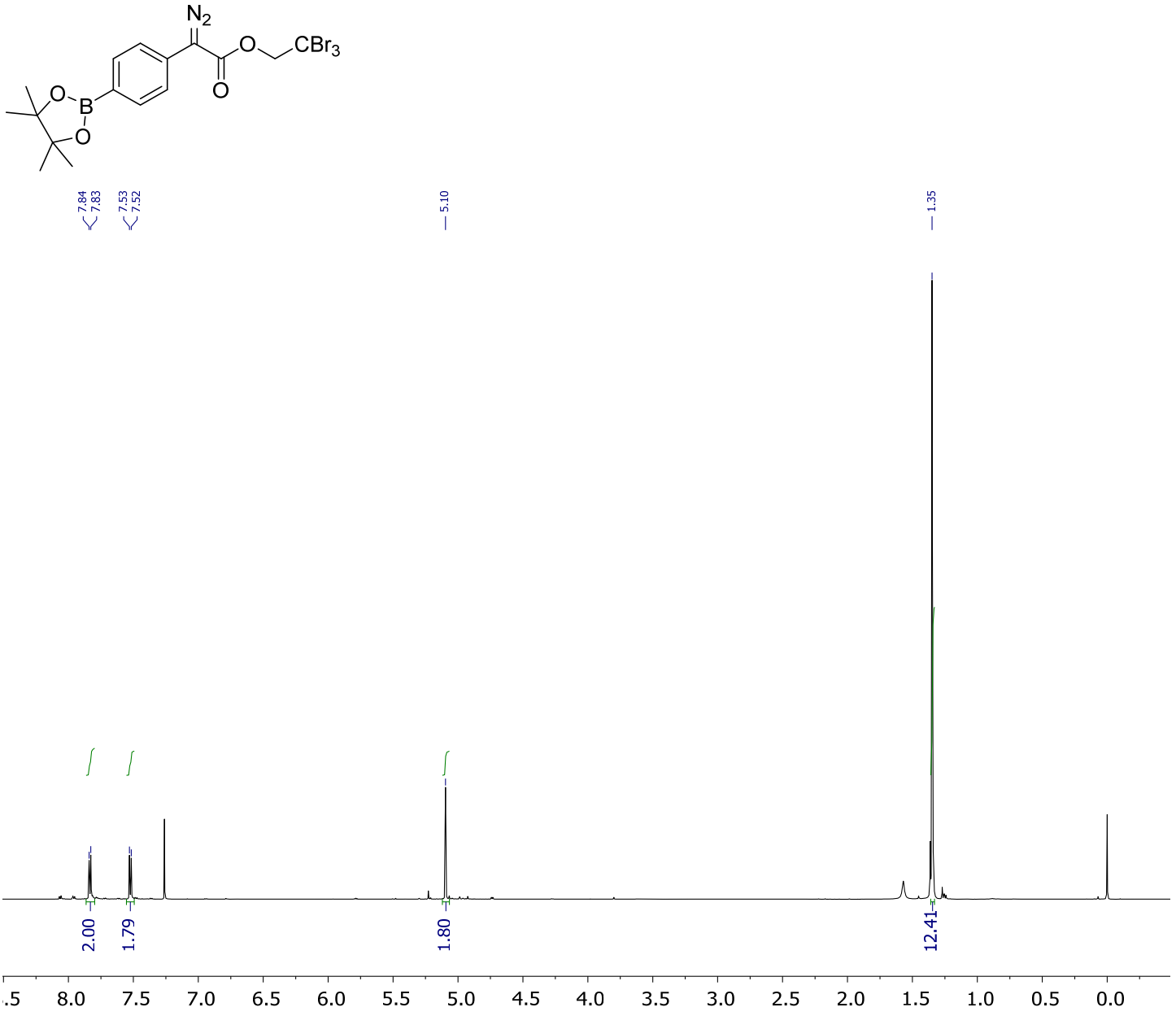
Ar= 2,4,6-tri-MeC_6H_2

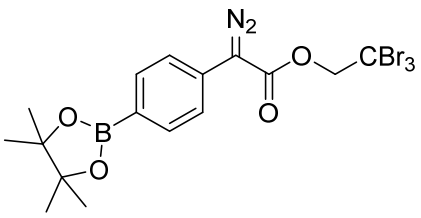
Rh_2(*R*-2,4,6-tri-MeC_6H_2-TPCP)$_4$

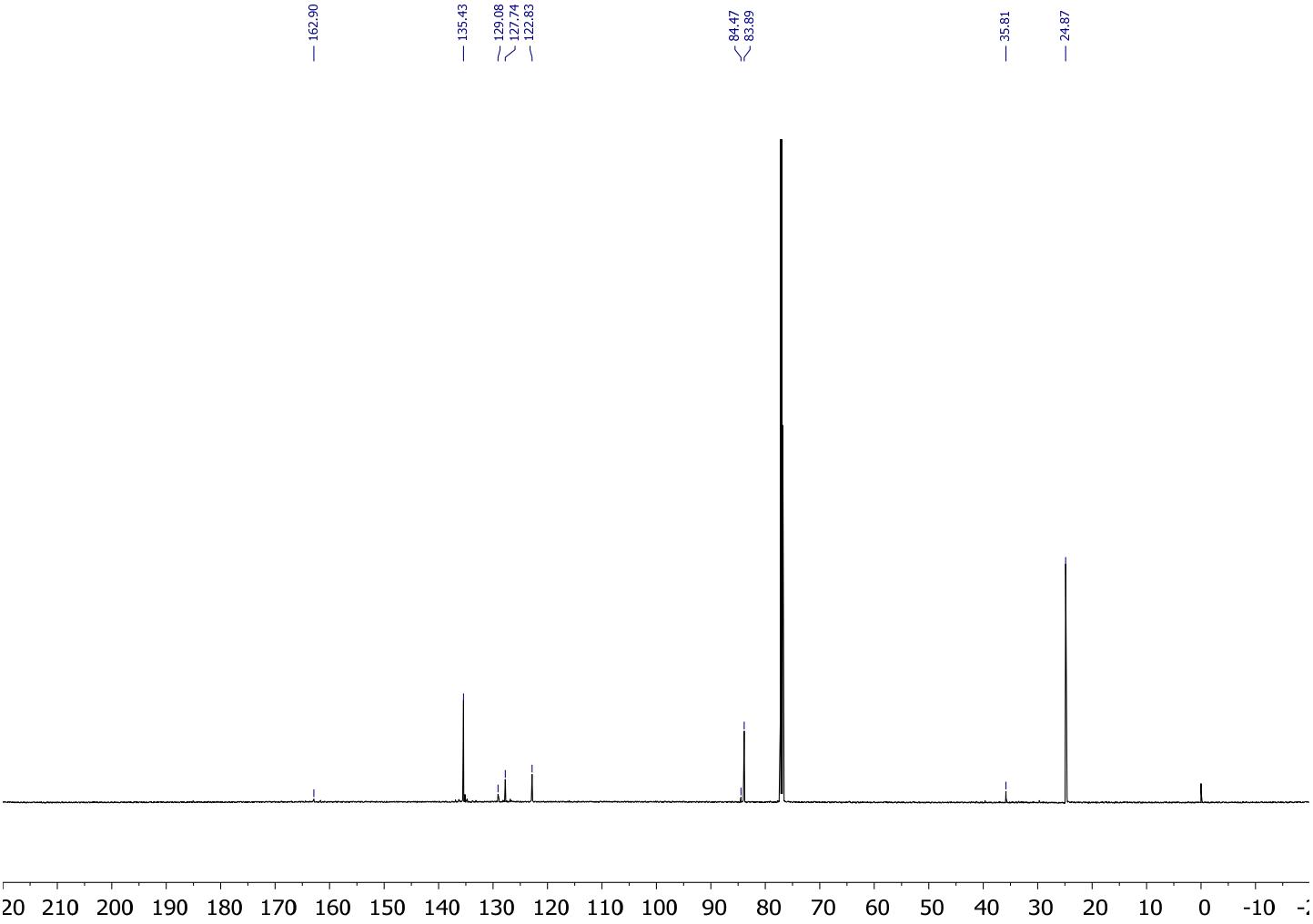
Q

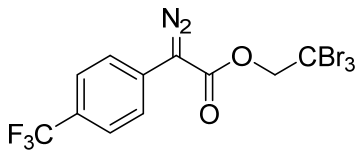


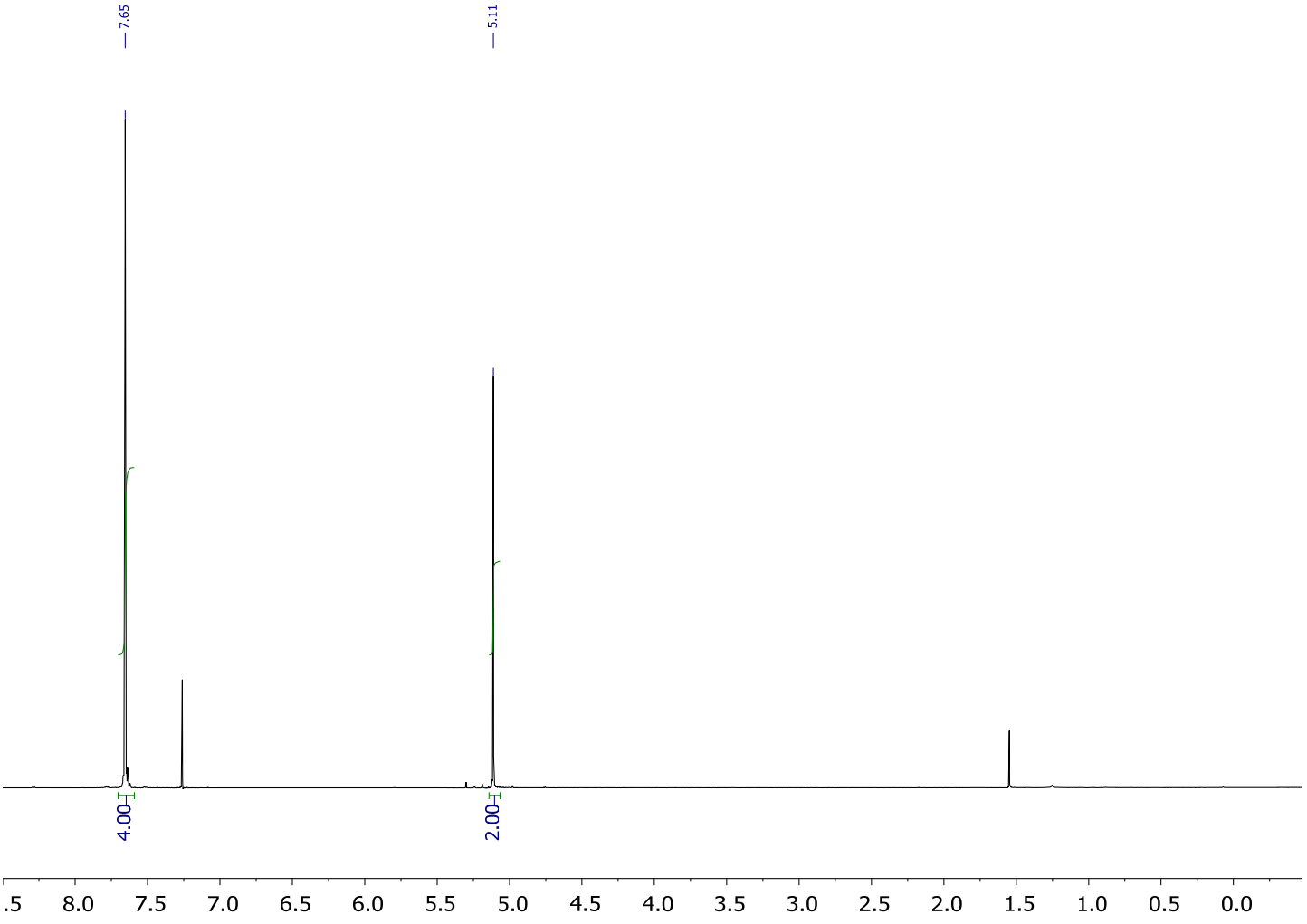
9.2 Diazo Compounds Preparation

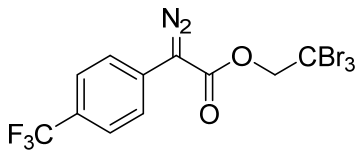


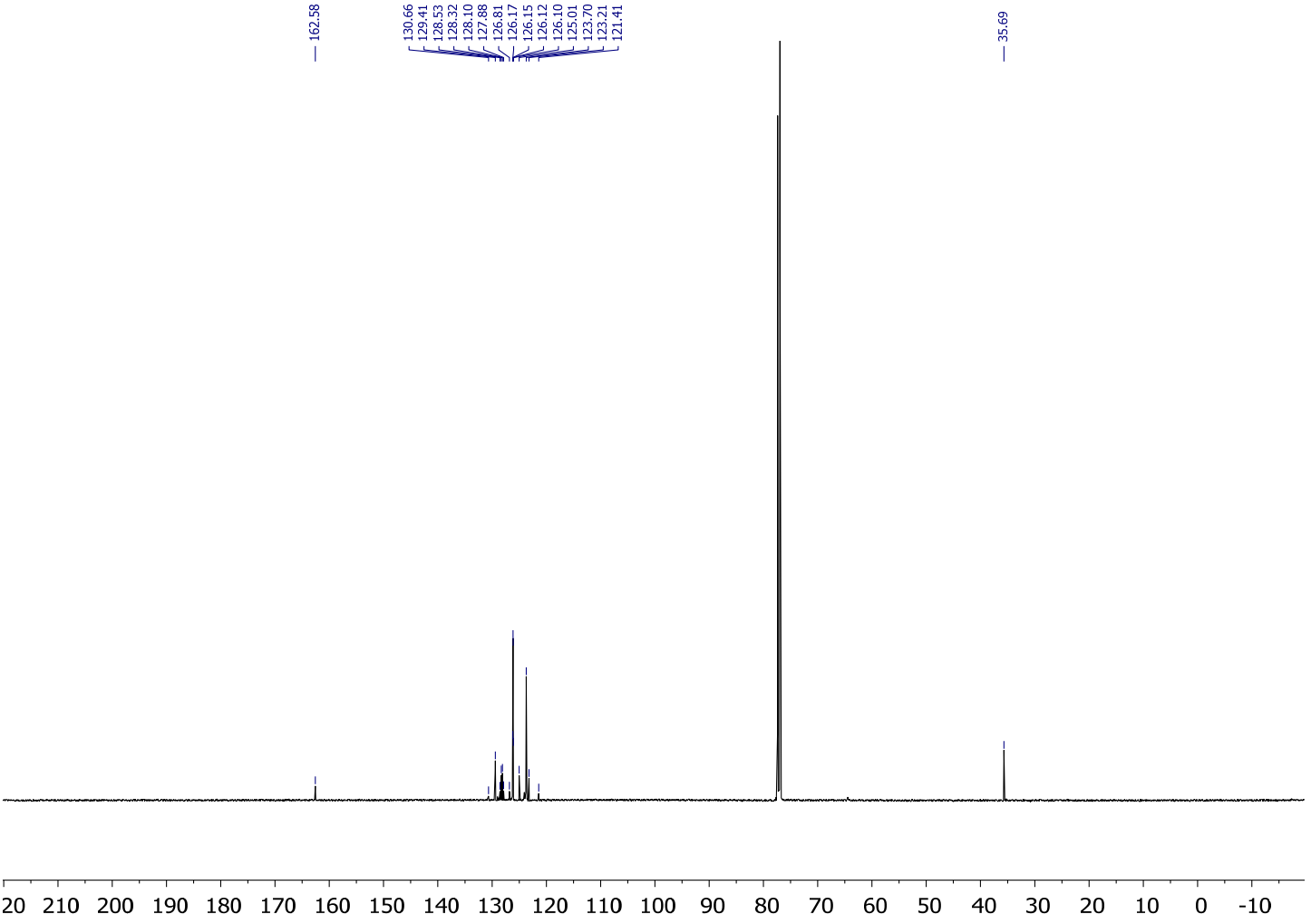

N2
O
CBr3
O
O
B
O


162.90
135.43
129.08
127.74
122.83
84.47
83.89
35.81
24.87
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

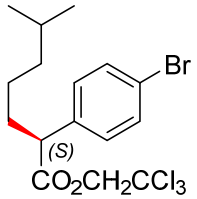

N2
O
CBr3
O
F3C

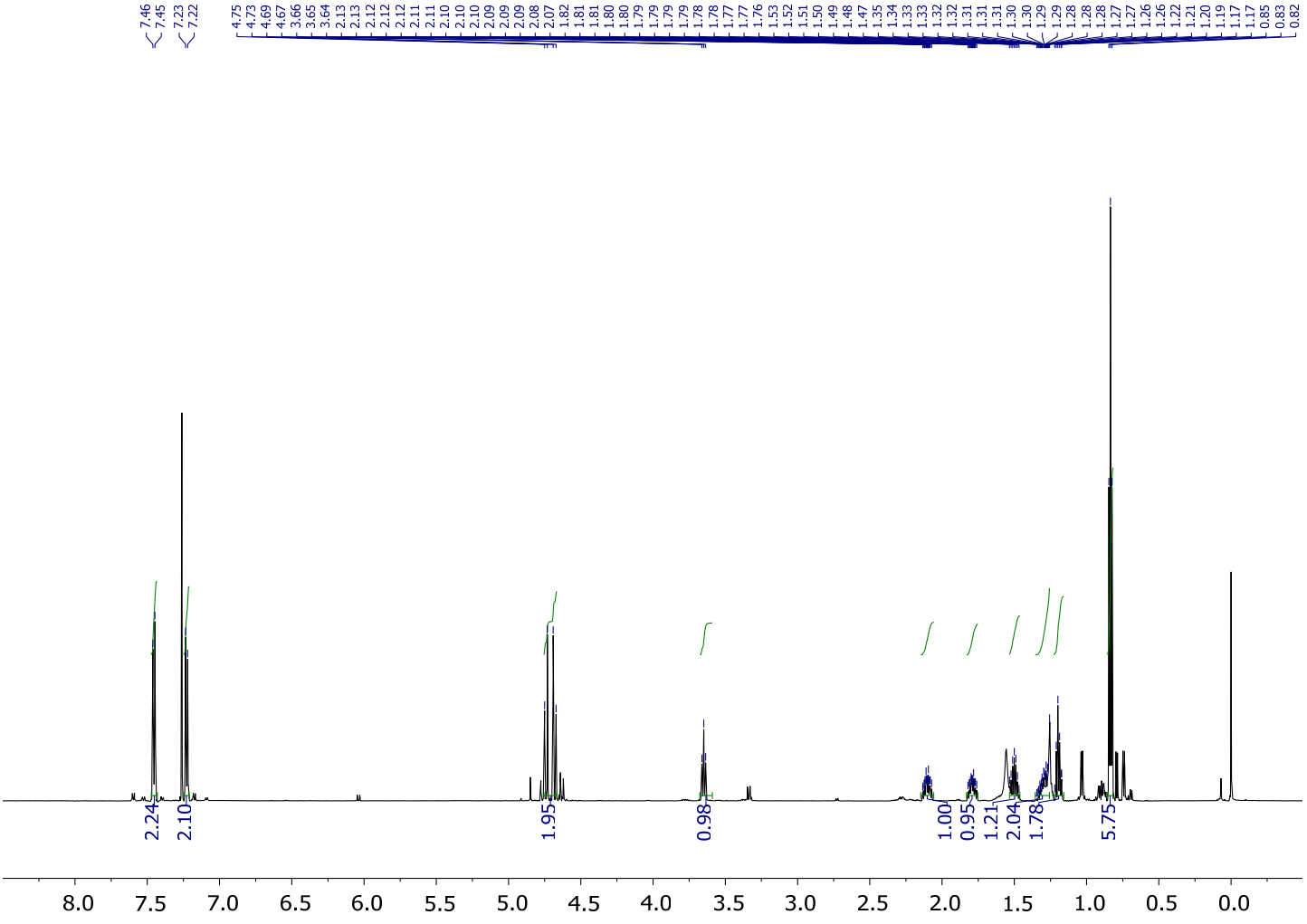

7.65
5.11
4.00
2.00
.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

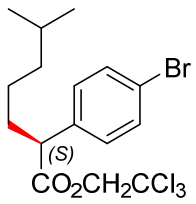

N2
O
CBr3
O
F3C

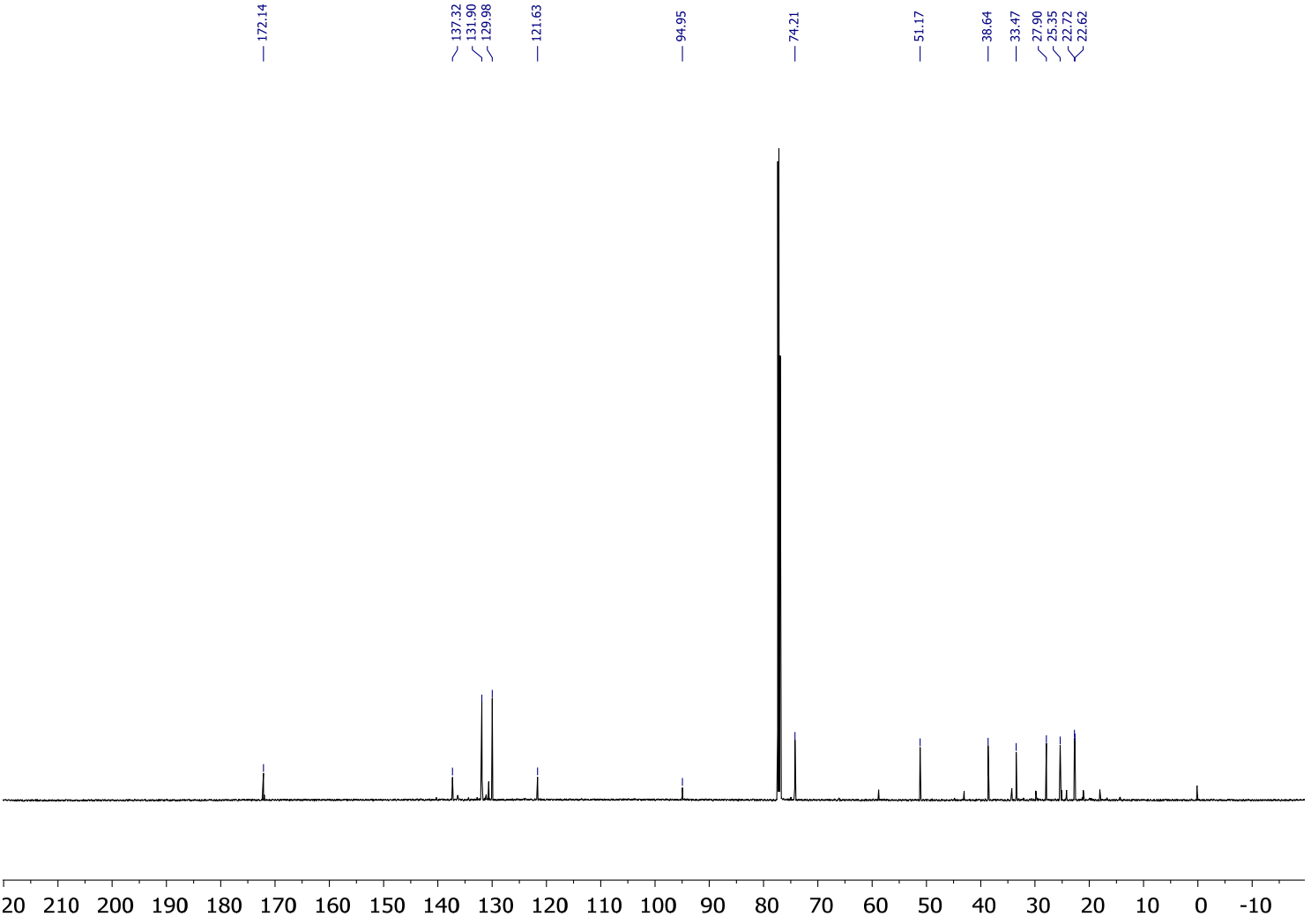

162.58
130.66
129.41
128.53
128.32
128.10
127.88
126.81
126.17
126.15
126.12
126.10
125.01
123.70
123.21
121.41
35.69
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

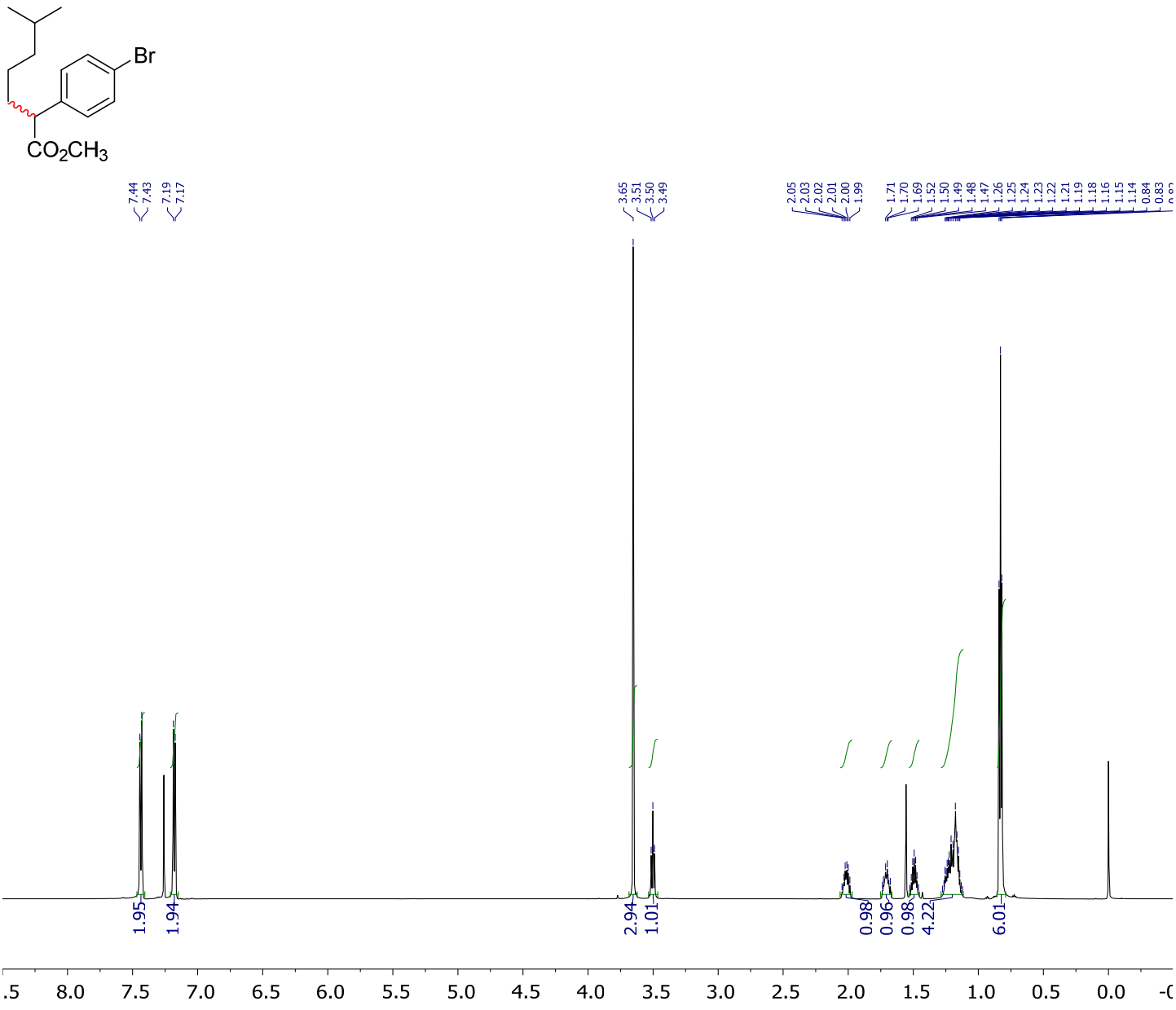
9.3 C–H Functionalization Products **5-29**

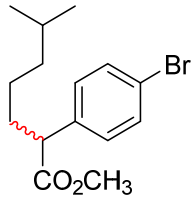


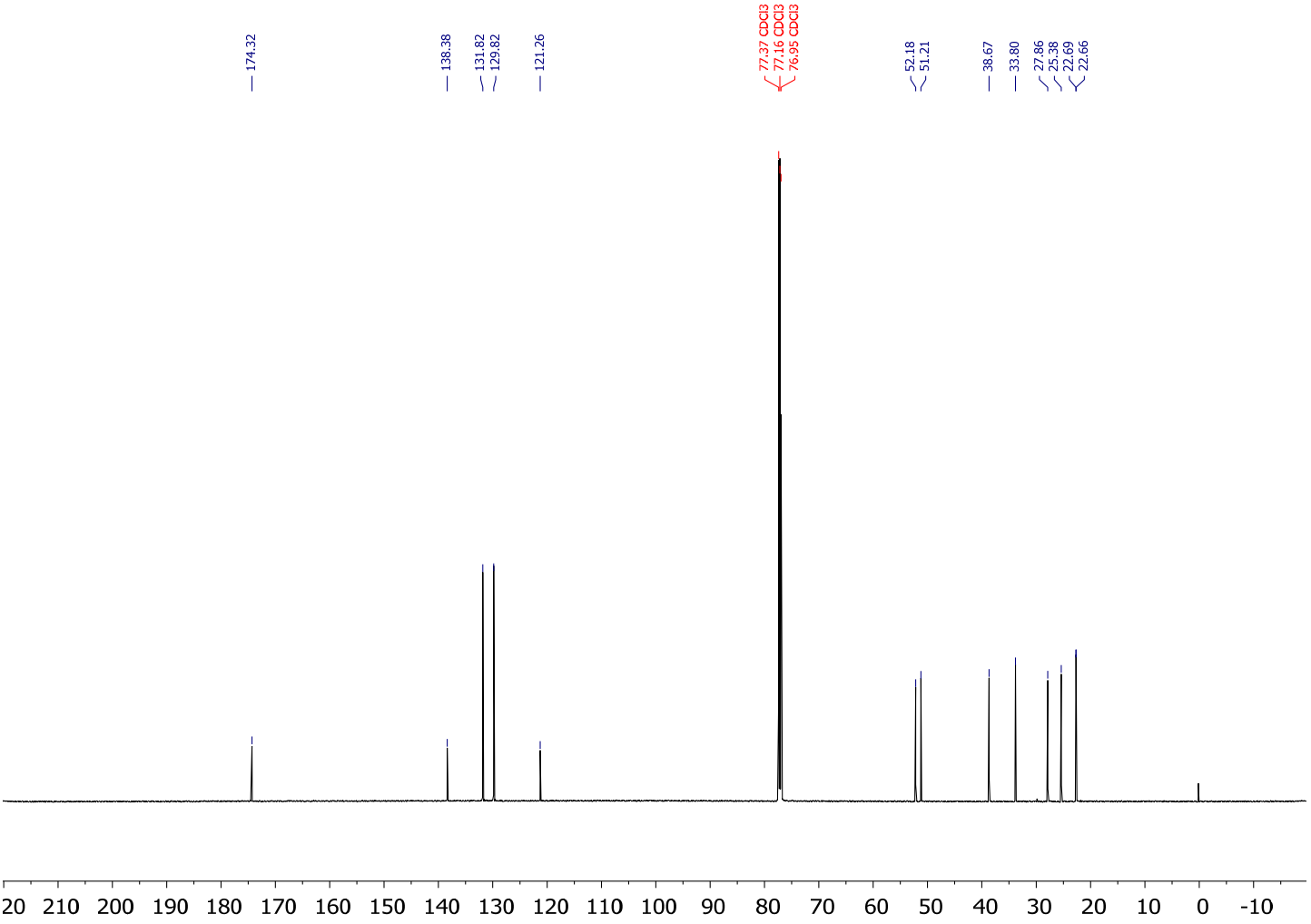


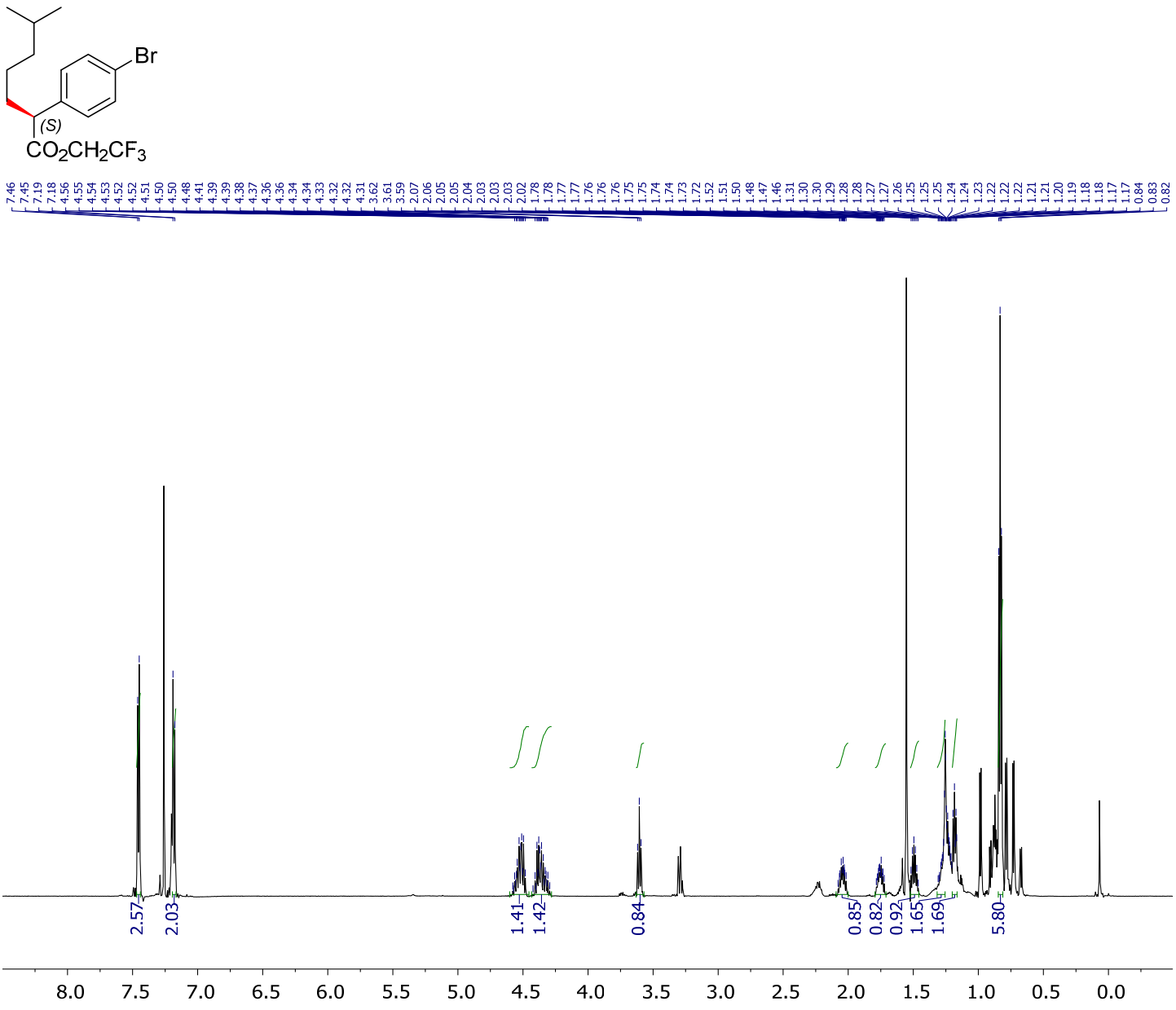

Br
(S)
CO2CH2CCl3

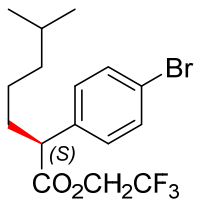

172.14
137.32
131.90
129.98
121.63
94.95
74.21
51.17
38.64
33.47
27.90
25.35
22.72
22.62
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

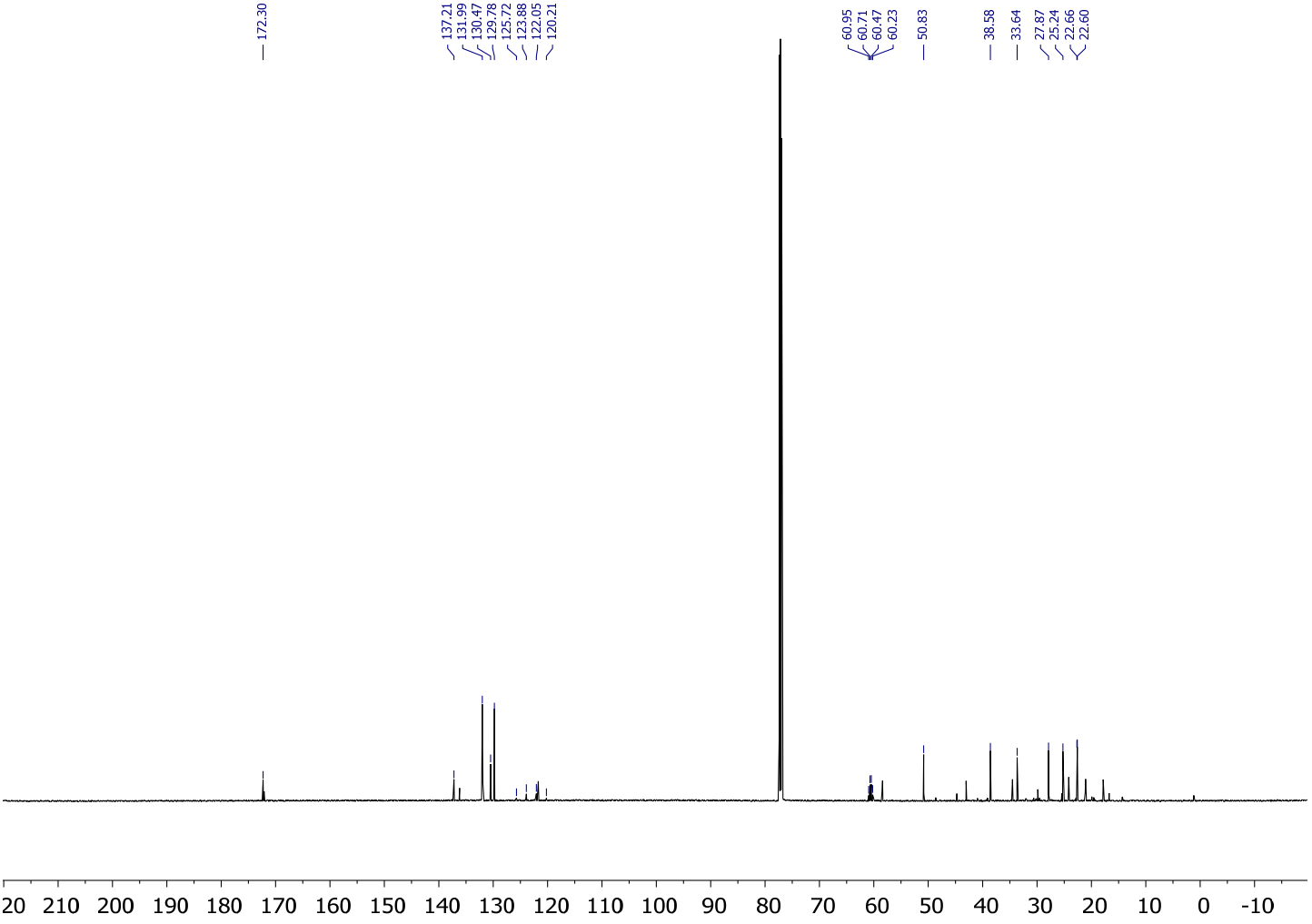

Br
CO2CH3
7.44
7.43
7.19
7.17
3.65
3.51
3.50
3.49
2.05
2.03
2.02
2.01
2.00
1.99
1.71
1.70
1.69
1.52
1.50
1.49
1.48
1.47
1.26
1.25
1.24
1.23
1.22
1.21
1.19
1.18
1.16
1.15
1.14
0.84
0.83
1.95
1.94
2.94
1.01
0.98
0.96
0.98
4.22
6.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

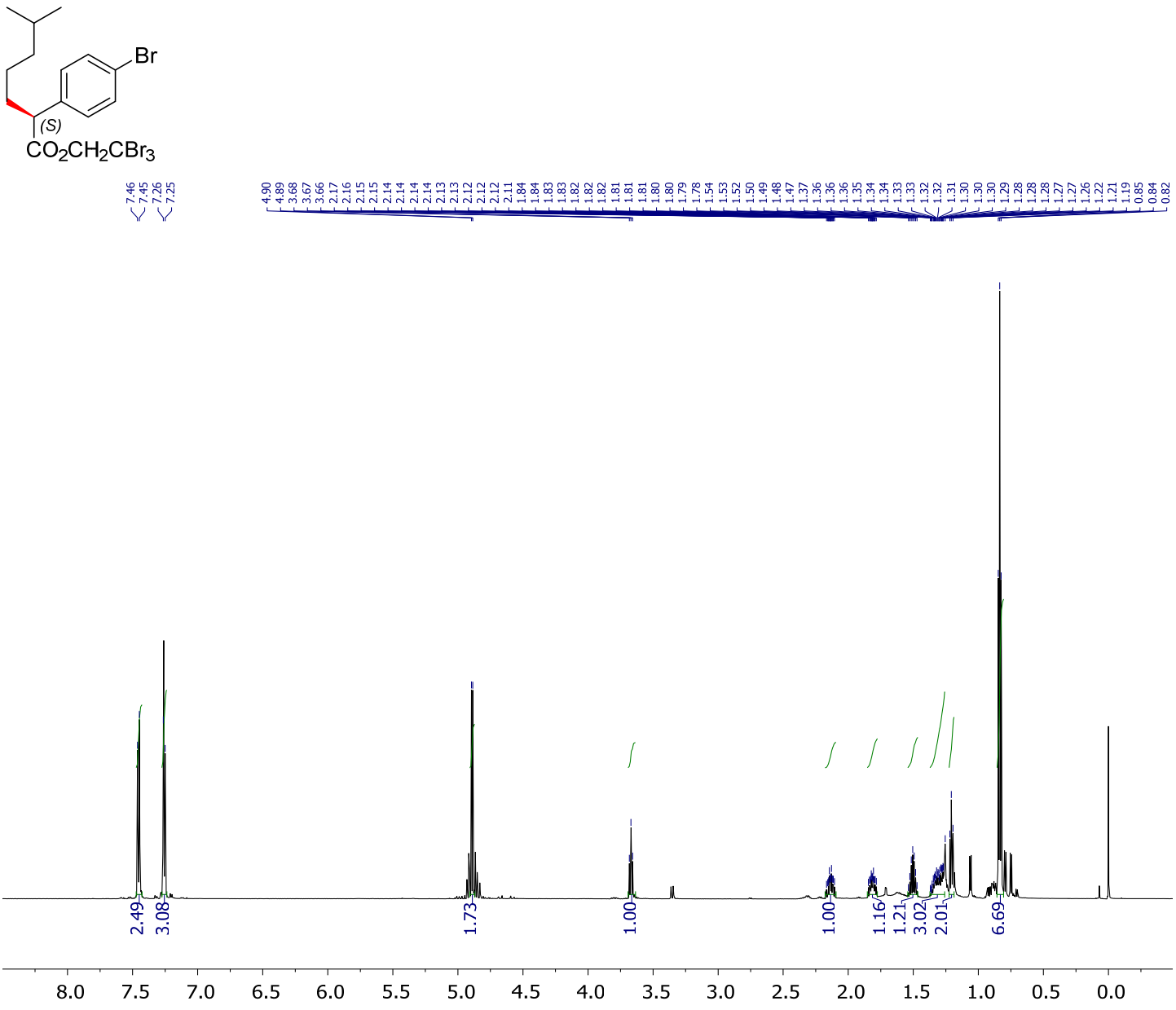

Br
CO2CH3

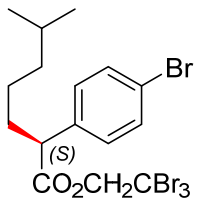

174.32
138.38
131.82
129.82
121.26
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
52.18
51.21
38.67
33.80
27.86
25.38
22.69
22.66
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

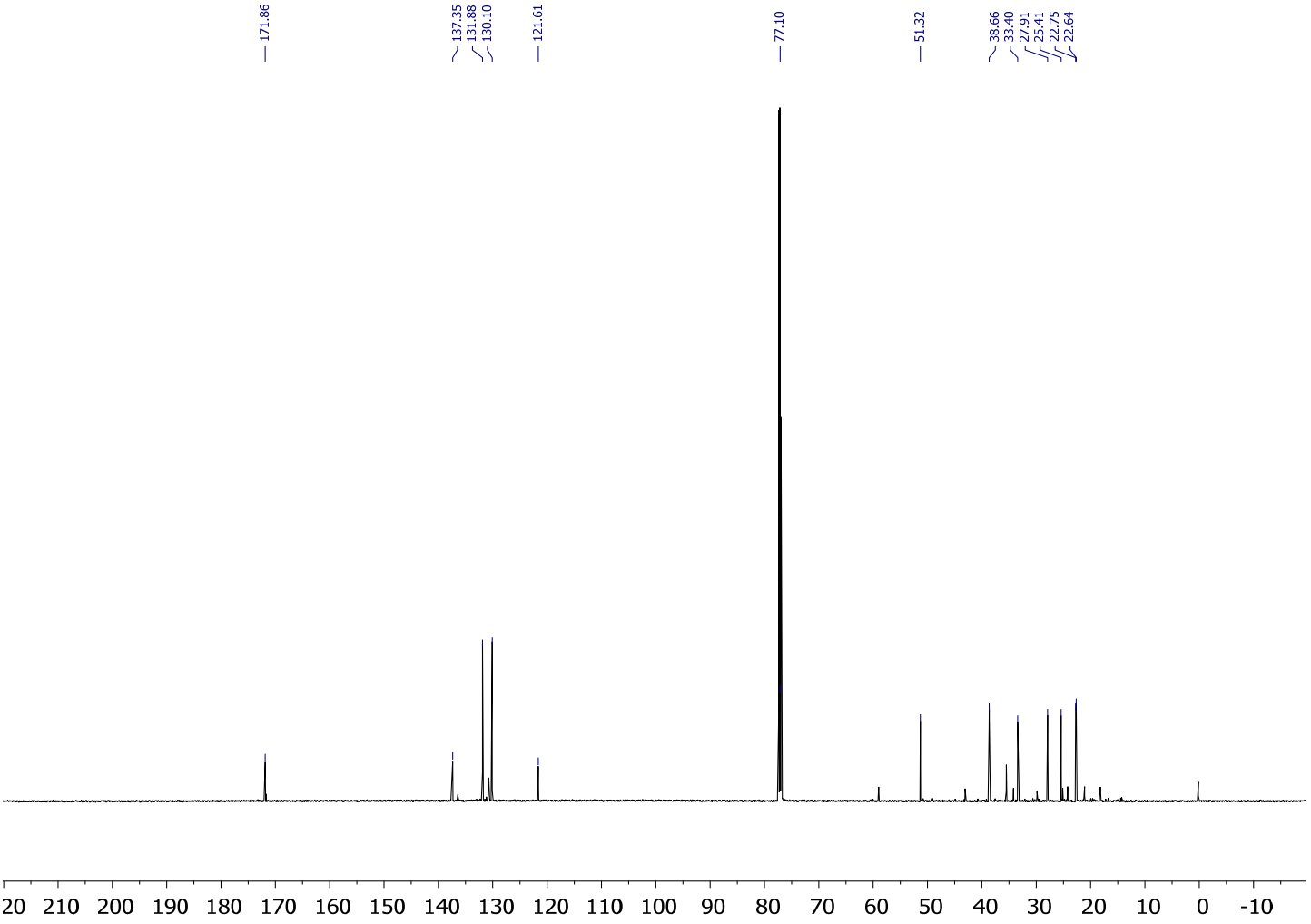

Br
(S)
CO2CH2CF3
2.57
2.03
1.41
1.42
0.84
0.85
0.82
0.92
1.65
1.69
5.80
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

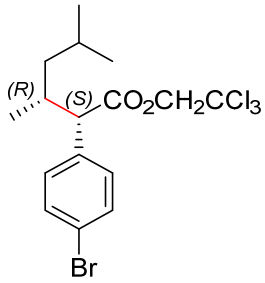

Br
(S)
CO2CH2CF3

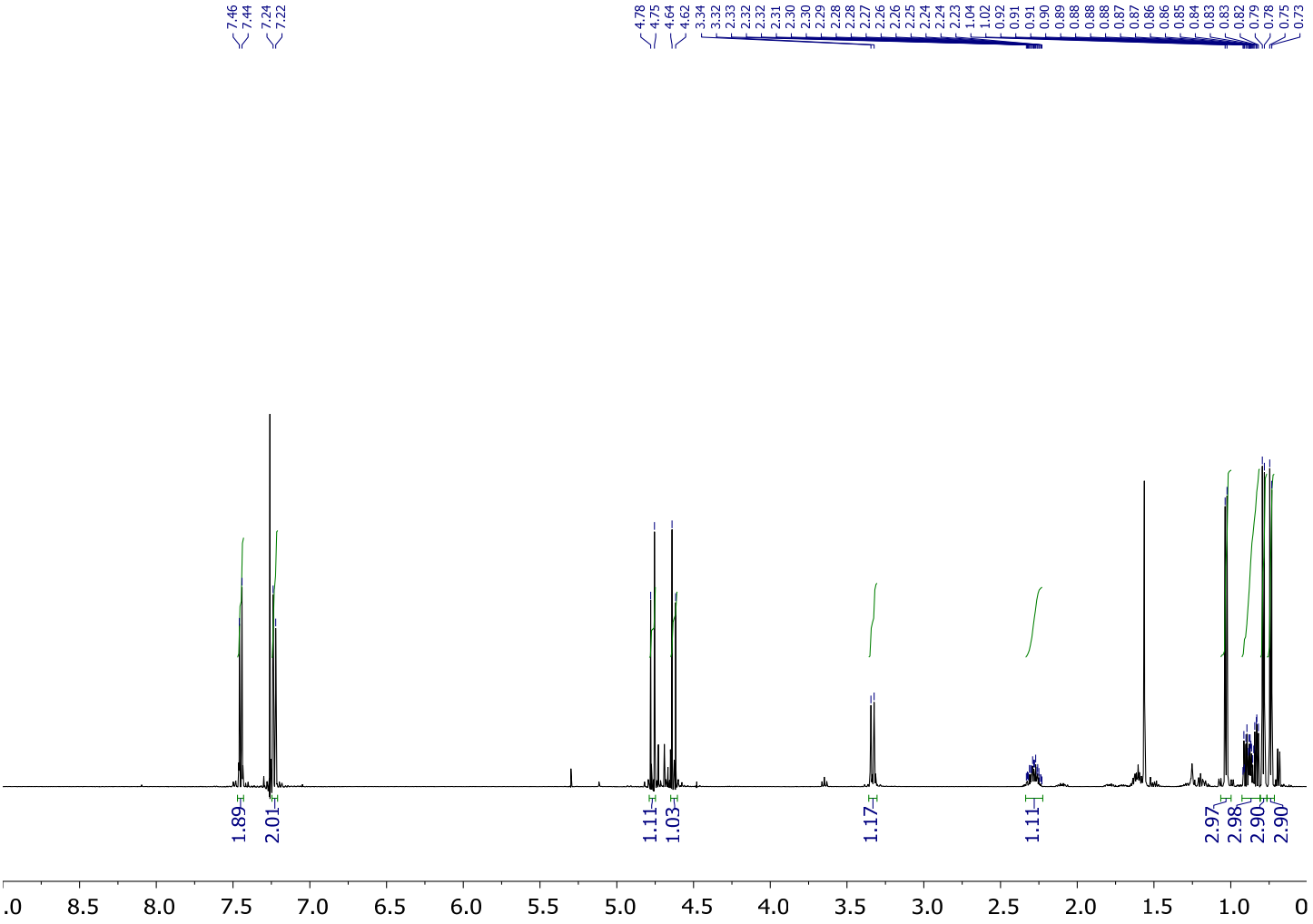

172.30
137.21
131.99
130.47
129.78
125.72
123.88
122.05
120.21
60.95
60.71
60.47
60.23
50.83
38.58
33.64
27.87
25.24
22.66
22.60
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


Br
(S)
CO2CH2CBr3
7.46
7.45
7.26
7.25
4.90
4.89
3.68
3.67
3.66
2.17
2.16
2.15
2.15
2.14
2.14
2.14
2.14
2.13
2.13
2.12
2.12
2.12
2.11
1.84
1.84
1.83
1.83
1.82
1.82
1.82
1.81
1.81
1.81
1.80
1.80
1.79
1.78
1.54
1.53
1.52
1.50
1.49
1.48
1.47
1.37
1.36
1.36
1.35
1.34
1.34
1.33
1.33
1.32
1.32
1.31
1.30
1.30
1.30
1.29
1.28
1.28
1.28
1.27
1.27
1.26
1.22
1.21
1.19
0.85
0.84
0.82
2.49
3.08
1.73
1.00
1.00
1.16
1.21
3.02
2.01
6.69
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


Br
(S)
CO2CH2CBr3


171.86
137.35
131.88
130.10
121.61
77.10
51.32
38.66
33.40
27.91
25.41
22.75
22.64
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


