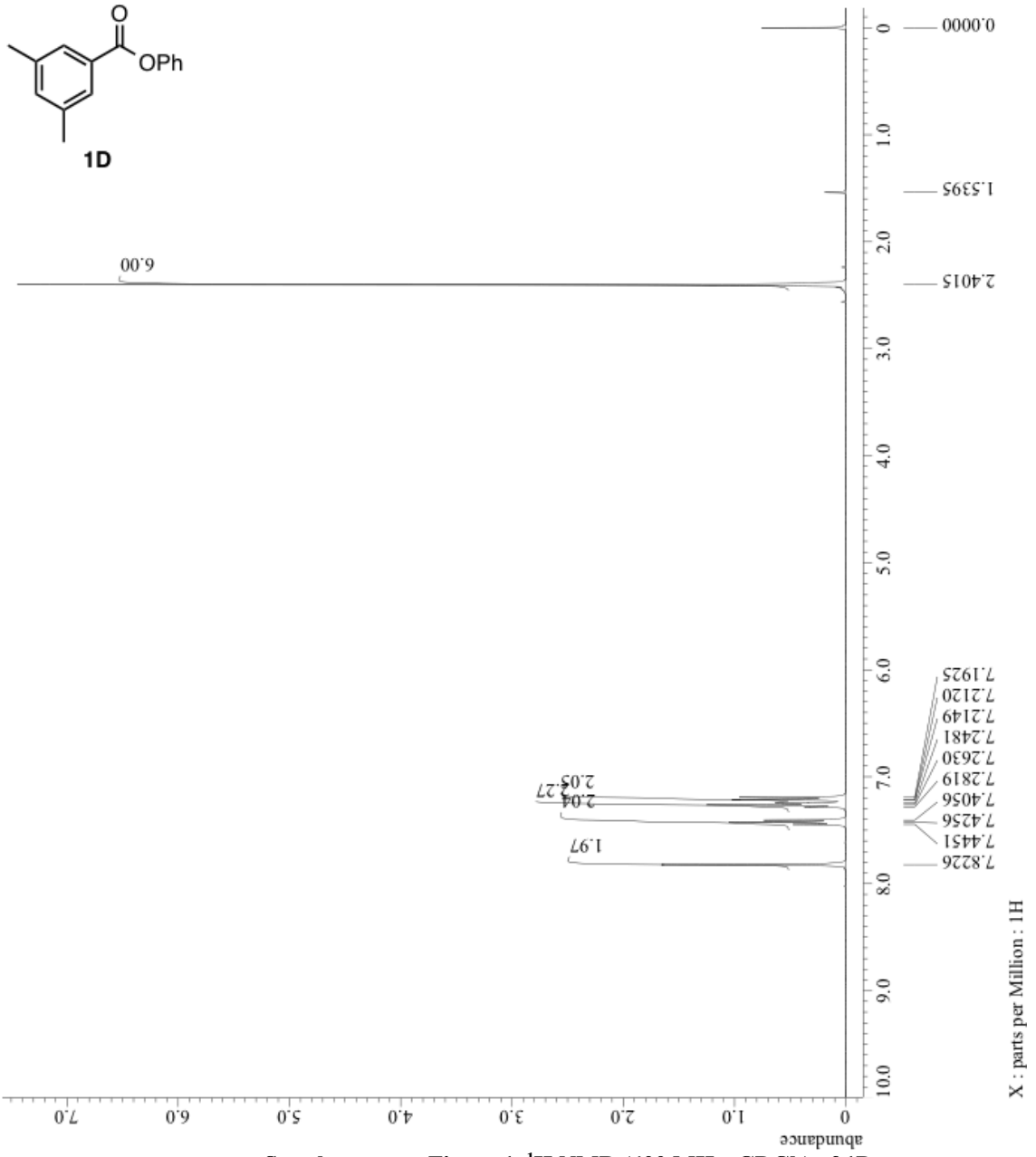
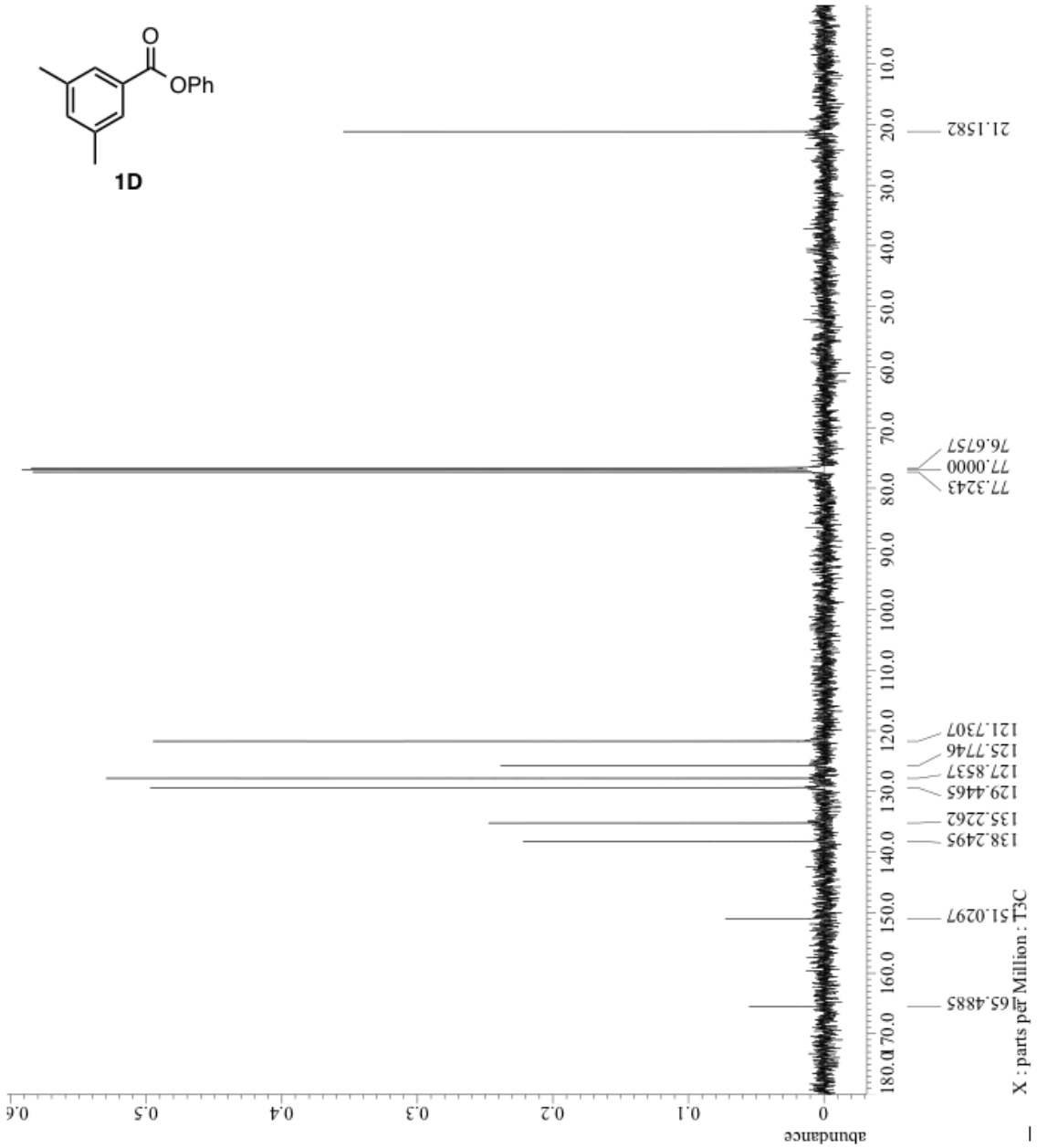