(R)
(S)
CO2CH2CCl3
Br


7.46
7.44
7.24
7.22
4.78
4.75
4.64
4.62
3.34
3.32
2.33
2.32
2.32
2.31
2.30
2.30
2.29
2.28
2.28
2.27
2.26
2.26
2.25
2.24
2.24
2.23
1.04
1.02
0.92
0.91
0.91
0.90
0.89
0.88
0.88
0.88
0.87
0.87
0.86
0.86
0.85
0.84
0.83
0.83
0.82
0.79
0.78
0.75
0.73
1.89
2.01
1.11
1.03
1.17
1.11
2.97
2.98
2.90
2.90
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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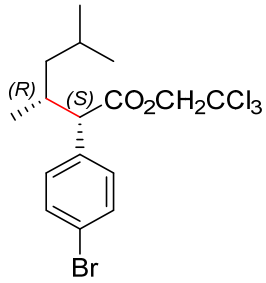
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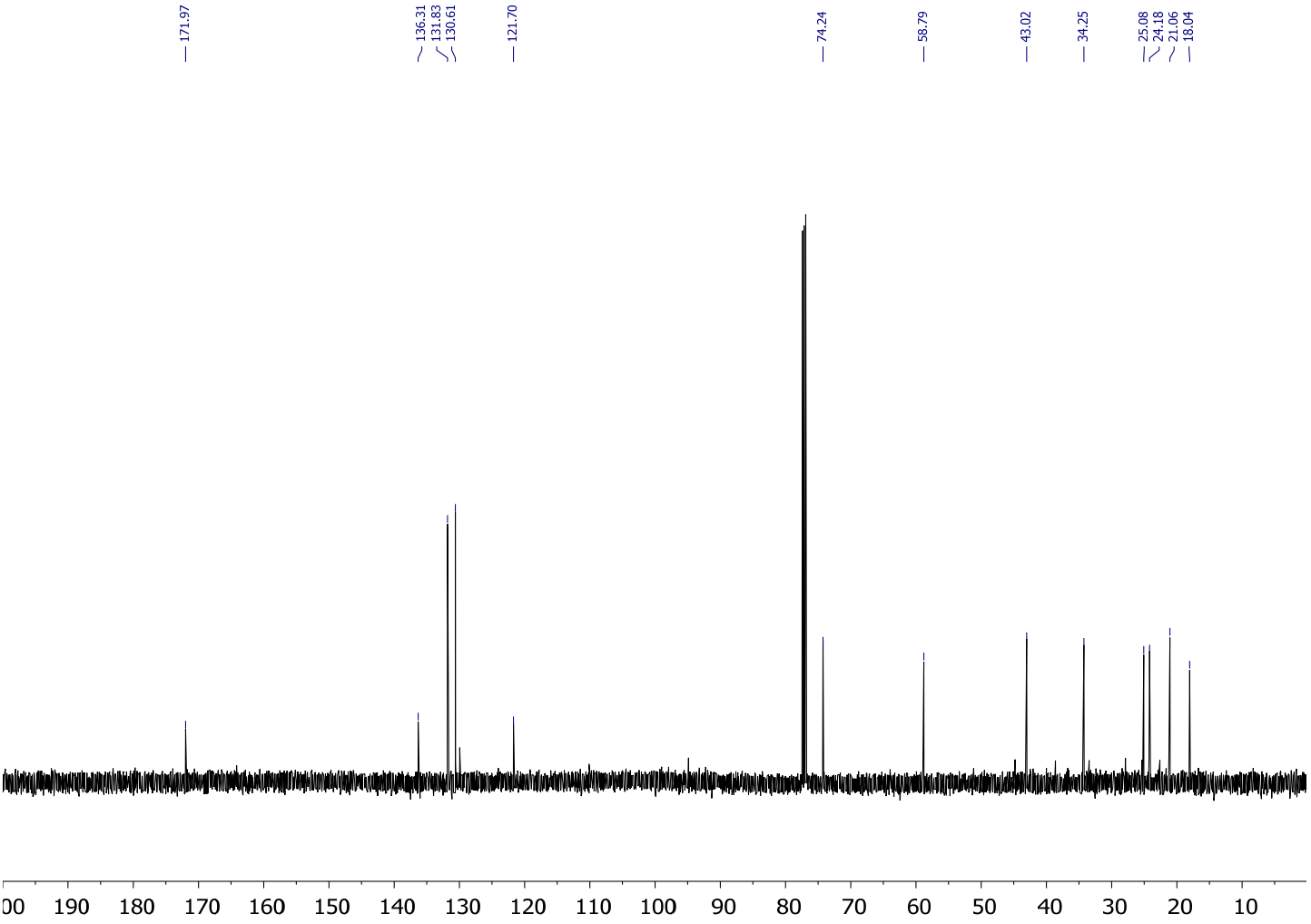
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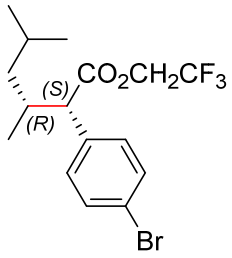
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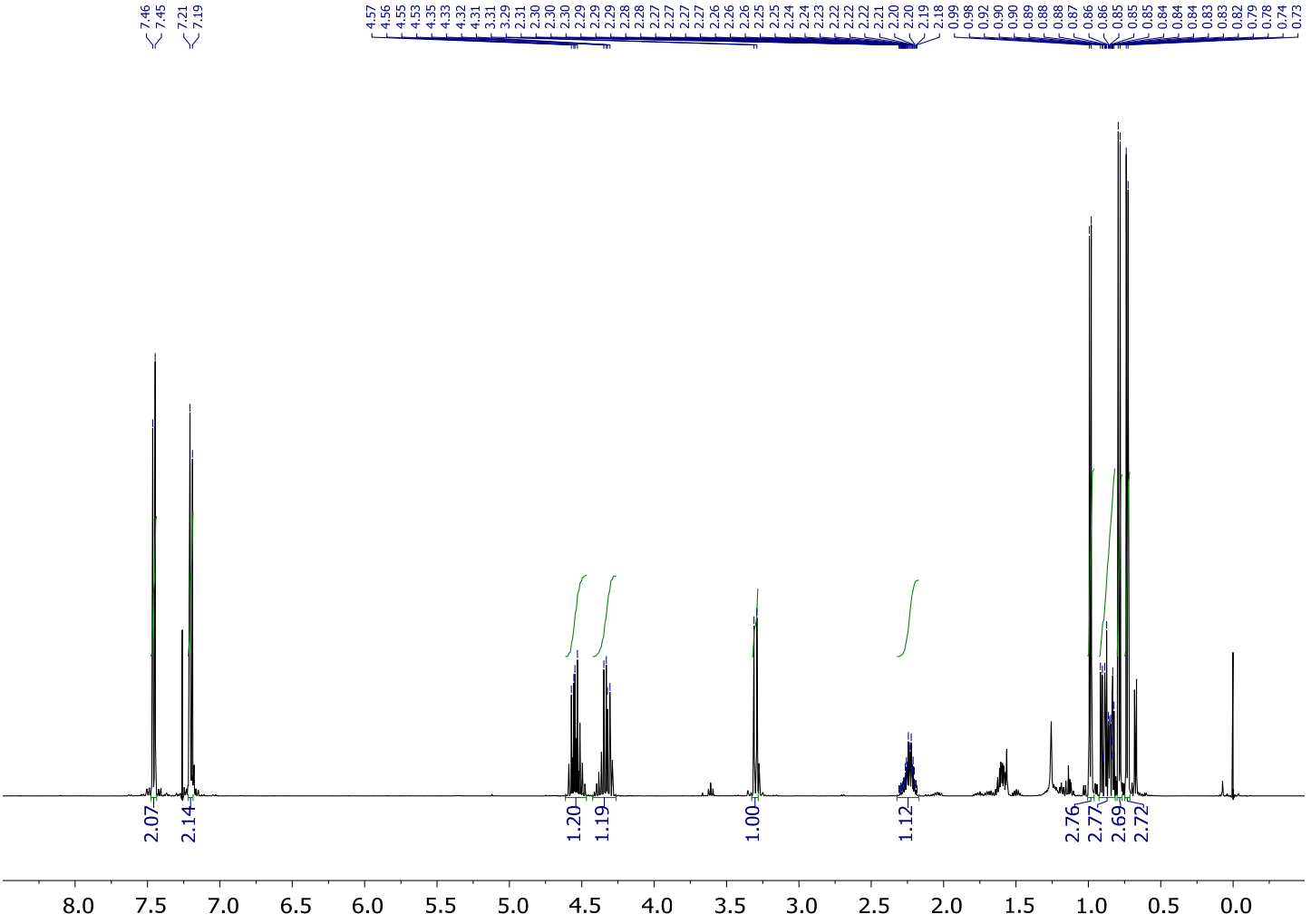
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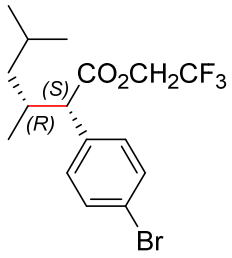
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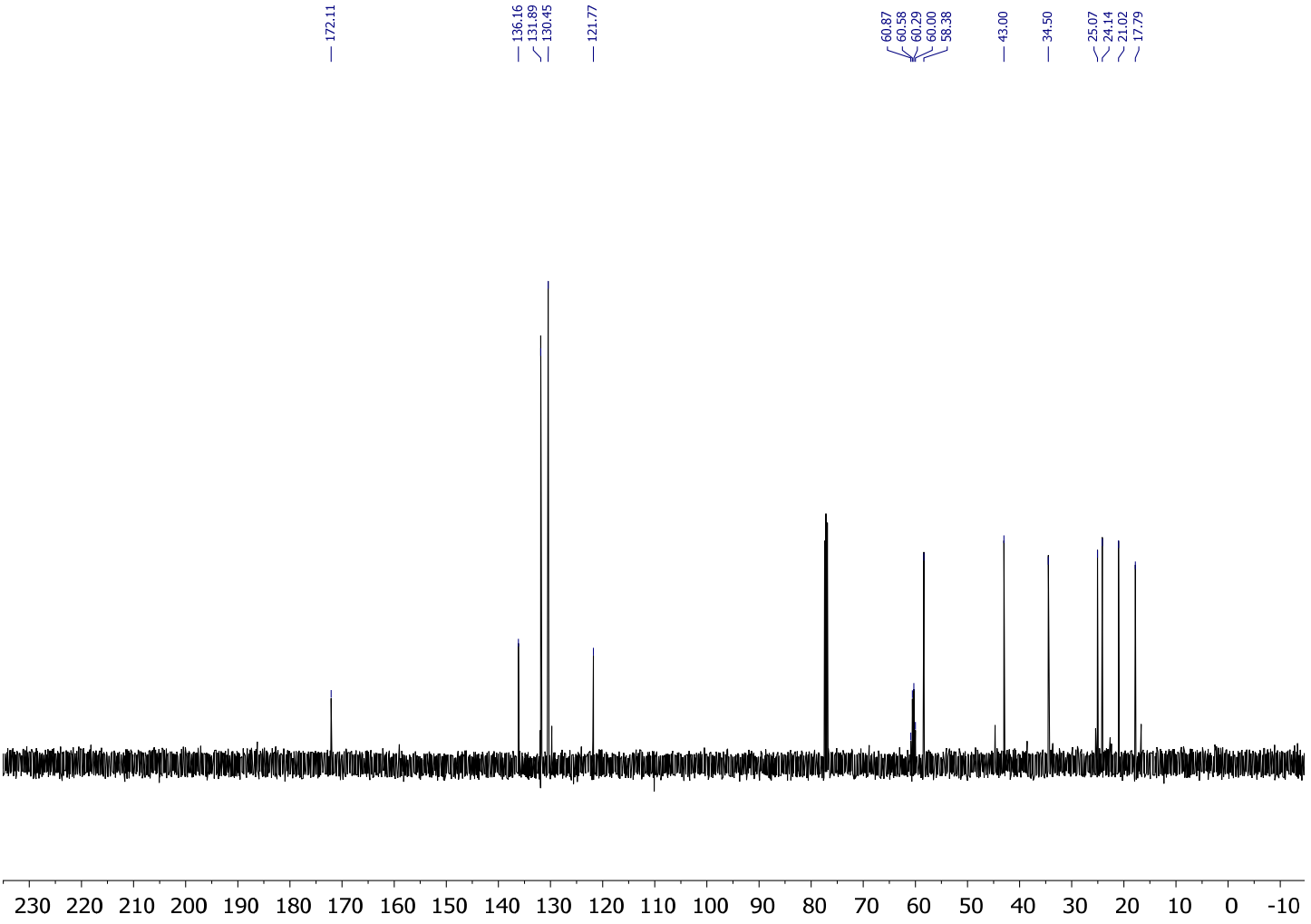
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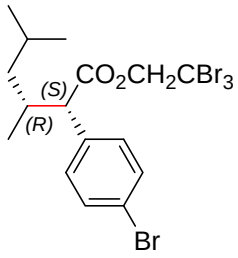
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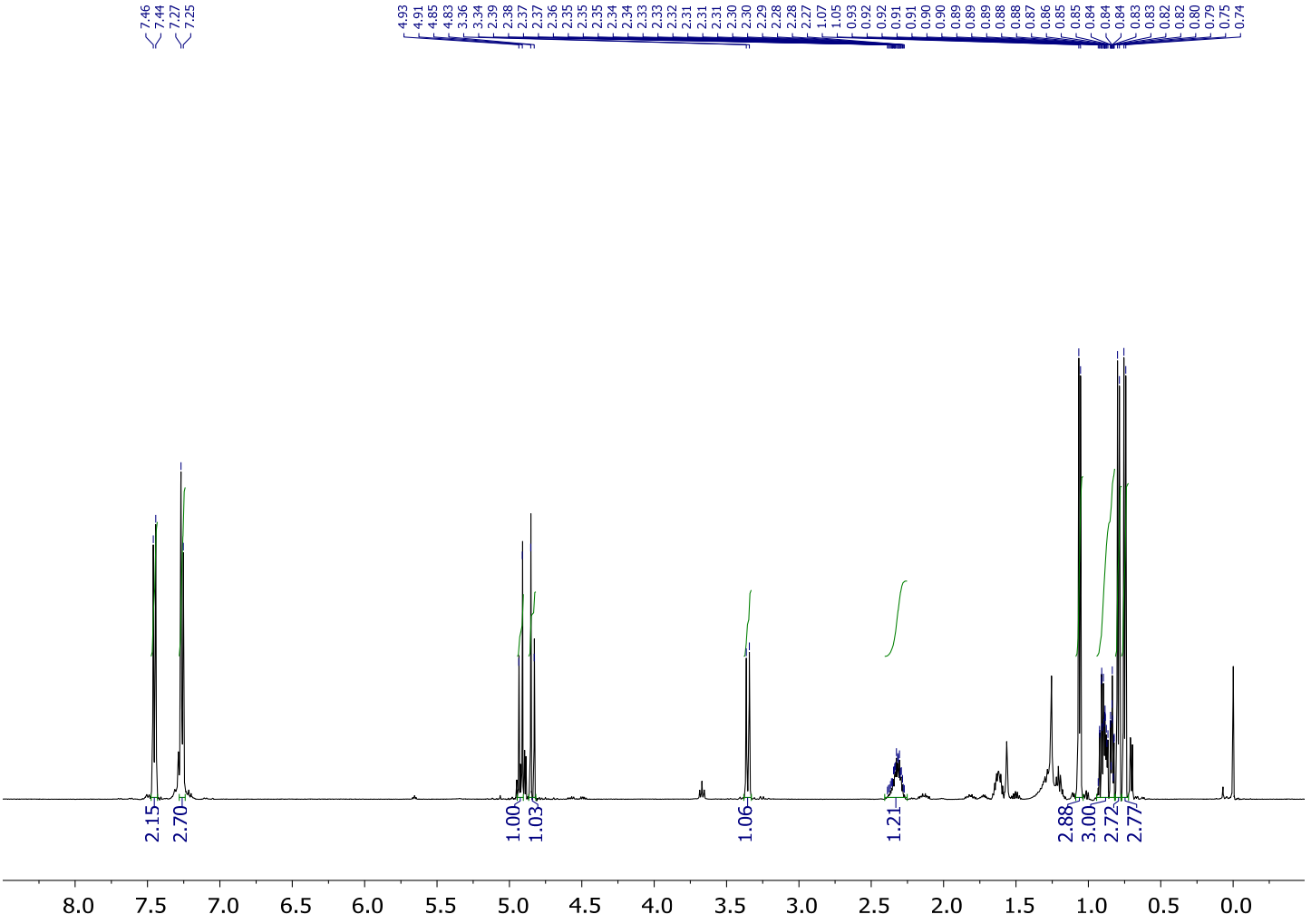
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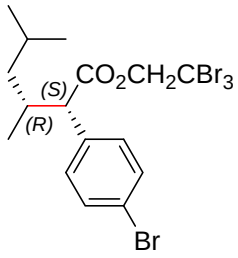
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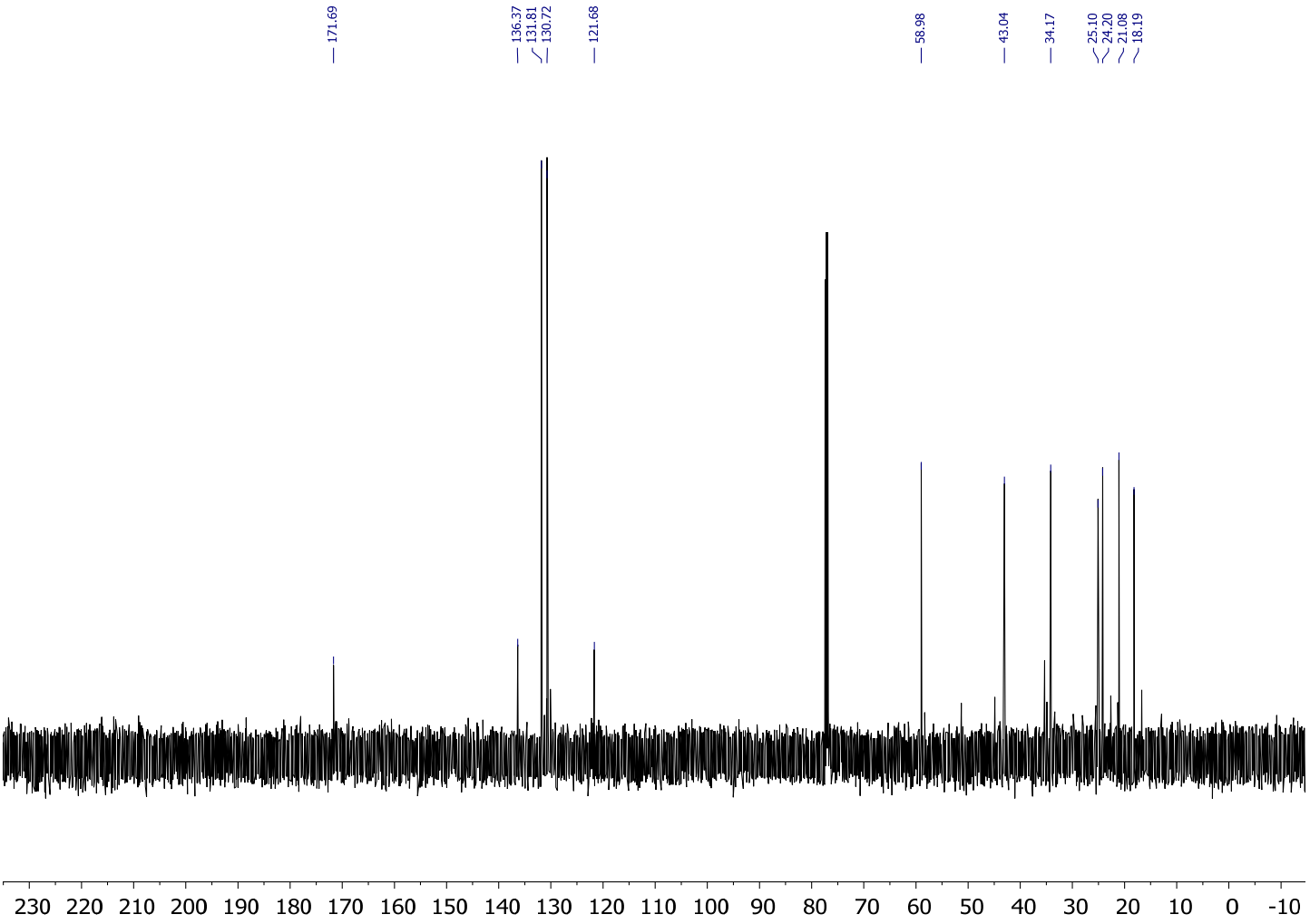
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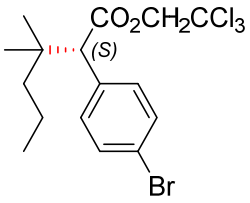
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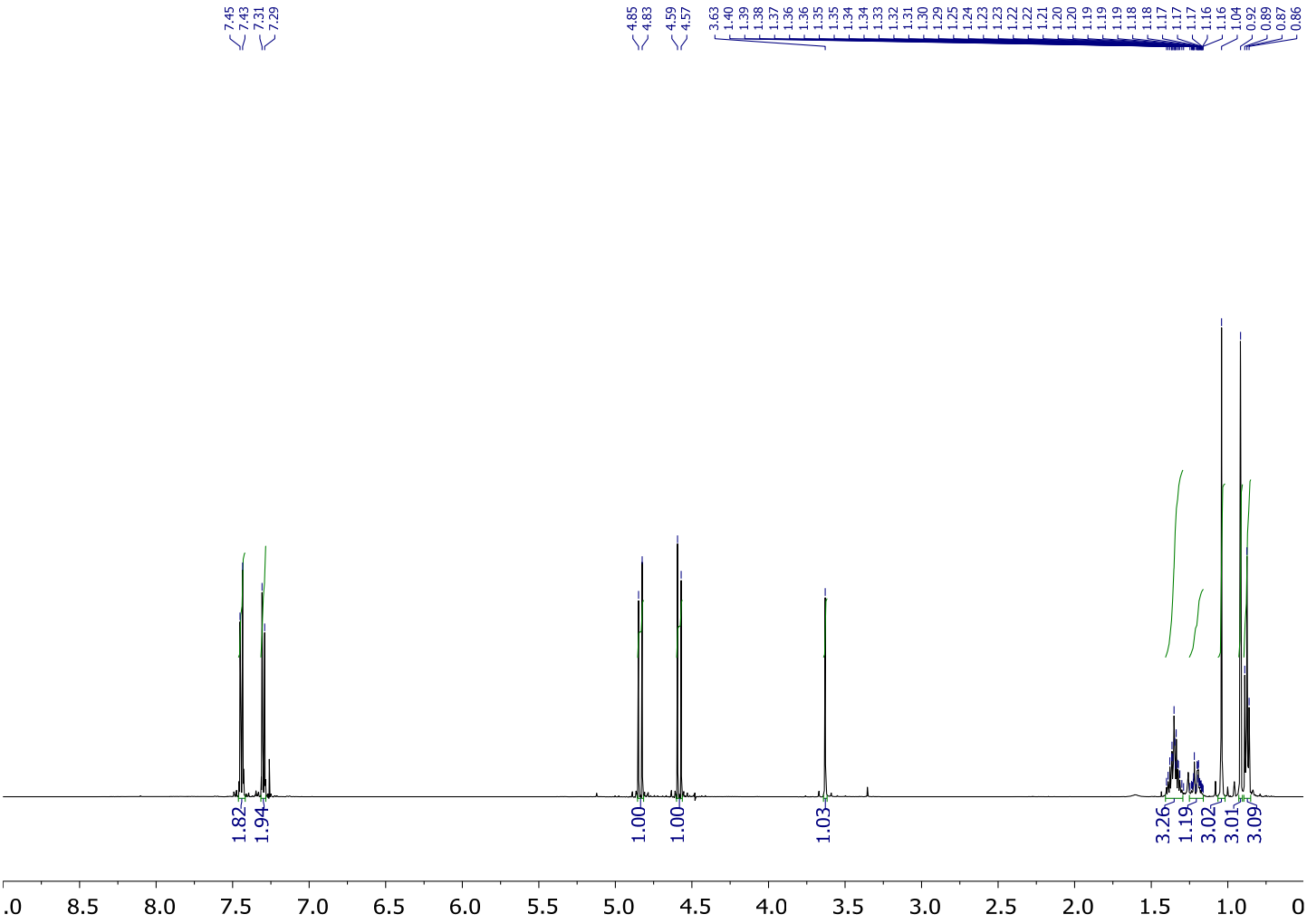
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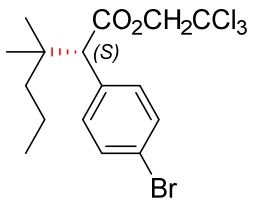
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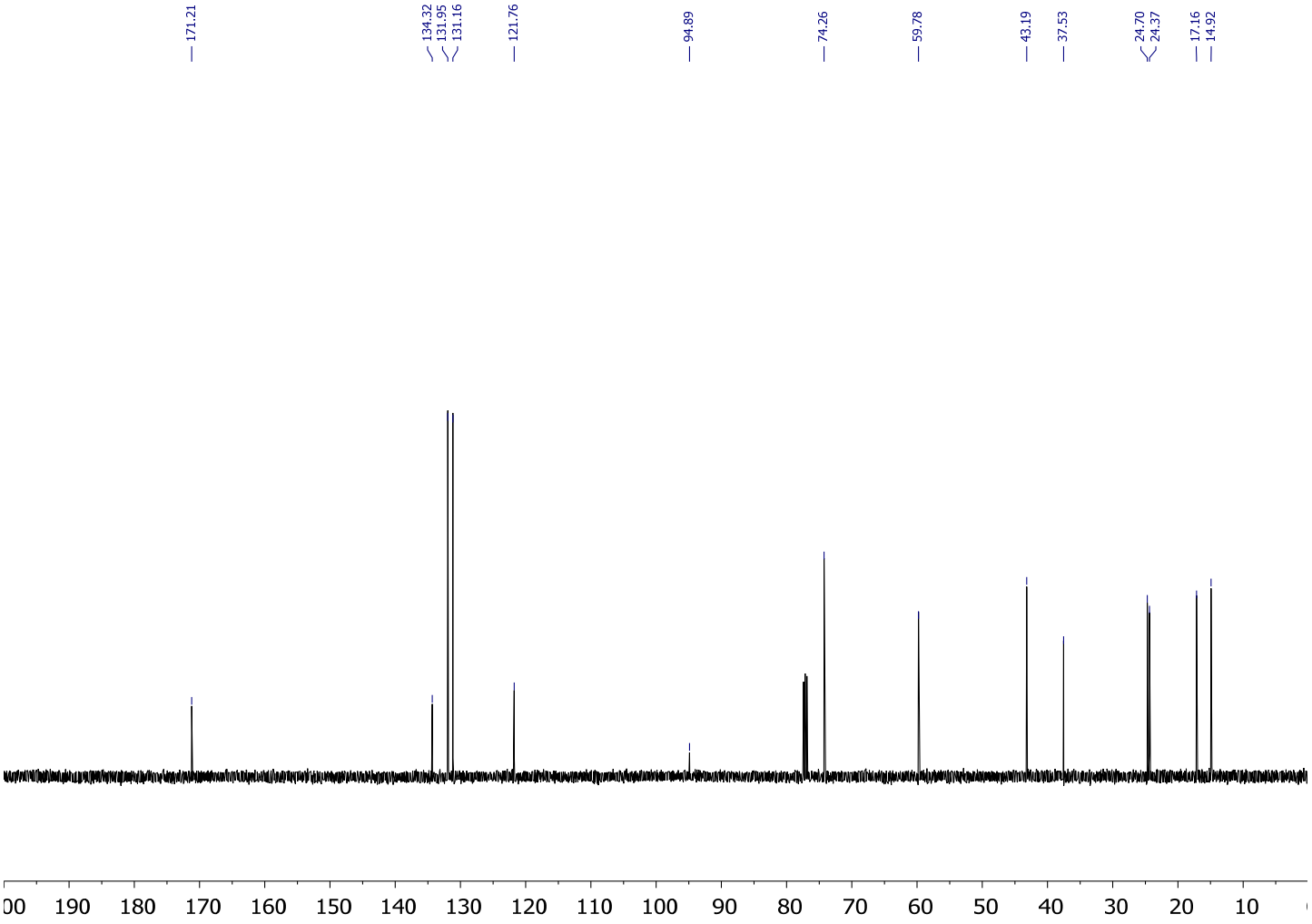
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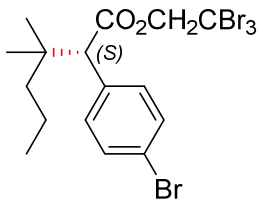
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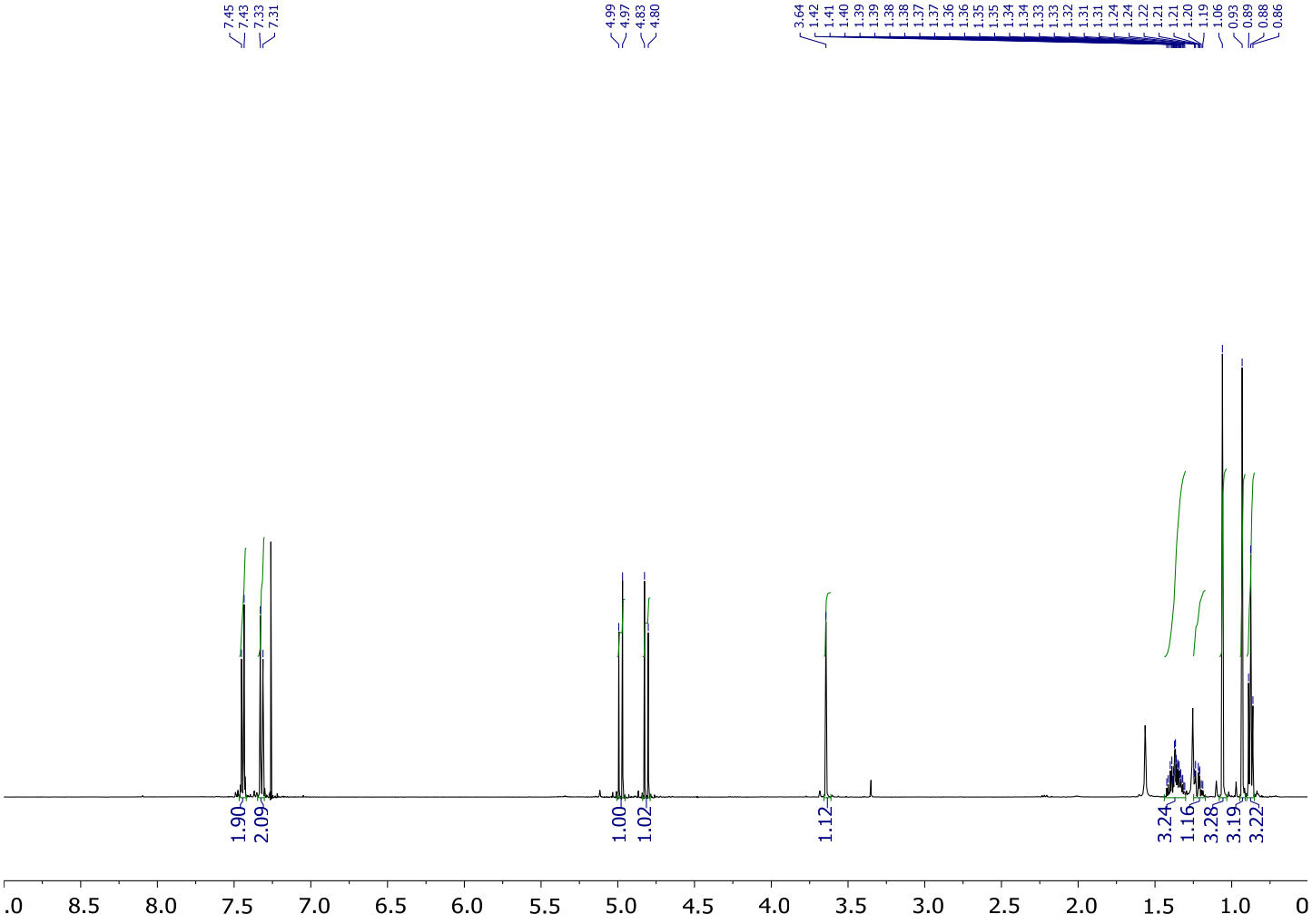
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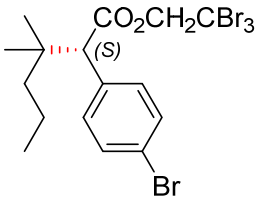
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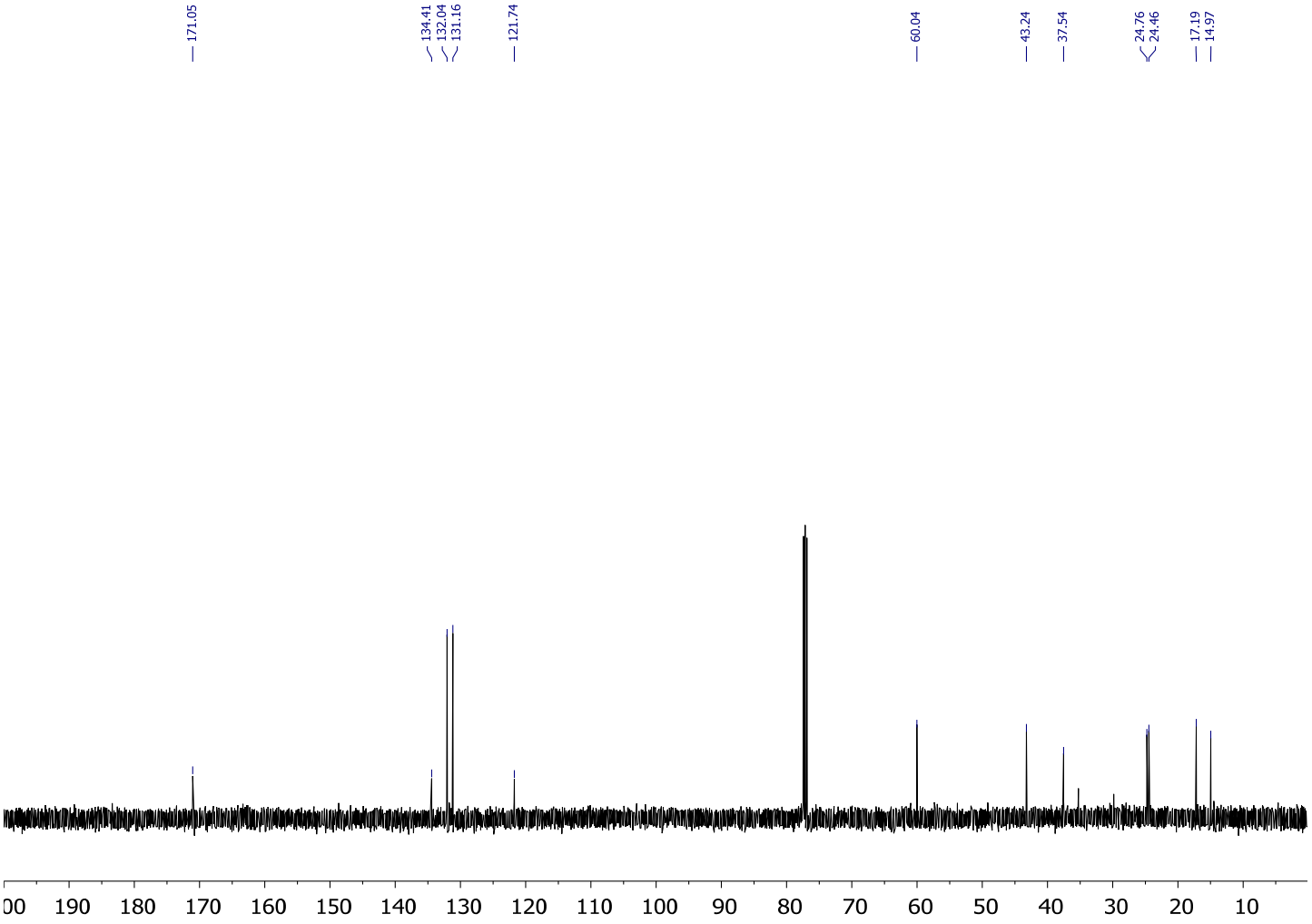
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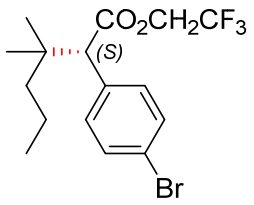
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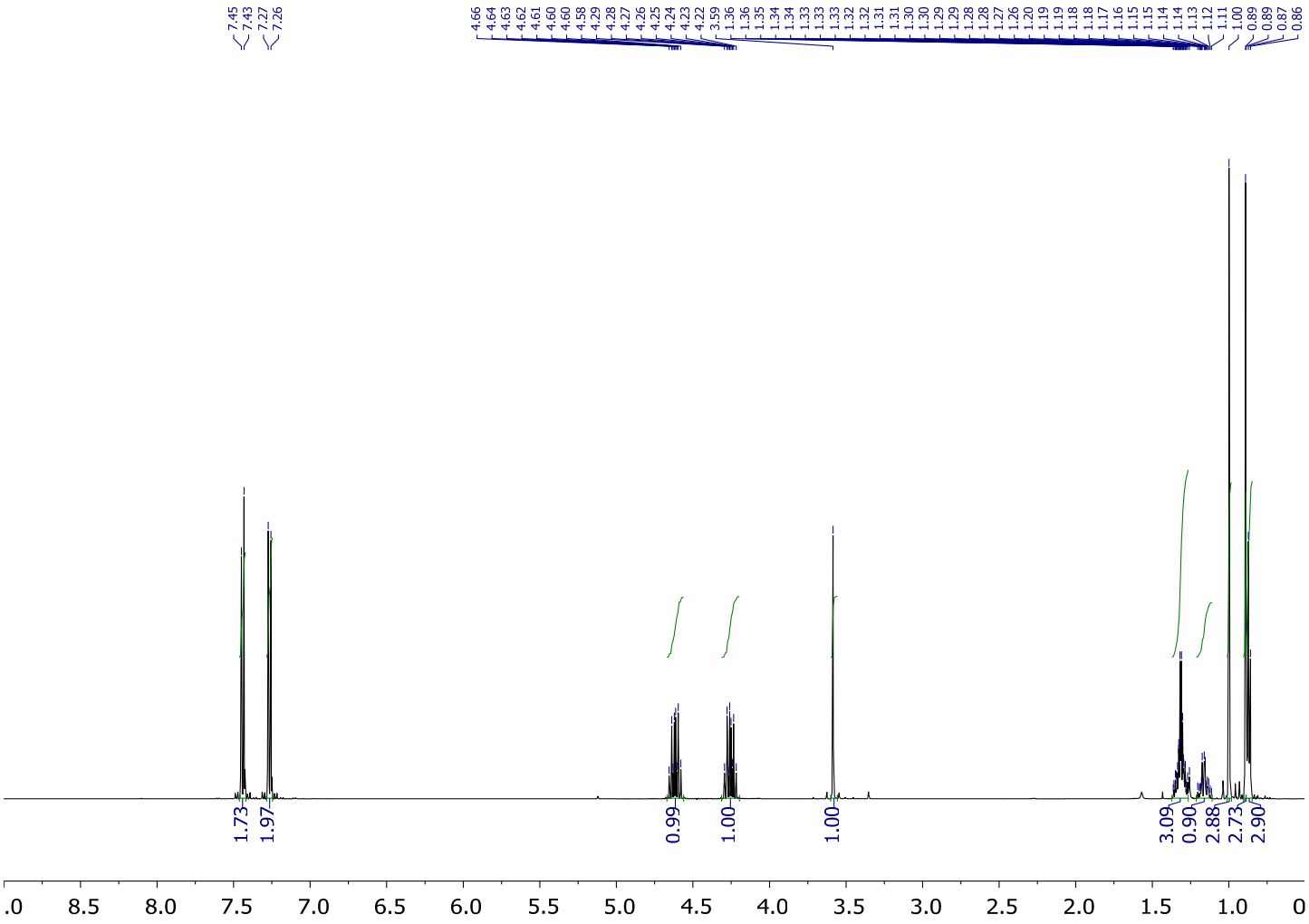
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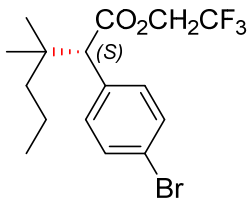
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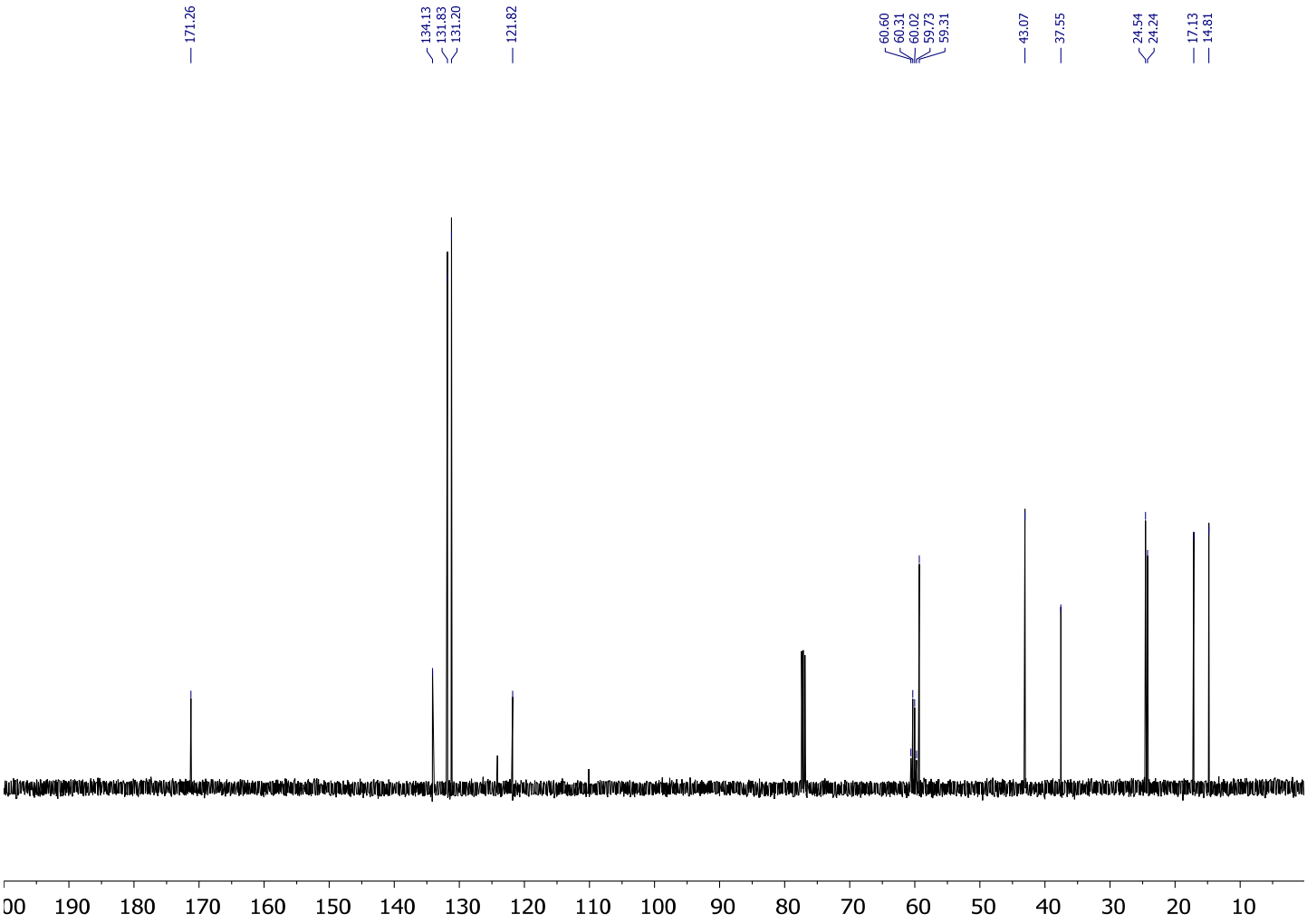
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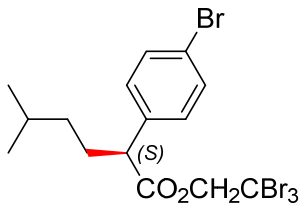
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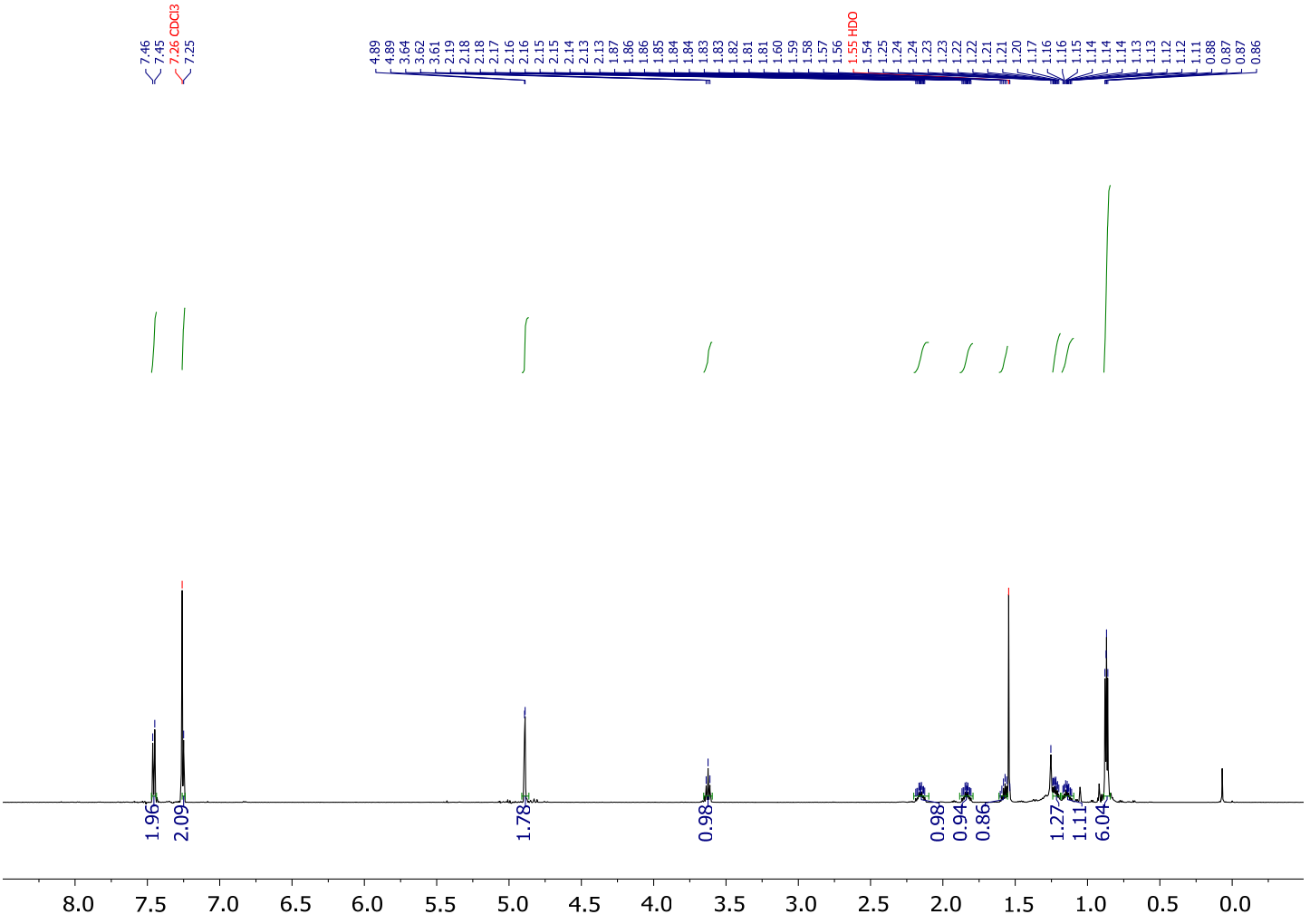
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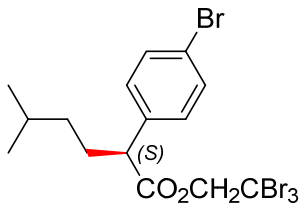
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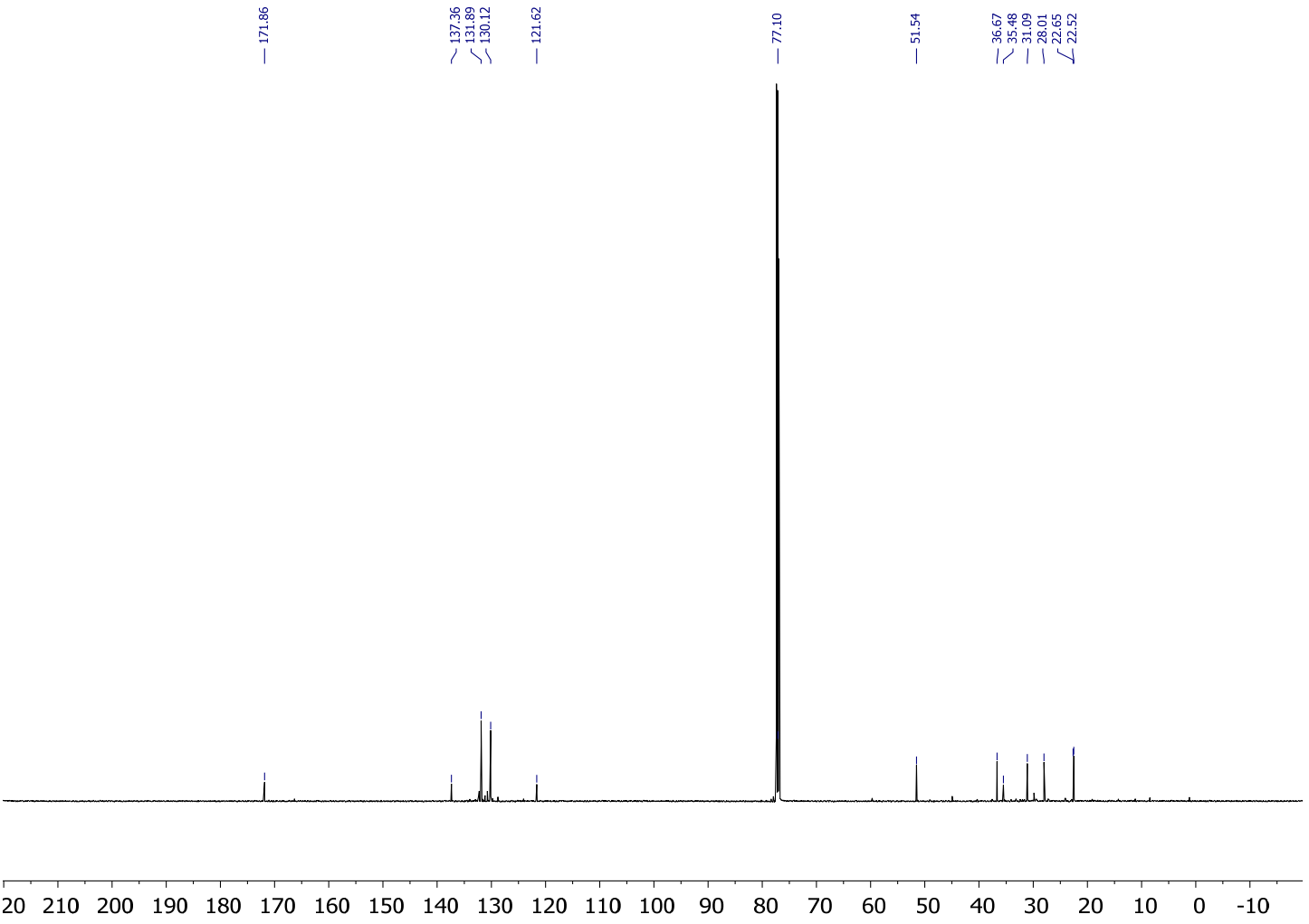
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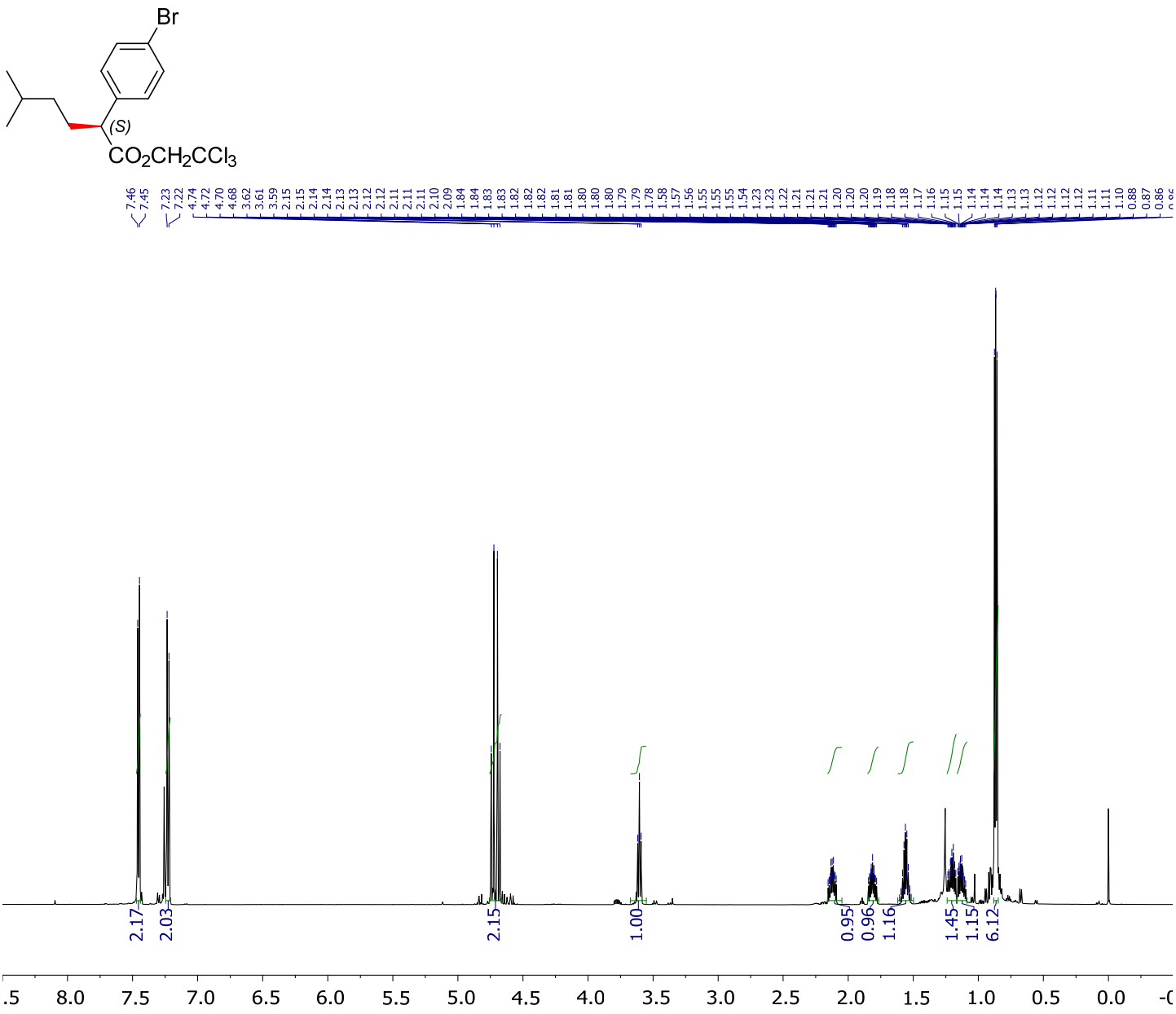
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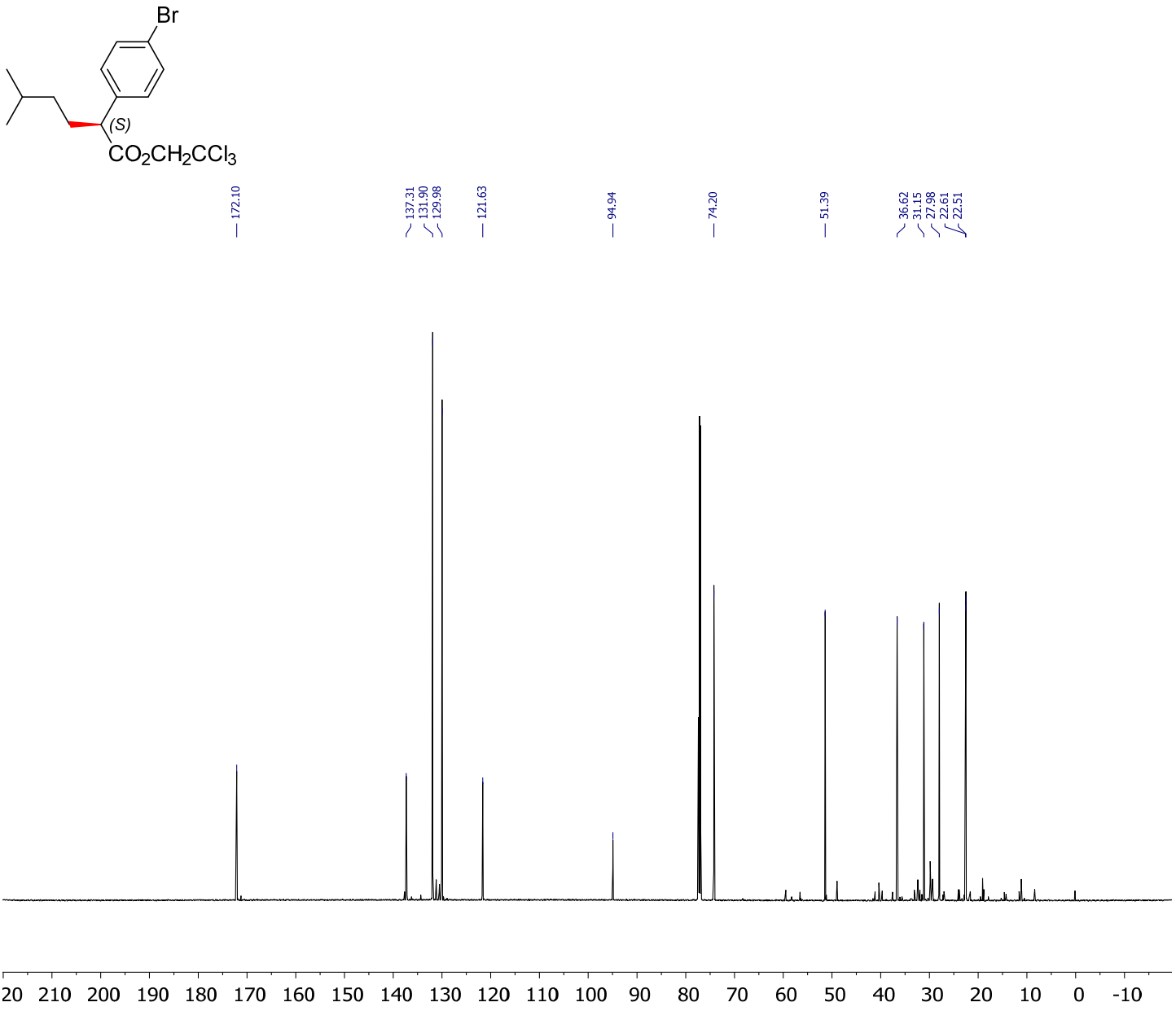
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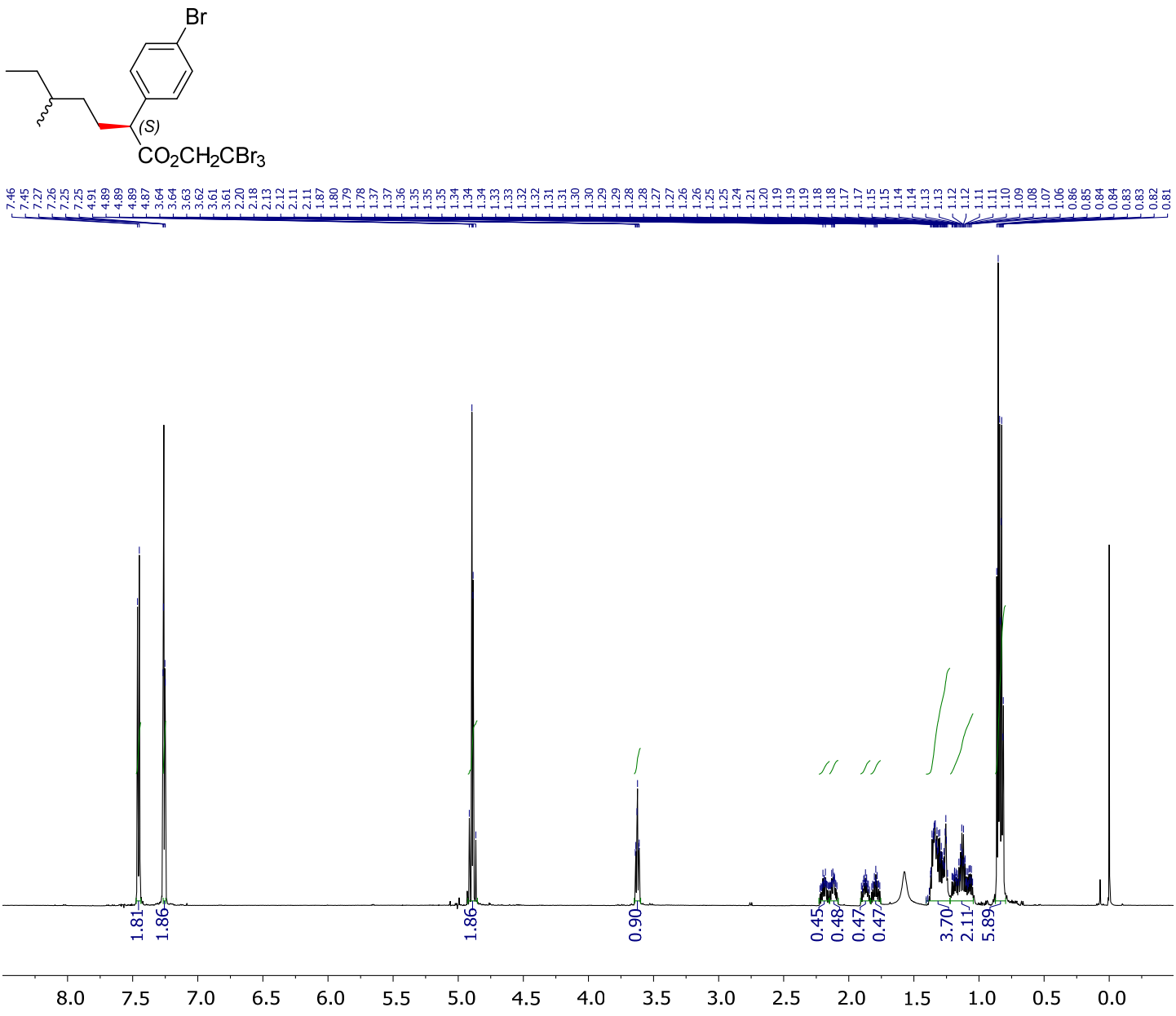
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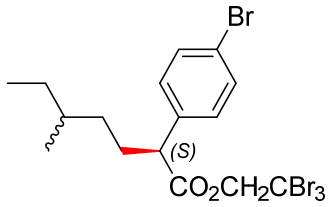
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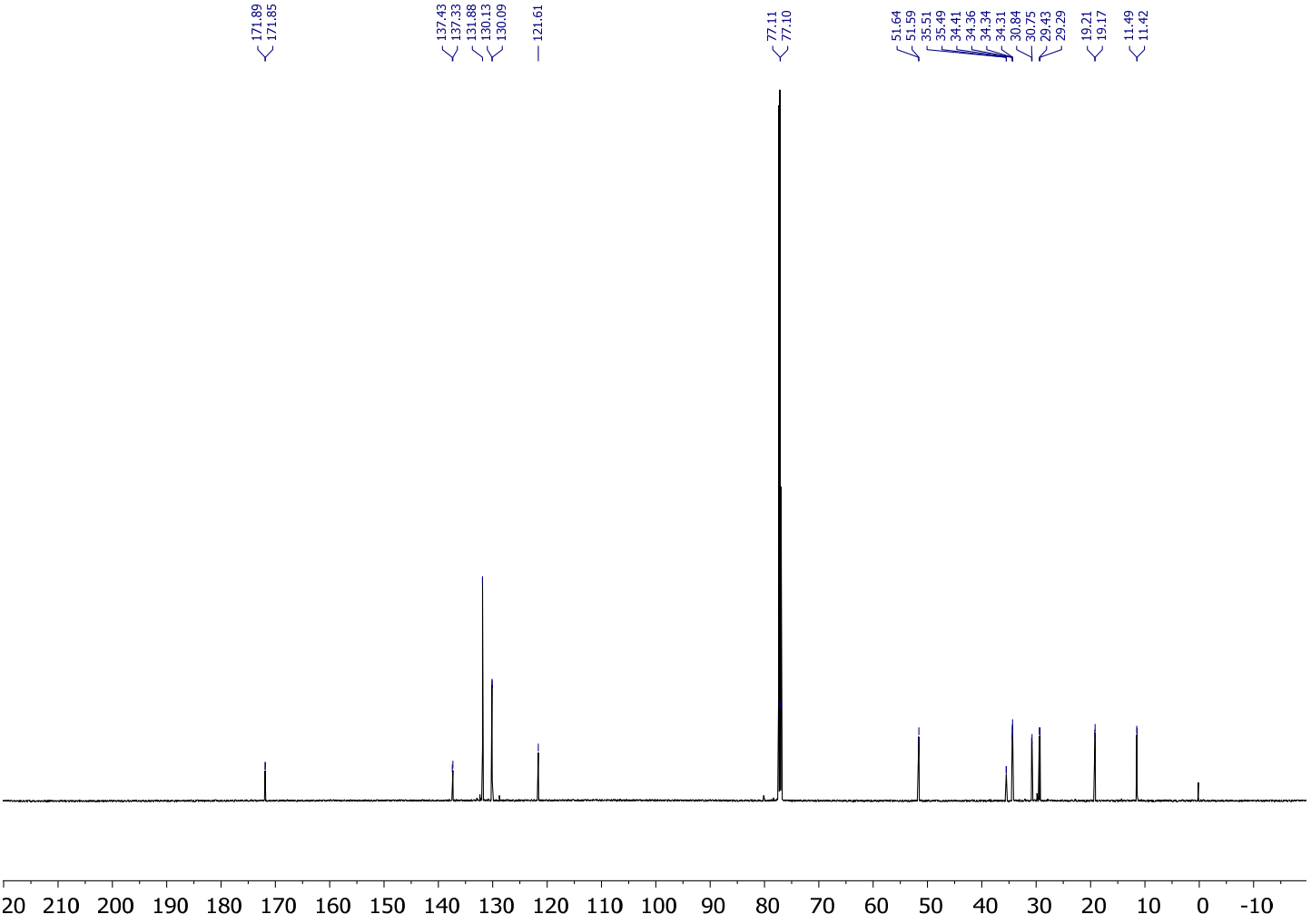
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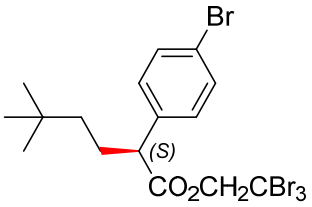
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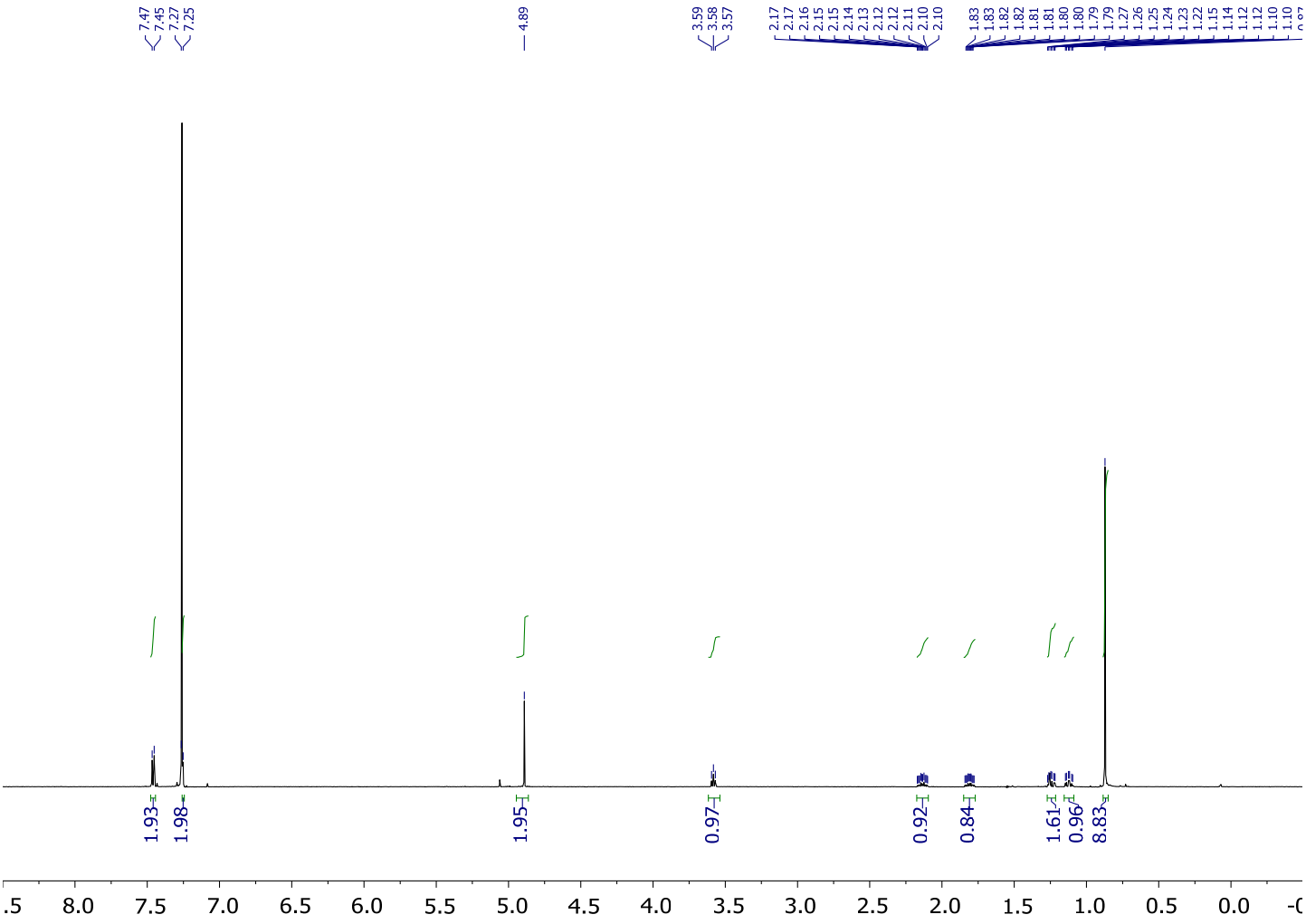
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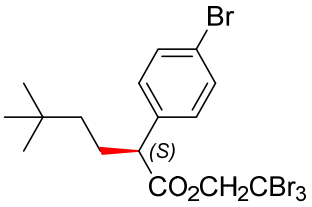
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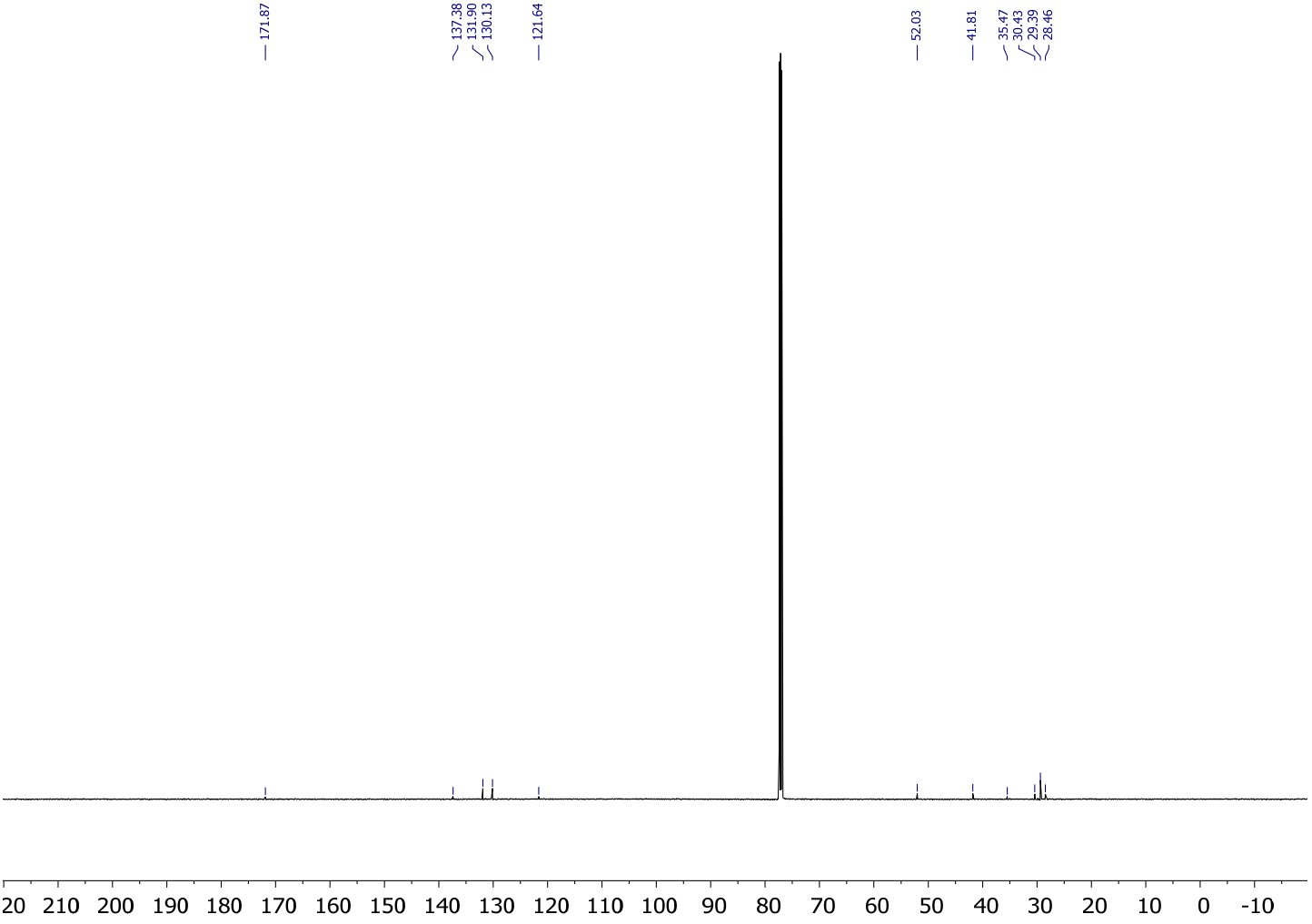
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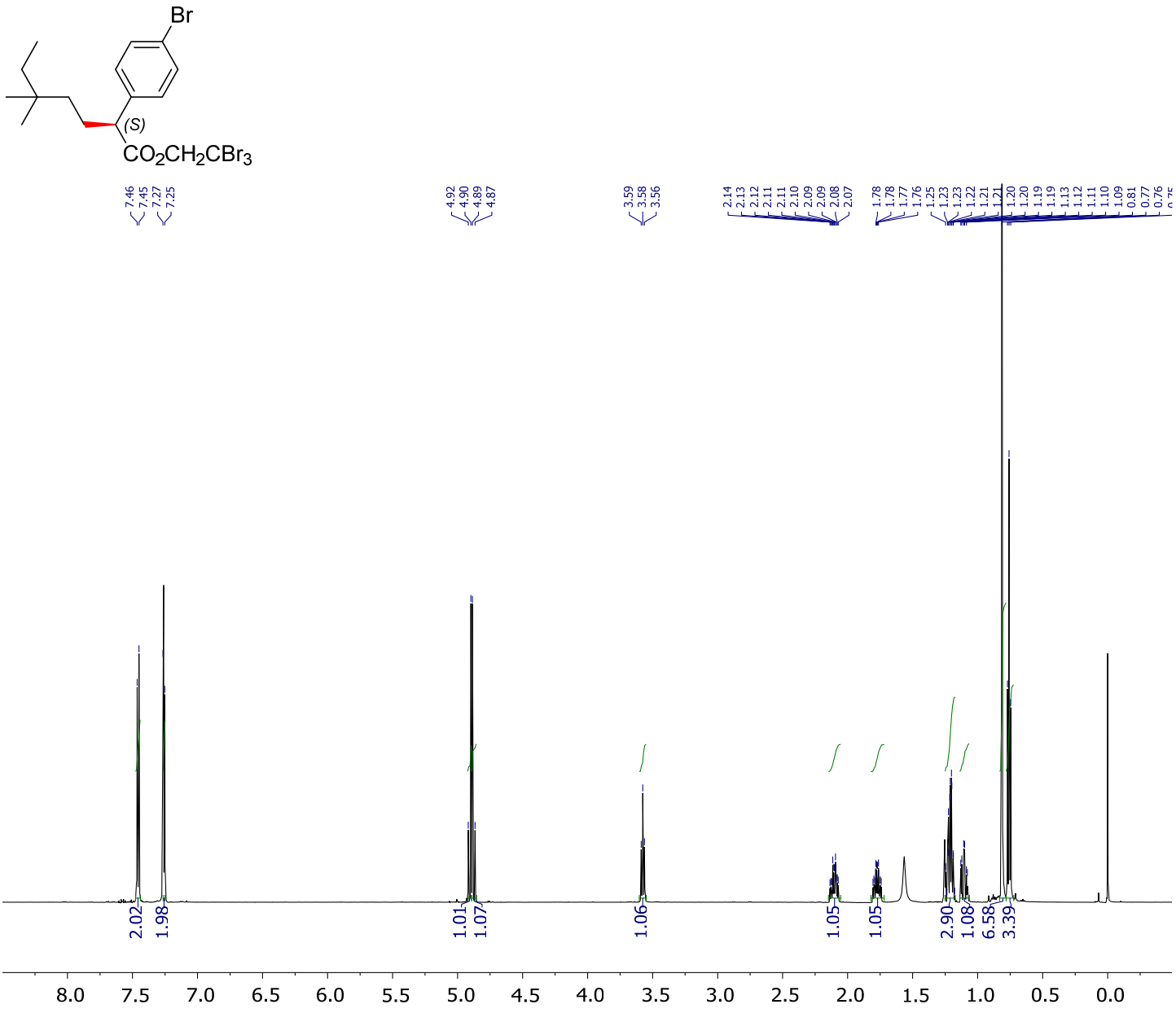
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2.11
2.10
2.09
2.09
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2.07
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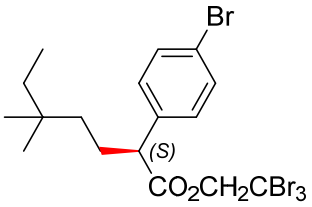
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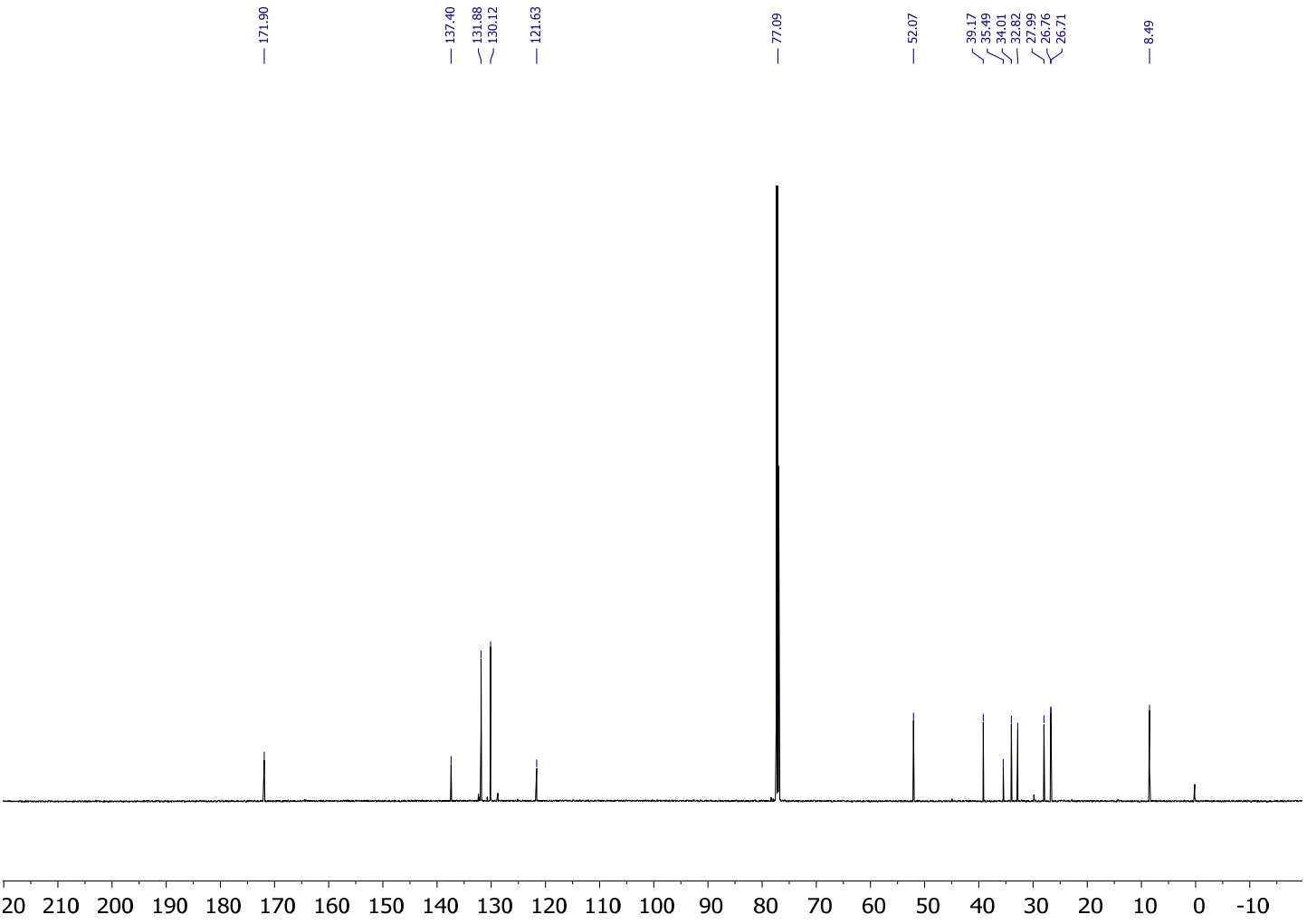
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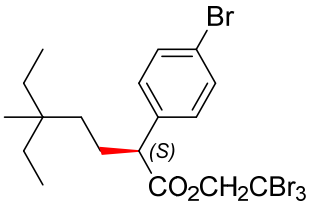
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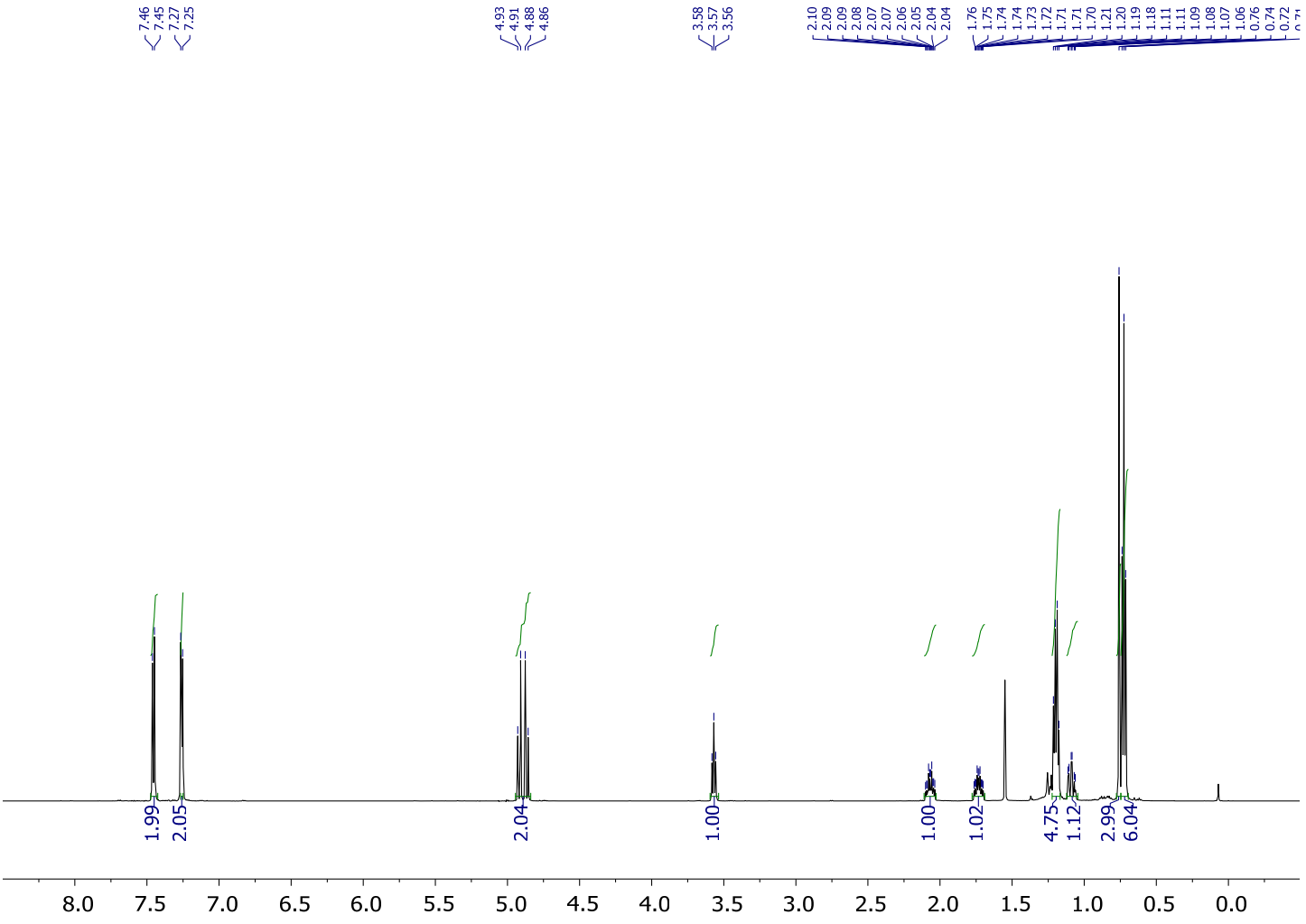
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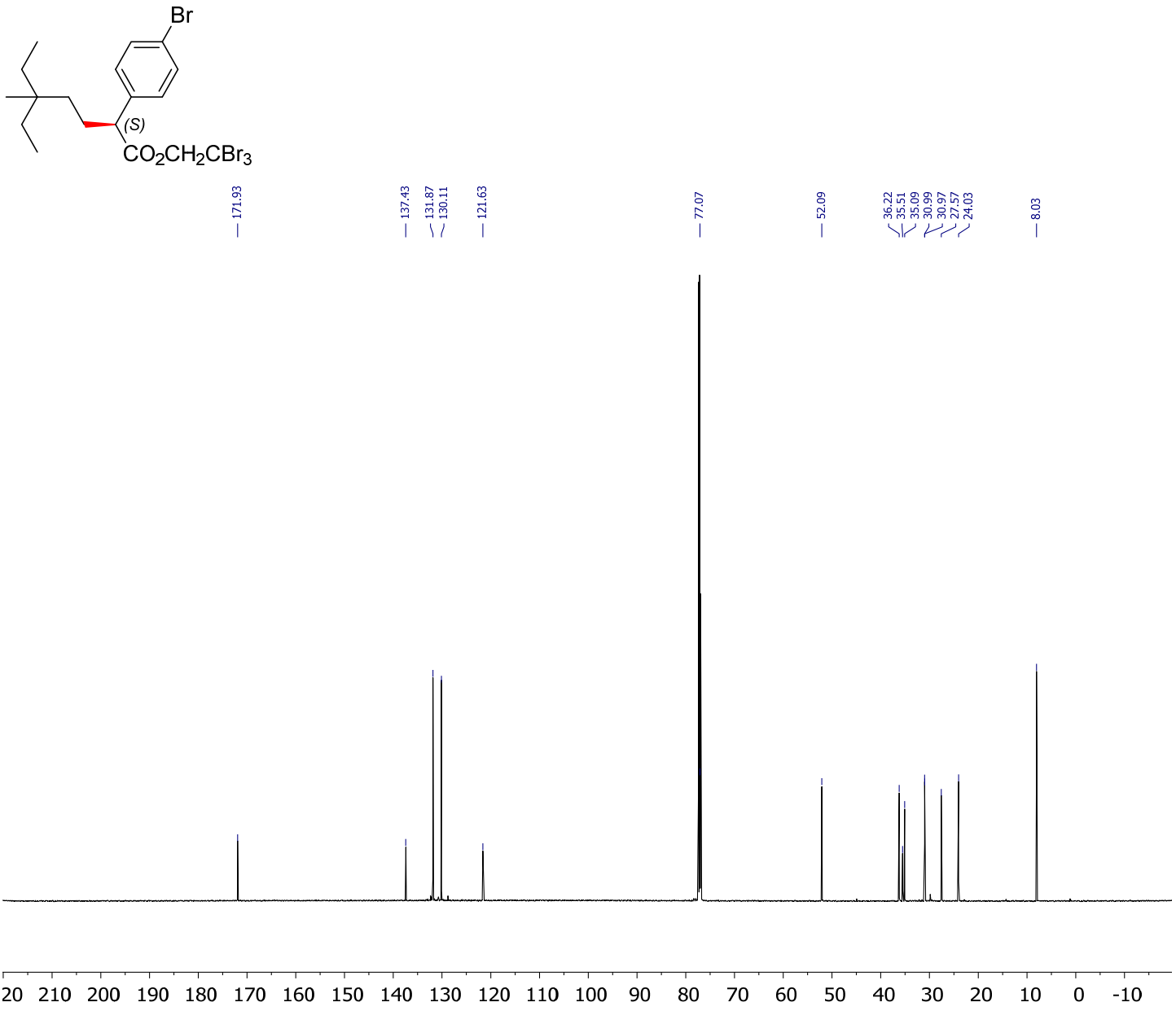
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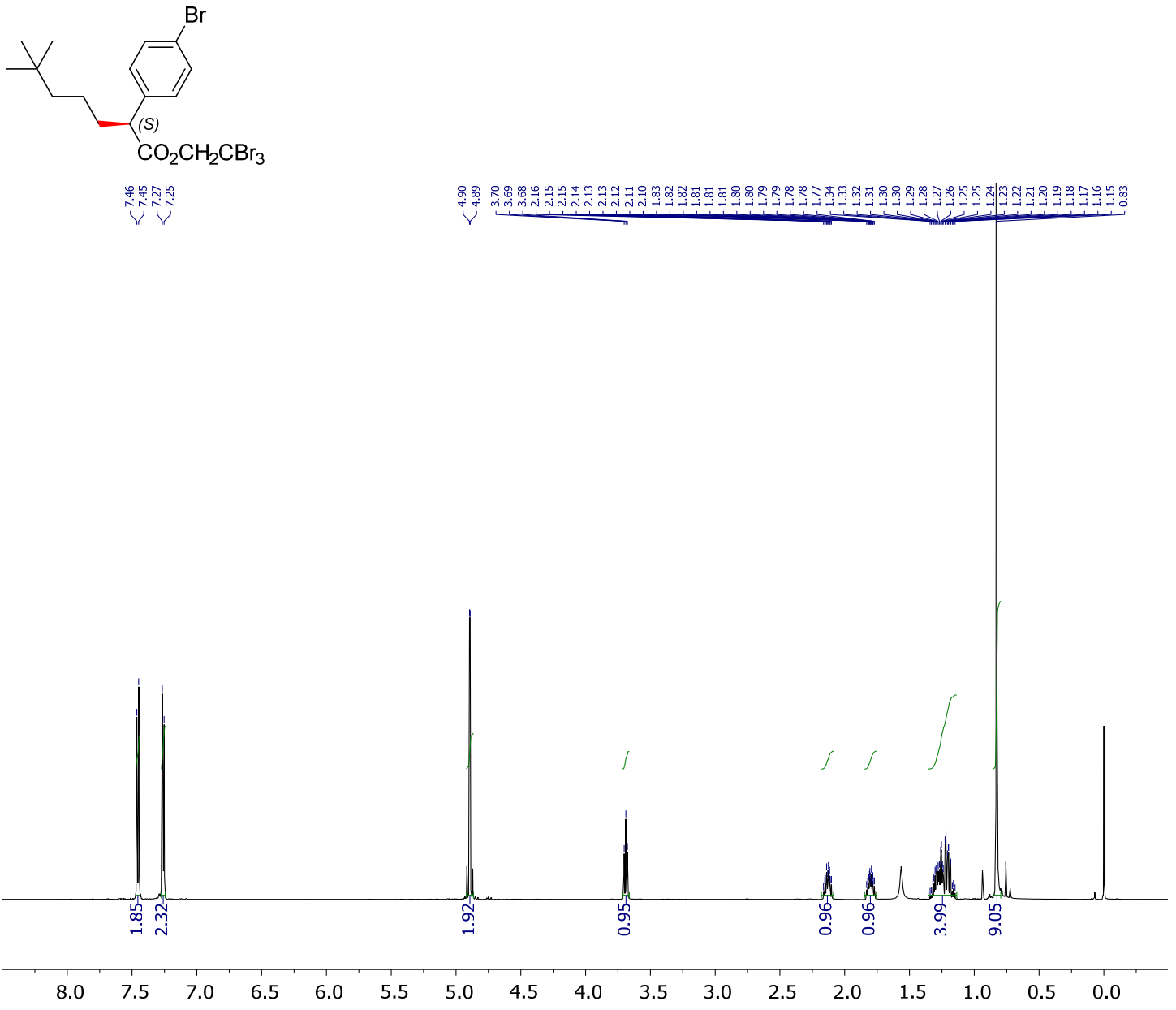
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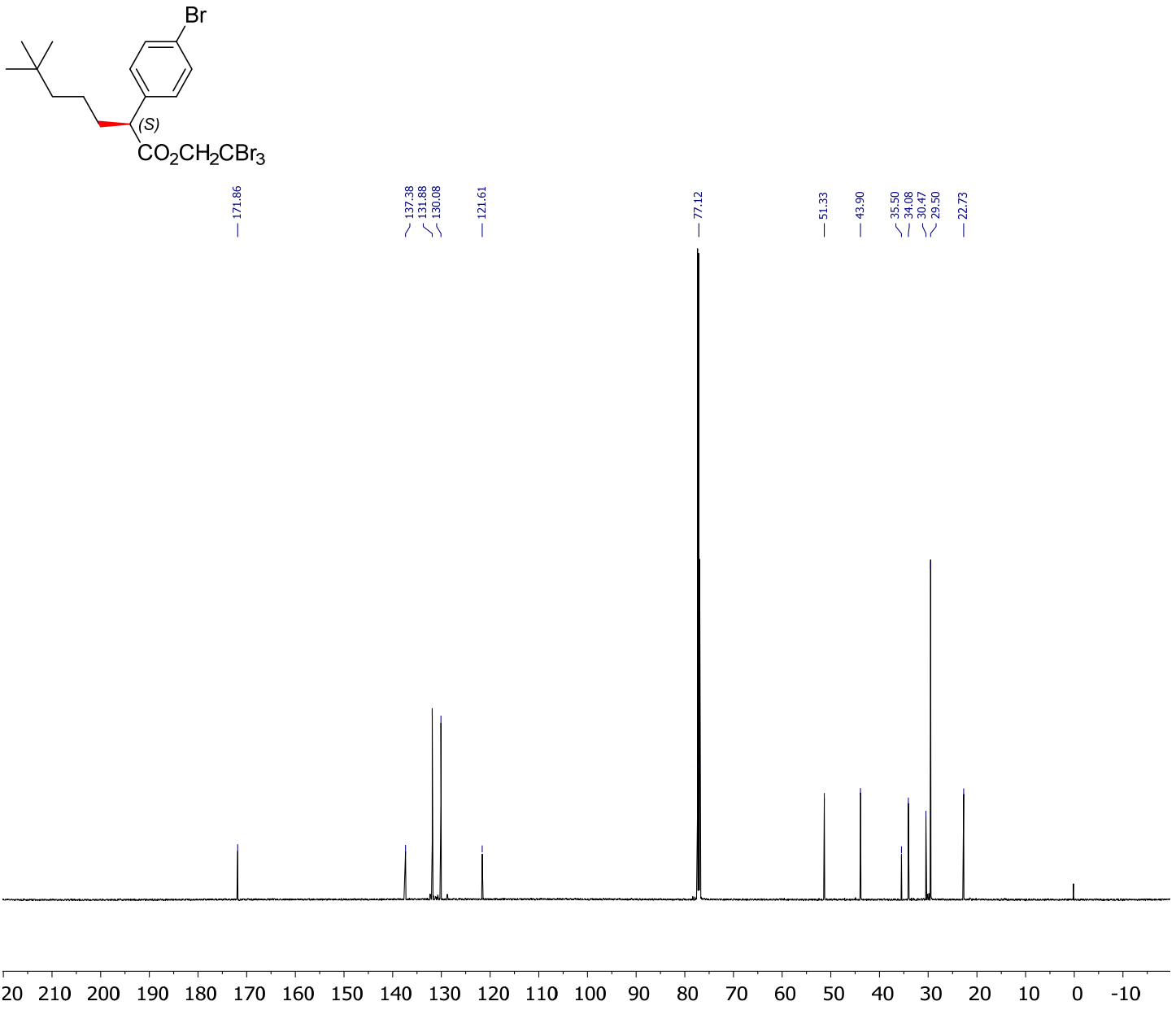
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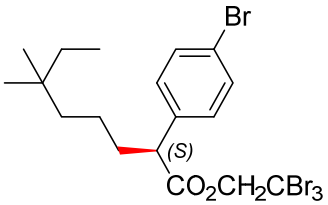
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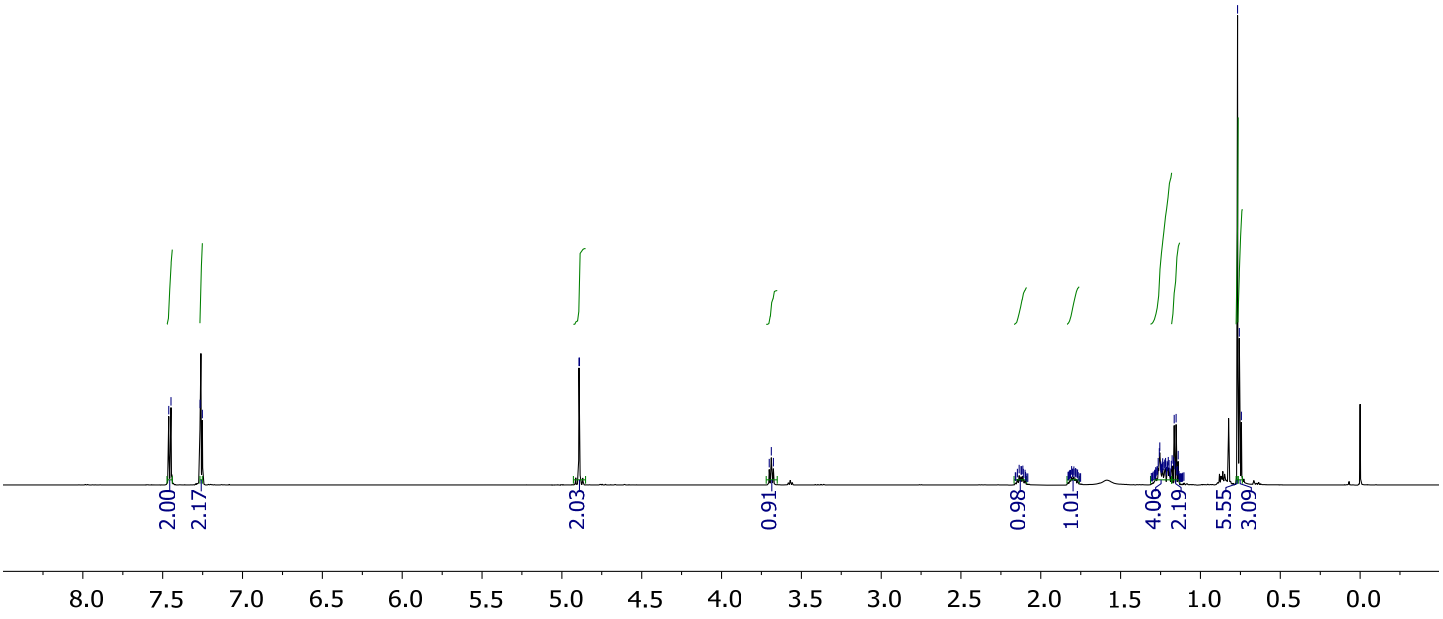
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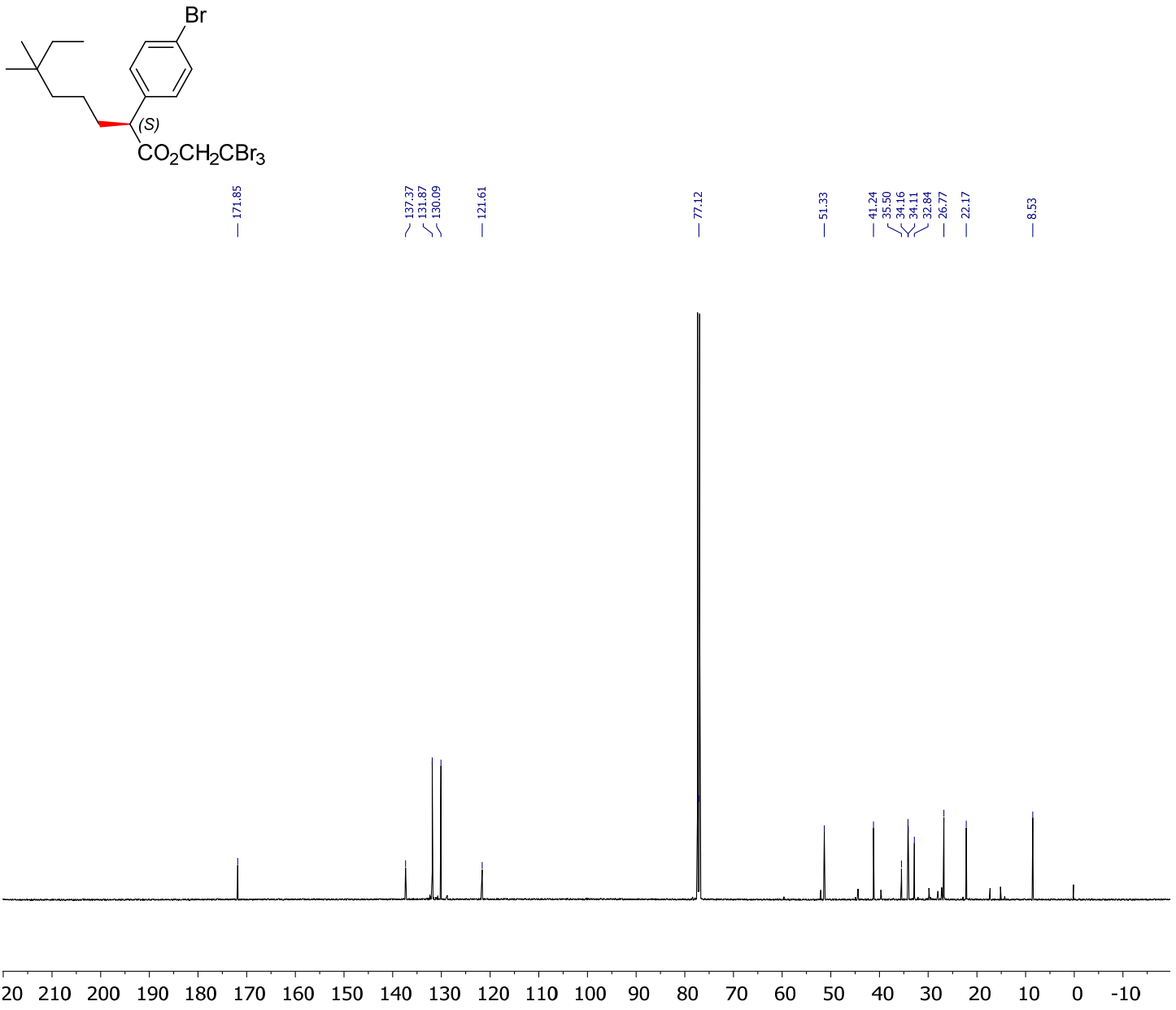
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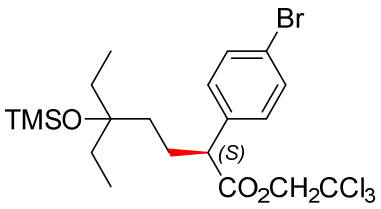
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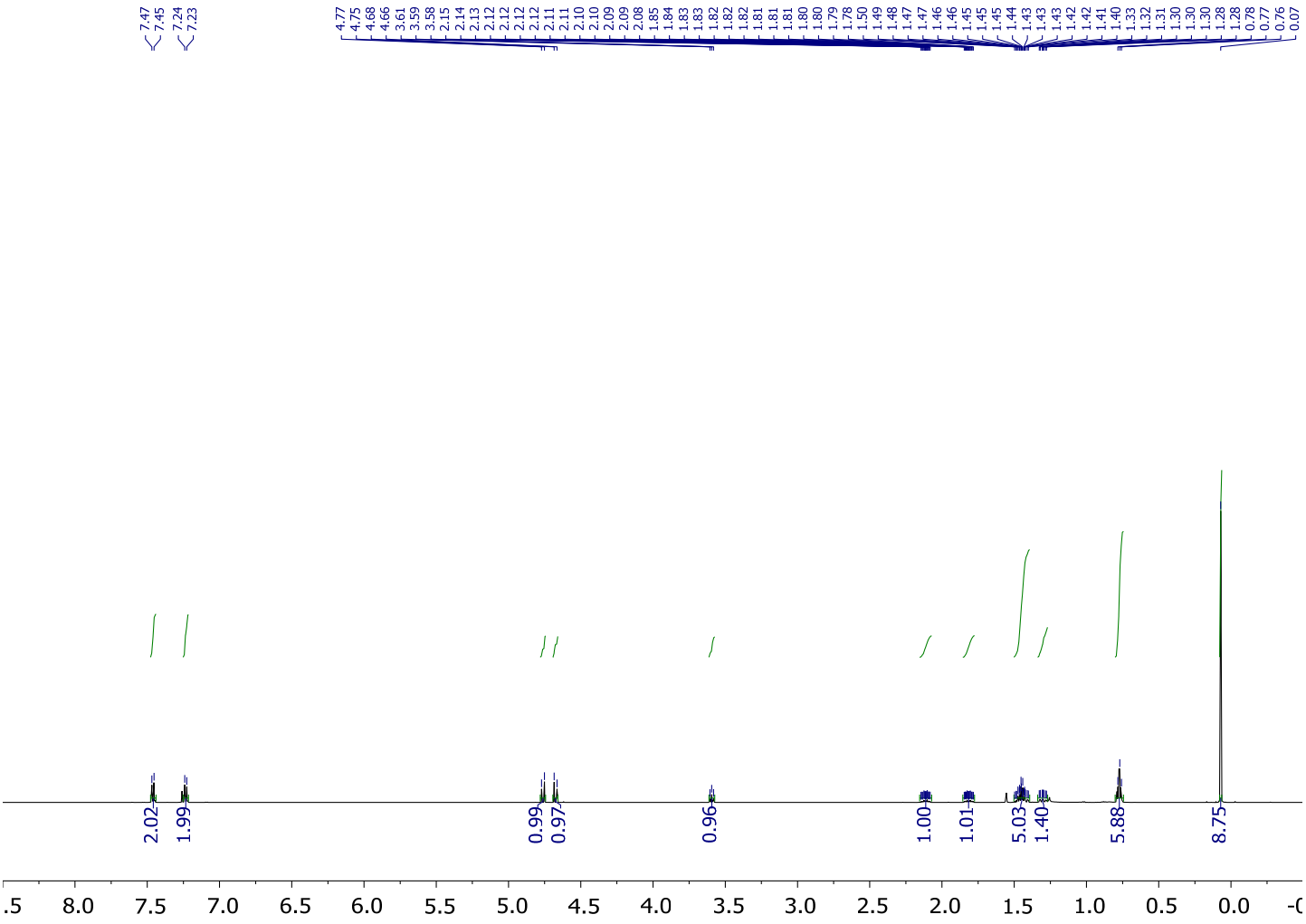
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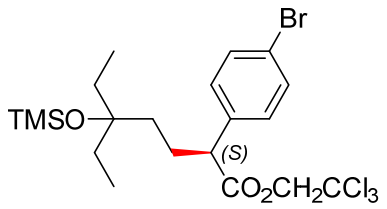
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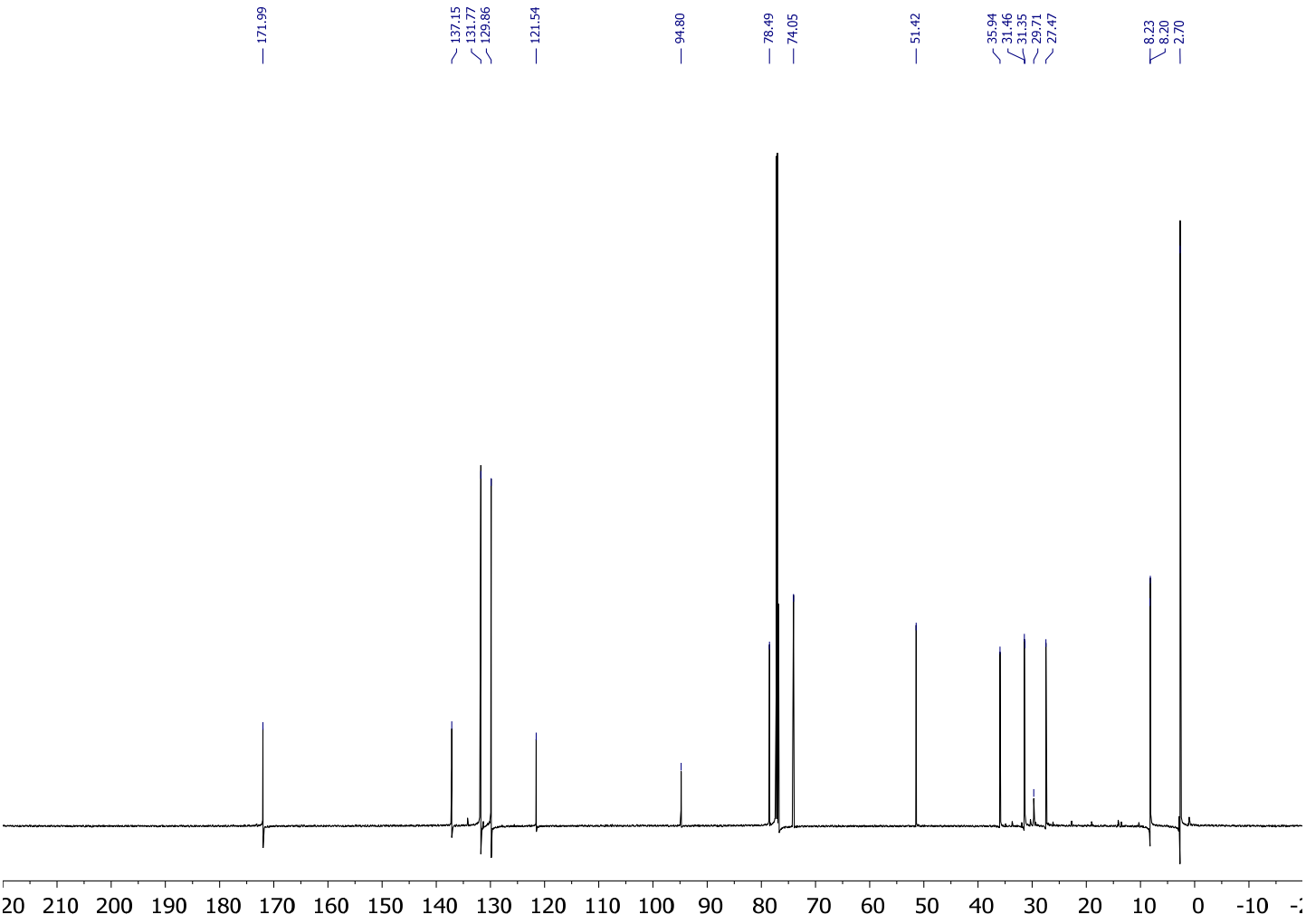
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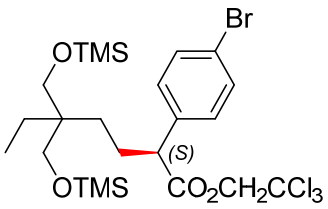
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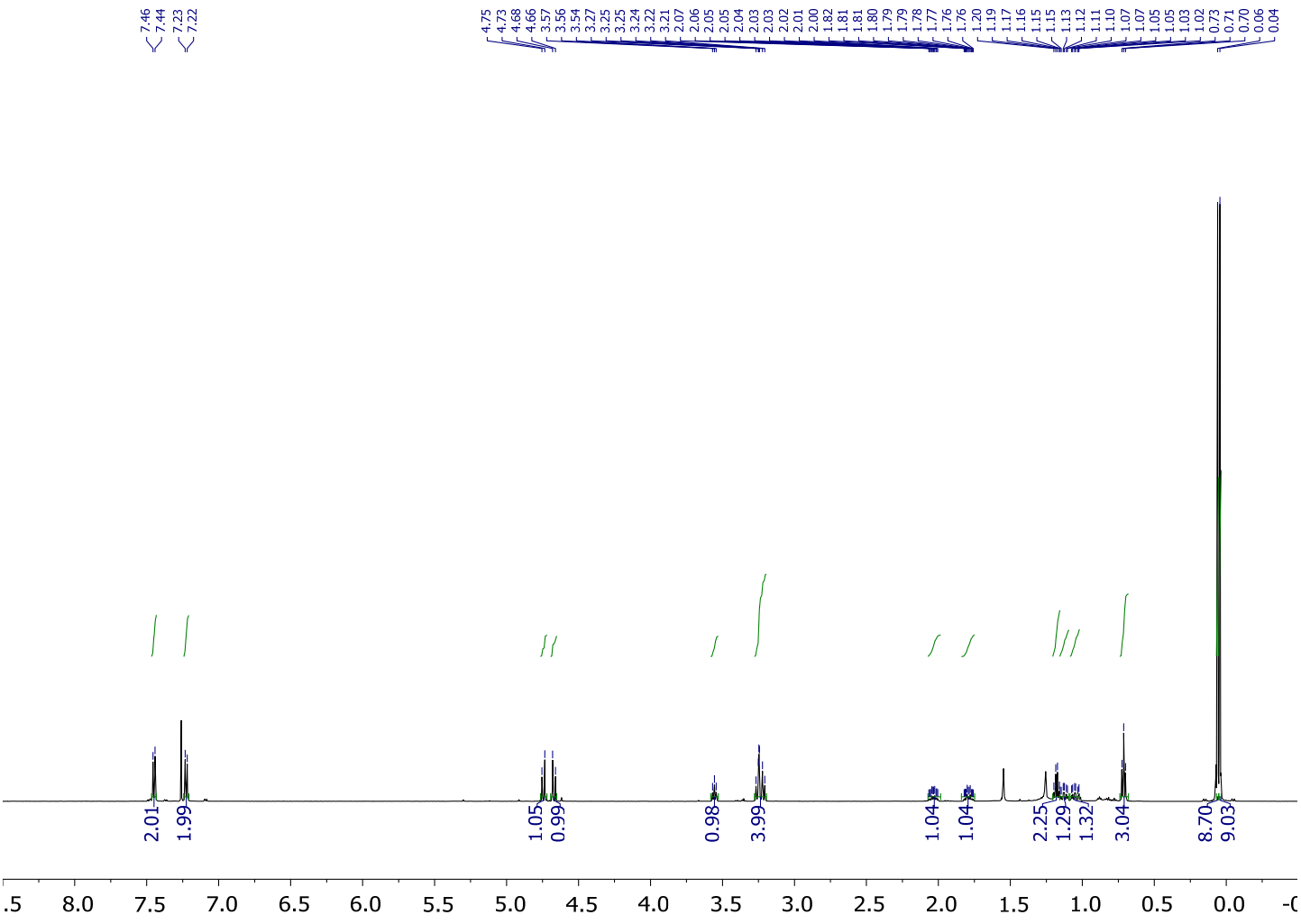
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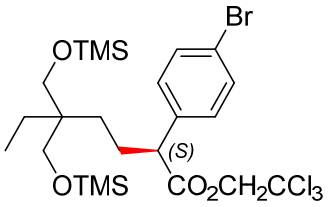
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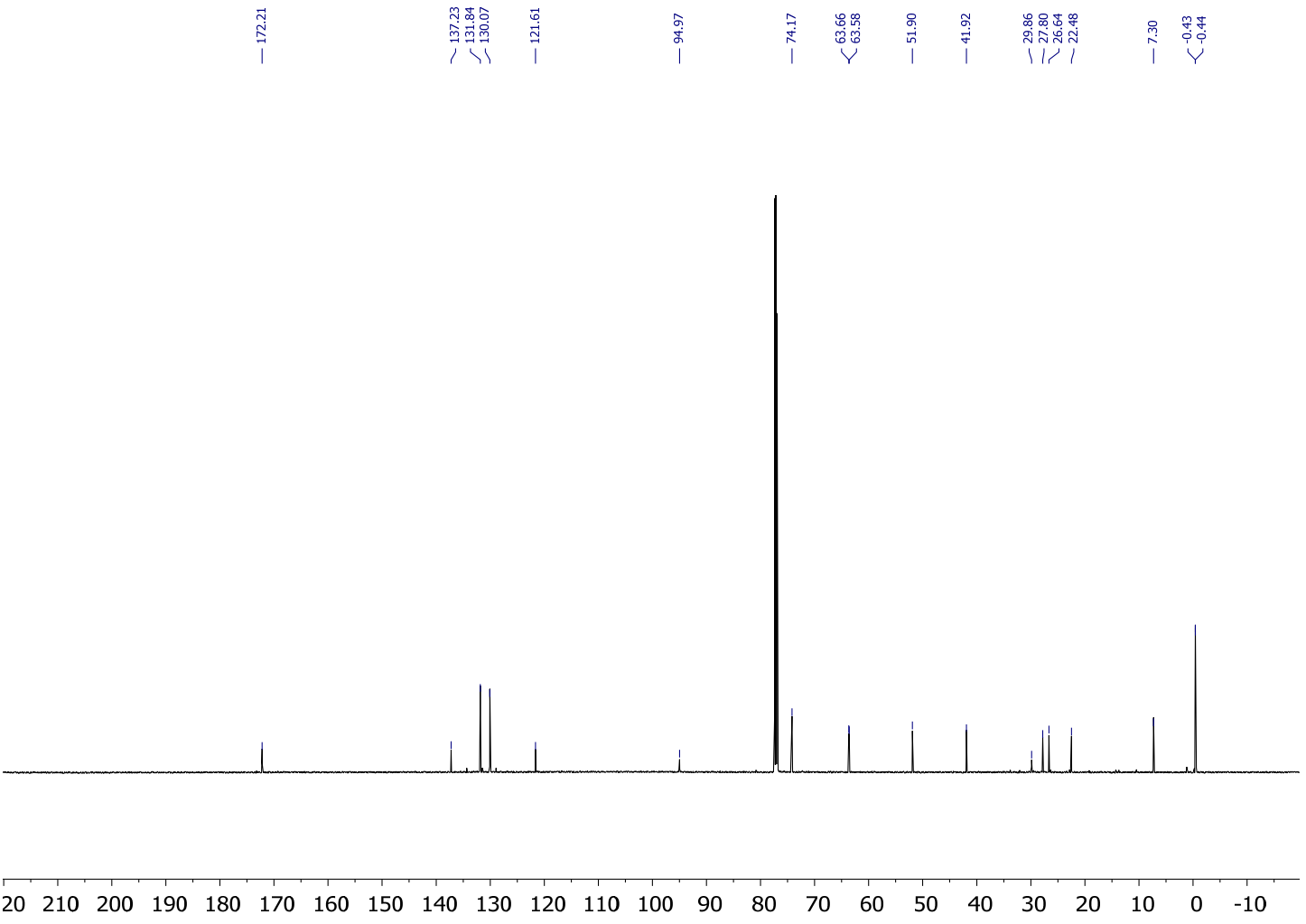
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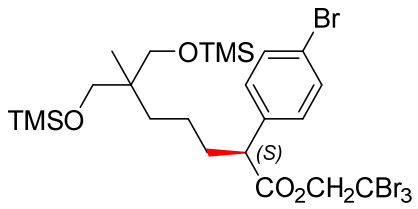
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TMSO
(S)
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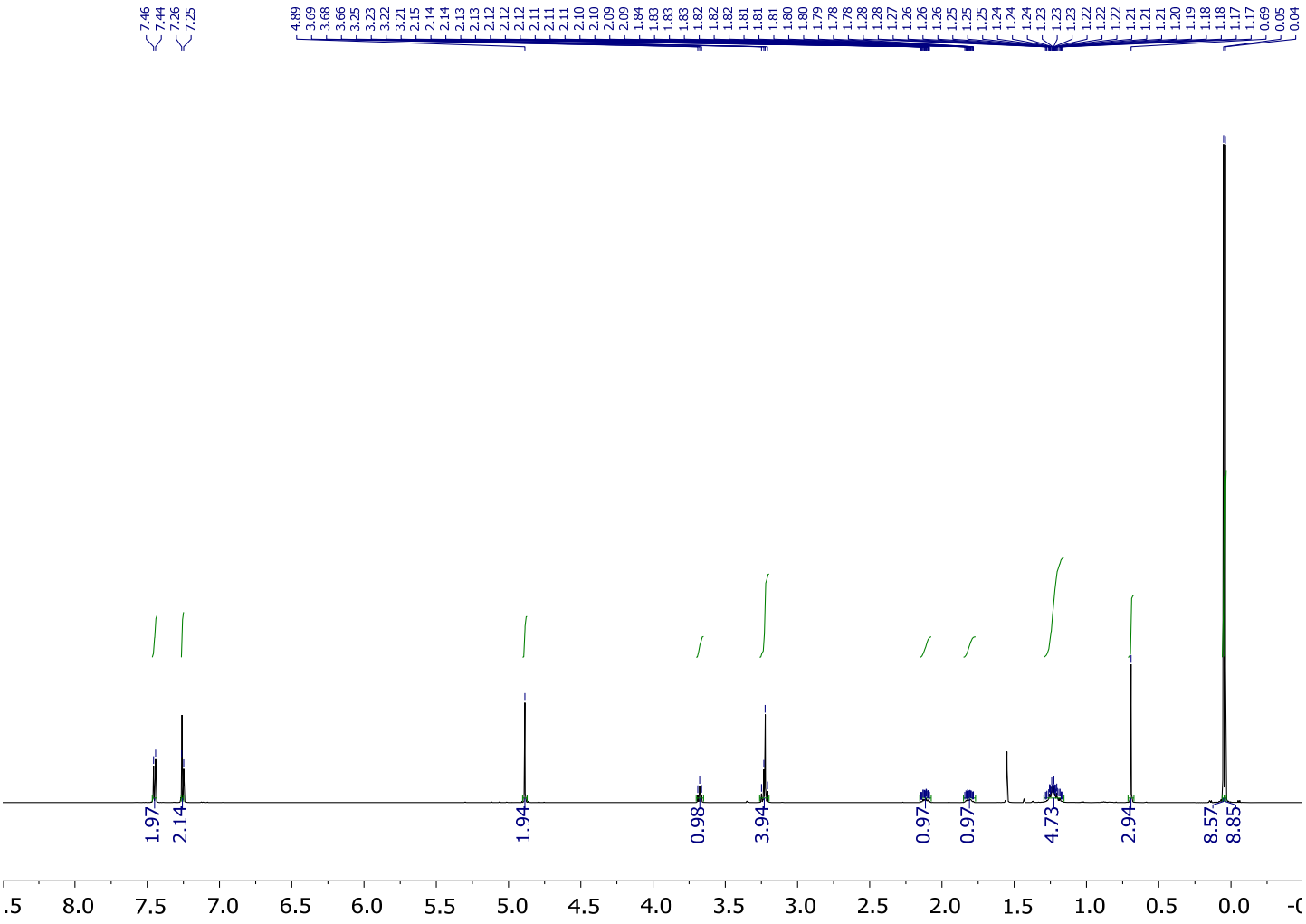
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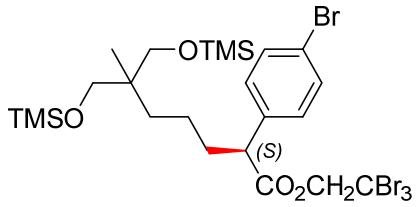
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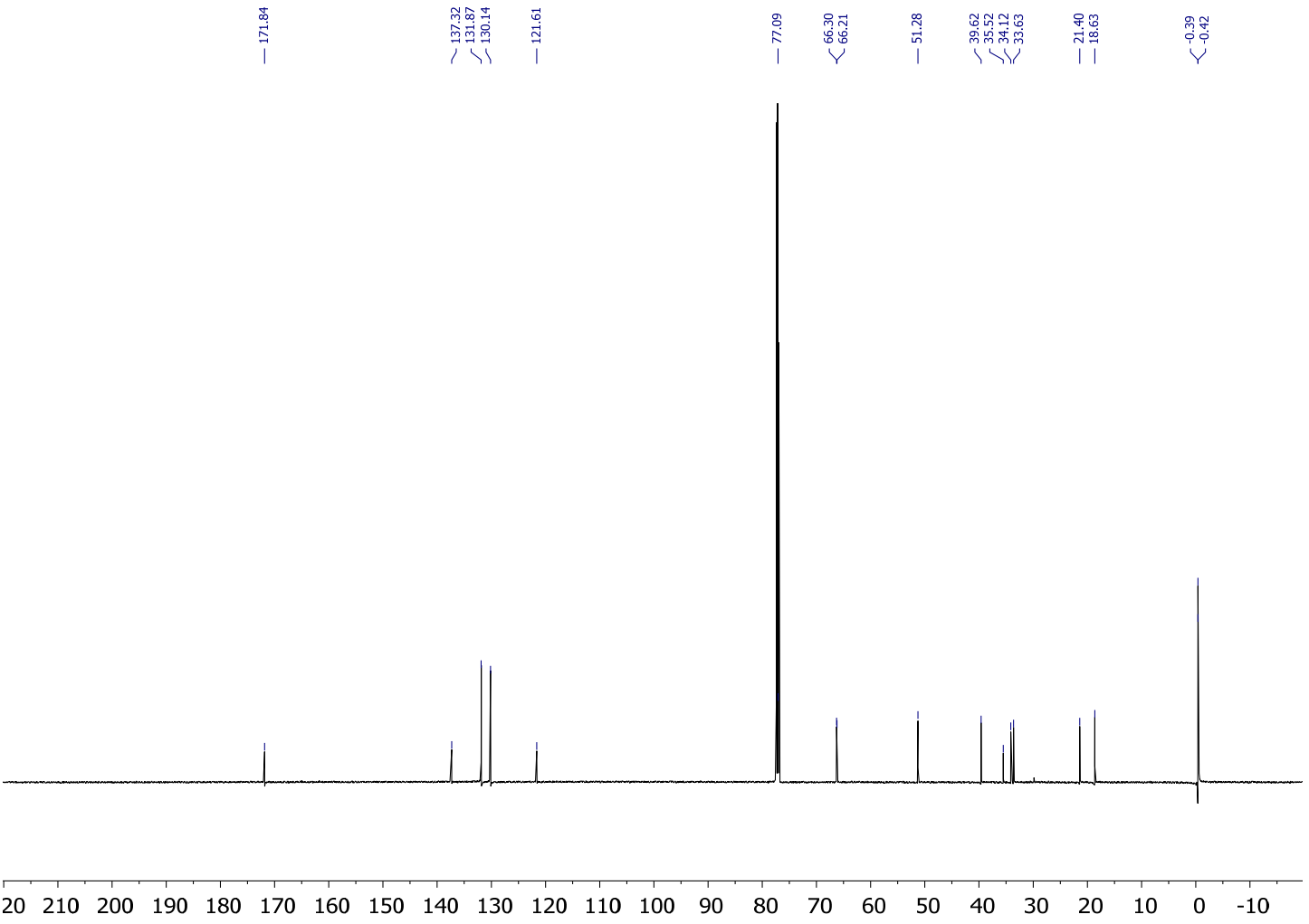
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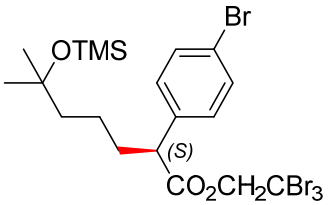
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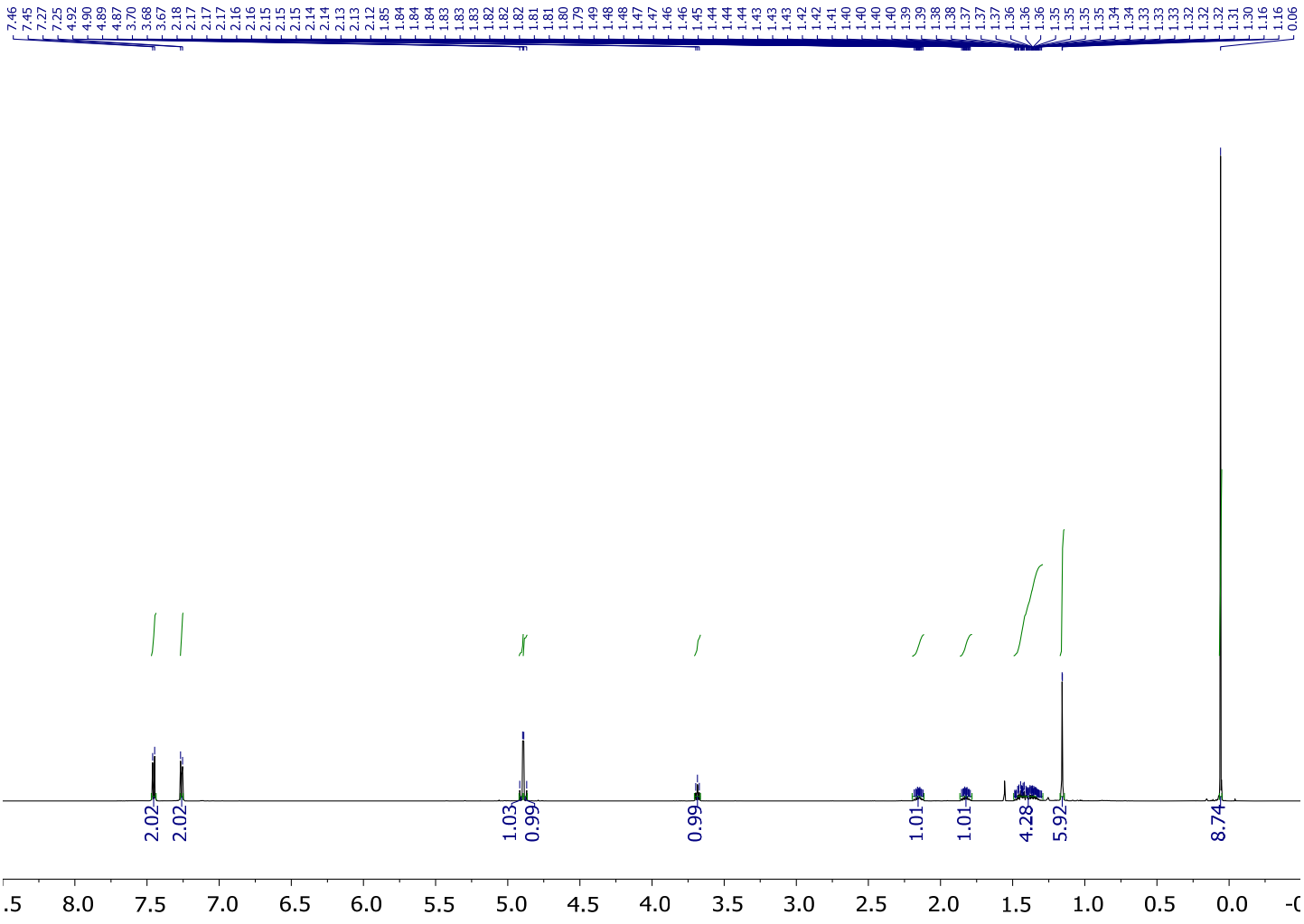
CO2CH2CBr3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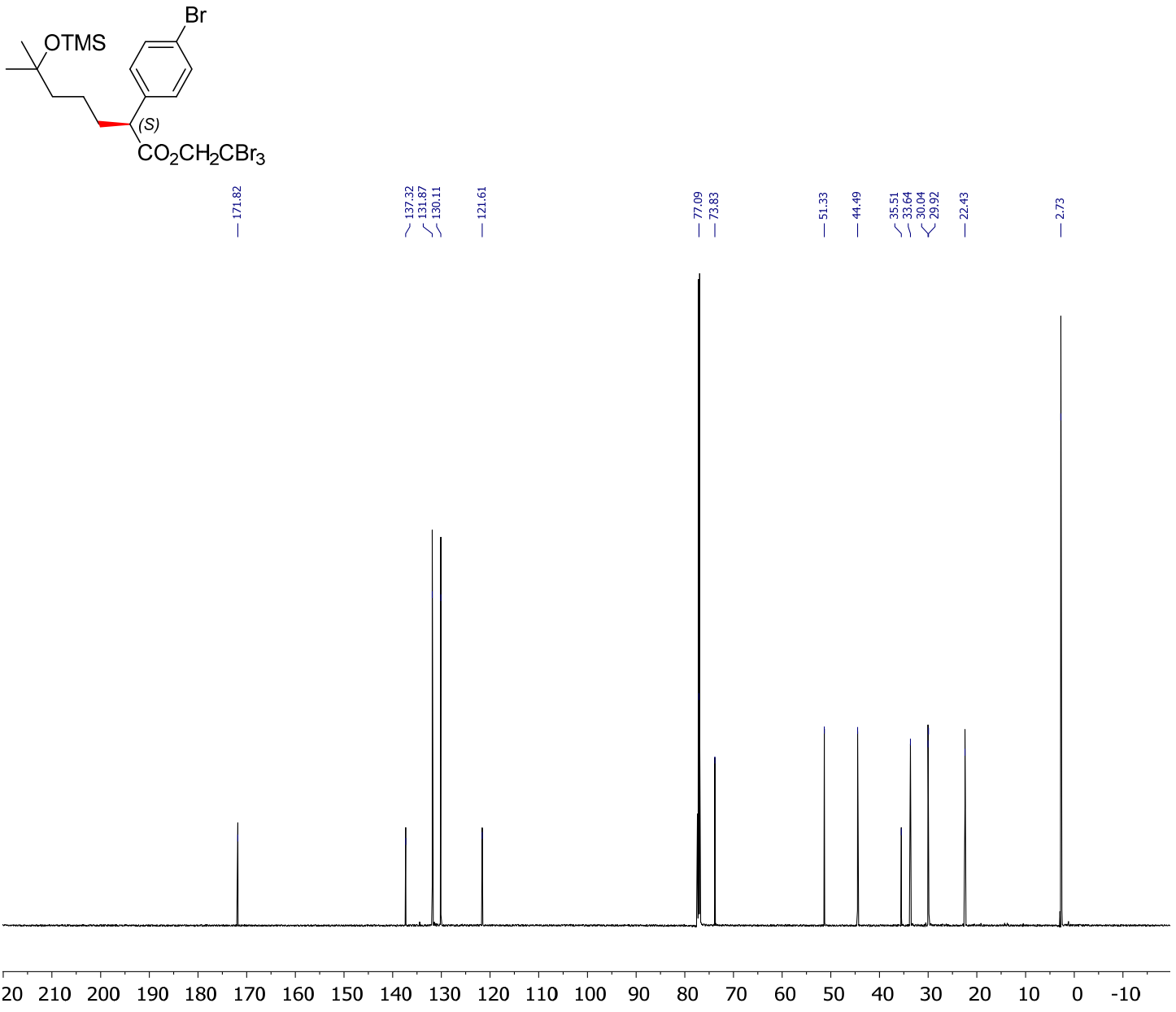
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CO2CH2CBr3
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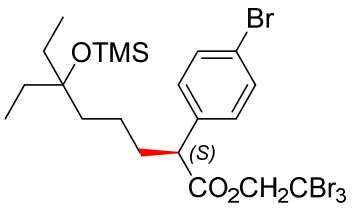
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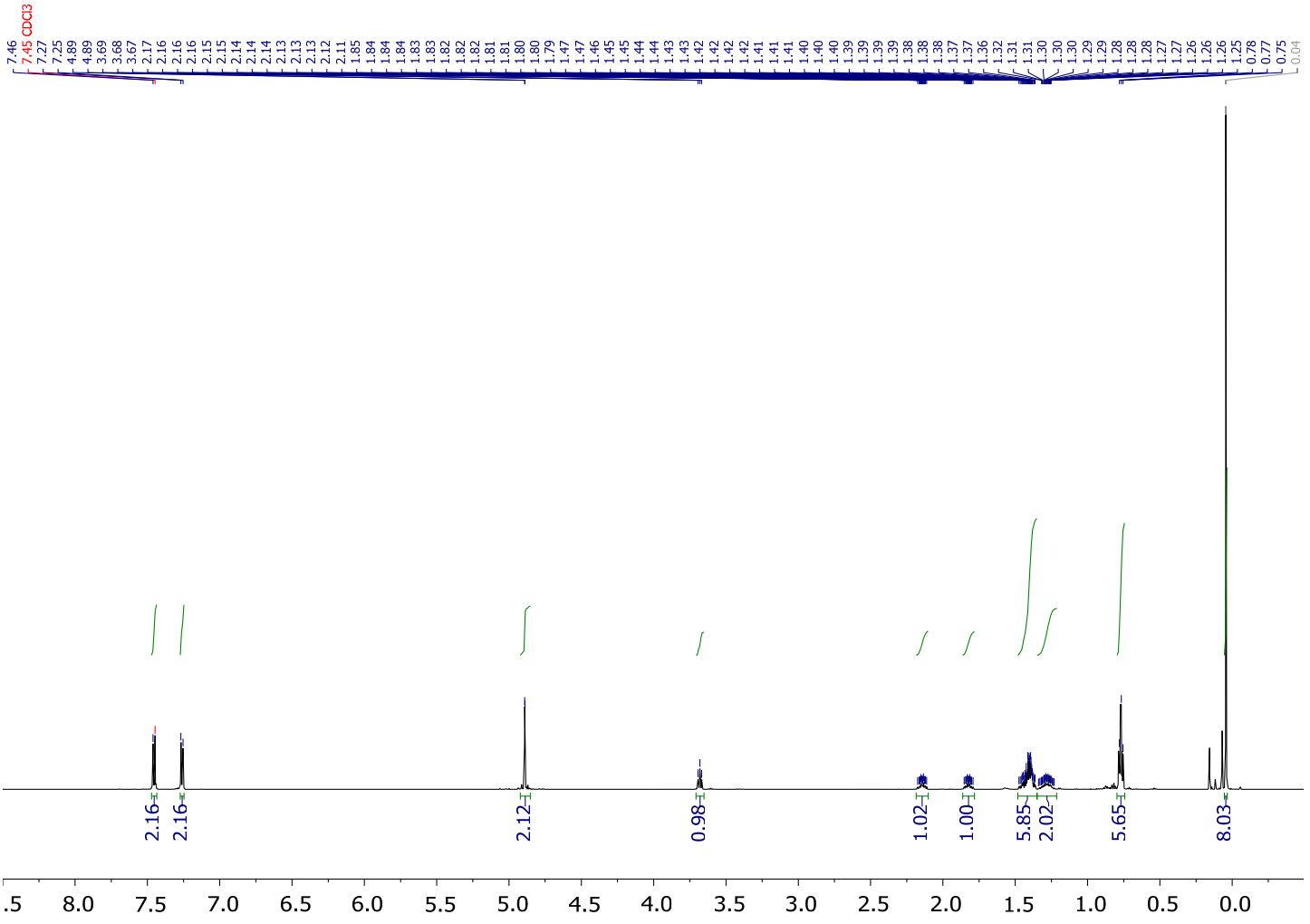
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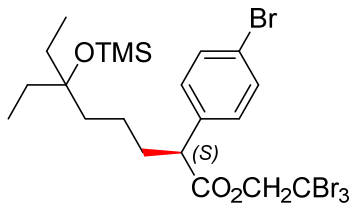
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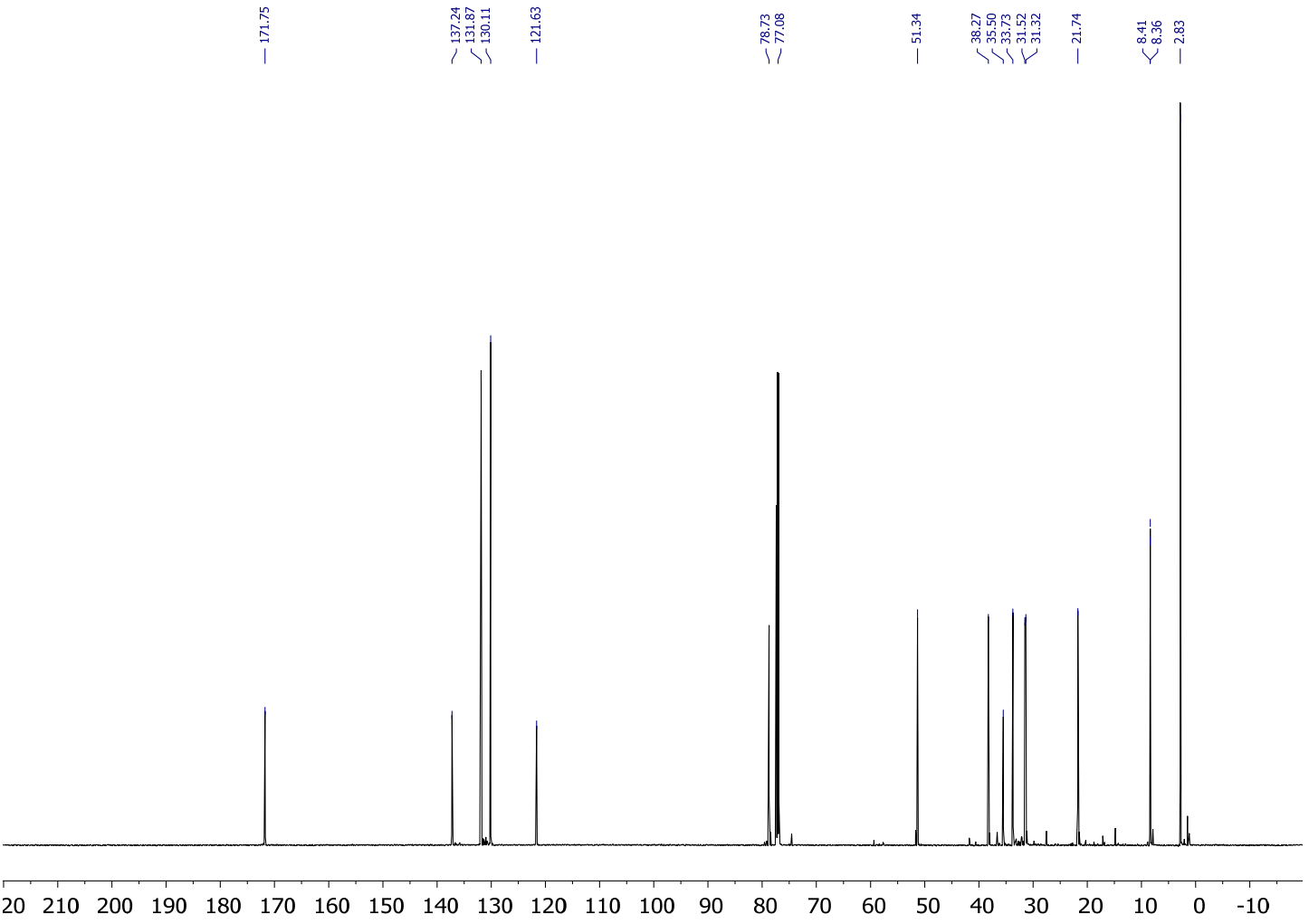
OTMS
(S)
CO2CH2CBr3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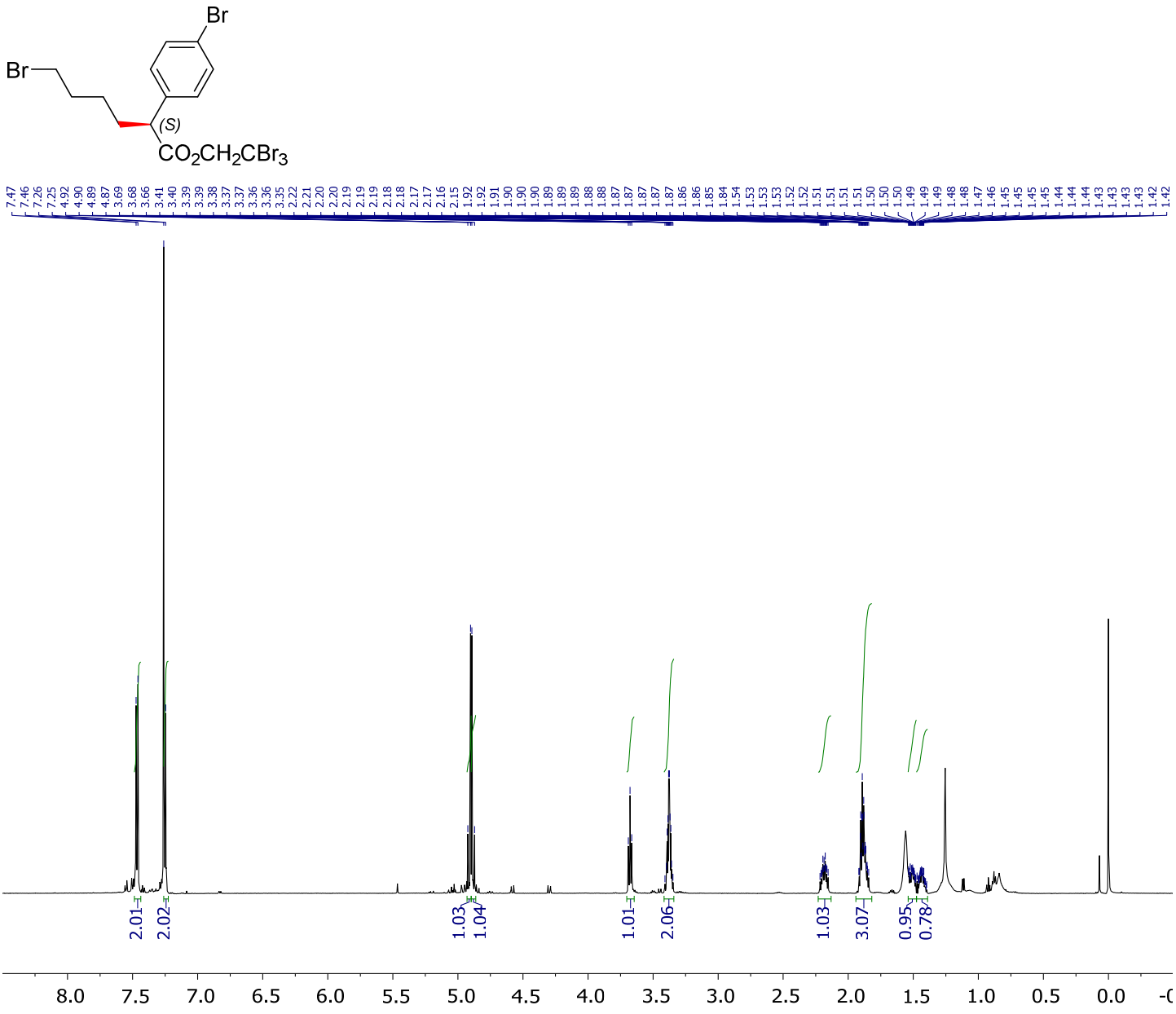
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Br
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CO2CH2CBr3
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1.04
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3.07
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0.78
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6.5
6.0
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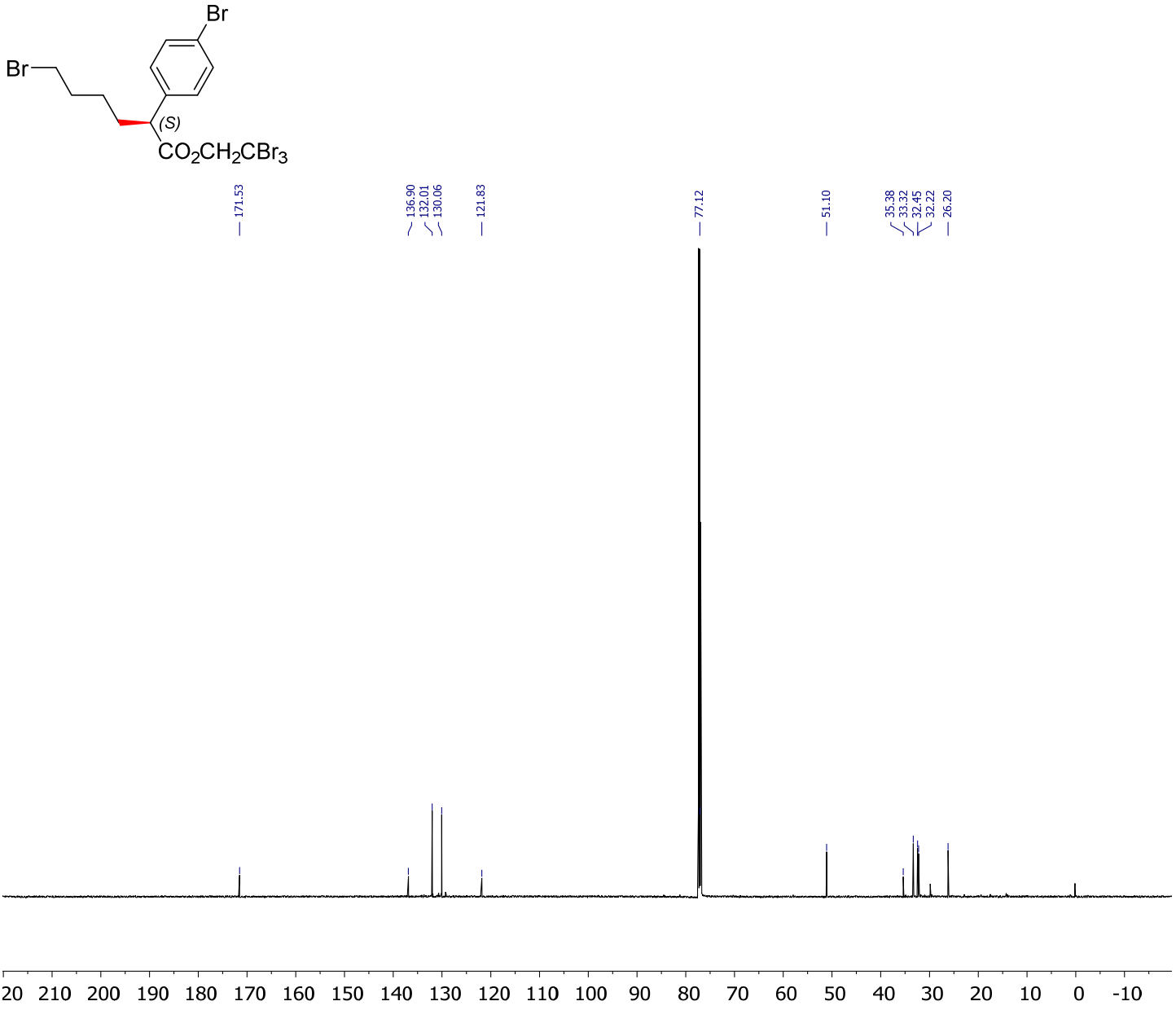
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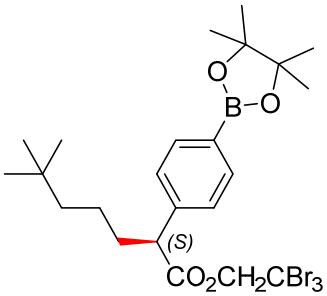
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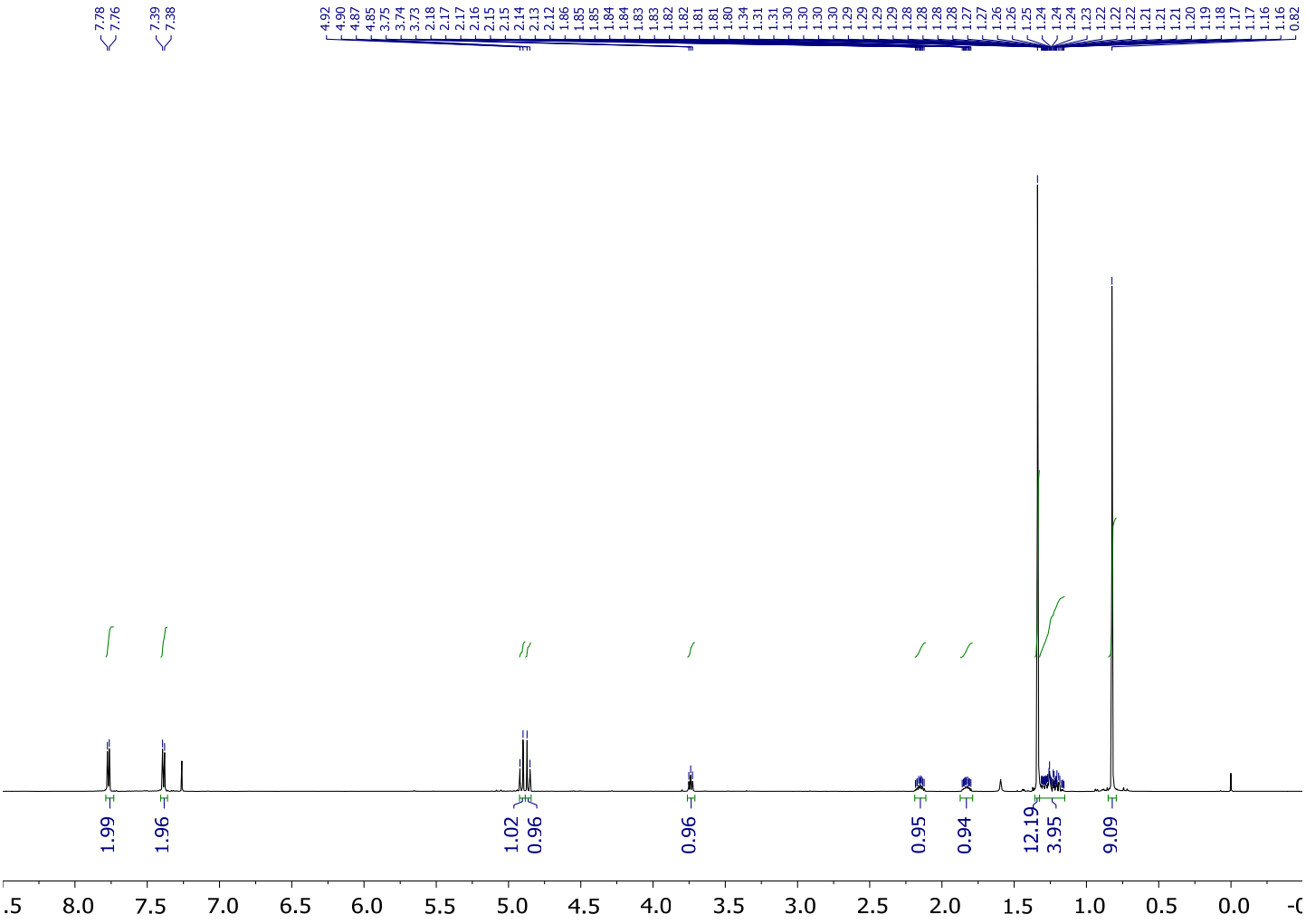
B–O
(S)
CO2CH2CBr3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0.94
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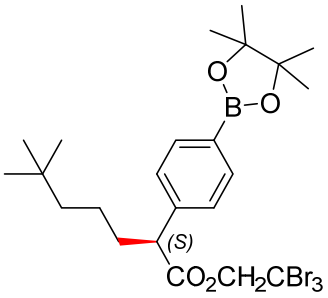
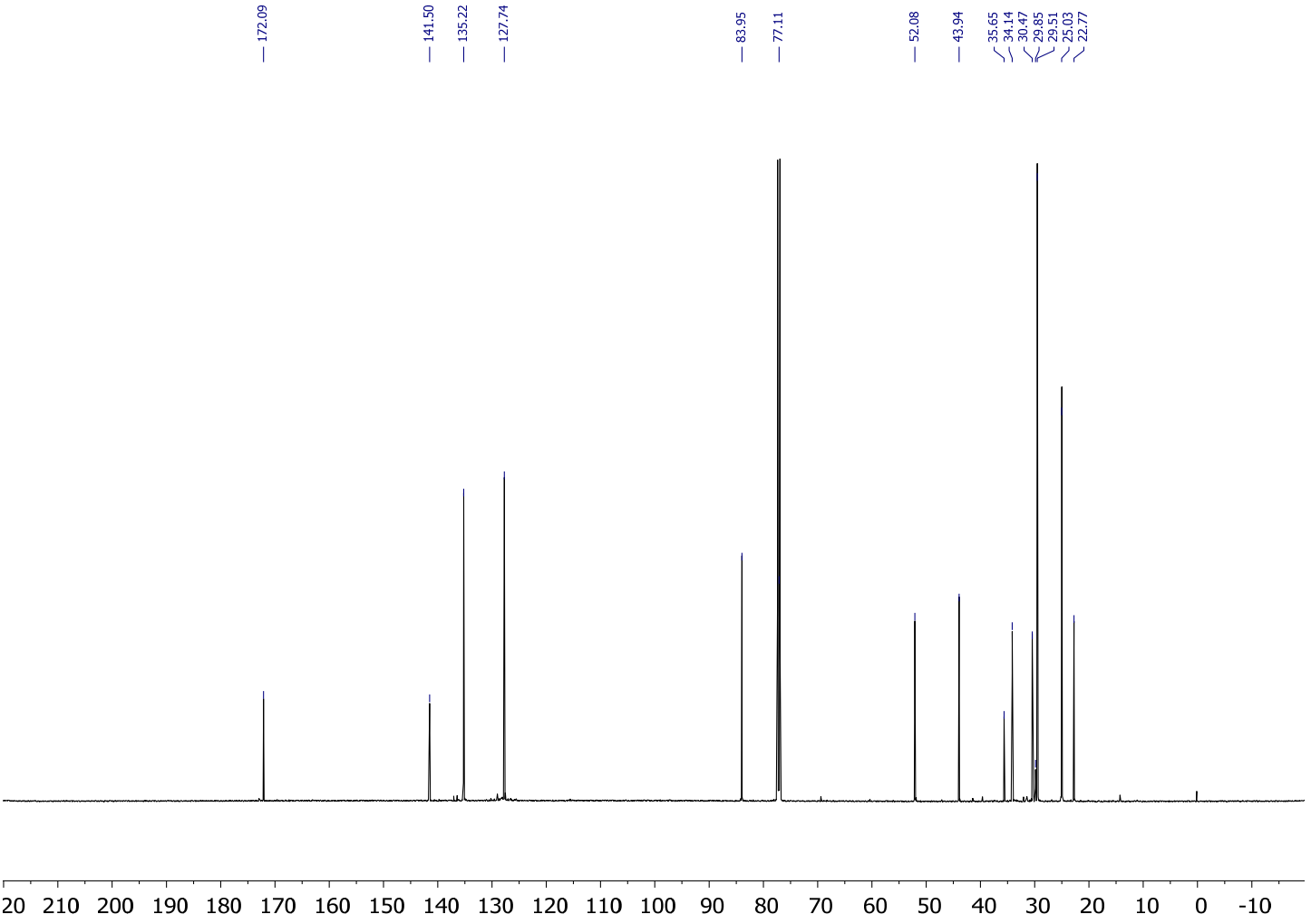

O
B–O
(S)
CO2CH2CBr3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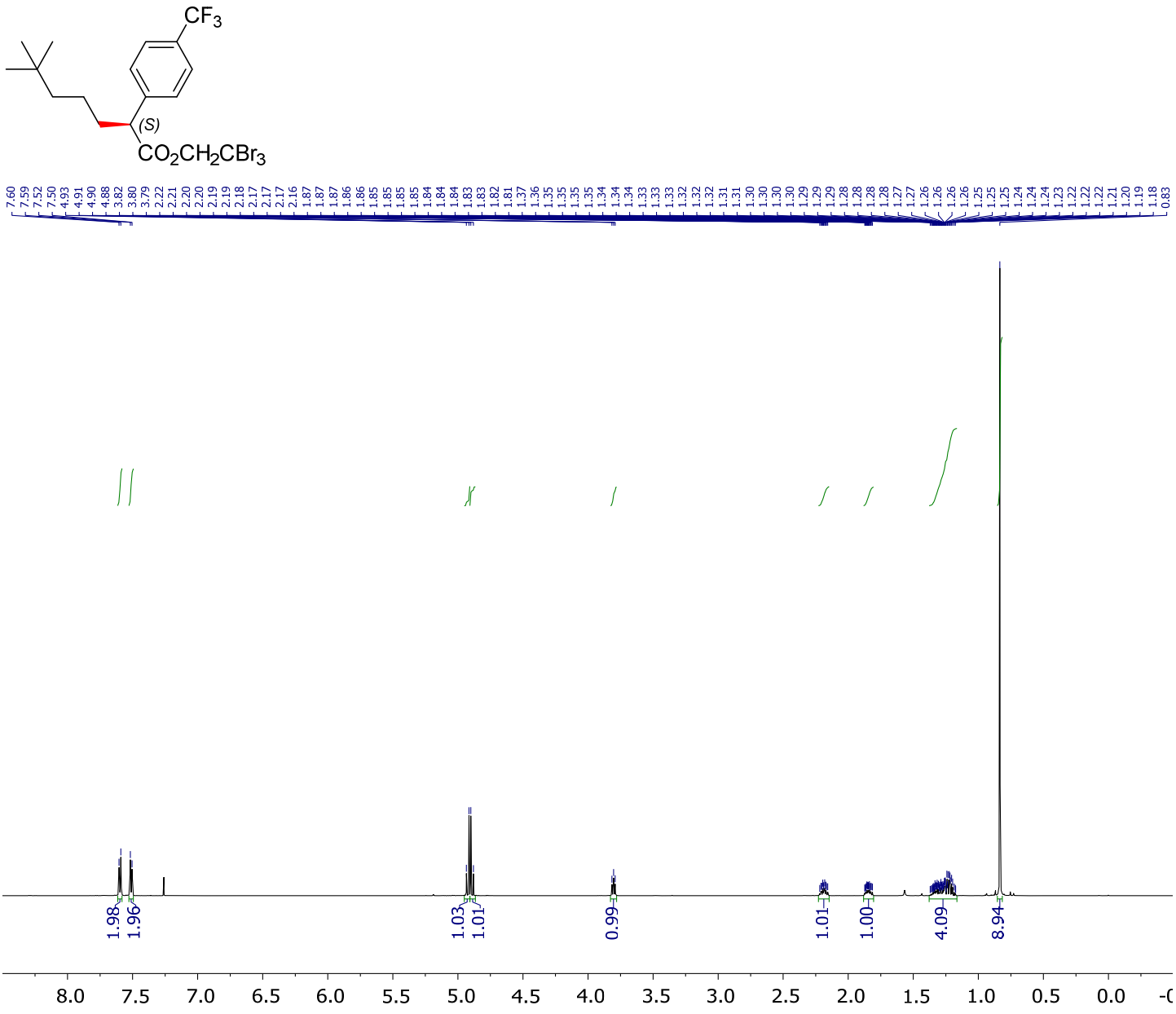
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0.99
1.01
1.00
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8.94
8.0
7.5
7.0
6.5
6.0
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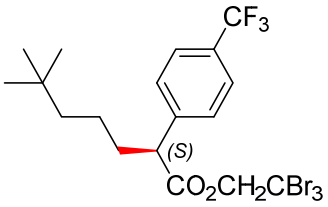
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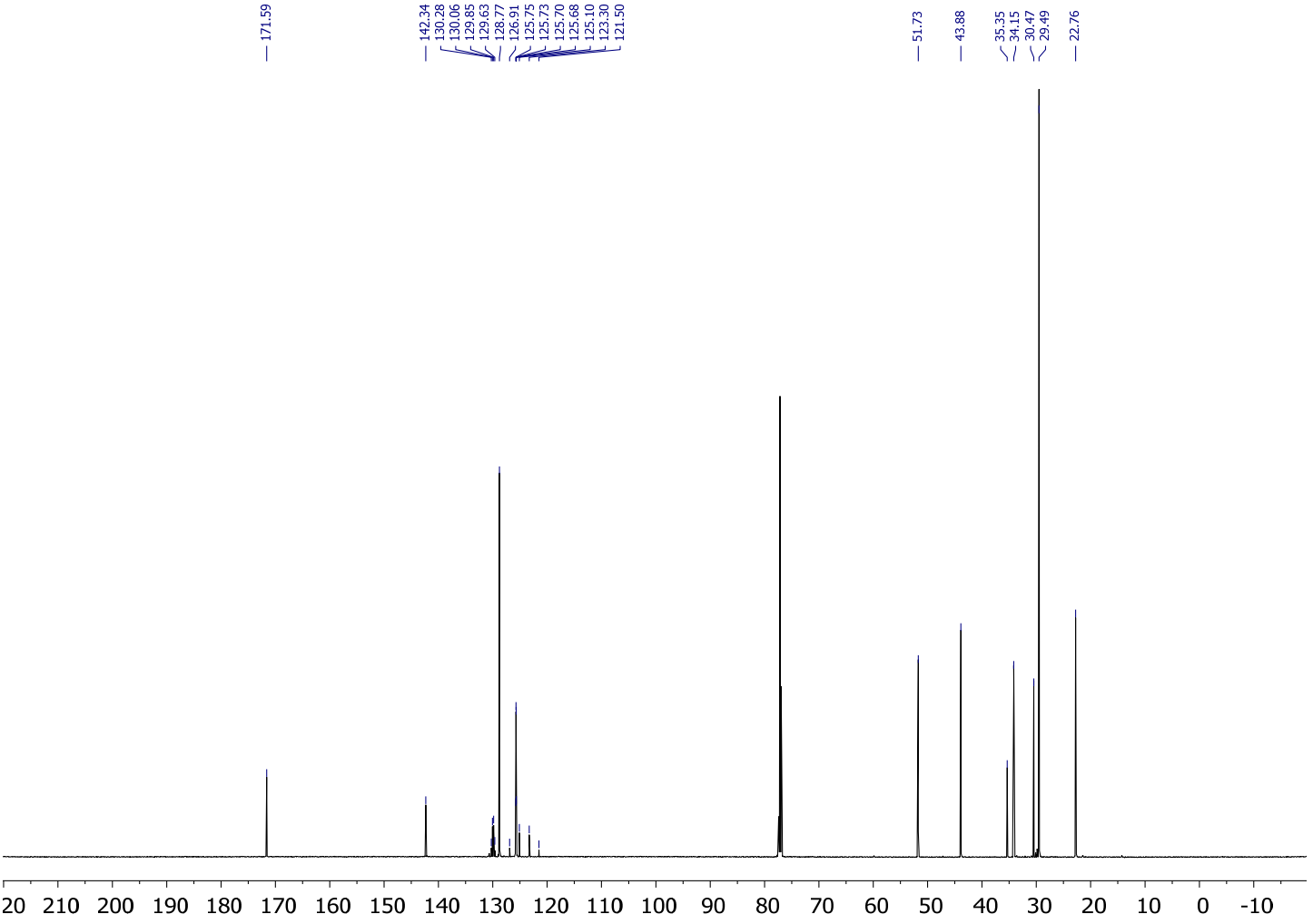
CO2CH2CBr3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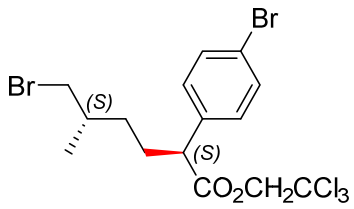
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(S)
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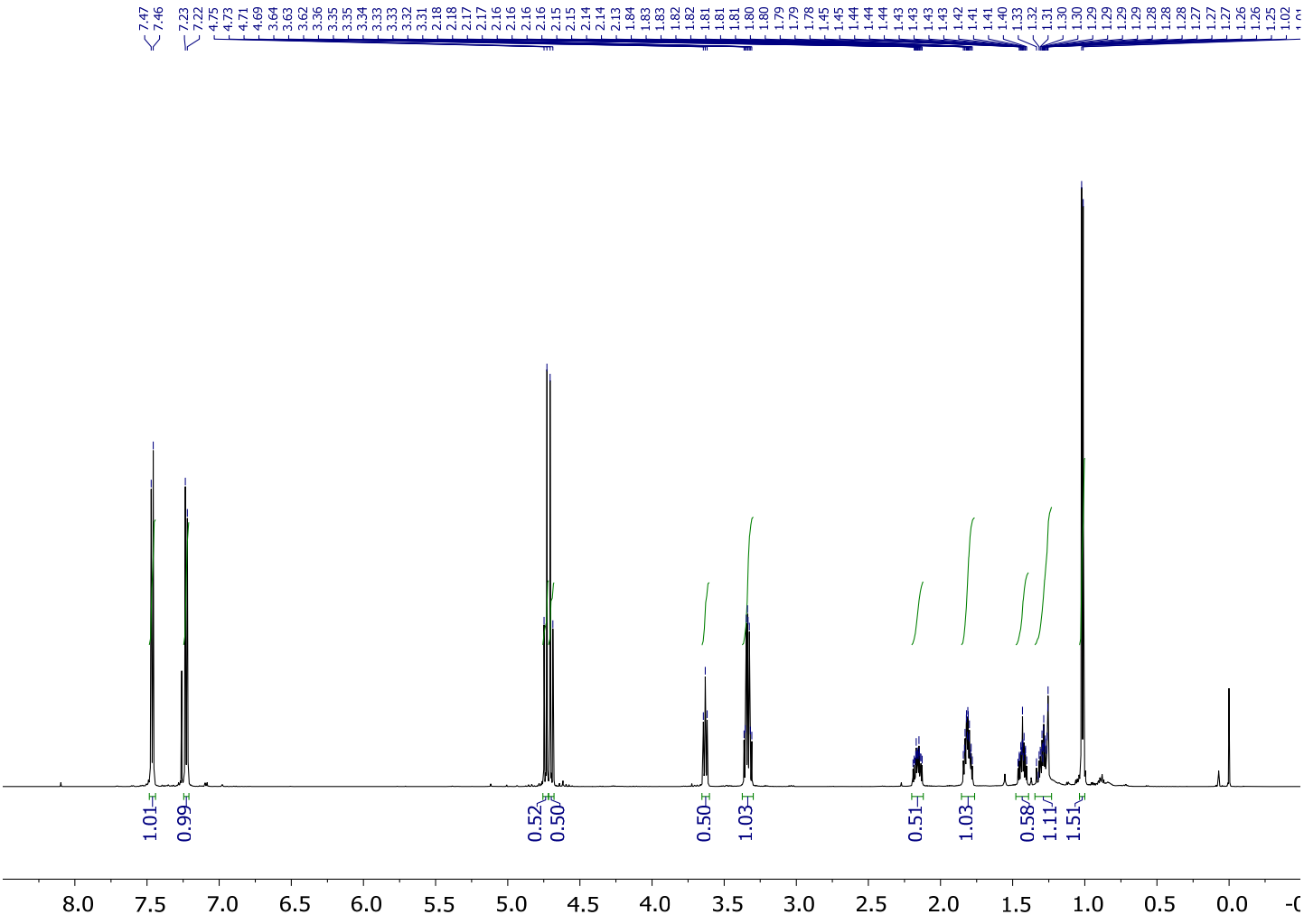
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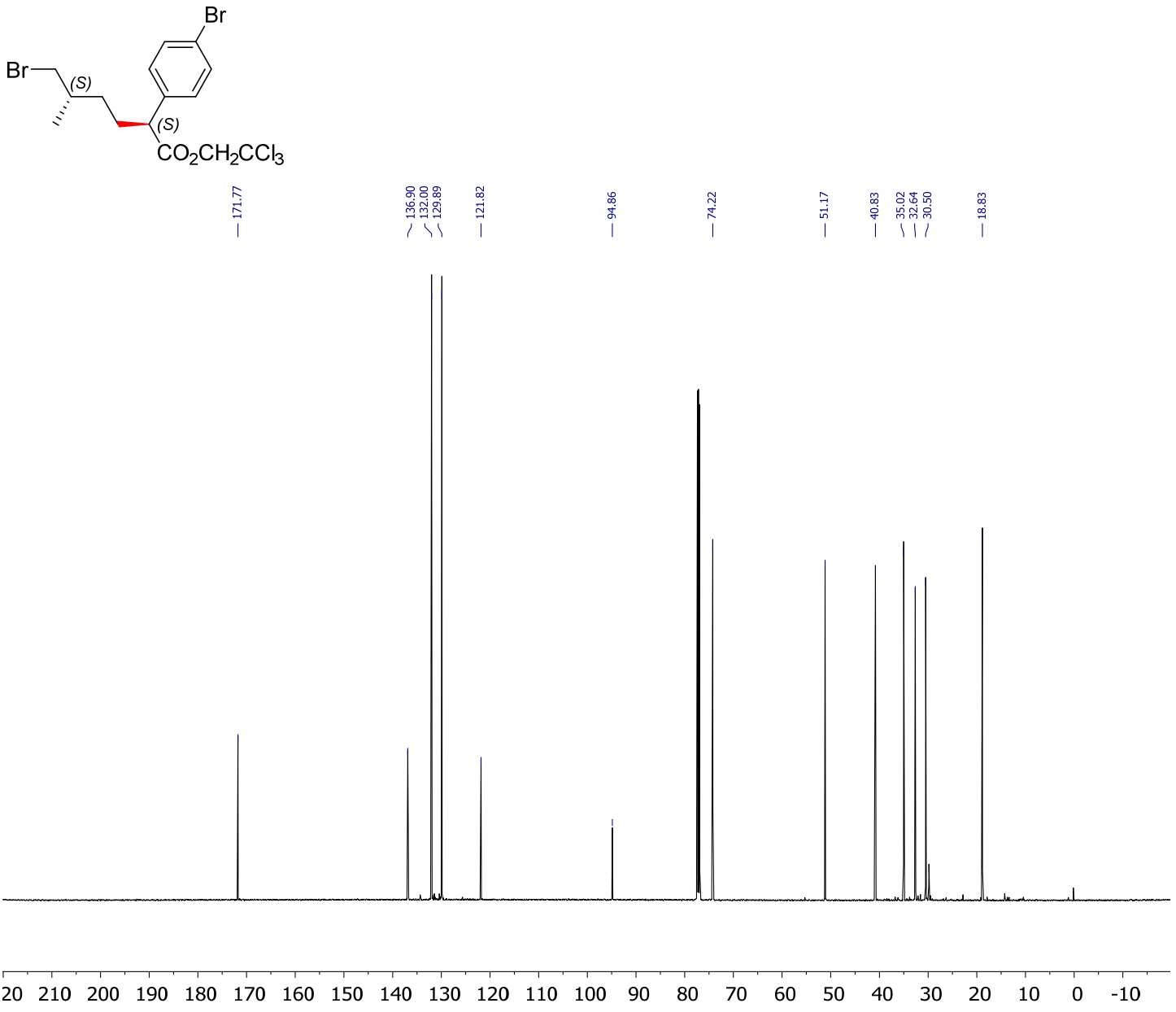
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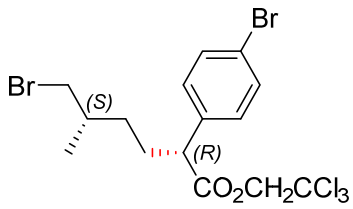
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(R)
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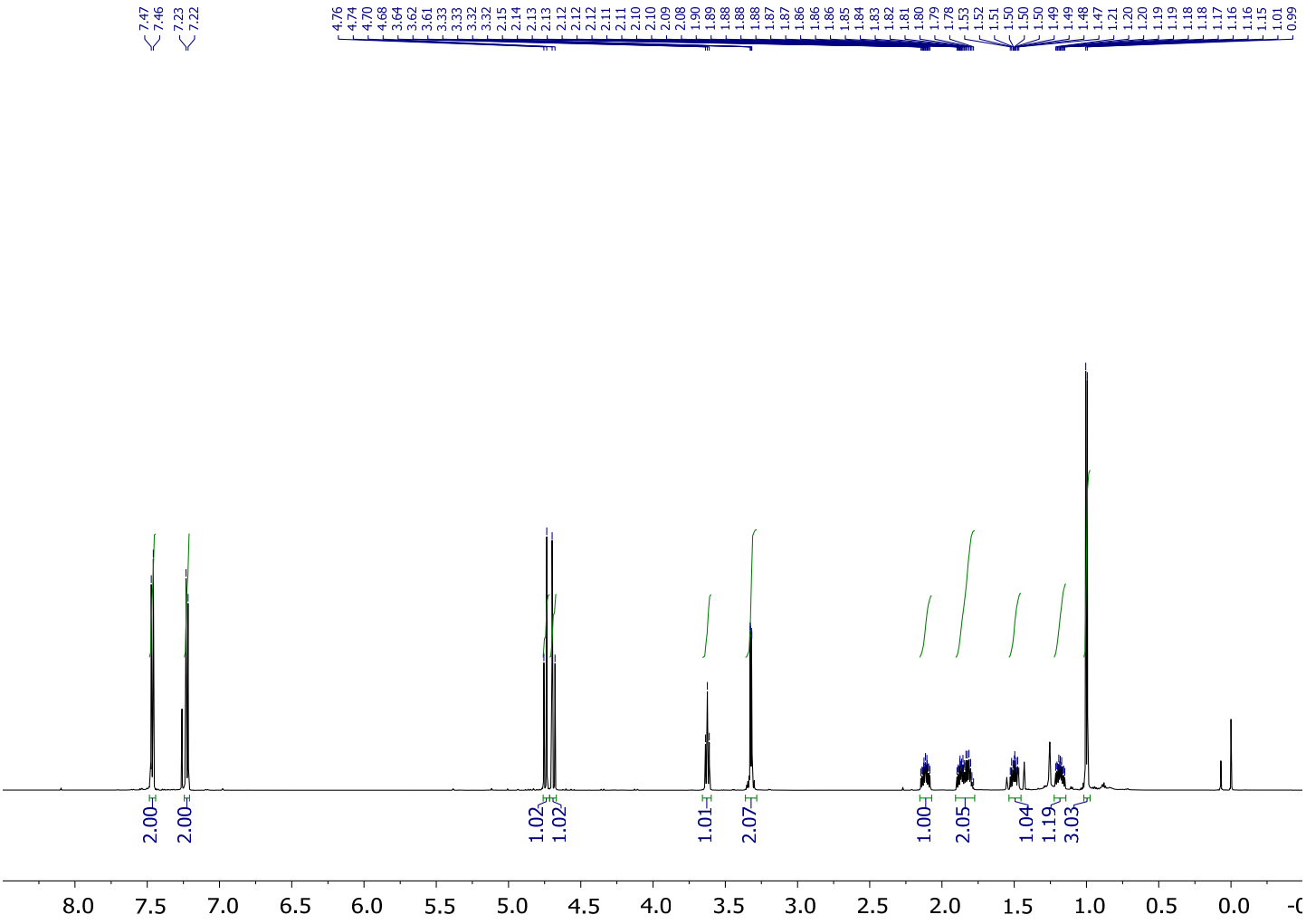
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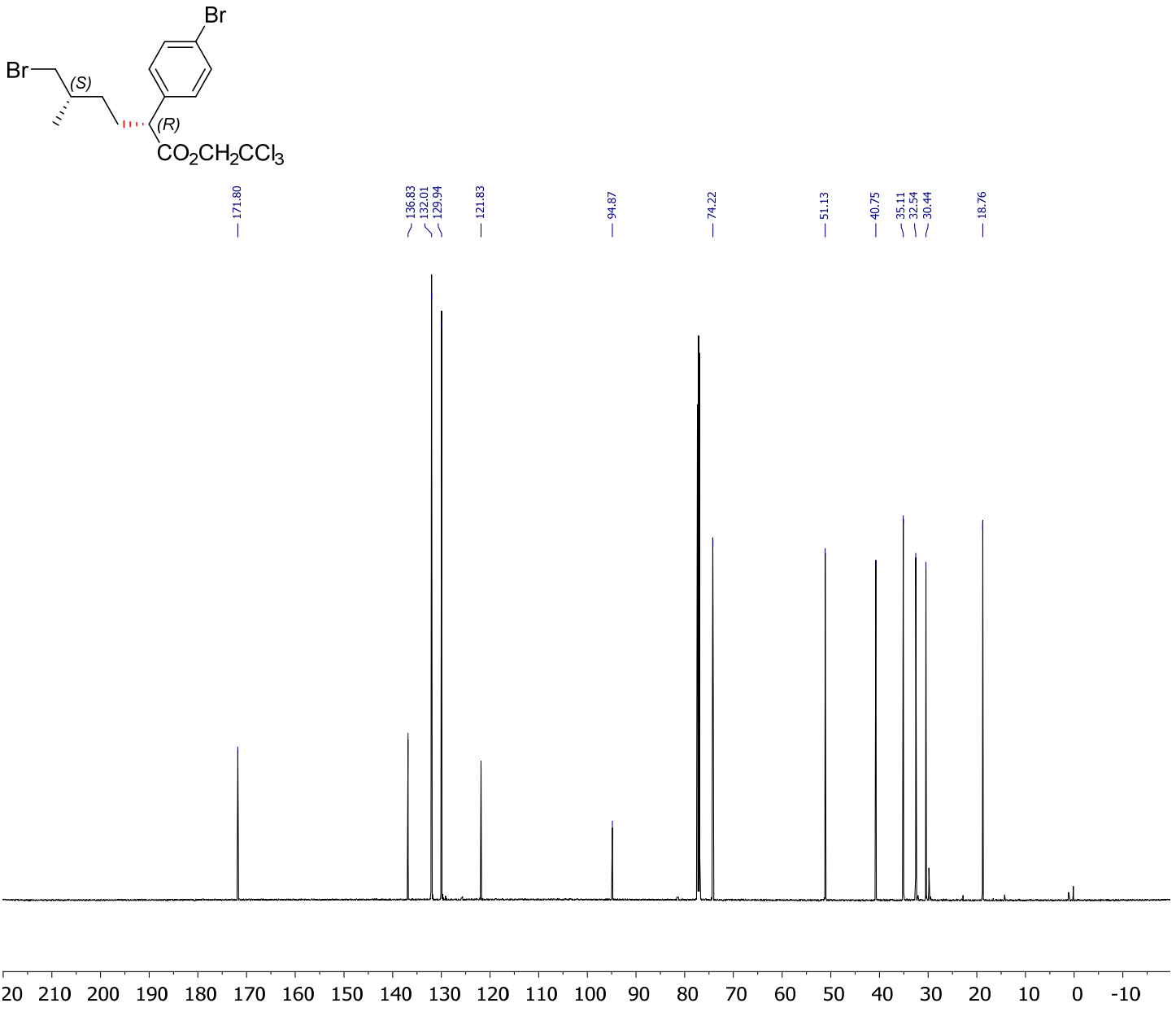
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Br
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(R)
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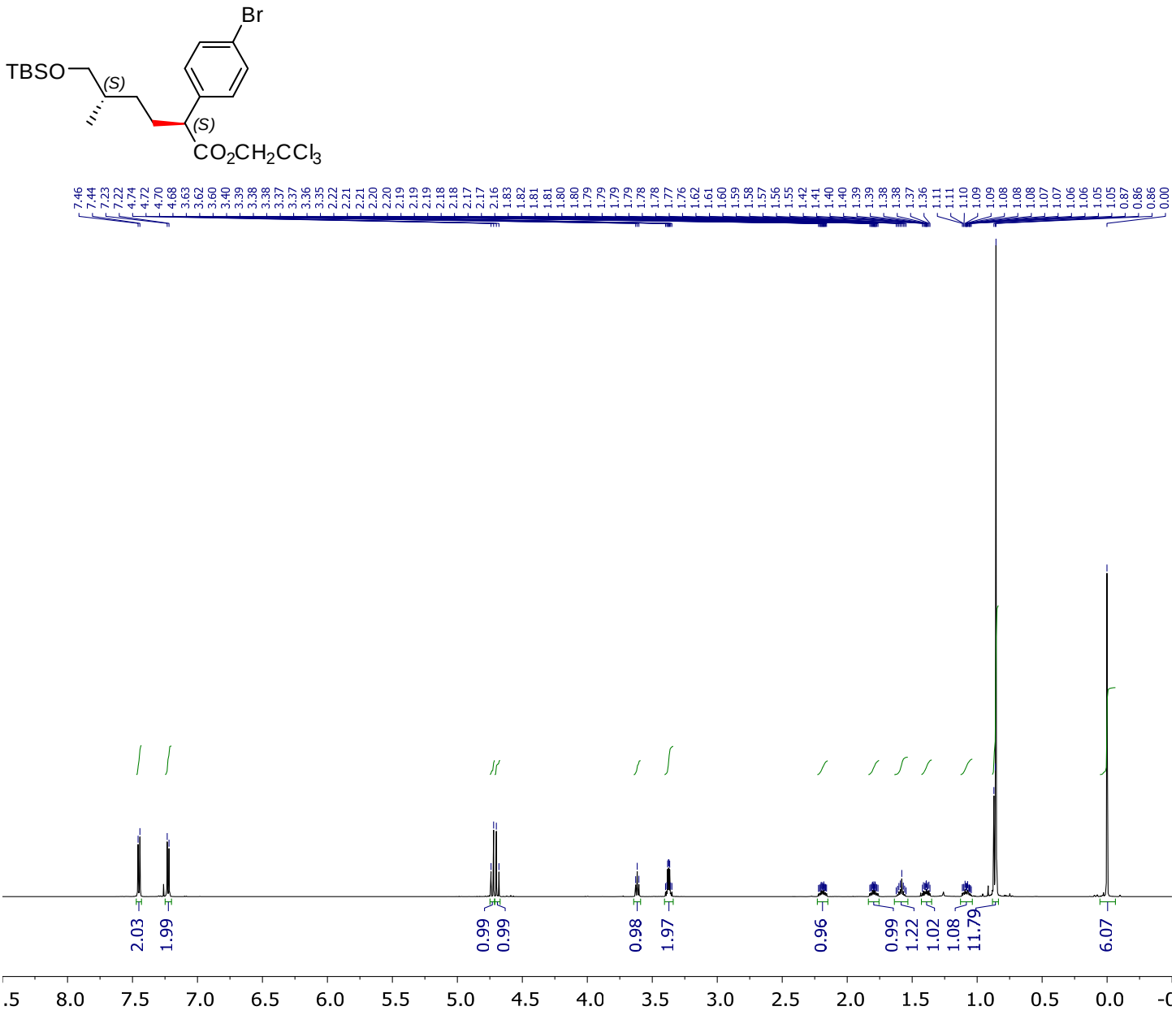
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TBSO
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(S)
CO2CH2CCl3
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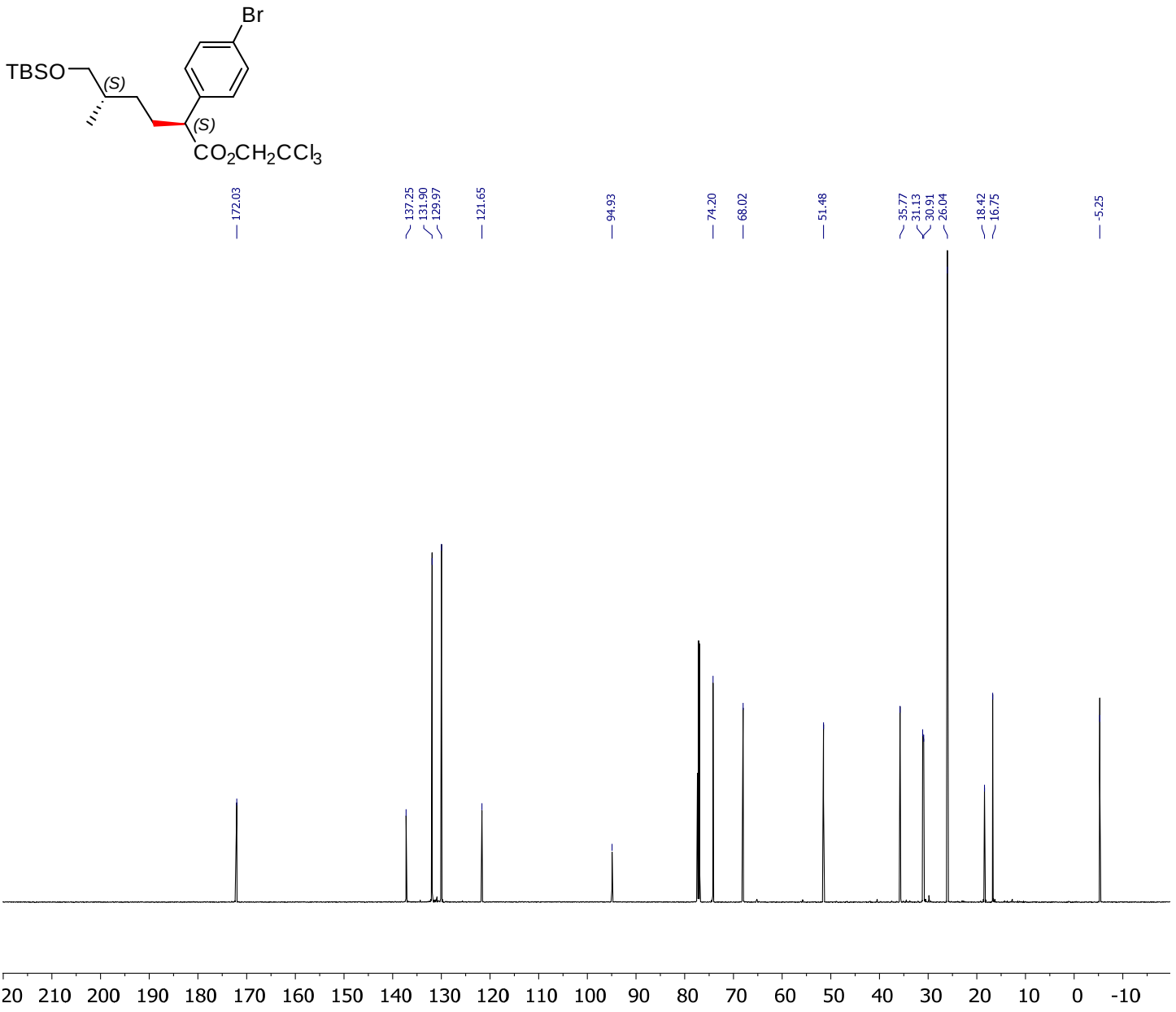
6.07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(S)
CO2CH2CCl3
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74.20
68.02
51.48
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16.75
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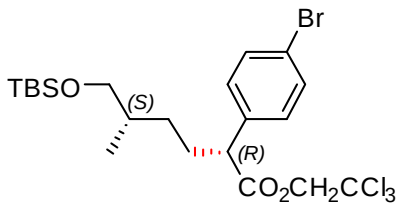
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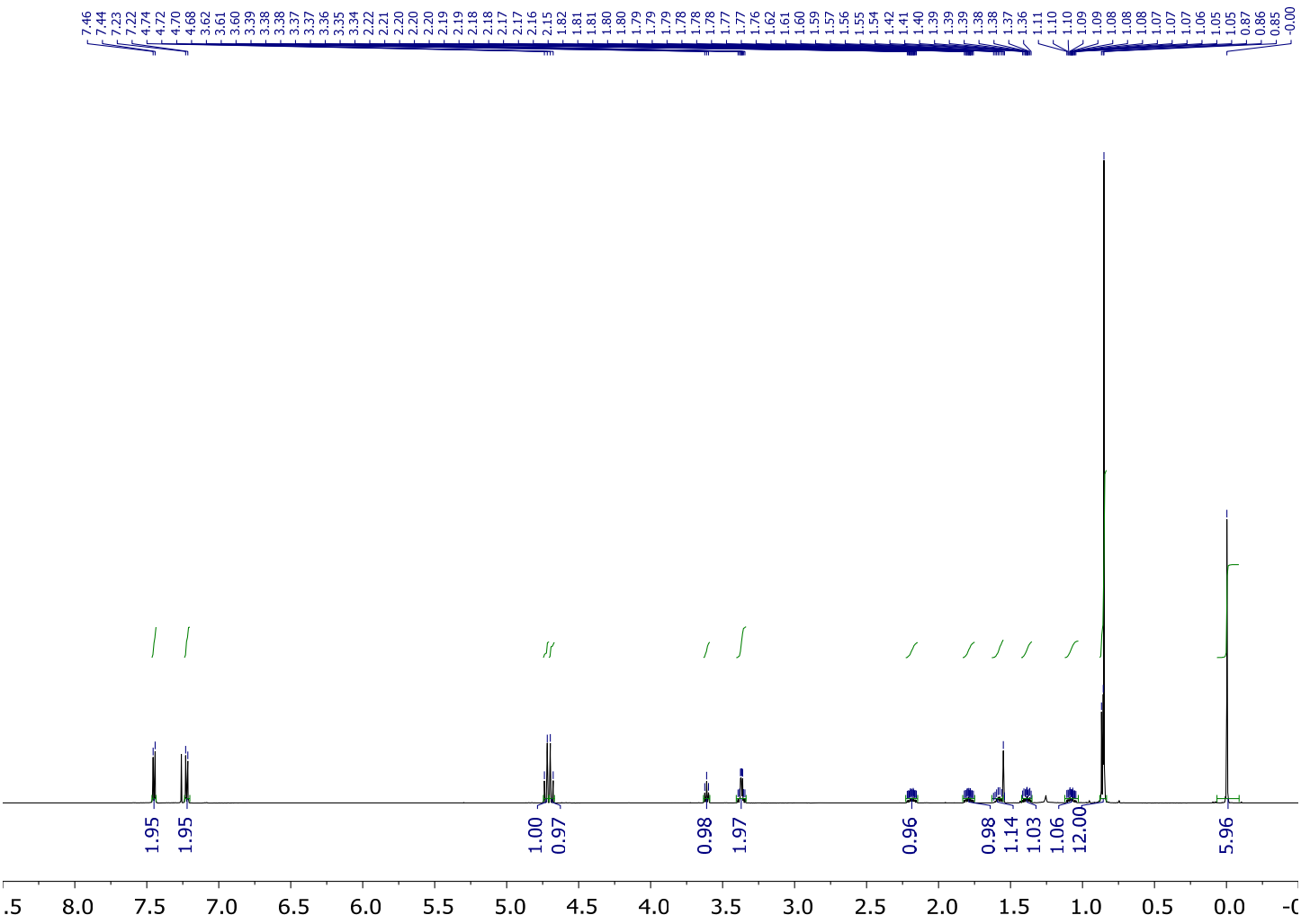
TBSO
(S)
(R)
CO2CH2CCl3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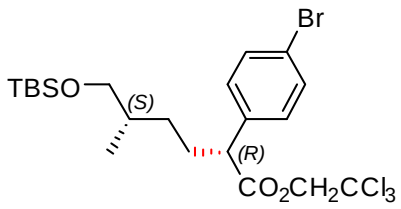
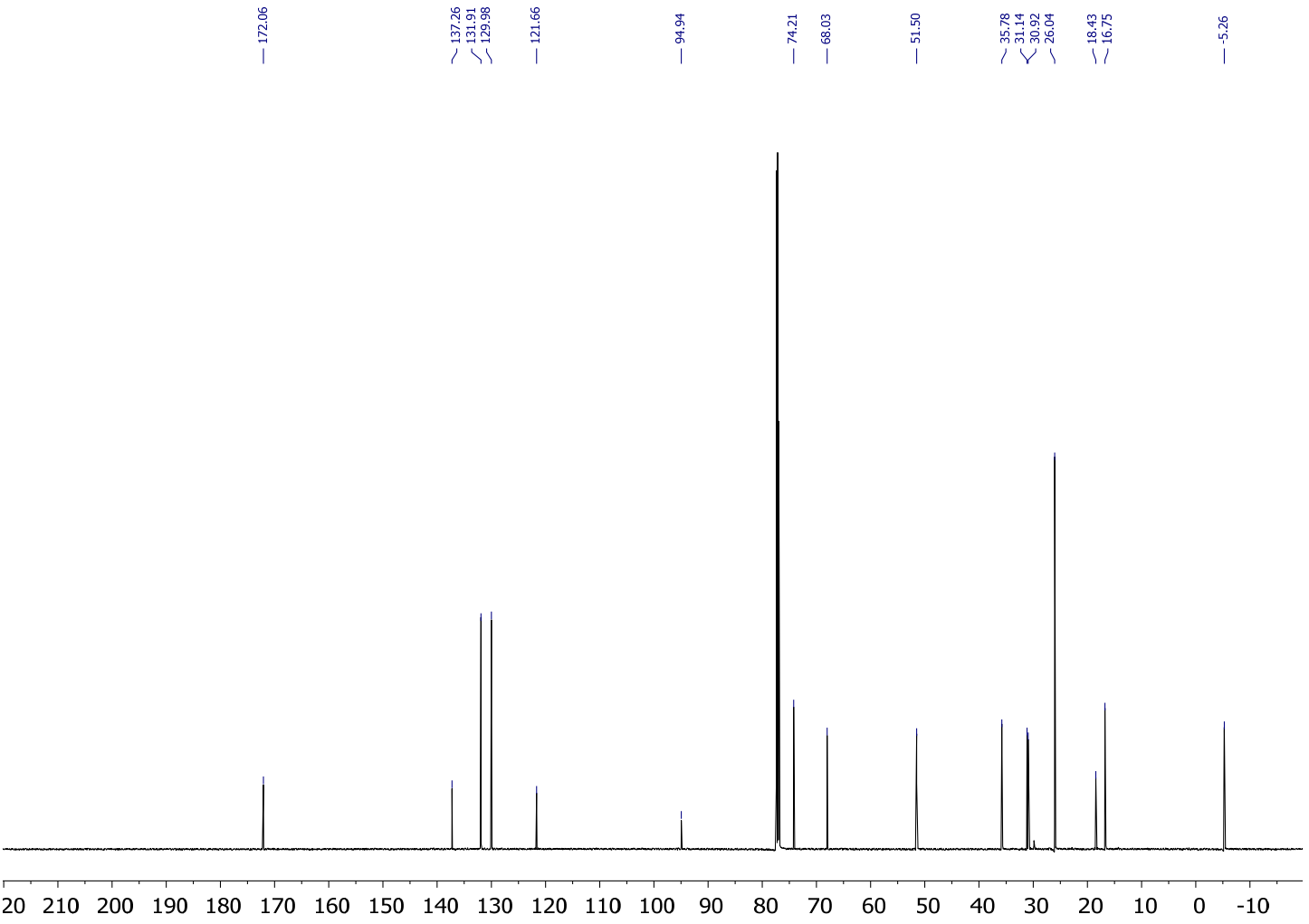

Br
TBSO
(S)
(R)
CO2CH2CCl3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26.04
18.43
16.75
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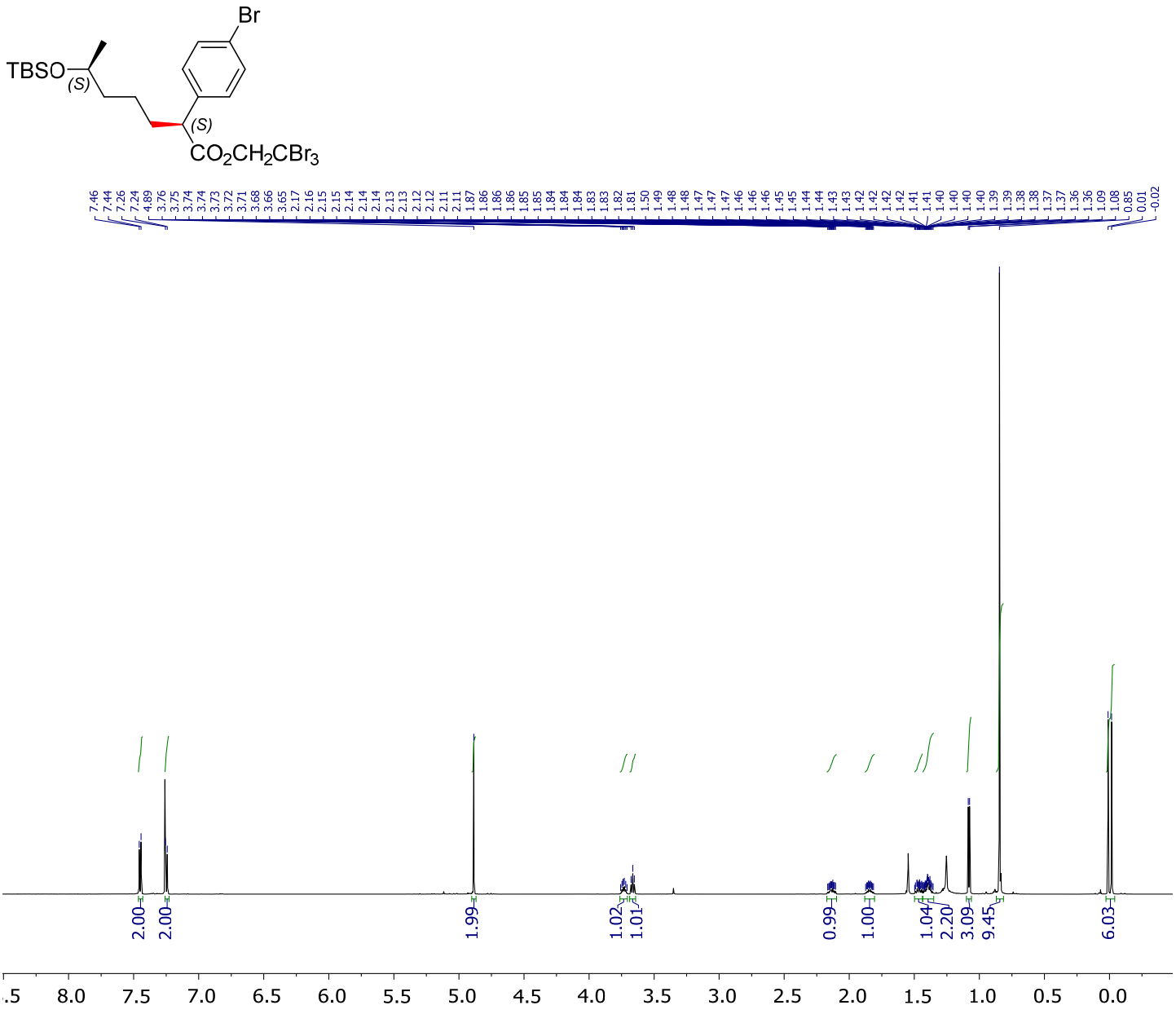
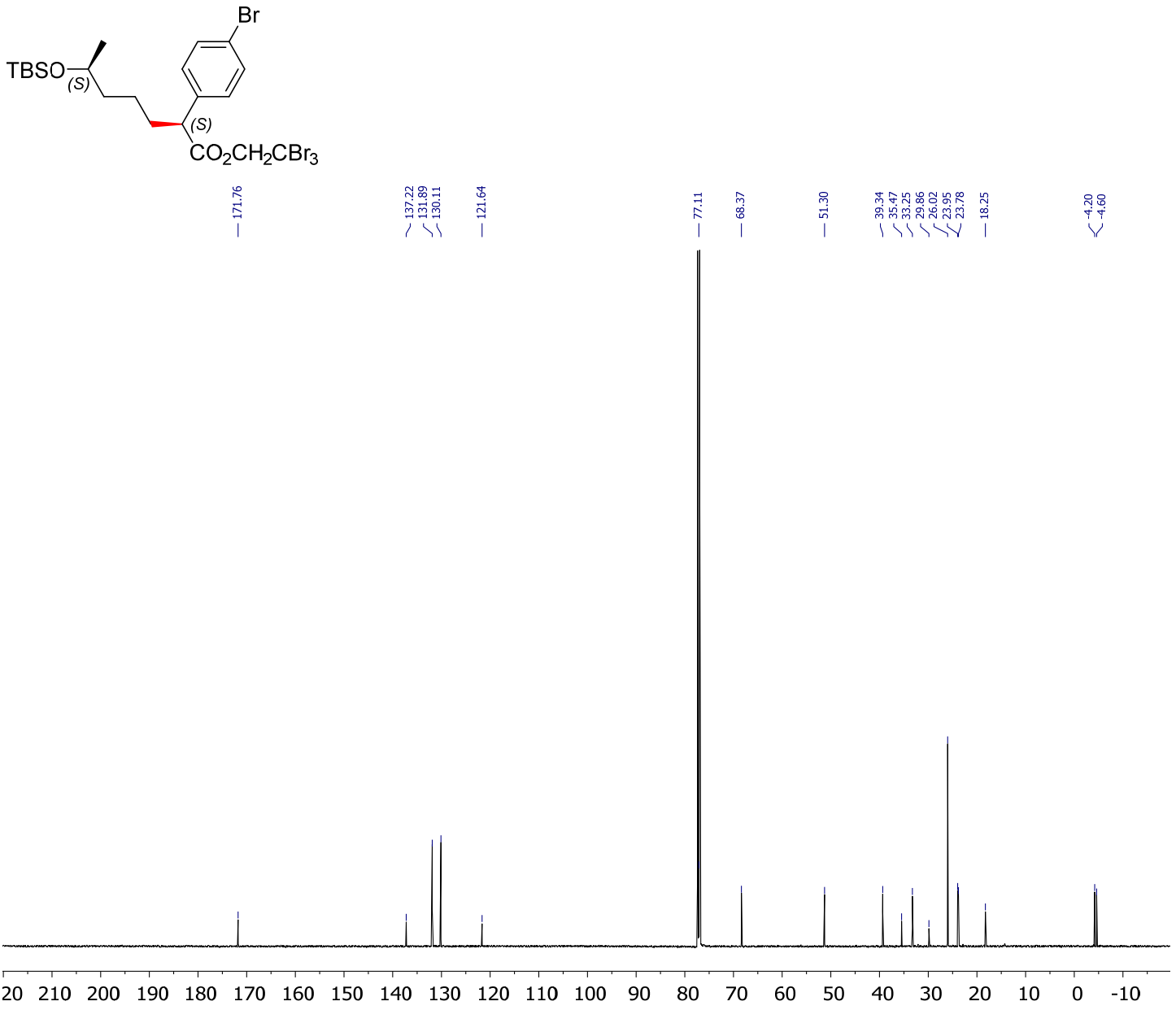
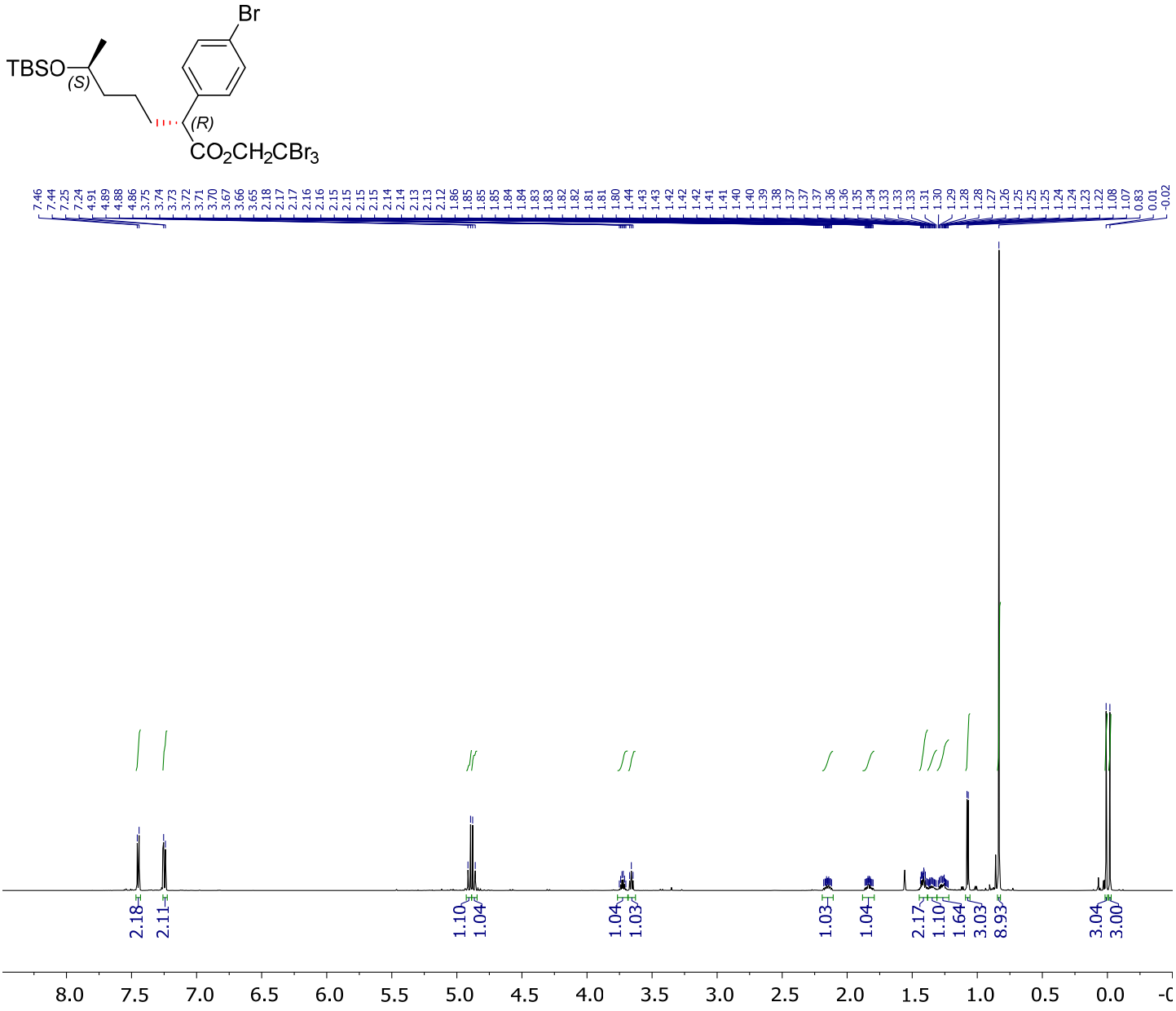
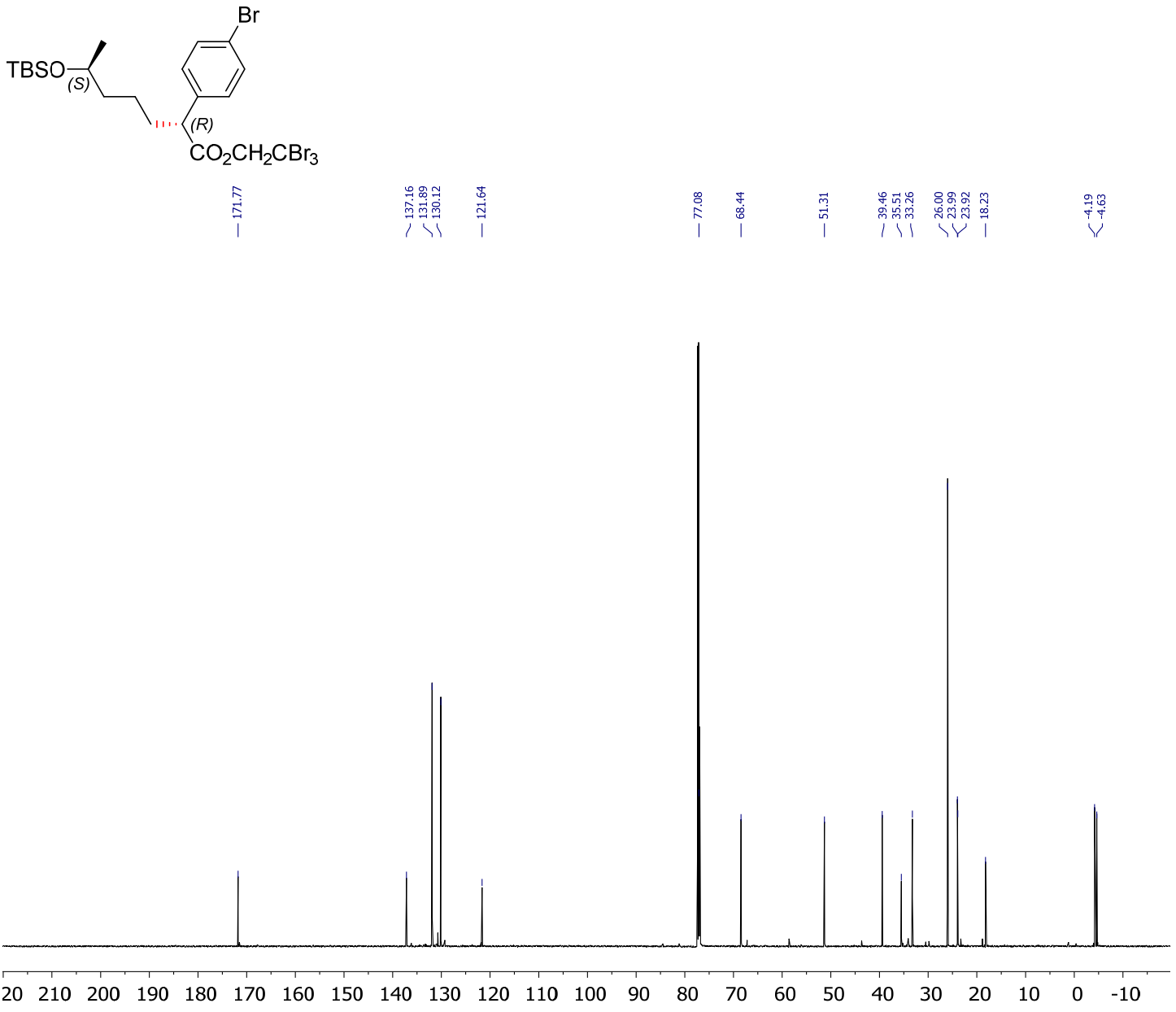
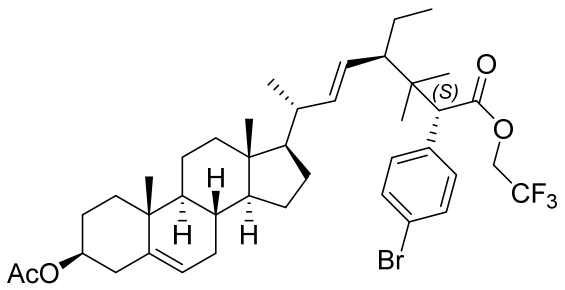
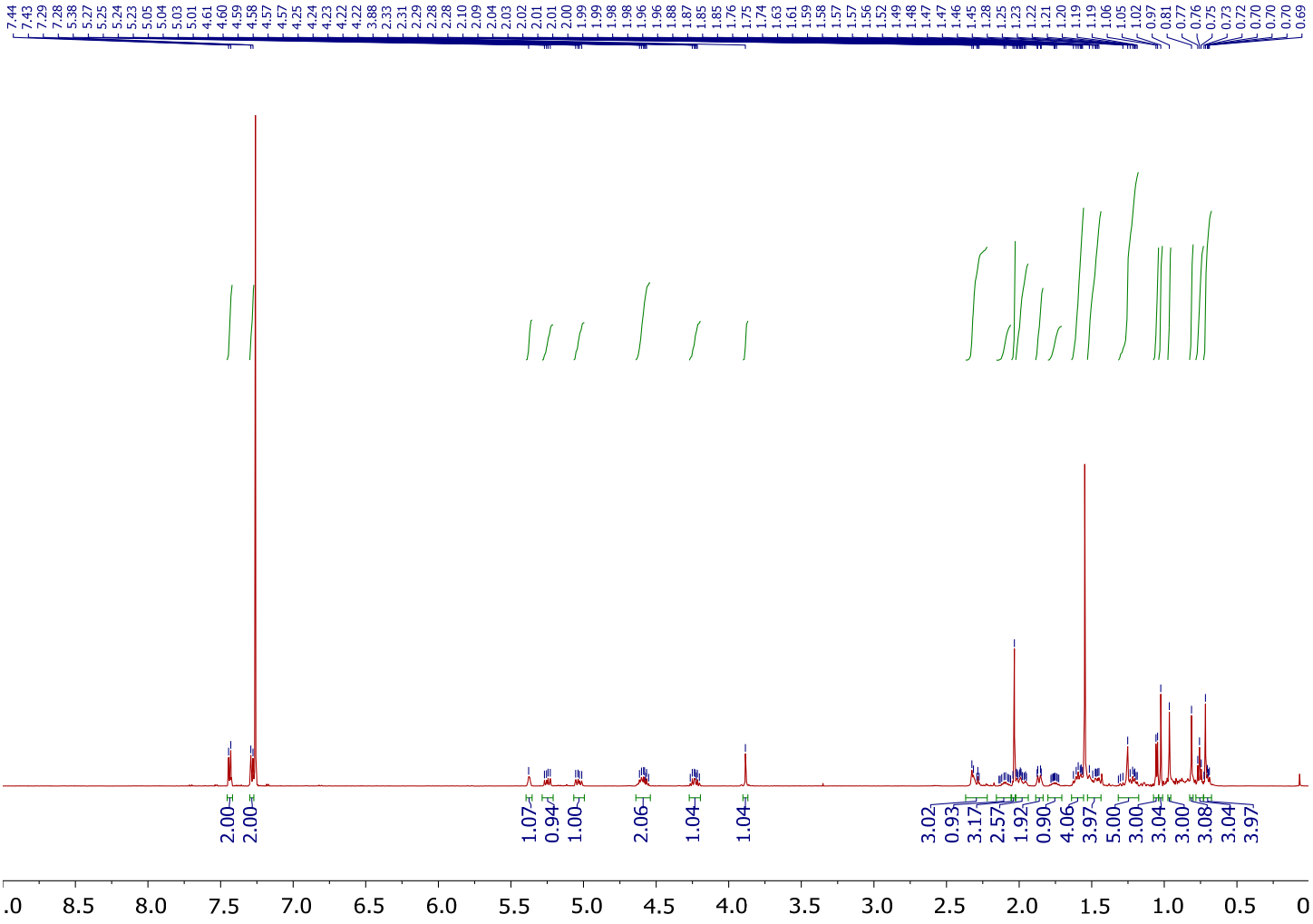

Br
TBSO
(S)
(S)
CO2CH2CBr3
7.46 7.44 7.26 7.24 4.89 3.76 3.75 3.74 3.74 3.73 3.72 3.71 3.68 3.66 3.65 2.17 2.16 2.15 2.14 2.14 2.14 2.13 2.13 2.12 2.12 2.11 2.11 1.87 1.86 1.86 1.86 1.85 1.85 1.84 1.84 1.84 1.83 1.83 1.82 1.81 1.50 1.49 1.48 1.48 1.47 1.47 1.47 1.46 1.46 1.46 1.45 1.45 1.44 1.44 1.43 1.43 1.42 1.42 1.42 1.42 1.41 1.41 1.40 1.40 1.40 1.40 1.39 1.39 1.38 1.38 1.37 1.37 1.36 1.36 1.09 1.08 0.85 0.01 -0.02
2.00 2.00 1.99 1.02 1.01 0.99 1.00 1.04 2.20 3.09 9.45 6.03
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

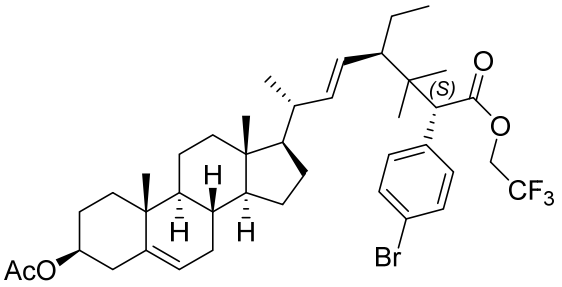

Br
TBSO
(S)
(S)
CO2CH2CBr3
171.76
137.22
131.89
130.11
121.64
77.11
68.37
51.30
39.34
35.47
33.25
29.86
26.02
23.95
23.78
18.25
-4.20
-4.60
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

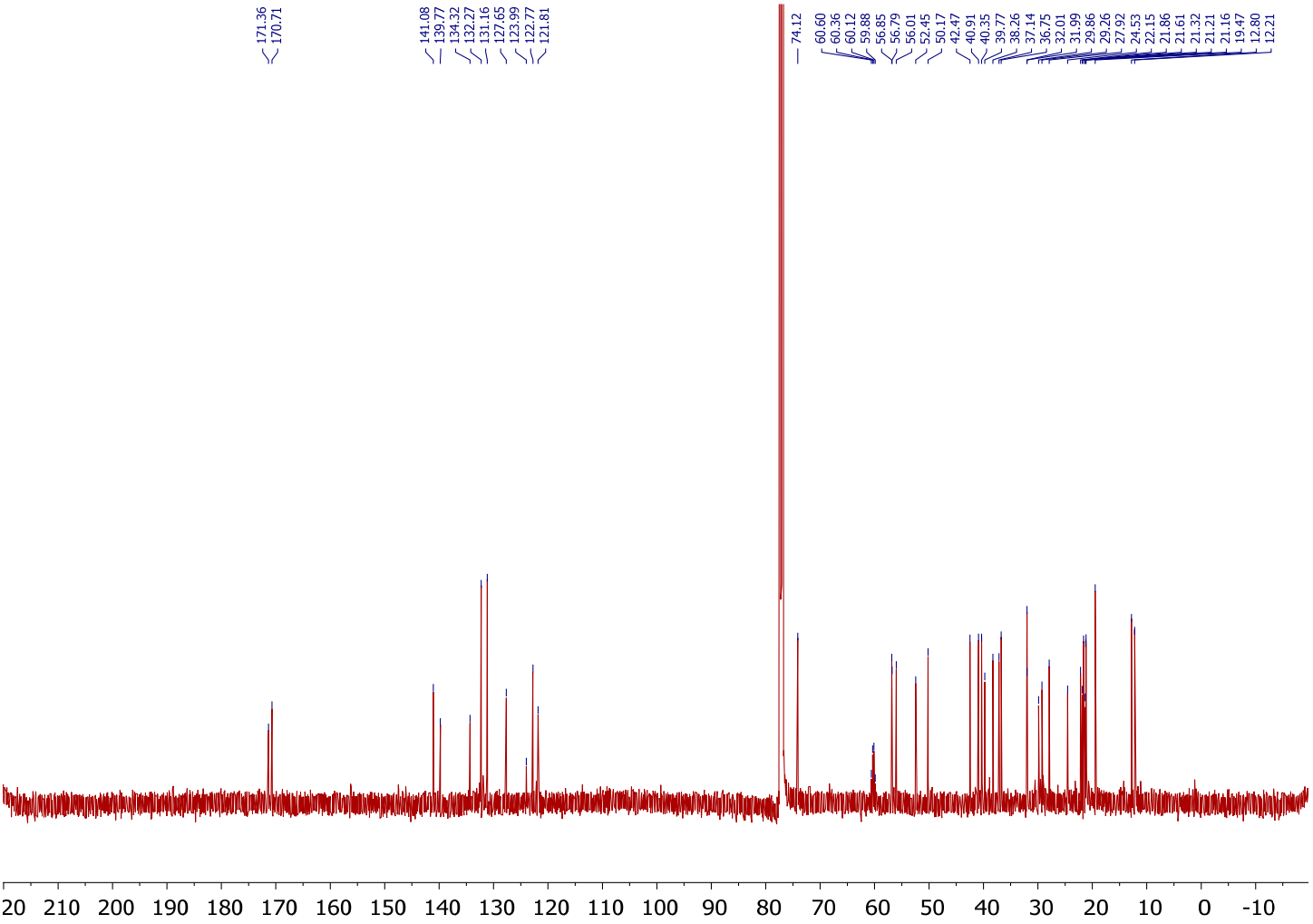

Br
TBSO
(S)
(R)
CO2CH2CBr3
2.18
2.11
1.10
1.04
1.04
1.03
1.03
1.04
2.17
1.10
1.64
3.03
8.93
3.04
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


Br
TBSO
(S)
(R)
CO2CH2CBr3
171.77
137.16
131.89
130.12
121.64
77.08
68.44
51.31
39.46
35.51
33.26
26.00
23.99
23.92
18.23
4.19
4.63
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


AcO
H
H
H
(S)
O
O
CF3
Br


7.44 7.43 7.29 7.28 5.38 5.27 5.25 5.24 5.23 5.05 5.04 5.03 5.01 4.61 4.60 4.59 4.58 4.57 4.57 4.25 4.24 4.23 4.22 4.22 3.88 2.33 2.31 2.29 2.28 2.28 2.10 2.09 2.04 2.03 2.02 2.01 2.01 2.00 1.99 1.99 1.98 1.98 1.96 1.96 1.88 1.87 1.85 1.85 1.76 1.75 1.74 1.63 1.61 1.59 1.58 1.57 1.57 1.56 1.52 1.49 1.48 1.47 1.47 1.46 1.45 1.28 1.25 1.23 1.22 1.21 1.20 1.19 1.19 1.06 1.05 1.02 0.97 0.81 0.77 0.76 0.75 0.73 0.72 0.70 0.70 0.70 0.69
2.00 2.00 1.07 0.94 1.00 2.06 1.04 1.04 3.02 0.93 3.17 2.57 1.92 0.90 4.06 3.97 5.00 3.00 3.04 3.00 3.08 3.04 3.97
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0


AcO
H
H
H
(S)
O
O
CF3
Br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170.71
141.08
139.77
134.32
132.27
131.16
127.65
123.99
122.77
121.81
74.12
60.60
60.36
60.12
59.88
56.85
56.79
56.01
52.45
50.17
42.47
40.91
40.35
39.77
38.26
37.14
36.75
32.01
31.99
29.86
29.26
27.92
24.53
22.15
21.86
21.61
21.32
21.21
21.16
19.47
12.80
12.21
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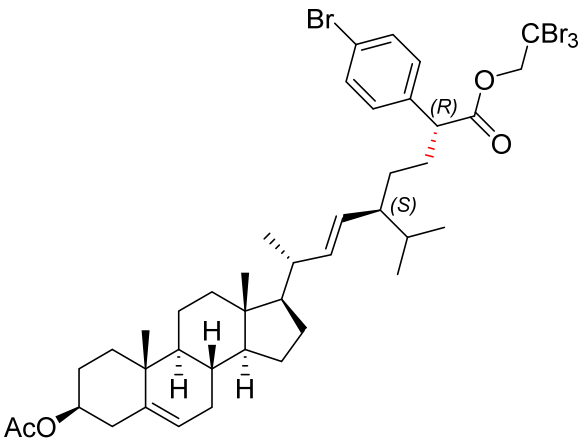
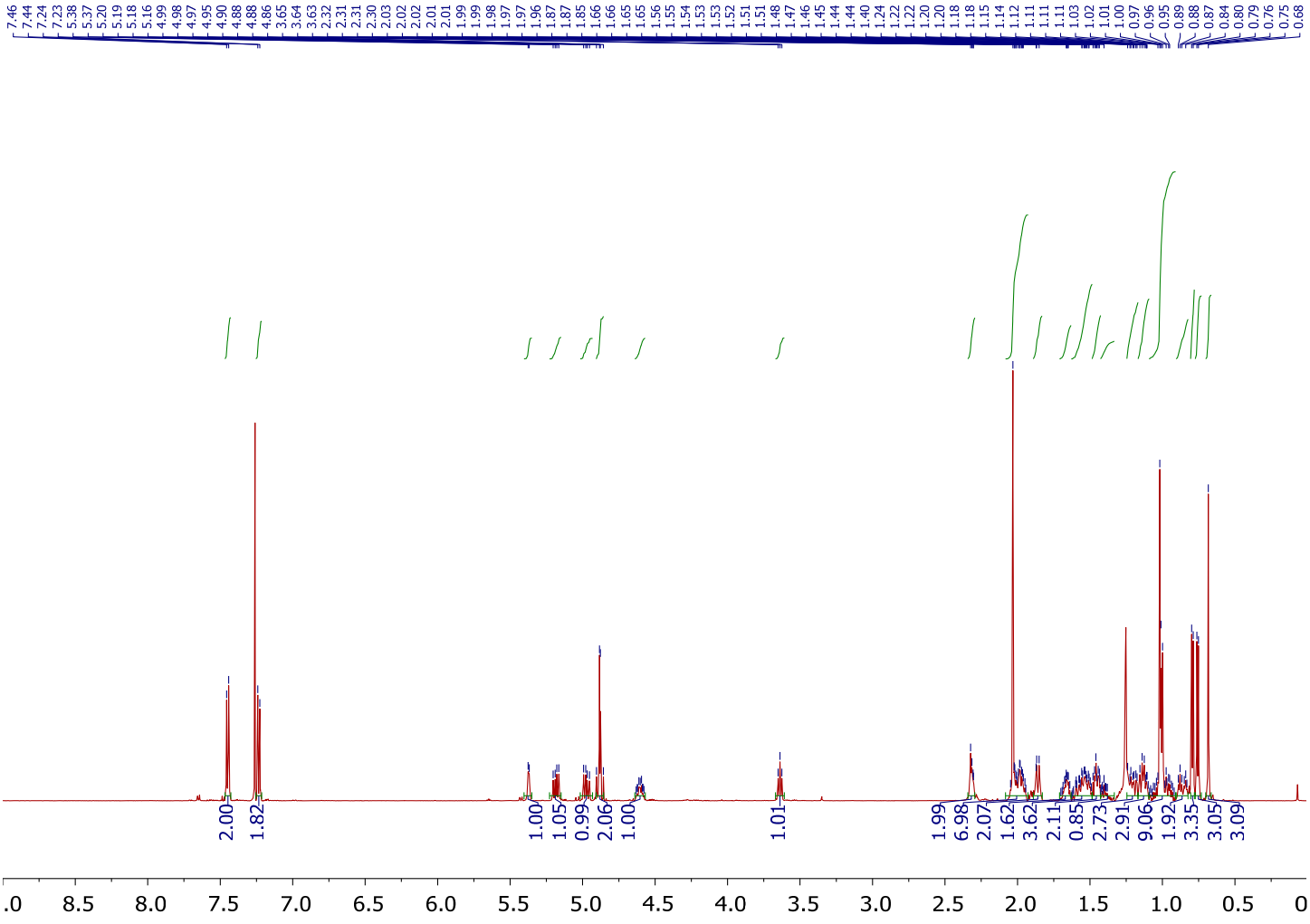
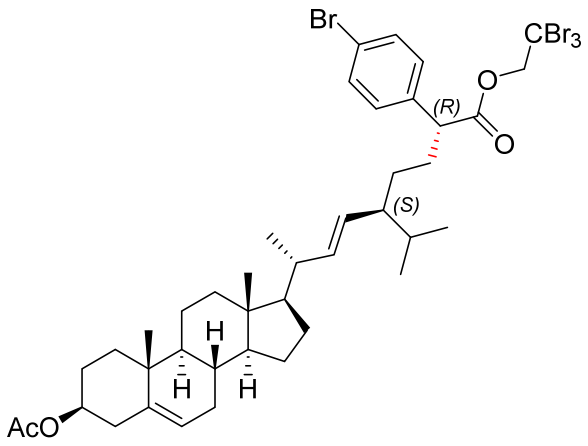
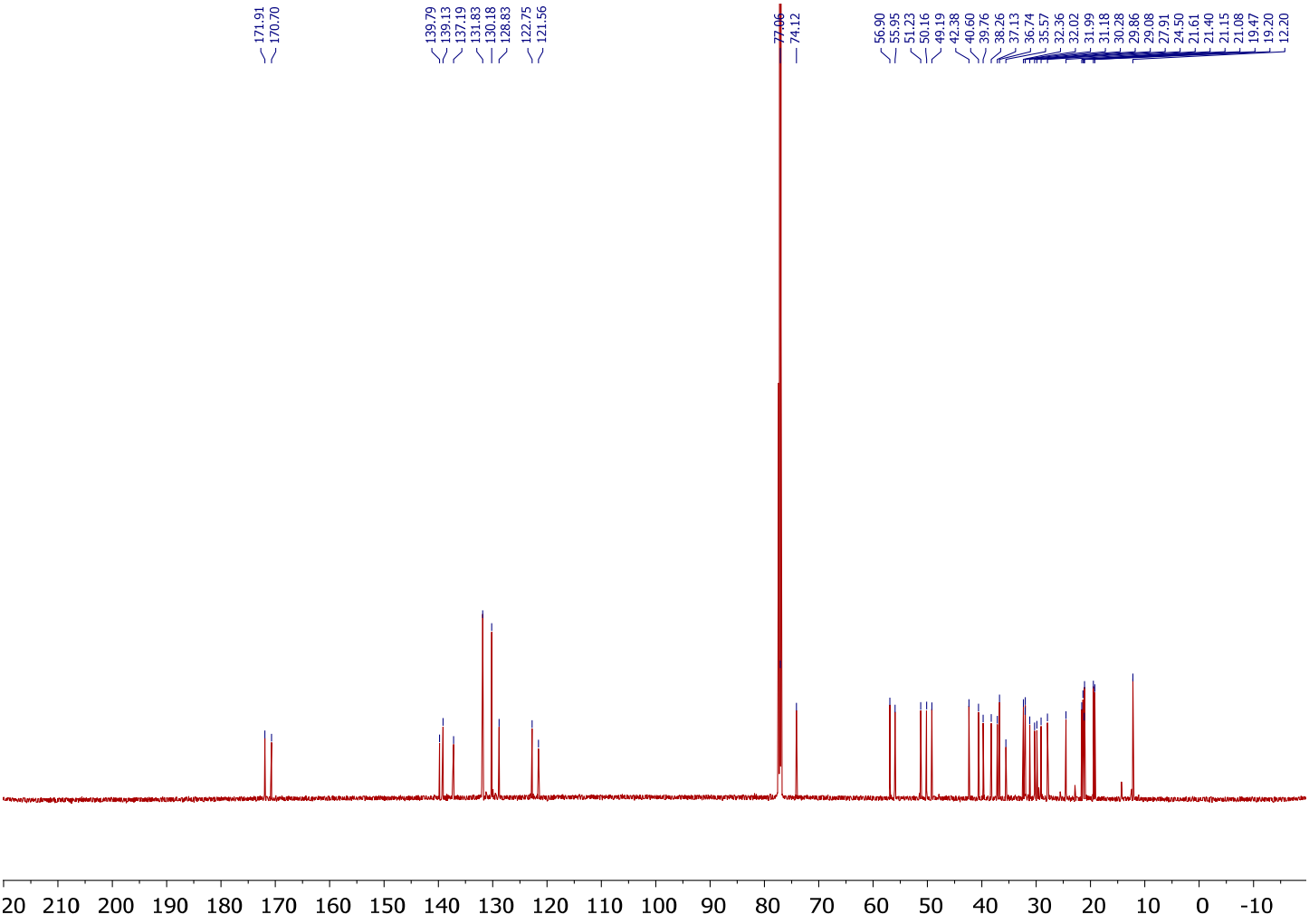

Br
CBr3
O
O
(R)
(S)
H
H
H
AcO


2.00
1.82
1.00
1.05
0.99
2.06
1.00
1.01
1.99
6.98
2.07
1.62
3.62
2.11
0.85
2.73
2.91
9.06
1.92
3.35
3.05
3.09
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0


Br
CBr3
O
O
(R)
(S)
H
H
H
AcO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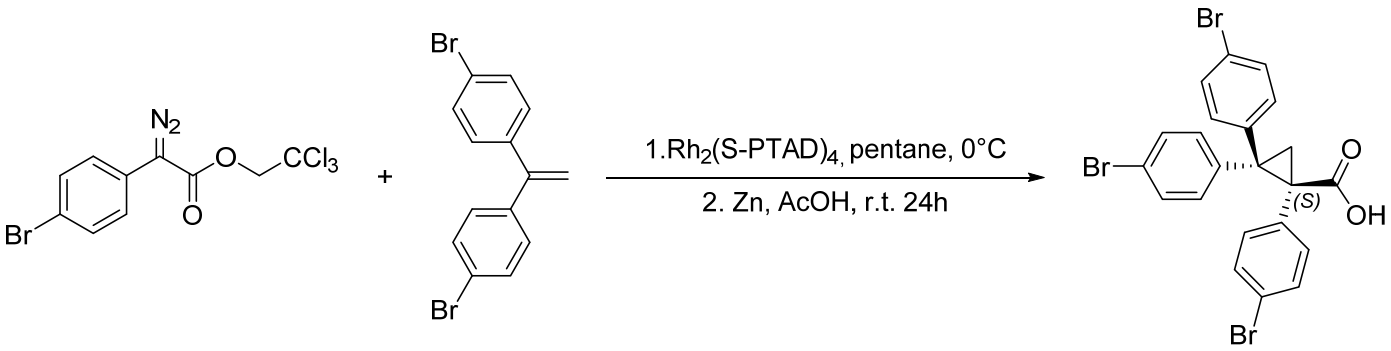
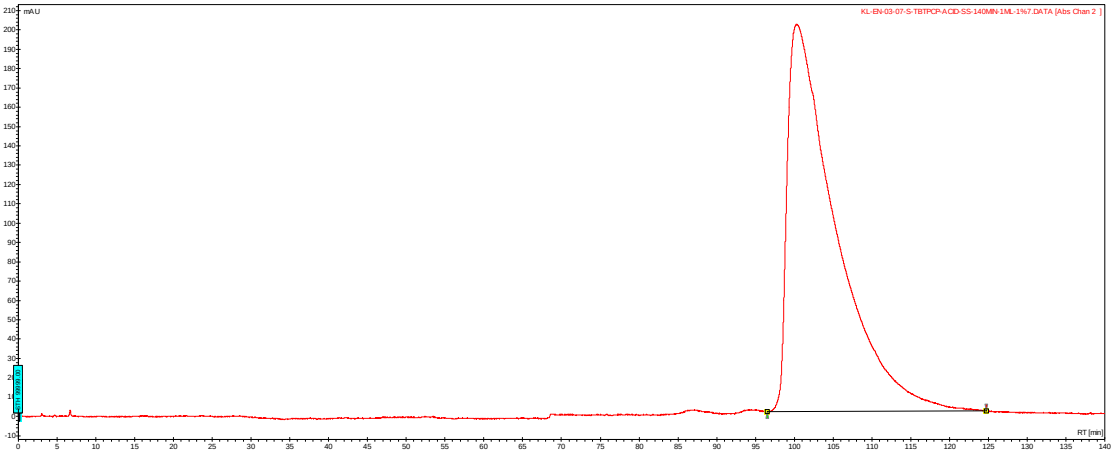
170.70
139.79
139.13
137.19
131.83
130.18
128.83
122.75
121.56
77.06
74.12
56.90
55.95
51.23
50.16
49.19
42.38
40.60
39.76
38.26
37.13
36.74
35.57
32.36
32.02
31.99
31.18
30.28
29.86
29.08
27.91
24.50
21.61
21.40
21.15
21.08
19.47
19.20
12.20
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

10 – HPLC Spectra for Enantiomeric Excess Determination

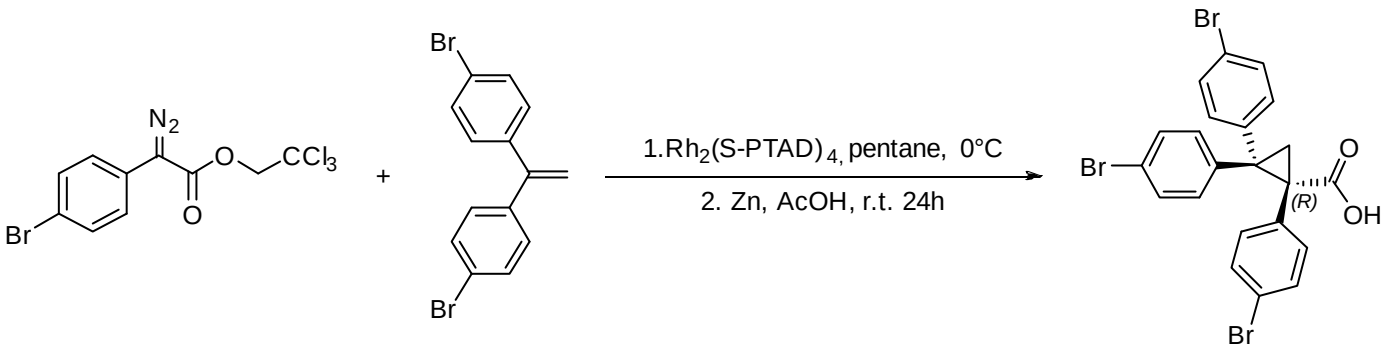
10.1 Catalyst preparation

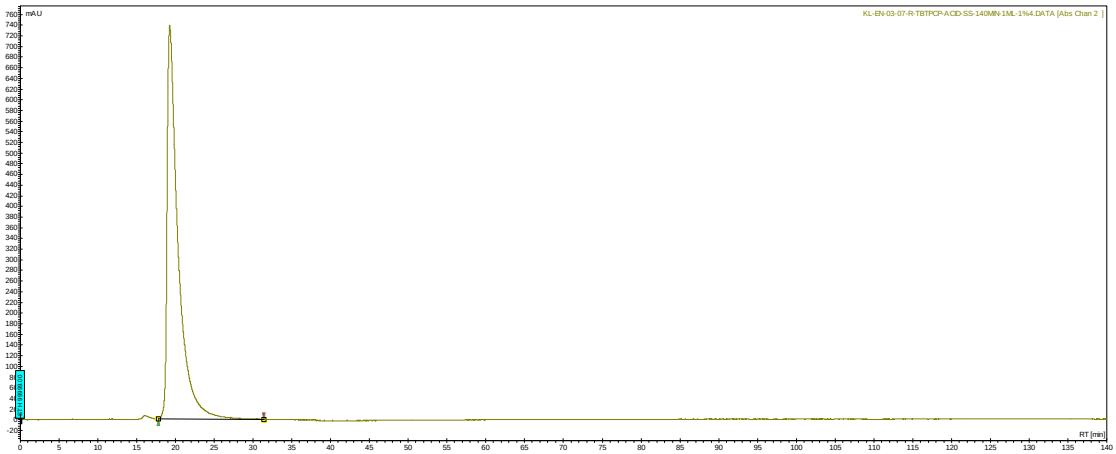




#	Time [Min]	Area % [%]
1	100.36	100.000

> 99% e.e.