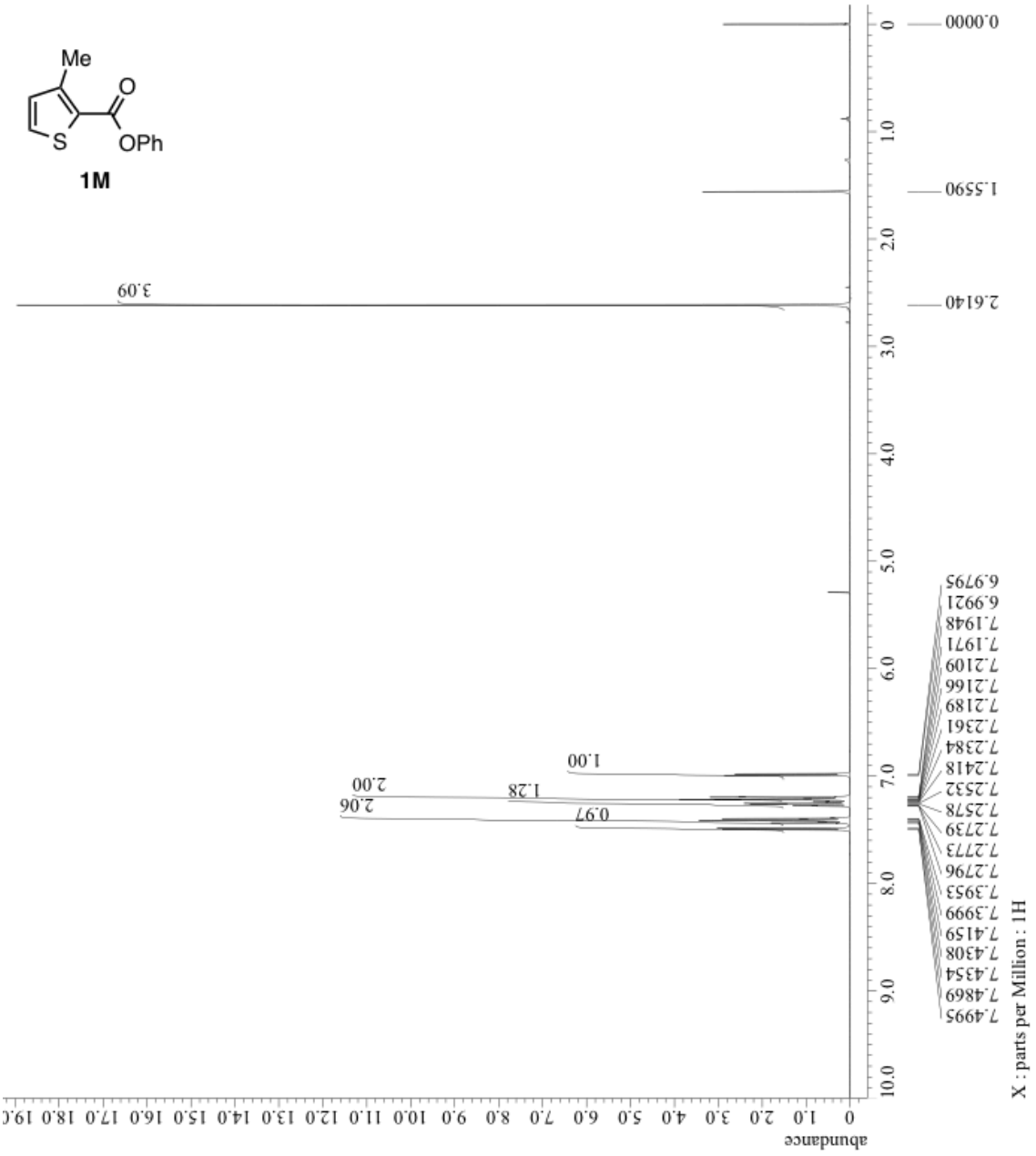


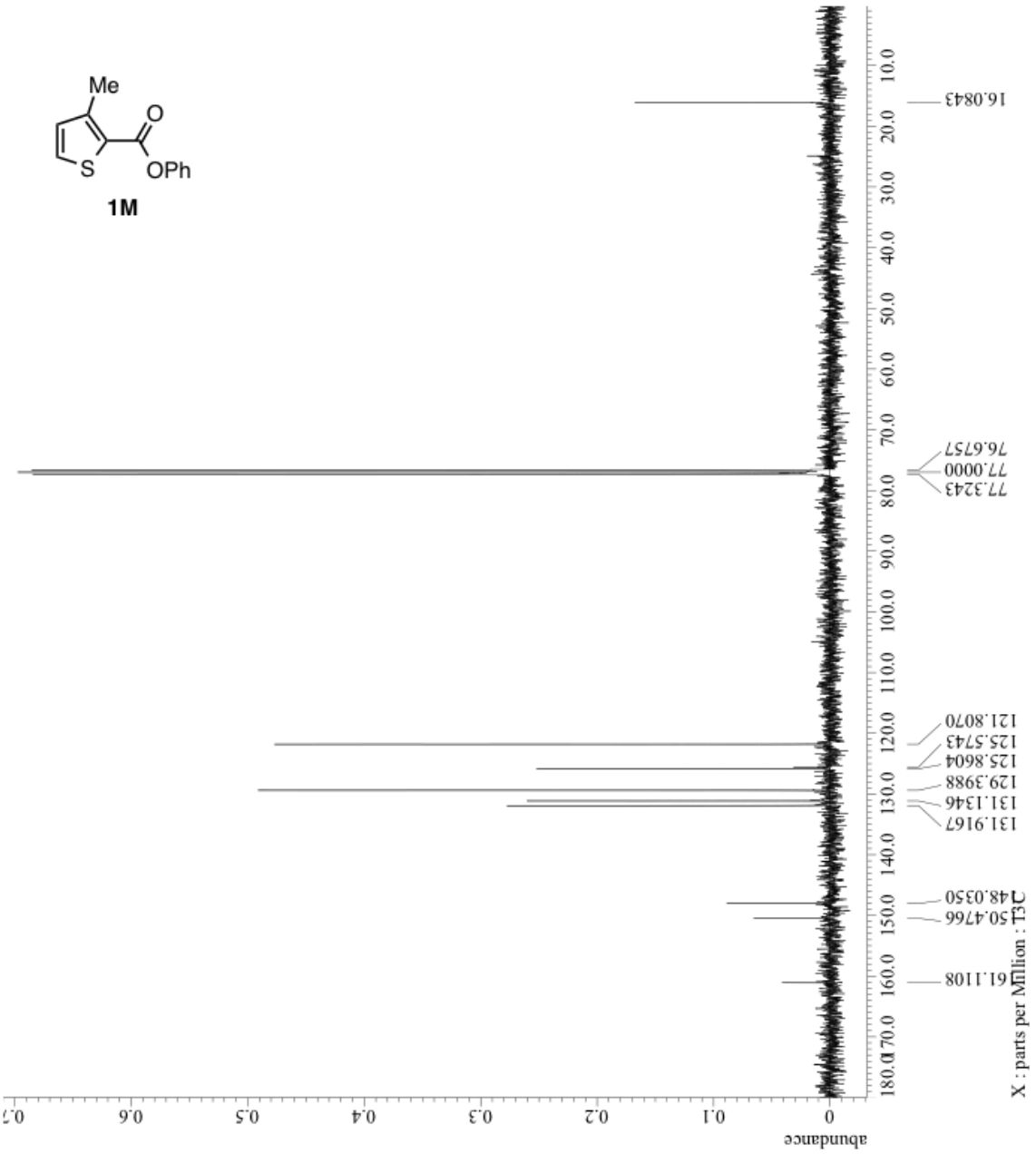