#	Time [Min]	Area % [%]
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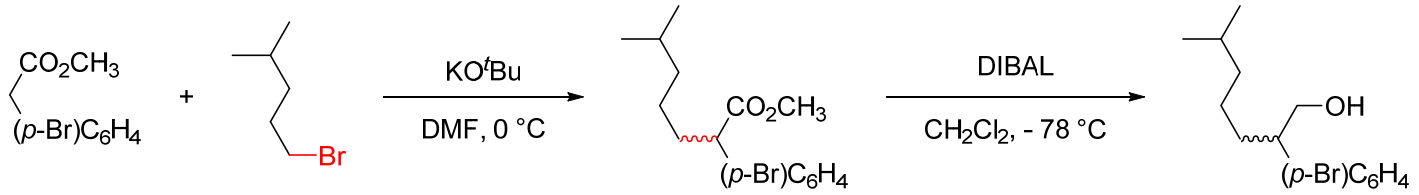
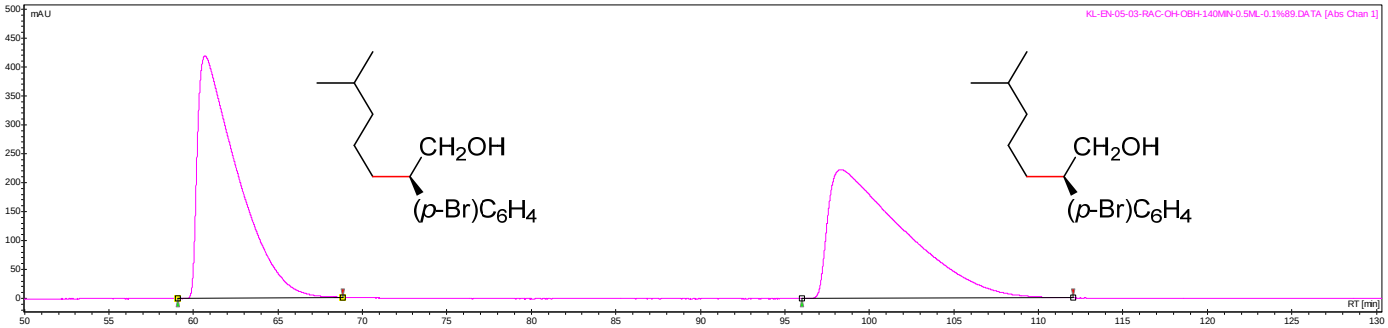
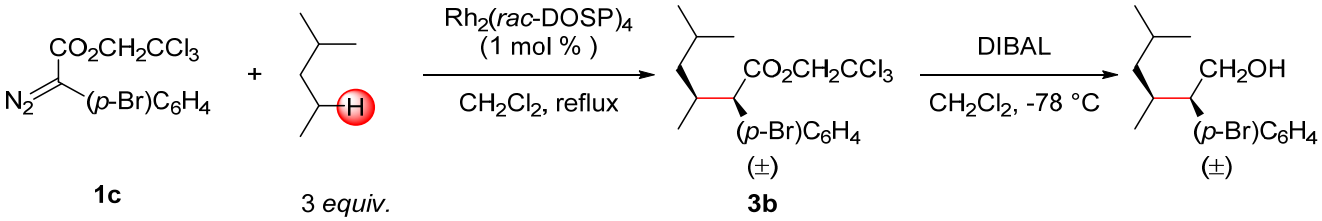
> 99% e.e.

10.2 C–H Functionalization Products of 2-Methylpentane

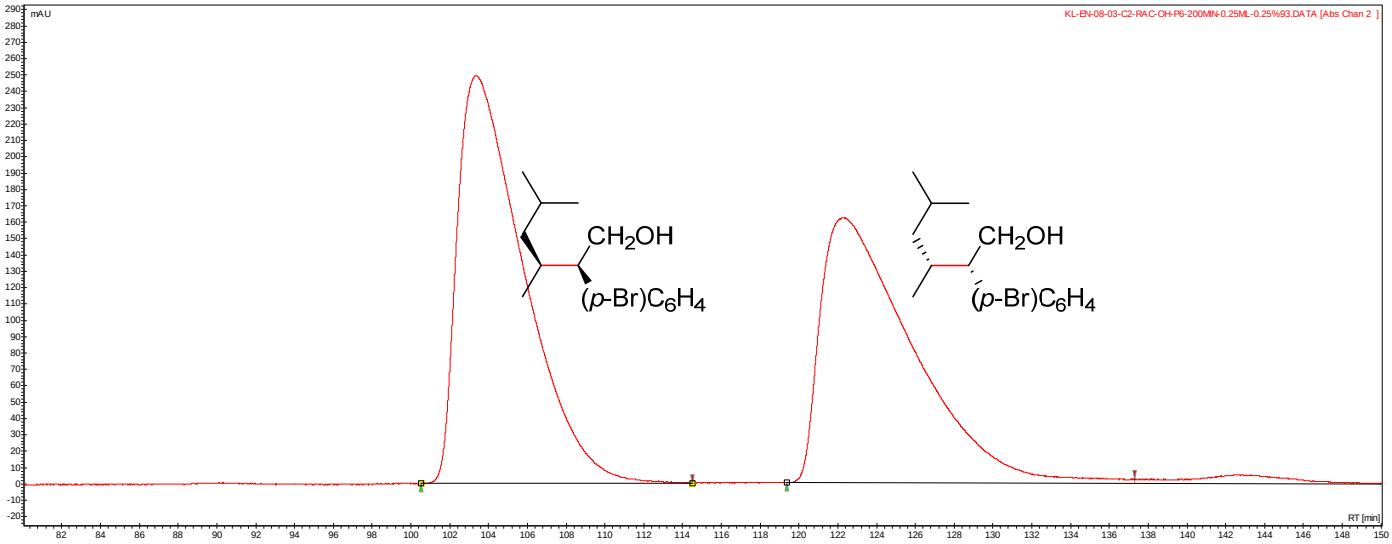




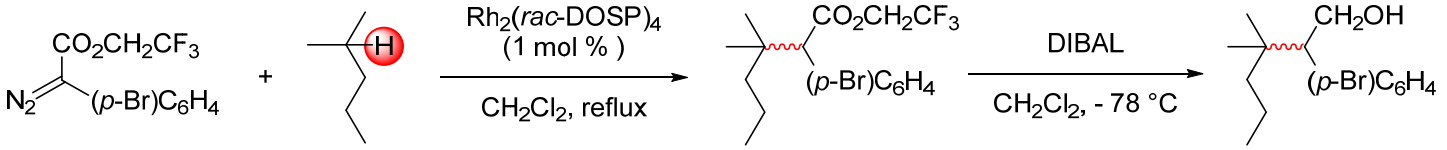
#	Time [Min]	Area% [%]
1	60.71	49.907
2	98.29	50.093

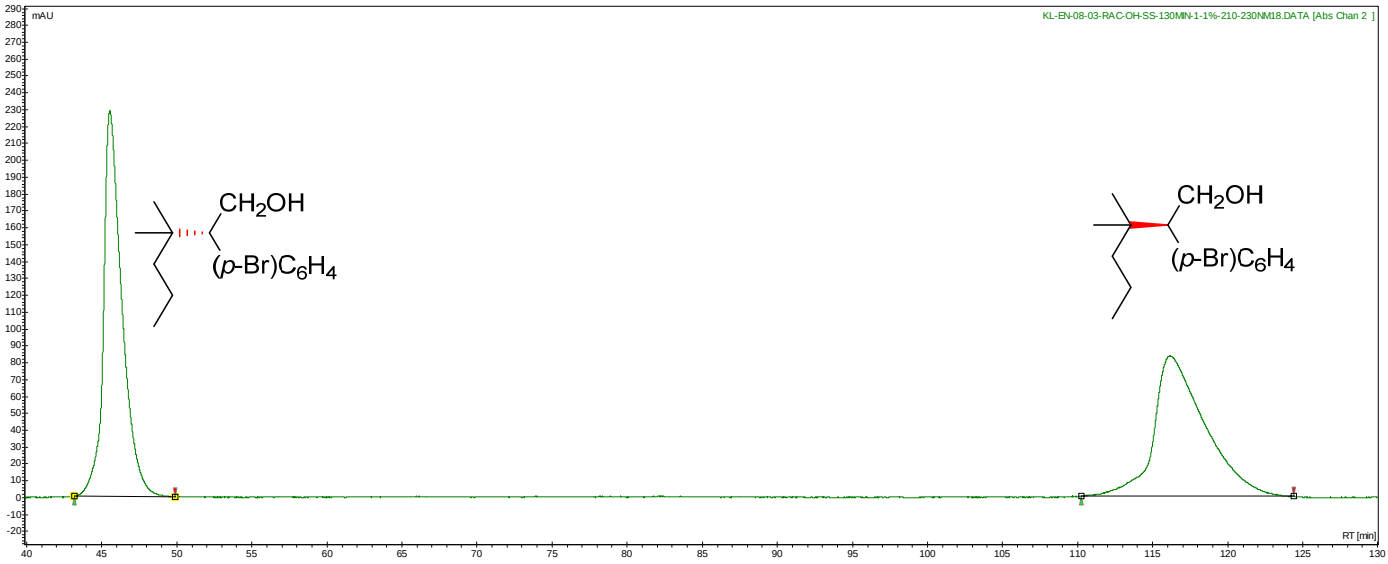


1c 3 *equiv.* **3b**



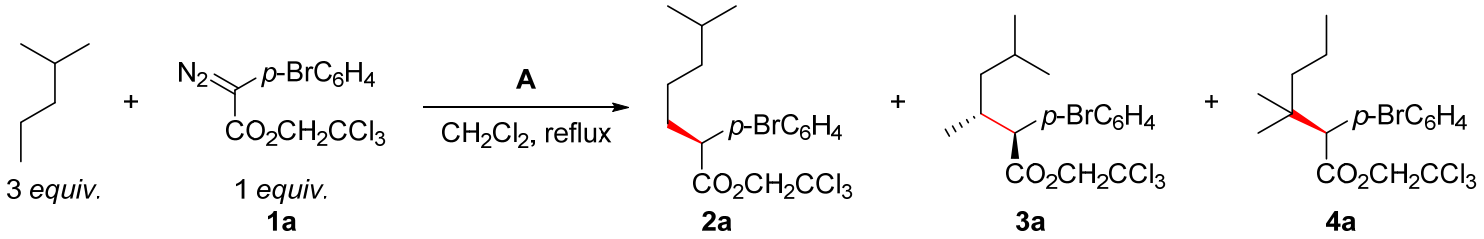
#	Time [Min]	Area% [%]
1	103.34	52.556
2	122.27	47.444

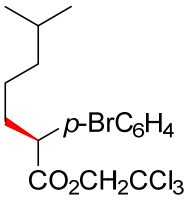




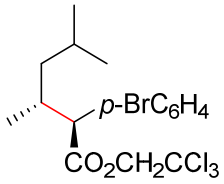
#	Time [Min]	Area% [%]
1	45.54	49.859
2	116.15	50.141

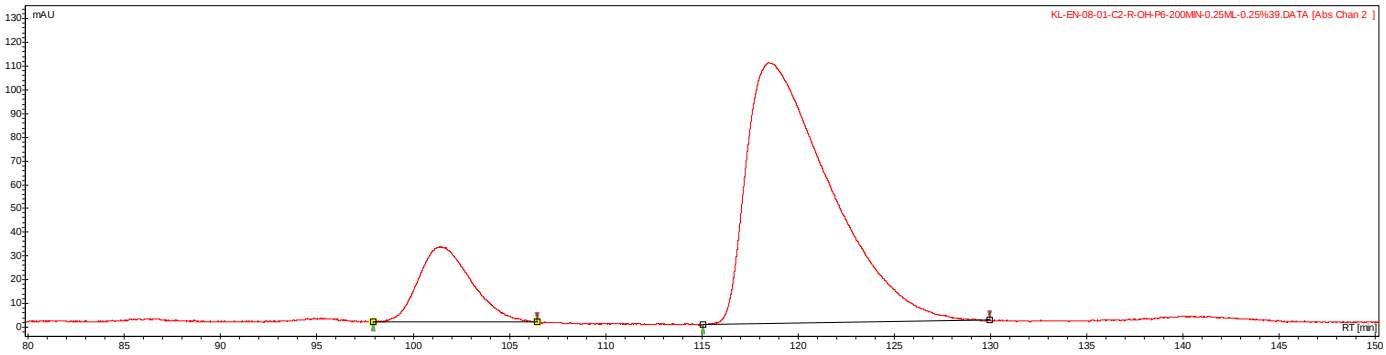
10.3 Catalyst Screen of 2-Methylpentane



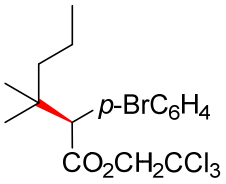


was not detected.

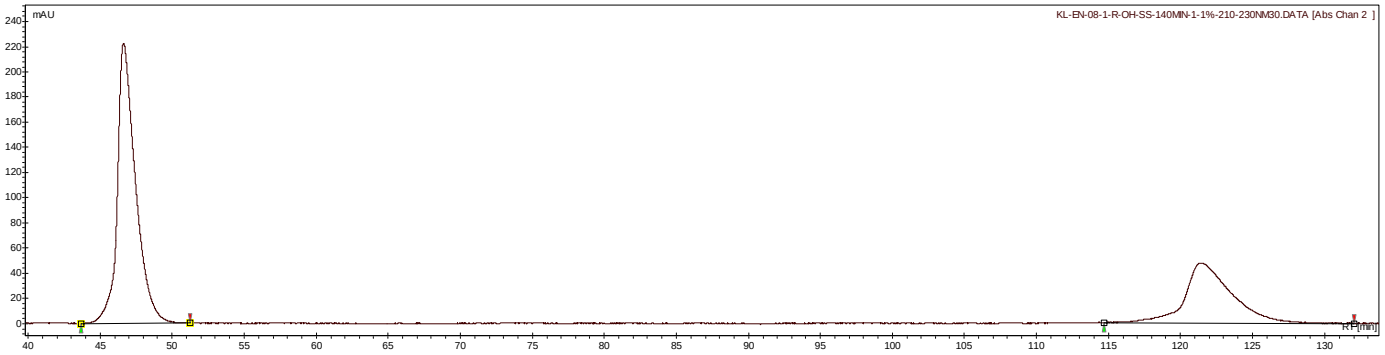




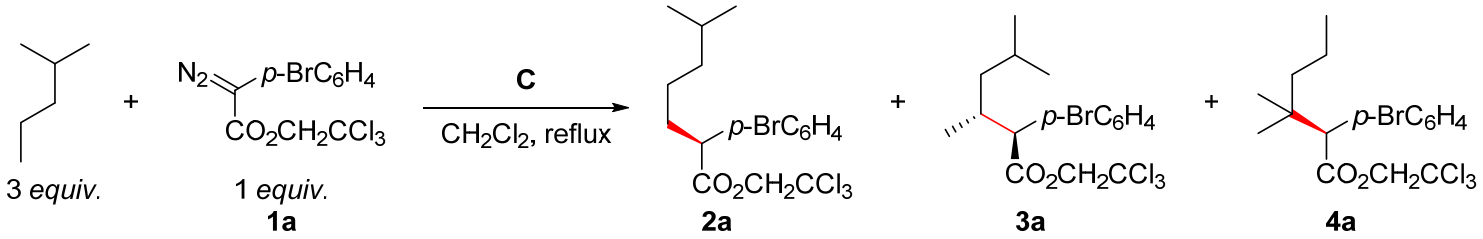
#	Time [Min]	Area% [%]
1	101.37	15.397
2	118.49	84.603
		69% *e.e.*

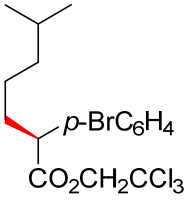


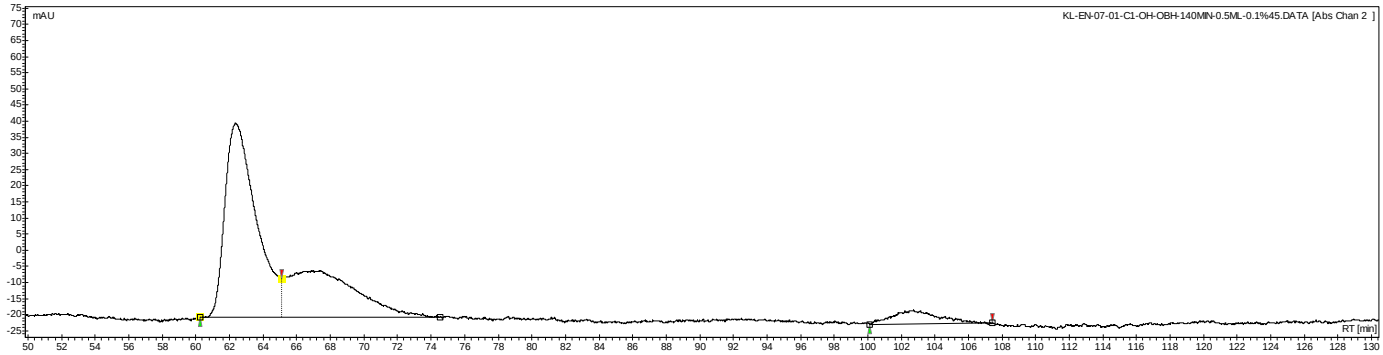
4a



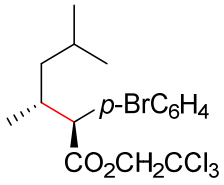
#	Time [Min]	Area% [%]
1	46.62	64.676
2	121.53	35.324
		29% *e.e.*

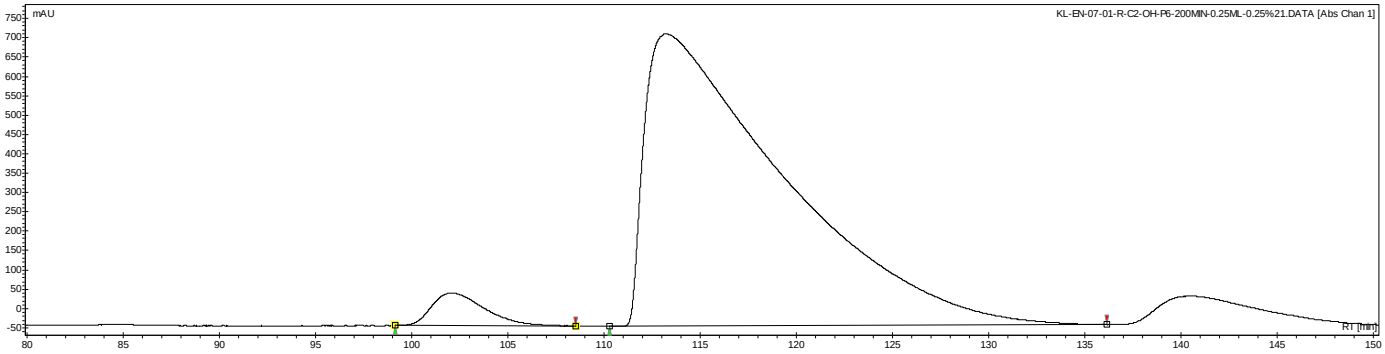




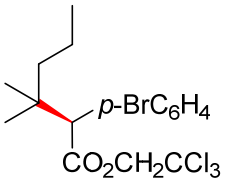


#	Time [Min]	Area% [%]
1	62.34	90.562
2	102.71	9.438
		81% *e.e.*

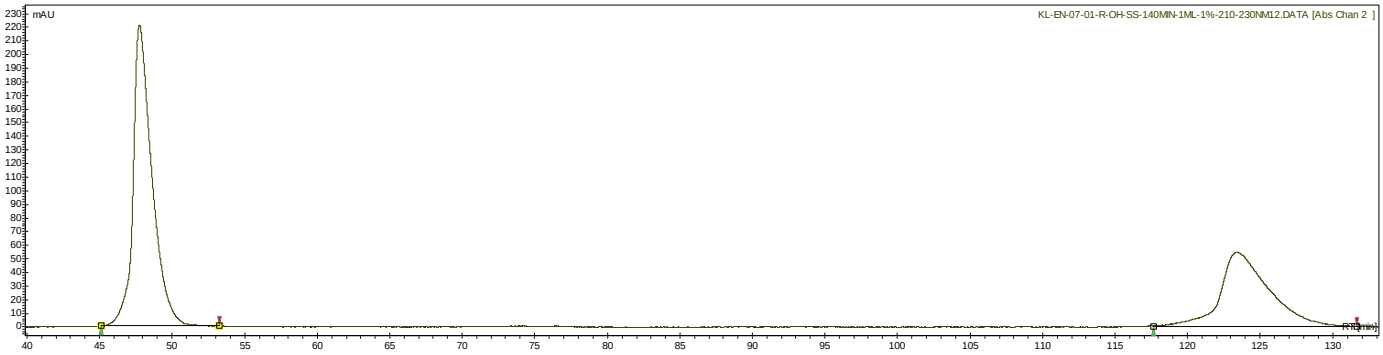




#	Time [Min]	Area% [%]
1	102.01	4.095
2	113.17	95.905
		92% *e.e.*



4a



#	Time [Min]	Area% [%]
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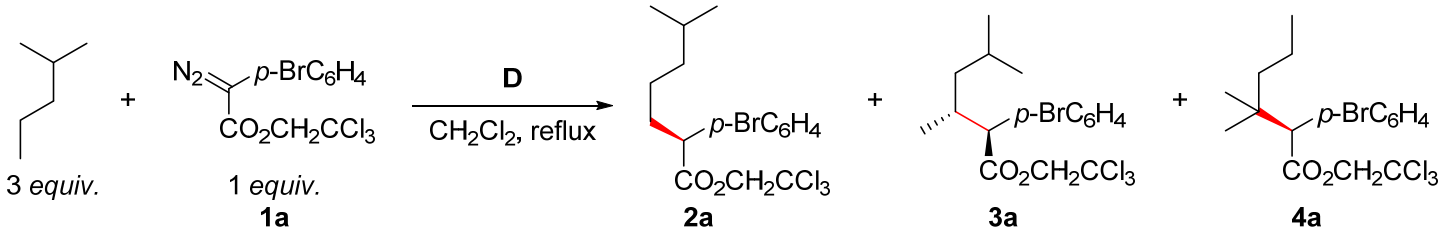
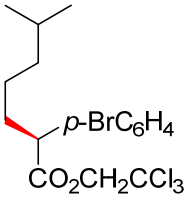
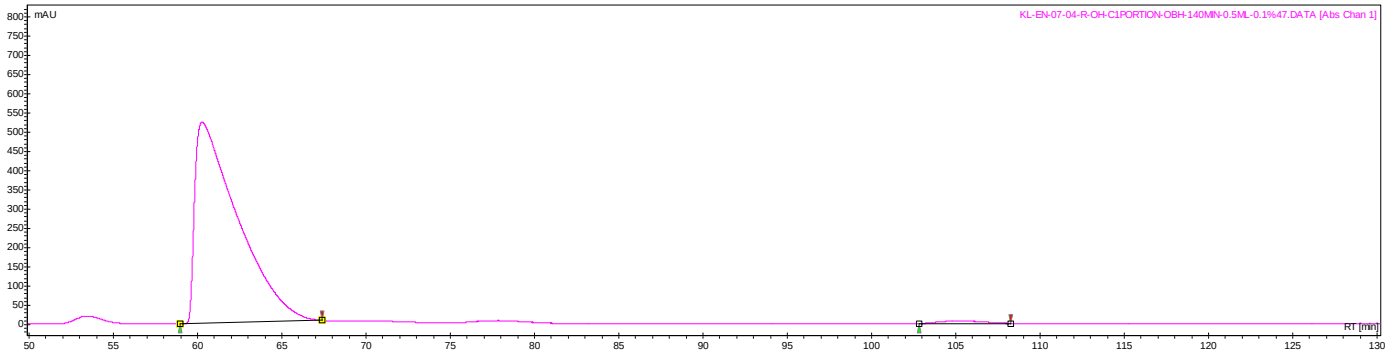
2	123.37	38.547
		23% *e.e.*

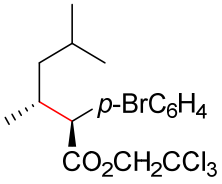




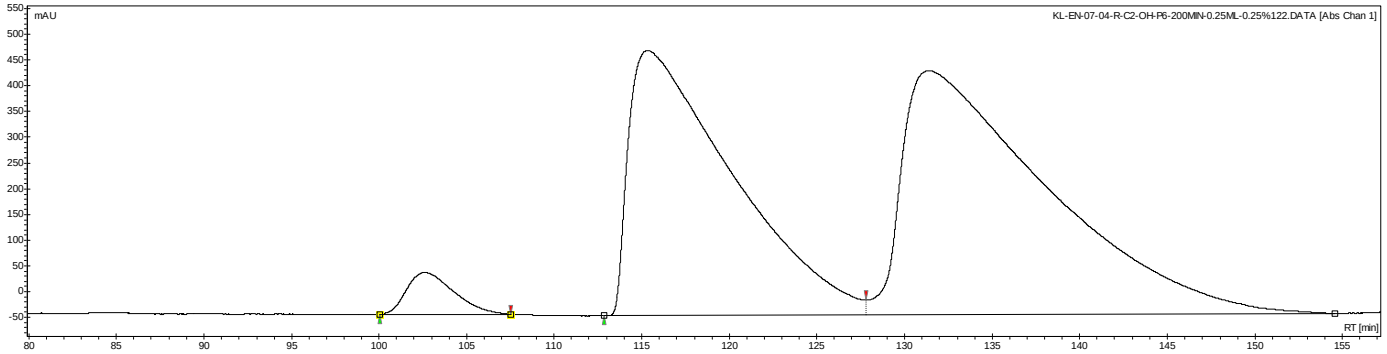
2a



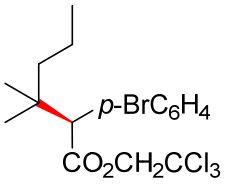
#	Time [Min]	Area% [%]
1	60.25	98.781
2	105.23	1.219
		97% *e.e.*



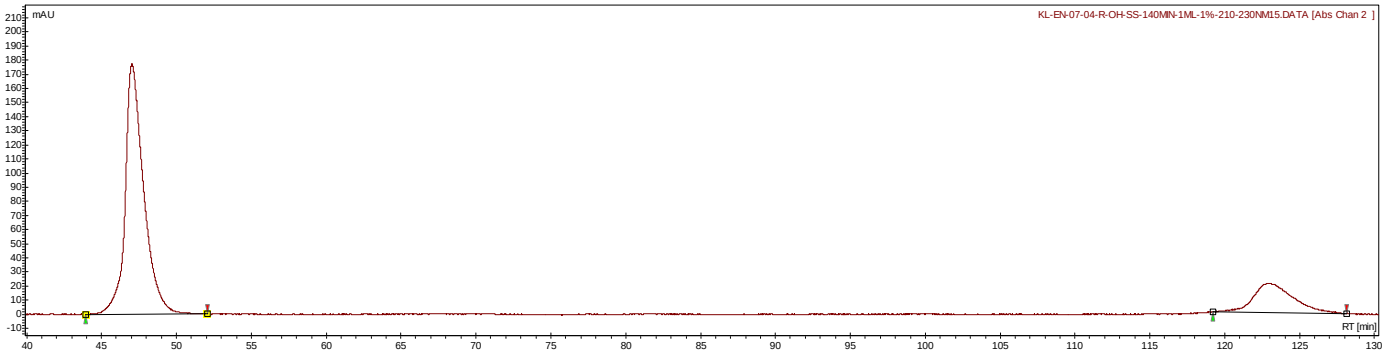
3a



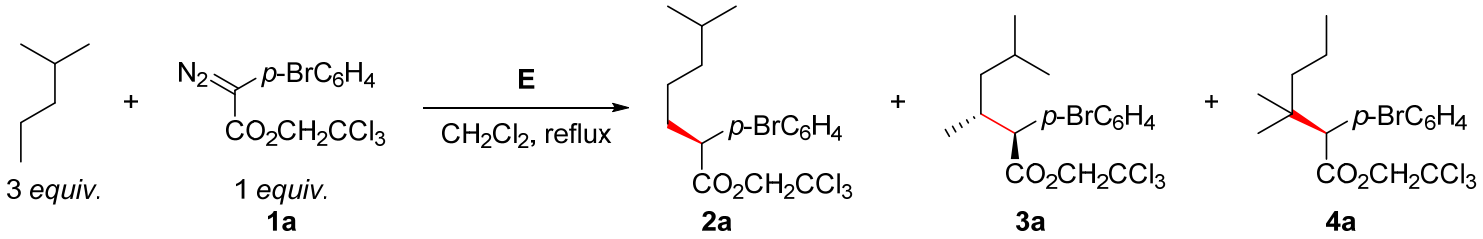
#	Time [Min]	Area% [%]
1	102.66	6.656
2	115.31	93.344
		87% *e.e.*

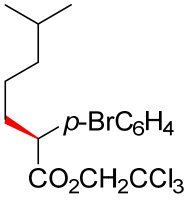


4a

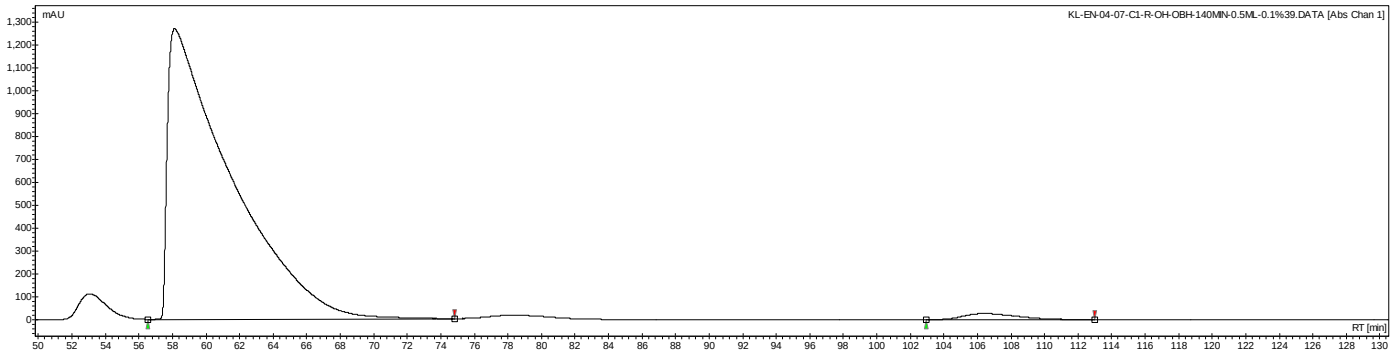


#	Time [Min]	Area% [%]
1	47.03	80.156
2	122.92	19.844
		60% *e.e.*

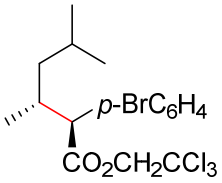




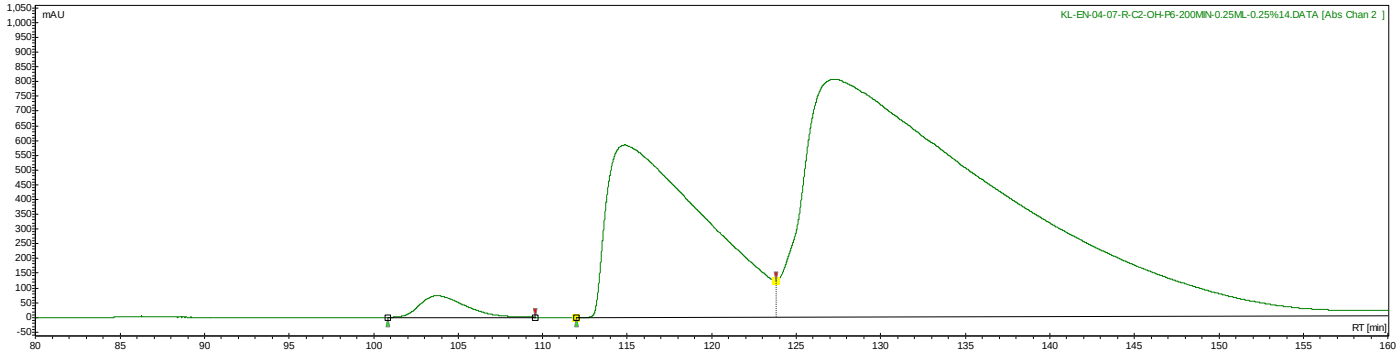
2a



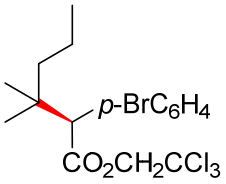
#	Time [Min]	Area% [%]
1	58.12	98.197
2	106.27	1.803
		96% *e.e.*



3a

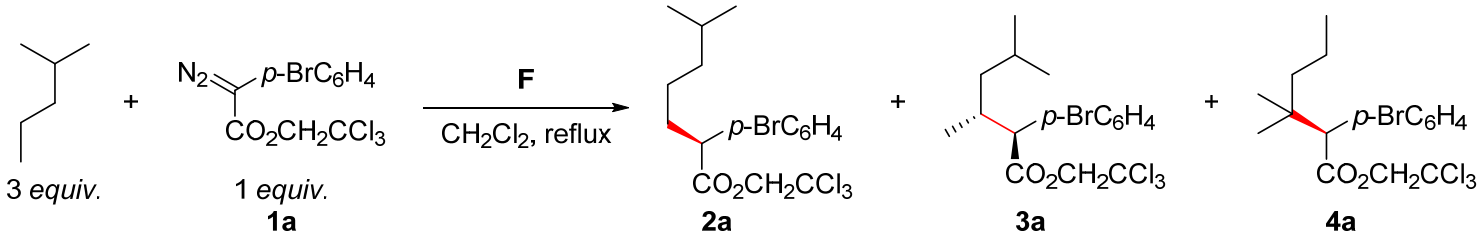


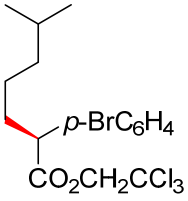
#	Time [Min]	Area% [%]
1	103.79	5.526
2	114.86	94.474
		89% *e.e.*

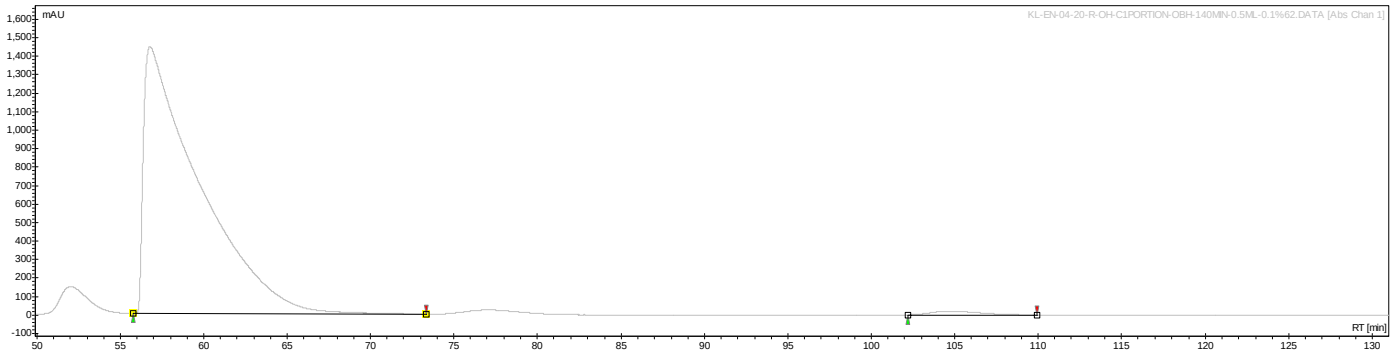


4a

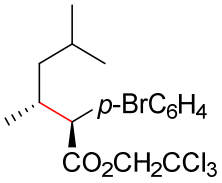
Enantiomeric excess was not determined.

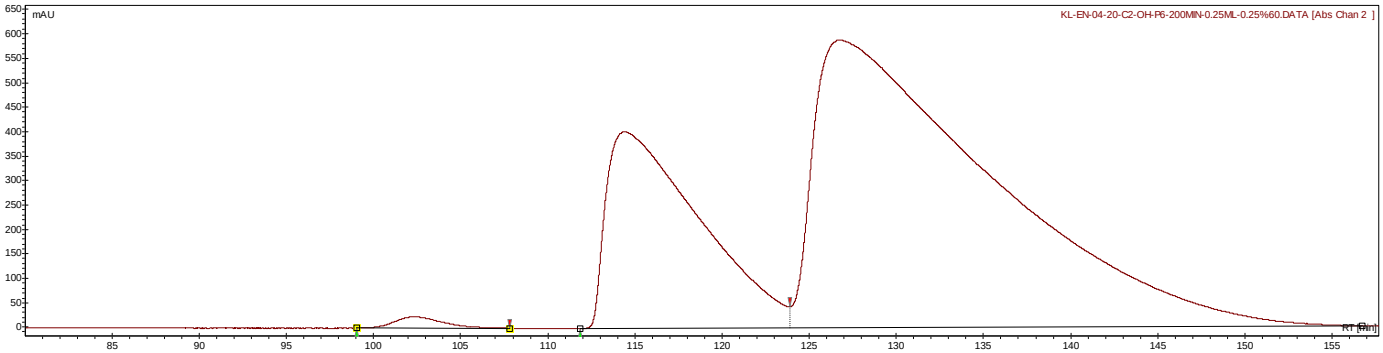




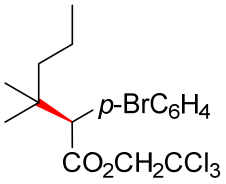


#	Time [Min]	Area% [%]
1	56.76	98.764
2	104.75	1.236
		98% *e.e.*



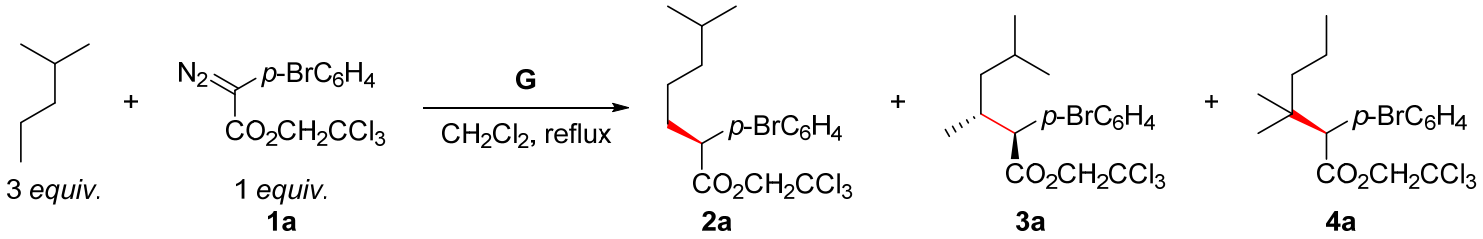


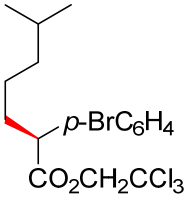
#	Time [Min]	Area% [%]
1	102.44	2.897
2	114.39	97.103
		94% *e.e.*

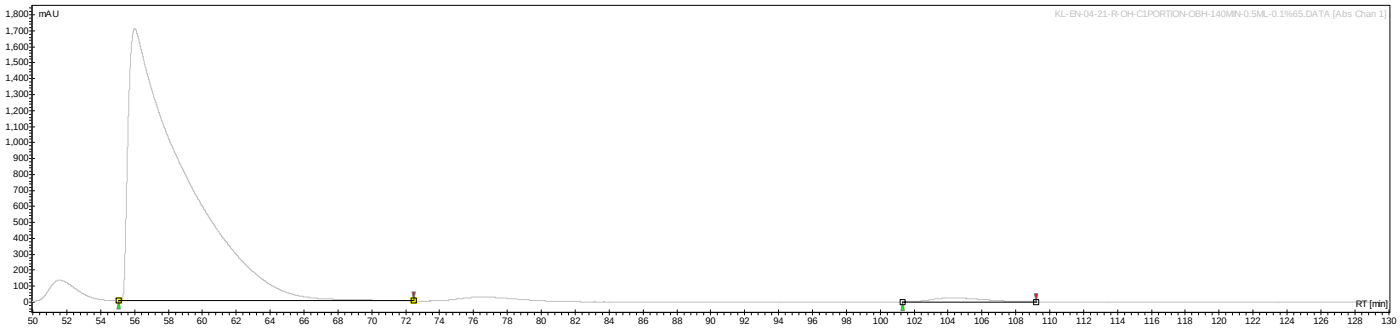


4a

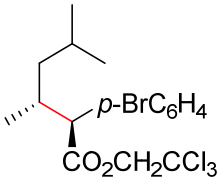
Enantiomeric excess was not determined.

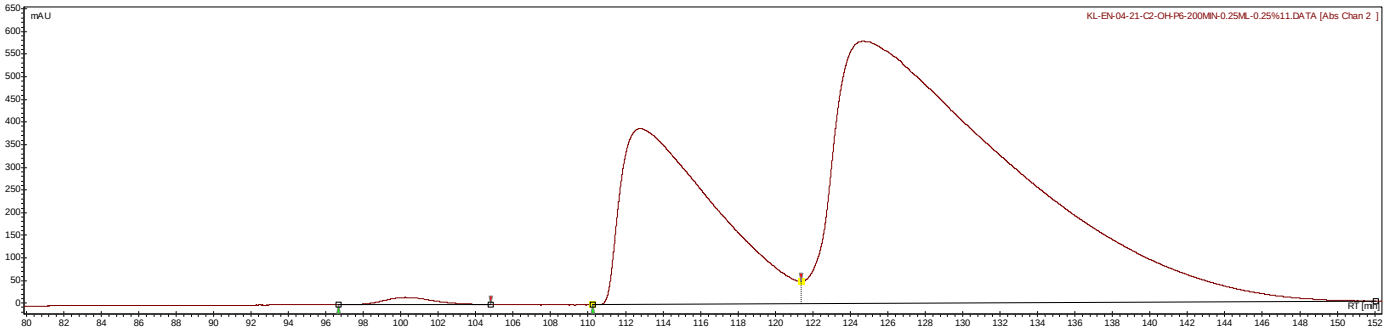




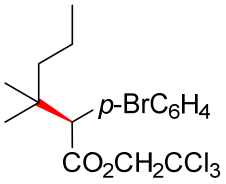


#	Time [Min]	Area% [%]
1	55.99	98.696
2	104.16	1.304
		97% *e.e.*



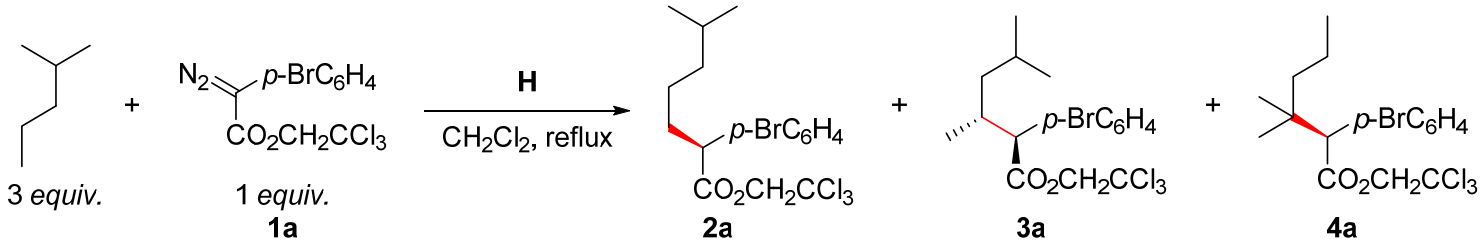


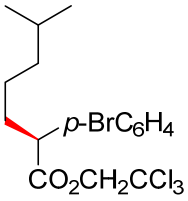
#	Time [Min]	Area% [%]
1	100.24	2.160
2	112.72	97.840
		96% *e.e.*

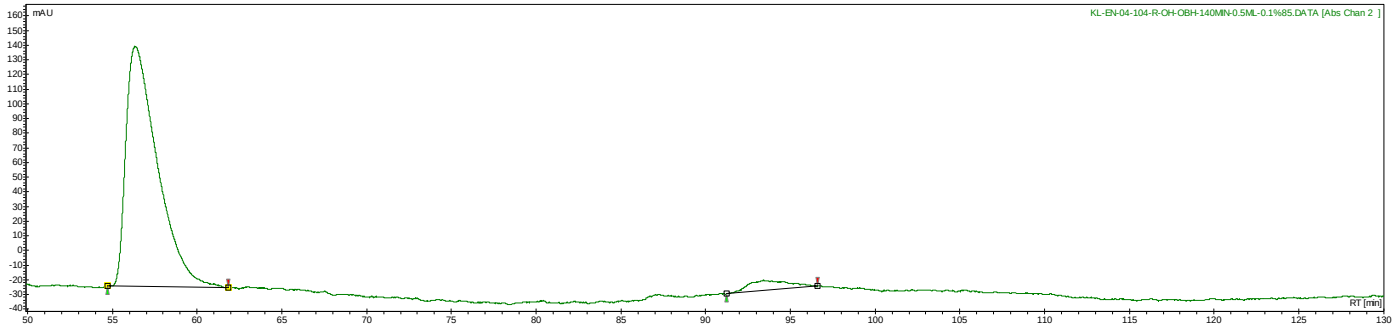


4a

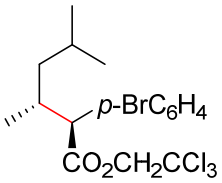
Enantiomeric excess was not determined.

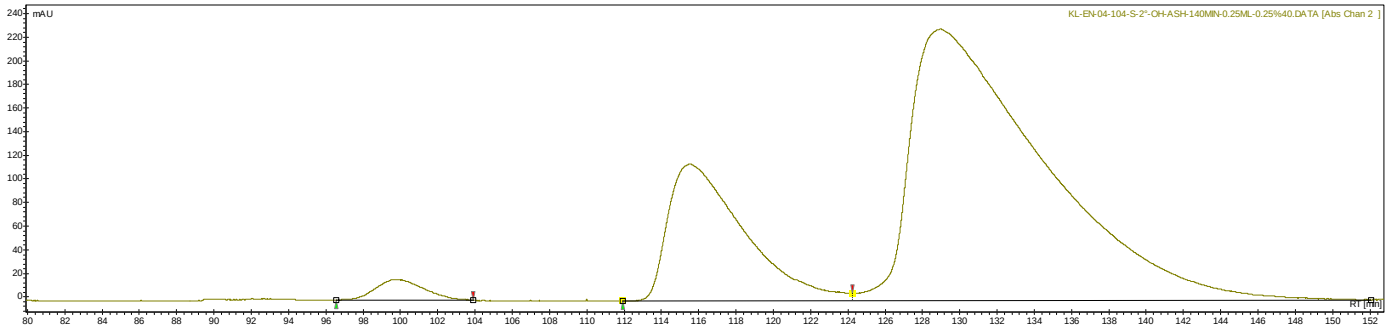




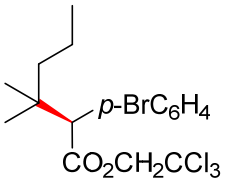


#	Time [Min]	Area% [%]
1	56.33	94.934
2	93.42	5.066
		90% *e.e.*

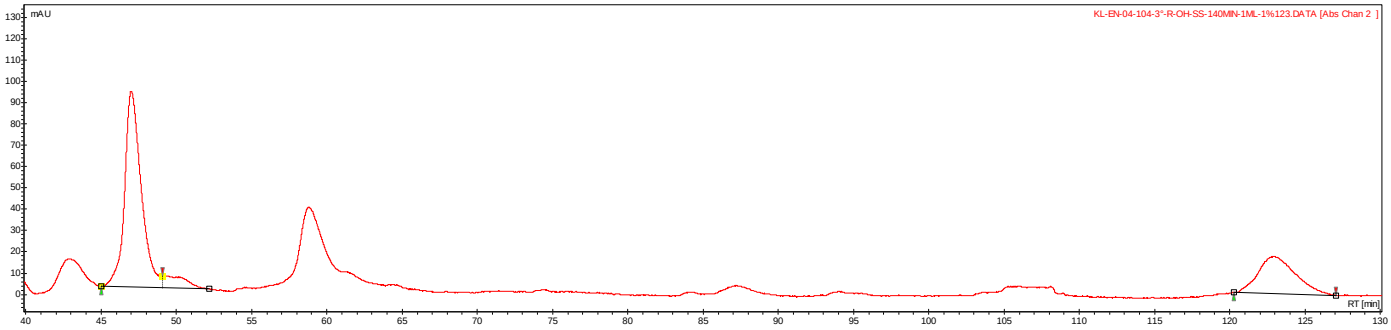




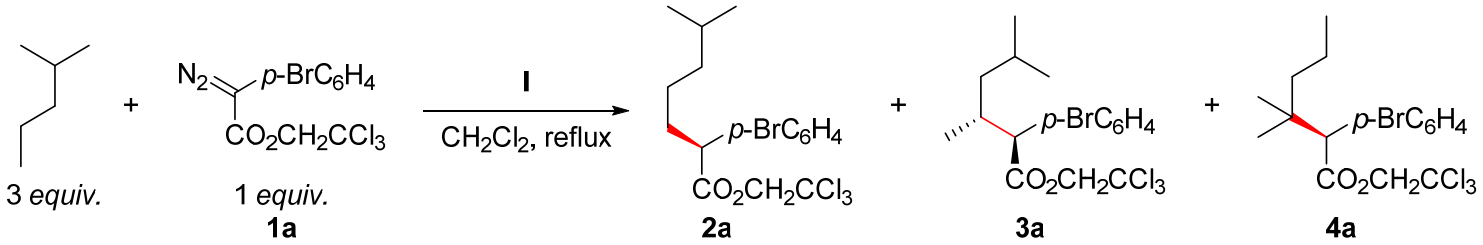
#	Time [Min]	Area% [%]
1	99.71	8.744
2	115.51	91.256
		83% *e.e.*

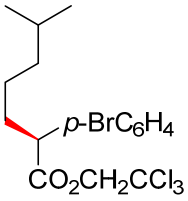


4a

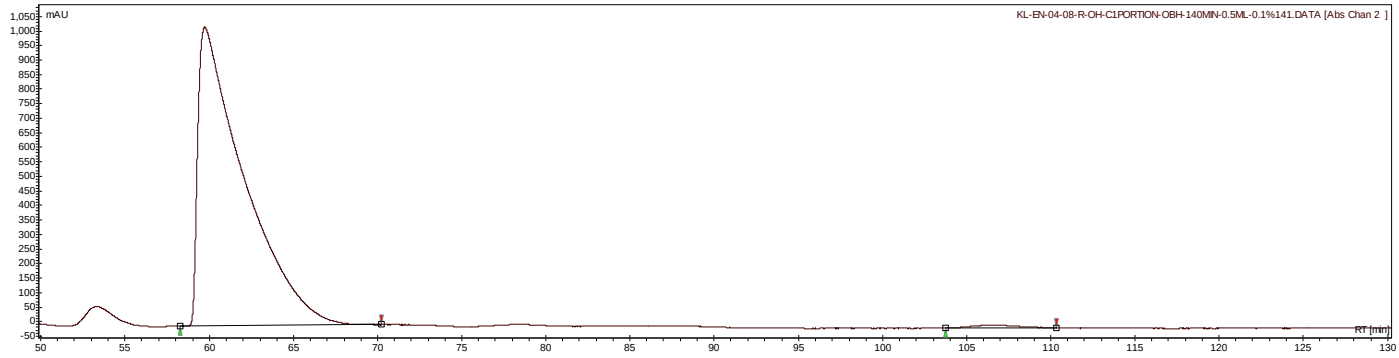


#	Time [Min]	Area% [%]
1	47.00	70.105
2	122.98	29.895
		40% *e.e.*

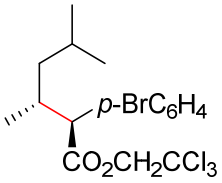




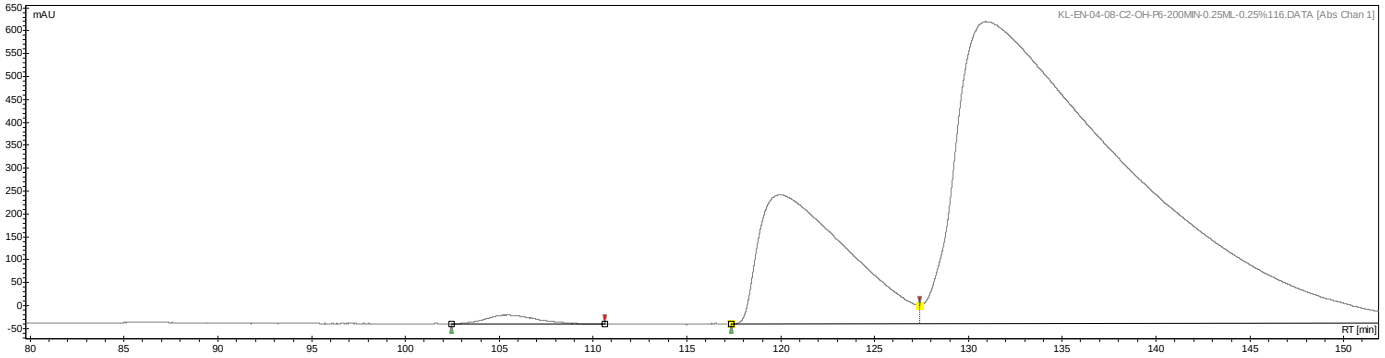
2a



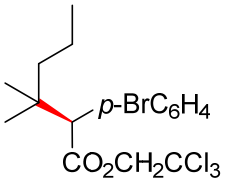
#	Time [Min]	Area% [%]
1	59.71	98.998
2	106.82	1.002
		98% *e.e.*



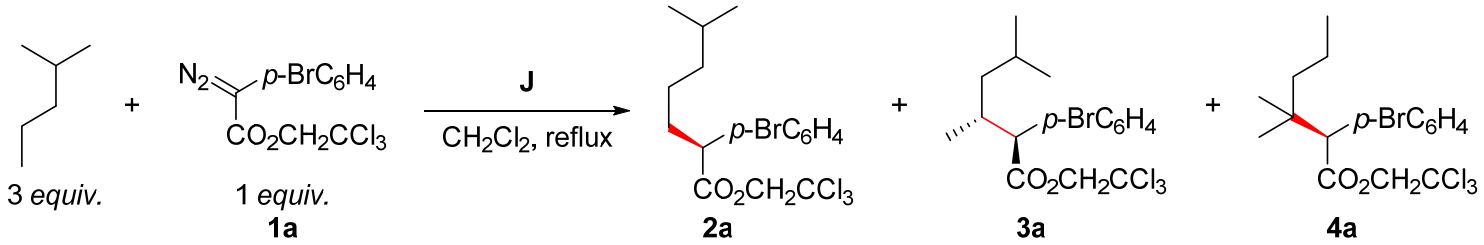
3a

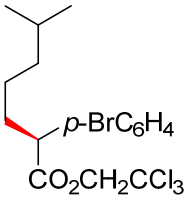


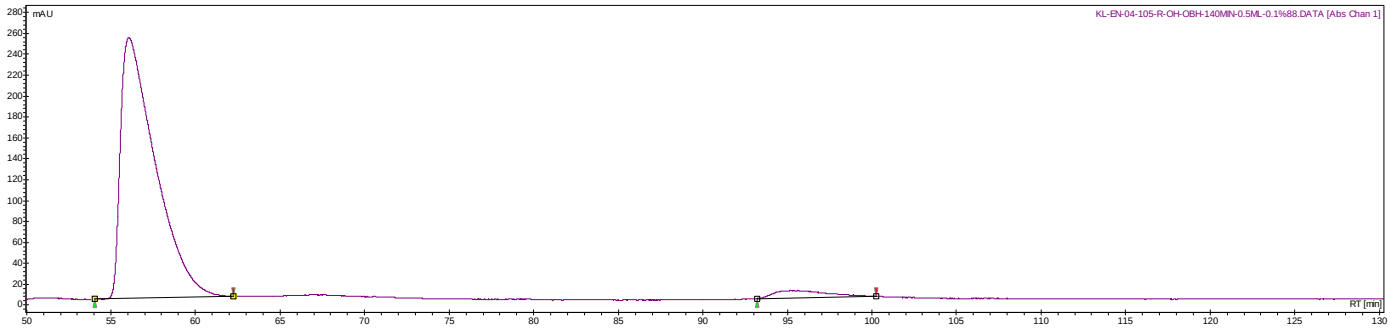
#	Time [Min]	Area% [%]
1	105.43	3.856
2	119.91	96.144
		92% *e.e.*



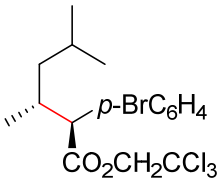
4a was not detected.

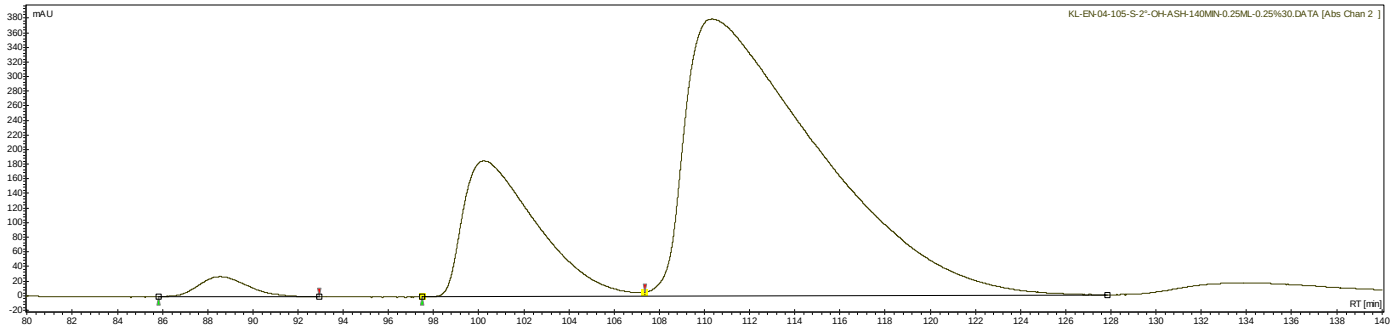




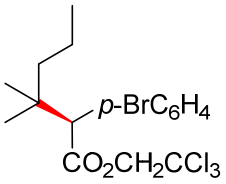


#	Time [Min]	Area% [%]
1	56.04	95.943
2	95.22	4.057
		92% *e.e.*

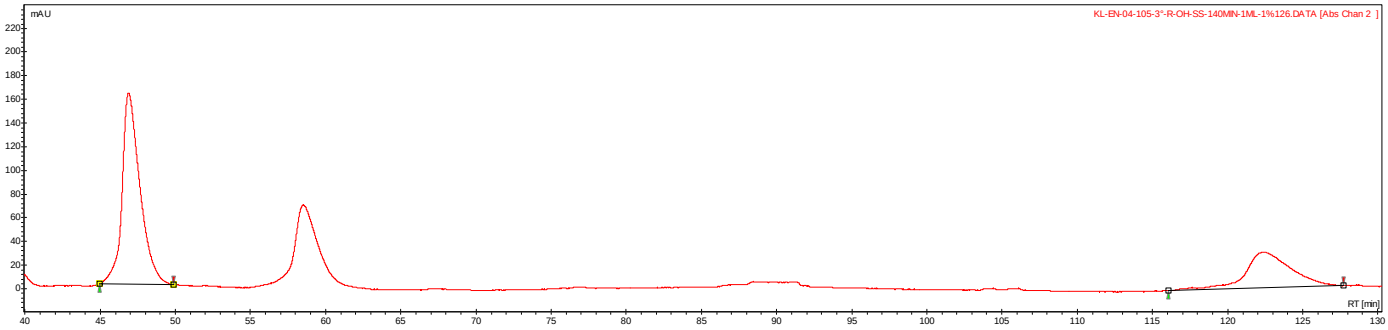




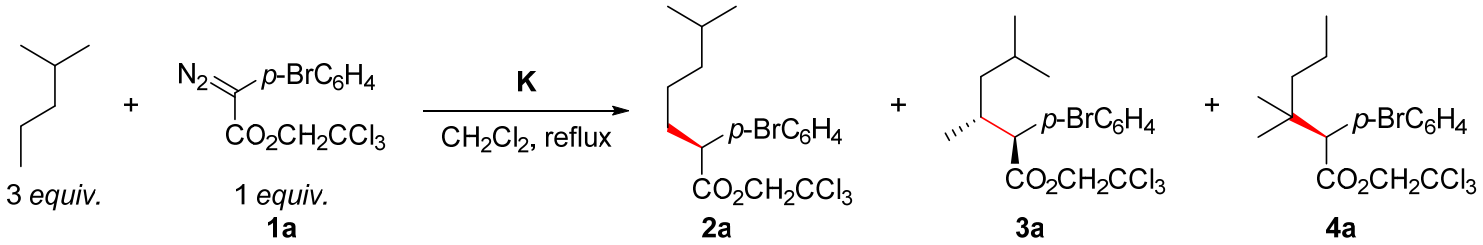
#	Time [Min]	Area% [%]
1	88.52	8.914
2	100.24	91.086
		82% *e.e.*

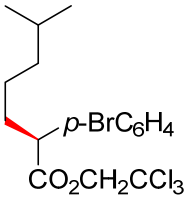


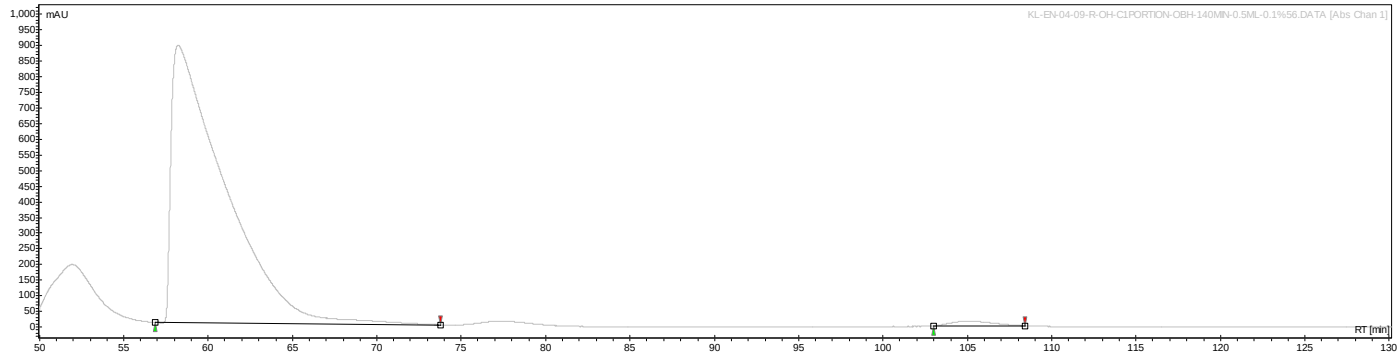
4a



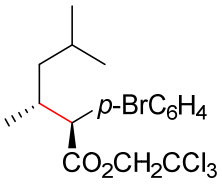
#	Time [Min]	Area% [%]
1	46.90	67.555
2	122.34	32.445
		35% *e.e.*

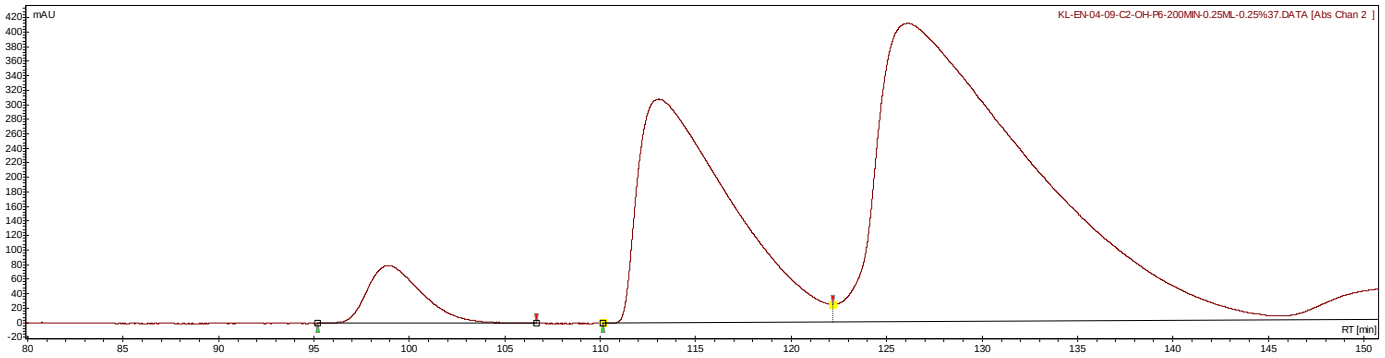




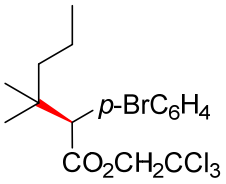


#	Time [Min]	Area% [%]
1	58.21	98.697
2	105.24	1.303
		97% *e.e.*

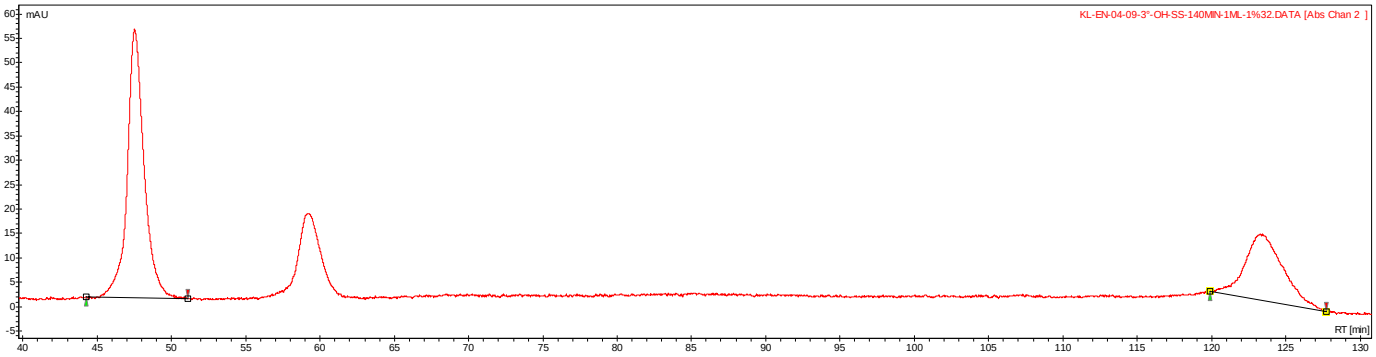




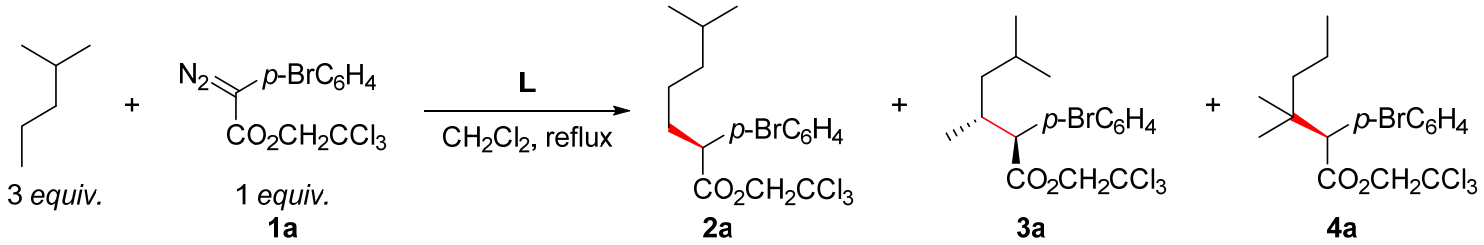
#	Time [Min]	Area% [%]
1	98.86	13.101
2	113.05	86.899
		74% *e.e.*

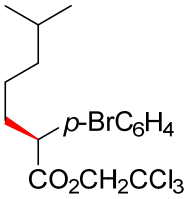


4a



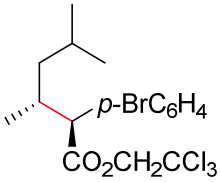
#	Time [Min]	Area% [%]
1	47.51	64.303
2	123.44	35.697
		29% *e.e.*



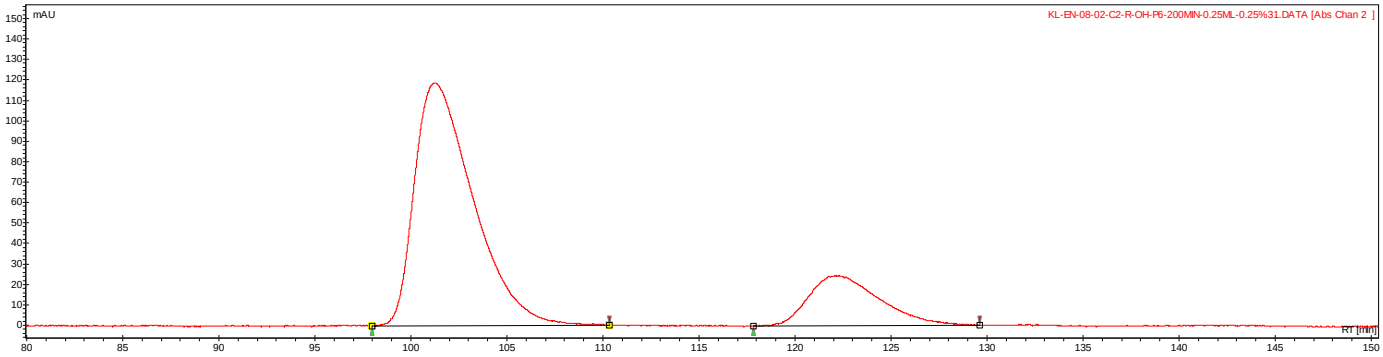


2a

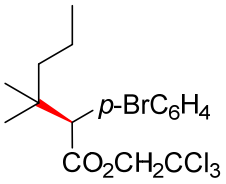
Enantiomeric excess was not determined.



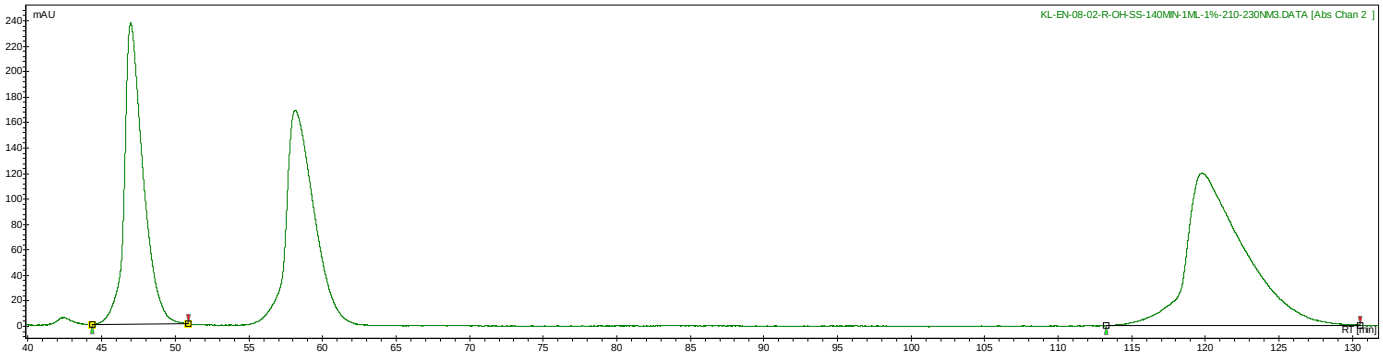
3a



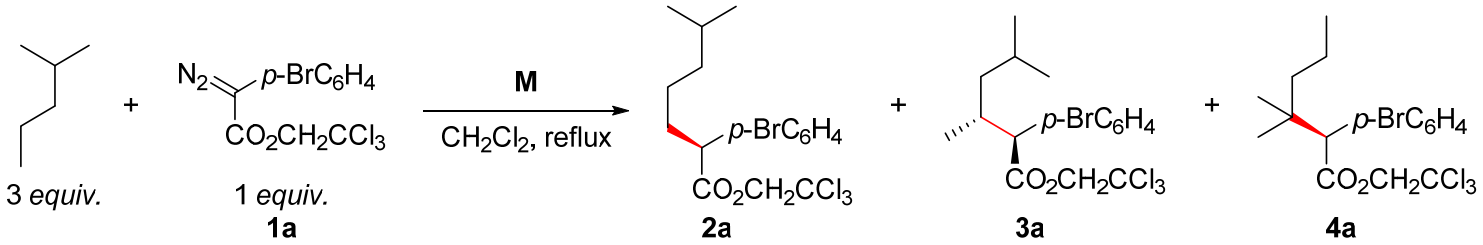
#	Time [Min]	Area% [%]
1	101.27	80.057
2	122.10	19.943
		-60% *e.e.*

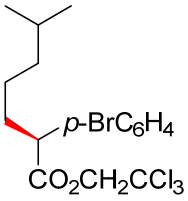


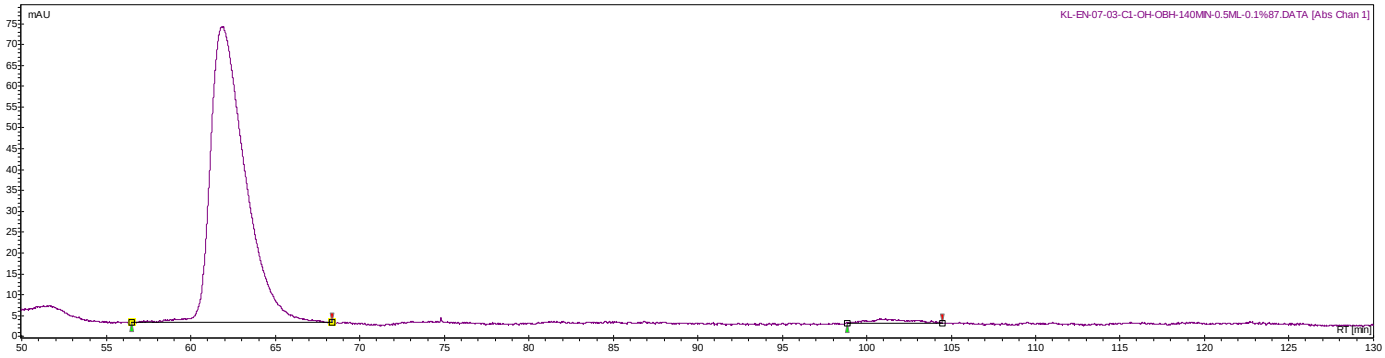
4a



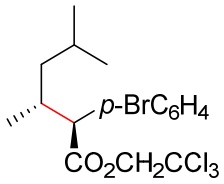
#	Time [Min]	Area% [%]
1	46.97	39.225
2	119.75	60.775
		-22% *e.e.*

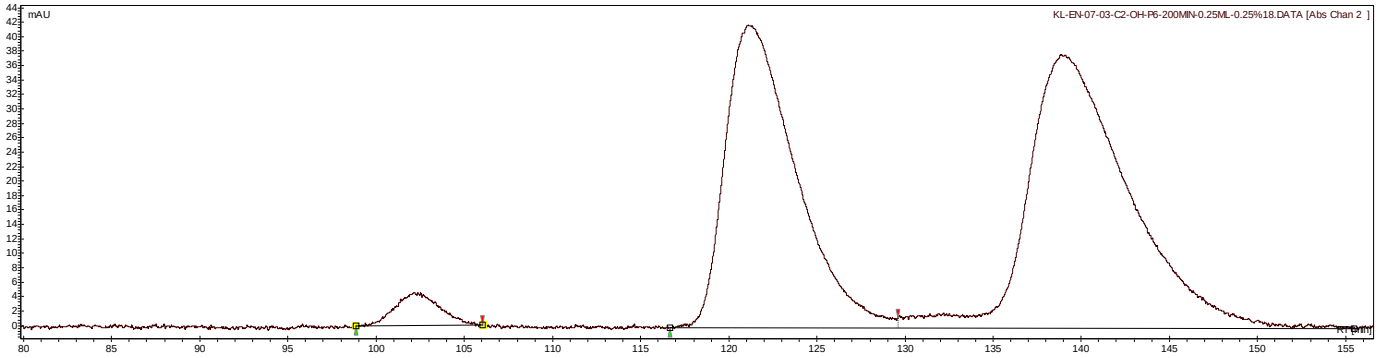




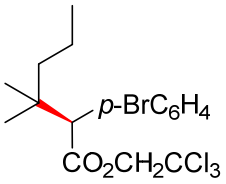


#	Time [Min]	Area% [%]
1	61.85	98.526
2	100.84	1.474
		97% *e.e.*

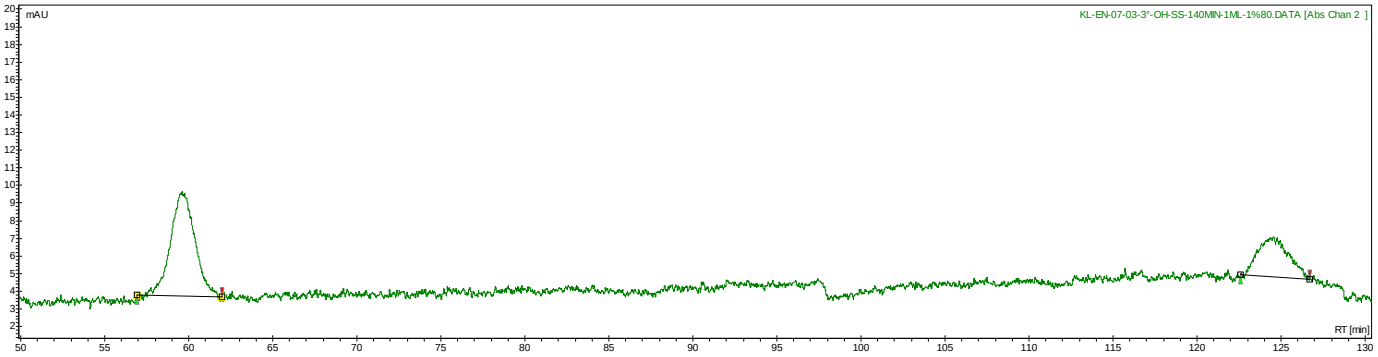




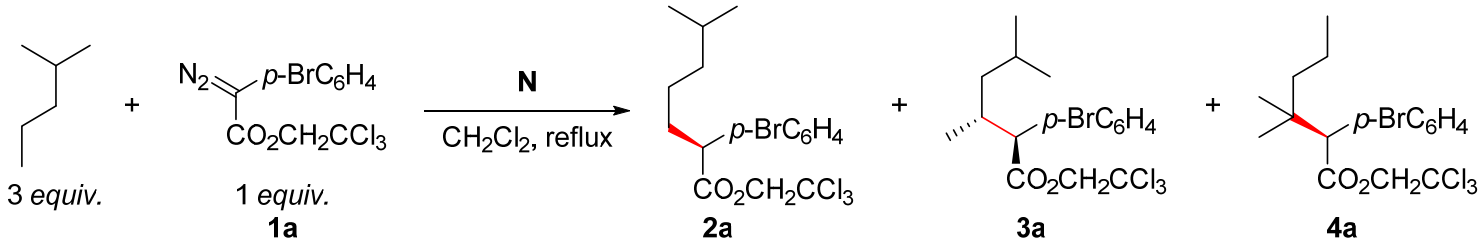
#	Time [Min]	Area% [%]
1	102.13	6.405
2	121.11	93.595
		87% *e.e.*

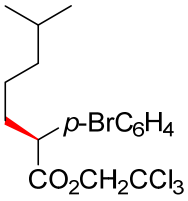


4a

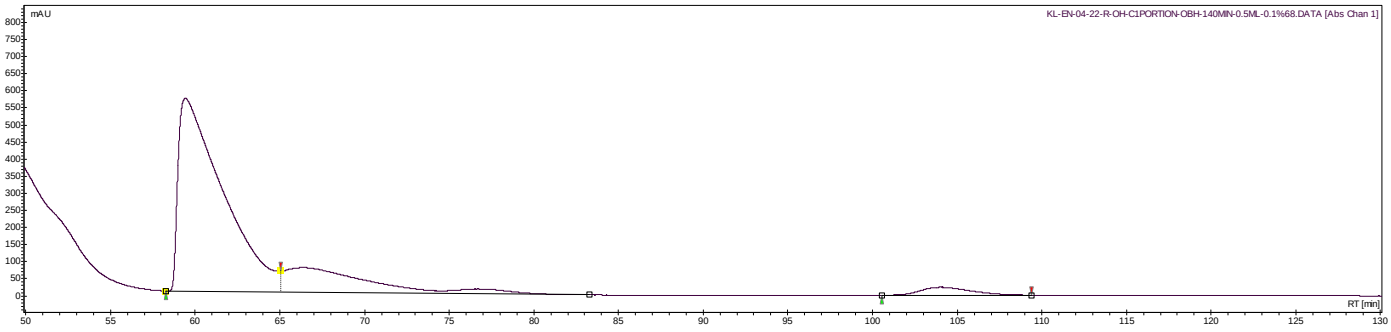


#	Time [Min]	Area% [%]
1	59.61	67.637
2	124.52	32.363
		35% *e.e.*

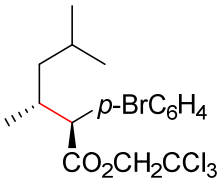




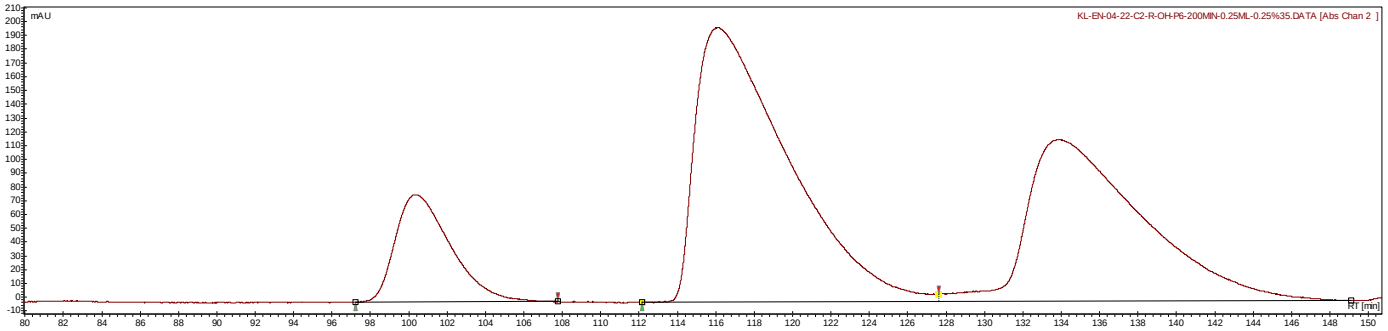
2a



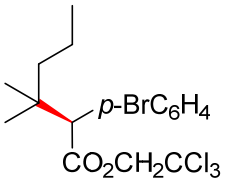
#	Time [Min]	Area% [%]
1	59.41	95.704
2	103.97	4.296
		91% *e.e.*



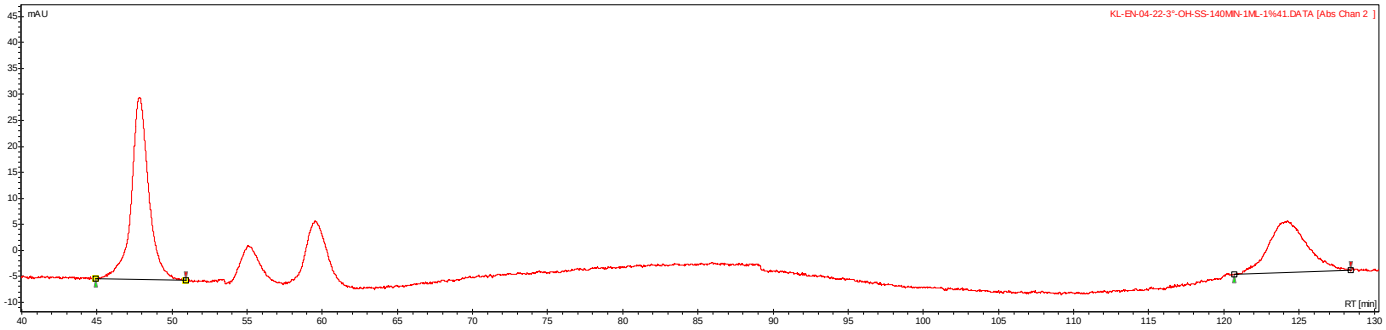
3a



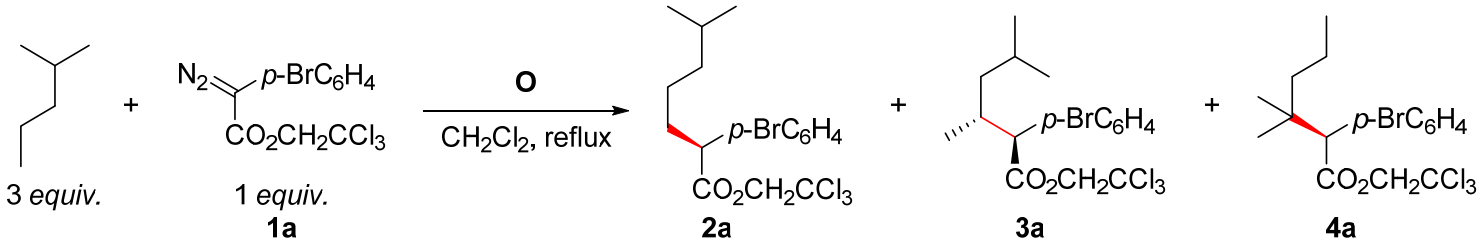
#	Time [Min]	Area% [%]
1	100.41	18.840
2	116.14	81.160
		62% *e.e.*

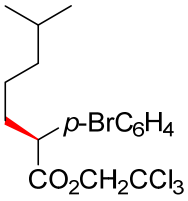


4a

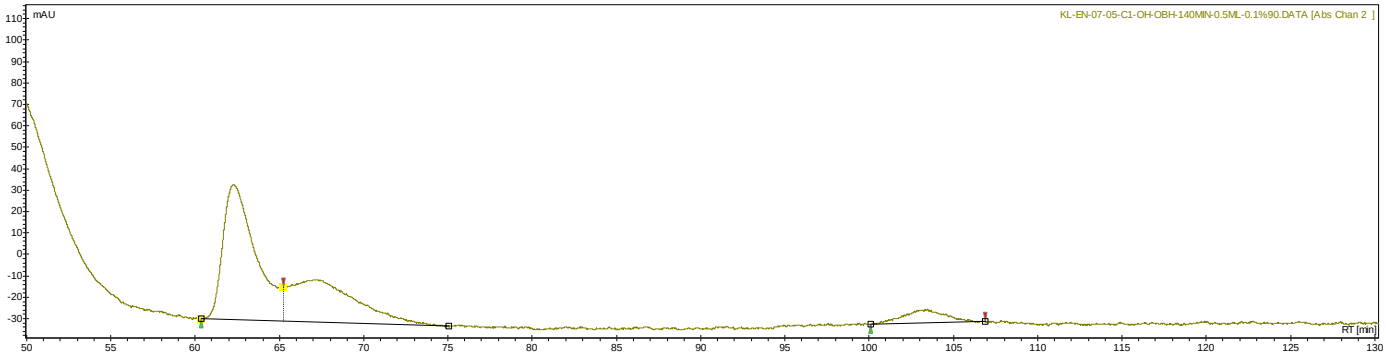


#	Time [Min]	Area% [%]
1	47.87	61.089
2	124.24	38.911
		14% *e.e.*

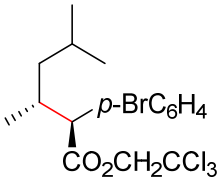




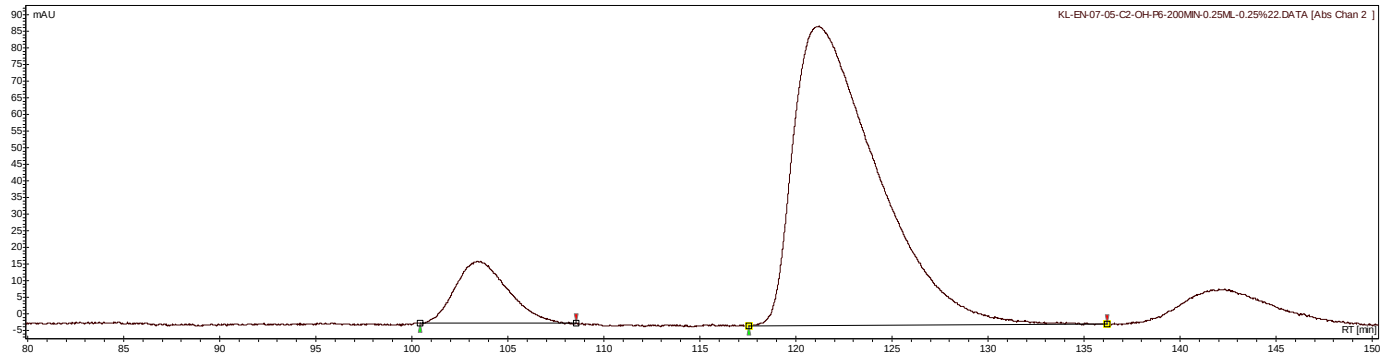
2a



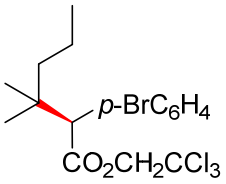
#	Time [Min]	Area% [%]
1	62.32	88.857
2	103.33	11.143
		78% *e.e.*



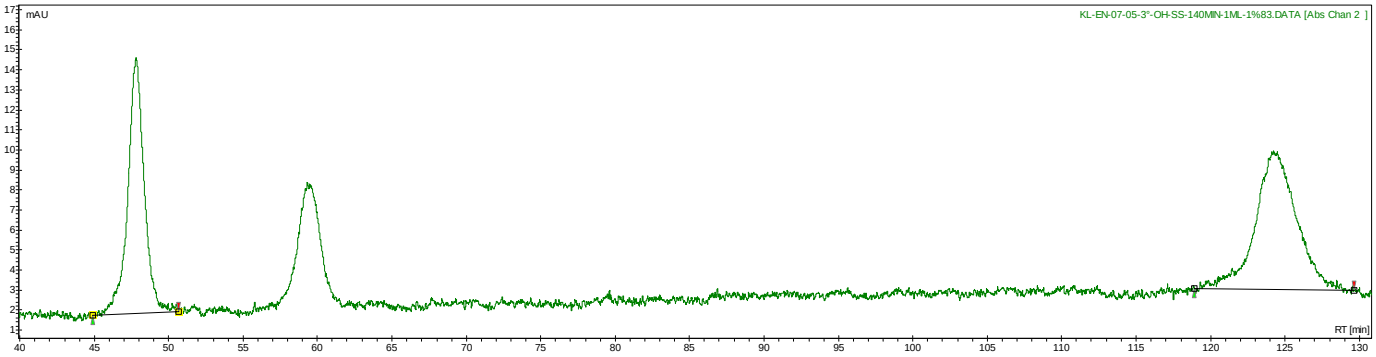
3a



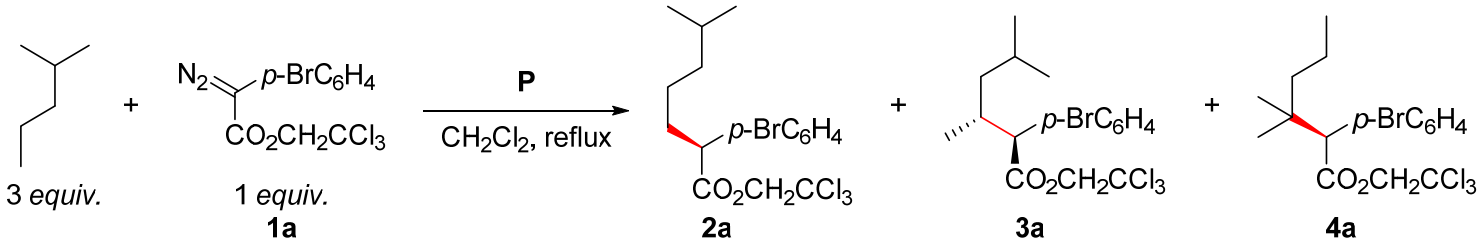
#	Time [Min]	Area% [%]
1	103.41	11.565
2	121.23	88.435
		77% *e.e.*

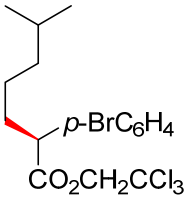


4a

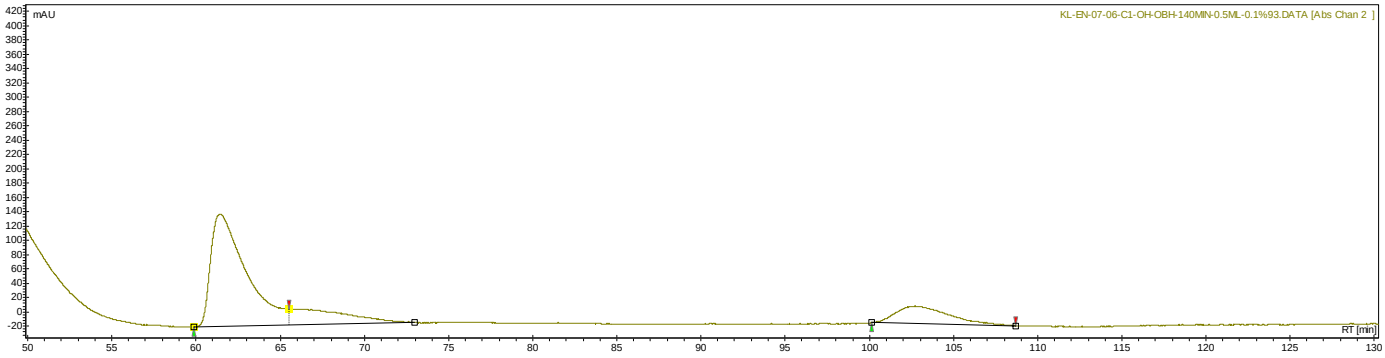


#	Time [Min]	Area% [%]
1	47.80	42.773
2	124.26	57.227
		14% *e.e.*

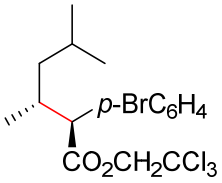




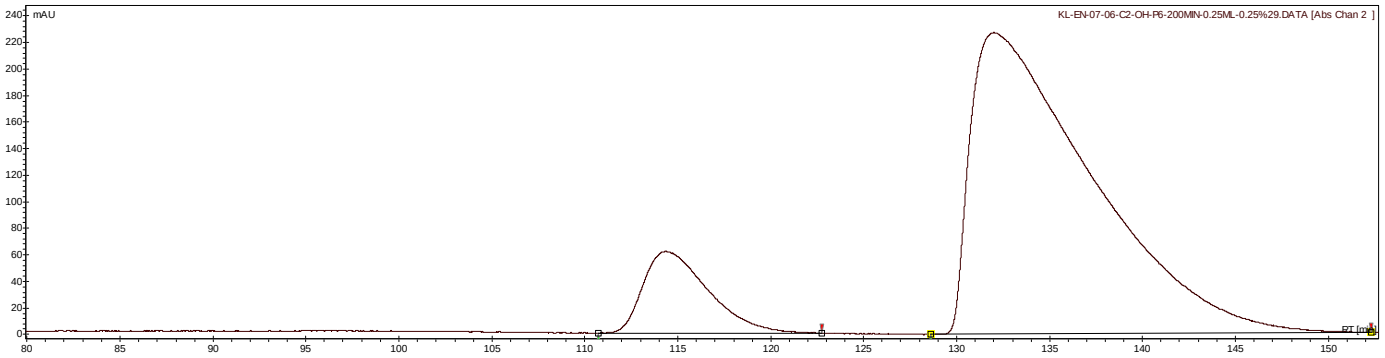
2a



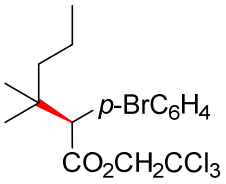
#	Time [Min]	Area% [%]
1	61.43	80.721
2	102.87	19.279
		62% *e.e.*



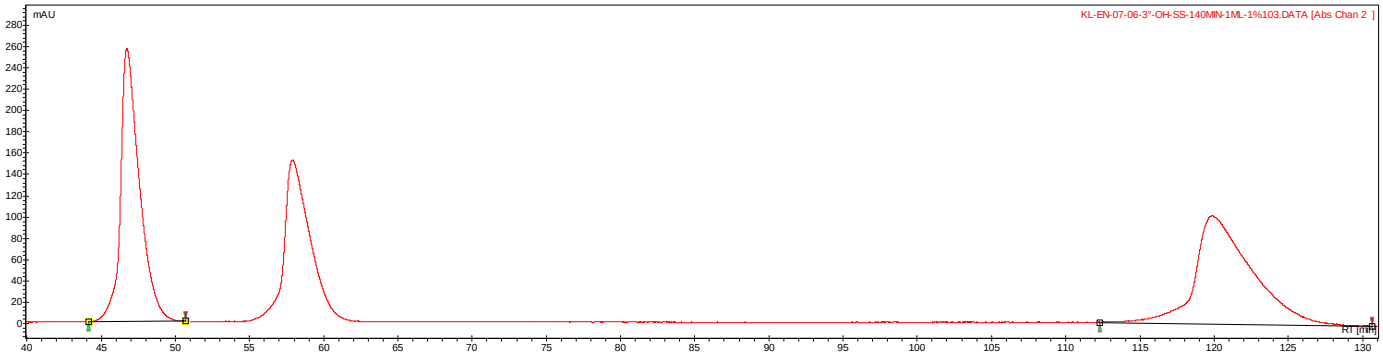
3a



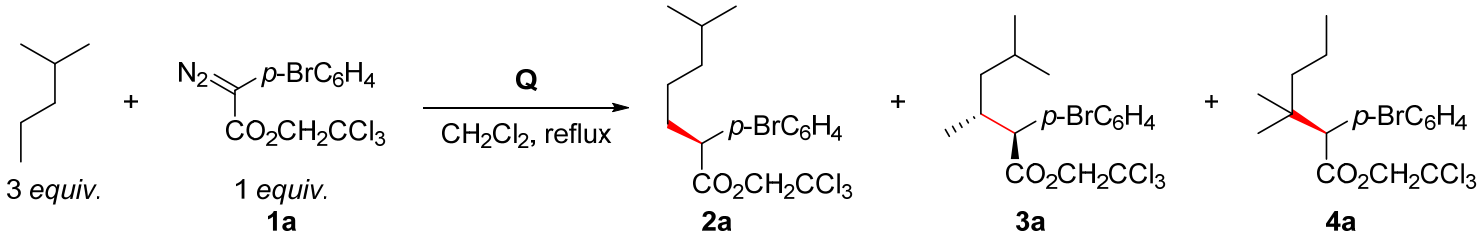
#	Time [Min]	Area% [%]
1	114.39	12.615
2	132.02	87.385
		>99% *e.e.*

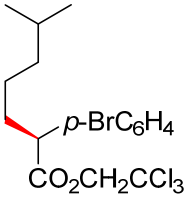


4a

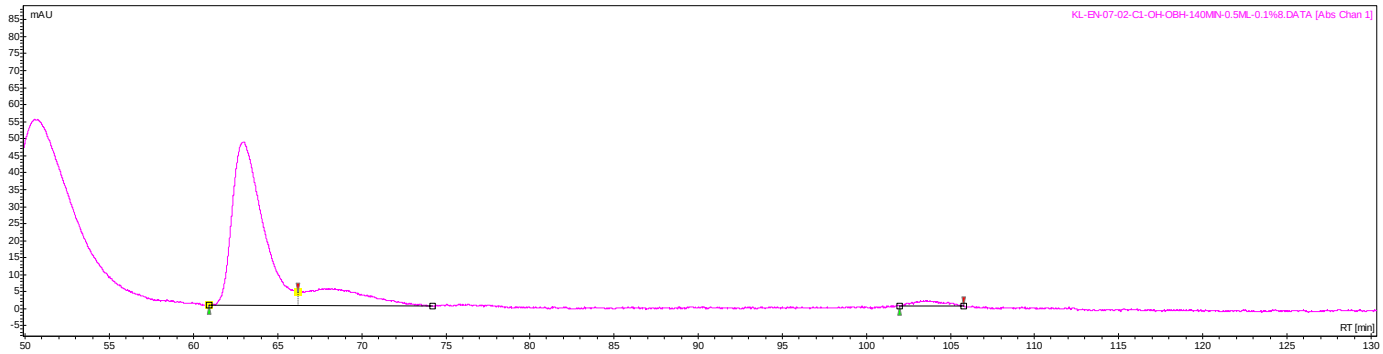


#	Time [Min]	Area% [%]
1	46.72	45.911
2	119.82	54.089
		8% *e.e.*

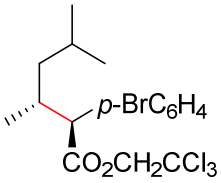




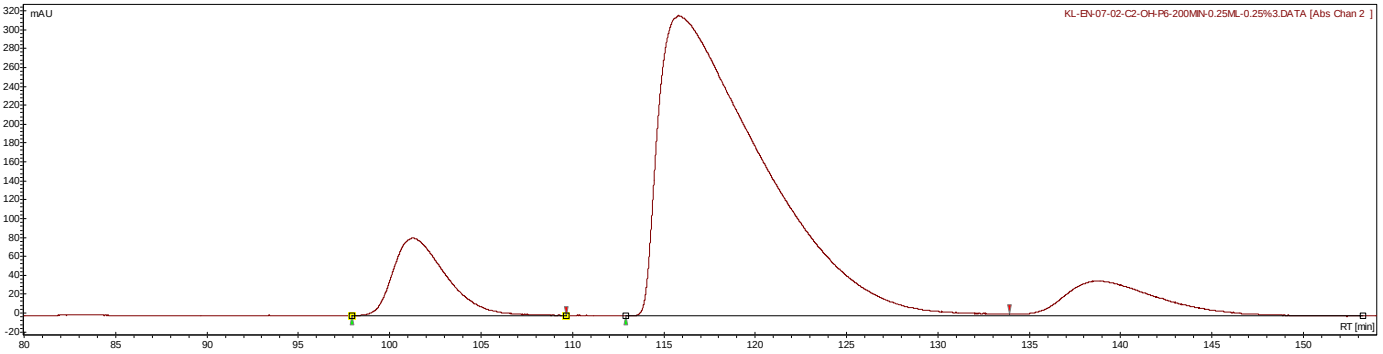
2a



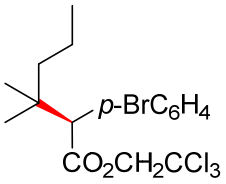
#	Time [Min]	Area% [%]
1	62.94	97.034
2	103.61	2.966
		94% *e.e.*



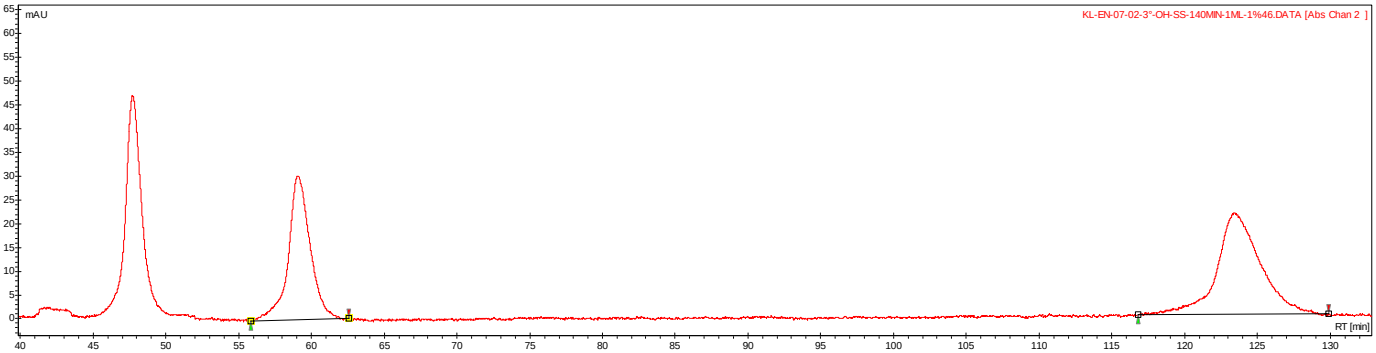
3a



#	Time [Min]	Area% [%]
1	101.22	11.581
2	115.80	88.419
		77% *e.e.*

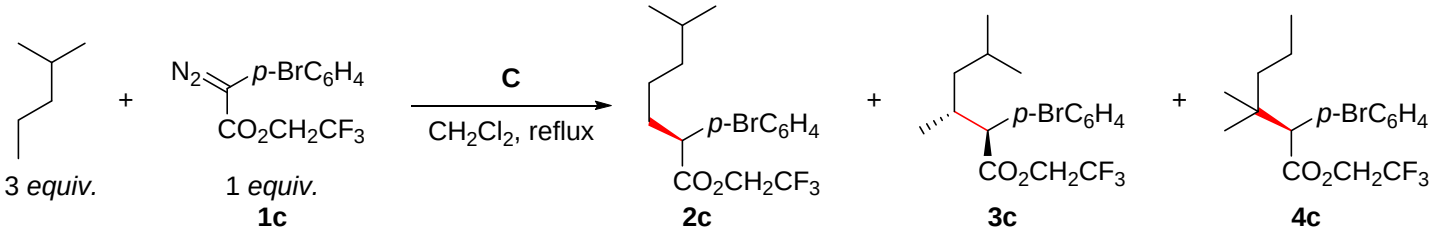


4a

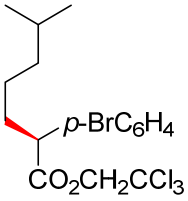


#	Time [Min]	Area% [%]
1	59.04	41.367
2	123.46	58.633
		17% *e.e.*

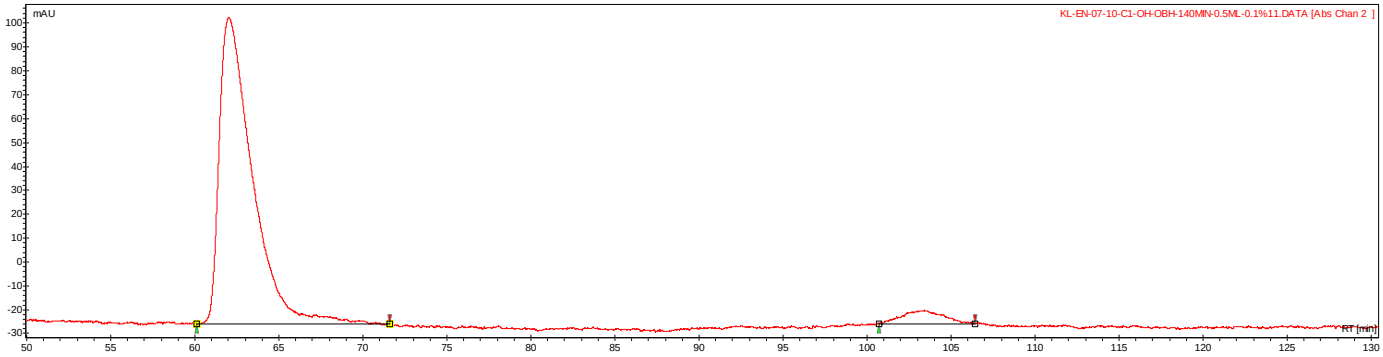
10.4 Diazo Screen of 2-Methylpentane



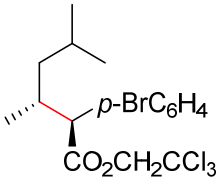
3 *equiv.* 1 *equiv.* **1c** **2c** **3c** **4c**



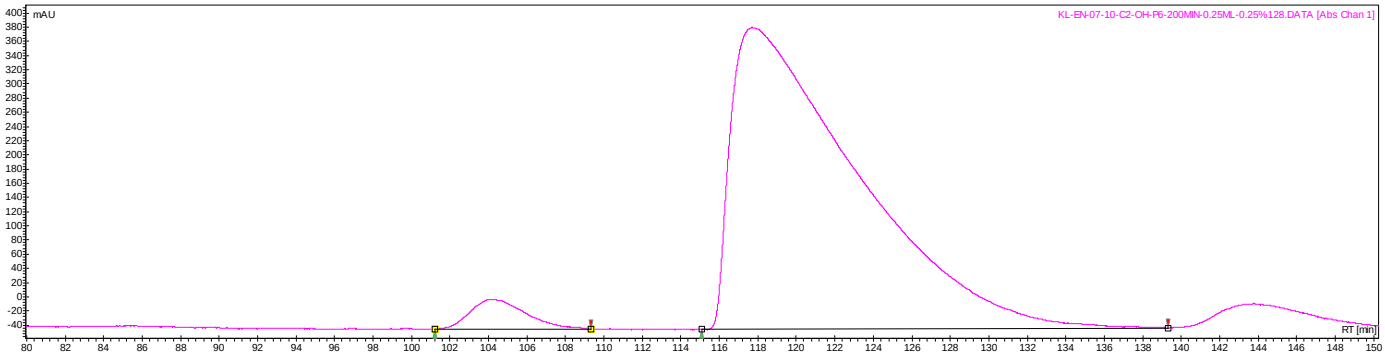
2c



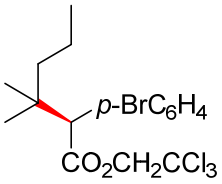
#	Time [Min]	Area% [%]
1	62.04	95.021
2	103.39	4.979
		90% *e.e.*



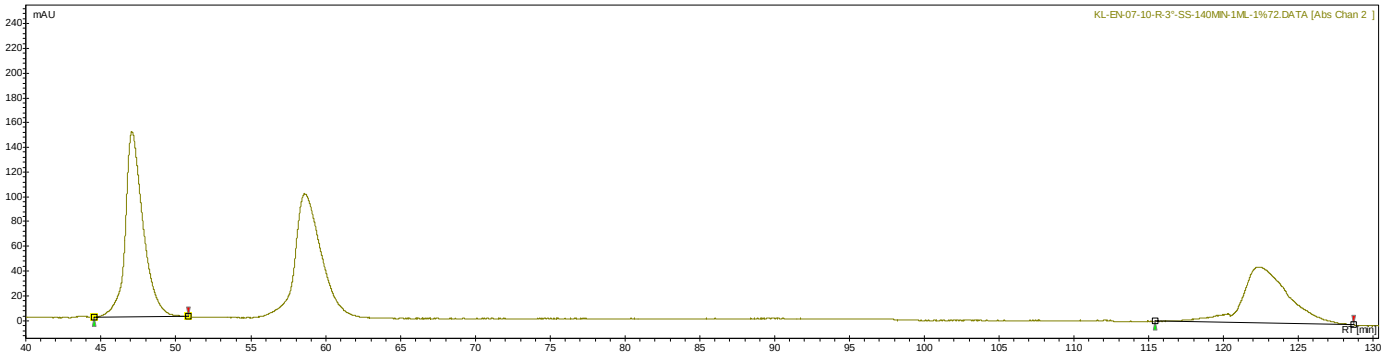
3c



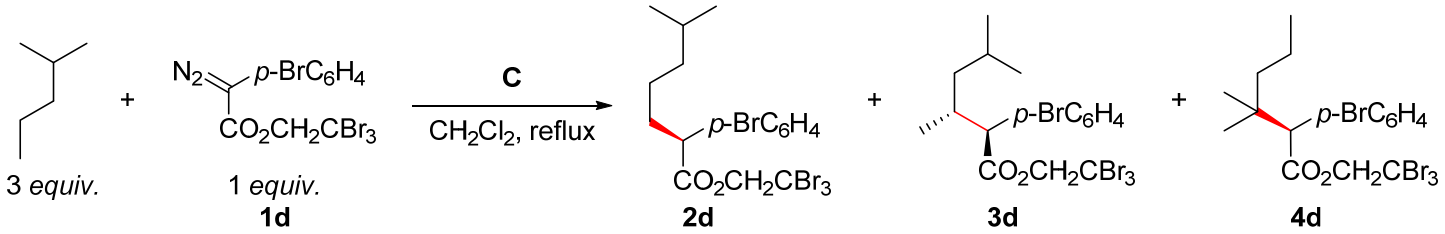
#	Time [Min]	Area% [%]
1	104.10	4.084
2	117.69	95.916
		92 *e.e.*

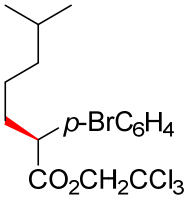


4c



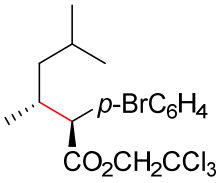
#	Time [Min]	Area% [%]
1	47.06	56.009
2	122.30	43.991
		12% *e.e.*



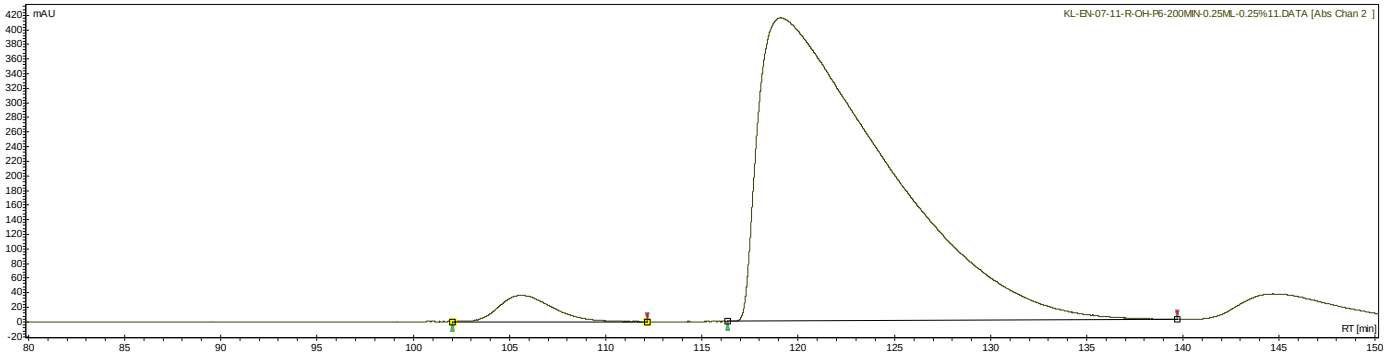


2d

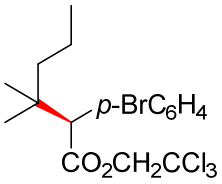
Enantiomeric excess was not determined.



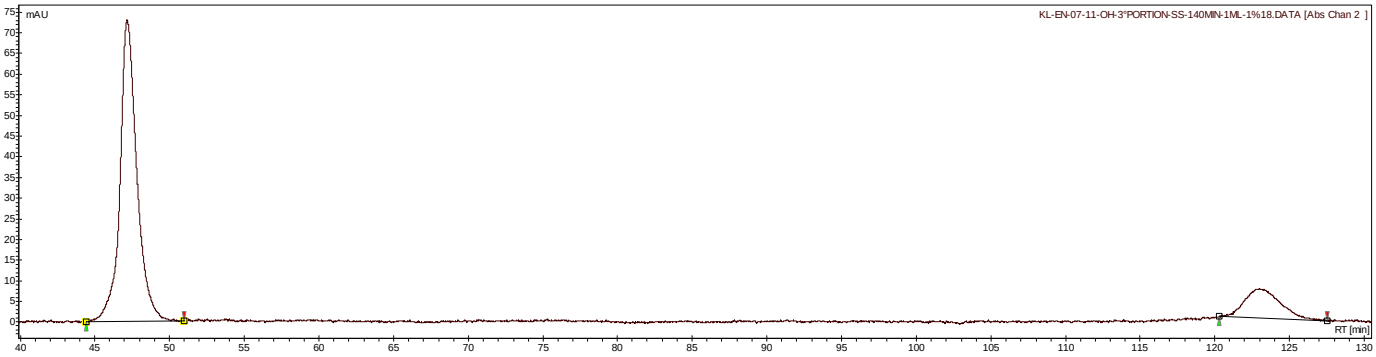
3d



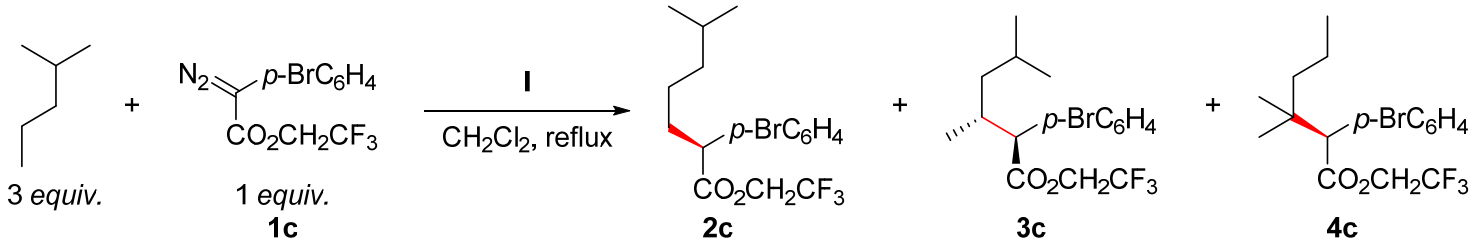
#	Time [Min]	Area% [%]
1	105.57	3.571
2	119.10	96.429
		93% *e.e.*

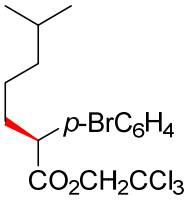


4d

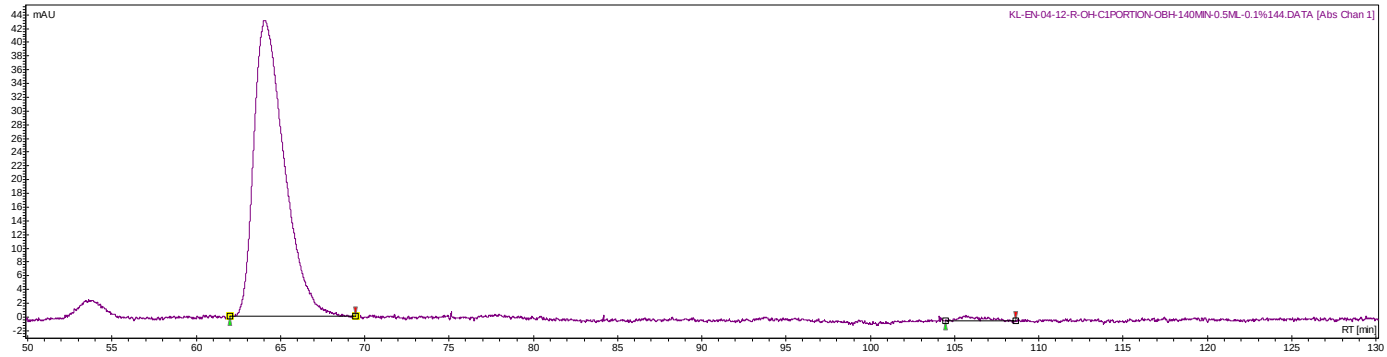


#	Time [Min]	Area% [%]
1	47.16	83.653
2	123.00	16.347
		67% *e.e.*

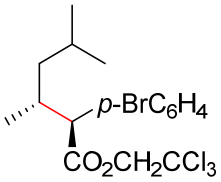




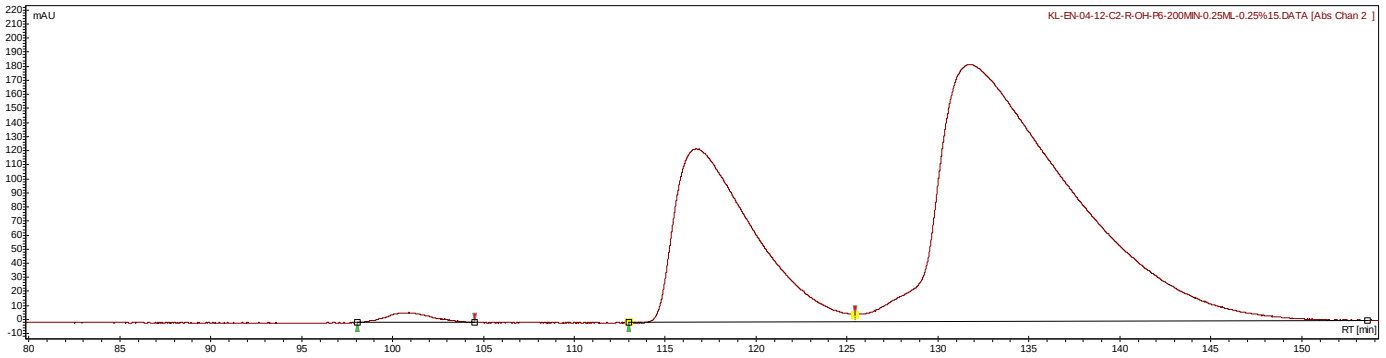
2c



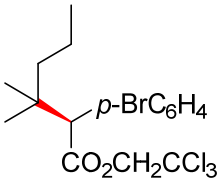
#	Time [Min]	Area% [%]
1	64.10	98.917
2	105.68	1.083
		98% *e.e.*



3c

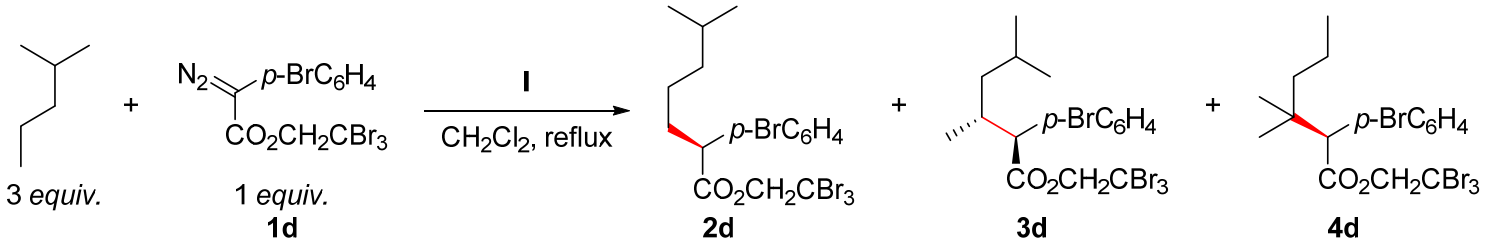


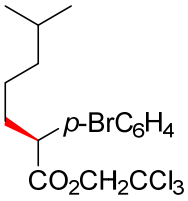
#	Time [Min]	Area% [%]
1	100.92	2.986
2	116.70	97.014
		94% *e.e.*



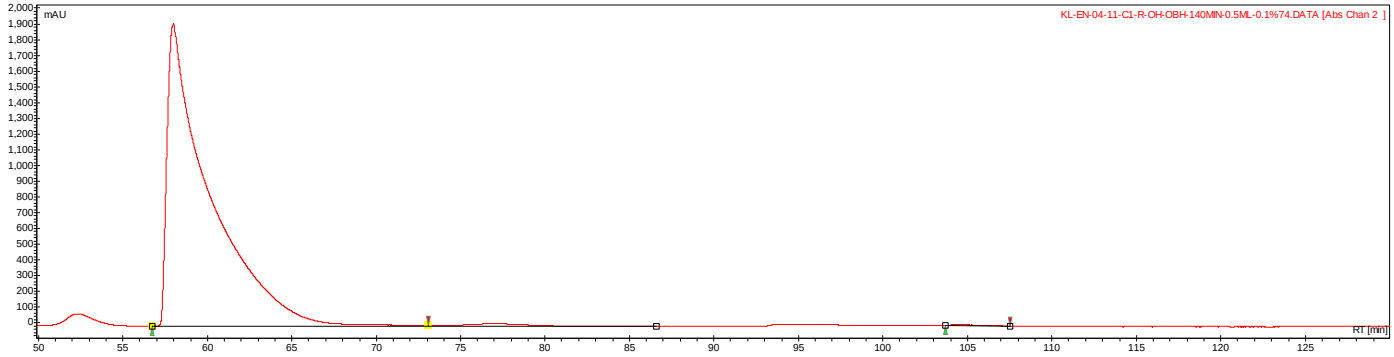
4c

Enantiomeric excess was not determined.

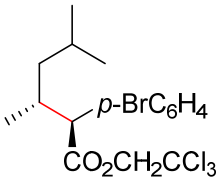




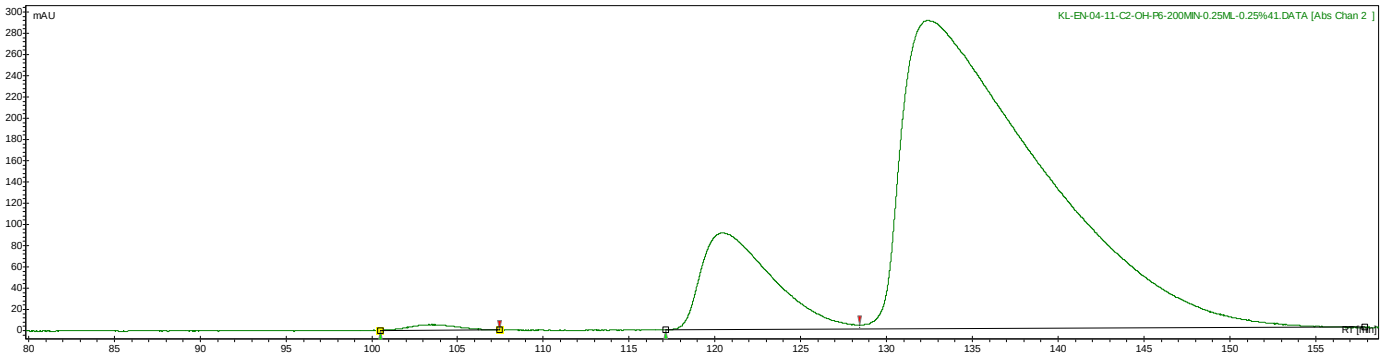
2d



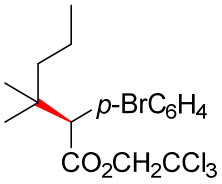
#	Time [Min]	Area% [%]
1	58.01	99.856
2	105.51	0.144
		>99% *e.e.*



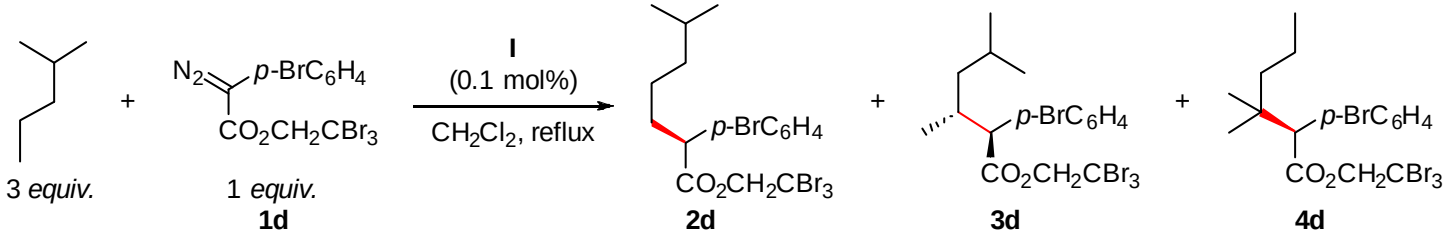
3d

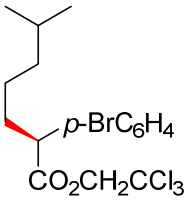


#	Time [Min]	Area% [%]
1	103.51	3.791
2	120.46	96.209
		92% *e.e.*

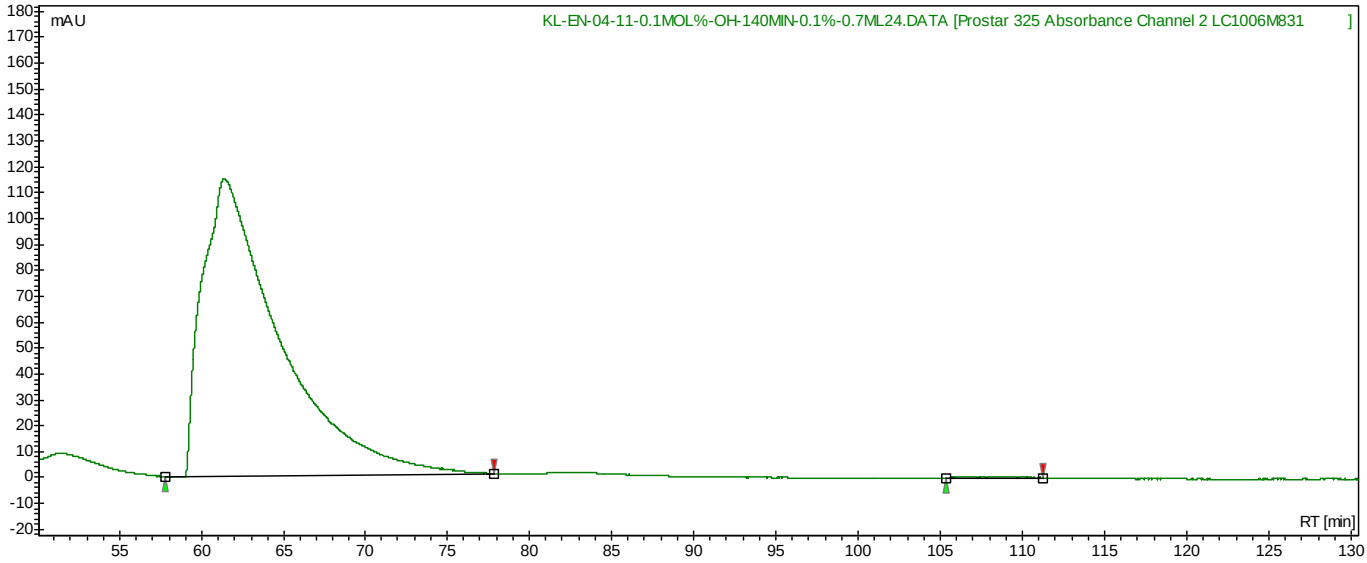


4d was not detected.



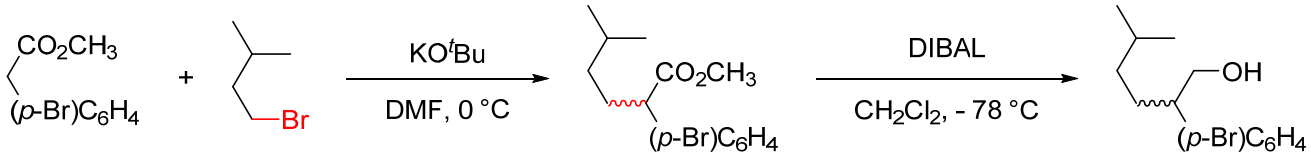


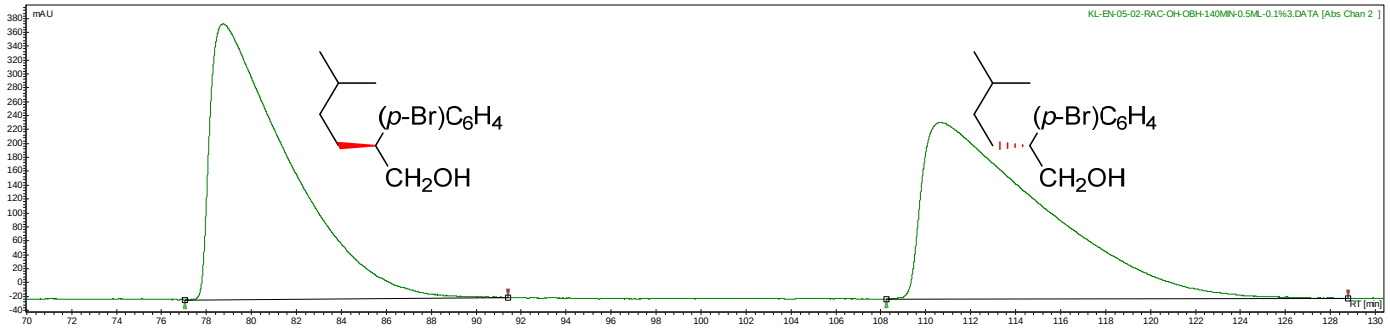
2d



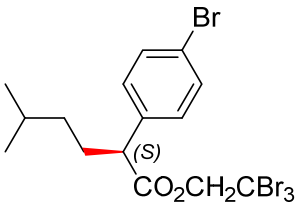
#	Time [Min]	Area% [%]
1	61.39	99.857
2	105.91	0.143
		>99% *e.e.*

10.5 C–H Functionalization Products **5-29**

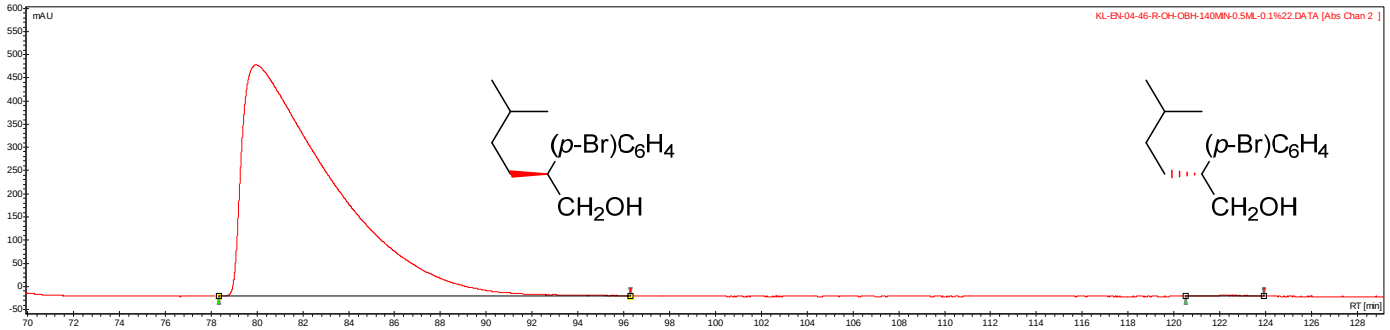




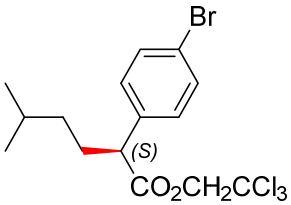
#	Time [Min]	Area% [%]
1	78.74	50.180
2	110.64	49.820



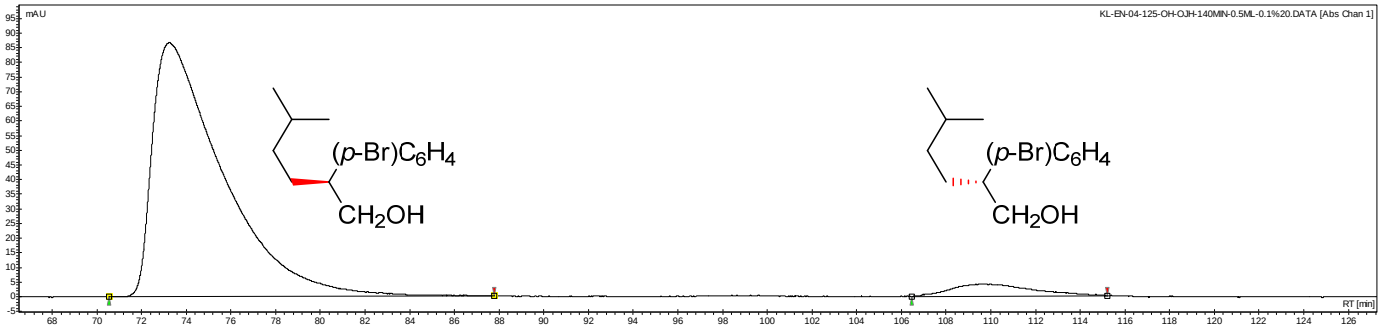
2,2,2-Tribromoethyl (*S*)-2-(4-bromophenyl)-5-methylhexanoate (**5**).



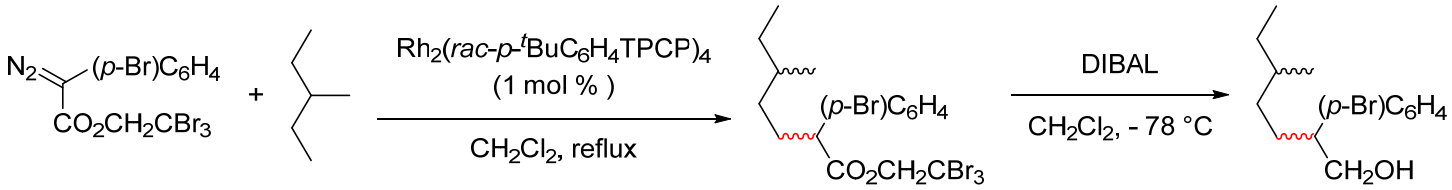
#	Time [Min]	Area% [%]
1	79.95	99.841
2	122.19	0.159
		>99% *e.e.*.

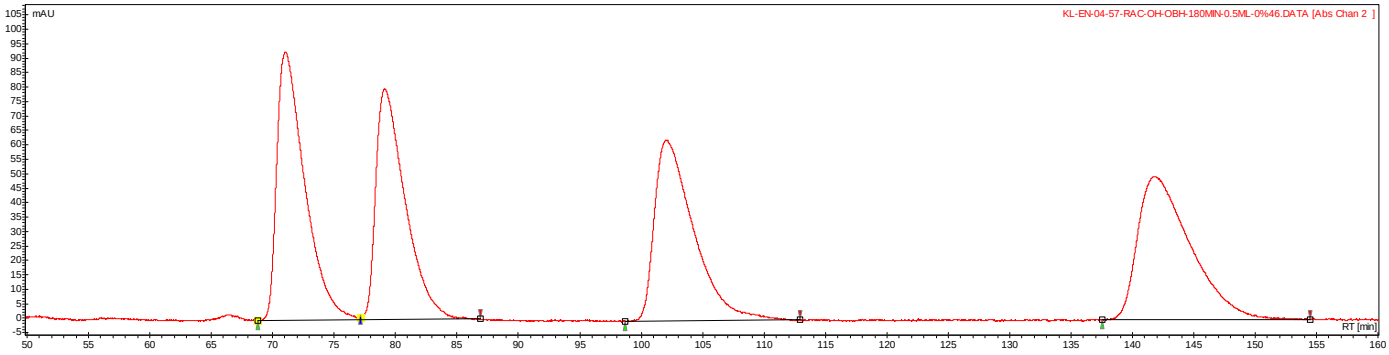


2,2,2-Trichloroethyl (*S*)-2-(4-bromophenyl)-5-methylhexanoate (**6**).

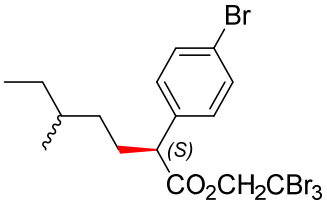


#	Time [Min]	Area% [%]
1	73.27	94.783
2	109.60	5.217
		90% *e.e.*.

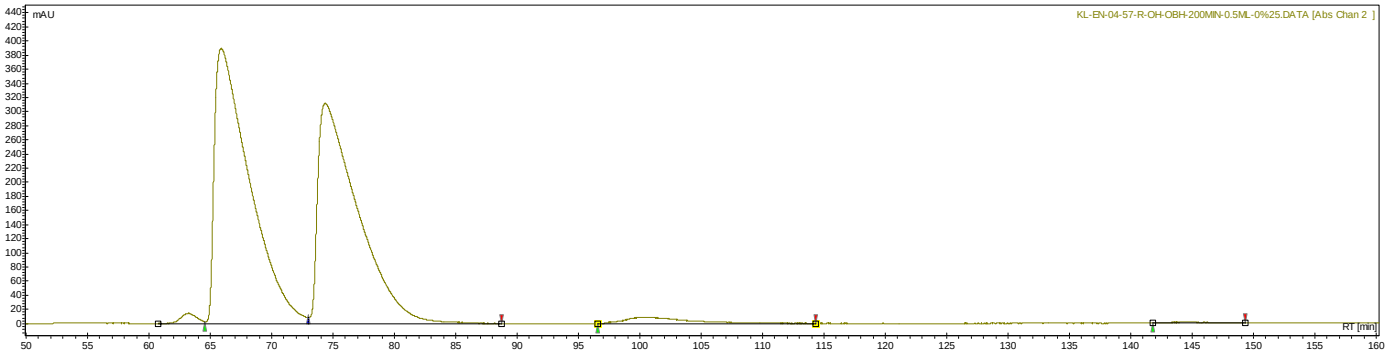




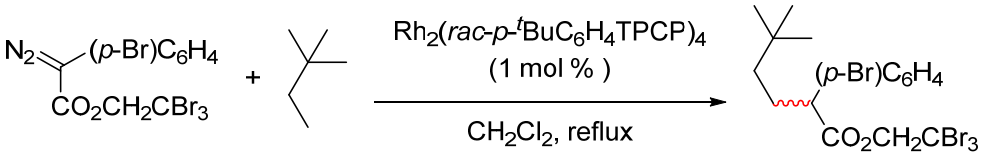
#	Time [Min]	Area% [%]
1	70.99	26.025
2	79.11	23.516
3	102.01	24.404
4	141.75	26.055

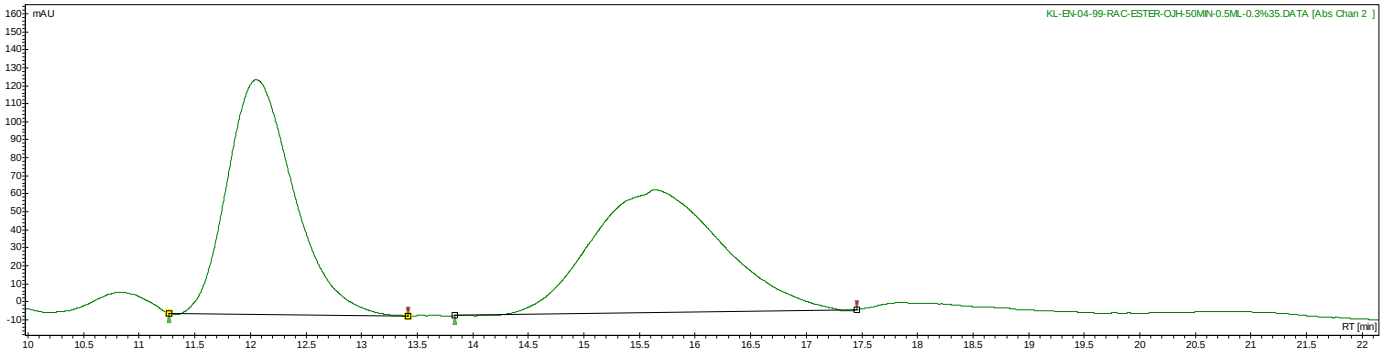


2,2,2-Tribromoethyl (2*S*)-2-(4-bromophenyl)-5-methylheptanoate (**7**).

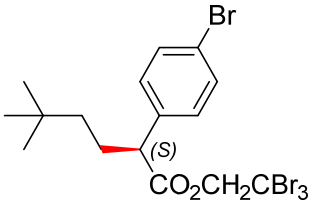


#	Time [Min]	Area% [%]
1	65.89	50.915
2	74.33	46.611
3	100.31	2.320
4	144.66	0.154
		>99% *e.e.*
		95% *e.e.*.

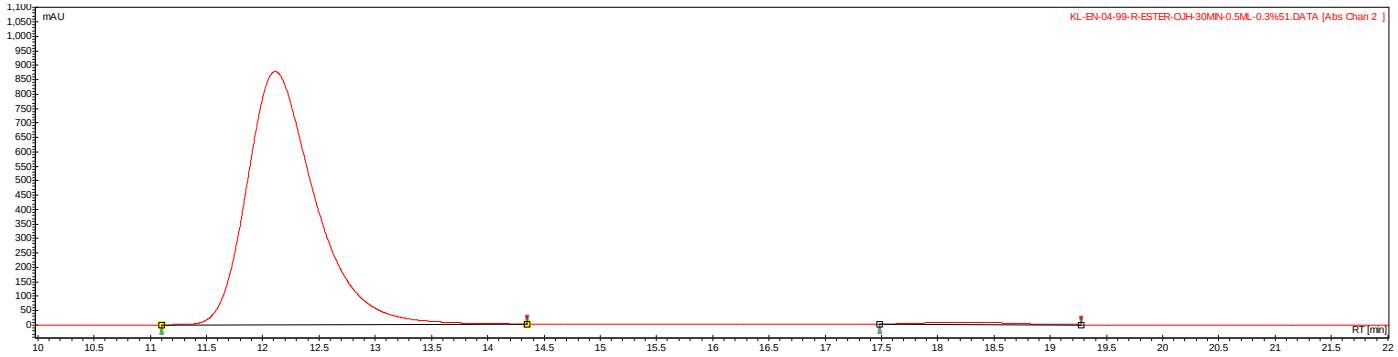




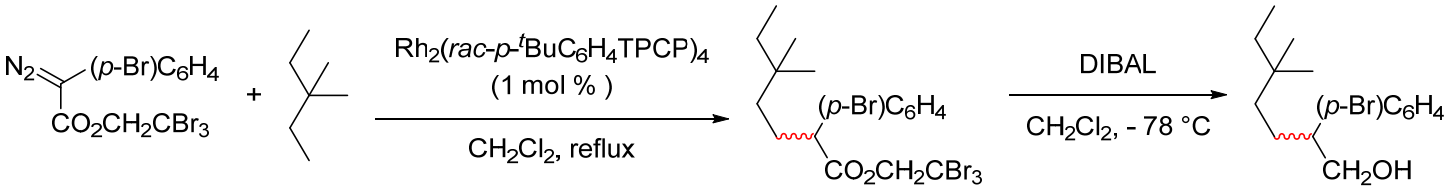
#	Time [Min]	Area% [%]
1	12.05	49.266
2	15.64	50.734

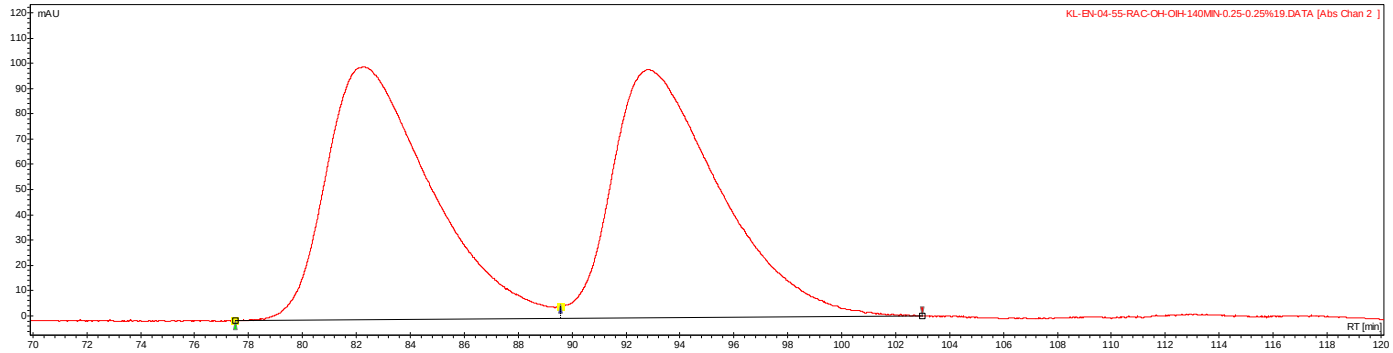


2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-5,5-dimethylhexanoate (**8**).

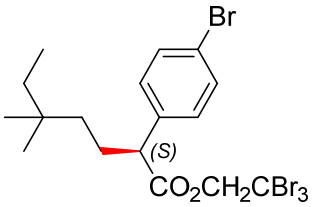


#	Time [Min]	Area% [%]
1	12.11	98.920
2	18.29	1.080
		98% *e.e.*.

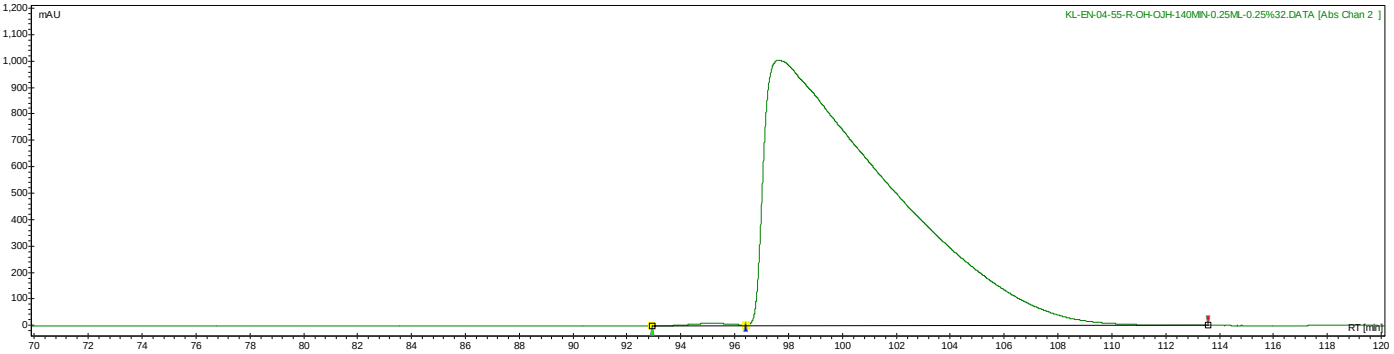




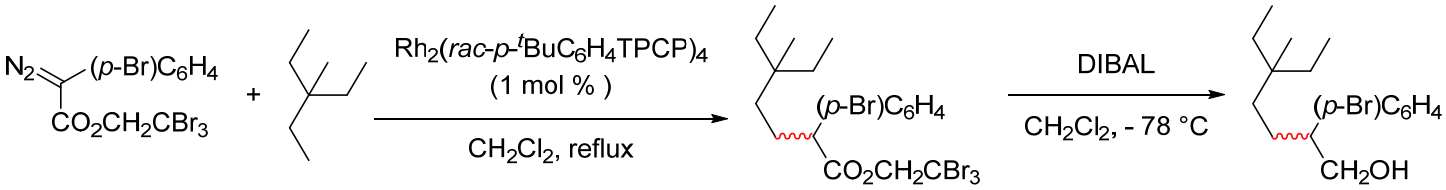
#	Time [Min]	Area% [%]
1	82.29	50.004
2	92.80	49.996

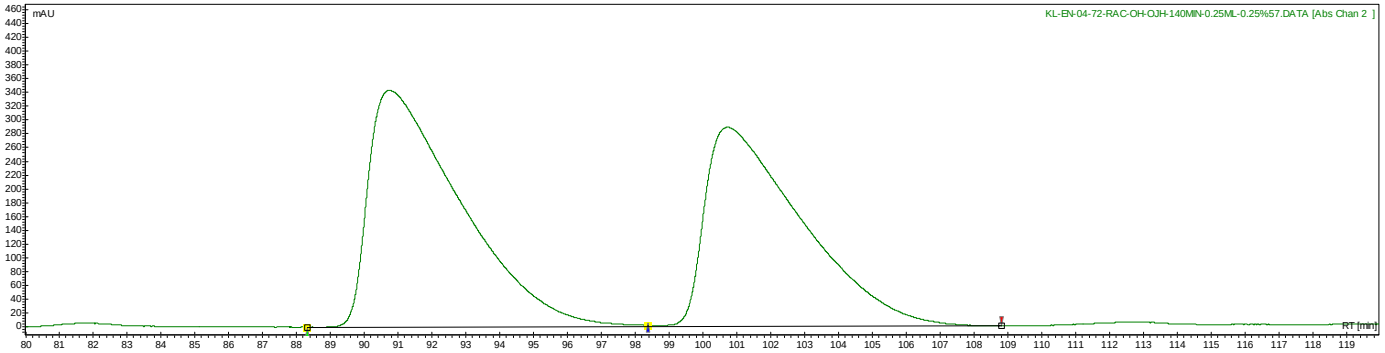


2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-5,5-dimethylheptanoate (**9**).

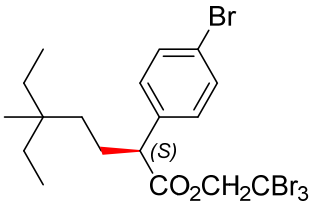


#	Time [Min]	Area% [%]
1	95.06	0.341
2	97.61	99.659
		>99% *e.e.*.

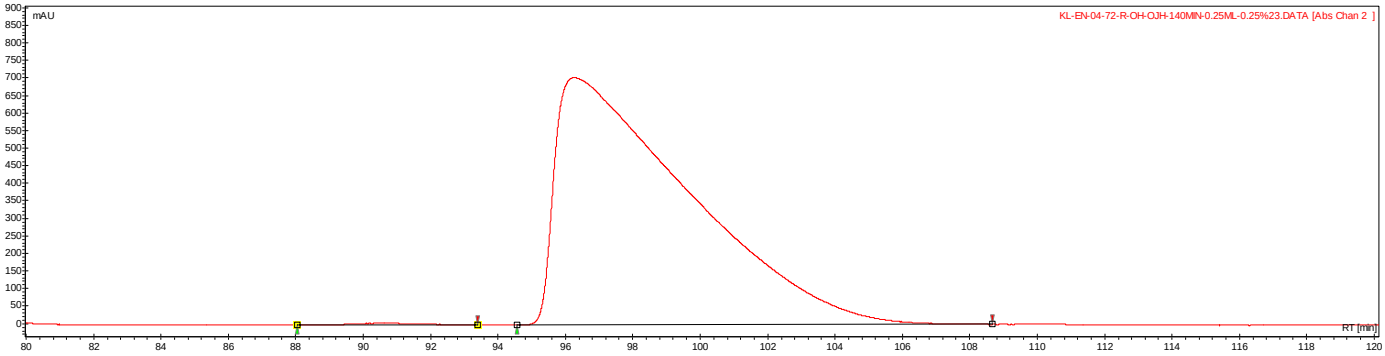




#	Time [Min]	Area% [%]
1	90.73	53.081
2	100.73	46.919

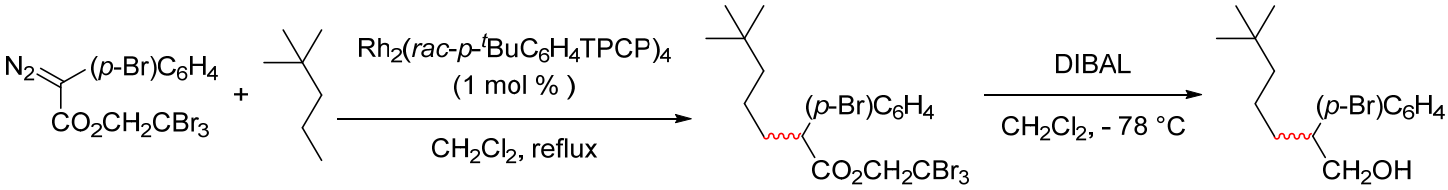


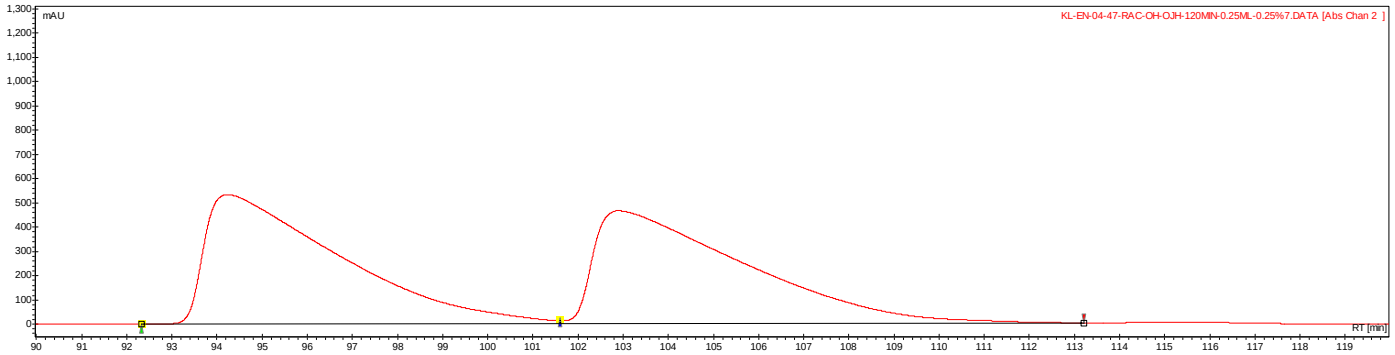
2,2,2-Tribromoethyl (*S*)-2-(4-bromophenyl)-5-ethyl-5-methylheptanoate (**10**).



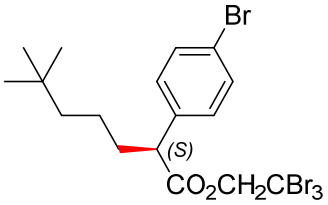
#	Time [Min]	Area% [%]
1	90.64	0.342
2	96.25	99.658

>99% *e.e.*.

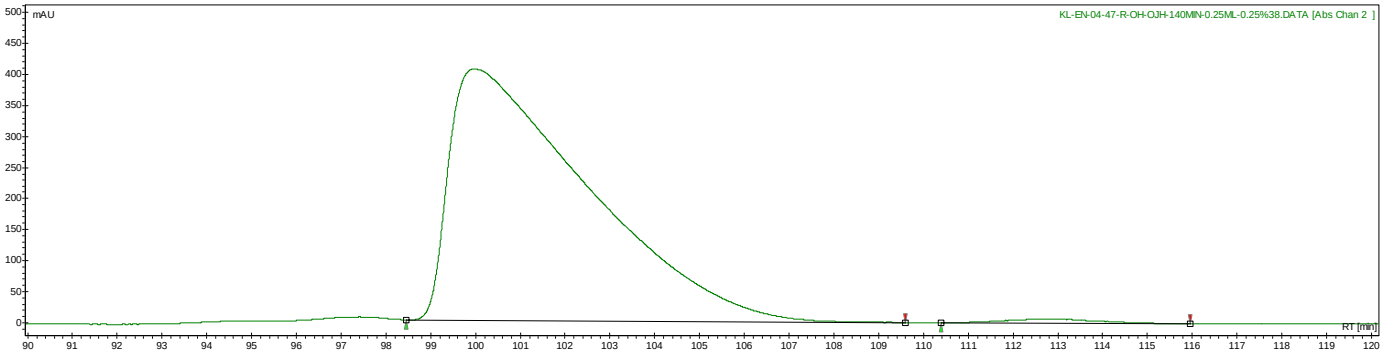




#	Time [Min]	Area% [%]
1	94.21	50.792
2	102.90	49.208

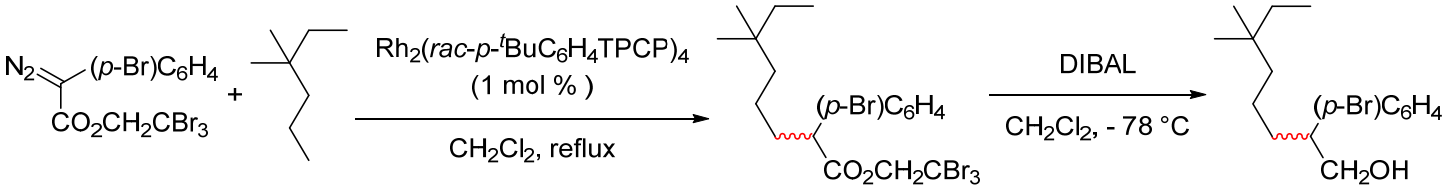


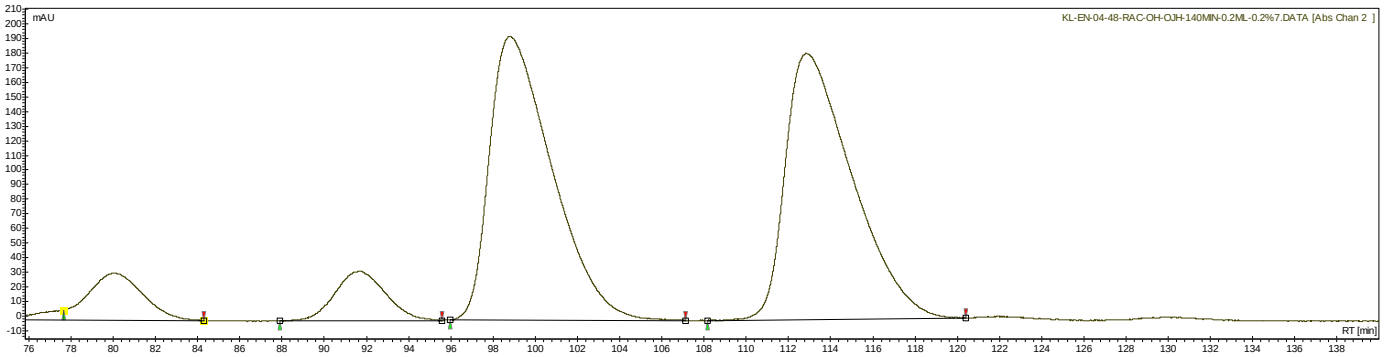
2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6,6-dimethylheptanoate (**11**).



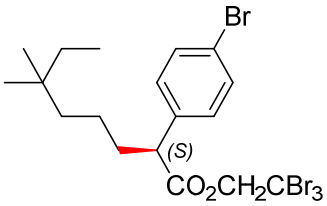
#	Time [Min]	Area% [%]
1	99.96	98.842
2	112.72	1.158

98% *e.e.*.

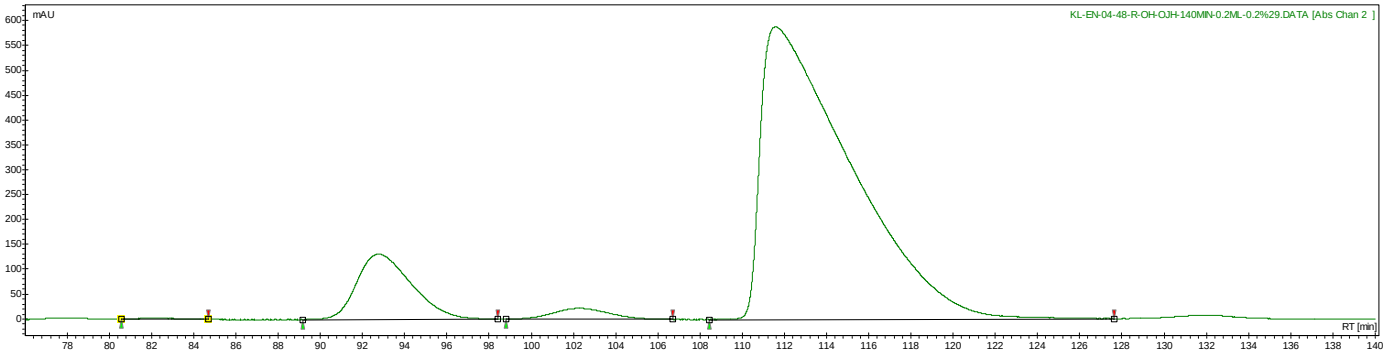




#	Time [Min]	Area% [%]
1	80.11	6.389
2	91.75	6.185
3	98.78	43.622
4	112.84	43.804



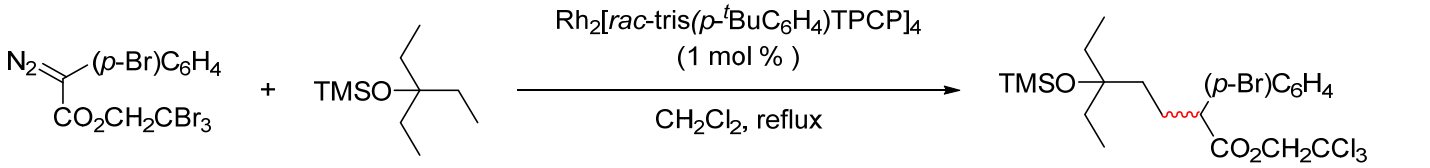
2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6,6-dimethyloctanoate (**12**).

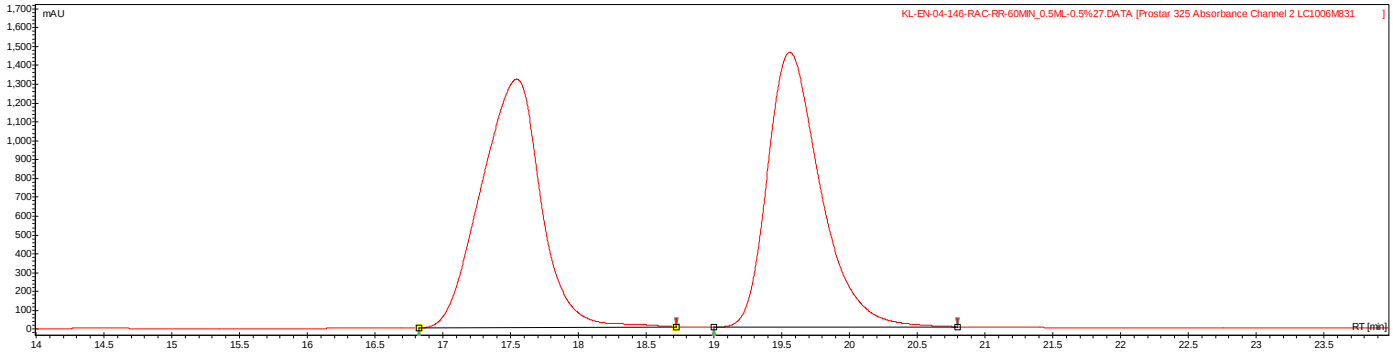


#	Time [Min]	Area% [%]
1	82.19	0.117
2	92.76	11.692
3	102.39	2.018
4	111.60	86.173

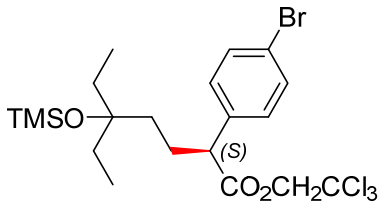
98% *e.e.*.

95% *e.e.*.

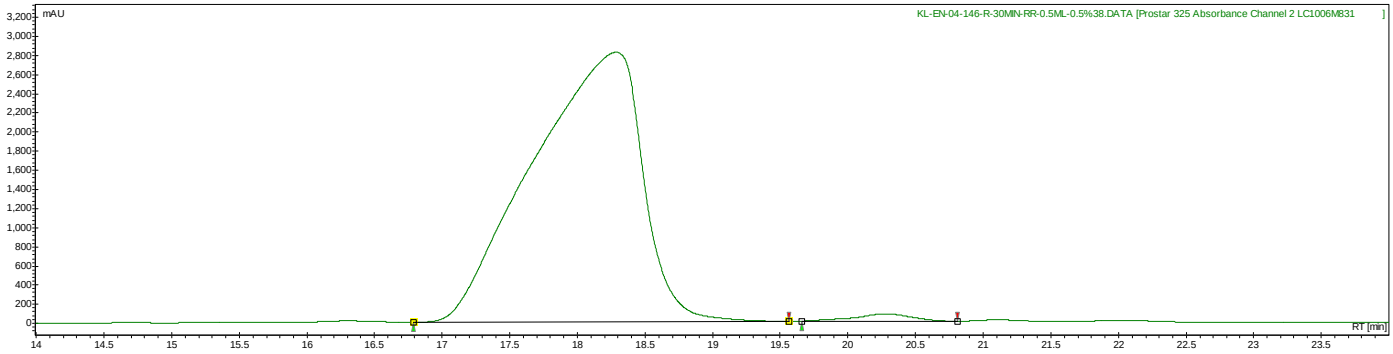




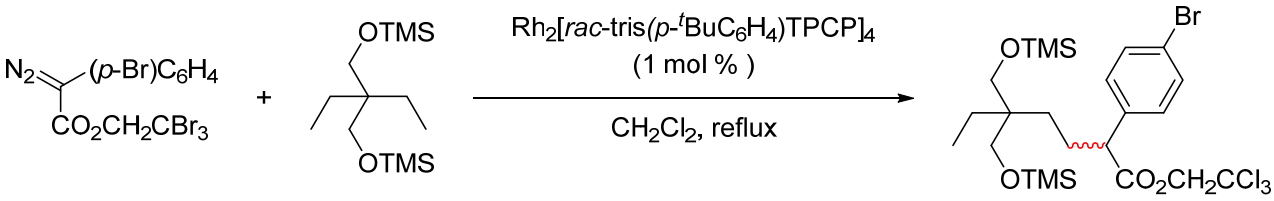
#	Time [Min]	Area% [%]
1	17.54	50.434
2	19.56	49.566

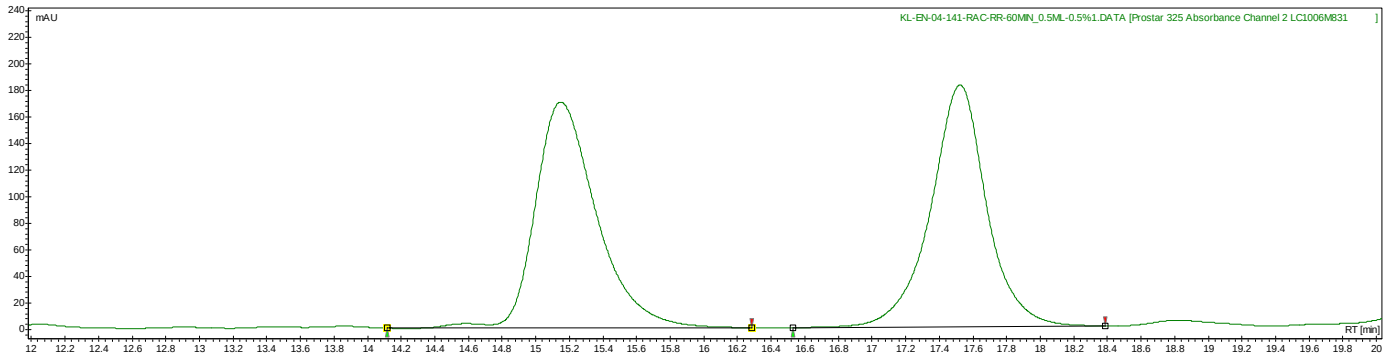


2,2,2-Trichloroethyl (S)-2-(4-bromophenyl)-5-ethyl-5-((trimethylsilyl)oxy)heptanoate (**13**).

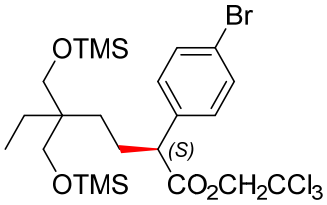


#	Time [Min]	Area% [%]
1	18.29	98.626
2	20.28	1.374
		97% *e.e.*.

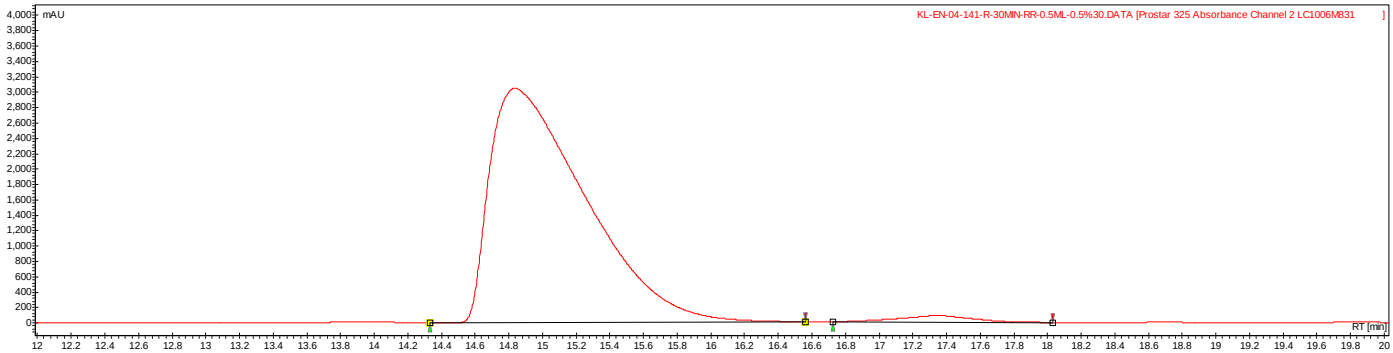




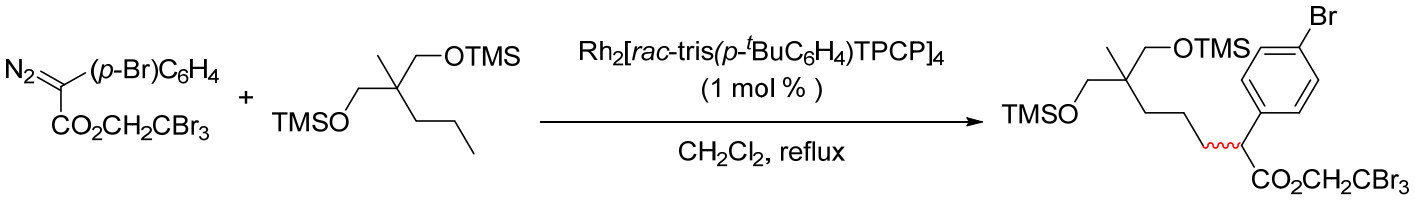
#	Time [Min]	Area% [%]
1	15.15	50.447
2	17.52	49.553

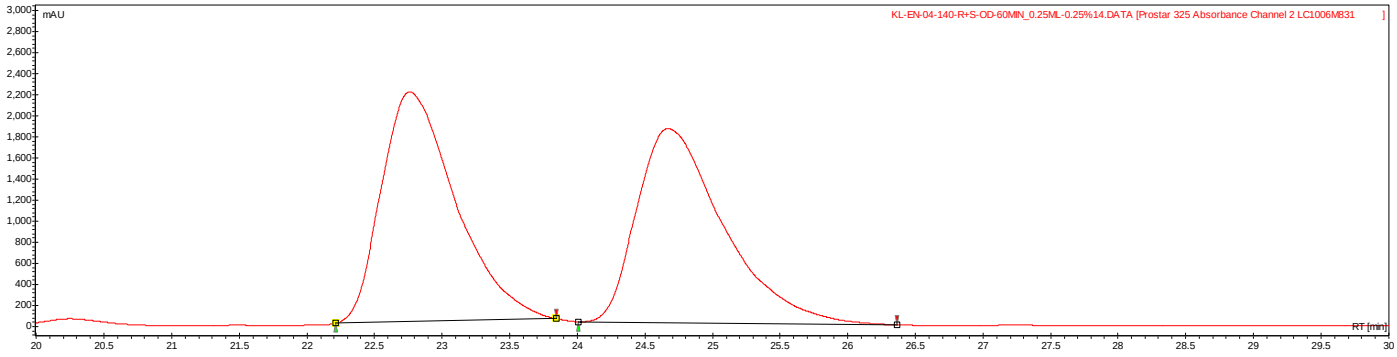


2,2,2-Trichloroethyl (S)-2-(4-bromophenyl)-5,5-bis(((trimethylsilyl)oxy)methyl)heptanoate (**14**).

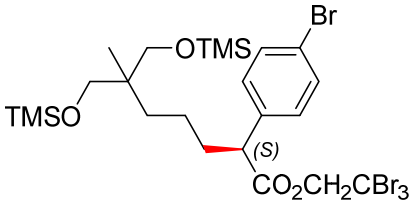


#	Time [Min]	Area% [%]
1	14.84	97.886
2	17.35	2.114
		96% *e.e.*.

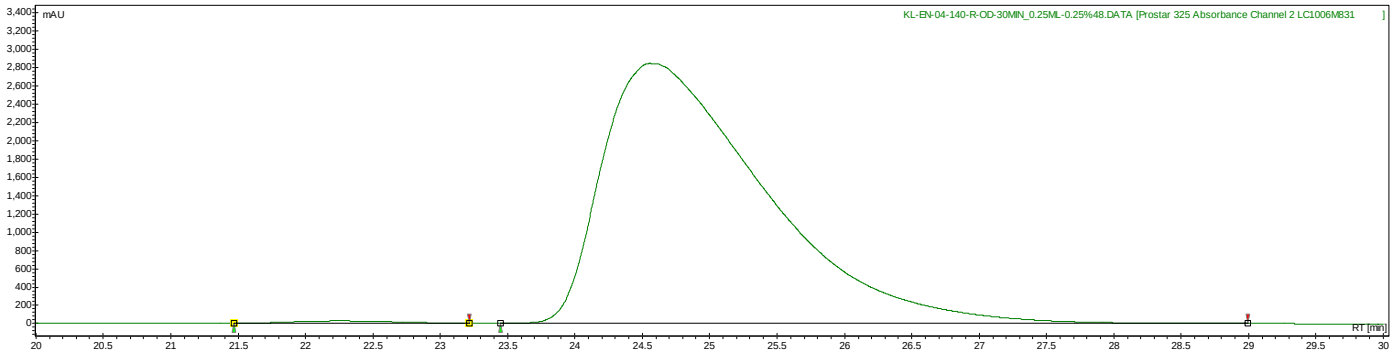




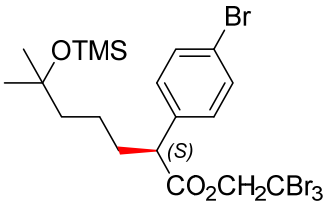
#	Time [Min]	Area% [%]
1	22.76	50.387
2	24.67	49.613



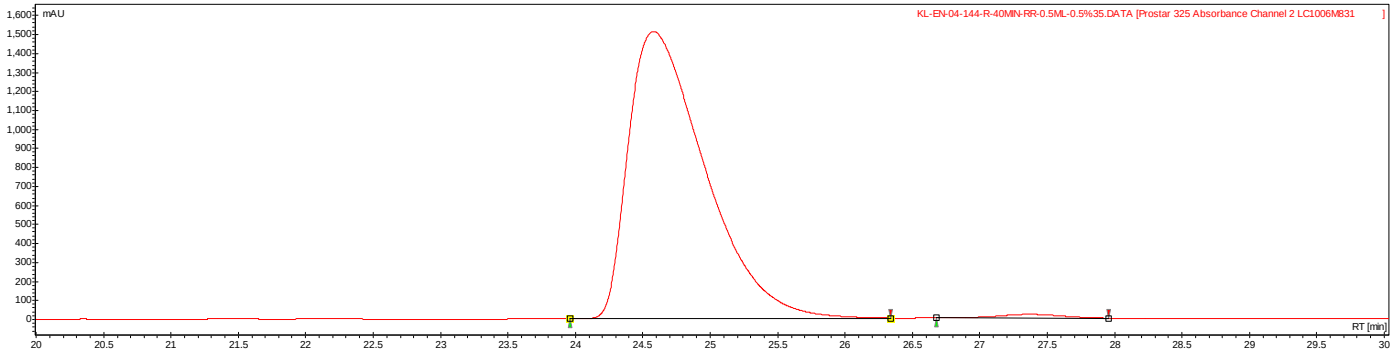
2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6-methyl-7-((trimethylsilyl)oxy)-6-(((trimethylsilyl)oxy)methyl)heptanoate (**15**).



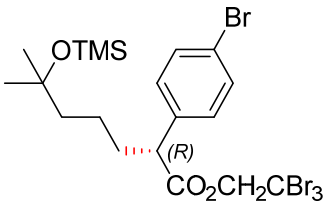
#	Time [Min]	Area% [%]
1	22.24	0.592
2	24.55	99.408
		99% *e.e.*.



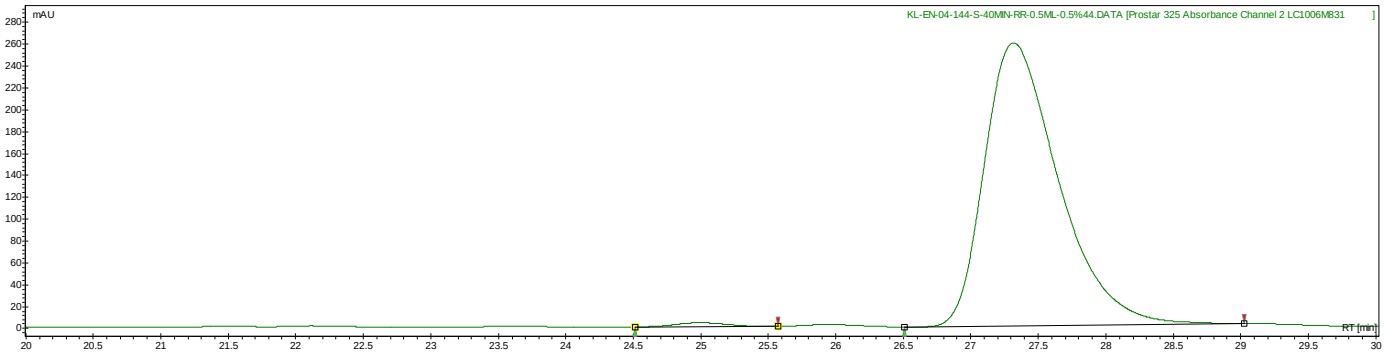
2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6-methyl-6-((trimethylsilyl)oxy)heptanoate (**16**).



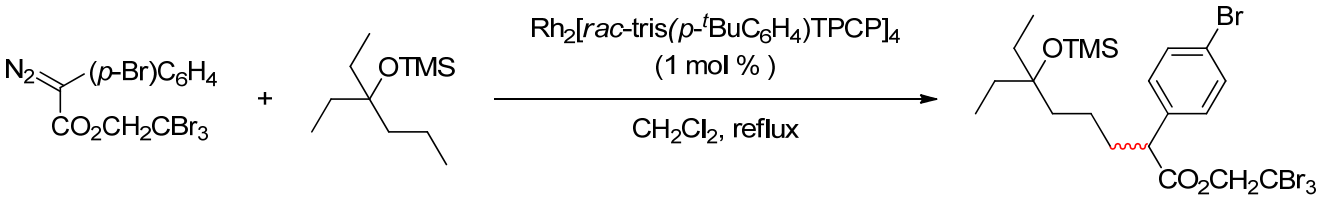
#	Time [Min]	Area% [%]
1	24.58	98.942
2	27.37	1.058
		98% *e.e.*.

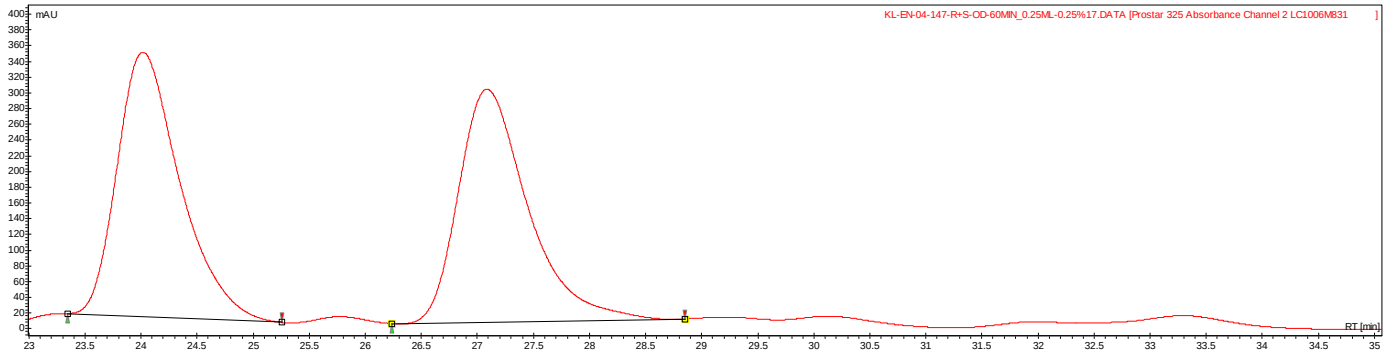


2,2,2-Tribromoethyl (R)-2-(4-bromophenyl)-6-methyl-6-((trimethylsilyl)oxy)heptanoate.

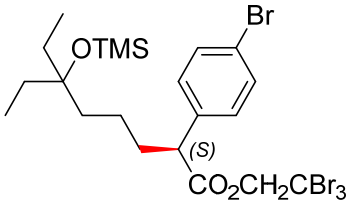


#	Time [Min]	Area% [%]
1	24.98	0.984
2	27.32	99.016
		98% *e.e.*.

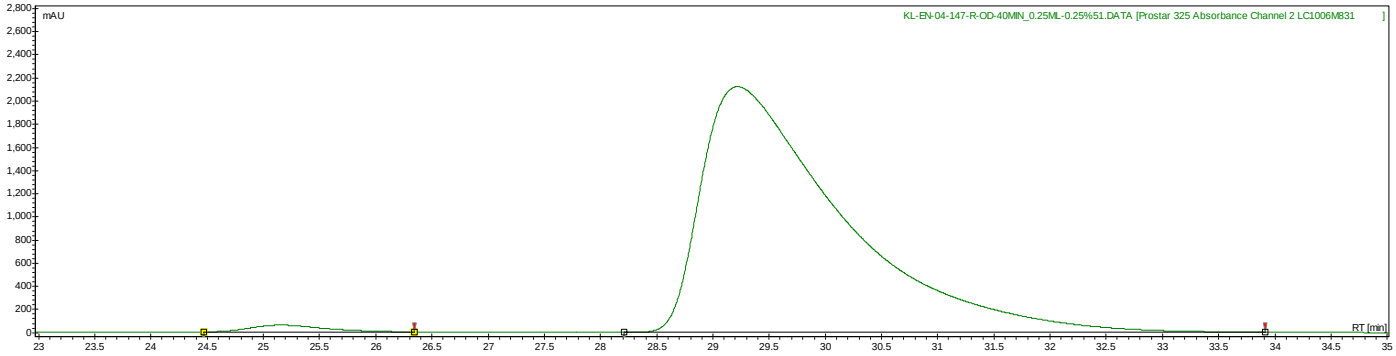




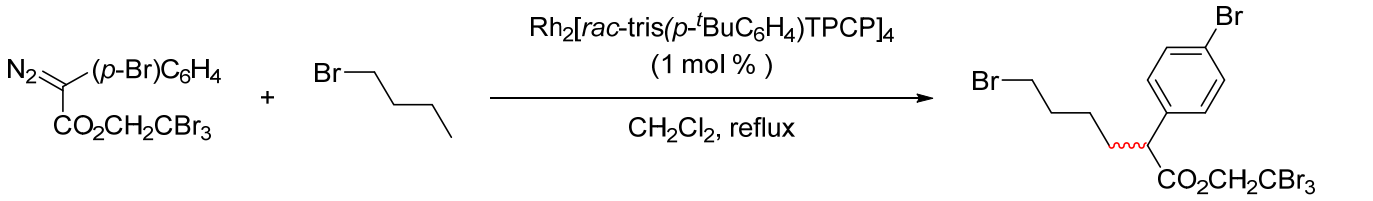
#	Time [Min]	Area% [%]
1	24.02	50.742
2	27.08	49.258

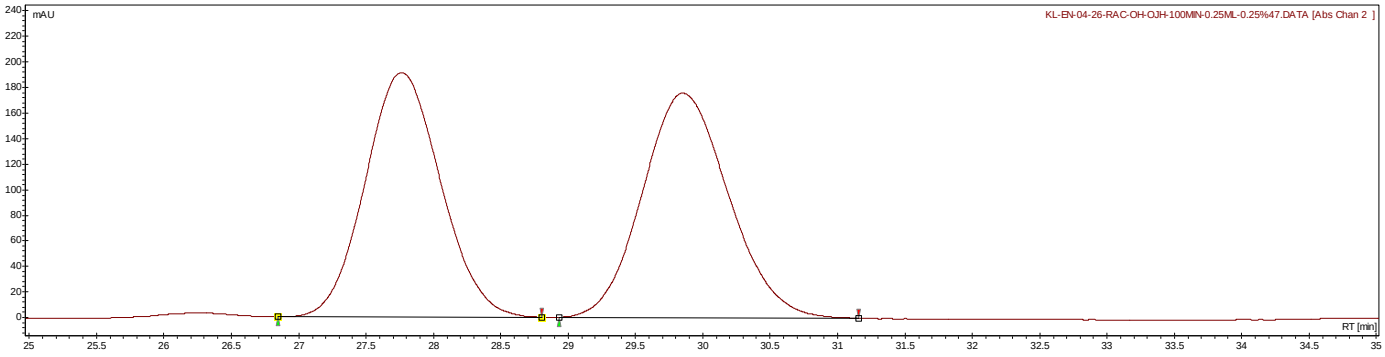


2,2,2-Tribromoethyl (S)-2-(4-bromophenyl)-6-ethyl-6-((trimethylsilyl)oxy)octanoate (**17**).

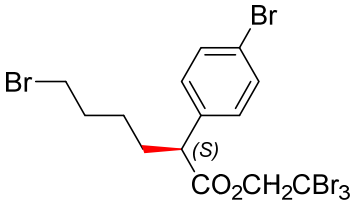


#	Time [Min]	Area% [%]
1	25.16	1.472
2	29.22	98.528
		97% *e.e.*.

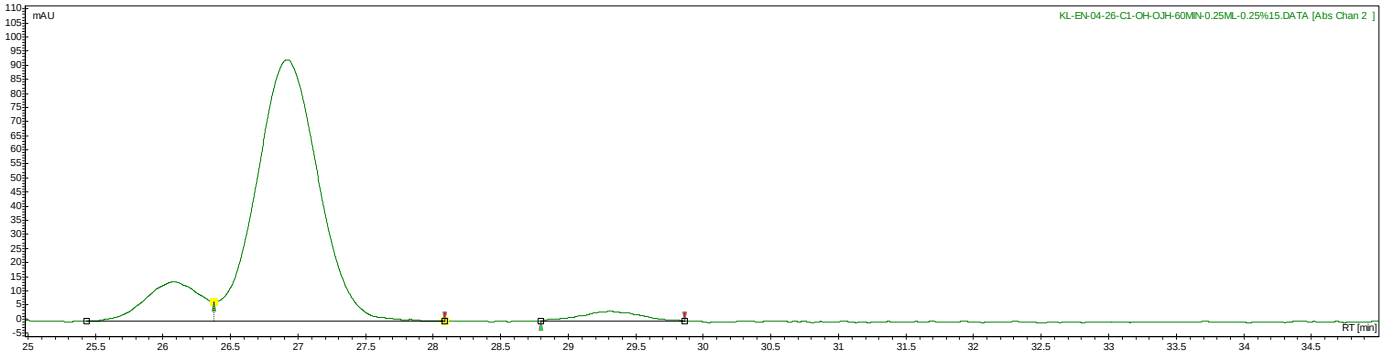




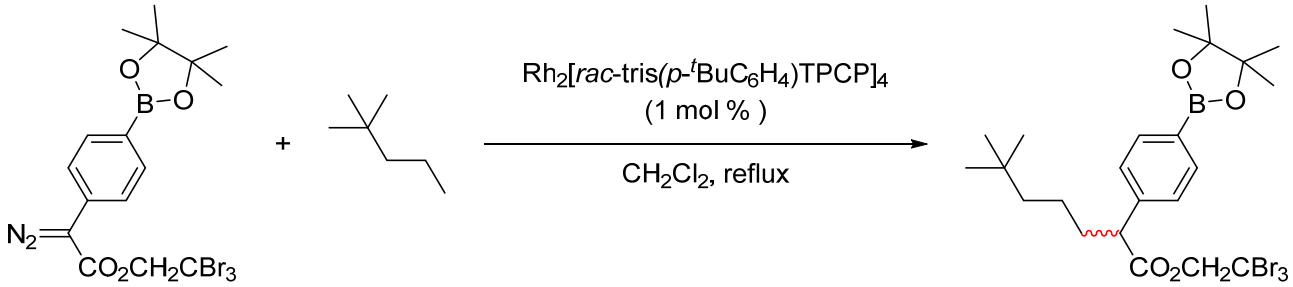
#	Time [Min]	Area% [%]
1	27.76	48.741
2	29.85	51.259

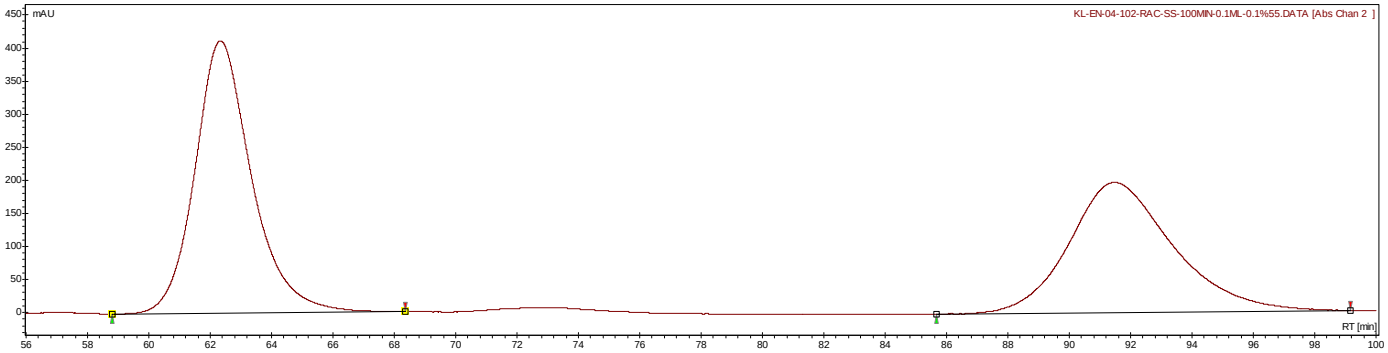


2,2,2-Tribromoethyl (S)-6-bromo-2-(4-bromophenyl)hexanoate (**18**).