Supplementary Figure 1. ^{1}H NMR (400 MHz, $CDCl_3$) of 1D



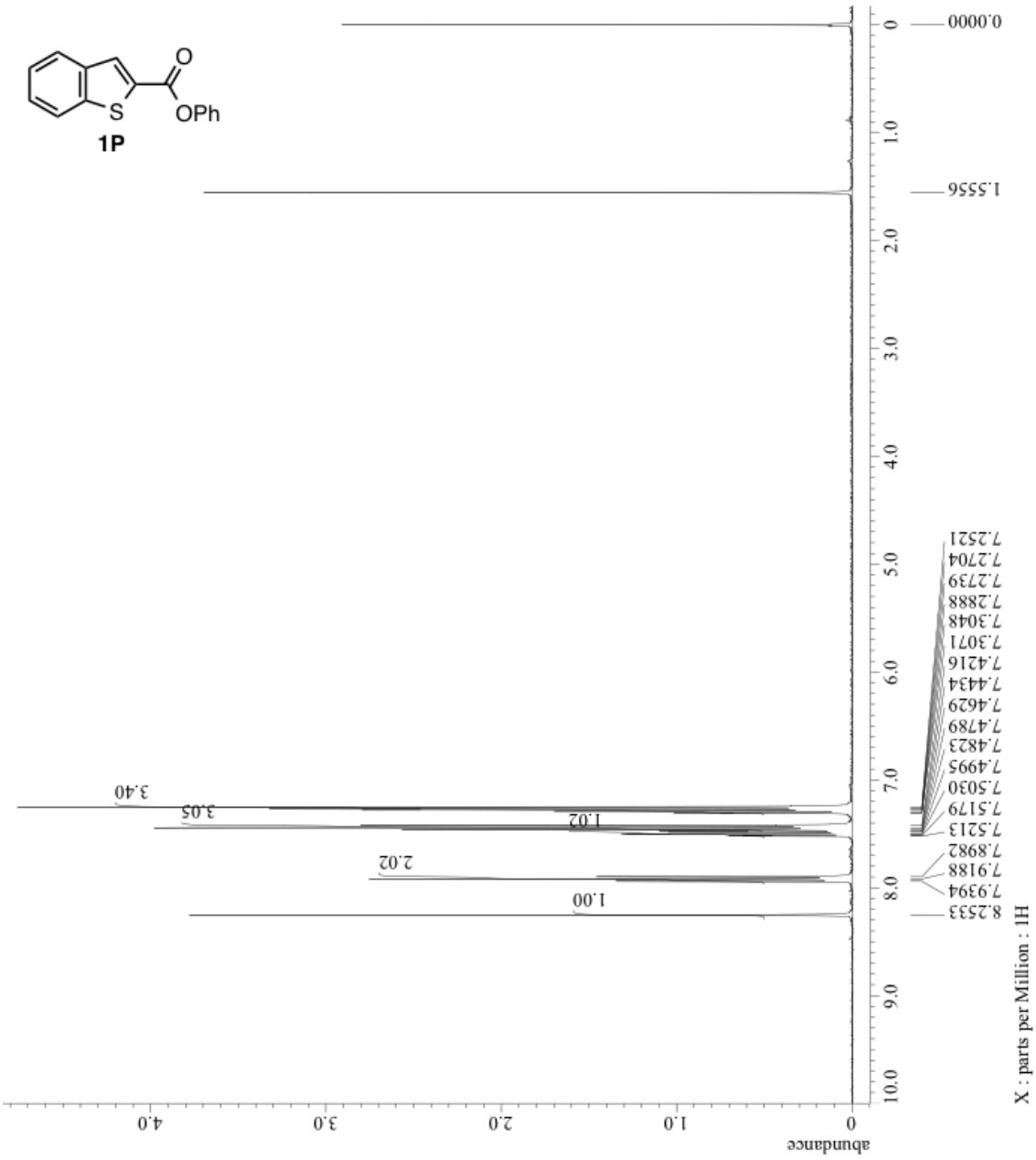
Supplementary Figure 2. ^{13}C NMR (100 MHz, $CDCl_3$) of 1D