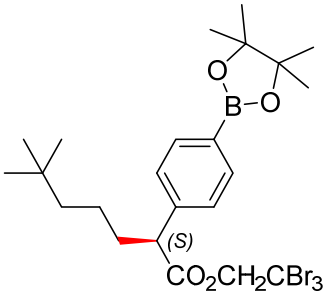


#	Time [Min]	Area% [%]
1	26.92	96.452
2	29.31	3.548
		93% *e.e.*.

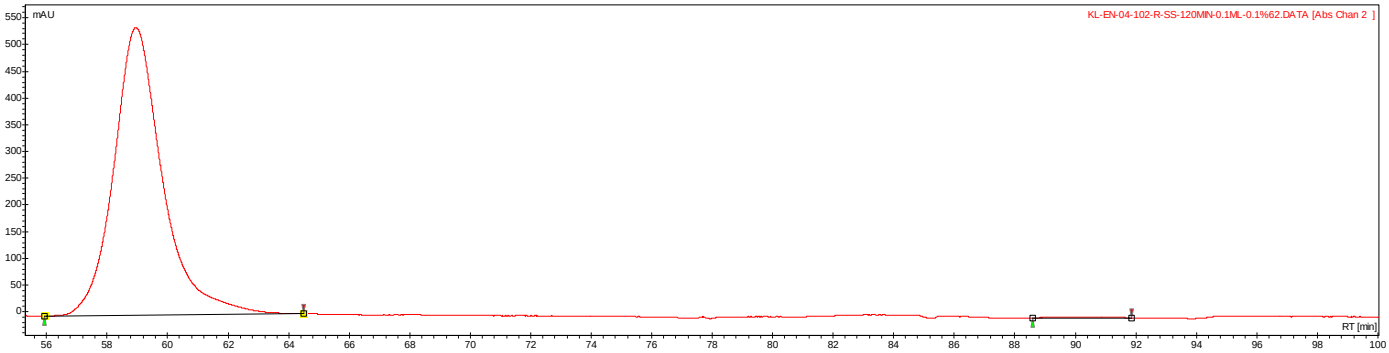




#	Time [Min]	Area% [%]
1	62.31	53.209
2	91.46	46.791

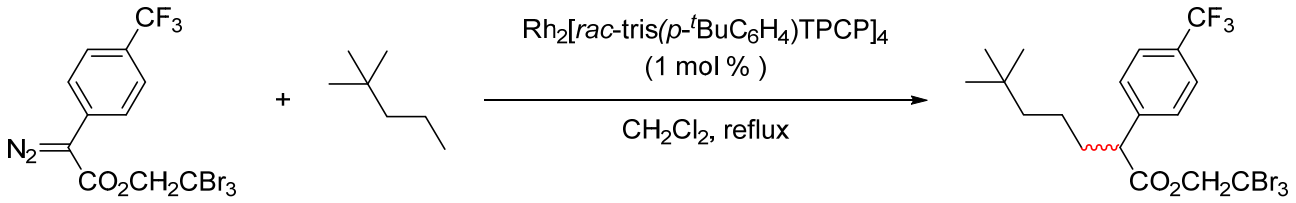


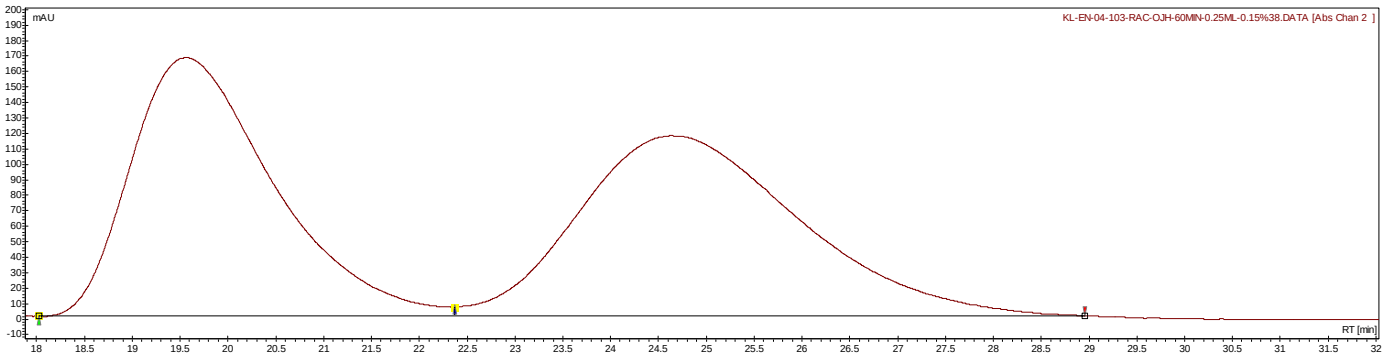
2,2,2-Tribromoethyl (S)-6,6-dimethyl-2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)heptanoate (**19**).



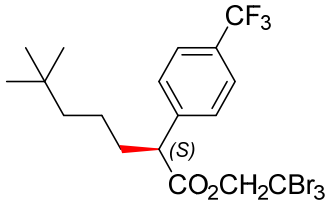
#	Time [Min]	Area% [%]
1	58.94	99.661
2	91.19	0.339

>99% *e.e.*.

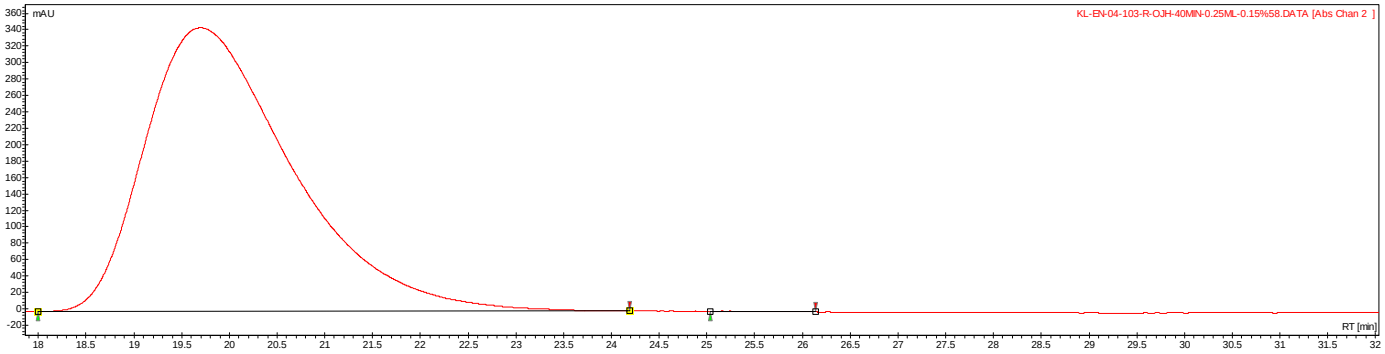




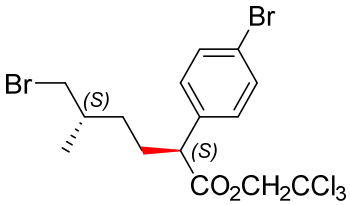
#	Time [Min]	Area% [%]
1	19.56	48.144
2	24.63	51.856



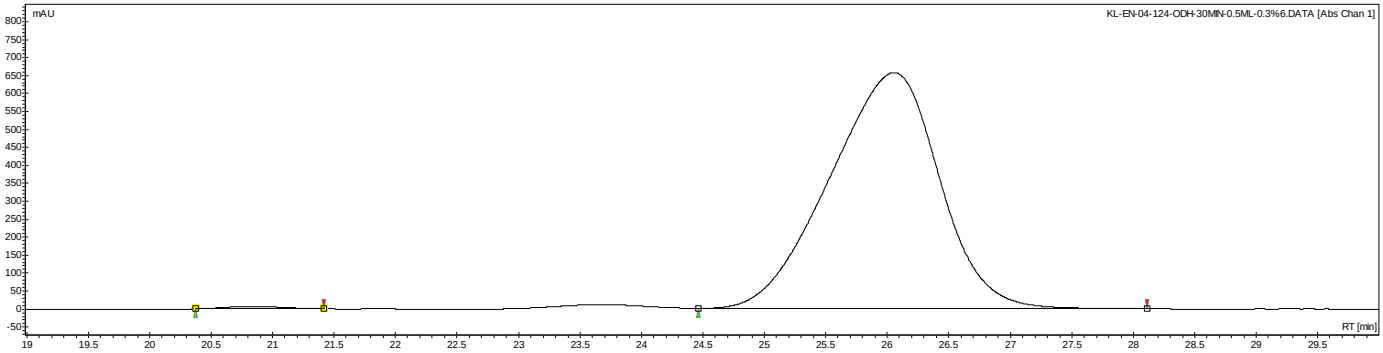
2,2,2-Tribromoethyl (S)-6,6-dimethyl-2-(4-(trifluoromethyl)phenyl)heptanoate (20).



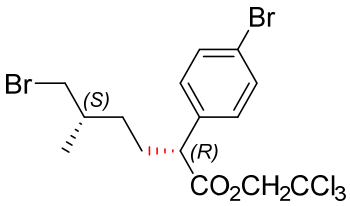
#	Time [Min]	Area% [%]
1	19.70	99.957
2	25.77	0.043
		>99% *e.e.*.



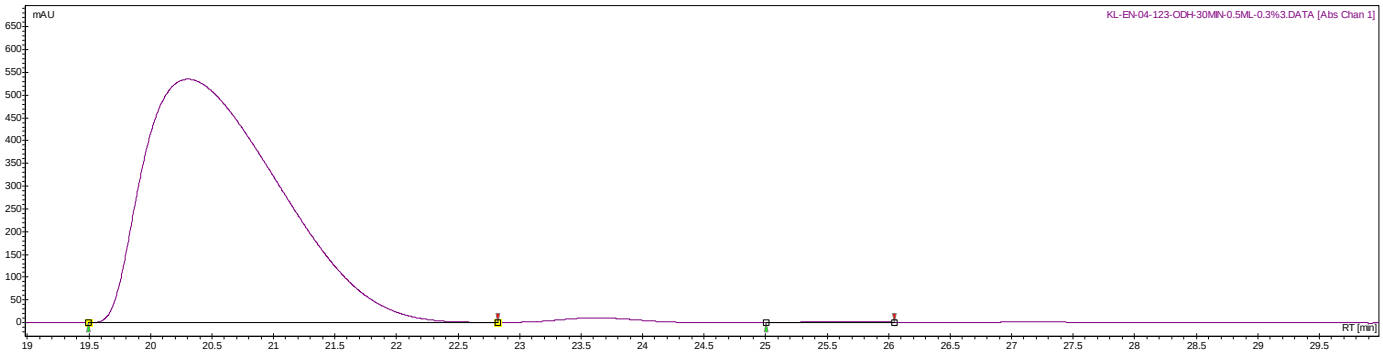
2,2,2-Trichloroethyl (2S,5S)-6-bromo-2-(4-bromophenyl)-5-methylhexanoate (**24**).



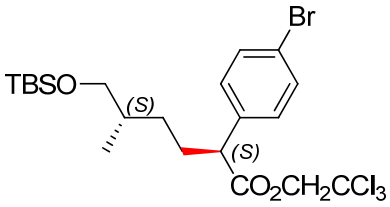
#	Time [Min]	Area% [%]
1	20.83	0.542
2	26.05	99.458
		>100:1 d.*r.*.



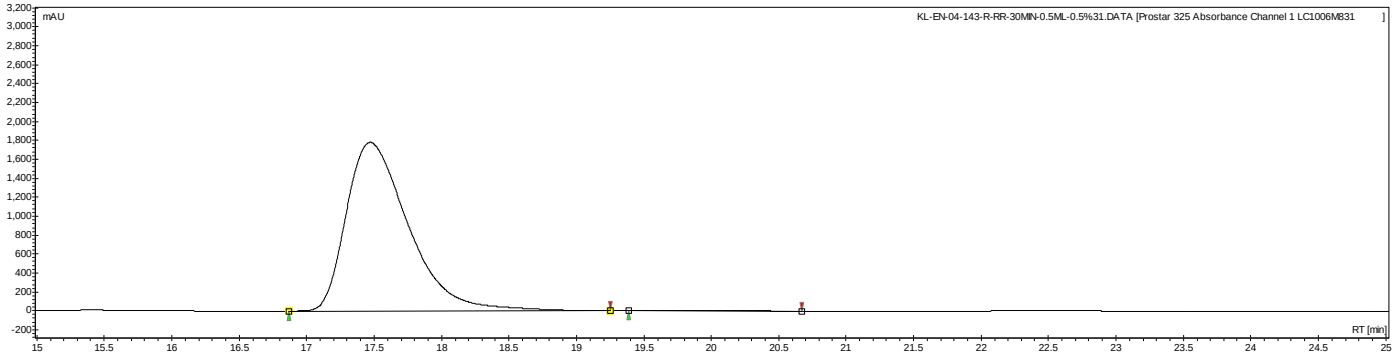
2,2,2-Trichloroethyl (2R,5S)-6-bromo-2-(4-bromophenyl)-5-methylhexanoate (**27**).



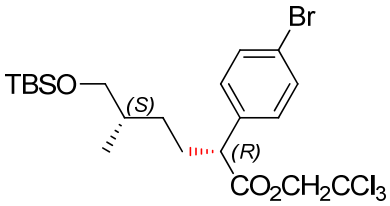
#	Time [Min]	Area% [%]
1	20.30	99.775
2	25.59	0.225
		>100:1 d.*r.*.



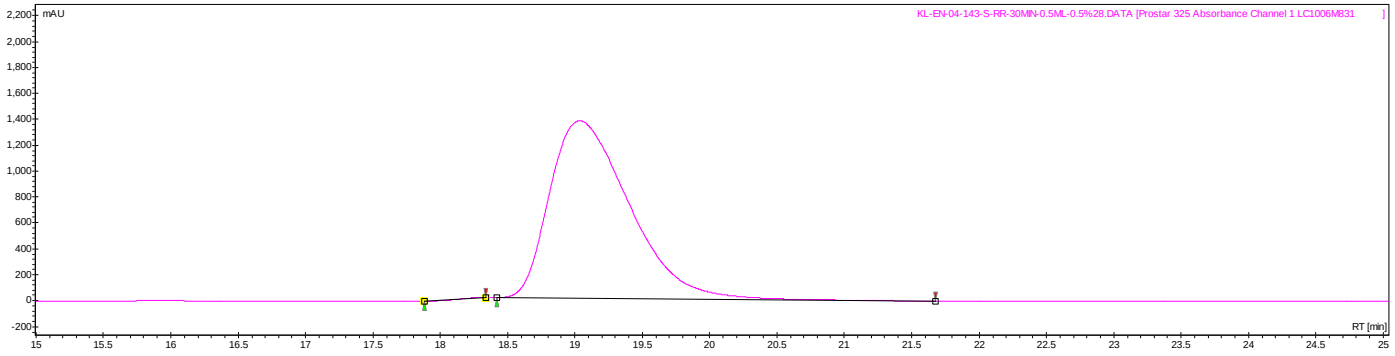
(2S,5S)-2,2,2-Trichloroethyl 2-(4-bromophenyl)-6-((tert-butyldimethylsilyl)oxy)-5-methylhexanoate (**25**).



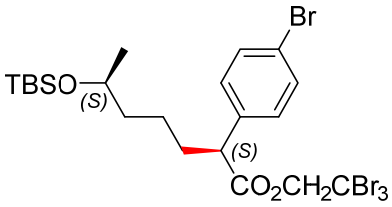
#	Time [Min]	Area% [%]
1	17.47	99.749
2	19.79	0.251
		>100:1 d.*r.*.



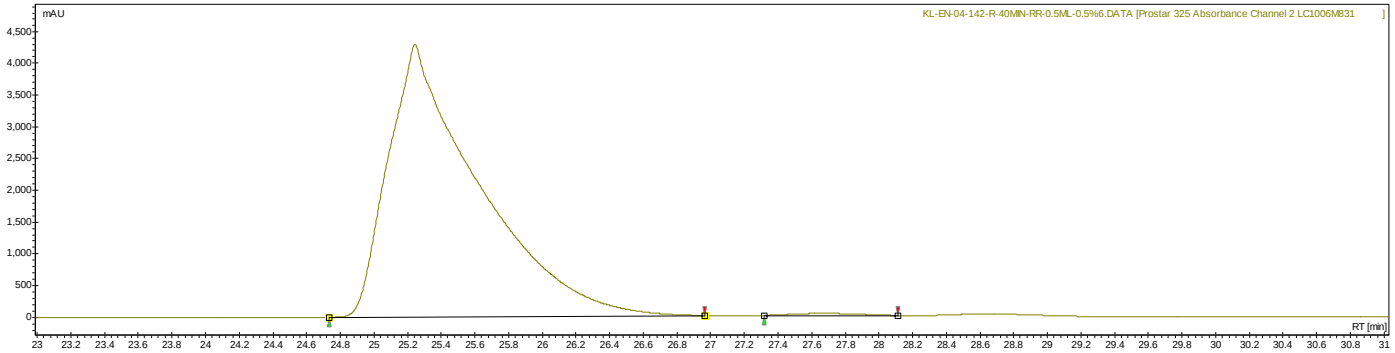
(2R,5S)-2,2,2-Trichloroethyl 2-(4-bromophenyl)-6-((tert-butyldimethylsilyl)oxy)-5-methylhexanoate (**28**).



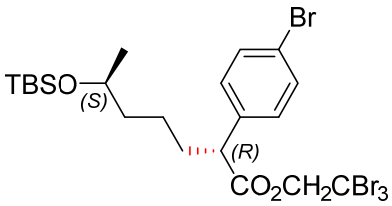
#	Time [Min]	Area% [%]
1	18.01	0.035
2	19.04	99.965
		>100:1 d.*r.*.



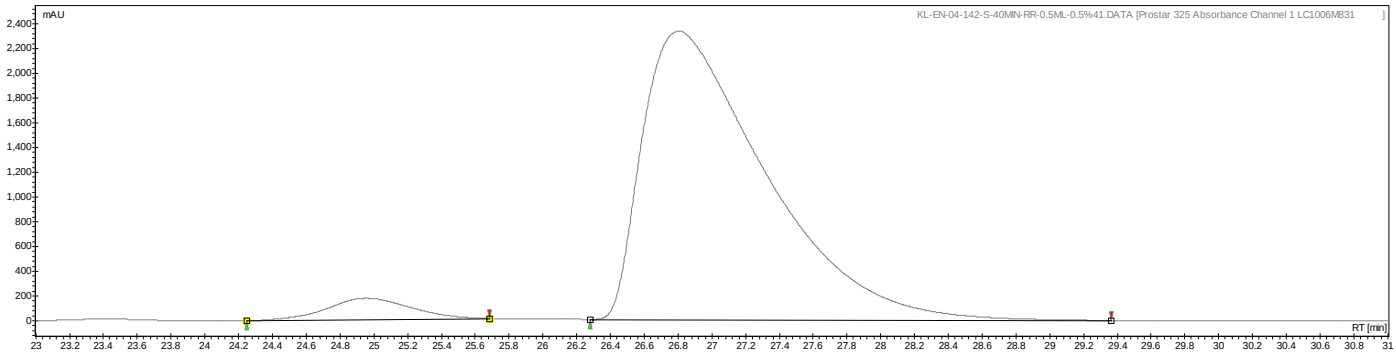
2,2,2-Tribromoethyl (2S,6S)-2-(4-bromophenyl)-6-((tert-butyldimethylsilyl)oxy)heptanoate (**26**).



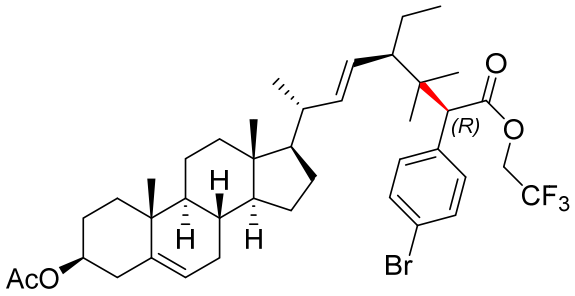
#	Time [Min]	Area% [%]
1	25.24	99.397
2	27.67	0.603
		>100:1 d.*r.*.

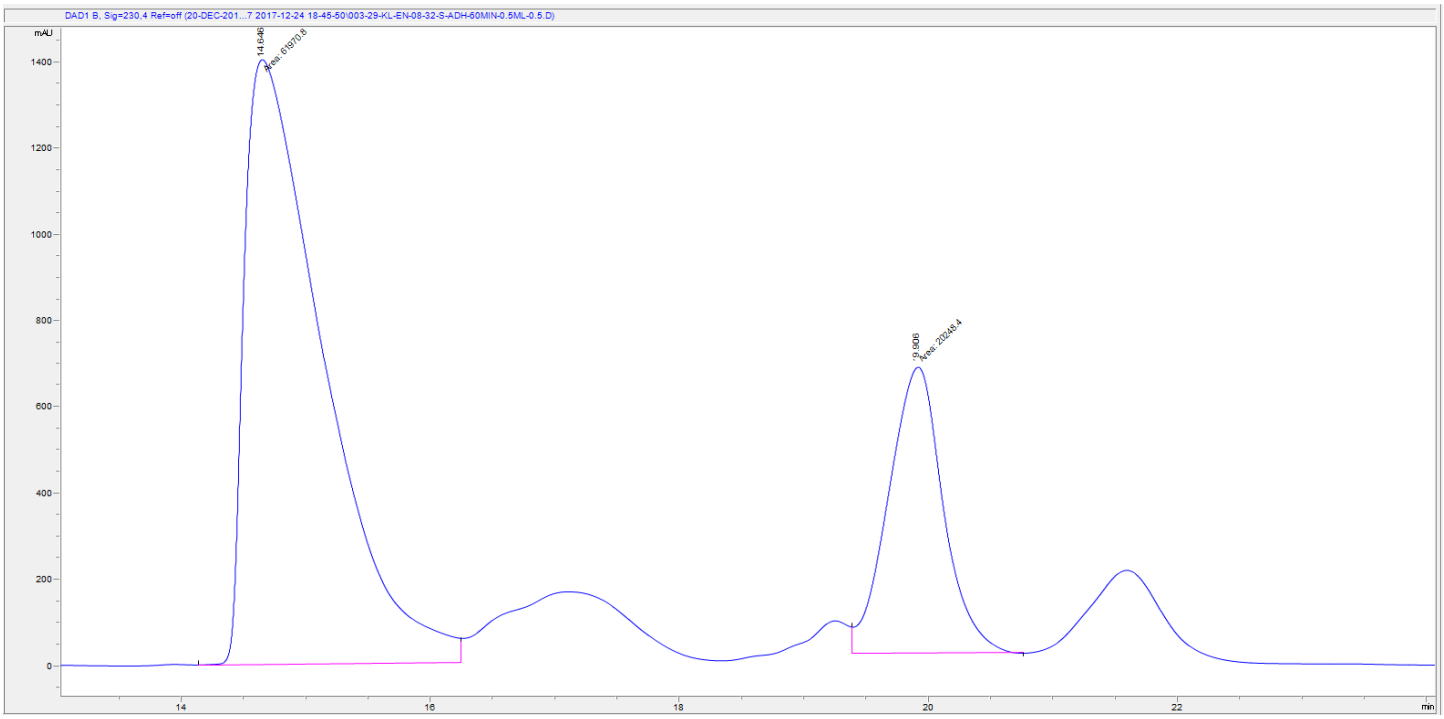


2,2,2-Tribromoethyl (2R,6S)-2-(4-bromophenyl)-6-((tert-butyldimethylsilyl)oxy)heptanoate (**29**).

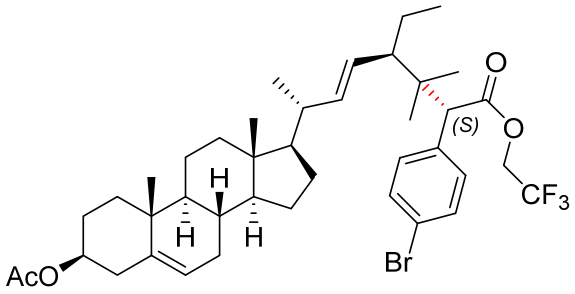


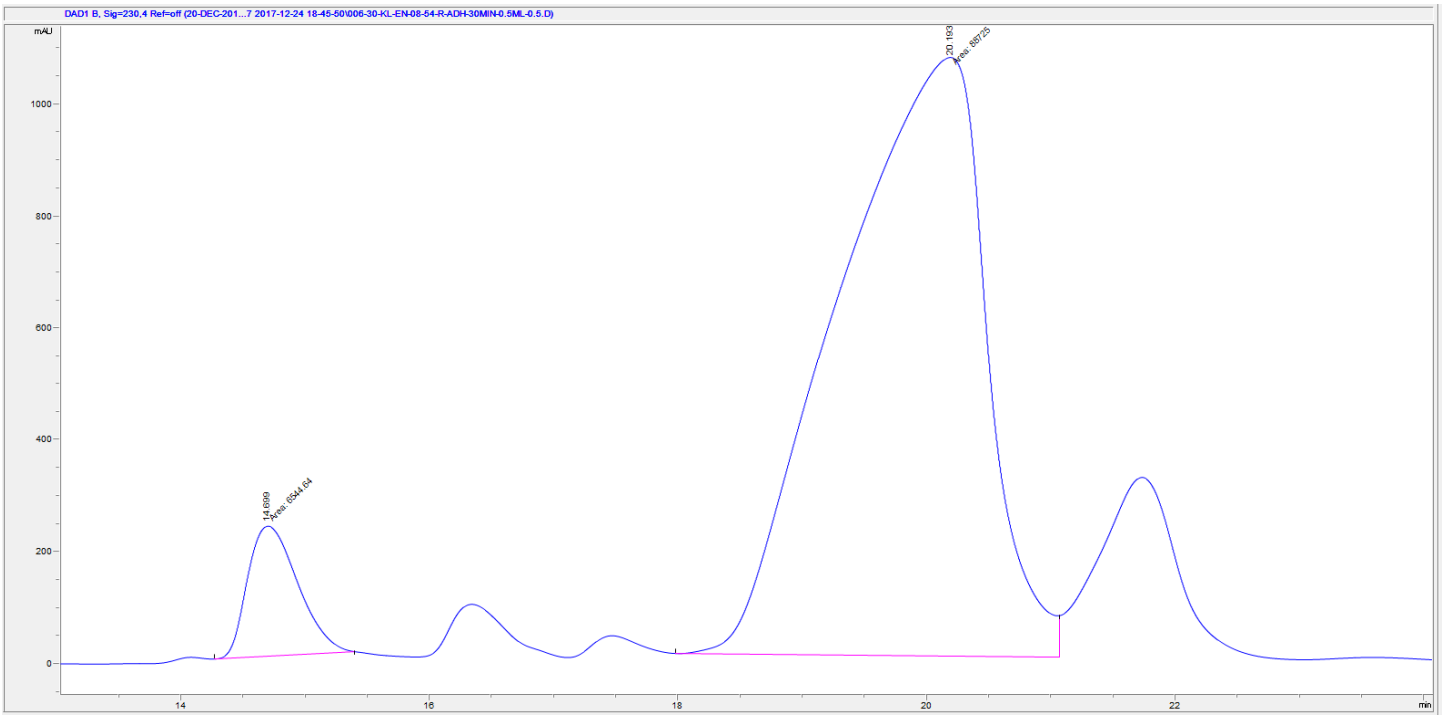
#	Time [Min]	Area% [%]
1	24.95	4.833
2	26.81	95.167
		20:1 d.*r.*.



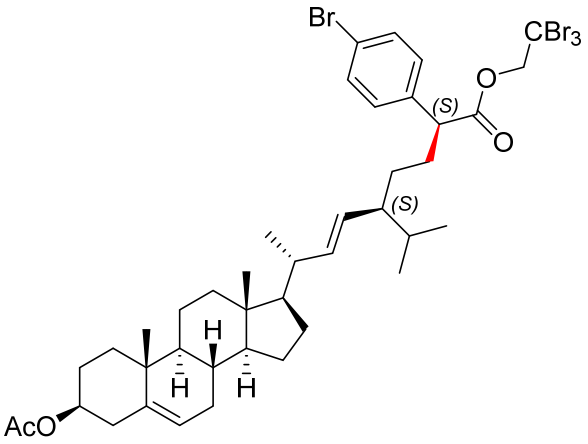


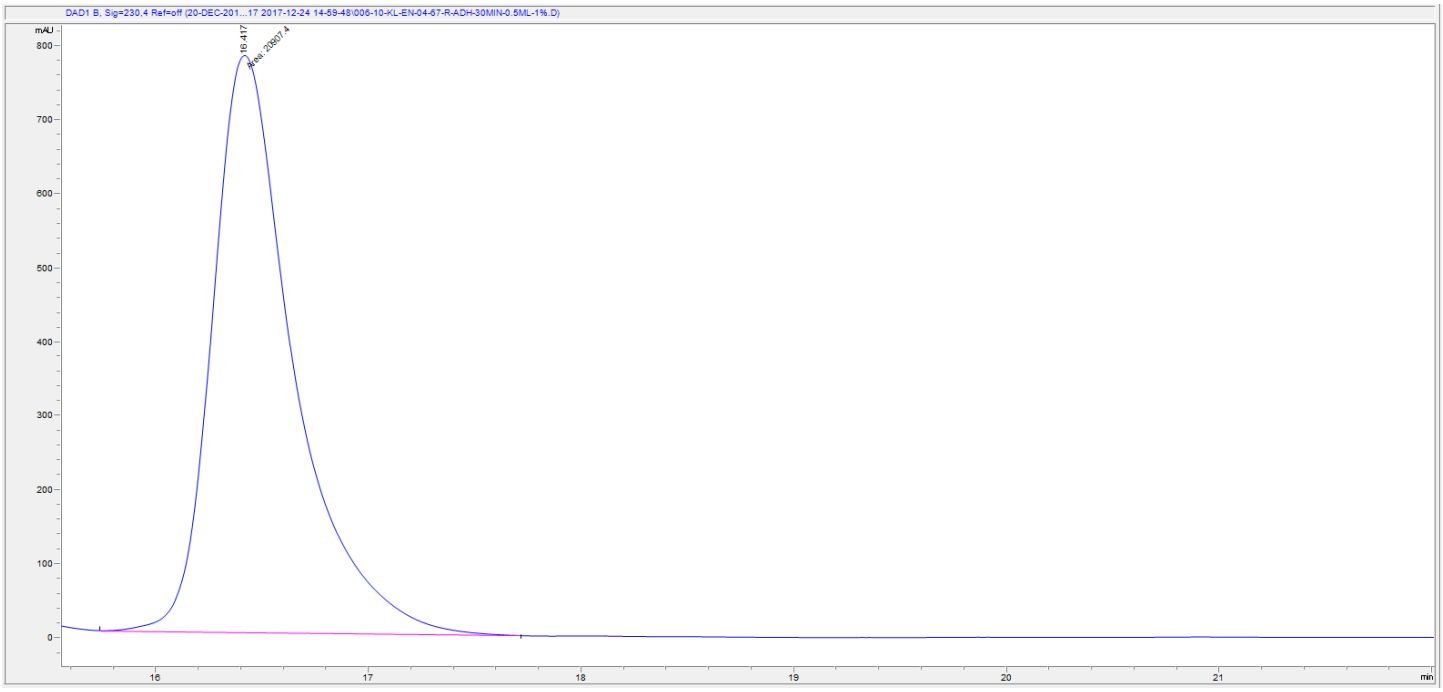
#	Time [Min]	Area% [%]
1	14.646	75.373
2	19.906	24.627
		3:1 d.*r.*.



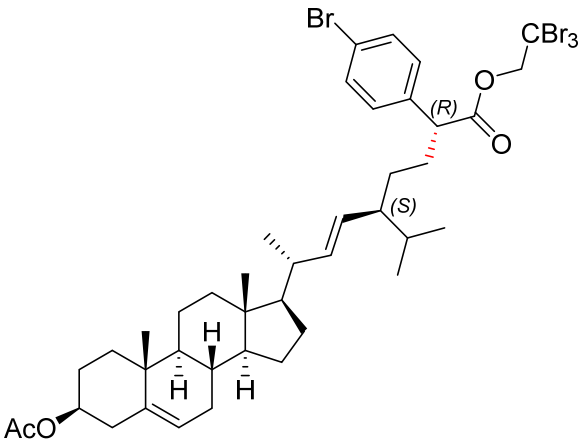


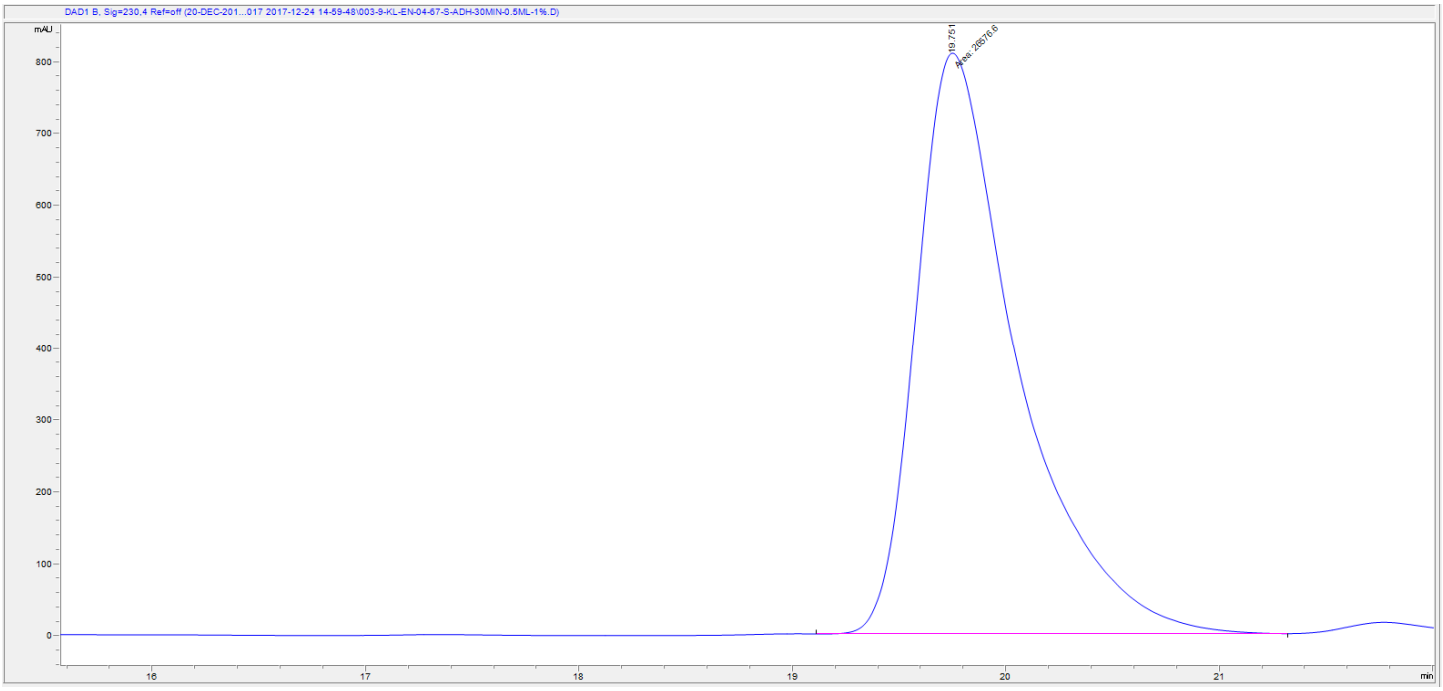
#	Time [Min]	Area% [%]
1	14.699	6.870
2	20.193	93.130
		14:1 d.*r*..





#	Time [Min]	Area% [%]
1	16.417	100
		>100:1 d.*r.*.





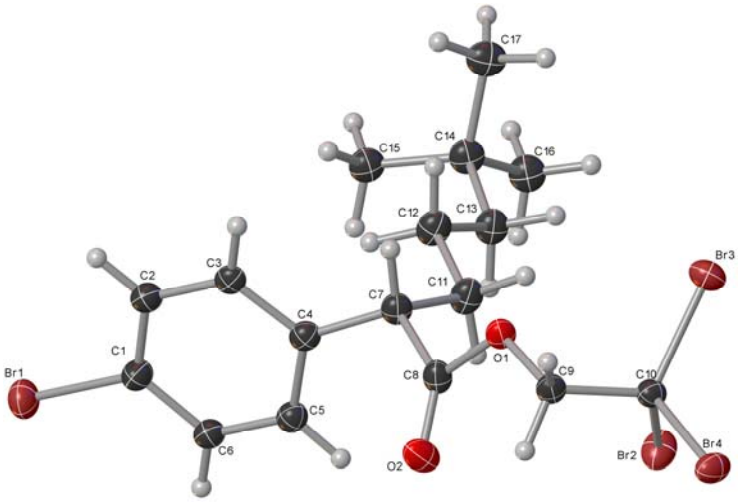
#	Time [Min]	Area% [%]
1	19.751	100
		>100:1 d.*r.*.

11 - X-Ray Crystallographic Data of Product **11**

Submitted by: **Kuangbiao Liao**
Davies Group, Emory University
Solved by: **John Bacsa**
Sample ID: **11**
CCDC number: 1551026

EMORY UNIVERSITY | X-ray Crystallography Center

Crystal Data and Experimental



Experimental. Single colourless needle-shaped crystals of (**11**) were recrystallised from hexane by slow evaporation. A suitable crystal (0.46×0.08×0.06 mm^3) was selected and mounted on a loop with paratone oil on a Bruker D8 Venture diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the **XT** (Sheldrick, 2015) structure solution program using the Intrinsic Phasing solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2014/7 of **XL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{17}H_{22}Br_4O_2$, M_r = 577.98, monoclinic, $P2_1$ (No. 4), a = 12.3961(10) Å, b = 5.9063(5) Å, c = 14.7231(11) Å, β = 110.981(4)°, $\alpha = \gamma = 90°$, V = 1006.48(14) Å^3, T = 100(2) K, Z = 2, Z' = 1, μ(CuK_α) = 9.807 mm^{-1}, 5488 reflections measured, 3186 unique (R_{int} = 0.0390) which were used in all calculations. The final wR_2 was 0.1304 (all data) and R_1 was 0.0512 (I > 2σ(I)).

Compound	**11**
Formula	$C_{17}H_{22}Br_4O_2$
$D_{calc.}$/ g cm^{-3}	1.907
μ/mm^{-1}	9.807
Formula Weight	577.98
Colour	colourless
Shape	needle
Size/mm^3	0.46×0.08×0.06
T/K	100(2)
Crystal System	monoclinic
Flack Parameter	0.18(8)
Hooft Parameter	0.24(3)
Space Group	$P2_1$
a/Å	12.3961(10)
b/Å	5.9063(5)
c/Å	14.7231(11)
α/°	90
β/°	110.981(4)
γ/°	90
V/Å^3	1006.48(14)
Z	2
Z'	1
Wavelength/Å	1.541840
Radiation type	CuK_α
Θ_{min}/°	3.215
Θ_{max}/°	70.313
Measured Refl.	5488
Independent Refl.	3186
Reflections with I > 2σ(I)	2871
R_{int}	0.0390
Parameters	212
Restraints	145
Largest Peak	1.366
Deepest Hole	-0.973
GooF	1.048
wR_2 (all data)	0.1304
wR_2	0.1216
R_1 (all data)	0.0630
R_1	0.0512

Structure Quality Indicators

Reflections: d min (Cu) 0.82 | I/σ 14.3 | Rint 3.90%

Refinement: Shift 0.000 | Max Peak 1.4 | Min Peak -1.0 | GooF 1.048

A colourless needle-shaped crystal with dimensions 0.46×0.08×0.06 mm^3 was mounted on a loop with paratone oil. Data were collected using a 'Bruker D8 Venture diffractometer equipped with a Oxford Cryosystems low-temperature device, operating at T = 100(2) K.

Data were measured using ϕ and ω scans with a narrow frame width of 0.50° per frame for 10.00 s using CuK_α radiation (microfocus sealed tube, 50 kV, 1 mA).The total number of runs and images was based on the strategy calculation from the program **APEX3** (Bruker). The maximum resolution that was achieved was Θ = 70.313°.

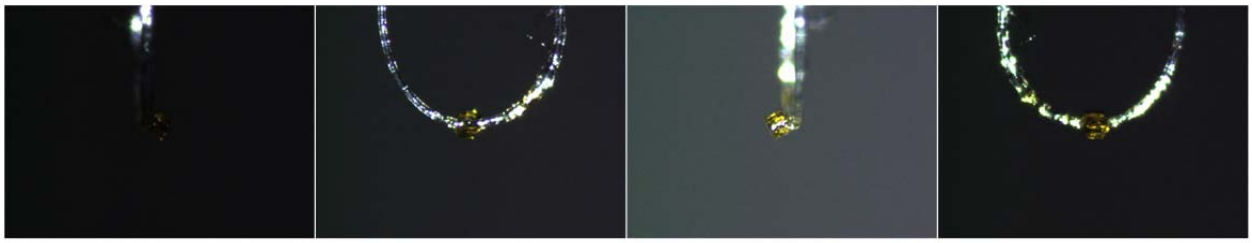
The diffraction patterns were indexed using **APEX3** (Bruker) and the unit cells were refined using SAINT (Bruker, V8.37A, 2015) on 8987 reflections. Data reduction, scaling and absorption corrections were performed using SAINT (Bruker, V8.37A, 2015) and SADABS-2016/2 (Bruker, 2016). The final completeness is 97.7% out to 70.313° in Θ. The absorption coefficient μ of this material is 9.807 mm^{-1} at this wavelength (λ = 1.54178 Å) and the minimum and maximum transmissions are 0.4475 and 0.7533.

The structure was solved and the space group $P2_1$ (# 4) determined by the XT (Sheldrick, 2015) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2014/7 of **XL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

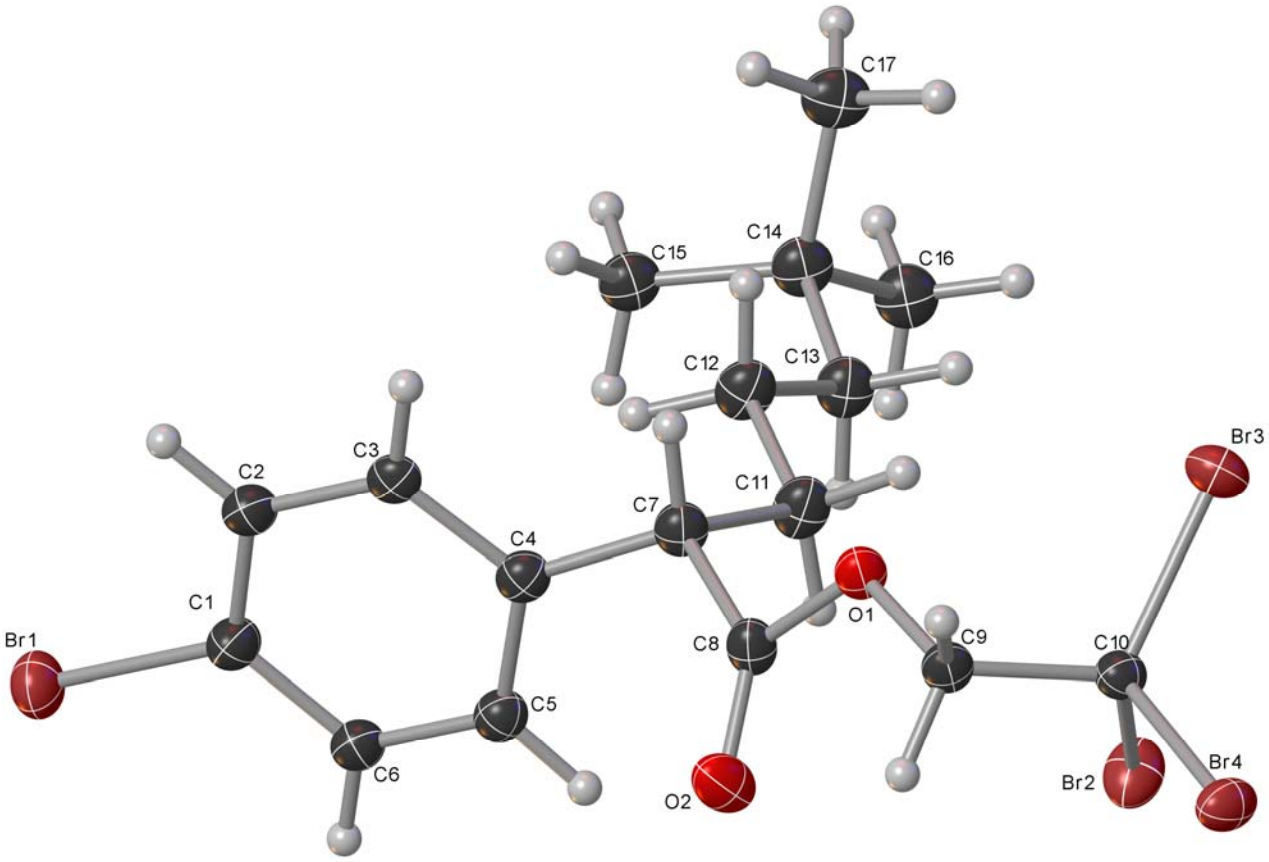
There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 2 and Z' is 1.

The Flack parameter was refined to 0.18(8). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in 0.24(3). Note: The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

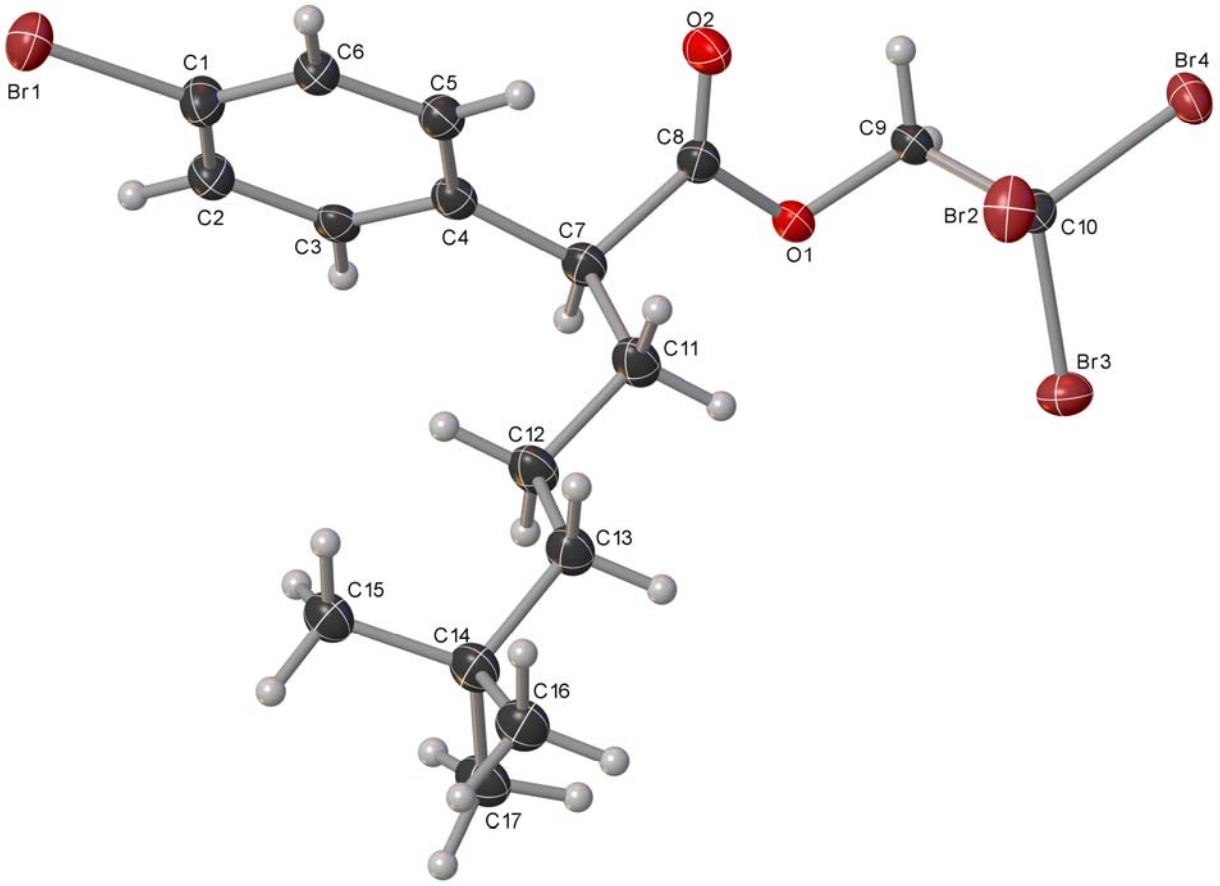
Images of the Crystal on the Diffractometer



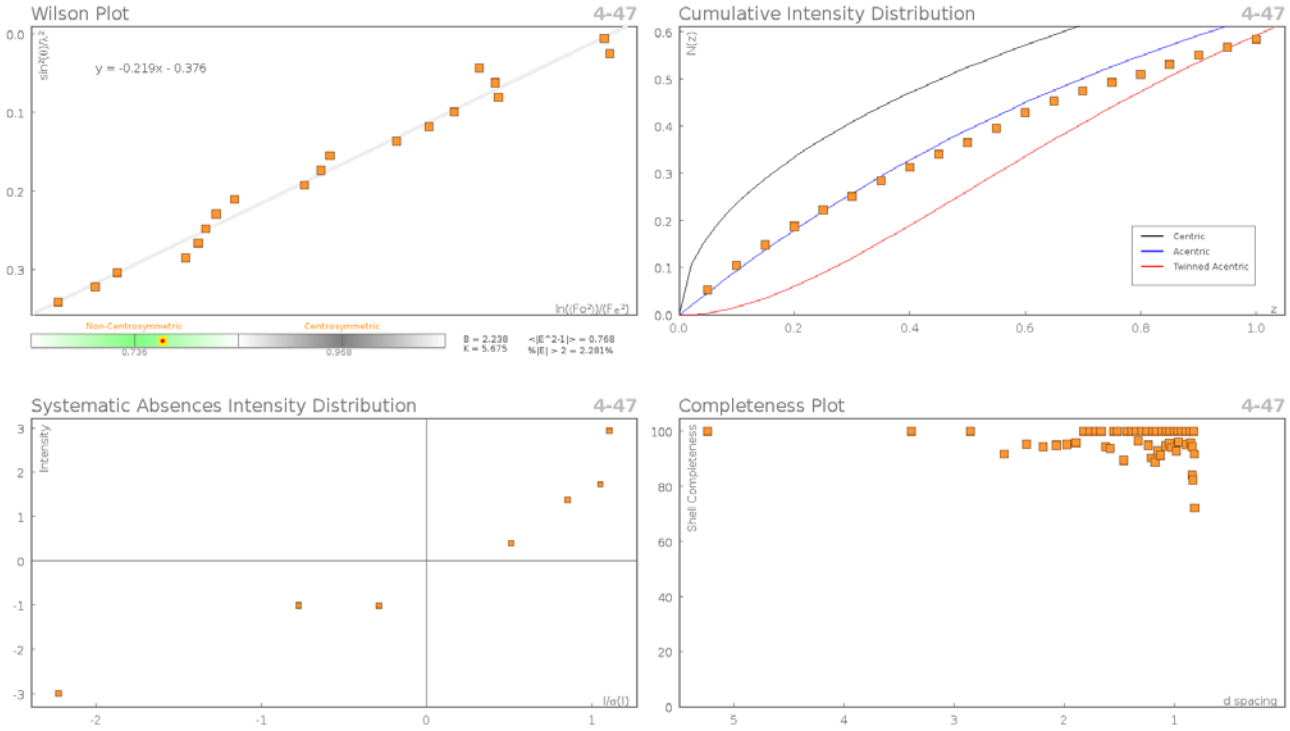
Supplementary Figure 3:

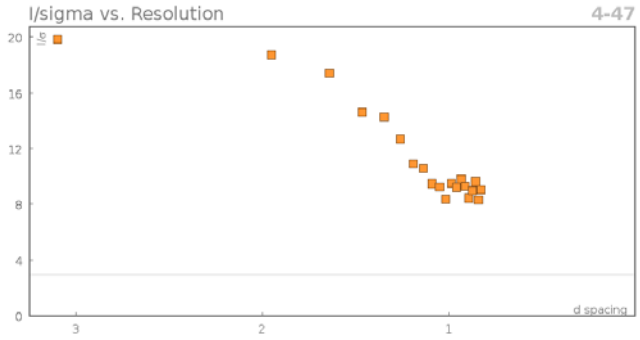


Supplementary Figure 4:

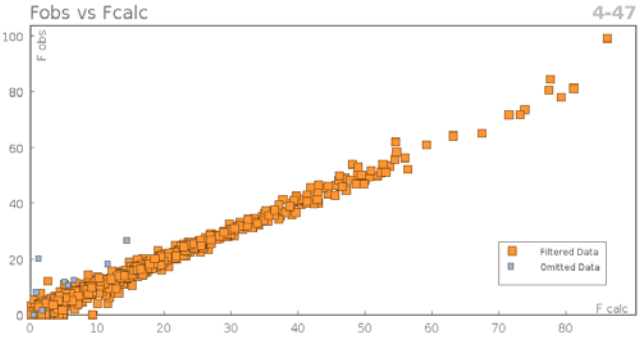


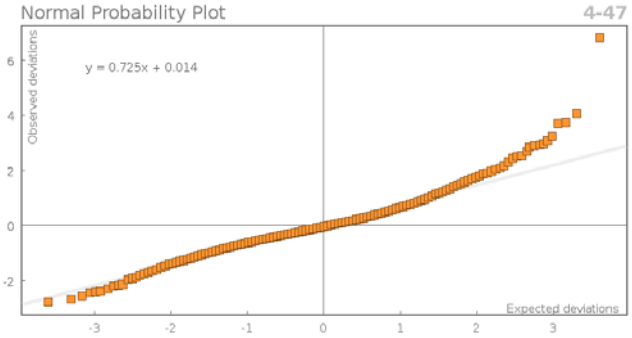
Data Plots: Diffraction Data





Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	5510	Unique reflections	3186
Completeness	0.831	Mean I/σ	14.29
hkl_{max} collected	(15, 7, 17)	hkl_{min} collected	(-15, -7, -14)
hkl_{max} used	(14, 7, 17)	hkl_{min} used	(-15, -7, 0)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.77
d_{max} used	13.75	d_{min} used	0.82
Friedel pairs	765	Friedel pairs merged	0
Inconsistent equivalents	10	R_{int}	0.039
R_{sigma}	0.0571	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	15
Multiplicity	(2347, 1330, 154, 9, 1)	Maximum multiplicity	5
Removed systematic absences	7	Filtered off (Shel/OMIT)	0

Supplementary Table 4: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **11**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Br3	3984.8(10)	-678(2)	4758.1(9)	27.1(3)
Br4	1697.8(11)	-719(2)	2882.2(8)	26.7(3)
Br1	12.6(12)	9973(2)	9050.1(10)	31.5(4)
Br2	2662.0(13)	3883(2)	3988.5(10)	30.7(3)
O2	808(7)	3900(20)	5343(6)	30.7(19)
O1	2199(7)	1231(16)	5674(6)	21.6(15)
C3	1691(9)	4720(20)	8263(8)	19.8(19)
C9	1682(10)	280(20)	4727(8)	21(2)
C7	2409(10)	3990(20)	6901(8)	22.3(18)
C4	1722(10)	5320(20)	7360(8)	21(2)
C11	3426(11)	5360(30)	6792(9)	27(3)
C15	5392(11)	9950(20)	9245(9)	27(2)
C10	2486(11)	690(20)	4146(8)	20.5(14)
C16	6699(12)	10740(30)	8323(10)	29(2)
C1	678(12)	8070(30)	8350(9)	27(2)
C6	673(10)	8700(20)	7449(8)	24(2)
C12	4224(12)	6250(20)	7756(9)	27(3)
C5	1171(11)	7380(20)	6944(9)	23(2)
C8	1666(11)	3060(20)	5885(9)	22(2)
C13	5097(11)	7940(20)	7653(9)	26(2)
C14	5993(11)	8910(30)	8597(8)	26.6(17)
C17	6826(12)	6950(30)	9154(10)	30(2)
C2	1177(11)	6060(20)	8764(9)	25(2)

Supplementary Table 5: Anisotropic Displacement Parameters ($\times 10^4$) **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br3	20.6(6)	26.6(8)	31.0(6)	0.7(6)	5.4(5)	2.2(6)
Br4	32.4(7)	25.3(7)	19.3(5)	-2.1(5)	5.5(5)	5.1(6)
Br1	35.1(8)	32.1(9)	32.0(7)	-2.5(6)	17.8(6)	3.4(6)
Br2	45.3(8)	17.8(7)	34.3(6)	2.2(6)	20.7(6)	-0.4(6)
O2	26(3)	36(5)	25(3)	-10(3)	3(2)	5(3)
O1	19(3)	26(3)	18(2)	-4(2)	4(2)	-2(2)
C3	15(4)	22(3)	19(3)	-2(3)	3(3)	-5(3)
C9	18(4)	25(5)	17(3)	-3(3)	4(3)	-2(3)
C7	21(3)	24(4)	21(3)	-4(3)	6(2)	-3(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C4	20(4)	22(4)	20(3)	-2(3)	5(3)	-3(3)
C11	25(4)	32(6)	23(4)	-5(3)	8(3)	-9(4)
C15	28(4)	26(5)	24(4)	-4(3)	7(3)	-3(4)
C10	21(3)	20(2)	20(2)	-0.4(17)	6.4(18)	2.4(18)
C16	28(4)	28(4)	30(4)	-5(3)	9(4)	-5(3)
C1	30(6)	29(3)	22(3)	2(3)	10(3)	6(4)
C6	23(5)	26(4)	20(3)	0(3)	6(3)	1(3)
C12	25(4)	30(5)	23(4)	-4(3)	6(3)	-8(4)
C5	22(5)	24(4)	21(3)	0(3)	7(3)	-1(3)
C8	19(3)	27(4)	22(3)	-5(2)	8(2)	-3(3)
C13	25(3)	27(4)	25(3)	-5(3)	8(3)	-6(3)
C14	26(3)	26(4)	25(3)	-5(3)	6(3)	-5(3)
C17	30(4)	26(4)	28(4)	-6(3)	4(3)	-3(3)
C2	25(5)	28(3)	21(3)	1(3)	7(3)	3(3)

Supplementary Table 6: Bond Lengths in Å for **11**.

Atom	Atom	Length/Å
Br3	C10	1.928(12)
Br4	C10	1.951(12)
Br1	C1	1.902(13)
Br2	C10	1.924(13)
O2	C8	1.185(16)
O1	C9	1.427(13)
O1	C8	1.360(15)
C3	C4	1.389(15)
C3	C2	1.383(17)
C9	C10	1.546(15)
C7	C4	1.486(16)
C7	C11	1.554(17)
C7	C8	1.550(16)
C4	C5	1.421(19)
C11	C12	1.504(17)
C15	C14	1.531(17)
C16	C14	1.531(19)
C1	C6	1.377(16)
C1	C2	1.38(2)
C6	C5	1.369(16)
C12	C13	1.519(18)
C13	C14	1.548(17)
C14	C17	1.57(2)

Supplementary Table 7: Bond Angles in ° for **11**.

Atom	Atom	Atom	Angle/°
C8	O1	C9	116.9(9)
C2	C3	C4	122.7(12)
O1	C9	C10	109.0(9)
C4	C7	C11	113.1(11)
C4	C7	C8	112.8(10)
C8	C7	C11	107.9(9)
C3	C4	C7	121.1(12)
C3	C4	C5	117.2(11)

Atom	Atom	Atom	Angle/°
C5	C4	C7	121.4(10)
C12	C11	C7	111.5(10)
Br3	C10	Br4	109.7(6)
Br2	C10	Br3	109.5(6)
Br2	C10	Br4	110.0(6)
C9	C10	Br3	112.3(8)
C9	C10	Br4	105.0(8)
C9	C10	Br2	110.1(8)
C6	C1	Br1	120.5(11)
C2	C1	Br1	118.9(9)
C2	C1	C6	120.6(12)
C5	C6	C1	121.3(13)
C11	C12	C13	112.7(11)
C6	C5	C4	119.8(11)
O2	C8	O1	124.9(11)
O2	C8	C7	125.5(12)
O1	C8	C7	109.4(10)
C12	C13	C14	117.6(11)
C15	C14	C16	109.5(12)
C15	C14	C13	110.8(10)
C15	C14	C17	110.1(10)
C16	C14	C13	108.7(10)
C16	C14	C17	109.1(11)
C13	C14	C17	108.6(12)
C1	C2	C3	118.5(12)

Supplementary Table 8: Torsion Angles in ° for **11**.

Atom	Atom	Atom	Atom	Angle/°
Br1	C1	C6	C5	178.5(10)
Br1	C1	C2	C3	-177.9(9)
O1	C9	C10	Br3	60.1(12)
O1	C9	C10	Br4	179.3(8)
O1	C9	C10	Br2	-62.3(11)
C3	C4	C5	C6	2.0(18)
C9	O1	C8	O2	0.4(18)
C9	O1	C8	C7	-174.7(9)
C7	C4	C5	C6	-171.5(11)
C7	C11	C12	C13	-169.6(12)
C4	C3	C2	C1	0(2)
C4	C7	C11	C12	56.9(15)
C4	C7	C8	O2	28.1(18)
C4	C7	C8	O1	-156.7(11)
C11	C7	C4	C3	-114.8(13)
C11	C7	C4	C5	58.5(15)
C11	C7	C8	O2	-97.5(15)
C11	C7	C8	O1	77.7(13)
C11	C12	C13	C14	-178.0(12)
C1	C6	C5	C4	-1.0(19)
C6	C1	C2	C3	1(2)
C12	C13	C14	C15	-53.8(17)
C12	C13	C14	C16	-174.2(12)
C12	C13	C14	C17	67.2(15)
C8	O1	C9	C10	112.0(11)
C8	C7	C4	C3	122.5(13)
C8	C7	C4	C5	-64.2(15)
C8	C7	C11	C12	-177.7(12)

Atom	Atom	Atom	Atom	Angle/°
C2	C3	C4	C7	172.1(11)
C2	C3	C4	C5	-1.4(18)
C2	C1	C6	C5	-1(2)

Supplementary Table 9: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **11**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H3	2039	3333	8549	24
H9A	921	988	4387	25
H9B	1563	-1369	4778	25
H7	2745	2664	7331	27
H11A	3867	4372	6506	32
H11B	3115	6642	6342	32
H15A	5972	10622	9822	40
H15B	4972	8759	9446	40
H15C	4848	11115	8881	40
H16A	6179	11928	7944	44
H16B	7112	10064	7934	44
H16C	7257	11401	8916	44
H6	317	10089	7171	28
H12A	4641	4962	8162	32
H12B	3759	6987	8096	32
H5	1148	7829	6319	27
H13A	4665	9219	7255	31
H13B	5525	7194	7281	31
H17A	7511	7597	9653	45
H17B	7062	6068	8692	45
H17C	6423	5960	9463	45
H2	1168	5598	9380	30

Citations

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O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

SAINT-8.37A-2015 - Software for the Integration of CCD Detector System Bruker Analytical X-ray Systems, Bruker axs, Madison, WI (2015).

Sheldrick, G.M., A short history of ShelX, *Acta Cryst.*, (2008), **A64**, 339-341.

#==========

Bond precision: C-C = 0.0183 A Wavelength=1.54178

Cell: a=12.3961(10) b=5.9063(5) c=14.7231(11)
alpha=90 beta=110.981(4) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1006.48(14)	1006.48(14)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C17 H22 Br4 O2	C17 H22 Br4 O2
Sum formula	C17 H22 Br4 O2	C17 H22 Br4 O2
Mr	577.95	577.98
Dx,g cm-3	1.907	1.907
Z	2	2
Mu (mm-1)	9.807	9.807
F000	560.0	560.0
F000'	555.42	
h,k,lmax	15,7,17	15,7,17
Nref	3833[2115]	3186
Tmin,Tmax	0.428,0.555	0.447,0.753
Tmin'	0.009	

Correction method= # Reported T Limits: Tmin=0.447 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.51/0.83 Theta(max)= 70.313

R(reflections)= 0.0512(2871) wR2(reflections)= 0.1304(3186)

S = 1.048 Npar= 212

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01831 Ang.
Author Response: We collected data on a copper source. The data is 97% complete to 0.85 A (130 degrees in 2theta, d=0.85 A). The data to parameter ratio is somewhat low resulting in somewhat large esd's for the carbon atoms in the presence of Br atoms but the R-indices, GOOF value and the thermal parameters are good and indicate a well refined structure.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.977 Why?
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 47 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 66 %
PLAT977_ALERT_2_C Check Negative Difference Density on H13A -0.34 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 23 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.78 Why ?
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 6 Report
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br2 ..Br4 3.59 Ang.

PLAT791_ALERT_4_G	Model has Chirality at C7 (Chiral SPGR) S Verify
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints ..... 145 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600 9 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ... 13 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

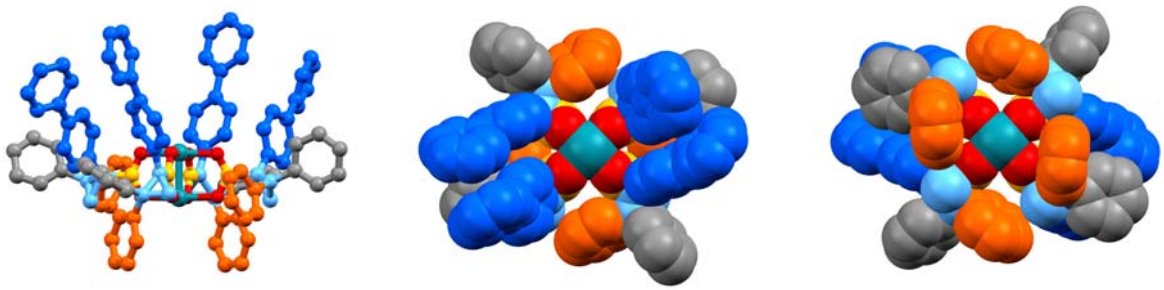
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 23/04/2018;
#==========

12 - X-Ray Crystallographic Data of **Catalyst D [Rh_2(*R*-*p*-PhTPCP)$_4$]**

The X-Ray Crystallographic Data of **Catalyst D [Rh_2(*R*-*p*-PhTPCP)$_4$]** was reported previously,[6] below is the side, top and bottom view of the structure.



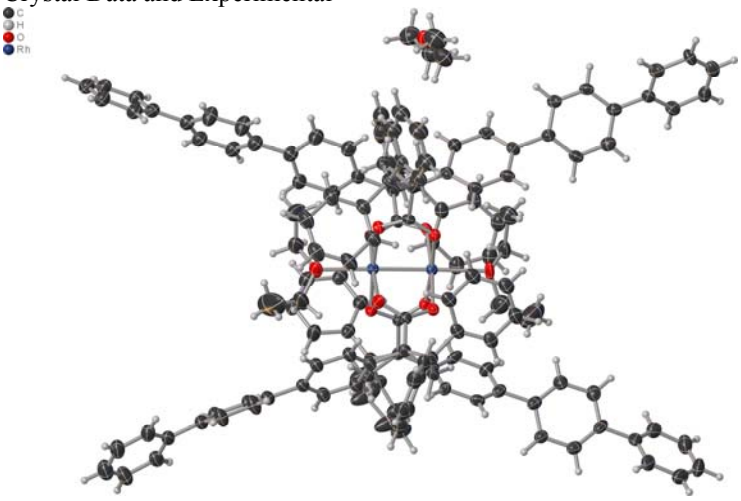
Supplementary Figure 5. Side, top and bottom view of the Catalyst D [Rh_2(*R*-*p*-PhTPCP)$_4$]

13 - X-Ray Crystallographic Data of **Catalyst F [Rh_2(*R*-*p*-$PhC_6H_4TPCP)_4$]**

Submitted by: **Kuangbiao Liao**
Davies Group, Emory University
Solved by: **John Bacsa**
Sample ID: **Rh_2(*R*-*p*-$PhC_6H_4TPCP)_4$**
CCDC number: 1552206

EMORY UNIVERSITY | X-ray Crystallography Center

Crystal Data and Experimental



Experimental. Single light green plate-shaped crystals of (**Rh_2(*R*-*p*-$PhC_6H_4TPCP)_4$**) were The crystal was chosen from the sample as supplied.. A suitable crystal (0.10×0.05×0.02 mm^3) was selected and mounted on a loop with paratone oil on an Bruker D8 VENTURE diffractometer diffractometer. The crystal was cooled to T = 100(2) K during data collection. The structure was solved with the XT (Sheldrick, 2015) structure solution program using the Intrinsic Phasing solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2014/7 of **XL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{148}H_{130}O_{11}Rh_2$, M_r = 2290.33, trigonal, $P3_1$ (No. 144), a = 14.66084(10) Å, b = 14.66084(10) Å, c = 48.6185(3) Å, α = 90.0°, β = 90.0°, γ = 120.0°, V = 9050.03(11) $Å^3$, T = 100(2) K, Z = 3, Z' = 1, $\mu(CuK_\alpha)$ = 2.696 mm^{-1}, 67340 reflections measured, 21512 unique (R_{int} = 0.0743) which were used in all calculations. The final wR_2 was 0.1472 (all data) and R_1 was 0.0565 (I > 2σ(I)).

Compound	**$Rh_2[R\text{-}p\text{-}PhC_6H_4TPCP]_4$**
Formula	$C_{148}H_{130}O_{11}Rh_2$
$D_{calc.}$/ g cm^{-3}	1.261
μ/mm^{-1}	2.696
Formula Weight	2290.33
Colour	light green
Shape	plate
Size/mm^3	0.10×0.05×0.02
T/K	100(2)
Crystal System	trigonal
Flack Parameter	-0.034(6)
Hooft Parameter	-0.017(5)
Space Group	$P3_1$
a/Å	14.66084(10)
b/Å	14.66084(10)
c/Å	48.6185(3)
α/°	90.0
β/°	90.0
γ/°	120.0
V/Å^3	9050.03(11)
Z	3
Z'	1
Wavelength/Å	1.541840
Radiation type	CuK_α
Θ_{min}/°	1.817
Θ_{max}/°	67.078
Measured Refl.	67340
Independent Refl.	21512
Reflections with I > 2σ(I)	19805
R_{int}	0.0743
Parameters	1457
Restraints	877
Largest Peak	1.140
Deepest Hole	-0.682
GooF	1.012
wR_2 (all data)	0.1465
wR_2	0.1416
R_1 (all data)	0.0620
R_1	0.0564

Structure Quality Indicators

Reflections:	d min (Cu) 0.84	I/σ 8.0	Rint 7.43%	complete at 2θ=134° 100%	
Refinement:	Shift -0.005	Max Peak 1.1	Min Peak -0.7	GooF 1.019	-0.034(6)

A light green plate-shaped crystal with dimensions 0.10×0.05×0.02 mm^3 was mounted on a loop with paratone oil. Data were collected using a Bruker D8 VENTURE diffractometer diffractometer equipped with a Oxford Cryosystems low-temperature device, operating at T = 100(2) K.

Data were measured using ϕ and ω scans with a narrow frame width of 0.5° per frame for 5.0 s using CuK_α radiation (microfocus sealed tube, 50 kV, 1 mA).The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker). The maximum resolution that was achieved was Θ = 67.078°.

The diffraction patterns were indexed using CrysAlisPro (Agilent) and the unit cells were refined using CrysAlisPro (Agilent) on 18119 reflections, 27 % of the observed reflections. Data reduction, scaling and absorption corrections were performed using CrysAlisPro (Agilent) and CrysAlisPro 1.171.39.9g (Rigaku Oxford Diffraction, 2015)Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.. The final completeness is 100.00 out to 67.078° in Θ. The absorption coefficient μ of this material is 2.696 at this wavelength (λ = 1.54184) and the minimum and maximum transmissions are 0.81432 and 1.00000.

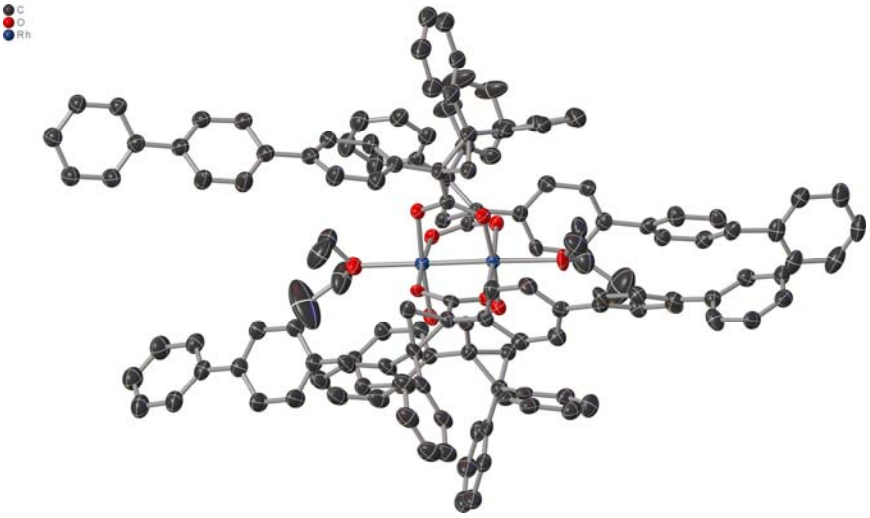
The structure was solved and the space group $P3_1$ (# 144) determined by the XT (Sheldrick, 2015) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2014/7 of **XL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

_refine_special_details: Refined as a 2-component twin.

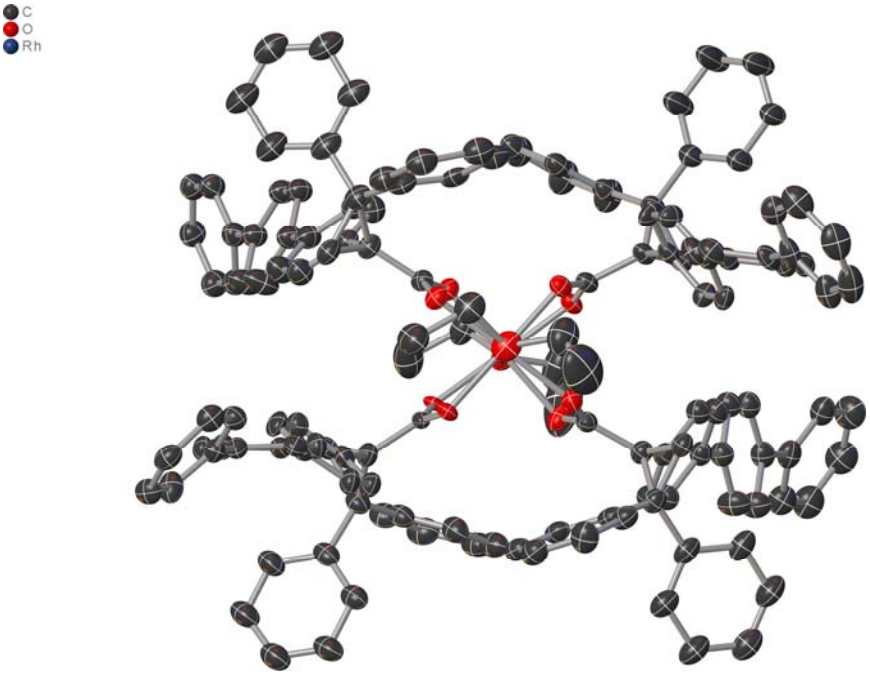
There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 3 and Z' is 1.

The Flack parameter was refined to -0.034(6). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in -0.017(5). Note: The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

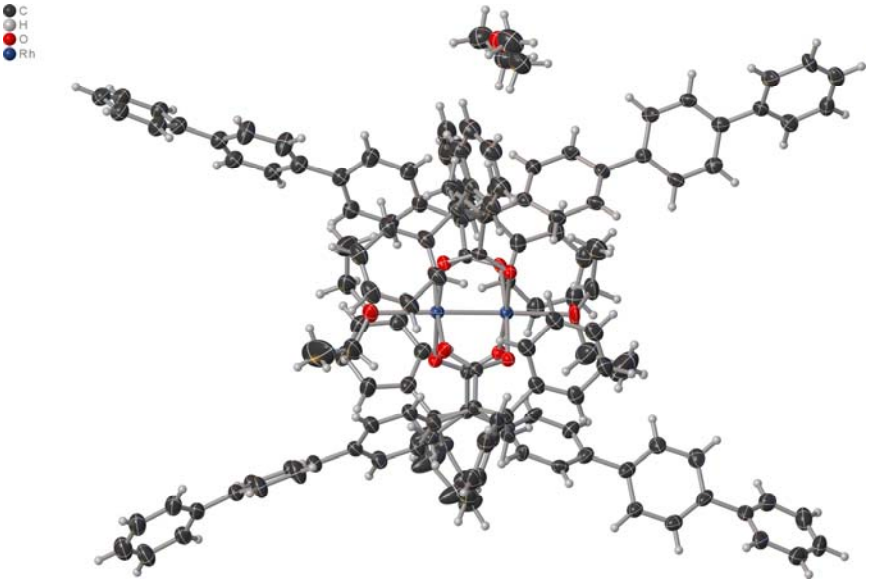
Supplementary Figure 6:



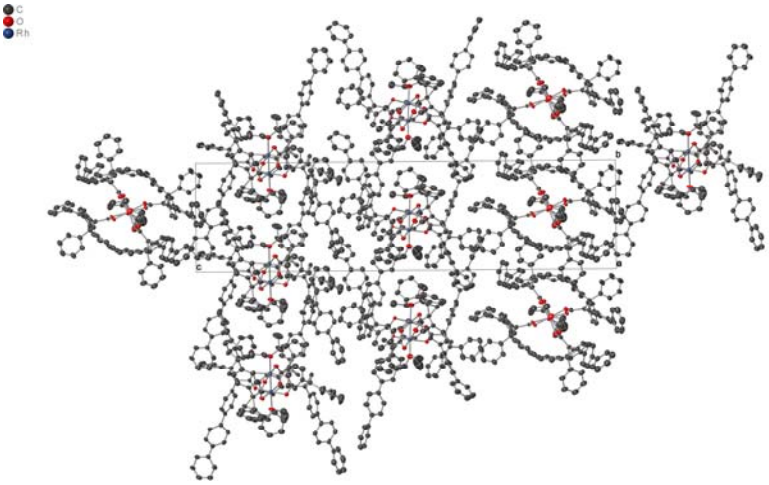
Supplementary Figure 7:



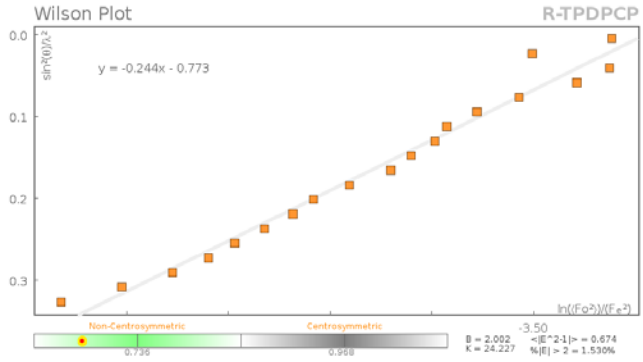
Supplementary Figure 8:

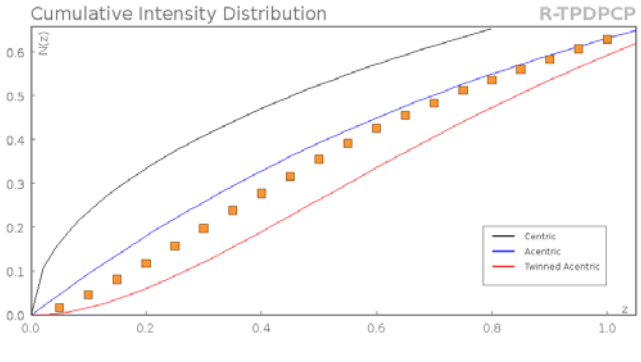


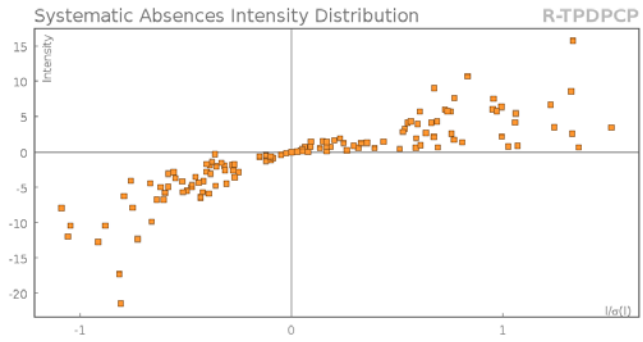
Supplementary Figure 9:

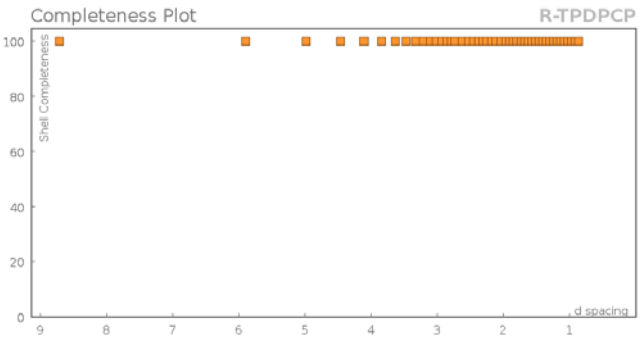


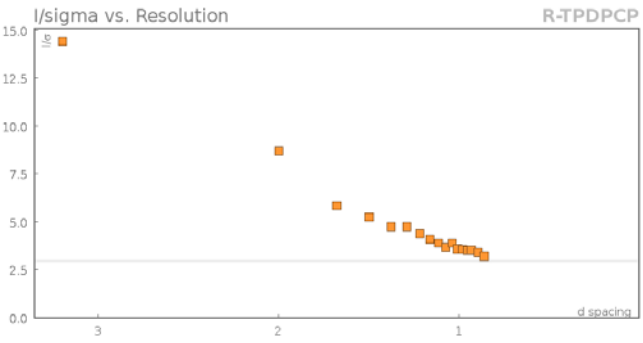
Data Plots: Diffraction Data



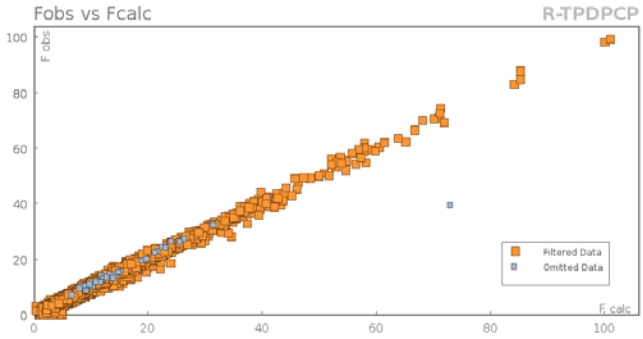


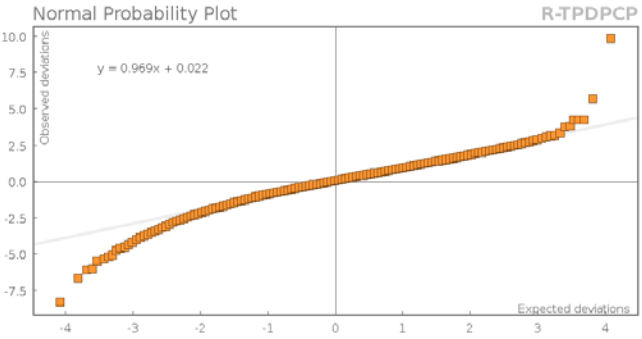






Data Plots: Refinement and Data





Reflection Statistics

Total reflections (after filtering)	67519	Unique reflections	21512
Completeness	0.997	Mean I/σ	8.04
hkl_{max} collected	(16, 17, 58)	hkl_{min} collected	(-17, -17, -58)
hkl_{max} used	(8, 17, 57)	hkl_{min} used	(-17, 0, -57)
Lim d_{max} collected	100.0	Lim d_{min} collected	0.77
d_{max} used	24.31	d_{min} used	0.84
Friedel pairs	17646	Friedel pairs merged	0
Inconsistent equivalents	3	R_{int}	0.0743
R_{sigma}	0.0977	Intensity transformed	0
Omitted reflections	0	Omitted by user (OMIT hkl)	179
Multiplicity	(28168, 14615, 3166, 137, 15)	Maximum multiplicity	10
Removed systematic absences	135	Filtered off (Shel/OMIT)	0

Supplementary Table 10: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Rh_2[*R*-*p*-PhC_6H_4TPCP]$_4$**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
Rh1	4427.0(5)	3708.1(5)	4929.1(2)	24.36(15)
Rh2	4350.7(6)	5287.2(6)	4914.8(2)	24.78(15)
O2	5726(5)	5948(5)	4695.6(12)	30.6(13)
O3	5941(6)	4555(6)	4788.7(13)	31.0(13)
O4	5069(5)	5670(5)	5285.6(11)	26.7(13)
O5	4831(5)	4032(5)	5331.9(11)	23.8(13)
O6	2983(5)	4515(5)	5131.7(13)	31.0(13)
O7	2920(5)	2952(5)	5062.8(12)	30.0(13)
O8	3640(5)	4826(5)	4543.4(12)	27.9(13)
O9	4023(5)	3514(5)	4523.2(11)	26.7(12)
O1	4313(6)	6844(6)	4894.9(15)	43.5(16)
O10	4526(6)	2193(6)	4935.8(14)	42.4(17)
C7	8043(8)	6958(8)	4501.3(19)	32.9(15)
C5	6190(7)	5419(8)	4668.7(16)	27.5(15)
C6	7097(8)	5799(8)	4471.3(18)	30.5(16)
C8	7261(8)	6676(8)	4273.3(18)	33.0(18)
C9	8001(8)	7628(8)	4731(2)	32.5(17)
C10	7917(8)	7323(9)	5002(2)	38(2)
C11	7979(9)	8009(10)	5211(2)	44(2)
C12	8130(10)	8982(10)	5145(2)	47(2)
C13	8194(10)	9289(10)	4877(3)	50(3)
C14	8132(9)	8612(9)	4669(2)	40(2)
C15	9146(8)	7161(8)	4442(2)	35.9(18)

Atom	x	y	z	U_{eq}
C16	9435(10)	6970(10)	4183(2)	48(2)
C17	10444(10)	7173(10)	4133(3)	55(3)
C18	11206(11)	7578(10)	4338(3)	57(3)
C19	10945(10)	7769(10)	4592(3)	52(2)
C20	9912(9)	7572(9)	4643(2)	41(2)
C21	7305(8)	4956(8)	4374.2(19)	31.4(16)
C22	6784(8)	4364(8)	4140.7(19)	34.4(18)
C23	6902(9)	3529(8)	4057(2)	36.0(19)
C24	7549(8)	3249(8)	4201.3(18)	31.4(16)
C25	8065(8)	3840(8)	4437.2(19)	34.2(18)
C26	7956(8)	4687(8)	4518.1(19)	34.8(19)
C27	7692(8)	2366(8)	4112.1(19)	34.1(17)
C28	6876(9)	1484(9)	3991(2)	38(2)
C29	7004(9)	638(9)	3900(2)	37.2(19)
C30	7978(9)	698(8)	3922.8(19)	34.8(17)
C31	8805(9)	1600(9)	4045(2)	44(2)
C32	8647(9)	2398(9)	4141(2)	44(2)
C33	8162(9)	-127(9)	3804(2)	38.5(19)
C34	8906(10)	-346(9)	3920(2)	44(2)
C35	9132(12)	-1085(10)	3800(3)	57(3)
C36	8565(12)	-1624(11)	3564(3)	62(3)
C37	7839(11)	-1423(10)	3448(3)	55(3)
C38	7624(9)	-678(9)	3570(2)	41(2)
C39	5037(7)	4924(7)	5424.4(16)	23.2(19)
C40	5264(8)	5117(8)	5730.8(18)	29(2)
C42	4867(8)	4130(8)	5904.6(18)	32(2)
C41	6035(8)	4806(8)	5860.5(18)	30.8(17)
C43	6554(8)	4346(8)	5686.1(19)	34.5(18)
C44	6459(9)	3400(9)	5766(2)	43(2)
C45	6999(11)	2993(11)	5614(3)	57(3)
C46	7605(10)	3540(11)	5390(3)	55(2)
C47	7711(10)	4494(11)	5312(2)	48(2)
C48	7180(9)	4900(10)	5460.8(19)	40(2)
C49	6741(9)	5446(9)	6095.5(19)	34.7(18)
C50	7686(9)	6340(9)	6047(2)	39(2)
C51	8414(10)	6871(11)	6253(2)	51(2)
C52	8166(11)	6486(12)	6519(2)	58(3)
C53	7229(11)	5599(13)	6575(2)	57(3)
C54	6511(10)	5073(11)	6364(2)	46(2)
C55	5140(8)	6003(8)	5839.5(17)	29(2)
C56	5818(8)	7051(8)	5770.8(18)	35(2)
C57	5629(8)	7854(9)	5856.5(18)	35(2)
C58	4749(8)	7619(8)	6018.0(17)	32(2)
C59	4087(8)	6584(9)	6090.0(19)	34(2)
C60	4269(8)	5793(9)	6000.8(19)	35(2)
C61	4542(8)	8468(8)	6112.6(19)	33(2)
C62	4758(9)	9328(9)	5947.1(18)	36(2)
C63	4609(9)	10147(9)	6042.2(19)	36(2)
C64	4243(8)	10119(9)	6312.7(19)	33(2)
C65	4012(8)	9254(9)	6471.2(19)	34(2)
C66	4138(8)	8427(9)	6376.9(19)	35(2)
C67	4138(8)	11001(9)	6420.7(19)	34(2)
C68	3684(8)	11473(8)	6272(2)	37(2)
C69	3560(9)	12270(9)	6380(2)	40(2)
C70	3934(9)	12655(9)	6643(2)	43(3)
C71	4411(9)	12219(9)	6794(2)	40(2)
C72	4507(9)	11392(9)	6688(2)	38(2)

Atom	x	y	z	U_{eq}
C73	2573(8)	3524(8)	5164.6(17)	28.4(15)
C74	1612(8)	2970(8)	5347.4(19)	33.1(16)
C76	1433(8)	3652(9)	5544.7(19)	35.9(19)
C75	682(9)	3186(9)	5309(2)	36.2(16)
C77	745(8)	3946(9)	5081(2)	36.2(18)
C78	979(8)	3836(9)	4817(2)	40(2)
C79	932(9)	4472(10)	4611(2)	44(2)
C80	679(10)	5248(10)	4679(3)	50(2)
C81	477(10)	5370(10)	4951(3)	49(2)
C82	514(8)	4720(9)	5152(2)	41(2)
C83	-443(9)	2296(9)	5358(2)	43(2)
C84	-809(10)	1833(10)	5614(3)	51(2)
C85	-1847(11)	1081(10)	5659(3)	60(3)
C86	-2549(10)	782(10)	5441(3)	59(3)
C87	-2215(10)	1207(11)	5180(3)	58(3)
C88	-1175(9)	1951(9)	5141(3)	47(2)
C89	1369(8)	1906(9)	5443(2)	35.8(18)
C90	1578(9)	1731(9)	5708(2)	45(2)
C91	1401(9)	738(9)	5796(2)	44(2)
C92	1032(9)	-102(9)	5606(2)	39(2)
C93	818(9)	78(9)	5339(2)	37(2)
C94	977(9)	1054(8)	5261(2)	37(2)
C95	898(9)	-1138(9)	5691(2)	40(2)
C96	172(9)	-2051(9)	5561(2)	41(2)
C97	45(9)	-3022(9)	5642(2)	40(2)
C98	638(9)	-3111(9)	5850(2)	38.6(19)
C99	1391(10)	-2179(9)	5975(2)	46(3)
C100	1514(11)	-1217(10)	5899(2)	51(3)
C101	480(9)	-4147(9)	5941.9(19)	36.2(18)
C102	-524(9)	-5030(9)	5952(2)	39.2(19)
C103	-660(10)	-5977(9)	6046(2)	42(2)
C104	192(9)	-6076(10)	6129(2)	43(2)
C105	1190(9)	-5193(9)	6115(2)	41(2)
C106	1342(9)	-4244(9)	6019(2)	40.0(19)
C107	3768(7)	4138(7)	4418.5(17)	26.2(16)
C108	3638(8)	4105(8)	4105.9(17)	29.0(16)
C110	4029(8)	3468(8)	3949.0(17)	30.8(16)
C109	2870(8)	3028(8)	3974.5(17)	30.8(15)
C111	2244(8)	2122(8)	4166.9(19)	35.6(18)
C112	1484(9)	2124(9)	4337.0(19)	36.6(19)
C113	860(9)	1265(9)	4501(2)	42(2)
C114	980(11)	386(10)	4499(3)	52(3)
C115	1735(12)	383(11)	4335(3)	60(3)
C116	2369(11)	1240(9)	4166(3)	50(3)
C117	2252(8)	2979(9)	3714.6(18)	37(2)
C118	2650(9)	3660(10)	3501(2)	43(2)
C119	2082(10)	3573(11)	3267(2)	51(3)
C120	1102(12)	2778(15)	3235(3)	92(6)
C121	676(13)	1948(16)	3438(3)	99(7)
C122	1246(11)	2089(12)	3676(2)	65(4)
C123	3797(8)	5125(8)	3990.5(17)	28.8(18)
C124	4778(8)	5900(8)	3903.6(18)	30(2)
C125	4959(8)	6873(8)	3816.2(18)	33(2)
C126	4134(8)	7102(8)	3819.8(17)	31(2)
C127	3154(9)	6323(9)	3914.2(19)	37(2)
C128	2985(8)	5368(9)	3998(2)	36(2)
C129	4306(8)	8150(8)	3727.4(19)	34(2)

Atom	x	y	z	U_{eq}
C130	4823(8)	8593(8)	3478.1(19)	33(2)
C131	4952(8)	9551(8)	3391.7(19)	37(2)
C132	4558(9)	10088(8)	3542(2)	38(2)
C133	4053(9)	9638(9)	3789(2)	39(2)
C134	3931(10)	8699(9)	3880(2)	41(3)
C135	4634(10)	11066(9)	3436.7(18)	39(3)
C136	3766(11)	11200(9)	3433(2)	46(3)
C137	3805(12)	12084(10)	3312(2)	54(3)
C138	4752(13)	12858(10)	3208(3)	59(4)
C139	5621(12)	12760(10)	3216(2)	54(3)
C140	5575(10)	11862(9)	3327(2)	45(3)
C1	3397(9)	6826(11)	5006(3)	51(3)
C2	3511(13)	6969(13)	5311(3)	66(4)
C3	4517(14)	7240(12)	4618(2)	82(3)
C4	5255(15)	8411(12)	4591(4)	97(4)
C141	5023(13)	2047(13)	4700(3)	73(3)
C142	5648(17)	1494(18)	4738(5)	109(5)
C143	3691(11)	1267(9)	5062(3)	57(3)
C144	3838(14)	1349(14)	5367(3)	79(5)
O11	3611(7)	4670(8)	6878.2(17)	54.6(19)
C145	4602(11)	5569(13)	6824(3)	66(3)
C146	5327(13)	5642(15)	7050(3)	84(5)
C147	2839(10)	4486(11)	6679(2)	56(3)
C148	1844(11)	3478(12)	6735(3)	64(3)

Supplementary Table 11: Anisotropic Displacement Parameters ($\times 10^4$) **Rh_2[*R*-*p*-PhC_6H_4TPCP]$_4$**. The anisotropic displacement factor exponent takes the form: : $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Rh1	24.8(3)	25.0(3)	23.9(3)	-0.2(2)	0.3(2)	13.0(3)
Rh2	26.5(4)	25.6(4)	24.0(3)	-1.4(2)	-1.0(2)	14.3(3)
O2	34(4)	31(3)	30(3)	-3(3)	-1(2)	19(3)
O3	32(4)	37(3)	32(3)	2(2)	4(2)	24(3)
O4	31(4)	29(3)	21(2)	-5(2)	-3(2)	15(3)
O5	24(3)	27(3)	19(2)	-7(2)	-8(2)	12(3)
O6	33(3)	34(3)	35(3)	-3(2)	4(3)	23(3)
O7	31(4)	28(3)	35(3)	1(2)	6(2)	17(3)
O8	32(4)	27(3)	26(2)	-3(2)	-7(2)	16(3)
O9	31(3)	28(3)	21(2)	-6(2)	-8(2)	15(3)
O1	44(4)	39(4)	63(3)	-13(3)	-7(3)	32(4)
O10	49(4)	26(3)	52(3)	2(3)	1(3)	18(3)
C7	31(3)	30(3)	37(3)	0(3)	5(3)	15(3)
C5	28(4)	32(3)	24(3)	-2(2)	-3(3)	16(3)
C6	31(4)	30(3)	30(3)	0(3)	2(3)	16(3)
C8	36(5)	30(4)	33(3)	2(3)	5(3)	17(4)
C9	22(5)	29(4)	42(3)	-5(3)	2(3)	10(4)
C10	31(5)	35(4)	40(3)	-5(3)	-1(3)	12(4)
C11	34(6)	49(5)	47(4)	-12(3)	-2(4)	21(5)
C12	39(6)	45(5)	55(4)	-18(4)	-4(4)	19(5)
C13	50(7)	41(5)	60(4)	-10(3)	4(4)	25(5)
C14	38(6)	36(4)	48(4)	-2(3)	4(4)	20(4)
C15	33(3)	24(5)	51(4)	4(3)	11(3)	14(3)
C16	47(5)	41(6)	56(4)	7(4)	24(3)	22(5)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C17	52(5)	43(6)	74(5)	19(5)	34(4)	28(5)
C18	47(5)	42(6)	89(5)	18(5)	27(4)	27(5)
C19	35(4)	42(6)	84(5)	10(5)	13(4)	22(5)
C20	33(4)	30(5)	62(4)	-1(4)	5(3)	18(4)
C21	32(4)	28(3)	33(3)	2(3)	6(3)	14(3)
C22	35(5)	33(4)	35(3)	-1(3)	2(3)	17(4)
C23	36(5)	36(4)	37(4)	-5(3)	-1(3)	18(4)
C24	26(4)	30(4)	35(3)	-2(3)	5(3)	12(3)
C25	32(5)	35(4)	36(3)	-4(3)	1(3)	18(4)
C26	38(5)	37(4)	32(3)	-5(3)	2(3)	20(4)
C27	33(4)	33(4)	37(4)	-7(3)	-2(3)	16(3)
C28	34(4)	37(4)	45(5)	-11(3)	-7(4)	19(3)
C29	39(4)	33(4)	39(4)	-9(4)	-4(3)	18(4)
C30	42(4)	31(4)	34(4)	-2(3)	-1(3)	20(3)
C31	40(4)	41(4)	55(5)	-15(4)	-8(4)	25(4)
C32	36(4)	39(5)	60(6)	-20(4)	-12(4)	21(4)
C33	47(5)	30(4)	40(4)	1(3)	5(3)	22(4)
C34	53(6)	36(5)	51(4)	5(4)	5(4)	27(5)
C35	72(8)	42(6)	71(6)	3(5)	9(5)	39(6)
C36	75(8)	44(7)	77(6)	-6(5)	10(5)	36(6)
C37	62(7)	39(6)	61(5)	-13(4)	6(5)	23(5)
C38	41(5)	32(5)	44(4)	-3(3)	6(3)	15(4)
C39	18(4)	34(5)	21(4)	-5(3)	-4(3)	15(4)
C40	35(5)	32(5)	28(4)	0(4)	2(4)	21(5)
C42	35(6)	31(5)	31(4)	1(4)	-1(4)	17(5)
C41	34(4)	34(4)	29(3)	3(3)	-1(3)	20(4)
C43	35(5)	35(4)	35(3)	-7(3)	-5(3)	19(4)
C44	39(6)	37(5)	57(5)	-5(3)	-10(4)	23(4)
C45	46(6)	50(6)	83(6)	-17(4)	-7(5)	30(5)
C46	44(6)	58(6)	67(5)	-28(4)	-14(4)	30(5)
C47	39(6)	66(6)	46(5)	-19(4)	-6(4)	32(5)
C48	42(5)	52(5)	34(4)	-2(3)	0(3)	30(5)
C49	39(4)	46(4)	31(3)	-5(3)	-3(3)	30(3)
C50	37(4)	48(5)	40(3)	-10(3)	-4(3)	27(3)
C51	47(5)	62(6)	53(4)	-22(4)	-15(3)	34(4)
C52	63(5)	79(7)	48(4)	-25(4)	-21(4)	48(5)
C53	67(5)	88(7)	34(3)	-10(4)	-12(4)	52(5)
C54	55(5)	64(6)	31(3)	-2(3)	-3(3)	38(4)
C55	32(5)	37(5)	24(4)	-2(4)	-2(4)	20(5)
C56	34(6)	40(6)	31(4)	-1(4)	7(4)	18(5)
C57	33(6)	44(6)	30(4)	1(4)	9(4)	21(5)
C58	37(6)	35(5)	27(4)	-4(4)	-2(4)	20(5)
C59	24(5)	45(6)	37(4)	1(4)	5(4)	19(5)
C60	34(6)	35(6)	38(4)	-3(4)	1(4)	18(5)
C61	30(5)	40(6)	32(4)	-1(4)	1(4)	20(5)
C62	47(6)	45(6)	27(4)	1(4)	4(4)	31(5)
C63	37(6)	38(6)	33(4)	2(4)	-2(4)	21(5)
C64	27(5)	39(6)	33(4)	-1(4)	-3(4)	18(5)
C65	35(6)	43(6)	33(4)	4(4)	8(4)	25(5)
C66	37(6)	45(6)	29(4)	4(4)	4(4)	25(5)
C67	32(6)	38(6)	33(4)	5(4)	6(4)	18(5)
C68	32(6)	34(6)	39(5)	0(4)	0(4)	11(5)
C69	40(6)	31(6)	49(5)	8(4)	1(5)	17(5)
C70	37(6)	34(6)	56(6)	1(5)	9(5)	17(5)
C71	37(6)	42(6)	44(5)	-8(5)	1(5)	22(5)
C72	36(6)	47(7)	38(5)	0(5)	4(4)	26(5)
C73	30(4)	35(3)	27(3)	-2(3)	-1(3)	21(3)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C74	32(4)	34(4)	35(4)	-2(3)	4(3)	18(3)
C76	34(5)	37(5)	39(3)	1(3)	10(3)	20(4)
C75	34(3)	34(4)	46(3)	-2(3)	6(3)	20(3)
C77	23(5)	35(4)	52(3)	0(3)	-1(3)	16(4)
C78	32(5)	40(5)	50(3)	-3(3)	-5(4)	18(4)
C79	31(6)	45(5)	54(4)	-1(4)	-9(4)	18(5)
C80	37(6)	47(6)	68(4)	5(4)	-5(5)	23(5)
C81	39(6)	41(6)	73(4)	6(4)	3(4)	25(5)
C82	26(5)	32(4)	64(4)	-2(4)	-1(4)	15(4)
C83	33(3)	36(5)	65(4)	-1(3)	11(3)	22(3)
C84	43(4)	39(5)	69(4)	2(4)	18(3)	20(4)
C85	44(5)	40(6)	93(6)	8(5)	24(4)	20(4)
C86	37(5)	41(6)	102(6)	0(4)	21(4)	21(5)
C87	34(4)	42(6)	96(6)	-4(5)	8(4)	17(4)
C88	33(4)	37(5)	76(5)	0(4)	4(3)	21(4)
C89	31(5)	36(3)	44(3)	2(2)	4(3)	19(3)
C90	47(7)	39(4)	46(3)	-3(3)	-7(4)	19(5)
C91	46(6)	43(4)	41(4)	-1(3)	-10(4)	21(4)
C92	35(5)	38(3)	41(3)	2(3)	-4(3)	16(4)
C93	34(5)	35(4)	39(3)	2(3)	-2(3)	14(4)
C94	35(5)	36(4)	37(3)	4(3)	1(4)	16(4)
C95	35(5)	39(3)	44(4)	5(3)	-5(4)	16(3)
C96	35(5)	40(4)	43(4)	3(3)	-7(4)	17(3)
C97	34(5)	40(4)	42(4)	6(3)	-2(3)	15(4)
C98	36(4)	37(3)	42(4)	1(3)	-5(3)	17(3)
C99	45(6)	36(4)	53(5)	2(3)	-16(4)	17(3)
C100	53(6)	36(4)	59(5)	-1(4)	-23(5)	18(4)
C101	38(4)	37(3)	33(4)	1(3)	-2(3)	19(3)
C102	39(4)	38(4)	38(4)	-1(3)	0(4)	17(3)
C103	42(4)	37(4)	42(5)	-2(4)	-4(4)	17(4)
C104	45(4)	46(4)	40(5)	1(4)	1(4)	24(3)
C105	43(4)	46(4)	38(4)	3(3)	-2(4)	26(3)
C106	42(4)	45(4)	37(4)	1(4)	-2(4)	25(4)
C107	27(5)	23(3)	25(2)	-3(2)	-5(3)	10(3)
C108	31(4)	29(3)	26(2)	-2(2)	-3(3)	15(3)
C110	37(4)	30(4)	25(3)	-2(3)	-3(3)	17(4)
C109	37(3)	31(3)	24(3)	-5(2)	-5(2)	17(3)
C111	39(5)	34(4)	31(3)	-1(3)	-6(3)	16(4)
C112	39(5)	32(4)	33(4)	0(3)	-3(3)	13(4)
C113	40(5)	35(4)	39(4)	4(3)	-3(3)	10(4)
C114	56(7)	37(5)	55(6)	10(4)	5(4)	17(5)
C115	68(8)	39(5)	70(7)	13(5)	15(5)	25(5)
C116	59(7)	35(4)	58(6)	6(4)	10(5)	24(5)
C117	34(4)	45(5)	28(3)	-1(3)	-4(3)	17(4)
C118	37(5)	50(5)	35(3)	7(3)	-4(3)	17(4)
C119	40(5)	63(7)	34(4)	11(4)	-6(4)	15(4)
C120	53(6)	112(10)	46(6)	27(6)	-16(5)	-8(6)
C121	53(7)	111(10)	55(6)	32(7)	-22(5)	-18(7)
C122	47(5)	67(6)	43(5)	11(5)	-13(4)	-1(5)
C123	33(5)	28(4)	23(3)	-4(3)	-6(3)	13(4)
C124	32(5)	28(5)	31(4)	3(4)	4(4)	15(4)
C125	32(5)	35(5)	28(4)	-1(4)	1(4)	15(5)
C126	32(5)	28(5)	28(4)	-2(4)	-4(4)	12(4)
C127	40(6)	38(6)	36(4)	6(4)	2(4)	22(5)
C128	24(5)	36(6)	40(5)	6(4)	1(4)	9(4)
C129	33(6)	33(6)	33(4)	0(4)	-4(4)	15(5)
C130	34(6)	28(5)	38(4)	-1(4)	-3(4)	16(5)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C131	33(6)	33(6)	33(4)	2(4)	-2(4)	9(5)
C132	45(6)	25(5)	37(5)	-2(4)	-9(4)	12(5)
C133	47(7)	38(6)	37(5)	-6(4)	-4(5)	25(5)
C134	48(7)	42(7)	32(4)	0(4)	0(4)	21(6)
C135	51(7)	31(6)	27(4)	-6(4)	-5(4)	13(5)
C136	58(8)	31(6)	50(6)	-1(5)	-4(5)	22(6)
C137	76(9)	41(7)	52(6)	-4(5)	-8(6)	35(7)
C138	91(11)	33(7)	54(6)	2(5)	-4(7)	32(7)
C139	76(10)	30(6)	47(6)	-2(5)	3(6)	20(6)
C140	57(8)	33(6)	38(5)	0(4)	3(5)	18(6)
C1	46(6)	56(7)	67(5)	-14(5)	-10(4)	38(6)
C2	69(10)	72(10)	64(5)	-9(6)	2(5)	40(8)
C3	84(4)	83(4)	77(3)	3(3)	3(3)	41(3)
C4	98(7)	88(5)	91(6)	15(4)	2(5)	37(4)
C141	73(4)	74(4)	73(4)	-5(3)	13(3)	37(3)
C142	110(7)	116(7)	127(8)	-6(5)	15(5)	76(6)
C143	62(7)	36(5)	71(6)	13(5)	13(5)	24(5)
C144	79(11)	72(11)	68(5)	19(6)	17(6)	23(9)
O11	61(4)	69(5)	48(4)	-2(4)	1(3)	43(4)
C145	62(5)	70(7)	74(7)	-14(6)	7(5)	39(4)
C146	70(7)	105(13)	86(8)	-35(9)	-11(7)	49(8)
C147	63(5)	76(7)	42(5)	7(5)	5(4)	46(5)
C148	61(5)	83(8)	55(6)	6(6)	0(5)	41(5)

Supplementary Table 12: Bond Lengths in Å for **Rh_2[*R*-*p*-PhC_6H_4TPCP]$_4$**.

Atom	Atom	Length/Å
Rh1	Rh2	2.3741(9)
Rh1	O3	2.044(7)
Rh1	O5	2.032(5)
Rh1	O7	2.020(7)
Rh1	O9	2.039(5)
Rh1	O10	2.297(7)
Rh2	O2	2.046(7)
Rh2	O4	2.021(6)
Rh2	O6	2.035(7)
Rh2	O8	2.024(6)
Rh2	O1	2.312(7)
O2	C5	1.268(12)
O3	C5	1.271(12)
O4	C39	1.267(11)
O5	C39	1.268(11)
O6	C73	1.274(12)
O7	C73	1.279(11)
O8	C107	1.268(11)
O9	C107	1.258(11)
O1	C1	1.436(8)
O1	C3	1.438(6)
O10	C141	1.432(11)
O10	C143	1.433(11)
C7	C6	1.573(14)
C7	C8	1.497(14)

Atom	Atom	Length/Å
C7	C9	1.509(13)
C7	C15	1.519(14)
C5	C6	1.503(13)
C6	C8	1.526(13)
C6	C21	1.491(14)
C9	C10	1.379(14)
C9	C14	1.391(15)
C10	C11	1.399(15)
C11	C12	1.368(18)
C12	C13	1.367(18)
C13	C14	1.389(15)
C15	C16	1.398(15)
C15	C20	1.380(16)
C16	C17	1.377(17)
C17	C18	1.39(2)
C18	C19	1.367(19)
C19	C20	1.414(15)
C21	C22	1.400(14)
C21	C26	1.391(15)
C22	C23	1.380(15)
C23	C24	1.395(15)
C24	C25	1.408(13)
C24	C27	1.477(14)
C25	C26	1.386(15)
C27	C28	1.379(14)
C27	C32	1.383(15)
C28	C29	1.414(15)
C29	C30	1.391(15)
C30	C31	1.403(15)
C30	C33	1.481(14)
C31	C32	1.383(15)
C33	C34	1.401(16)
C33	C38	1.390(15)
C34	C35	1.408(17)
C35	C36	1.41(2)
C36	C37	1.36(2)
C37	C38	1.410(16)
C39	C40	1.522(11)
C40	C42	1.518(13)
C40	C41	1.549(13)
C40	C55	1.495(13)
C42	C41	1.504(15)
C41	C43	1.505(14)
C41	C49	1.512(13)
C43	C44	1.378(16)
C43	C48	1.398(15)
C44	C45	1.415(17)
C45	C46	1.38(2)
C46	C47	1.381(19)
C47	C48	1.397(15)
C49	C50	1.371(16)
C49	C54	1.389(14)
C50	C51	1.387(15)
C51	C52	1.381(18)
C52	C53	1.37(2)
C53	C54	1.394(17)
C55	C56	1.390(15)

Atom	Atom	Length/Å
C55	C60	1.395(14)
C56	C57	1.400(15)
C57	C58	1.398(14)
C58	C59	1.376(15)
C58	C61	1.494(14)
C59	C60	1.384(15)
C61	C62	1.392(14)
C61	C66	1.404(13)
C62	C63	1.402(15)
C63	C64	1.413(13)
C64	C65	1.373(15)
C64	C67	1.474(15)
C65	C66	1.392(15)
C67	C68	1.380(15)
C67	C72	1.416(14)
C68	C69	1.372(16)
C69	C70	1.395(16)
C70	C71	1.372(16)
C71	C72	1.387(15)
C73	C74	1.513(13)
C74	C76	1.501(13)
C74	C75	1.557(14)
C74	C89	1.489(14)
C76	C75	1.495(15)
C75	C77	1.542(15)
C75	C83	1.525(16)
C77	C78	1.361(15)
C77	C82	1.381(15)
C78	C79	1.392(15)
C79	C80	1.402(17)
C80	C81	1.383(18)
C81	C82	1.387(16)
C83	C84	1.390(17)
C83	C88	1.405(17)
C84	C85	1.379(18)
C85	C86	1.39(2)
C86	C87	1.39(2)
C87	C88	1.375(17)
C89	C90	1.379(15)
C89	C94	1.398(15)
C90	C91	1.411(16)
C91	C92	1.410(15)
C92	C93	1.395(14)
C92	C95	1.488(15)
C93	C94	1.383(15)
C95	C96	1.377(16)
C95	C100	1.402(15)
C96	C97	1.397(15)
C97	C98	1.382(14)
C98	C99	1.396(16)
C98	C101	1.486(15)
C99	C100	1.380(17)
C101	C102	1.392(15)
C101	C106	1.393(15)
C102	C103	1.378(16)
C103	C104	1.388(16)
C104	C105	1.387(17)

Atom	Atom	Length/Å
C105	C106	1.375(16)
C107	C108	1.530(11)
C108	C110	1.522(13)
C108	C109	1.546(13)
C108	C123	1.502(13)
C110	C109	1.491(14)
C109	C111	1.504(14)
C109	C117	1.535(12)
C111	C112	1.389(15)
C111	C116	1.392(16)
C112	C113	1.382(15)
C113	C114	1.384(18)
C114	C115	1.366(19)
C115	C116	1.396(17)
C117	C118	1.355(15)
C117	C122	1.410(17)
C118	C119	1.377(14)
C119	C120	1.331(19)
C120	C121	1.44(2)
C121	C122	1.381(17)
C123	C124	1.380(14)
C123	C128	1.404(15)
C124	C125	1.381(14)
C125	C126	1.408(15)
C126	C127	1.392(15)
C126	C129	1.496(14)
C127	C128	1.356(15)
C129	C130	1.405(14)
C129	C134	1.393(15)
C130	C131	1.384(15)
C131	C132	1.395(16)
C132	C133	1.391(15)
C132	C135	1.474(15)
C133	C134	1.369(16)
C135	C136	1.381(18)
C135	C140	1.392(16)
C136	C137	1.399(16)
C137	C138	1.38(2)
C138	C139	1.35(2)
C139	C140	1.393(17)
C1	C2	1.497(17)
C3	C4	1.510(7)
C141	C142	1.507(7)
C143	C144	1.496(19)
O11	C145	1.416(18)
O11	C147	1.411(15)
C145	C146	1.494(15)
C147	C148	1.493(15)

Supplementary Table 13: Bond Angles in ° for **Rh_2[*R*-*p*-PhC_6H_4TPCP]$_4$**.

Atom	Atom	Atom	Angle/°
O3	Rh1	Rh2	87.9(2)
O3	Rh1	O10	91.1(3)
O5	Rh1	Rh2	87.19(18)
O5	Rh1	O3	94.5(3)
O5	Rh1	O9	174.7(3)

Atom	Atom	Atom	Angle/°
O5	Rh1	O10	93.4(3)
O7	Rh1	Rh2	88.45(19)
O7	Rh1	O3	176.3(3)
O7	Rh1	O5	85.9(3)
O7	Rh1	O9	94.2(3)
O7	Rh1	O10	92.6(3)
O9	Rh1	Rh2	87.48(18)
O9	Rh1	O3	85.0(3)
O9	Rh1	O10	91.9(3)
O10	Rh1	Rh2	178.84(18)
O2	Rh2	Rh1	87.77(19)
O2	Rh2	O1	90.9(3)
O4	Rh2	Rh1	88.45(19)
O4	Rh2	O2	94.6(3)
O4	Rh2	O6	85.6(3)
O4	Rh2	O8	176.6(3)
O4	Rh2	O1	91.7(3)
O6	Rh2	Rh1	87.47(19)
O6	Rh2	O2	175.2(3)
O6	Rh2	O1	93.9(3)
O8	Rh2	Rh1	88.12(19)
O8	Rh2	O2	85.1(3)
O8	Rh2	O6	94.4(3)
O8	Rh2	O1	91.8(3)
O1	Rh2	Rh1	178.6(2)
C5	O2	Rh2	117.9(6)
C5	O3	Rh1	116.3(6)
C39	O4	Rh2	116.5(5)
C39	O5	Rh1	118.3(5)
C73	O6	Rh2	118.1(6)
C73	O7	Rh1	116.7(6)
C107	O8	Rh2	115.9(6)
C107	O9	Rh1	117.5(5)
C1	O1	Rh2	116.8(7)
C1	O1	C3	111.3(11)
C3	O1	Rh2	109.5(8)
C141	O10	Rh1	114.6(7)
C141	O10	C143	117.2(10)
C143	O10	Rh1	119.1(7)
C8	C7	C6	59.5(6)
C8	C7	C9	116.9(9)
C8	C7	C15	120.4(8)
C9	C7	C6	118.1(8)
C9	C7	C15	113.6(9)
C15	C7	C6	118.1(9)
O2	C5	O3	125.9(9)
O2	C5	C6	119.0(9)
O3	C5	C6	115.0(9)
C5	C6	C7	118.7(8)
C5	C6	C8	116.9(9)
C8	C6	C7	57.7(6)
C21	C6	C7	119.3(8)
C21	C6	C5	113.8(9)
C21	C6	C8	119.2(8)
C7	C8	C6	62.7(7)
C10	C9	C7	121.6(9)
C10	C9	C14	119.3(9)

Atom	Atom	Atom	Angle/°
C14	C9	C7	119.0(9)
C9	C10	C11	119.9(11)
C12	C11	C10	119.9(11)
C13	C12	C11	121.0(11)
C12	C13	C14	119.5(12)
C13	C14	C9	120.5(11)
C16	C15	C7	122.1(10)
C20	C15	C7	120.3(9)
C20	C15	C16	117.6(11)
C17	C16	C15	121.0(13)
C16	C17	C18	121.0(12)
C19	C18	C17	119.2(12)
C18	C19	C20	119.8(13)
C15	C20	C19	121.4(11)
C22	C21	C6	119.8(9)
C26	C21	C6	122.0(9)
C26	C21	C22	118.1(9)
C23	C22	C21	121.1(10)
C22	C23	C24	121.2(9)
C23	C24	C25	117.6(9)
C23	C24	C27	121.7(9)
C25	C24	C27	120.7(9)
C26	C25	C24	121.0(10)
C25	C26	C21	120.9(9)
C28	C27	C24	120.7(10)
C28	C27	C32	117.6(10)
C32	C27	C24	121.7(9)
C27	C28	C29	121.4(10)
C30	C29	C28	120.2(10)
C29	C30	C31	117.9(10)
C29	C30	C33	121.2(10)
C31	C30	C33	120.7(10)
C32	C31	C30	120.6(11)
C31	C32	C27	122.2(10)
C34	C33	C30	120.7(10)
C38	C33	C30	120.8(10)
C38	C33	C34	118.5(10)
C33	C34	C35	121.3(12)
C36	C35	C34	118.1(13)
C37	C36	C35	121.6(12)
C36	C37	C38	119.7(12)
C33	C38	C37	120.8(12)
O4	C39	O5	126.1(7)
O4	C39	C40	116.8(8)
O5	C39	C40	117.2(8)
C39	C40	C41	117.9(8)
C42	C40	C39	115.0(8)
C42	C40	C41	58.7(6)
C55	C40	C39	113.4(8)
C55	C40	C42	118.5(8)
C55	C40	C41	122.4(8)
C41	C42	C40	61.7(7)
C42	C41	C40	59.6(6)
C42	C41	C43	116.7(9)
C42	C41	C49	120.1(8)
C43	C41	C40	120.6(8)
C43	C41	C49	111.2(8)

Atom	Atom	Atom	Angle/°
C49	C41	C40	119.9(8)
C44	C43	C41	118.2(9)
C44	C43	C48	120.7(10)
C48	C43	C41	120.9(10)
C43	C44	C45	118.8(12)
C46	C45	C44	120.0(13)
C47	C46	C45	121.3(12)
C46	C47	C48	119.0(12)
C47	C48	C43	120.2(11)
C50	C49	C41	120.9(9)
C50	C49	C54	118.0(10)
C54	C49	C41	120.6(11)
C49	C50	C51	122.5(11)
C52	C51	C50	118.5(13)
C53	C52	C51	120.6(12)
C52	C53	C54	120.1(12)
C49	C54	C53	120.4(13)
C56	C55	C40	123.1(9)
C56	C55	C60	116.6(9)
C60	C55	C40	120.1(9)
C55	C56	C57	121.7(9)
C58	C57	C56	120.4(10)
C57	C58	C61	120.9(10)
C59	C58	C57	118.0(10)
C59	C58	C61	121.1(9)
C58	C59	C60	121.3(9)
C59	C60	C55	122.0(10)
C62	C61	C58	121.9(8)
C62	C61	C66	117.9(10)
C66	C61	C58	120.2(9)
C61	C62	C63	121.5(9)
C62	C63	C64	120.1(10)
C63	C64	C67	120.7(9)
C65	C64	C63	117.7(10)
C65	C64	C67	121.6(9)
C64	C65	C66	122.7(9)
C65	C66	C61	120.0(10)
C68	C67	C64	122.9(9)
C68	C67	C72	117.4(10)
C72	C67	C64	119.7(9)
C69	C68	C67	122.0(10)
C68	C69	C70	120.1(10)
C71	C70	C69	119.3(11)
C70	C71	C72	120.6(10)
C71	C72	C67	120.5(10)
O6	C73	O7	125.7(9)
O6	C73	C74	117.9(8)
O7	C73	C74	116.3(9)
C73	C74	C75	119.7(9)
C76	C74	C73	116.3(9)
C76	C74	C75	58.5(7)
C89	C74	C73	114.6(9)
C89	C74	C76	118.0(8)
C89	C74	C75	118.3(9)
C75	C76	C74	62.6(7)
C76	C75	C74	58.8(6)
C76	C75	C77	117.1(9)

Atom	Atom	Atom	Angle/°
C76	C75	C83	120.5(9)
C77	C75	C74	119.3(9)
C83	C75	C74	119.4(9)
C83	C75	C77	112.2(9)
C78	C77	C75	121.5(10)
C78	C77	C82	120.9(11)
C82	C77	C75	117.6(10)
C77	C78	C79	120.1(11)
C78	C79	C80	119.6(11)
C81	C80	C79	119.5(12)
C80	C81	C82	120.0(12)
C77	C82	C81	119.8(11)
C84	C83	C75	123.0(11)
C84	C83	C88	117.2(11)
C88	C83	C75	119.8(11)
C85	C84	C83	122.3(14)
C84	C85	C86	118.7(14)
C85	C86	C87	121.0(13)
C88	C87	C86	119.0(14)
C87	C88	C83	121.7(13)
C90	C89	C74	121.8(10)
C90	C89	C94	117.1(10)
C94	C89	C74	121.0(9)
C89	C90	C91	122.1(11)
C92	C91	C90	119.7(10)
C91	C92	C95	120.6(9)
C93	C92	C91	117.9(10)
C93	C92	C95	121.5(10)
C94	C93	C92	120.9(10)
C93	C94	C89	122.2(9)
C96	C95	C92	120.7(10)
C96	C95	C100	117.8(11)
C100	C95	C92	121.5(10)
C95	C96	C97	120.4(10)
C98	C97	C96	122.2(11)
C97	C98	C99	117.0(11)
C97	C98	C101	122.2(10)
C99	C98	C101	120.8(10)
C100	C99	C98	121.3(10)
C99	C100	C95	121.2(11)
C102	C101	C98	120.9(10)
C102	C101	C106	119.1(11)
C106	C101	C98	120.0(10)
C103	C102	C101	120.2(11)
C102	C103	C104	121.1(11)
C105	C104	C103	118.2(11)
C106	C105	C104	121.5(11)
C105	C106	C101	119.9(11)
O8	C107	C108	115.8(8)
O9	C107	O8	126.9(8)
O9	C107	C108	117.2(8)
C107	C108	C109	117.3(8)
C110	C108	C107	116.0(8)
C110	C108	C109	58.1(6)
C123	C108	C107	112.6(8)
C123	C108	C110	120.3(8)
C123	C108	C109	122.3(8)

Atom	Atom	Atom	Angle/°
C109	C110	C108	61.7(6)
C110	C109	C108	60.1(6)
C110	C109	C111	119.6(8)
C110	C109	C117	118.0(8)
C111	C109	C108	117.1(7)
C111	C109	C117	112.7(8)
C117	C109	C108	119.9(8)
C112	C111	C109	120.2(10)
C112	C111	C116	118.8(10)
C116	C111	C109	120.8(10)
C113	C112	C111	120.6(11)
C112	C113	C114	120.6(12)
C115	C114	C113	119.3(12)
C114	C115	C116	121.0(13)
C111	C116	C115	119.8(12)
C118	C117	C109	124.8(10)
C118	C117	C122	116.4(9)
C122	C117	C109	118.2(9)
C117	C118	C119	123.2(11)
C120	C119	C118	120.9(12)
C119	C120	C121	118.9(12)
C122	C121	C120	118.1(14)
C121	C122	C117	121.7(12)
C124	C123	C108	120.9(9)
C124	C123	C128	117.8(9)
C128	C123	C108	120.9(9)
C123	C124	C125	121.9(10)
C124	C125	C126	119.9(10)
C125	C126	C129	121.1(9)
C127	C126	C125	117.8(10)
C127	C126	C129	121.1(10)
C128	C127	C126	121.8(10)
C127	C128	C123	120.9(10)
C130	C129	C126	120.6(9)
C134	C129	C126	121.4(9)
C134	C129	C130	118.0(10)
C131	C130	C129	119.9(10)
C130	C131	C132	121.9(9)
C131	C132	C135	121.0(9)
C133	C132	C131	117.2(10)
C133	C132	C135	121.7(10)
C134	C133	C132	121.7(10)
C133	C134	C129	121.2(10)
C136	C135	C132	121.0(11)
C136	C135	C140	118.2(11)
C140	C135	C132	120.7(11)
C135	C136	C137	121.5(12)
C138	C137	C136	118.4(14)
C139	C138	C137	121.1(12)
C138	C139	C140	120.6(13)
C135	C140	C139	120.0(13)
O1	C1	C2	109.3(10)
O1	C3	C4	115.2(12)
O10	C141	C142	118.4(14)
O10	C143	C144	109.1(12)
C147	O11	C145	113.7(11)
O11	C145	C146	107.0(13)

Atom	Atom	Atom	Angle/°
O11	C147	C148	110.9(11)

Supplementary Table 14: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Rh_2[*R*-*p*-PhC_6H_4TPCP]$_4$**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	x	y	z	U_{eq}
H8A	7498.7	6648.78	4084.46	40
H8B	6763.28	6945.36	4285.44	40
H10	7818.28	6649.26	5047.63	45
H11	7915.92	7798.83	5398.25	52
H12	8191.32	9452.11	5288.08	57
H13	8279.8	9958.85	4833.59	60
H14	8180.12	8823.68	4481.91	48
H16	8926.59	6695.77	4039.97	58
H17	10620.34	7034	3956.33	65
H18	11901.82	7720.53	4300.79	69
H19	11455.27	8032.71	4735.31	63
H20	9741.7	7726.34	4818.94	49
H22	6343.04	4540.41	4038	41
H23	6536.35	3137.46	3898.99	43
H25	8494.17	3654.5	4542.55	41
H26	8332.45	5089.53	4674.15	42
H28	6213.23	1443.59	3968.31	45
H29	6422.56	27.54	3824.06	45
H31	9479.84	1662.46	4061.97	53
H32	9212.28	2988.1	4228.77	53
H34	9264.71	10.53	4083.02	53
H35	9652.18	-1215.46	3876.33	68
H36	8691.68	-2140.39	3483.45	75
H37	7478.61	-1782.64	3285.67	66
H38	7104.86	-550.92	3491.21	49
H42A	4588.4	4133.71	6089.73	38
H42B	4501.14	3442.41	5808.82	38
H44	6037.98	3028.15	5919.67	51
H45	6945.25	2343.52	5666.18	69
H46	7956.23	3254.48	5287.44	65
H47	8138.9	4867.92	5158.78	58
H48	7243.65	5553.92	5408.98	48
H50	7849.4	6606.89	5864.28	47
H51	9067.05	7484.06	6213.54	61
H52	8651.22	6842.57	6663.34	69
H53	7067.12	5340.02	6757.82	68
H54	5860.94	4455.72	6403.86	55
H56	6424	7227.15	5662.99	42
H57	6101.47	8562.09	5804.62	42
H59	3493.62	6408.98	6203.21	41
H60	3786.88	5084.95	6050.85	42
H62	5011.94	9360.89	5765.46	43
H63	4754.5	10722.1	5924.69	43
H65	3755.95	9219.05	6652.6	41
H66	3949.83	7834.14	6491.59	42
H68	3448.66	11238.91	6090.29	44
H69	3219.91	12560.14	6275.1	48
H70	3858.8	13213.86	6717.22	51
H71	4678.02	12486.17	6971.76	48

Atom	x	y	z	U_{eq}
H72	4822.73	11084.65	6796.72	46
H76A	1169.19	3365.16	5730.51	43
H76B	1937.32	4418.97	5539.75	43
H78	1173.63	3325.77	4772.42	48
H79	1071.45	4380.42	4425.2	52
H80	647.15	5686.83	4540.53	60
H81	312.11	5899	4999.05	59
H82	380.3	4806.56	5338.97	49
H84	-327.48	2042.74	5763.01	61
H85	-2076.5	773.85	5835.26	72
H86	-3269.97	278.23	5470.41	71
H87	-2698.79	987.27	5031.42	70
H88	-944.21	2240.3	4962.64	56
H90	1850.9	2296.71	5835.71	54
H91	1529.05	634.7	5981.35	53
H93	559.8	-477.33	5207.82	44
H94	815.01	1149.66	5077.54	44
H96	-245.13	-2020.45	5415.85	49
H97	-467.59	-3641.97	5551.55	48
H99	1826.68	-2207.55	6115.75	56
H100	2026.54	-596.44	5990.16	61
H102	-1115.44	-4978.93	5894.09	47
H103	-1349.6	-6572.88	6053.87	50
H104	95.69	-6730.04	6193.19	51
H105	1780.75	-5245.53	6172.79	49
H106	2033.96	-3655.79	6006.16	48
H11A	4352.18	3732.61	3766.31	37
H11B	4349.25	3127.69	4056.92	37
H112	1392.04	2720.97	4340.31	44
H113	344.08	1277.16	4617.02	50
H114	541.59	-207.77	4609.55	63
H115	1830.4	-212.03	4335.77	72
H116	2883.04	1222.59	4050.78	60
H118	3355.75	4224.96	3512.71	51
H119	2393.58	4088.6	3126.23	61
H120	690.46	2757.24	3082.18	110
H121	22.61	1321.28	3408.07	119
H122	952.58	1574.21	3817.21	78
H124	5344.74	5760.89	3904	37
H125	5638.92	7387.22	3753.69	39
H127	2588.68	6464.5	3920.14	44
H128	2307.14	4857.42	4062.75	43
H130	5084.31	8236.44	3368.84	39
H131	5320.37	9850.32	3225.19	44
H133	3784.72	9990.46	3897.33	47
H134	3584.92	8416.87	4049.85	49
H136	3127.84	10678.68	3514.9	56
H137	3193.21	12149.22	3301.91	65
H138	4794.56	13470.44	3128.56	70
H139	6268.83	13309.27	3145.65	65
H140	6185.24	11792.8	3327.93	54
H1A	2760.42	6145.8	4961.59	61
H1B	3315.53	7397.93	4922.63	61
H2A	4167.75	7617.76	5353.96	99
H2B	3525.74	6366.83	5394	99
H2C	2913.35	7014.28	5385.34	99
H3A	3838.48	7061.67	4530.36	98

Atom	x	y	z	U_{eq}
H3B	4817.88	6870.35	4514.05	98
H4A	5811.94	8543.17	4458.64	145
H4B	5571.19	8702.98	4770.5	145
H4C	4861.25	8748.03	4526.73	145
H14A	5500.05	2749.88	4620.46	88
H14B	4468.94	1647.28	4561.61	88
H14C	5345.37	859.01	4623.32	164
H14D	5624.99	1297.99	4931.34	164
H14E	6381.01	1966.72	4682.98	164
H14F	3699.68	634.95	4993.25	68
H14G	3003.25	1197.63	5013.78	68
H14H	4553.94	1505	5411.71	119
H14I	3327.24	680.32	5452.47	119
H14J	3729.78	1914.67	5436.65	119
H14K	4538.36	6210.06	6819.93	79
H14L	4875.12	5497.63	6643.71	79
H14M	5603.87	5171.39	7009.5	127
H14N	4940.09	5435.1	7224.07	127
H14O	5911.65	6368.5	7063.59	127
H14P	3106.32	4453.77	6494.02	67
H14Q	2692.95	5076.38	6679.56	67
H14R	1318.43	3369.78	6594.49	96
H14S	1575.05	3512.39	6916.73	96
H14T	1984.48	2891.79	6729.71	96

Citations

APEX2 suite for crystallographic software, Bruker axs, Madison, WI (2015).

O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.