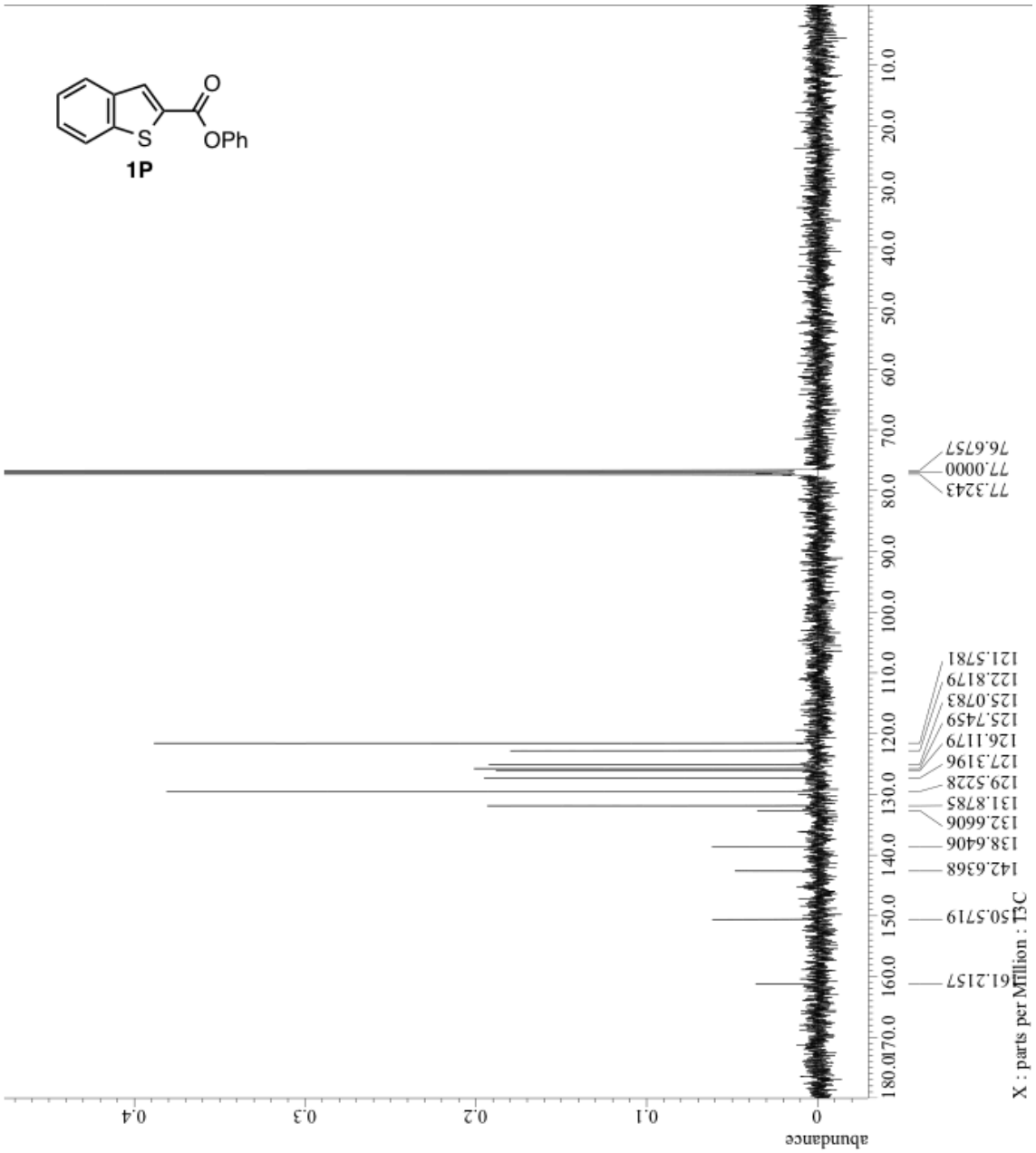
Supplementary Figure 3. ^{1}H