Sheldrick, G.M., A short history of ShelX, *Acta Cryst.*, (2008), **A64**, 339-341.

```
#==============================================================================
Bond precision:  C-C = 0.0173 A          Wavelength=1.54184

Cell:            a=14.66084(10)    b=14.66084(10)     c=48.6185(3)
                 alpha=90          beta=90            gamma=120

Temperature: 100 K

                   Calculated                  Reported
Volume             9050.03(16)                 9050.03(11)
Space group        P 31                        P 31
Hall group         P 31                        P 31
Moiety formula     C144 H120 O10 Rh2, C4 H10   C144 H120 O10 Rh2, C4 H10
                   O                           O
Sum formula        C148 H130 O11 Rh2           C148 H130 O11 Rh2
Mr                 2290.35                     2290.33
Dx,g cm-3          1.261                       1.261
Z                  3                           3
Mu (mm-1)          2.696                       2.696
F000               3588.0                      3588.0
F000'              3597.90
h,k,lmax           17,17,58                    17,17,58
Nref               21580[ 10790]               21511
Tmin,Tmax          0.851,0.948                 0.814,1.000
Tmin'              0.764

Correction method= # Reported T Limits: Tmin=0.814 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.99/1.00 Theta(max)= 67.078

R(reflections)= 0.0564( 19805) wR2(reflections)= 0.1465( 21511)

S = 1.012                       Npar= 1457
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT601 ALERT 2 B Structure Contains Solvent Accessible VOIDS of . 103 Ang**3

Author Response: The large structure and its bowl shaped cavity are ideal for diffuse solvent. The solvent could not be detected from the electron density and the BYPASS procedure (SQUEEZE) could not implemented because the structure was refined using a twin law.

Alert level C

PLAT090 ALERT 3 C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.39 Note
PLAT220 ALERT 2 C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT222 ALERT 3 C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio
PLAT241 ALERT 2 C High 'MainMol' Ueq as Compared to Neighbors of C120 Check
PLAT241 ALERT 2 C High 'MainMol' Ueq as Compared to Neighbors of C121 Check
PLAT242 ALERT 2 C Low 'MainMol' Ueq as Compared to Neighbors of C119 Check
PLAT342 ALERT 3 C Low Bond Precision on C-C Bonds ..... 0.01732 Ang.
PLAT911 ALERT 3 C Missing FCF Refl Between Thmin & STh/L= 0.597 16 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 120 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..... 0.00030 Ang.
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 5 Units
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 14 Report
PLAT791_ALERT_4_G Model has Chirality at C6 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G Model has Chirality at C40 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G Model has Chirality at C74 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G Model has Chirality at C108 (Chiral SPGR) R Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 877 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 78% Note
PLAT931_ALERT_5_G Found Twin Law (1-2 0)[ ] Est. BASF 0.12 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 47 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
11 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to

CIF submission.

PLATON version of 23/04/2018; check.def file version of 23/

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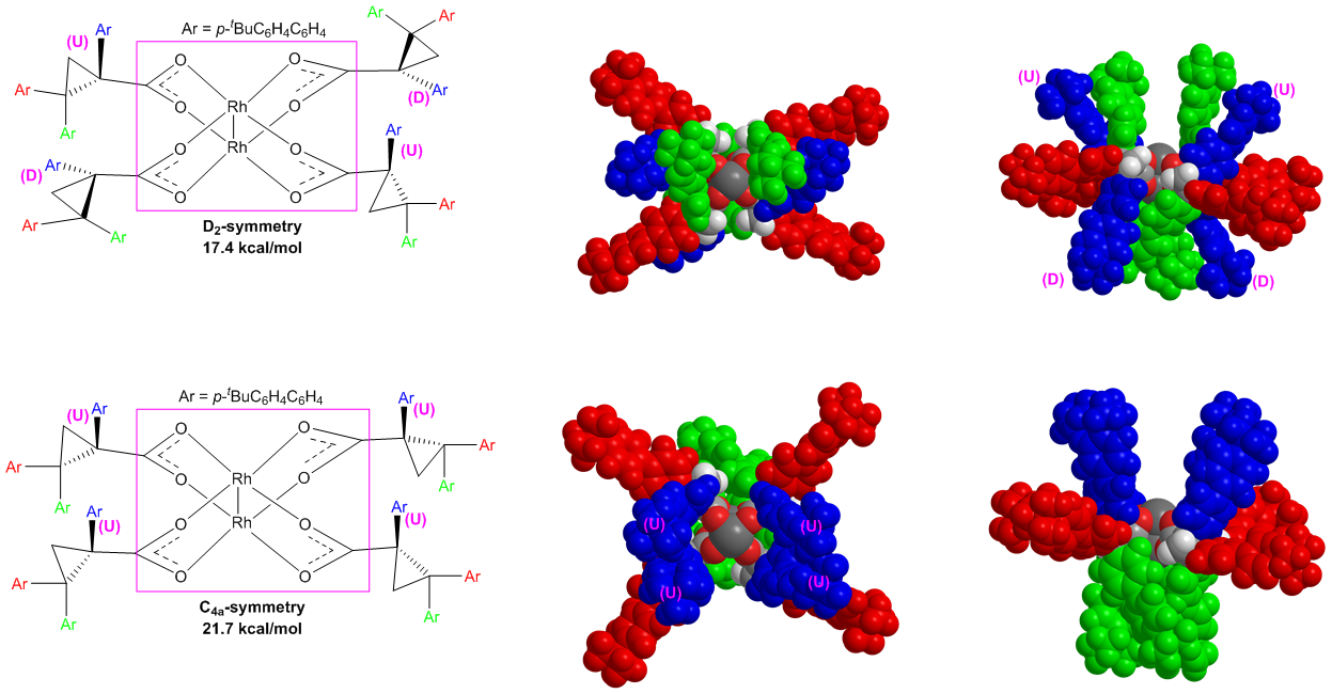
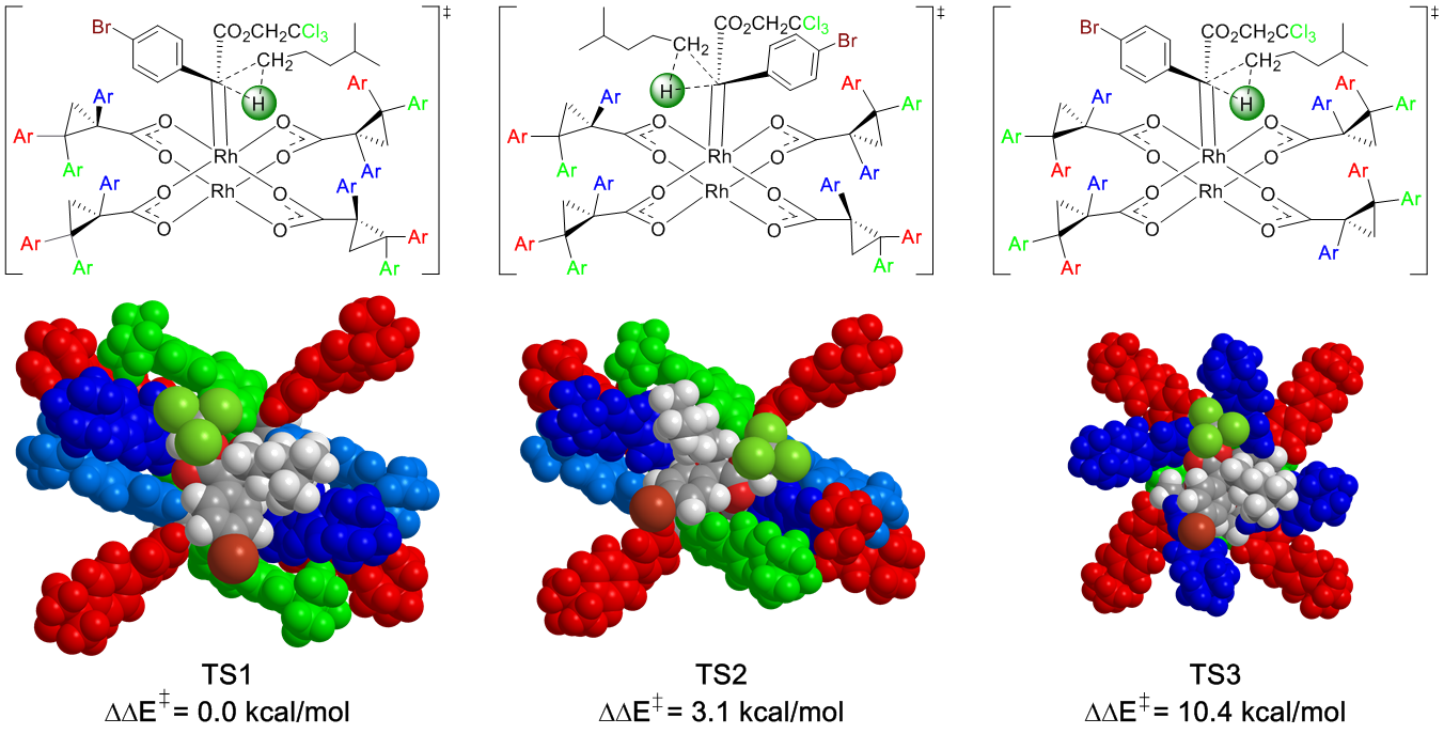
14 - Computational Study

Computational Details

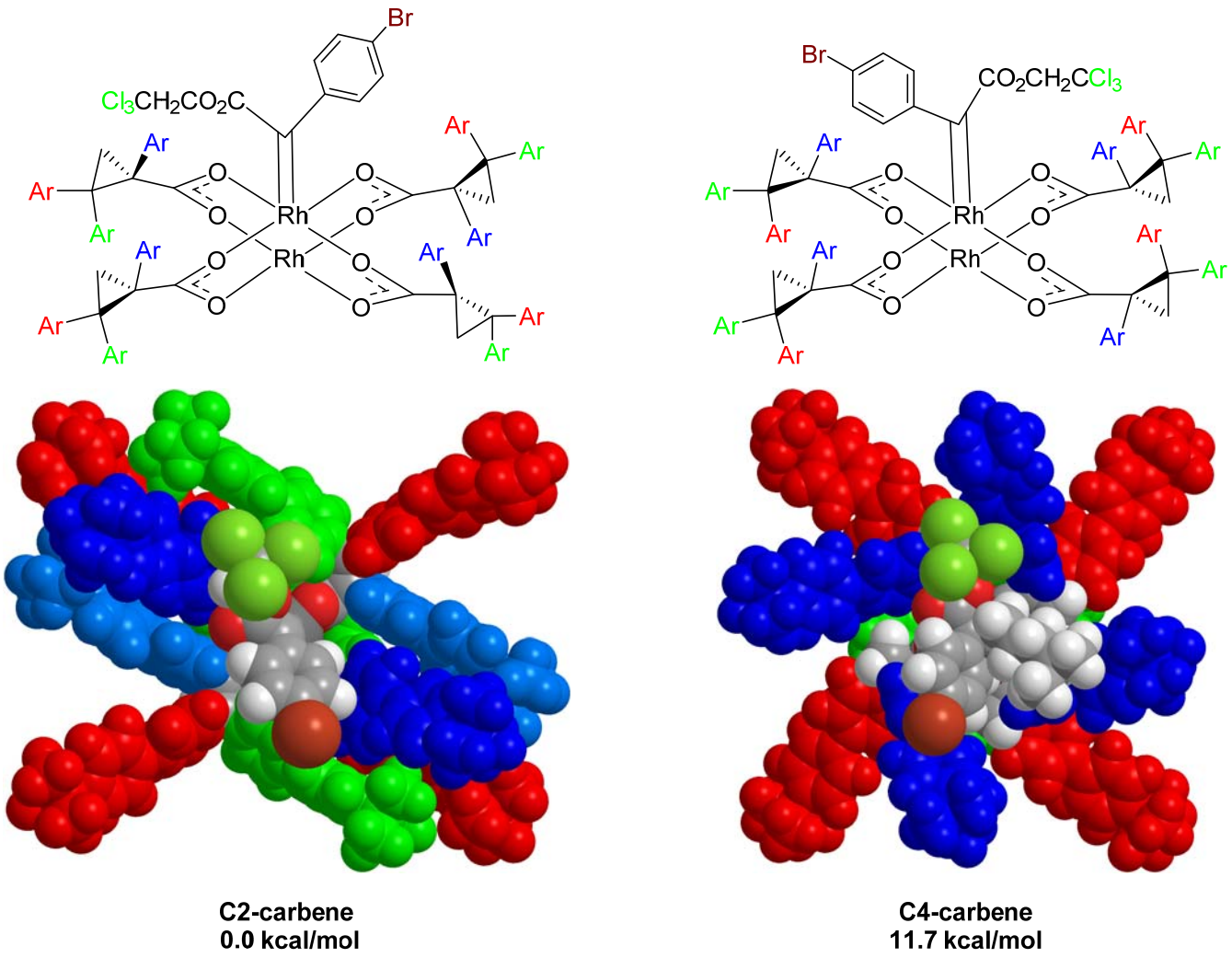
All calculations were performed using Gaussian 09.[7] Performing DFT calculations on the complete dirhodium complex (approximately 500 atoms) is impractical, so we employed a two-layer ONIOM[7] (B3LYP[9-11]:UFF[12]) approach to study this reaction. The ONIOM partitioning of the catalyst system that was used is shown in Supplementary Figure 10. ONIOM partitioning of the catalyst with the atoms inside the purple rectangle modeled with DFT and the atoms outside modeled with the UFF. The carbene and the 2-methylpentane substrate are also included in the QM part. For the QM part, the LANL2DZ basis set[13-14] was used for Rh, Br, and Cl atoms, and the 6-31G(d)[15-17] basis set was used for all other atoms. The solvation free-energy corrections were computed with the SMD model[18] on gas-phase optimized geometries, and dichloromethane was chosen as the solvent for consistency with the experiment. Extensive conformational searches for catalysts and transition states have been conducted, but only the most stable conformers are discussed here.



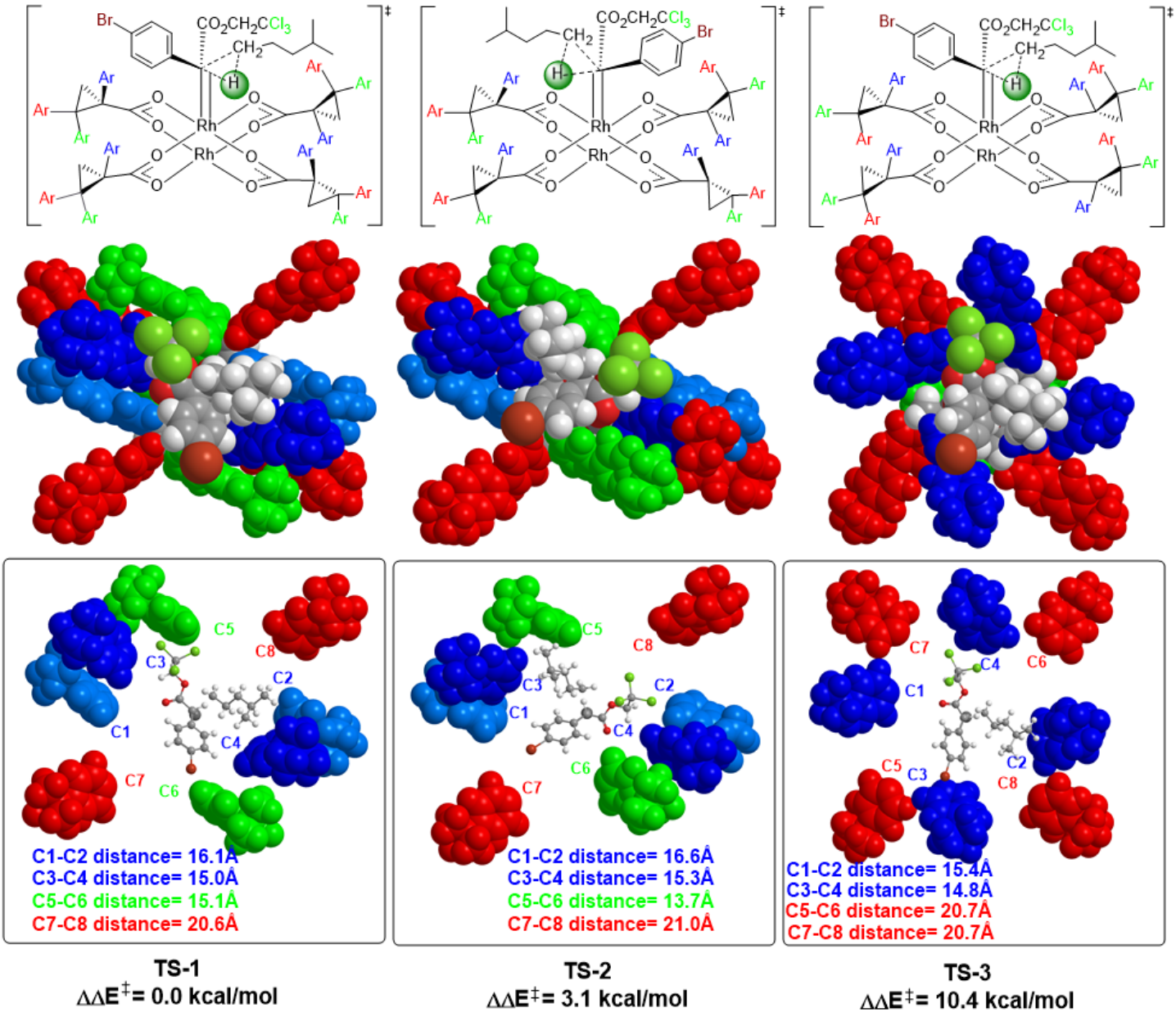
Supplementary Figure 10. Structural information about the dirhodium catalyst I. a, ONIOM partitioning of the catalyst with the atoms inside the purple rectangle modeled with DFT and the atoms outside modeled with the UFF, along with the relative energies of the D2 and C4a conformations. b, Top and side views of the D2 and C4a conformations.



Supplementary Figure 11. ONIOM transition structures for carbene insertion into the least hindered primary C–H bond with C_2 and C_4-catalyst.



Supplementary Figure 12. Structural information about the dirhodium catalyst I. a, ONIOM partitioning of the catalyst with the atoms inside the purple rectangle modeled with DFT and the atoms outside modeled with the UFF, along with the relative energies of the C2-carbene and C4-carbene conformations. b, Top views of the C2-carbene and C4-carbene conformations.



Supplementary Figure 13. Optimized geometries of the primary and primary enantiomeric C–H bond activation transition states.

Cartesian coordinates of the structures

catalyst I (C_2) (E = -973.3576356 a.u. ; Esol = -973.46376139 a.u.)

C	-2.3845	-1.09716	0.773495	H
C	-3.7764	-1.72575	0.80406	L
C	-3.76185	-3.05216	1.573852	L
H	-4.35373	-3.8901	1.17446	L
H	-2.83663	-3.27817	2.147002	L
C	-4.59135	-1.88782	2.131799	L
C	-4.06959	-1.17053	3.351925	L
C	-3.62471	-1.8889	4.471446	L
H	-3.72905	-2.96614	4.507735	L
C	-2.98727	-1.22602	5.524292	L
H	-2.61111	-1.80466	6.357754	L
C	-2.7877	0.164534	5.472675	L
C	-3.29938	0.888645	4.382782	L
H	-3.18029	1.963791	4.331722	L
C	-3.95402	0.227792	3.341235	L
H	-4.30578	0.795215	2.490087	L
C	-6.09548	-2.04461	2.007165	L
C	-6.86988	-0.9772	1.532331	L
H	-6.43311	0.005277	1.412443	L
C	-8.17098	-1.20195	1.08303	L
H	-8.71649	-0.39381	0.620771	L
C	-8.74064	-2.48115	1.15901	L
C	-8.02758	-3.50592	1.802622	L
H	-8.45031	-4.49751	1.89808	L
C	-6.71568	-3.28639	2.232266	L
H	-6.1591	-4.11095	2.65929	L
C	-4.60959	-1.60196	-0.46787	L
C	-5.08777	-2.71273	-1.17719	L
H	-4.78905	-3.70291	-0.91595	L
C	-6.0066	-2.55985	-2.21429	L
H	-6.39837	-3.44898	-2.68655	L
C	-6.45259	-1.28311	-2.59071	L
C	-5.89479	-0.16351	-1.94959	L
H	-6.18346	0.833919	-2.24325	L
C	-4.98127	-0.32191	-0.90362	L
H	-4.60755	0.552957	-0.38816	L
C	1.116363	-2.40601	0.799821	H
C	1.921154	-3.6915	0.832104	L
C	1.240882	-5.06775	0.569446	L
C	1.592083	-4.62863	1.997338	L
H	0.725421	-4.32146	2.622935	L
H	2.451432	-5.15057	2.463728	L
C	3.382275	-3.55727	0.455368	L

C	3.725787	-3.35351	-0.88761	L
H	2.954178	-3.2666	-1.64146	L
C	5.062786	-3.25309	-1.27221	L
H	5.28486	-3.08055	-2.31717	L
C	6.091651	-3.31676	-0.31408	L
C	5.741285	-3.47002	1.040422	L
H	6.501251	-3.51986	1.80897	L
C	4.401136	-3.56988	1.422535	L
H	4.167076	-3.65516	2.475171	L
C	2.086354	-6.18925	-0.00288	L
C	2.395064	-6.18767	-1.3709	L
H	2.032565	-5.39516	-2.01178	L
C	3.164029	-7.21116	-1.92787	L
H	3.39139	-7.17726	-2.98601	L
C	3.608647	-8.28163	-1.13387	L
C	3.243737	-8.31751	0.223305	L
H	3.562334	-9.13402	0.858971	L
C	2.477377	-7.28955	0.779668	L
H	2.191462	-7.35805	1.821019	L
C	-0.24275	-5.2012	0.31915	L
C	-1.00088	-6.08133	1.109208	L
H	-0.5582	-6.55332	1.977623	L
C	-2.3119	-6.41035	0.753475	L
H	-2.85578	-7.11515	1.368897	L
C	-2.89322	-5.87332	-0.40825	L
C	-2.13495	-4.97489	-1.18672	L
H	-2.55491	-4.51855	-2.07361	L
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H	-0.2381	-4.0223	-1.49057	L
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C	3.826622	1.672136	0.728661	L
C	3.815123	3.024488	1.447607	L
H	4.41606	3.827071	0.988635	L
H	2.878985	3.288931	1.985324	L
C	4.615104	1.871506	2.069572	L
C	4.056419	1.196461	3.29823	L
C	3.581744	1.951055	4.381176	L
H	3.685939	3.028875	4.38474	L
C	2.916975	1.322533	5.438746	L
H	2.520448	1.928265	6.243301	L
C	2.719867	-0.06968	5.4289	L
C	3.258293	-0.82857	4.375762	L
H	3.142772	-1.90536	4.356823	L
C	3.938235	-0.20213	3.329436	L
H	4.310599	-0.79967	2.50712	L
C	6.122972	2.037121	2.000781	L

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H	6.134267	4.139783	2.531939	L
C	8.05714	3.500391	1.844727	L
H	8.463563	4.501446	1.905005	L
C	8.823339	2.443583	1.326747	L
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H	8.857037	0.317062	0.945489	L
C	6.937726	0.947764	1.659647	L
H	6.521698	-0.04814	1.590941	L
C	4.69122	1.510477	-0.51529	L
C	5.040612	2.591087	-1.33845	L
H	4.595443	3.554626	-1.19454	L
C	6.005706	2.445416	-2.33768	L
H	6.272946	3.309909	-2.932	L
C	6.629868	1.204192	-2.55179	L
C	6.196985	0.099038	-1.80022	L
H	6.652134	-0.868	-1.94098	L
C	5.224362	0.248139	-0.80679	L
H	4.944034	-0.60538	-0.20416	L
C	-1.1384	2.37637	0.696433	H
C	-1.96493	3.652054	0.694375	L
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C	-1.64507	4.609124	1.848448	L
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C	-3.43925	3.491211	0.376408	L
C	-3.85533	3.357171	-0.95476	L
H	-3.1262	3.32895	-1.75324	L
C	-5.21276	3.248188	-1.26937	L
H	-5.48954	3.146089	-2.30993	L
C	-6.18726	3.215108	-0.25258	L
C	-5.75883	3.30846	1.085716	L
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C	-4.40278	3.427219	1.395715	L
H	-4.11122	3.472289	2.436521	L
C	-2.16067	6.14393	-0.16477	L
C	-2.57499	7.238954	0.613663	L
H	-2.29975	7.313462	1.65736	L
C	-3.33957	8.262187	0.0471	L
H	-3.64684	9.091815	0.671466	L
C	-3.67553	8.231334	-1.31737	L
C	-3.20901	7.166279	-2.10663	L
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C	-2.44477	6.144889	-1.53825	L
H	-2.06819	5.354897	-2.17422	L
C	0.176944	5.178138	0.168597	L

C	0.766634	4.614098	-0.96899	L
H	0.190663	3.973295	-1.62333	L
C	2.089271	4.918808	-1.30388	L
H	2.515925	4.452237	-2.18183	L
C	2.844479	5.815052	-0.5193	L
C	2.245225	6.377197	0.621509	L
H	2.780752	7.089289	1.235694	L
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H	0.472781	6.55277	1.811959	L
O	0.936376	-1.81779	1.910242	H
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O	1.806407	0.956651	1.798357	H
O	1.949056	0.723957	-0.43292	H
O	-0.9358	1.834276	1.826983	H
O	-0.79539	1.892887	-0.4264	H
O	-1.78195	-0.93458	1.875385	H
O	-1.90454	-0.8053	-0.36733	H
C	-7.63427	3.036648	-0.58049	L
C	-8.48522	2.343274	0.295314	L
C	-8.17839	3.541456	-1.77449	L
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C	-9.52785	3.343714	-2.08993	L
H	-7.56689	4.106921	-2.46518	L
C	-10.3858	2.638483	-1.21454	L
H	-10.4401	1.603649	0.694224	L
H	-9.8805	3.754496	-3.02402	L
C	7.514225	-3.15254	-0.72408	L
C	8.421049	-2.46436	0.096826	L
C	7.962402	-3.62475	-1.9687	L
C	9.732449	-2.23623	-0.32285	L
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C	9.269896	-3.38437	-2.39764	L
H	7.300938	-4.18313	-2.61859	L
C	10.18279	-2.67288	-1.58647	L
H	10.39114	-1.69834	0.345021	L
H	9.544635	-3.76408	-3.37013	L
C	7.757827	1.073946	-3.51615	L
C	8.686682	2.115229	-3.66573	L
C	7.941757	-0.10028	-4.26445	L
C	9.767481	1.990555	-4.53876	L
H	8.597479	3.021806	-3.08459	L
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H	7.240899	-0.92151	-4.18477	L
C	9.955149	0.823157	-5.30833	L
H	10.46034	2.818201	-4.60602	L

H	9.102615	-1.15299	-5.69282	L
C	-7.53484	-1.12347	-3.60074	L
C	-8.48063	-0.0946	-3.47039	L
C	-7.66616	-2.02264	-4.67201	L
C	-9.5301	0.027899	-4.37943	L
H	-8.43588	0.599112	-2.64168	L
C	-8.73032	-1.91362	-5.57175	L
H	-6.94363	-2.81433	-4.82206	L
C	-9.69399	-0.88801	-5.4381	L
H	-10.2264	0.839448	-4.23927	L
H	-8.78042	-2.64466	-6.36457	L
C	4.437328	-9.36228	-1.72503	L
C	5.461939	-9.05756	-2.6334	L
C	4.209562	-10.7045	-1.38876	L
C	6.242062	-10.0709	-3.19644	L
H	5.672794	-8.02873	-2.89842	L
C	4.986314	-11.7199	-1.95115	L
H	3.415313	-10.9735	-0.70365	L
C	6.019804	-11.4285	-2.86839	L
H	7.015923	-9.76831	-3.88565	L
H	4.769421	-12.7403	-1.66598	L
C	-4.29669	-6.20935	-0.7872	L
C	-4.67797	-6.27544	-2.13736	L
C	-5.29315	-6.33645	0.195411	L
C	-6.02373	-6.3888	-2.4951	L
H	-3.93715	-6.20766	-2.92367	L
C	-6.6402	-6.4515	-0.16033	L
H	-5.04292	-6.28014	1.2469	L
C	-7.03912	-6.4499	-1.51666	L
H	-6.26867	-6.39652	-3.54833	L
H	-7.35639	-6.51074	0.644978	L
C	-10.0137	-2.76812	0.458722	L
C	-10.9959	-3.57977	1.040678	L
C	-10.2165	-2.28287	-0.84061	L
C	-12.1554	-3.90983	0.331965	L
H	-10.8645	-3.96427	2.044494	L
C	-11.3642	-2.61954	-1.55492	L
H	-9.46372	-1.67442	-1.3231	L
C	-12.3606	-3.44174	-0.98812	L
H	-12.873	-4.54263	0.831778	L
H	-11.4602	-2.24147	-2.56341	L
C	-4.49326	9.315876	-1.91765	L
C	-5.59291	9.84573	-1.22645	L
C	-4.18143	9.828864	-3.1852	L
C	-6.36589	10.86557	-1.78812	L
H	-5.86844	9.458188	-0.25339	L

C	-4.95106	10.84884	-3.74878	L
H	-3.32835	9.453948	-3.73676	L
C	-6.06092	11.39163	-3.06506	L
H	-7.20052	11.22579	-1.20582	L
H	-4.66902	11.2146	-4.7266	L
C	4.255258	6.142884	-0.87722	L
C	5.224434	6.332037	0.122328	L
C	4.662337	6.193372	-2.22061	L
C	6.567278	6.520281	-0.21083	L
H	4.95712	6.28791	1.170071	L
C	6.007468	6.369014	-2.55601	L
H	3.941177	6.083405	-3.02018	L
C	6.994898	6.516281	-1.55545	L
H	7.276193	6.647842	0.595723	L
H	6.25374	6.378158	-3.60695	L
C	10.13451	2.710751	0.692186	L
C	11.05651	3.590739	1.27491	L
C	10.41798	2.168425	-0.56854	L
C	12.23255	3.936558	0.601568	L
H	10.8614	4.021834	2.249023	L
C	11.57815	2.529288	-1.25239	L
H	9.715306	1.500013	-1.04992	L
C	12.51155	3.422552	-0.68728	L
H	12.8998	4.624038	1.099022	L
H	11.73355	2.117235	-2.2392	L
C	1.94897	-0.73028	6.508254	L
C	0.984318	-1.70109	6.204188	L
C	2.186259	-0.40768	7.849761	L
C	0.291946	-2.35738	7.224791	L
H	0.766336	-1.95497	5.17376	L
C	1.494012	-1.0601	8.873535	L
H	2.937088	0.328284	8.108303	L
C	0.541379	-2.06473	8.584109	L
H	-0.42842	-3.11297	6.943158	L
H	1.737489	-0.77868	9.886629	L
C	-2.03515	0.857072	6.543916	L
C	-1.04846	1.800558	6.226183	L
C	-2.30554	0.585502	7.890137	L
C	-0.36169	2.4763	7.23766	L
H	-0.80672	2.015536	5.192187	L
C	-1.61695	1.254981	8.905151	L
H	-3.07629	-0.12637	8.157425	L
C	-0.63765	2.229386	8.600988	L
H	0.377845	3.208816	6.945175	L
H	-1.88228	1.008766	9.922051	L
C	6.852022	-12.5799	-3.47007	L

C	5.92032	-13.539	-4.24254	L
H	5.371933	-12.9881	-5.03715	L
H	6.503783	-14.3548	-4.72204	L
H	5.175524	-14.0145	-3.57077	L
C	7.557429	-13.3536	-2.335	L
H	8.199892	-12.6677	-1.74136	L
H	6.826072	-13.8282	-1.64797	L
H	8.19824	-14.1627	-2.74815	L
C	7.942654	-12.0912	-4.45365	L
H	8.666039	-11.4203	-3.94166	L
H	8.517689	-12.9501	-4.86334	L
H	7.488249	-11.5543	-5.31434	L
C	-8.51978	-6.48422	-1.9537	L
C	-9.5032	-6.55612	-0.7616	L
H	-10.5568	-6.56954	-1.11725	L
H	-9.33721	-7.47925	-0.16552	L
H	-9.38808	-5.67021	-0.10413	L
C	-8.84957	-5.20374	-2.7523	L
H	-8.24738	-5.13521	-3.68228	L
H	-9.92144	-5.18421	-3.04614	L
H	-8.64313	-4.30325	-2.13614	L
C	-8.77037	-7.72126	-2.84241	L
H	-8.17937	-7.67724	-3.78077	L
H	-8.49398	-8.65007	-2.29802	L
H	-9.84242	-7.78962	-3.12905	L
C	-13.6052	-3.80467	-1.8217	L
C	-13.1664	-4.58136	-3.08225	L
H	-12.5068	-3.96917	-3.73141	L
H	-12.6121	-5.50135	-2.79536	L
H	-14.049	-4.87936	-3.68875	L
C	-14.34	-2.51219	-2.24201	L
H	-15.2677	-2.75129	-2.80578	L
H	-14.6188	-1.91739	-1.3453	L
H	-13.7103	-1.87607	-2.89774	L
C	-14.6139	-4.68931	-1.05095	L
H	-14.1514	-5.65752	-0.76063	L
H	-14.9806	-4.16886	-0.13984	L
H	-15.4986	-4.92039	-1.68336	L
C	-10.9033	-0.74412	-6.38408	L
C	-10.9405	-1.82759	-7.4882	L
H	-11.01	-2.84397	-7.04338	L
H	-11.8268	-1.69033	-8.14537	L
H	-10.036	-1.76847	-8.1315	L
C	-12.2096	-0.86117	-5.56798	L
H	-12.2974	-0.05067	-4.81447	L
H	-13.0978	-0.79469	-6.23294	L

H	-12.2446	-1.83595	-5.03699	L
C	-10.855	0.634357	-7.07836	L
H	-10.9432	1.464414	-6.34653	L
H	-9.89797	0.755334	-7.6305	L
H	-11.6921	0.740699	-7.80218	L
C	-11.8817	2.400991	-1.51172	L
C	-12.3324	2.990371	-2.87006	L
H	-13.4118	2.79139	-3.0472	L
H	-12.1895	4.092385	-2.89039	L
H	-11.7696	2.534739	-3.71082	L
C	-12.7344	3.065797	-0.40933	L
H	-13.8187	2.943809	-0.62222	L
H	-12.5389	2.614995	0.586071	L
H	-12.51	4.15285	-0.34982	L
C	-12.1734	0.883361	-1.53356	L
H	-11.5257	0.373437	-2.2751	L
H	-11.9945	0.416717	-0.54245	L
H	-13.2333	0.687191	-1.80514	L
C	0.089933	3.048058	9.688692	L
C	-0.33473	2.659455	11.12554	L
H	0.217637	3.264716	11.87702	L
H	-1.41956	2.843842	11.28227	L
H	-0.11038	1.589603	11.32878	L
C	-0.22592	4.546987	9.494476	L
H	-1.32393	4.717642	9.524346	L
H	0.243811	5.157069	10.2964	L
H	0.159321	4.921645	8.52303	L
C	1.614066	2.831477	9.580364	L
H	1.863649	1.765891	9.758021	L
H	2.003485	3.124843	8.583672	L
H	2.151674	3.438885	10.34048	L
C	-0.18201	-2.86941	9.685235	L
C	0.214566	-2.43144	11.11594	L
H	-0.33344	-3.02862	11.87703	L
H	1.301202	-2.58588	11.29134	L
H	-0.0373	-1.36198	11.28651	L
C	0.170271	-4.36552	9.537205	L
H	-0.29618	-4.96378	10.34988	L
H	-0.19348	-4.77579	8.571859	L
H	1.271358	-4.50999	9.585678	L
C	-1.7089	-2.69146	9.552078	L
H	-1.98431	-1.62708	9.694525	L
H	-2.07854	-3.02453	8.560552	L
H	-2.24229	-3.28782	10.32382	L
C	8.495076	6.673774	-1.8798	L
C	8.808132	6.522656	-3.38814	L

H	9.901186	6.604703	-3.575	L
H	8.47655	5.52961	-3.76165	L
H	8.313339	7.322666	-3.9798	L
C	9.305705	5.595767	-1.12731	L
H	10.37002	5.599322	-1.44666	L
H	9.297154	5.769709	-0.03227	L
H	8.882754	4.58876	-1.32337	L
C	8.968868	8.071485	-1.43185	L
H	8.386337	8.862282	-1.95219	L
H	8.841451	8.210066	-0.33734	L
H	10.04562	8.215941	-1.66795	L
C	11.14731	0.740017	-6.28439	L
C	12.46889	0.83172	-5.49254	L
H	13.34264	0.776537	-6.17738	L
H	12.54339	1.785443	-4.93019	L
H	12.54386	-0.00664	-4.76946	L
C	11.07286	1.909443	-7.29155	L
H	11.88917	1.836715	-8.04271	L
H	10.10065	1.894088	-7.8302	L
H	11.17788	2.892653	-6.78749	L
C	11.17411	-0.57484	-7.10015	L
H	11.28193	-1.45636	-6.43403	L
H	10.24779	-0.68347	-7.7048	L
H	12.0363	-0.58544	-7.80202	L
C	11.62754	-2.36414	-2.02778	L
C	11.9395	-2.8508	-3.4626	L
H	11.8495	-3.95605	-3.53616	L
H	11.25105	-2.37679	-4.19382	L
H	12.97792	-2.58171	-3.75483	L
C	12.61661	-3.05567	-1.06638	L
H	13.66644	-2.87241	-1.38294	L
H	12.5081	-2.67508	-0.02901	L
H	12.4409	-4.15317	-1.0551	L
C	11.86194	-0.83916	-1.99241	L
H	11.11214	-0.3201	-2.62796	L
H	11.78551	-0.43875	-0.96084	L
H	12.8779	-0.58504	-2.36424	L
C	-6.88473	12.51802	-3.72305	L
C	-7.47134	12.01353	-5.05947	L
H	-8.09782	11.11107	-4.8901	L
H	-8.105	12.79516	-5.53218	L
H	-6.67194	11.75192	-5.78379	L
C	-8.06433	13.00007	-2.84452	L
H	-7.69753	13.40779	-1.87771	L
H	-8.63015	13.81022	-3.35417	L
H	-8.7767	12.16991	-2.64742	L

C	-5.97197	13.73463	-3.99041	L
H	-5.50695	14.08415	-3.04321	L
H	-5.16065	13.48743	-4.70648	L
H	-6.55369	14.57621	-4.42545	L
C	13.76489	3.815426	-1.49434	L
C	14.57335	2.54659	-1.84612	L
H	14.84046	1.989978	-0.92185	L
H	14.00082	1.866005	-2.51027	L
H	15.51248	2.812088	-2.37833	L
C	14.70447	4.773803	-0.72453	L
H	15.59947	5.023091	-1.33522	L
H	14.1887	5.72937	-0.48709	L
H	15.06165	4.304466	0.217625	L
C	13.33209	4.524811	-2.79613	L
H	12.72783	5.427925	-2.56224	L
H	14.2195	4.841397	-3.38596	L
H	12.7227	3.858728	-3.44154	L
Rh	0.010128	-0.03252	-0.47018	H
Rh	0.01106	0.015653	1.910576	H

catalyst I (C_4) (E = -973.3335121 a.u. ; Esol = -973.44765145 a.u.)

C	2.567274	0.550416	-1.63035	H
C	4.057398	0.825628	-1.61683	L
C	4.393344	2.292991	-1.88974	L
H	5.274984	2.486308	-2.53476	L
H	3.519912	2.978396	-1.91954	L
C	4.712108	1.705711	-0.50846	L
C	3.869722	2.211853	0.641697	L
C	3.715913	3.586551	0.869276	L
H	4.174565	4.304749	0.201254	L
C	2.972315	4.046081	1.962253	L
H	2.885311	5.114155	2.108203	L
C	2.363036	3.137962	2.852973	L
C	2.567394	1.760562	2.642131	L
H	2.107892	1.020539	3.282247	L
C	3.348374	1.310232	1.577169	L
H	3.520013	0.248338	1.461026	L
C	6.186381	1.537107	-0.21053	L
C	7.095656	2.575871	-0.46939	L
H	6.759626	3.501482	-0.91956	L
C	8.447811	2.430004	-0.14816	L
H	9.131236	3.23447	-0.38894	L
C	8.913063	1.252783	0.463999	L
C	7.992316	0.234019	0.763111	L
H	8.311718	-0.66805	1.269894	L
C	6.642086	0.38306	0.441139	L
H	5.949438	-0.3977	0.715792	L
C	4.90695	-0.22464	-2.29777	L
C	5.060884	-1.46879	-1.67194	L
H	4.614851	-1.64567	-0.70329	L
C	5.767431	-2.49834	-2.29396	L
H	5.888153	-3.43855	-1.77097	L
C	6.308915	-2.31534	-3.57694	L
C	6.123141	-1.08007	-4.22286	L
H	6.495539	-0.92274	-5.22734	L
C	5.414452	-0.04998	-3.59669	L
H	5.243827	0.868487	-4.14171	L
C	-0.55332	2.548168	-1.62526	H
C	-0.83411	4.037285	-1.60849	L
C	-1.70753	4.688055	-0.49238	L
C	-2.3053	4.366926	-1.86843	L
H	-2.98674	3.490338	-1.89256	L
H	-2.50867	5.248124	-2.51096	L
C	0.204123	4.890436	-2.30289	L
C	0.013761	5.389395	-3.60294	L

H	-0.90978	5.212168	-4.13723	L
C	1.034863	6.096712	-4.2449	L
H	0.865626	6.461767	-5.25018	L
C	2.276821	6.289097	-3.61421	L
C	2.475252	5.757234	-2.32954	L
H	3.421331	5.882923	-1.81828	L
C	1.454248	5.052662	-1.69129	L
H	1.64325	4.612932	-0.72212	L
C	-1.54281	6.162886	-0.1959	L
C	-2.58819	7.067392	-0.44474	L
H	-3.5165	6.727232	-0.88619	L
C	-2.44556	8.420137	-0.12447	L
H	-3.25543	9.099907	-0.35743	L
C	-1.26481	8.890632	0.476849	L
C	-0.23906	7.974458	0.766135	L
H	0.666116	8.29781	1.264705	L
C	-0.38485	6.623592	0.445168	L
H	0.4013	5.934234	0.712761	L
C	-2.20363	3.844043	0.661156	L
C	-3.57642	3.689735	0.900333	L
H	-4.30037	4.14899	0.238983	L
C	-4.02659	2.945204	1.996701	L
H	-5.09334	2.858177	2.152122	L
C	-3.11079	2.335617	2.879309	L
C	-1.73531	2.539708	2.65634	L
H	-0.98992	2.079826	3.289832	L
C	-1.29416	3.321845	1.588367	L
H	-0.23353	3.494519	1.463714	L
C	-2.54834	-0.567	-1.6138	H
C	-4.03857	-0.842	-1.59129	L
C	-4.37461	-2.31099	-1.85524	L
H	-5.25765	-2.50708	-2.49755	L
H	-3.50048	-2.99512	-1.88513	L
C	-4.68871	-1.71712	-0.47603	L
C	-3.84149	-2.21737	0.673268	L
C	-3.68879	-3.59091	0.908867	L
H	-4.1524	-4.31254	0.248014	L
C	-2.94017	-4.04476	2.000975	L
H	-2.85468	-5.112	2.153762	L
C	-2.32436	-3.13194	2.882429	L
C	-2.52671	-1.75562	2.663008	L
H	-2.06181	-1.01224	3.295158	L
C	-3.31329	-1.31081	1.599941	L
H	-3.48412	-0.24951	1.478228	L
C	-6.16149	-1.54524	-0.17282	L
C	-6.61105	-0.39173	0.484044	L

H	-5.91457	0.385173	0.760048	L
C	-7.95994	-0.2383	0.809445	L
H	-8.27444	0.663382	1.319888	L
C	-8.88557	-1.25219	0.508793	L
C	-8.4263	-2.42954	-0.1077	L
H	-9.11343	-3.23054	-0.34948	L
C	-7.07537	-2.57993	-0.4322	L
H	-6.74423	-3.50583	-0.88537	L
C	-4.89109	0.200356	-2.28023	L
C	-5.38588	0.018559	-3.58304	L
H	-5.20441	-0.90065	-4.12347	L
C	-6.09538	1.042167	-4.2187	L
H	-6.45746	0.879437	-5.22612	L
C	-6.29467	2.278161	-3.57831	L
C	-5.76608	2.468349	-2.291	L
H	-5.89679	3.40958	-1.77213	L
C	-5.05863	1.445122	-1.65953	L
H	-4.62095	1.628376	-0.68847	L
C	0.566757	-2.56654	-1.61984	H
C	0.833305	-4.05824	-1.60352	L
C	1.70899	-4.71794	-0.4944	L
C	2.299091	-4.40234	-1.87499	L
H	2.988991	-3.53246	-1.90464	L
H	2.486192	-5.28406	-2.52182	L
C	-0.21612	-4.90035	-2.29438	L
C	-1.45984	-5.06447	-1.67066	L
H	-1.63591	-4.63608	-0.69418	L
C	-2.49307	-5.75169	-2.30803	L
H	-3.4343	-5.87809	-1.78807	L
C	-2.31449	-6.26169	-3.6044	L
C	-1.07811	-6.06887	-4.24595	L
H	-0.92365	-6.41706	-5.25955	L
C	-0.04417	-5.3802	-3.60411	L
H	0.87458	-5.20017	-4.14585	L
C	1.525911	-6.1903	-0.1956	L
C	0.371695	-6.63216	0.465188	L
H	-0.39648	-5.9296	0.749892	L
C	0.205478	-7.98165	0.781506	L
H	-0.69696	-8.29029	1.294205	L
C	1.207181	-8.91602	0.467498	L
C	2.386427	-8.46474	-0.15133	L
H	3.178388	-9.15874	-0.40309	L
C	2.54962	-7.11307	-0.46669	L
H	3.47624	-6.78863	-0.92318	L
C	2.217944	-3.87699	0.655828	L
C	1.317784	-3.346	1.58718	L

H	0.255284	-3.51272	1.470314	L
C	1.770383	-2.5593	2.646942	L
H	1.031634	-2.09125	3.282198	L
C	3.148367	-2.35939	2.857974	L
C	4.054784	-2.98006	1.973269	L
H	5.123058	-2.89716	2.12009	L
C	3.593101	-3.7288	0.88455	L
H	4.309879	-4.19463	0.220038	L
O	-0.12011	2.028056	-0.55657	H
O	-0.70291	1.941916	-2.73291	H
O	-2.02196	-0.13794	-0.5465	H
O	-1.94714	-0.71738	-2.72415	H
O	0.14499	-2.04105	-0.54922	H
O	0.71313	-1.96368	-2.72981	H
O	2.047105	0.125686	-0.55827	H
O	1.960186	0.695829	-2.73808	H
C	-3.42568	-6.96	-4.29767	L
C	-3.17947	-8.10609	-5.06743	L
C	-4.74072	-6.48197	-4.19795	L
C	-4.22414	-8.76392	-5.72248	L
H	-2.17663	-8.50657	-5.15038	L
C	-5.78643	-7.13616	-4.85221	L
H	-4.96071	-5.5878	-3.62754	L
C	-5.55436	-8.29201	-5.62941	L
H	-3.96797	-9.64259	-6.29496	L
H	-6.78246	-6.72784	-4.74883	L
C	3.371947	7.013541	-4.30596	L
C	4.693029	6.547844	-4.23245	L
C	3.104158	8.173674	-5.04694	L
C	5.72369	7.227784	-4.88443	L
H	4.929284	5.643924	-3.68437	L
C	4.133716	8.857499	-5.6992	L
H	2.096159	8.564918	-5.10887	L
C	5.469931	8.398333	-5.63237	L
H	6.72518	6.828118	-4.8022	L
H	3.861233	9.745966	-6.24856	L
C	-7.0243	3.375352	-4.2617	L
C	-8.18068	3.10725	-5.0085	L
C	-6.56846	4.699004	-4.17295	L
C	-8.87052	4.13882	-5.65121	L
H	-8.56474	2.097282	-5.08207	L
C	-7.25471	5.731763	-4.81499	L
H	-5.66765	4.936072	-3.62013	L
C	-8.42166	5.477623	-5.56838	L
H	-9.75573	3.865845	-6.20557	L
H	-6.86299	6.735305	-4.72042	L

C	7.03891	-3.41898	-4.24972	L
C	6.574534	-4.7397	-4.16133	L
C	8.204753	-3.16013	-4.98501	L
C	7.261894	-5.77869	-4.7921	L
H	5.666513	-4.9697	-3.6174	L
C	8.895776	-4.19803	-5.61632	L
H	8.595375	-2.15265	-5.058	L
C	8.43862	-5.53403	-5.53333	L
H	6.863498	-6.77966	-4.6982	L
H	9.78856	-3.93217	-6.16191	L
Rh	0.006047	-0.01074	-2.83561	H
Rh	0.013203	-0.00628	-0.46515	H
C	10.34989	1.092253	0.802444	L
C	10.99686	-0.13544	0.599663	L
C	11.0846	2.163767	1.331429	L
C	12.34808	-0.28846	0.917373	L
H	10.46145	-0.97676	0.177341	L
C	12.43658	2.013556	1.651777	L
H	10.6082	3.118547	1.516385	L
C	13.10029	0.780869	1.450871	L
H	12.80401	-1.25279	0.739446	L
H	12.94275	2.875646	2.059243	L
C	1.494243	3.615629	3.972891	L
C	1.347401	2.858949	5.148827	L
C	0.75814	4.807182	3.856816	L
C	0.463555	3.255142	6.154925	L
H	1.91853	1.955332	5.303085	L
C	-0.12586	5.205672	4.860333	L
H	0.825515	5.419911	2.971156	L
C	-0.31093	4.429405	6.022864	L
H	0.39427	2.619303	7.024695	L
H	-0.67884	6.123073	4.711787	L
C	3.628229	-1.48302	3.971179	L
C	4.823857	-0.75418	3.851144	L
C	2.869772	-1.32142	5.144127	L
C	5.224673	0.137022	4.847375	L
H	5.438483	-0.83324	2.96786	L
C	3.268092	-0.43004	6.142765	L
H	1.963265	-1.88688	5.302011	L
C	4.446737	0.336965	6.006307	L
H	6.145383	0.683659	4.695951	L
H	2.630762	-0.34951	7.01046	L
C	1.02574	-10.3529	0.79506	L
C	2.089521	-11.1104	1.307242	L
C	-0.21433	-10.9775	0.59723	L
C	1.919685	-12.4629	1.615655	L

H	3.053728	-10.6517	1.488022	L
C	-0.38701	-12.329	0.903179	L
H	-1.05035	-10.4243	0.187526	L
C	0.674422	-13.1041	1.419274	L
H	2.776837	-12.9873	2.010224	L
H	-1.36036	-12.7671	0.72956	L
C	-1.45169	-3.6034	4.002058	L
C	-1.29731	-2.83773	5.171249	L
C	-0.71968	-4.79812	3.892479	L
C	-0.41003	-3.22818	6.176513	L
H	-1.86545	-1.93158	5.321089	L
C	0.167493	-5.19112	4.89546	L
H	-0.79296	-5.41803	3.012345	L
C	0.360168	-4.40587	6.050718	L
H	-0.33508	-2.58549	7.040726	L
H	0.716809	-6.11154	4.752214	L
C	-10.3212	-1.08631	0.849758	L
C	-11.0604	-2.15653	1.375165	L
C	-10.9627	0.1452	0.652661	L
C	-12.4114	-2.00136	1.697372	L
H	-10.5883	-3.11424	1.555839	L
C	-12.3129	0.303227	0.97242	L
H	-10.4239	0.98576	0.233178	L
C	-13.0695	-0.7648	1.502143	L
H	-12.9212	-2.86276	2.101764	L
H	-12.7644	1.27042	0.798998	L
C	-3.57865	1.468388	4.004547	L
C	-2.81219	1.324439	5.174494	L
C	-4.77123	0.732131	3.900319	L
C	-3.20063	0.444258	6.186781	L
H	-1.90728	1.895768	5.319581	L
C	-5.16221	-0.14801	4.910307	L
H	-5.39114	0.797149	3.019462	L
C	-4.37685	-0.32925	6.067374	L
H	-2.55774	0.377605	7.051517	L
H	-6.0814	-0.70049	4.771471	L
C	-1.10775	10.3281	0.814083	L
C	0.114899	10.98086	0.599707	L
C	-2.1777	11.0578	1.353113	L
C	0.264452	12.3329	0.915727	L
H	0.954732	10.44939	0.169542	L
C	-2.03092	12.41057	1.671801	L
H	-3.12841	10.57693	1.547129	L
C	-0.8034	13.08013	1.459091	L
H	1.22485	12.7934	0.728597	L
H	-2.89154	12.91271	2.08727	L

C	-14.5587	-0.54826	1.842546	L
C	-15.3244	-0.13789	0.565795	L
H	-15.2058	-0.91341	-0.22169	L
H	-16.4091	-0.01799	0.777713	L
H	-14.9568	0.828327	0.16153	L
C	-15.2415	-1.81481	2.412871	L
H	-14.7518	-2.13789	3.356982	L
H	-16.3108	-1.61624	2.643679	L
H	-15.2089	-2.6477	1.677514	L
C	-14.6878	0.570009	2.899642	L
H	-14.1065	0.309401	3.81054	L
H	-14.3146	1.541758	2.51421	L
H	-15.7504	0.714954	3.192762	L
C	-9.15091	6.647521	-6.26108	L
C	-10.4094	6.200437	-7.04329	L
H	-10.1414	5.481974	-7.84794	L
H	-11.1527	5.730904	-6.36311	L
H	-10.9038	7.071549	-7.526	L
C	-8.19417	7.329677	-7.26308	L
H	-8.7116	8.149882	-7.80663	L
H	-7.31519	7.774092	-6.75123	L
H	-7.82736	6.592582	-8.0099	L
C	-9.59955	7.675318	-5.19947	L
H	-10.2557	7.189822	-4.44492	L
H	-8.73176	8.122042	-4.67077	L
H	-10.1657	8.507847	-5.67095	L
C	-4.82541	-1.33995	7.142683	L
C	-6.18031	-0.8914	7.729499	L
H	-6.97348	-0.87434	6.952701	L
H	-6.51147	-1.58571	8.532074	L
H	-6.09499	0.12873	8.162718	L
C	-4.98172	-2.7413	6.509322	L
H	-4.0316	-3.06201	6.033294	L
H	-5.25499	-3.49415	7.280176	L
H	-5.77902	-2.75749	5.7377	L
C	-3.81936	-1.46617	8.312133	L
H	-2.82401	-1.79577	7.942903	L
H	-3.71086	-0.49933	8.849473	L
H	-4.16799	-2.21839	9.052831	L
C	-1.32753	4.884838	7.089662	L
C	-0.88493	6.245785	7.666913	L
H	-0.8662	7.032398	6.883523	L
H	-1.58377	6.582069	8.463391	L
H	0.133372	6.166656	8.105573	L
C	-2.72618	5.03236	6.448282	L
H	-3.04207	4.077646	5.978223	L

H	-3.48349	5.309807	7.213244	L
H	-2.74063	5.823384	5.670178	L
C	-1.45682	3.888596	8.267112	L
H	-1.78287	2.889451	7.905148	L
H	-0.49208	3.786655	8.809496	L
H	-2.21295	4.242068	9.001495	L
C	1.379798	-4.85575	7.11695	L
C	2.77517	-5.01348	6.470891	L
H	3.534749	-5.2874	7.234868	L
H	2.783507	-5.81085	5.699206	L
H	3.092367	-4.06369	5.991783	L
C	1.517632	-3.84995	8.285298	L
H	2.275866	-4.19966	9.019319	L
H	1.845331	-2.85499	7.913279	L
H	0.555678	-3.74021	8.831093	L
C	0.935007	-6.2102	7.70765	L
H	-0.08112	-6.12379	8.149966	L
H	0.910147	-7.00333	6.931028	L
H	1.636091	-6.54218	8.503962	L
C	4.90544	1.360591	7.06496	L
C	5.062439	2.752542	6.411323	L
H	5.341951	3.515269	7.170123	L
H	5.855698	2.755538	5.635366	L
H	4.11083	3.069366	5.935636	L
C	3.90726	1.506128	8.238894	L
H	3.798703	0.546945	8.789767	L
H	4.263291	2.266903	8.967228	L
H	2.910771	1.834432	7.871727	L
C	6.262522	0.915541	7.649427	L
H	6.17658	-0.09827	8.097108	L
H	7.050823	0.885215	6.868097	L
H	6.600966	1.619659	8.440329	L
C	0.441747	-14.5944	1.743964	L
C	1.702738	-15.2985	2.300464	L
H	1.492535	-16.3679	2.520181	L
H	2.532491	-15.2674	1.561509	L
H	2.036026	-14.8234	3.248444	L
C	-0.67305	-14.7222	2.804873	L
H	-0.40135	-14.1543	3.721003	L
H	-1.64209	-14.3332	2.428313	L
H	-0.82925	-15.7862	3.086688	L
C	0.016345	-15.3406	0.460646	L
H	-0.94734	-14.9571	0.065219	L
H	0.789489	-15.2223	-0.3292	L
H	-0.11543	-16.4262	0.660883	L
C	-6.73788	-8.98453	-6.33645	L

C	-7.40168	-7.99455	-7.31831	L
H	-8.23156	-8.48494	-7.87211	L
H	-7.82928	-7.11797	-6.78833	L
H	-6.6577	-7.6265	-8.05766	L
C	-7.77404	-9.43527	-5.2839	L
H	-8.61716	-9.97567	-5.7666	L
H	-7.30111	-10.1159	-4.54314	L
H	-8.20424	-8.57018	-4.73735	L
C	-6.31475	-10.2349	-7.14454	L
H	-5.59141	-9.96399	-7.94385	L
H	-5.85928	-11.0007	-6.47998	L
H	-7.1951	-10.7027	-7.6369	L
C	9.169093	-6.71071	-6.21305	L
C	10.43919	-6.27389	-6.98224	L
H	10.93421	-7.14969	-7.45571	L
H	10.18465	-5.55716	-7.79279	L
H	11.17707	-5.80582	-6.29525	L
C	9.599487	-7.73699	-5.1424	L
H	8.723083	-8.17686	-4.62224	L
H	10.16641	-8.5745	-5.60403	L
H	10.24948	-7.25229	-4.38202	L
C	8.220114	-7.39124	-7.2235	L
H	7.866346	-6.65495	-7.97736	L
H	8.738968	-8.2166	-7.75783	L
H	7.332623	-7.82847	-6.72021	L
C	6.637352	9.11978	-6.33724	L
C	7.298844	8.160215	-7.3503	L
H	8.11695	8.67208	-7.90219	L
H	7.741502	7.275712	-6.84648	L
H	6.549536	7.802241	-8.08922	L
C	7.681968	9.556555	-5.28713	L
H	8.513183	10.11736	-5.7672	L
H	7.211325	10.2142	-4.52451	L
H	8.128195	8.683467	-4.76681	L
C	6.191365	10.38438	-7.1102	L
H	5.461279	10.12479	-7.90712	L
H	5.735983	11.12919	-6.42216	L
H	7.060722	10.87311	-7.60168	L
C	14.59077	0.569836	1.788981	L
C	15.26802	1.836964	2.364625	L
H	16.33846	1.642363	2.59376	L
H	15.23097	2.673054	1.63313	L
H	14.7775	2.153392	3.310546	L
C	15.35717	0.169091	0.509646	L
H	16.44263	0.053216	0.720057	L
H	14.99371	-0.79689	0.101123	L

H	15.23436	0.947772	-0.27404	L
C	14.72622	-0.55271	2.840743	L
H	14.14437	-0.29922	3.753313	L
H	14.35751	-1.52448	2.451079	L
H	15.7897	-0.69382	3.132335	L
C	-0.59641	14.57173	1.79475	L
C	0.535363	14.71299	2.835806	L
H	1.50518	14.34886	2.437067	L
H	0.674062	15.77723	3.125759	L
H	0.293335	14.13021	3.750891	L
C	-0.21151	15.33965	0.511454	L
H	-0.99702	15.21288	-0.26476	L
H	-0.09884	16.42571	0.720458	L
H	0.752253	14.98068	0.093855	L
C	-1.8613	15.24306	2.382158	L
H	-2.70409	15.20174	1.658614	L
H	-2.1664	14.75133	3.33117	L
H	-1.66973	16.31451	2.609137	L

catalyst I (C_{4a}) (E = -973.31373745 a.u. ; Esol = -973.42920947 a.u.)

C	1.69699	-0.08292	2.076376	H
C	2.77181	-0.162	3.161899	L
C	2.291863	-0.97636	4.364202	L
H	2.516664	-0.52913	5.354296	L
H	1.359631	-1.56	4.215004	L
C	3.495814	-1.48365	3.560389	L
C	3.325553	-2.65458	2.626562	L
C	2.783595	-3.86702	3.071783	L
H	2.436463	-3.96916	4.092042	L
C	2.720782	-4.96634	2.208911	L
H	2.328683	-5.90159	2.581439	L
C	3.213104	-4.87607	0.893318	L
C	3.763494	-3.66061	0.45718	L
H	4.150436	-3.5602	-0.54841	L
C	3.827671	-2.56577	1.321019	L
H	4.279009	-1.64451	0.982095	L
C	4.82093	-1.42239	4.299641	L
C	5.99895	-1.07821	3.618633	L
H	5.979233	-0.85812	2.561588	L
C	7.222533	-1.03322	4.290667	L
H	8.112424	-0.75974	3.737688	L
C	7.301373	-1.36791	5.653037	L
C	6.132748	-1.77306	6.320243	L
H	6.160808	-2.04432	7.368043	L
C	4.909467	-1.81477	5.646693	L
H	4.031203	-2.15232	6.181944	L
C	3.532701	1.122117	3.415172	L
C	4.502386	1.509249	2.479849	L
H	4.740079	0.864564	1.643714	L
C	5.135572	2.745864	2.581355	L
H	5.870036	3.020648	1.834666	L
C	4.776428	3.645988	3.595575	L
C	3.782333	3.274935	4.518412	L
H	3.478234	3.957645	5.302016	L
C	3.15929	2.024882	4.424908	L
H	2.363159	1.782971	5.116345	L
C	-2.17647	-0.05565	1.643602	H
C	-3.5086	-0.05357	2.399543	L
C	-3.94904	-1.28642	3.238472	L
C	-4.56318	-1.02054	1.858193	L
H	-4.22191	-1.6996	1.054385	L
H	-5.61132	-0.65605	1.862578	L
C	-4.064	1.318885	2.749102	L
C	-4.93701	1.981961	1.869973	L

H	-5.30736	1.487461	0.983631	L
C	-5.30948	3.306917	2.098994	L
H	-5.96122	3.789872	1.384119	L
C	-4.79987	4.014605	3.200929	L
C	-3.92613	3.350007	4.082189	L
H	-3.51654	3.858917	4.945047	L
C	-3.54798	2.024701	3.845824	L
H	-2.81203	1.567138	4.492084	L
C	-4.86573	-1.07356	4.424219	L
C	-4.337	-0.57587	5.623561	L
H	-3.28362	-0.34119	5.699906	L
C	-5.15547	-0.39723	6.741283	L
H	-4.71811	-0.00913	7.652616	L
C	-6.51539	-0.74894	6.693118	L
C	-7.03137	-1.30297	5.50868	L
H	-8.07271	-1.59186	5.442122	L
C	-6.21128	-1.47834	4.391124	L
H	-6.63056	-1.93493	3.504134	L
C	-3.09488	-2.5284	3.284737	L
C	-3.63576	-3.7627	2.893933	L
H	-4.6562	-3.82451	2.536101	L
C	-2.86731	-4.92492	2.961215	L
H	-3.31628	-5.86208	2.657019	L
C	-1.54538	-4.87947	3.438546	L
C	-1.01785	-3.64368	3.858291	L
H	-0.00437	-3.57338	4.225944	L
C	-1.78918	-2.48006	3.790584	L
H	-1.36647	-1.53992	4.123093	L
C	-1.74616	0.391846	-1.89316	H
C	-2.79075	0.56003	-2.99874	L
C	-2.27674	0.05861	-4.3497	L
H	-2.50904	0.705328	-5.22033	L
H	-1.32856	-0.51756	-4.32361	L
C	-3.47544	-0.64938	-3.70394	L
C	-3.27181	-2.0099	-3.08571	L
C	-3.79489	-2.27157	-1.81105	L
H	-4.29533	-1.48571	-1.26197	L
C	-3.68463	-3.54396	-1.24537	L
H	-4.09353	-3.72162	-0.25914	L
C	-3.05567	-4.58106	-1.95091	L
C	-2.53973	-4.31907	-3.2334	L
H	-2.08375	-5.11127	-3.8116	L
C	-2.65842	-3.04683	-3.80182	L
H	-2.29232	-2.87646	-4.80612	L
C	-4.79689	-0.44606	-4.42216	L
C	-4.8718	-0.53028	-5.82318	L

H	-3.98471	-0.726	-6.41195	L
C	-6.09254	-0.35924	-6.48086	L
H	-6.11128	-0.39175	-7.56292	L
C	-7.27101	-0.13036	-5.75002	L
C	-7.20405	-0.10399	-4.34666	L
H	-8.1009	0.027098	-3.75423	L
C	-5.98297	-0.27793	-3.69122	L
H	-5.97047	-0.29535	-2.61134	L
C	-3.5725	1.858601	-2.96849	L
C	-3.23422	2.959043	-3.77478	L
H	-2.43777	2.888739	-4.50324	L
C	-3.89634	4.182001	-3.61383	L
H	-3.60905	5.020867	-4.23545	L
C	-4.88091	4.334647	-2.62136	L
C	-5.20335	3.237163	-1.80865	L
H	-5.96283	3.322528	-1.04254	L
C	-4.54419	2.019979	-1.97182	L
H	-4.77179	1.202528	-1.30124	L
C	2.096141	0.477258	-1.42775	H
C	3.413094	0.735977	-2.16515	L
C	3.927468	-0.24884	-3.25408	L
C	4.529176	-0.25989	-1.8433	L
H	4.237949	-1.12978	-1.22547	L
H	5.552846	0.159377	-1.757	L
C	3.869574	2.186704	-2.21794	L
C	3.271484	3.069096	-3.12943	L
H	2.528187	2.710505	-3.82829	L
C	3.590602	4.429581	-3.11786	L
H	3.125843	5.080156	-3.84789	L
C	4.491875	4.944807	-2.16938	L
C	5.065856	4.067589	-1.23414	L
H	5.733742	4.439683	-0.46708	L
C	4.746312	2.70742	-1.24888	L
H	5.16832	2.067989	-0.48647	L
C	4.830485	0.276085	-4.35043	L
C	6.194778	-0.05864	-4.39442	L
H	6.634816	-0.68867	-3.63242	L
C	7.007801	0.416161	-5.42664	L
H	8.062727	0.172804	-5.41366	L
C	6.467425	1.209013	-6.45393	L
C	5.090978	1.492999	-6.43892	L
H	4.63695	2.064062	-7.23903	L
C	4.279626	1.01486	-5.40718	L
H	3.216161	1.209338	-5.44153	L
C	3.131168	-1.48387	-3.59435	L
C	1.83793	-1.37297	-4.12241	L

H	1.384476	-0.39851	-4.25642	L
C	1.120611	-2.51974	-4.4737	L
H	0.118405	-2.40731	-4.86149	L
C	1.688663	-3.79727	-4.31432	L
C	2.995415	-3.90011	-3.80532	L
H	3.473788	-4.86544	-3.69619	L
C	3.713025	-2.75378	-3.46128	L
H	4.725891	-2.85587	-3.09153	L
O	-1.76288	-1.11709	1.080092	H
O	-1.57799	1.064663	1.603055	H
O	-1.21727	-0.74609	-1.70571	H
O	-1.46244	1.441156	-1.23388	H
O	1.73458	-0.71372	-1.17061	H
O	1.45563	1.518106	-1.08061	H
O	1.213361	-1.15299	1.597103	H
O	1.344966	1.090387	1.734764	H
C	4.805732	6.39666	-2.13436	L
C	3.794999	7.349153	-2.33155	L
C	6.116124	6.841317	-1.9039	L
C	4.086818	8.715386	-2.31402	L
H	2.769502	7.03798	-2.48743	L
C	6.412222	8.207064	-1.89051	L
H	6.920388	6.131035	-1.75792	L
C	5.406701	9.176269	-2.1011	L
H	3.262882	9.394141	-2.47446	L
H	7.439419	8.50173	-1.72426	L
C	-5.12945	5.455212	3.388003	L
C	-6.39629	5.954555	3.043318	L
C	-4.16584	6.351933	3.876098	L
C	-6.68892	7.315266	3.169317	L
H	-7.17178	5.291242	2.682208	L
C	-4.46063	7.70933	4.017218	L
H	-3.16952	6.012097	4.127742	L
C	-5.72376	8.225646	3.657547	L
H	-7.67966	7.63278	2.880827	L
H	-3.68594	8.357959	4.402578	L
C	-5.54708	5.641286	-2.40461	L
C	-5.7361	6.134327	-1.10514	L
C	-6.007	6.398468	-3.49041	L
C	-6.38461	7.352005	-0.89422	L
H	-5.36821	5.583604	-0.24871	L
C	-6.66214	7.61598	-3.28284	L
H	-5.88021	6.036458	-4.50336	L
C	-6.87155	8.117666	-1.97631	L
H	-6.50457	7.691573	0.125559	L
H	-7.00212	8.146007	-4.15971	L

C	5.390785	4.992894	3.633015	L
C	4.593637	6.134843	3.790532	L
C	6.769885	5.148707	3.438462	L
C	5.157702	7.411467	3.719016	L
H	3.523388	6.041805	3.928612	L
C	7.338332	6.421721	3.37768	L
H	7.410189	4.282089	3.327451	L
C	6.543706	7.583062	3.49326	L
H	4.487537	8.251012	3.826104	L
H	8.405843	6.492665	3.220351	L
Rh	-0.0091	-1.01319	-0.05915	H
Rh	-0.06391	1.340286	0.266684	H
C	-8.56703	0.0689	-6.44703	L
C	-9.47465	1.040566	-5.99983	L
C	-8.90476	-0.70664	-7.56572	L
C	-10.6929	1.236014	-6.65597	L
H	-9.23426	1.666508	-5.14929	L
C	-10.122	-0.51475	-8.22292	L
H	-8.23377	-1.47683	-7.92506	L
C	-11.0445	0.460726	-7.78536	L
H	-11.3435	2.003135	-6.26395	L
H	-10.3394	-1.13914	-9.0787	L
C	-2.99074	-5.94925	-1.38346	L
C	-1.82413	-6.71194	-1.5074	L
C	-4.11252	-6.5241	-0.76931	L
C	-1.79874	-8.0469	-1.10123	L
H	-0.93202	-6.27387	-1.93057	L
C	-4.08449	-7.85525	-0.34494	L
H	-5.02858	-5.95792	-0.65591	L
C	-2.93812	-8.65833	-0.53404	L
H	-0.8873	-8.59259	-1.26761	L
H	-4.97993	-8.26386	0.10278	L
C	-7.38655	-0.55529	7.880001	L
C	-8.32929	-1.52859	8.241821	L
C	-7.28095	0.605753	8.660114	L
C	-9.14746	-1.34579	9.358779	L
H	-8.4231	-2.44389	7.670871	L
C	-8.0993	0.792533	9.777461	L
H	-6.57405	1.382501	8.395633	L
C	-9.05298	-0.18207	10.15298	L
H	-9.85597	-2.12617	9.600586	L
H	-7.97036	1.709744	10.33202	L
C	-0.71875	-6.1137	3.485217	L
C	0.188517	-6.33496	4.532867	L
C	-0.81576	-7.07187	2.465684	L
C	1.002054	-7.47076	4.541698	L

H	0.274271	-5.62808	5.348214	L
C	-0.00826	-8.21005	2.476153	L
H	-1.48916	-6.92349	1.631694	L
C	0.931406	-8.42883	3.506824	L
H	1.7043	-7.5845	5.35595	L
H	-0.10899	-8.88687	1.645082	L
C	3.205227	-6.06576	0.00522	L
C	4.318521	-6.37622	-0.7897	L
C	2.10465	-6.93076	-0.01071	L
C	4.345079	-7.54994	-1.54789	L
H	5.18785	-5.73083	-0.79692	L
C	2.137497	-8.11542	-0.7481	L
H	1.216589	-6.68882	0.553901	L
C	3.264364	-8.45886	-1.52651	L
H	5.231961	-7.75721	-2.13077	L
H	1.27886	-8.75978	-0.68015	L
C	8.599617	-1.30504	6.371221	L
C	8.95812	-2.30173	7.29051	L
C	9.48817	-0.24326	6.145404	L
C	10.17673	-2.23772	7.969755	L
H	8.3024	-3.14371	7.473932	L
C	10.70772	-0.17559	6.824321	L
H	9.231505	0.550158	5.454278	L
C	11.07988	-1.17376	7.754604	L
H	10.41029	-3.03104	8.666574	L
H	11.34289	0.670209	6.608427	L
C	0.926627	-5.018	-4.68301	L
C	1.017536	-6.17674	-3.8991	L
C	0.101191	-5.03492	-5.81792	L
C	0.289832	-7.31975	-4.2324	L
H	1.628362	-6.19189	-3.00583	L
C	-0.62505	-6.18036	-6.15614	L
H	0.025085	-4.16402	-6.45661	L
C	-0.54912	-7.35031	-5.36536	L
H	0.375818	-8.17935	-3.58562	L
H	-1.24066	-6.1277	-7.04131	L
C	7.332656	1.726414	-7.54425	L
C	7.169284	3.034396	-8.02411	L
C	8.330386	0.919234	-8.10992	L
C	7.98611	3.52801	-9.04501	L
H	6.418562	3.686784	-7.59537	L
C	9.147291	1.408915	-9.13132	L
H	8.469978	-0.10075	-7.77421	L
C	8.996427	2.72417	-9.6225	L
H	7.811745	4.544345	-9.36454	L
H	9.9004	0.748016	-9.53813	L

C	-6.00288	9.734423	3.816966	L
C	-7.40785	10.14715	3.315544	L
H	-7.53114	9.900926	2.239507	L
H	-8.2042	9.640024	3.901913	L
H	-7.56139	11.24244	3.428434	L
C	-4.96134	10.54376	3.011827	L
H	-5.19632	11.62995	3.038778	L
H	-3.9383	10.4196	3.423665	L
H	-4.94923	10.21396	1.951913	L
C	-5.90301	10.11637	5.308915	L
H	-4.88459	9.928162	5.709229	L
H	-6.12721	11.19537	5.455129	L
H	-6.62742	9.523958	5.908836	L
C	-7.60138	9.448103	-1.69884	L
C	-8.83898	9.18193	-0.81362	L
H	-8.55412	8.766264	0.175224	L
H	-9.40121	10.12287	-0.62831	L
H	-9.52118	8.459095	-1.31118	L
C	-8.08857	10.15409	-2.98689	L
H	-7.23196	10.4085	-3.64792	L
H	-8.80482	9.511814	-3.54363	L
H	-8.61264	11.10352	-2.74159	L
C	-6.64654	10.41459	-0.96706	L
H	-5.73422	10.59307	-1.57635	L
H	-7.14058	11.39266	-0.77978	L
H	-6.33402	10.00646	0.014467	L
C	5.778623	10.67418	-2.11278	L
C	6.431427	11.05974	-0.76783	L
H	7.401903	10.54162	-0.62576	L
H	6.635124	12.15168	-0.72491	L
H	5.760506	10.79633	0.078224	L
C	6.775972	10.94342	-3.25996	L
H	6.333823	10.6436	-4.23475	L
H	7.036049	12.02307	-3.31104	L
H	7.721225	10.37846	-3.11857	L
C	4.557012	11.60115	-2.32283	L
H	4.072267	11.40345	-3.30332	L
H	3.812419	11.46374	-1.50901	L
H	4.866229	12.66911	-2.31643	L
C	7.201535	8.970125	3.350184	L
C	6.186223	10.13504	3.437056	L
H	5.681288	10.14847	4.427071	L
H	6.697746	11.11431	3.312457	L
H	5.421363	10.05311	2.634604	L
C	7.903394	9.063527	1.977435	L
H	8.754031	8.354662	1.902174	L

H	7.184402	8.828462	1.163477	L
H	8.309454	10.08437	1.808106	L
C	8.241939	9.164421	4.473318	L
H	8.709214	10.17097	4.40712	L
H	7.757634	9.068084	5.469162	L
H	9.05638	8.412766	4.408492	L
C	12.41434	-1.13872	8.528135	L
C	13.28654	0.091228	8.178606	L
H	13.55308	0.094164	7.099511	L
H	12.75783	1.036158	8.429782	L
H	14.23655	0.077851	8.75611	L
C	12.12901	-1.09482	10.04516	L
H	11.59739	-2.00711	10.38757	L
H	13.07631	-1.02589	10.62291	L
H	11.50238	-0.21132	10.29491	L
C	13.23485	-2.40433	8.197091	L
H	13.41252	-2.47394	7.102024	L
H	14.22075	-2.38066	8.71028	L
H	12.71261	-3.32733	8.524848	L
C	9.922115	3.227415	-10.7496	L
C	9.627879	4.687541	-11.1704	L
H	8.589479	4.787762	-11.554	L
H	9.773358	5.383164	-10.3157	L
H	10.31534	5.009923	-11.9826	L
C	9.745665	2.335396	-11.9977	L
H	10.37204	2.705064	-12.8385	L
H	10.04699	1.286258	-11.7962	L
H	8.683768	2.336564	-12.3263	L
C	11.39084	3.163063	-10.2768	L
H	12.07446	3.561509	-11.0577	L
H	11.52609	3.766476	-9.35314	L
H	11.70552	2.120637	-10.0613	L
C	-12.3773	0.642481	-8.54108	L
C	-13.2722	1.750837	-7.93576	L
H	-13.5417	1.512188	-6.88414	L
H	-12.7597	2.736569	-7.9698	L
H	-14.2202	1.848755	-8.50836	L
C	-12.0887	1.023248	-10.0096	L
H	-11.5402	0.217409	-10.5404	L
H	-13.0355	1.201624	-10.5642	L
H	-11.4771	1.950319	-10.0551	L
C	-13.1761	-0.6785	-8.50131	L
H	-13.3554	-0.98986	-7.44942	L
H	-14.1609	-0.55926	-9.00322	L
H	-12.6366	-1.49812	-9.02025	L
C	-9.97548	-0.01931	11.37894	L

C	-9.74681	1.309678	12.13863	L
H	-8.70587	1.372123	12.52339	L
H	-9.94894	2.18219	11.48033	L
H	-10.4298	1.38681	13.01257	L
C	-11.4501	-0.04976	10.92153	L
H	-11.7157	-1.02502	10.46277	L
H	-12.1339	0.108751	11.78365	L
H	-11.6392	0.750695	10.1738	L
C	-9.72229	-1.17553	12.37077	L
H	-10.3459	-1.05613	13.28335	L
H	-9.97385	-2.15993	11.92377	L
H	-8.65405	-1.1943	12.67753	L
C	1.889718	-9.63681	3.514446	L
C	1.71029	-10.4348	4.824607	L
H	2.355472	-11.3401	4.826832	L
H	1.987692	-9.83202	5.714053	L
H	0.653006	-10.759	4.936928	L
C	1.648662	-10.6133	2.33734	L
H	0.61088	-11.0111	2.358923	L
H	1.8306	-10.1136	1.363203	L
H	2.34228	-11.4801	2.39506	L
C	3.343748	-9.12859	3.413759	L
H	4.057893	-9.97995	3.384803	L
H	3.479374	-8.52677	2.4884	L
H	3.613057	-8.49337	4.283641	L
C	3.357759	-9.78061	-2.31682	L
C	2.095	-10.6669	-2.17563	L
H	1.19247	-10.1428	-2.55273	L
H	2.203338	-11.6039	-2.76399	L
H	1.930142	-10.9576	-1.11561	L
C	4.560004	-10.5998	-1.79946	L
H	5.519641	-10.068	-1.96811	L
H	4.454979	-10.7931	-0.70961	L
H	4.625529	-11.5782	-2.32324	L
C	3.555271	-9.4745	-3.81728	L
H	4.508017	-8.93594	-4.00197	L
H	3.583086	-10.4138	-4.41108	L
H	2.72338	-8.84732	-4.19932	L
C	-1.33247	-8.63719	-5.69579	L
C	-2.22793	-8.4952	-6.94963	L
H	-2.7794	-9.43966	-7.14964	L
H	-2.98196	-7.69098	-6.80696	L
H	-1.6166	-8.27183	-7.85059	L
C	-0.33706	-9.78915	-5.95376	L
H	0.275281	-10.0087	-5.05397	L
H	-0.87643	-10.7222	-6.22633	L

H	0.351049	-9.52624	-6.78613	L
C	-2.24603	-9.00843	-4.50695	L
H	-2.89962	-8.15104	-4.23531	L
H	-2.89283	-9.87663	-4.75869	L
H	-1.6517	-9.2952	-3.61651	L
C	-2.97535	-10.1513	-0.1475	L
C	-1.65856	-10.9002	-0.47246	L
H	-1.73389	-11.9718	-0.18669	L
H	-1.43759	-10.8599	-1.56095	L
H	-0.8023	-10.4714	0.086712	L
C	-4.10863	-10.8536	-0.92765	L
H	-4.12528	-11.9427	-0.70509	L
H	-5.10538	-10.4467	-0.65797	L
H	-3.96227	-10.7228	-2.02205	L
C	-3.23749	-10.2845	1.367534	L
H	-2.45211	-9.75447	1.94593	L
H	-4.22262	-9.85721	1.648912	L
H	-3.23549	-11.3527	1.675289	L

catalyst I (D_2) (E = -973.32267634 a.u. ; Esol = -973.43603127 a.u.)

C	1.885099	-0.50154	-2.21495	H
C	2.915017	-1.06182	-3.19961	L
C	2.754694	-0.52566	-4.62553	L
H	2.864445	-1.28333	-5.42784	L
H	2.031734	0.309862	-4.74662	L
C	4.024727	-0.1741	-3.83803	L
C	4.159352	1.263404	-3.40854	L
C	4.234093	2.287143	-4.36627	L
H	4.143062	2.055679	-5.42029	L
C	4.455432	3.610802	-3.96858	L
H	4.521091	4.385723	-4.72207	L
C	4.577624	3.929058	-2.6054	L
C	4.483799	2.901887	-1.6569	L
H	4.554844	3.124026	-0.60816	L
C	4.329038	1.577012	-2.054	L
H	4.314188	0.797026	-1.30234	L
C	5.309491	-0.83237	-4.30517	L
C	6.311791	-1.1266	-3.36836	L
H	6.169885	-0.88786	-2.32266	L
C	7.510689	-1.71877	-3.77056	L
H	8.261585	-1.93919	-3.02219	L
C	7.749628	-1.99453	-5.12733	L
C	6.772806	-1.64027	-6.07393	L
H	6.931409	-1.83008	-7.12802	L
C	5.572299	-1.05058	-5.66899	L
H	4.855333	-0.76242	-6.42603	L
C	3.213875	-2.54579	-3.07186	L
C	4.086741	-2.98507	-2.06481	L
H	4.553923	-2.27218	-1.3988	L
C	4.339013	-4.34636	-1.88499	L
H	5.016259	-4.65598	-1.09869	L
C	3.67802	-5.30093	-2.67388	L
C	2.766238	-4.86529	-3.65048	L
H	2.23448	-5.58163	-4.26427	L
C	2.526122	-3.50083	-3.83919	L
H	1.790902	-3.19483	-4.57206	L
C	-1.84699	-0.20768	-1.82108	H
C	-3.03383	-0.56158	-2.71142	L
C	-3.34979	-2.03496	-3.12479	L
C	-2.52578	-1.12944	-4.04266	L
H	-1.43266	-1.32797	-4.08413	L
H	-3.04867	-0.7597	-4.95061	L
C	-4.04121	0.558058	-2.90225	L
C	-3.74447	1.629191	-3.76481	L
H	-2.86289	1.60233	-4.39279	L

C	-4.53096	2.781056	-3.76786	L
H	-4.23838	3.608644	-4.40206	L
C	-5.61566	2.90475	-2.88519	L
C	-5.93777	1.822714	-2.04932	L
H	-6.76961	1.890056	-1.35927	L
C	-5.15302	0.665563	-2.05388	L
H	-5.37842	-0.11131	-1.34298	L
C	-4.73497	-2.38506	-3.6333	L
C	-5.81814	-2.47812	-2.74559	L
H	-5.68642	-2.28893	-1.69178	L
C	-7.08746	-2.83678	-3.2047	L
H	-7.90769	-2.86763	-2.49857	L
C	-7.2963	-3.1422	-4.56012	L
C	-6.20188	-3.0998	-5.44051	L
H	-6.32195	-3.36886	-6.48247	L
C	-4.93278	-2.74142	-4.97868	L
H	-4.1032	-2.75241	-5.67399	L
C	-2.60835	-3.1191	-2.37044	L
C	-1.53105	-3.80501	-2.95386	L
H	-1.27867	-3.65713	-3.99588	L
C	-0.72477	-4.63659	-2.17473	L
H	0.131636	-5.11578	-2.62941	L
C	-1.00228	-4.82389	-0.81086	L
C	-2.15298	-4.24106	-0.26033	L
H	-2.39497	-4.3786	0.785732	L
C	-2.95186	-3.39962	-1.03656	L
H	-3.78137	-2.89352	-0.56749	L
C	-1.48043	1.157275	1.473545	H
C	-2.70131	1.403387	2.350767	L
C	-2.44404	2.406886	3.473814	L
H	-2.87584	2.152566	4.462451	L
H	-1.47502	2.947622	3.407633	L
C	-3.45967	2.763477	2.378467	L
C	-3.08039	3.857601	1.413037	L
C	-3.3525	3.697124	0.04667	L
H	-3.711	2.747969	-0.3301	L
C	-3.19115	4.763987	-0.83701	L
H	-3.43378	4.616935	-1.87979	L
C	-2.79041	6.0257	-0.36781	L
C	-2.5052	6.181848	1.001135	L
H	-2.18374	7.138798	1.392199	L
C	-2.65674	5.108726	1.884604	L
H	-2.48224	5.264806	2.941805	L
C	-4.91108	2.785887	2.816151	L
C	-5.29317	3.408509	4.015819	L
H	-4.54972	3.839015	4.674326	L

C	-6.64195	3.495008	4.371034	L
H	-6.90472	3.957066	5.314278	L
C	-7.63885	2.986365	3.519975	L
C	-7.25655	2.398443	2.302383	L
H	-8.00193	2.033485	1.606851	L
C	-5.90864	2.313276	1.949827	L
H	-5.64671	1.899695	0.986825	L
C	-3.54203	0.173096	2.631641	L
C	-3.55765	-0.47367	3.878767	L
H	-2.98336	-0.091	4.710549	L
C	-4.29461	-1.65164	4.053704	L
H	-4.26965	-2.14347	5.01776	L
C	-5.01434	-2.21244	2.981128	L
C	-4.9794	-1.56708	1.734379	L
H	-5.53489	-1.95679	0.891516	L
C	-4.2288	-0.40683	1.559569	L
H	-4.17264	0.046849	0.581688	L
C	2.173251	1.054212	1.296334	H
C	3.010127	1.486858	2.489336	L
C	2.857308	0.79095	3.874999	L
C	2.122182	2.101568	3.578707	L
H	1.029112	2.018771	3.396106	L
H	2.520527	2.981653	4.123993	L
C	4.277661	2.254877	2.165748	L
C	5.375159	1.560067	1.634926	L
H	5.338456	0.483396	1.527863	L
C	6.498747	2.250167	1.170693	L
H	7.318944	1.688179	0.74187	L
C	6.535866	3.655188	1.203594	L
C	5.449876	4.351541	1.757029	L
H	5.436919	5.434337	1.763907	L
C	4.322067	3.661999	2.207363	L
H	3.467321	4.239718	2.530493	L
C	3.984478	0.906883	4.879707	L
C	3.77714	1.556992	6.10727	L
H	2.81631	1.999563	6.338469	L
C	4.808652	1.647414	7.045333	L
H	4.629215	2.184419	7.968193	L
C	6.062382	1.067002	6.785508	L
C	6.252816	0.377035	5.575857	L
H	7.194264	-0.11378	5.363181	L
C	5.219254	0.286063	4.640605	L
H	5.382131	-0.28285	3.73714	L
C	2.024593	-0.47169	3.948293	L
C	2.560037	-1.68354	3.478446	L
H	3.550893	-1.71707	3.044578	L

C	1.799067	-2.85214	3.537474	L
H	2.208928	-3.77832	3.153071	L
C	0.504241	-2.81019	4.074337	L
C	0.004117	-1.59405	4.572992	L
H	-0.98025	-1.55957	5.022553	L
C	0.741094	-0.47169	4.528307	L
H	0.328283	0.437689	4.945866	L
O	-1.23339	0.869488	-2.10274	H
O	-1.55144	-0.98345	-0.86432	H
O	-1.16237	1.99755	0.582405	H
O	-0.88372	0.05167	1.678154	H
O	1.701486	1.982013	0.568246	H
O	1.976302	-0.18647	1.12057	H
O	1.622097	0.73999	-2.21612	H
O	1.344703	-1.35621	-1.4433	H
C	7.635773	4.398322	0.544164	L
C	8.18745	5.540547	1.139971	L
C	8.09975	4.000833	-0.7178	L
C	9.194068	6.264616	0.495088	L
H	7.846169	5.869629	2.113745	L
C	9.098709	4.726764	-1.36839	L
H	7.669901	3.140939	-1.21686	L
C	9.670979	5.874646	-0.77821	L
H	9.583872	7.128951	1.011044	L
H	9.420251	4.384147	-2.34229	L
C	-6.31806	4.20463	-2.75332	L
C	-6.62493	4.969464	-3.88749	L
C	-6.59624	4.733708	-1.48444	L
C	-7.18044	6.244942	-3.75892	L
H	-6.42754	4.582135	-4.87948	L
C	-7.14049	6.012408	-1.35205	L
H	-6.34821	4.177874	-0.58865	L
C	-7.43923	6.801378	-2.48471	L
H	-7.3856	6.784556	-4.67108	L
H	-7.30919	6.389298	-0.35259	L
C	-5.78193	-3.47506	3.147358	L
C	-5.8238	-4.42532	2.114463	L
C	-6.48903	-3.73599	4.330429	L
C	-6.56966	-5.59652	2.252933	L
H	-5.26578	-4.27268	1.199342	L
C	-7.23604	-4.90921	4.472424	L
H	-6.48906	-3.0182	5.140986	L
C	-7.29977	-5.86404	3.430553	L
H	-6.57696	-6.29201	1.425016	L
H	-7.76632	-5.04319	5.403069	L
C	3.908994	-6.74716	-2.44889	L

C	2.830351	-7.64029	-2.38736	L
C	5.210162	-7.24318	-2.29404	L
C	3.047242	-9.00692	-2.19194	L
H	1.813494	-7.27841	-2.47931	L
C	5.431615	-8.60993	-2.11056	L
H	6.06135	-6.57518	-2.34327	L
C	4.357354	-9.5256	-2.06093	L
H	2.174624	-9.64121	-2.15469	L
H	6.45445	-8.9493	-2.02244	L
Rh	0.264207	1.473185	-0.82834	H
Rh	0.236536	-0.69728	0.136804	H
C	7.16409	1.171079	7.775891	L
C	8.480726	1.410999	7.355333	L
C	6.907962	1.033947	9.147984	L
C	9.519841	1.513978	8.284063	L
H	8.706828	1.538361	6.303848	L
C	7.944378	1.135021	10.07864	L
H	5.905668	0.830336	9.503661	L
C	9.274053	1.378158	9.670207	L
H	10.50857	1.704223	7.894643	L
H	7.698247	1.018711	11.12524	L
C	-0.31512	-4.03511	4.152811	L
C	-1.62286	-4.04411	3.656271	L
C	0.189602	-5.1846	4.77066	L
C	-2.42241	-5.18001	3.793824	L
H	-2.02446	-3.16923	3.16074	L
C	-0.60935	-6.32097	4.916003	L
H	1.19155	-5.18795	5.180136	L
C	-1.93947	-6.34159	4.434902	L
H	-3.42958	-5.14035	3.40965	L
H	-0.17306	-7.16502	5.427147	L
C	-0.0501	-5.56064	0.04609	L
C	-0.49535	-6.53405	0.947714	L
C	1.317708	-5.27345	-0.02627	L
C	0.417871	-7.24142	1.735524	L
H	-1.55053	-6.76248	1.024327	L
C	2.232011	-5.97348	0.759224	L
H	1.677768	-4.49687	-0.68851	L
C	1.806793	-6.98301	1.648816	L
H	0.017227	-7.99259	2.399023	L
H	3.279557	-5.72691	0.657442	L
C	-8.64589	-3.52051	-5.05112	L
C	-9.47447	-4.35937	-4.29144	L
C	-9.11561	-3.04405	-6.28406	L
C	-10.7438	-4.71369	-4.7538	L
H	-9.13444	-4.75877	-3.3441	L

C	-10.3857	-3.39571	-6.749	L
H	-8.50552	-2.38116	-6.88511	L
C	-11.2302	-4.2408	-5.99222	L
H	-11.3444	-5.36587	-4.13462	L
H	-10.6878	-2.9914	-7.70328	L
C	9.019155	-2.63594	-5.55319	L
C	9.687771	-2.20299	-6.70741	L
C	9.570479	-3.68857	-4.80767	L
C	10.88106	-2.80852	-7.10729	L
H	9.297349	-1.38121	-7.29463	L
C	10.76349	-4.29764	-5.20587	L
H	9.067818	-4.05586	-3.92136	L
C	11.44731	-3.86983	-6.36764	L
H	11.36214	-2.43752	-8.00193	L
H	11.1312	-5.10484	-4.59054	L
C	-9.07352	3.090609	3.88769	L
C	-9.95242	2.025285	3.642183	L
C	-9.57604	4.258004	4.480606	L
C	-11.3045	2.121968	3.982361	L
H	-9.59021	1.105468	3.199713	L
C	-10.9268	4.358393	4.820444	L
H	-8.92748	5.105258	4.665335	L
C	-11.8232	3.294184	4.580151	L
H	-11.926	1.265122	3.770468	L
H	-11.2683	5.280116	5.271307	L
C	-2.74386	7.185384	-1.29453	L
C	-3.21294	8.442174	-0.88514	L
C	-2.28578	7.032508	-2.61204	L
C	-3.2378	9.516712	-1.77568	L
H	-3.5973	8.589018	0.116327	L
C	-2.31637	8.104306	-3.50774	L
H	-1.90128	6.079576	-2.9539	L
C	-2.80649	9.370156	-3.11164	L
H	-3.62455	10.46112	-1.41798	L
H	-1.95887	7.917146	-4.50903	L
C	4.846246	5.31602	-2.16172	L
C	4.159011	5.856022	-1.06583	L
C	5.834976	6.08477	-2.78901	L
C	4.458255	7.137065	-0.59776	L
H	3.386861	5.283282	-0.5664	L
C	6.138828	7.36531	-2.32173	L
H	6.396258	5.682898	-3.62358	L
C	5.460739	7.921012	-1.21413	L
H	3.896216	7.491279	0.253048	L
H	6.91459	7.918919	-2.83093	L
C	-2.87714	-7.55052	4.627575	L

C	-4.07283	-7.1241	5.505676	L
H	-4.69414	-6.35731	4.998131	L
H	-4.72617	-7.99276	5.735055	L
H	-3.71349	-6.69983	6.468118	L
C	-2.18473	-8.74945	5.319194	L
H	-1.31309	-9.09896	4.723978	L
H	-1.84656	-8.47695	6.342277	L
H	-2.88682	-9.60564	5.419949	L
C	-3.39446	-8.03981	3.256866	L
H	-4.05556	-8.92462	3.379497	L
H	-3.98293	-7.2578	2.733831	L
H	-2.54461	-8.33555	2.606629	L
C	2.85731	-7.77056	2.456077	L
C	2.232139	-8.83262	3.39163	L
H	3.021993	-9.37547	3.955019	L
H	1.55951	-8.35674	4.135777	L
H	1.660607	-9.58769	2.809689	L
C	3.680394	-6.7991	3.329819	L
H	4.416577	-7.35468	3.950295	L
H	4.249423	-6.0729	2.712976	L
H	3.012805	-6.23023	4.00933	L
C	3.800808	-8.50301	1.4793	L
H	3.216473	-9.1813	0.82103	L
H	4.359478	-7.79103	0.836201	L
H	4.549257	-9.1091	2.034162	L
C	-8.1462	-7.15071	3.525474	L
C	-7.24193	-8.38767	3.334407	L
H	-7.83351	-9.32496	3.419569	L
H	-6.75517	-8.39315	2.337236	L
H	-6.44971	-8.40823	4.11011	L
C	-9.22556	-7.13353	2.421737	L
H	-9.87764	-8.03108	2.493297	L
H	-9.86431	-6.22909	2.519828	L
H	-8.77159	-7.13116	1.40856	L
C	-8.8657	-7.30359	4.887034	L
H	-8.13067	-7.34073	5.720199	L
H	-9.57411	-6.46439	5.058185	L
H	-9.45438	-8.24629	4.918206	L
C	4.646993	-11.0337	-1.90504	L
C	3.361859	-11.8933	-1.83612	L
H	2.769948	-11.7988	-2.77212	L
H	3.61324	-12.969	-1.71015	L
H	2.732189	-11.593	-0.97052	L
C	5.446567	-11.2873	-0.6079	L
H	6.424134	-10.7627	-0.6166	L
H	4.871908	-10.9434	0.276502	L

H	5.655016	-12.3719	-0.481	L
C	5.474229	-11.5192	-3.11465	L
H	5.662591	-12.613	-3.05084	L
H	4.930927	-11.3133	-4.06231	L
H	6.461048	-11.0126	-3.16168	L
C	-12.6388	-4.65526	-6.46617	L
C	-13.6885	-4.17933	-5.43849	L
H	-14.7165	-4.42944	-5.77998	L
H	-13.5408	-4.66215	-4.44995	L
H	-13.6239	-3.07804	-5.30215	L
C	-13.0192	-4.05185	-7.83982	L
H	-13.0206	-2.9411	-7.79798	L
H	-12.314	-4.38955	-8.6299	L
H	-14.0388	-4.37473	-8.14363	L
C	-12.7072	-6.19262	-6.59468	L
H	-11.9283	-6.55631	-7.29939	L
H	-12.5519	-6.69194	-5.61557	L
H	-13.7009	-6.51269	-6.9767	L
C	-13.3081	3.446181	4.970387	L
C	-13.9221	4.638865	4.205341	L
H	-15.0044	4.741684	4.437965	L
H	-13.4318	5.596295	4.479285	L
H	-13.8128	4.492003	3.108949	L
C	-13.4178	3.700353	6.489618	L
H	-12.9231	4.650104	6.781827	L
H	-14.4824	3.770693	6.801995	L
H	-12.9417	2.870423	7.055425	L
C	-14.1535	2.192077	4.641741	L
H	-14.1397	1.979667	3.550781	L
H	-13.7769	1.304336	5.194478	L
H	-15.2145	2.343092	4.937994	L
C	10.38948	1.48549	10.73074	L
C	10.07019	2.646187	11.69797	L
H	9.128718	2.46479	12.25731	L
H	10.88256	2.770653	12.44662	L
H	9.964044	3.599264	11.13584	L
C	10.4734	0.164106	11.52543	L
H	10.6605	-0.68894	10.83776	L
H	11.29993	0.202191	12.26794	L
H	9.535377	-0.03743	12.08363	L
C	11.78533	1.754818	10.1186	L
H	12.08446	0.930136	9.43601	L
H	11.79453	2.716139	9.560667	L
H	12.55823	1.824773	10.91482	L
C	12.76647	-4.5123	-6.84454	L
C	13.24988	-5.65995	-5.92535	L

H	14.20096	-6.09414	-6.3037	L
H	13.44014	-5.28893	-4.89499	L
H	12.50093	-6.48046	-5.88873	L
C	13.87777	-3.44067	-6.87997	L
H	14.84946	-3.88983	-7.17996	L
H	13.64599	-2.63539	-7.60791	L
H	14.00127	-2.979	-5.87637	L
C	12.57212	-5.09655	-8.26071	L
H	11.74562	-5.83985	-8.26179	L
H	12.3296	-4.30463	-8.99975	L
H	13.49832	-5.60332	-8.6089	L
C	-8.0045	8.224047	-2.29512	L
C	-6.97751	9.081755	-1.52625	L
H	-7.3485	10.12154	-1.3965	L
H	-6.77347	8.669314	-0.51596	L
H	-6.02007	9.12142	-2.08681	L
C	-8.3061	8.941252	-3.63321	L
H	-7.38056	9.062719	-4.2364	L
H	-9.05862	8.375576	-4.2241	L
H	-8.71807	9.957827	-3.45151	L
C	-9.32235	8.156395	-1.49276	L
H	-10.055	7.498571	-2.00855	L
H	-9.15875	7.761537	-0.46851	L
H	-9.77317	9.167239	-1.38868	L
C	-2.90305	10.56836	-4.0777	L
C	-2.06016	11.74137	-3.5319	L
H	-1.00312	11.42612	-3.3945	L
H	-2.07965	12.6018	-4.23556	L
H	-2.44597	12.10293	-2.55601	L
C	-2.3898	10.24306	-5.50111	L
H	-2.47546	11.13175	-6.16372	L
H	-1.31875	9.946718	-5.4777	L
H	-2.98769	9.426631	-5.96109	L
C	-4.37853	11.00851	-4.2006	L
H	-5.00571	10.16132	-4.55339	L
H	-4.78349	11.35899	-3.22825	L
H	-4.48172	11.84525	-4.92509	L
C	5.832924	9.334853	-0.7222	L
C	7.31168	9.352186	-0.28145	L
H	7.990558	9.103771	-1.12255	L
H	7.599906	10.35775	0.094472	L
H	7.47801	8.615811	0.533258	L
C	4.979615	9.803152	0.481195	L
H	3.901386	9.835486	0.213038	L
H	5.121777	9.129868	1.354244	L
C	5.626278	10.35111	-1.86651	L

H	5.8401	11.38531	-1.51928	L
H	6.300413	10.14478	-2.72378	L
H	4.576532	10.31483	-2.23024	L
C	10.7822	6.641137	-1.52501	L
C	10.24665	7.136336	-2.88612	L
H	11.02615	7.713058	-3.42973	L
H	9.3674	7.797169	-2.73817	L
C	11.98383	5.700575	-1.76059	L
H	12.81688	6.241941	-2.25946	L
H	12.35705	5.300748	-0.79289	L
H	11.70933	4.842753	-2.40952	L
C	11.29678	7.87564	-0.74608	L
H	10.47631	8.604171	-0.57017	L
H	11.73568	7.574074	0.229528	L
H	12.09106	8.400817	-1.32003	L
H	5.275532	10.82643	0.799802	L
H	9.942311	6.29243	-3.53948	L

C2-carbene (E = -1566.43496410 a.u. ; Esol = -1566.54538324 a.u.)

C	-2.42202	-0.97019	1.230636
C	-3.81127	-1.60652	1.242971
C	-3.76994	-2.97776	1.928052
H	-4.35048	-3.79513	1.471283
H	-2.83432	-3.22538	2.475081
C	-4.6086	-1.86389	2.567701
C	-4.08386	-1.20522	3.819499
C	-3.6008	-1.97482	4.888173
H	-3.67821	-3.05464	4.864289
C	-2.95999	-1.35693	5.966338
H	-2.55511	-1.97188	6.75946
C	-2.79365	0.038667	5.989875
C	-3.3438	0.81081	4.953165
H	-3.25096	1.889807	4.961483
C	-4.00303	0.19456	3.887713
H	-4.38353	0.802496	3.077373
C	-6.11211	-2.04083	2.453435
C	-6.91427	-0.95529	2.076369
H	-6.49747	0.041321	2.02739
C	-8.21934	-1.16886	1.632874
H	-8.78776	-0.33687	1.245434
C	-8.76343	-2.4614	1.617221
C	-8.02122	-3.51922	2.166359
H	-8.42491	-4.52339	2.187372
C	-6.70672	-3.30796	2.592418
H	-6.12935	-4.15202	2.947413
C	-4.66496	-1.41343	-0.00472
C	-5.10296	-2.48268	-0.79593
H	-4.7395	-3.47051	-0.62746
C	-6.05576	-2.2922	-1.79545
H	-6.40963	-3.15735	-2.33566
C	-6.57013	-1.01187	-2.05695
C	-6.04651	0.076906	-1.33831
H	-6.38175	1.079721	-1.54832
C	-5.09981	-0.12149	-0.32909
H	-4.7496	0.724995	0.246322
C	1.039412	-2.34829	1.298432
C	1.817226	-3.65053	1.302915
C	1.124751	-5.00592	0.972073
C	1.439062	-4.61845	2.424804
H	0.559047	-4.31461	3.033118
H	2.289411	-5.14276	2.904957
C	3.28051	-3.53634	0.937387
C	3.630035	-3.33768	-0.40372
H	2.861324	-3.2453	-1.15866

C	4.967537	-3.25942	-0.78579
H	5.193484	-3.09535	-1.83133
C	5.992459	-3.3365	0.17478
C	5.637525	-3.48604	1.529083
H	6.396001	-3.54823	2.29829
C	4.294496	-3.57107	1.907816
H	4.053182	-3.66457	2.958161
C	1.966607	-6.13086	0.396167
C	2.279921	-6.12441	-0.97134
H	1.92043	-5.32955	-1.61096
C	3.053593	-7.14388	-1.52939
H	3.287278	-7.10402	-2.58594
C	3.497103	-8.21667	-0.73811
C	3.122951	-8.2611	0.61606
H	3.439009	-9.08047	1.249324
C	2.352039	-7.23741	1.173571
H	2.059048	-7.31549	2.212052
C	-0.34836	-5.09317	0.652318
C	-1.15608	-5.98573	1.374248
H	-0.7621	-6.49526	2.244991
C	-2.45166	-6.28236	0.943868
H	-3.03183	-7.00104	1.507727
C	-2.97187	-5.69336	-0.22249
C	-2.16318	-4.78271	-0.93402
H	-2.53297	-4.286	-1.82187
C	-0.86031	-4.50173	-0.51095
H	-0.23719	-3.86216	-1.12171
C	2.438302	1.110873	1.2092
C	3.847205	1.712288	1.263768
C	3.837003	3.051369	2.011438
H	4.445331	3.869049	1.590871
H	2.90112	3.306541	2.5541
C	4.625888	1.879887	2.613751
C	4.055568	1.167519	3.816237
C	3.574955	1.888099	4.919612
H	3.679023	2.965261	4.957069
C	2.907418	1.226482	5.955576
H	2.508371	1.806471	6.777832
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C	3.253503	-0.89016	4.827367
H	3.140022	-1.96593	4.775328
C	3.934491	-0.23118	3.802418
H	4.307437	-0.80323	2.962723
C	6.13729	2.014605	2.543414
C	6.76182	3.25932	2.736797
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C	8.098737	3.440201	2.376049
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C	8.259798	1.093398	1.812209
H	8.825375	0.246283	1.450733
C	6.924665	0.912952	2.177389
H	6.484134	-0.07088	2.088334
C	4.73045	1.54366	0.032317
C	5.220735	2.63113	-0.70525
H	4.874853	3.624326	-0.51392
C	6.180492	2.447203	-1.70203
H	6.535275	3.313718	-2.24411
C	6.670808	1.163301	-1.995
C	6.12339	0.066687	-1.30779
H	6.480398	-0.9316	-1.50139
C	5.154005	0.254356	-0.31752
H	4.783573	-0.60041	0.232457
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C	-1.92074	3.7669	1.149535
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H	-5.58148	3.359531	-1.70489
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C	-5.68946	3.404209	1.703752
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C	-3.30861	8.342317	0.409942
H	-3.63113	9.17407	1.023695
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O	0.8734	-1.77149	2.40871
O	0.715223	-1.88866	0.156816
O	1.812752	0.994865	2.294263
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C	-7.64067	3.191547	0.118476
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C	-9.60184	3.55104	-1.28907
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H	-10.377	1.679243	1.450811
H	-9.99859	4.000247	-2.18707
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C	7.856748	-3.69531	-1.4741
C	9.652322	-2.32474	0.158857
H	8.031896	-2.10991	1.532244
C	9.16984	-3.48946	-1.90243
H	7.184837	-4.24754	-2.1186
C	10.09665	-2.78975	-1.0971
H	10.32094	-1.79183	0.820891
H	9.437916	-3.88731	-2.86949
C	7.76814	0.974171	-2.9865
C	8.774646	1.942449	-3.12711
C	7.836862	-0.1811	-3.78286
C	9.818947	1.764849	-4.03374
H	8.775791	2.832352	-2.51566
C	8.884125	-0.36333	-4.69176
H	7.069945	-0.94237	-3.72089
C	9.89787	0.611525	-4.84128
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C	-8.8404	-1.49706	-5.07242
H	-7.0312	-2.3993	-4.3885
C	-9.83041	-0.50923	-4.86836
H	-10.406	1.116836	-3.55402
H	-8.87203	-2.17241	-5.9141
C	4.337242	-9.28945	-1.3275
C	5.368964	-8.97394	-2.22408
C	4.11691	-10.6344	-0.9972
C	6.164842	-9.97924	-2.77955
H	5.574198	-7.94271	-2.48419
C	4.909496	-11.6417	-1.5519
H	3.317562	-10.9118	-0.32143
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C	-11.4076	-2.46685	-1.07737
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H	-11.5168	-2.02837	-2.05982
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C	-6.3825	10.8618	-1.46138
H	-5.85622	9.485236	0.091225
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H	4.020234	5.995322	-2.64097
C	7.073025	6.421999	-1.17177
H	7.342662	6.640905	0.973939
H	6.343152	6.215932	-3.22195
C	10.15828	2.613115	1.211237
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C	10.44587	2.035138	-0.03306
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H	9.74269	1.35825	-0.5012
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C	0.995648	-1.83577	6.634143
C	2.190853	-0.58125	8.314251
C	0.318694	-2.53462	7.636542
H	0.775594	-2.05987	5.597273
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C	-11.0439	-0.33128	-5.80303
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H	-12.4513	0.225663	-4.1909
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H	11.04002	-1.73	-6.01897
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H	12.90428	-2.8107	-3.251
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H	13.57362	-3.06818	-0.87286
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H	12.31662	-4.31349	-0.52774
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H	11.08027	-0.47872	-2.16966
H	11.75589	-0.58667	-0.50283
H	12.84018	-0.77985	-1.90782
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H	14.04816	1.646592	-1.91991
H	15.55926	2.599082	-1.8206
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C	0.156142	-0.21525	-2.03104
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O	1.780373	1.149458	-2.98027
C	3.118718	1.466578	-3.34011
H	3.423439	2.321577	-2.73768
H	3.774121	0.611966	-3.16491
C	-0.82992	-0.81586	-2.87383
C	-2.19624	-0.45578	-2.74489
C	-0.47354	-1.8183	-3.81757
C	-3.16029	-1.05763	-3.53941
H	-2.47283	0.31963	-2.04245
C	-1.44813	-2.48685	-4.5424
H	0.567125	-2.10609	-3.92016
C	-2.78087	-2.09288	-4.39564
H	-4.19442	-0.74428	-3.48699
H	-1.18185	-3.2903	-5.21945
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C	0.433927	-5.10421	0.162979
C	1.127585	-4.50523	1.368652
C	2.496443	-4.71485	1.58981
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C	3.140037	-4.10846	2.674191
H	4.197269	-4.29221	2.809159
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C	1.040338	-3.12918	3.367532
H	0.449694	-2.48612	4.004668
C	0.395581	-3.77617	2.31243
H	-0.67251	-3.65558	2.193124
C	-0.1804	-6.471	0.356926
C	0.510584	-7.63419	-0.02041
H	1.481524	-7.56963	-0.49471
C	-0.04164	-8.89514	0.219929
H	0.499992	-9.77314	-0.10869
C	-1.2826	-9.01936	0.869332
C	-1.95098	-7.85439	1.28374
H	-2.88829	-7.91712	1.822245
C	-1.39686	-6.59582	1.041606
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C	-1.31568	-4.58216	-1.81829
C	-2.62799	-4.65741	-1.33151
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C	-3.708	-4.76906	-2.21119
H	-4.71094	-4.80627	-1.80453
C	-3.49936	-4.76515	-3.60094
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C	-1.107	-4.60245	-3.20985
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C	2.59456	-0.00551	-0.77309
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C	4.969272	-3.6879	-1.41287
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O	0.317401	-2.06548	-1.8877
C	-6.00836	4.739952	-3.52461
C	-7.12439	4.722388	-4.37359
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C	-3.79593	-11.838	1.22137
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C	-1.60715	-12.6834	1.80501
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C	-2.99235	-12.9192	1.644654
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C	3.129421	-2.50931	4.636952
C	2.45954	-2.13538	5.815414
C	4.460419	-2.09059	4.470811
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C	5.085212	-1.28814	5.42587
H	5.015751	-2.34104	3.579986
C	4.406834	-0.87473	6.590819
H	2.505307	-1.07663	7.649666
H	6.103645	-0.97739	5.236616
C	-2.2611	-3.38883	4.789155
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C	0.204585	11.27297	2.069895
C	2.43492	10.66028	1.377387
C	0.646323	12.5668	2.359359
H	-0.83379	11.02441	2.250787
C	2.879335	11.95273	1.664529
H	3.141399	9.941447	0.981214
C	1.996888	12.93688	2.161225
H	-0.08691	13.2616	2.740229
H	3.922277	12.17983	1.490882
C	2.129713	3.127049	4.860454
C	1.847724	2.399952	6.030703
C	1.637472	4.440339	4.763382
C	1.066818	2.949306	7.049962
H	2.231503	1.400003	6.170642
C	0.858109	4.992177	5.780989
H	1.811806	5.038324	3.881741
C	0.536035	4.253832	6.938231
H	0.882613	2.329178	7.9143
H	0.493932	6.001636	5.647716
C	10.32192	-1.05583	1.64156
C	10.7345	-2.36489	1.353522
C	11.23554	-0.17588	2.240538
C	12.03216	-2.78415	1.654751
H	10.058	-3.06287	0.876015
C	12.53428	-0.59265	2.544535
H	10.94065	0.835468	2.491511
C	12.96309	-1.90921	2.256366
H	12.30554	-3.80121	1.409181
H	13.1862	0.132515	3.007761
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C	3.100427	14.97534	1.170986
H	2.321926	15.00371	0.378052
H	3.450271	16.0145	1.354495
H	3.966825	14.39661	0.788207
C	1.43493	15.30975	2.99983
H	1.008573	14.92906	3.953132
H	1.858152	16.31752	3.203552
H	0.618721	15.43582	2.255896
C	3.6415	14.26983	3.529513
H	3.256592	13.78524	4.452882
H	4.511992	13.68493	3.16584
H	4.010549	15.28433	3.795051
C	8.188827	6.206717	-6.33805
C	8.036884	7.33247	-7.38926
H	7.197769	7.114302	-8.08486
H	7.861269	8.313351	-6.89681
H	8.96029	7.427762	-8.00116
C	8.475296	4.892412	-7.09703
H	9.348939	5.010244	-7.77429
H	8.705814	4.059596	-6.40029
H	7.594748	4.600221	-7.70946
C	9.398606	6.558494	-5.44538
H	9.191062	7.480006	-4.85942
H	9.633968	5.739082	-4.73455
H	10.30639	6.733866	-6.06267
C	-0.35975	4.887569	8.02224
C	0.350691	6.124877	8.609988
H	0.519025	6.902284	7.835277
H	-0.25973	6.582937	9.418321
H	1.336655	5.838324	9.035887
C	-1.70719	5.319751	7.40008
H	-2.21232	4.453488	6.924258
H	-2.38592	5.732821	8.177481
H	-1.5716	6.107888	6.630841
C	-0.67409	3.920449	9.189052
H	-1.19427	3.010595	8.818261
H	0.255657	3.622312	9.720032
H	-1.3393	4.40629	9.935682
C	5.122142	0.04421	7.601992
C	6.365345	-0.68034	8.160551
H	7.100646	-0.90387	7.359336
H	6.879495	-0.05224	8.920152
H	6.070782	-1.63871	8.640505
C	5.5634	1.346963	6.897049
H	4.690454	1.85687	6.438336
H	6.034421	2.047024	7.62068

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C	4.226888	0.439553	8.801161
H	3.320688	0.983056	8.457712
H	3.919442	-0.45812	9.379921
H	4.77478	1.111112	9.497442
C	-5.06458	-0.42957	7.90669
C	-5.53789	-1.74206	7.241244
H	-5.96472	-2.43603	7.997463
H	-6.32682	-1.55758	6.483014
H	-4.68939	-2.2538	6.741036
C	-4.10357	-0.81011	9.05882
H	-4.6067	-1.48445	9.785536
H	-3.21074	-1.34475	8.66846
H	-3.7762	0.092766	9.618218
C	-6.27886	0.296242	8.523174
H	-5.96244	1.258819	8.9803
H	-7.05396	0.512564	7.758159
H	-6.75155	-0.32736	9.312819
C	0.262636	-5.26123	7.858916
C	1.587381	-5.70015	7.194147
H	2.278637	-6.14019	7.945279
H	1.420493	-6.46916	6.411806
H	2.093978	-4.83137	6.724395
C	0.621038	-4.32402	9.037421
H	-0.29044	-4.02316	9.59775
H	1.296849	-4.83572	9.756769
H	1.1462	-3.41443	8.672694
C	-0.45225	-6.49992	8.438207
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H	0.170766	-6.98415	9.221294
C	-14.451	2.298707	2.671738
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H	-16.3828	1.578726	3.447693
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H	-14.9606	0.739709	4.144008
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H	-13.8447	2.997858	4.660869
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C	-7.96926	-4.42181	-7.38265
C	-7.78983	-5.27568	-8.66091
H	-8.65605	-5.14683	-9.34591
H	-6.87713	-4.96931	-9.21664
H	-7.72252	-6.35629	-8.40951
C	-9.27453	-4.87551	-6.6939
H	-9.52279	-4.23121	-5.82472
H	-10.1313	-4.82546	-7.40052
H	-9.17799	-5.92323	-6.33533
C	-8.10624	-2.94707	-7.82062
H	-7.1598	-2.59119	-8.28174
H	-8.92265	-2.83136	-8.5662
H	-8.34557	-2.28555	-6.96209
C	7.751026	-8.568	-5.03534
C	6.829431	-8.96124	-6.21031
H	7.198812	-9.88315	-6.70986
H	5.793122	-9.16243	-5.86725
H	6.795264	-8.1451	-6.96421
C	7.736288	-9.68985	-3.97424
H	8.137655	-10.637	-4.3959
H	8.3615	-9.4036	-3.10087
H	6.70736	-9.89743	-3.61322
C	9.193813	-8.46102	-5.58551
H	9.257912	-7.68845	-6.38208
H	9.910287	-8.21226	-4.77291
H	9.518409	-9.42645	-6.03138
C	-3.64215	-14.2927	1.912789
C	-2.62544	-15.3666	2.369681
H	-3.13355	-16.3388	2.551209
H	-1.85119	-15.5362	1.590398
H	-2.13218	-15.0666	3.319539
C	-4.31566	-14.8047	0.620968
H	-4.75453	-15.814	0.778308
H	-5.13701	-14.1333	0.294462
H	-3.57155	-14.8718	-0.20208

C	-4.70515	-14.1511	3.023928
H	-4.24441	-13.7426	3.949398
H	-5.52951	-13.4741	2.716936
H	-5.1577	-15.1375	3.264893
C	0.113201	-0.2087	-4.0772
C	-0.8122	-0.699	-5.04864
C	-0.39498	-1.04354	-6.36903
C	-2.18404	-0.88436	-4.7174
C	-1.28819	-1.55795	-7.29386
H	0.645059	-0.92606	-6.65353
C	-3.08502	-1.39035	-5.64149
H	-2.51905	-0.63296	-3.71981
C	-2.62494	-1.72825	-6.91581
H	-0.95964	-1.82804	-8.29073
H	-4.12728	-1.52908	-5.37788
C	1.53485	-0.09367	-4.4846
O	2.252962	-1.06737	-4.55678
O	1.935901	1.192379	-4.66143
C	3.343397	1.404955	-4.68542
H	3.85923	0.475319	-4.44896
H	3.573313	2.175281	-3.9462
C	3.827028	1.885711	-6.0505
Cl	3.464904	0.656481	-7.35458
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Cl	3.065329	3.475111	-6.50851
Br	-3.88559	-2.46523	-8.20831
C	14.38771	-2.41117	2.570885
C	15.07704	-2.85676	1.262836
H	16.12169	-3.18274	1.458687
H	14.54636	-3.71006	0.791293
H	15.10375	-2.01711	0.534905
C	14.30889	-3.60861	3.542711
H	15.32675	-3.96094	3.817883
H	13.77683	-3.31597	4.47377
H	13.77171	-4.46786	3.089678
C	15.28079	-1.33108	3.227832
H	15.4019	-0.45437	2.55535
H	14.84979	-0.99568	4.195943
H	16.29621	-1.73283	3.437007

TS-1 (E = -1803.50394123 a.u. ; Esol = -1803.61965564 a.u.)

C	2.333803	1.137197	1.507836	H
C	3.74371	1.727998	1.535696	L
C	3.785129	3.063541	2.283602	L
H	4.41584	3.864945	1.871546	L
H	2.863599	3.340228	2.83999	L
C	4.557902	1.869316	2.864489	L
C	3.992477	1.217968	4.101659	L
C	3.597027	1.997161	5.198333	L
H	3.774442	3.065473	5.203705	L
C	2.911153	1.412304	6.265268	L
H	2.57019	2.041658	7.076341	L
C	2.615562	0.038389	6.254468	L
C	3.079647	-0.75247	5.189005	L
H	2.885456	-1.81785	5.167658	L
C	3.781251	-0.1693	4.130789	L
H	4.093236	-0.78464	3.29711	L
C	6.068833	1.939541	2.735427	L
C	6.779613	0.818442	2.283838	L
H	6.295579	-0.14727	2.216404	L
C	8.067058	0.969677	1.768032	L
H	8.558044	0.122265	1.315747	L
C	8.684677	2.228699	1.749432	L
C	8.050744	3.303697	2.394624	L
H	8.515511	4.27881	2.432941	L
C	6.752986	3.157672	2.892789	L
H	6.250453	4.022787	3.306427	L
C	4.573965	1.554425	0.269446	L
C	5.091677	2.631889	-0.46759	L
H	4.853485	3.644459	-0.2166	L
C	5.956819	2.412788	-1.54006	L
H	6.372673	3.27103	-2.05011	L
C	6.301838	1.106649	-1.92342	L
C	5.738253	0.0301	-1.21997	L
H	5.97186	-0.98546	-1.49101	L
C	4.878858	0.25084	-0.14524	L
H	4.482377	-0.59825	0.396914	L
C	-1.16263	2.468154	1.39686	H
C	-1.97271	3.750432	1.346488	L
C	-1.27417	5.124179	1.132369	L
C	-1.75173	4.702141	2.527266	L
H	-0.94031	4.412468	3.23013	L
H	-2.64689	5.233677	2.906479	L
C	-3.38064	3.609408	0.806688	L
C	-3.56159	3.328408	-0.55478	L
H	-2.70596	3.202398	-1.20603	L

C	-4.84238	3.199913	-1.09049	L
H	-4.9355	2.96062	-2.14155	L
C	-5.97902	3.324182	-0.26985	L
C	-5.79253	3.570594	1.103916	L
H	-6.6374	3.678246	1.770796	L
C	-4.50826	3.690176	1.639348	L
H	-4.40454	3.840703	2.705164	L
C	-2.06412	6.235063	0.467802	L
C	-2.26614	6.203795	-0.92004	L
H	-1.86028	5.395743	-1.51392	L
C	-2.98479	7.217265	-1.55686	L
H	-3.12972	7.160881	-2.62844	L
C	-3.48555	8.305641	-0.82262	L
C	-3.2278	8.369368	0.557996	L
H	-3.59284	9.199234	1.149853	L
C	-2.51136	7.351849	1.194065	L
H	-2.30898	7.439881	2.253477	L
C	0.222859	5.227192	0.977543	L
C	0.956667	6.09115	1.809274	L
H	0.47913	6.56785	2.656295	L
C	2.289611	6.402754	1.514856	L
H	2.81767	7.098074	2.154384	L
C	2.909173	5.866547	0.37281	L
C	2.176412	4.976668	-0.43262	L
H	2.631377	4.52659	-1.29755	L
C	0.846464	4.672019	-0.14489	L
H	0.289723	4.048572	-0.83204	L
C	-2.49958	-1.00241	1.412888	H
C	-3.91553	-1.59303	1.46624	L
C	-3.96305	-2.84909	2.347201	L
H	-4.58698	-3.69506	2.018324	L
H	-3.05219	-3.06757	2.945086	L
C	-4.74342	-1.60394	2.795791	L
C	-4.19622	-0.82391	3.965844	L
C	-3.81157	-1.48023	5.143853	L
H	-3.97914	-2.54402	5.257757	L
C	-3.15232	-0.77889	6.156541	L
H	-2.82232	-1.31653	7.035604	L
C	-2.87335	0.591162	6.00933	L
C	-3.32708	1.260621	4.859383	L
H	-3.14901	2.321461	4.732232	L
C	-3.99932	0.561317	3.853977	L
H	-4.30414	1.083962	2.956494	L
C	-6.25309	-1.70509	2.678913	L
C	-6.92377	-2.90018	2.99133	L
H	-6.40054	-3.71821	3.469958	L

C	-8.24636	-3.09127	2.585555	L
H	-8.70325	-4.05947	2.74303	L
C	-8.9268	-2.07884	1.888011	L
C	-8.30669	-0.82924	1.73116	L
H	-8.82852	-0.02218	1.237857	L
C	-6.98646	-0.63699	2.141828	L
H	-6.50919	0.316023	1.953664	L
C	-4.74742	-1.55295	0.185899	L
C	-5.27683	-2.70689	-0.41416	L
H	-5.00843	-3.6831	-0.07179	L
C	-6.17123	-2.6164	-1.48012	L
H	-6.54976	-3.53272	-1.91347	L
C	-6.55748	-1.36506	-1.98738	L
C	-5.98194	-0.21096	-1.42791	L
H	-6.25704	0.767135	-1.78889	L
C	-5.0824	-0.30547	-0.36046	L
H	-4.68844	0.59906	0.083381	L
C	1.054654	-2.33647	1.480638	H
C	1.871938	-3.61727	1.533494	L
C	1.192382	-5.00628	1.357501	L
C	1.5904	-4.50607	2.750771	L
H	0.743272	-4.18234	3.39417	L
H	2.472793	-4.99562	3.209186	L
C	3.323986	-3.49732	1.119652	L
C	3.651826	-3.43638	-0.24001	L
H	2.871175	-3.42706	-0.98789	L
C	4.985397	-3.39454	-0.64871	L
H	5.19198	-3.3547	-1.70756	L
C	6.028199	-3.35833	0.296746	L
C	5.689304	-3.37164	1.664544	L
H	6.452027	-3.36244	2.430923	L
C	4.35406	-3.42045	2.069785	L
H	4.131346	-3.40878	3.128635	L
C	2.019428	-6.14564	0.790745	L
C	2.497078	-7.18752	1.604668	L
H	2.282994	-7.20665	2.664899	L
C	3.250892	-8.22751	1.054148	L
H	3.611132	-9.0136	1.705916	L
C	3.512768	-8.26732	-0.3263	L
C	2.979177	-7.25942	-1.14716	L
H	3.155316	-7.26499	-2.21544	L
C	2.225527	-6.22176	-0.59521	L
H	1.803138	-5.47381	-1.25304	L
C	-0.29541	-5.1355	1.150327	L
C	-0.8879	-4.64792	-0.02007	L
H	-0.31396	-4.05645	-0.7213	L

C	-2.20707	-4.98112	-0.33188	L
H	-2.63178	-4.59566	-1.24413	L
C	-2.9607	-5.8206	0.510042	L
C	-2.36798	-6.29115	1.694362	L
H	-2.90729	-6.95433	2.358074	L
C	-1.04657	-5.95879	2.005567	L
H	-0.59131	-6.38618	2.890445	L
O	-1.03194	1.917352	2.529497	H
O	-0.77713	1.992384	0.283443	H
O	-1.88771	-0.87081	2.509755	H
O	-2.01857	-0.71166	0.269666	H
O	0.852122	-1.74989	2.580748	H
O	0.72476	-1.90389	0.327398	H
O	1.696513	1.059207	2.59144	H
O	1.890843	0.776085	0.367593	H
C	7.453893	-3.25743	-0.14023	L
C	8.397436	-2.58309	0.651105	L
C	7.884215	-3.81223	-1.35884	L
C	9.72295	-2.45236	0.23552	L
H	8.113442	-2.13424	1.591762	L
C	9.21262	-3.68194	-1.77869	L
H	7.200746	-4.36626	-1.98852	L
C	10.16347	-2.9962	-0.98812	L
H	10.40539	-1.91922	0.883255	L
H	9.475509	-4.13022	-2.72502	L
C	-7.34486	3.136267	-0.83623	L
C	-8.36131	2.543249	-0.07152	L
C	-7.63247	3.502129	-2.16176	L
C	-9.62343	2.308636	-0.61831	L
H	-8.17885	2.235022	0.948185	L
C	-8.89074	3.25606	-2.71631	L
H	-6.8862	3.98842	-2.77642	L
C	-9.91501	2.647221	-1.95625	L
H	-10.3713	1.850205	0.014102	L
H	-9.04119	3.555613	-3.74246	L
C	-7.56259	-1.26995	-3.08453	L
C	-8.60873	-2.20251	-3.17605	L
C	-7.48909	-0.25188	-4.04949	L
C	-9.54385	-2.13157	-4.20816	L
H	-8.72027	-2.9853	-2.43941	L
C	-8.42853	-0.17499	-5.08261	L
H	-6.68805	0.475602	-4.02674	L
C	-9.47222	-1.12327	-5.19169	L
H	-10.3256	-2.87838	-4.23342	L
H	-8.31059	0.627917	-5.79458	L
C	7.268645	0.865802	-3.0274	L

C	8.156168	-0.21952	-2.97047	L
C	7.327961	1.724357	-4.13679	L
C	9.07879	-0.43936	-3.99057	L
H	8.163002	-0.88707	-2.12012	L
C	8.26782	1.517943	-5.15035	L
H	6.639394	2.554195	-4.2315	L
C	9.172994	0.433357	-5.09307	L
H	9.732404	-1.2933	-3.90373	L
H	8.267806	2.219395	-5.97092	L
C	-4.26318	9.37482	-1.49827	L
C	-5.21527	9.052792	-2.4769	L
C	-4.06069	10.72324	-1.17061	L
C	-5.95008	10.05507	-3.11577	L
H	-5.40611	8.019151	-2.7383	L
C	-4.79228	11.72754	-1.80844	L
H	-3.32102	11.00549	-0.43184	L
C	-5.75379	11.41858	-2.79549	L
H	-6.66951	9.739376	-3.85617	L
H	-4.59772	12.75304	-1.52566	L
C	4.318476	6.201467	0.019616	L
C	4.71363	6.270416	-1.32658	L
C	5.303285	6.326815	1.013035	L
C	6.061342	6.368836	-1.67155	L
H	3.981482	6.212356	-2.12144	L
C	6.655584	6.433533	0.66957	L
H	5.038959	6.273481	2.061348	L
C	7.066597	6.42605	-0.68394	L
H	6.314815	6.367015	-2.72273	L
H	7.366456	6.4854	1.480371	L
C	9.906277	2.442169	0.936571	L
C	10.9481	3.262603	1.388011	L
C	9.994079	1.87942	-0.34547	L
C	12.05568	3.518185	0.572564	L
H	10.90575	3.709157	2.373629	L
C	11.08764	2.145189	-1.16734	L
H	9.192333	1.264771	-0.73179	L
C	12.14707	2.966388	-0.72814	L
H	12.82489	4.159037	0.976147	L
H	11.09273	1.711711	-2.15815	L
C	4.328791	-9.36277	-0.90835	L
C	5.479173	-9.82162	-0.24979	L
C	3.967397	-9.9541	-2.12765	L
C	6.254024	-10.8479	-0.79679	L
H	5.793007	-9.37253	0.684437	L
C	4.738726	-10.981	-2.6763	L
H	3.07553	-9.63448	-2.65204	L

C	5.90008	-11.452	-2.02564	L
H	7.129184	-11.1507	-0.24194	L
H	4.417929	-11.4082	-3.61651	L
C	-4.36247	-6.18117	0.155296	L
C	-5.35284	-6.27486	1.146782	L
C	-4.74508	-6.32457	-1.1891	L
C	-6.69571	-6.43994	0.799167	L
H	-5.10228	-6.15949	2.193292	L
C	-6.08772	-6.48113	-1.5391	L
H	-4.00706	-6.29242	-1.98048	L
C	-7.09831	-6.5123	-0.55199	L
H	-7.42453	-6.47906	1.59715	L
H	-6.31409	-6.55674	-2.59188	L
C	-10.2094	-2.36863	1.202734	L
C	-11.192	-3.16569	1.806604	L
C	-10.4047	-1.93784	-0.1174	L
C	-12.3357	-3.54537	1.09656	L
H	-11.0701	-3.5069	2.82704	L
C	-11.5329	-2.33293	-0.83451	L
H	-9.65663	-1.33569	-0.61735	L
C	-12.5222	-3.14908	-0.24921	L
H	-13.0517	-4.16636	1.613353	L
H	-11.6175	-2.01237	-1.86296	L
C	-2.09799	1.314912	7.044727	L
C	-1.07312	2.200102	6.681328	L
C	-2.37797	1.124054	8.403537	L
C	-0.35822	2.897413	7.658539	L
H	-0.8207	2.350539	5.638582	L
C	-1.66297	1.81651	9.383739	L
H	-3.17475	0.457169	8.707864	L
C	-0.64413	2.732184	9.032199	L
H	0.413309	3.580533	7.330814	L
H	-1.9381	1.633908	10.41132	L
C	1.804184	-0.56039	7.339574	L
C	0.755228	-1.44144	7.042872	L
C	2.066855	-0.24499	8.678301	L
C	-0.00568	-2.00843	8.068127	L
H	0.517642	-1.68658	6.014669	L
C	1.303795	-0.8041	9.706196	L
H	2.8834	0.419401	8.931639	L
C	0.2554	-1.71075	9.424302	L
H	-0.79611	-2.69286	7.792834	L
H	1.562739	-0.52429	10.71608	L
C	-6.54008	12.55797	-3.47662	L
C	-5.55456	13.50711	-4.19254	L
H	-4.94727	12.94506	-4.93476	L

H	-6.10173	14.3135	-4.72756	L
H	-4.86304	13.99552	-3.47465	L
C	-7.32974	13.34786	-2.41026	L
H	-8.01414	12.66994	-1.85563	L
H	-6.65263	13.83497	-1.67788	L
H	-7.9387	14.14872	-2.88321	L
C	-7.55321	12.0506	-4.53107	L
H	-8.31219	11.38638	-4.06386	L
H	-8.09697	12.9013	-4.99675	L
H	-7.03482	11.50086	-5.34629	L
C	8.549103	6.432978	-1.11182	L
C	9.526978	6.531839	0.082329	L
H	10.5816	6.543659	-0.27019	L
H	9.353206	7.465001	0.660334	L
H	9.417348	5.658005	0.754919	L
C	8.861586	5.123523	-1.86838	L
H	8.272595	5.042947	-2.8061	L
H	9.936507	5.070782	-2.1424	L
H	8.620371	4.246198	-1.23138	L
C	8.821688	7.639407	-2.03674	L
H	8.242927	7.572768	-2.98112	L
H	8.548736	8.587491	-1.52486	L
H	9.897317	7.688349	-2.31368	L
C	13.33729	3.234364	-1.67129	L
C	12.83601	3.966296	-2.93482	L
H	12.08777	3.361204	-3.48841	L
H	12.36622	4.934852	-2.65913	L
H	13.67883	4.174138	-3.62917	L
C	13.98532	1.892774	-2.08078	L
H	14.88918	2.064395	-2.70463	L
H	14.28688	1.317416	-1.17878	L
H	13.28944	1.267803	-2.6782	L
C	14.43704	4.109353	-1.02402	L
H	14.03933	5.11154	-0.75391	L
H	14.8474	3.619043	-0.11478	L
H	15.28117	4.267599	-1.73009	L
C	10.24987	0.181476	-6.16665	L
C	10.22834	1.230923	-7.30341	L
H	10.41591	2.251095	-6.90375	L
H	11.02042	1.015823	-8.05338	L
H	9.25283	1.217686	-7.83603	L
C	11.64798	0.228369	-5.51023	L
H	11.77503	-0.57831	-4.7585	L
H	12.44647	0.099331	-6.27263	L
H	11.80406	1.204594	-5.00218	L
C	10.02726	-1.20771	-6.80339	L

H	10.14495	-2.02281	-6.05898	L
H	9.005217	-1.27507	-7.23545	L
H	10.76367	-1.39157	-7.61555	L
C	11.64365	-2.84409	-1.3972	L
C	11.96169	-3.47688	-2.77352	L
H	13.03336	-3.33604	-3.03375	L
H	11.76371	-4.57046	-2.7621	L
H	11.36014	-3.00561	-3.57863	L
C	12.53743	-3.53699	-0.34608	L
H	13.60858	-3.47601	-0.63739	L
H	12.43653	-3.06164	0.652099	L
H	12.26157	-4.60956	-0.25072	L
C	12.0139	-1.34589	-1.46978	L
H	11.34653	-0.81442	-2.17797	L
H	11.92908	-0.85232	-0.47931	L
H	13.06219	-1.21523	-1.81513	L
C	-0.5717	-2.39871	10.53094	L
C	-0.14785	-1.97368	11.95767	L
H	-0.76976	-2.48719	12.723	L
H	0.912187	-2.24453	12.15364	L
H	-0.28037	-0.87905	12.10052	L
C	-0.39454	-3.92902	10.42482	L
H	0.681325	-4.19931	10.49599	L
H	-0.93948	-4.4476	11.24337	L
H	-0.78978	-4.31946	9.463726	L
C	-2.06474	-2.04594	10.36508	L
H	-2.21328	-0.95125	10.46518	L
H	-2.45693	-2.36758	9.37829	L
H	-2.67603	-2.54755	11.14638	L
C	0.119448	3.57054	10.07943	L
C	-0.31651	3.26776	11.53353	L
H	0.261956	3.884778	12.25522	L
H	-1.39232	3.5039	11.68271	L
H	-0.13527	2.200326	11.78662	L
C	-0.13416	5.070393	9.814946	L
H	0.367431	5.697428	10.5838	L
H	0.258579	5.381065	8.824079	L
H	-1.2237	5.28888	9.842788	L
C	1.632426	3.285047	9.979658	L
H	1.833026	2.211386	10.17203	L
H	2.035679	3.54918	8.9807	L
H	2.195225	3.879666	10.73161	L
C	-8.59826	-6.61035	-0.8986	L
C	-8.87378	-6.56366	-2.42122	L
H	-9.96595	-6.60257	-2.62641	L
H	-8.48247	-5.62173	-2.86376	L

H	-8.41142	-7.433	-2.93641	L
C	-9.35563	-5.42851	-0.25543	L
H	-10.4158	-5.40569	-0.58765	L
H	-9.36435	-5.50357	0.850806	L
H	-8.87778	-4.46648	-0.53615	L
C	-9.16345	-7.93705	-0.35179	L
H	-8.61761	-8.79979	-0.79132	L
H	-9.06873	-7.99246	0.753242	L
H	-10.2415	-8.03863	-0.60385	L
C	-10.5016	-1.10922	-6.34093	L
C	-11.9261	-0.96061	-5.76383	L
H	-12.6813	-0.94959	-6.57933	L
H	-12.1843	-1.7974	-5.08174	L
H	-12.016	-0.01019	-5.19966	L
C	-10.4069	-2.43455	-7.12823	L
H	-11.1038	-2.43011	-7.99444	L
H	-9.37425	-2.58331	-7.51175	L
H	-10.6725	-3.30612	-6.49402	L
C	-10.2763	0.048372	-7.34302	L
H	-10.363	1.034028	-6.83808	L
H	-9.27655	-0.03153	-7.82215	L
H	-11.0375	0.021968	-8.15296	L
C	-11.3181	2.358204	-2.52601	L
C	-11.4487	2.719914	-4.02458	L
H	-11.2955	3.808763	-4.1858	L
H	-10.7109	2.151711	-4.6305	L
H	-12.4629	2.469322	-4.40489	L
C	-12.3656	3.180226	-1.74634	L
H	-13.3846	3.009979	-2.15692	L
H	-12.385	2.898701	-0.6724	L
H	-12.1362	4.265501	-1.81755	L
C	-11.6364	0.855236	-2.37793	L
H	-10.8457	0.244178	-2.86306	L
H	-11.7052	0.557362	-1.31186	L
H	-12.613	0.60762	-2.84693	L
C	6.725434	-12.587	-2.66671	L
C	7.223594	-12.1387	-4.05796	L
H	7.82718	-11.2093	-3.9711	L
H	7.857649	-12.9251	-4.52215	L
H	6.378853	-11.9422	-4.75072	L
C	7.965262	-12.9836	-1.82935	L
H	7.663882	-13.349	-0.8238	L
H	8.530538	-13.8025	-2.32542	L
H	8.65856	-12.1223	-1.71549	L
C	5.841256	-13.8438	-2.81901	L
H	5.439092	-14.1552	-1.83062	L

H	4.985294	-13.6611	-3.50168	L
H	6.427136	-14.6896	-3.24006	L
C	-13.7362	-3.58561	-1.0931	L
C	-14.5009	-2.33569	-1.58178	L
H	-14.8145	-1.7119	-0.7169	L
H	-13.8767	-1.71071	-2.25422	L
H	-15.4102	-2.62722	-2.15093	L
C	-14.7322	-4.47112	-0.30723	L
H	-15.5931	-4.76045	-0.94851	L
H	-14.2431	-5.40848	0.035963	L
H	-15.1388	-3.92508	0.571387	L
C	-13.247	-4.39652	-2.31379	L
H	-12.6571	-5.27815	-1.98159	L
H	-14.1077	-4.75913	-2.91652	L
H	-12.6082	-3.78347	-2.98366	L
Rh	-0.04874	0.051439	0.198556	H
Rh	-0.09953	0.085851	2.624969	H
C	-0.0099	0.171152	-2.15703	H
C	-1.39416	-0.20125	-2.51448	H
O	-2.31011	0.587289	-2.62318	H
O	-1.56592	-1.55638	-2.65974	H
C	-2.88011	-1.98681	-2.95958	H
H	-3.23078	-2.61843	-2.14752	H
H	-3.54442	-1.1291	-3.08073	H
C	0.584934	1.379698	-2.75931	H
C	1.949655	1.672237	-2.5485	H
C	-0.1513	2.259348	-3.58278	H
C	2.574523	2.731317	-3.20073	H
H	2.521964	1.069821	-1.85649	H
C	0.450515	3.361053	-4.18573	H
H	-1.20937	2.094005	-3.73349	H
C	1.813924	3.571499	-4.00735	H
H	3.630498	2.923561	-3.054	H
H	-0.138	4.034306	-4.79892	H
Br	2.684829	5.100931	-4.88362	H
C	-2.88805	-2.80997	-4.24209	H
Cl	-2.34862	-1.79638	-5.66676	H
Cl	-1.78526	-4.26481	-4.10324	H
Cl	-4.59865	-3.38735	-4.52421	H
H	0.714519	-0.73087	-1.99676	H
C	1.17301	-1.60527	-3.09259	H
H	0.535525	-1.54153	-3.9679	H
H	0.914453	-2.44128	-2.44271	H
C	2.622361	-1.29178	-3.28285	H
H	2.730023	-0.32377	-3.77925	H
H	3.137448	-1.23415	-2.31689	H

C	3.307669	-2.38169	-4.15265	H
H	2.754096	-2.50639	-5.09364	H
H	3.251284	-3.34312	-3.62642	H
C	4.787225	-2.06174	-4.47185	H
C	5.4851	-3.30072	-5.05264	H
H	6.545496	-3.09567	-5.24084	H
H	5.424984	-4.15313	-4.3657	H
H	5.029805	-3.60239	-6.00456	H
C	4.948978	-0.85548	-5.40877	H
H	6.009038	-0.67732	-5.62315	H
H	4.442104	-1.02924	-6.3667	H
H	4.54579	0.067268	-4.97706	H
H	5.288824	-1.8161	-3.5282	H

TS-2 (E = -1803.4996243 a.u. ; Esol = -1803.61469965 a.u.)

C	-2.08631	-1.36432	0.970013
C	-3.4411	-2.07569	0.94436
C	-3.40391	-3.39941	1.713471
H	-3.96462	-4.24796	1.296634
H	-2.4867	-3.59861	2.308588
C	-4.28473	-2.26385	2.251021
C	-3.82444	-1.55309	3.497462
C	-3.76307	-0.15289	3.514211
H	-4.08989	0.416851	2.653326
C	-3.20693	0.512561	4.607738
H	-3.13057	1.590799	4.582699
C	-2.73598	-0.20801	5.718071
C	-2.89035	-1.60538	5.738045
H	-2.55923	-2.18418	6.58948
C	-3.42905	-2.27356	4.634204
H	-3.50362	-3.35374	4.651068
C	-5.77626	-2.50724	2.119048
C	-6.33506	-3.75584	2.442774
H	-5.72945	-4.52706	2.90205
C	-7.66003	-4.04402	2.10477
H	-8.05143	-5.033	2.307095
C	-8.44141	-3.08939	1.434196
C	-7.91211	-1.81017	1.20797
H	-8.50087	-1.0547	0.705071
C	-6.60773	-1.50682	1.596744
H	-6.22283	-0.51209	1.418329
C	-4.26618	-1.95543	-0.33327
C	-4.76616	-3.0685	-1.02949
H	-4.44267	-4.06273	-0.7955
C	-5.77348	-2.91554	-1.98395
H	-6.20617	-3.80323	-2.42459
C	-6.27825	-1.64084	-2.28882
C	-5.66641	-0.51874	-1.70787
H	-5.99797	0.478036	-1.96102
C	-4.6745	-0.67575	-0.7383
H	-4.29262	0.200286	-0.23051
C	1.651726	-2.02982	1.080922
C	2.613829	-3.21423	1.115008
C	2.123601	-4.67741	0.896142
C	2.387174	-4.15106	2.309613
H	1.474258	-3.9524	2.912976
H	3.309204	-4.5069	2.811936
C	4.068121	-2.89977	0.817097
C	4.513386	-2.85868	-0.5084
H	3.825983	-3.07214	-1.31242

C	5.840488	-2.53758	-0.80935
H	6.149216	-2.55251	-1.84595
C	6.747102	-2.19874	0.213384
C	6.290235	-2.228	1.545375
H	6.93783	-1.94177	2.363315
C	4.971469	-2.58058	1.842196
H	4.654047	-2.58368	2.876104
C	3.111066	-5.70353	0.369111
C	3.71877	-6.65299	1.210256
H	3.493777	-6.68649	2.2675
C	4.618673	-7.58719	0.690465
H	5.076578	-8.30162	1.363103
C	4.902362	-7.6177	-0.68578
C	4.24019	-6.7144	-1.53421
H	4.427184	-6.71768	-2.60063
C	3.340507	-5.78295	-1.01229
H	2.820857	-5.11911	-1.68901
C	0.673653	-4.98413	0.610876
C	-0.00174	-5.93566	1.391716
H	0.471371	-6.35228	2.27242
C	-1.26289	-6.40439	1.011071
H	-1.73585	-7.16449	1.618534
C	-1.87715	-5.93334	-0.16389
C	-1.19942	-4.96568	-0.93172
H	-1.64249	-4.56539	-1.8306
C	0.067972	-4.51068	-0.55808
H	0.596736	-3.82555	-1.20705
C	2.226872	1.669424	1.279938
C	3.585672	2.377244	1.420341
C	3.529263	3.607462	2.339134
H	4.145633	4.492818	2.106897
H	2.572669	3.757617	2.884362
C	4.335067	2.38185	2.793206
C	3.764674	1.557638	3.921617
C	3.310662	2.157107	5.105946
H	3.405652	3.226097	5.249631
C	2.689548	1.383066	6.09264
H	2.312511	1.87234	6.980591
C	2.517623	-0.00146	5.909228
C	3.043792	-0.6039	4.754188
H	2.956883	-1.67207	4.599297
C	3.670109	0.169477	3.777186
H	4.021744	-0.29666	2.870326
C	5.846087	2.498688	2.758198
C	6.495264	3.636329	3.260996
H	5.926195	4.442781	3.705559

C	7.886353	3.747025	3.183025
H	8.363882	4.638039	3.571345
C	8.655703	2.708531	2.62927
C	8.00813	1.550129	2.171254
H	8.575852	0.736141	1.739066
C	6.617766	1.44436	2.24423
H	6.13837	0.548419	1.877654
C	4.487314	2.395314	0.186406
C	4.712293	1.180394	-0.48398
H	4.221996	0.271151	-0.15814
C	5.59089	1.112331	-1.5613
H	5.725182	0.167975	-2.06275
C	6.324208	2.237838	-1.95508
C	6.112466	3.453408	-1.28989
H	6.651491	4.343495	-1.5877
C	5.177991	3.542868	-0.25623
H	5.029961	4.511053	0.190943
C	-1.41202	2.287367	1.194428
C	-2.23085	3.560133	1.279458
C	-1.64838	4.917306	0.793177
C	-1.64759	4.55738	2.283628
H	-0.65854	4.278399	2.707969
H	-2.38843	5.095782	2.910026
C	-3.73277	3.372887	1.298921
C	-4.47009	3.331787	2.495113
H	-3.9902	3.511779	3.446839
C	-5.83571	3.021932	2.475664
H	-6.37899	2.994472	3.411543
C	-6.48784	2.744278	1.26011
C	-5.74511	2.793445	0.06978
H	-6.20674	2.56462	-0.88095
C	-4.38182	3.079086	0.097159
H	-3.81767	3.041012	-0.81853
C	-2.60445	6.028364	0.399504
C	-3.31366	5.958906	-0.81008
H	-3.187	5.119326	-1.47679
C	-4.18321	6.984835	-1.18565
H	-4.71726	6.899281	-2.12383
C	-4.33712	8.122184	-0.37531
C	-3.58304	8.219602	0.806844
H	-3.67403	9.085896	1.449888
C	-2.71526	7.190585	1.182001
H	-2.13174	7.303791	2.086675
C	-0.31453	4.909277	0.078009
C	0.817502	5.509127	0.651481
H	0.781665	5.899302	1.660466

C	1.99732	5.647654	-0.08699
H	2.854432	6.105511	0.38905
C	2.059277	5.223857	-1.42832
C	0.925317	4.614217	-1.99278
H	0.922186	4.307697	-3.02938
C	-0.24503	4.458014	-1.24784
H	-1.11281	4.019164	-1.72091
O	1.372032	-1.50334	2.196723
O	1.273542	-1.60223	-0.05761
O	1.557793	1.457677	2.332567
O	1.864283	1.323698	0.109261
O	-1.24565	1.663475	2.283244
O	-1.00096	1.925294	0.049381
O	-1.49394	-1.25431	2.074846
O	-1.63618	-0.93681	-0.14728
C	-7.91736	2.338655	1.225558
C	-8.4402	1.472844	2.197679
C	-8.75231	2.758683	0.178992
C	-9.74808	0.989183	2.093621
H	-7.82001	1.121402	3.012755
C	-10.061	2.284084	0.077147
H	-8.39126	3.452855	-0.56952
C	-10.5768	1.357663	1.008366
H	-10.0792	0.301193	2.856798
H	-10.6631	2.633283	-0.75028
C	8.146292	-1.77828	-0.10245
C	8.445667	-1.0951	-1.29374
C	9.194743	-2.02712	0.800274
C	9.736264	-0.63469	-1.55287
H	7.685932	-0.8947	-2.03086
C	10.49094	-1.57338	0.539766
H	9.021249	-2.58379	1.711663
C	10.78874	-0.85795	-0.64218
H	9.904816	-0.09615	-2.47545
H	11.24521	-1.79181	1.280571
C	7.319834	2.136212	-3.04443
C	7.014515	1.448149	-4.2262
C	8.589475	2.70938	-2.89978
C	7.956597	1.343003	-5.25196
H	6.036303	1.005586	-4.36508
C	9.532625	2.609295	-3.92356
H	8.858717	3.225603	-1.98637
C	9.238528	1.927719	-5.12498
H	7.657613	0.805341	-6.13896
H	10.49896	3.068461	-3.76765
C	-7.5071	-1.48976	-3.11128

C	-8.48089	-0.54087	-2.75859
C	-7.7587	-2.33842	-4.19878
C	-9.68144	-0.45177	-3.46551
H	-8.33608	0.109759	-1.90472
C	-8.95747	-2.24912	-4.90972
H	-7.02932	-3.07543	-4.50271
C	-9.95339	-1.31452	-4.55141
H	-10.3874	0.295294	-3.13835
H	-9.10379	-2.92391	-5.74194
C	5.875683	-8.59629	-1.23389
C	5.623863	-9.25475	-2.44639
C	7.067827	-8.87499	-0.54902
C	6.542998	-10.171	-2.96239
H	4.705244	-9.0749	-2.99072
C	7.989894	-9.79056	-1.06297
H	7.298524	-8.36898	0.38032
C	7.747319	-10.4609	-2.28439
H	6.3033	-10.656	-3.89877
H	8.889021	-9.95577	-0.48876
C	-3.22848	-6.41775	-0.57631
C	-3.5871	-6.4762	-1.93443
C	-4.20705	-6.72842	0.38402
C	-4.90532	-6.7371	-2.3172
H	-2.85367	-6.29483	-2.7095
C	-5.52644	-6.98382	0.003118
H	-3.97779	-6.7002	1.441031
C	-5.91528	-6.95274	-1.35274
H	-5.11632	-6.74669	-3.37535
H	-6.2512	-7.17379	0.782993
C	-9.78148	-3.43827	0.9168
C	-10.7096	-4.11578	1.717057
C	-10.1308	-3.10494	-0.39727
C	-11.9764	-4.43507	1.218655
H	-10.4613	-4.38212	2.737056
C	-11.3894	-3.42822	-0.90063
H	-9.42062	-2.60678	-1.04332
C	-12.3457	-4.09362	-0.10445
H	-12.652	-4.94788	1.886333
H	-11.6111	-3.14855	-1.91987
C	-5.27116	9.20723	-0.76946
C	-6.52796	8.903027	-1.31343
C	-4.91498	10.55354	-0.60374
C	-7.41175	9.920504	-1.68289
H	-6.83784	7.87268	-1.4376
C	-5.7953	11.57282	-0.97345
H	-3.94521	10.82158	-0.20342

C	-7.0641	11.28179	-1.52071
H	-8.36452	9.618364	-2.0908
H	-5.47447	12.59559	-0.83039
C	3.27383	5.471685	-2.25657
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C	3.663984	4.563101	-3.25404
C	5.160314	6.88266	-2.8712
H	3.757099	7.374629	-1.33847
C	4.784017	4.809111	-4.05269
H	3.115114	3.646378	-3.40899
C	5.557717	5.979364	-3.88017
H	5.712207	7.79608	-2.69686
H	5.030946	4.064414	-4.79441
C	10.13046	2.830283	2.547541
C	10.95755	1.765928	2.931969
C	10.72043	4.02364	2.109121
C	12.34747	1.90548	2.912546
H	10.52856	0.83447	3.280484
C	12.11025	4.160348	2.071706
H	10.10318	4.854016	1.78844
C	12.95721	3.1061	2.486154
H	12.94542	1.068418	3.245574
H	12.50041	5.105386	1.725449
C	1.774847	-0.8173	6.901534
C	0.882112	-1.81223	6.475232
C	1.964141	-0.62367	8.276125
C	0.214763	-2.61677	7.401065
H	0.695874	-1.96889	5.419533
C	1.293302	-1.42359	9.204942
H	2.657026	0.127078	8.634361
C	0.408692	-2.44318	8.790482
H	-0.44173	-3.3766	7.005671
H	1.486958	-1.25283	10.25471
C	-2.06627	0.500099	6.836179
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C	-2.34418	0.163938	8.167394
C	-0.54689	2.230576	7.62146
H	-0.89801	1.79572	5.555418
C	-1.73917	0.86078	9.216565
H	-3.05515	-0.61921	8.398467
C	-0.8324	1.914743	8.969632
H	0.13395	3.023227	7.351418
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C	8.736698	-11.4785	-2.88926
C	9.193673	-10.9877	-4.28024
H	9.659099	-9.98139	-4.201

H	9.940662	-11.6847	-4.71864
H	8.343107	-10.9234	-4.99054
C	8.041684	-12.8501	-3.03213
H	7.667645	-13.1982	-2.04495
H	7.182458	-12.8019	-3.73319
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C	10.00349	-11.6821	-2.02348
H	9.736897	-12.0686	-1.01599
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C	-7.39952	-7.14742	-1.72773
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H	-8.90956	-8.73855	-1.59595
H	-7.22094	-9.3308	-1.81526
H	-7.76501	-8.70958	-0.2153
C	-8.26606	-6.10032	-0.991
H	-7.90635	-5.07279	-1.21015
H	-9.3298	-6.17061	-1.30672
H	-8.24322	-6.25118	0.107257
C	-7.66698	-6.98532	-3.2438
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C	-13.7296	-4.42242	-0.69924
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H	-12.9774	-4.85467	-2.73041
H	-13.0195	-6.27791	-1.62967
H	-14.5432	-5.63315	-2.34548
C	-14.4249	-3.11568	-1.1403
H	-15.4424	-3.32472	-1.53619
H	-14.5222	-2.42103	-0.27811
H	-13.8575	-2.5998	-1.94312
C	-14.666	-5.13706	0.304177
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H	-10.3355	-1.66072	-7.30319
H	-11.9115	-0.81302	-7.40267
H	-10.4425	0.082842	-6.86603
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H	-12.9389	-2.61411	-5.83866
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H	-13.2177	-0.22521	-5.38113
C	-11.9978	0.790104	0.811498
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H	-13.3571	-0.74643	1.6173
H	-11.6172	-1.16426	1.749809
H	-12.3579	0.06085	2.862157
C	-12.1289	0.190353	-0.60736
H	-13.1038	-0.32658	-0.73352
H	-12.0774	0.97383	-1.39103
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C	-0.22318	2.691942	10.15549
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H	-0.94264	3.957861	11.8046
H	-1.96464	4.015803	10.32152
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C	0.748284	3.812097	9.711388
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H	1.170316	4.340496	10.5939
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H	1.398121	1.258975	10.50064
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C	-0.27619	-3.33649	9.846089
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H	0.334878	-4.76883	11.39993
H	1.454046	-4.67736	9.9905
H	1.442632	-3.3719	11.23129
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H	-1.69144	-5.0157	10.01743
H	-2.02567	-3.91929	8.639169
H	-0.64468	-5.09243	8.565126
C	-1.12684	-2.46646	10.79594
H	-0.51085	-1.7097	11.32425
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H	-1.61842	-3.095	11.56987
C	6.793383	6.300131	-4.74643
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H	7.988907	5.47984	-6.4031
H	7.302862	4.236006	-5.31289

H	6.242463	5.091865	-6.50563
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H	10.61093	1.067639	-8.27177
H	9.550377	0.044191	-7.25331
H	8.932576	1.604742	-7.94016
C	11.54699	1.102526	-5.69795
H	12.32717	1.018316	-6.48528
H	12.00016	1.631185	-4.83321
H	11.2674	0.077006	-5.37434
C	10.70982	3.273516	-6.66816
H	9.819007	3.835502	-7.02176
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C	12.1974	-0.3192	-0.96281
C	12.1429	1.220374	-1.06544
H	11.47112	1.548718	-1.88483
H	11.77122	1.659687	-0.11482
H	13.15092	1.637825	-1.27546
C	12.68522	-0.90631	-2.30525
H	13.71753	-0.56337	-2.53458
H	12.68604	-2.01704	-2.26412
H	12.03888	-0.59021	-3.1481
C	13.24556	-0.68797	0.112542
H	12.96854	-0.25902	1.097488
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H	14.24637	-0.28767	-0.15884
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C	-9.35635	11.94888	-2.49549
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C	-8.31725	13.29653	-0.66939
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H	16.22575	2.2472	1.57485
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C	0.059137	0.282502	-2.53282
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C	-2.22194	1.26593	-2.67811
C	-0.52364	2.131272	-4.16011
C	-3.16833	2.10636	-3.25783
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C	-1.44782	3.017645	-4.7068
H	0.497275	2.156479	-4.51783
C	-2.76339	2.989621	-4.25322
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TS-3 (E = -1803.47796546 a.u. ; Esol = -1803.60304243 a.u.)

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H	4.533643	6.950859	2.039255
C	2.797737	6.029475	1.193388
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C	2.436844	4.186675	-1.61137
C	3.64792	3.806151	-1.01757
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H	1.499113	4.74808	-3.48671
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H	-0.1539	-2.14892	4.26079
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C	-4.7082	-4.52308	-2.81261
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H	-5.62531	-3.62213	-1.06613
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C	2.559807	-0.62479	-0.56451
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