NMR (400 MHz, $CDCl_3$) of 1M



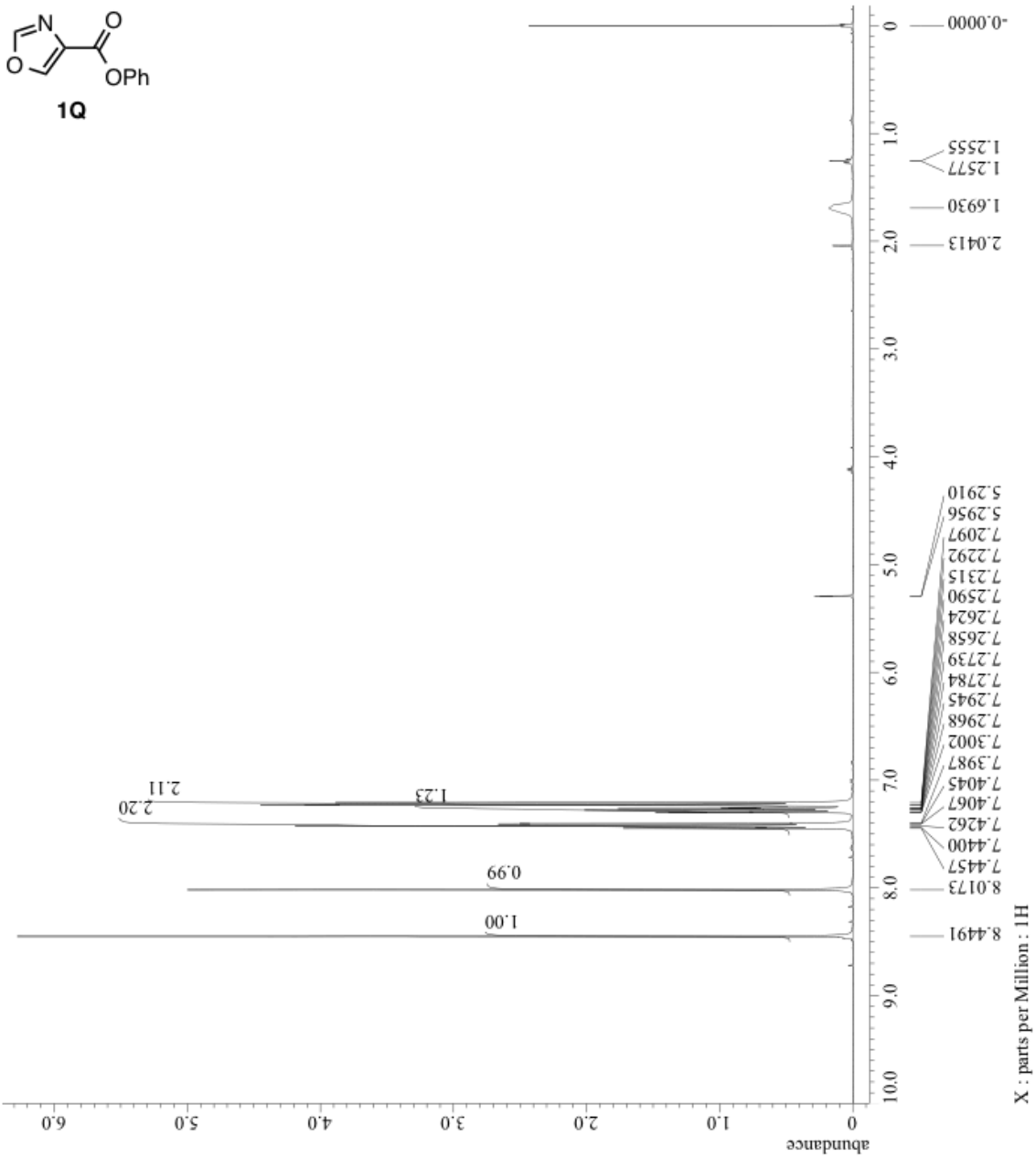
Supplementary Figure 4. ^{13}C NMR (100 MHz, $CDCl_3$) of 1M



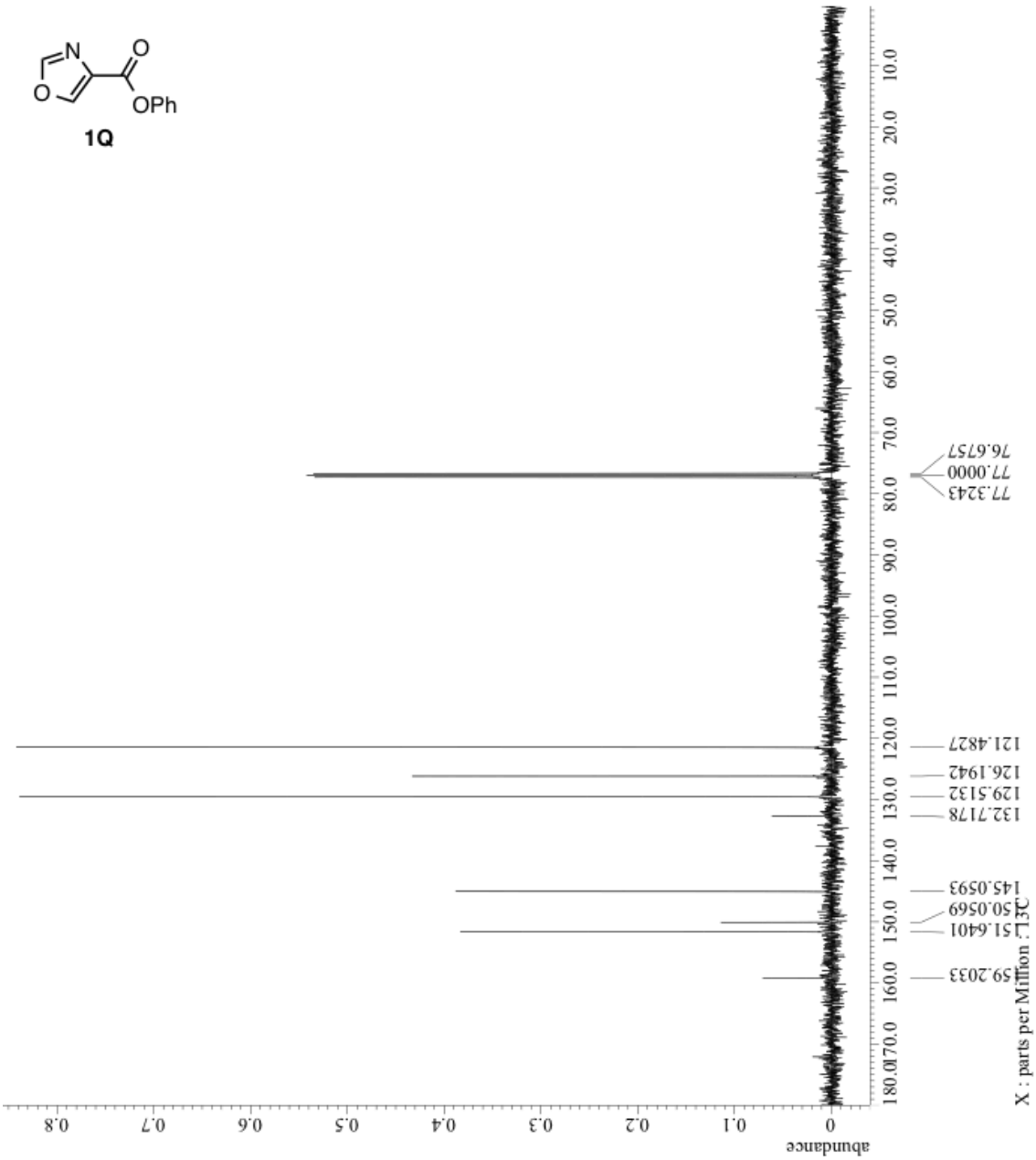
Supplementary Figure 5. ^{1}H NMR (400 MHz, $CDCl_3$) of 1P



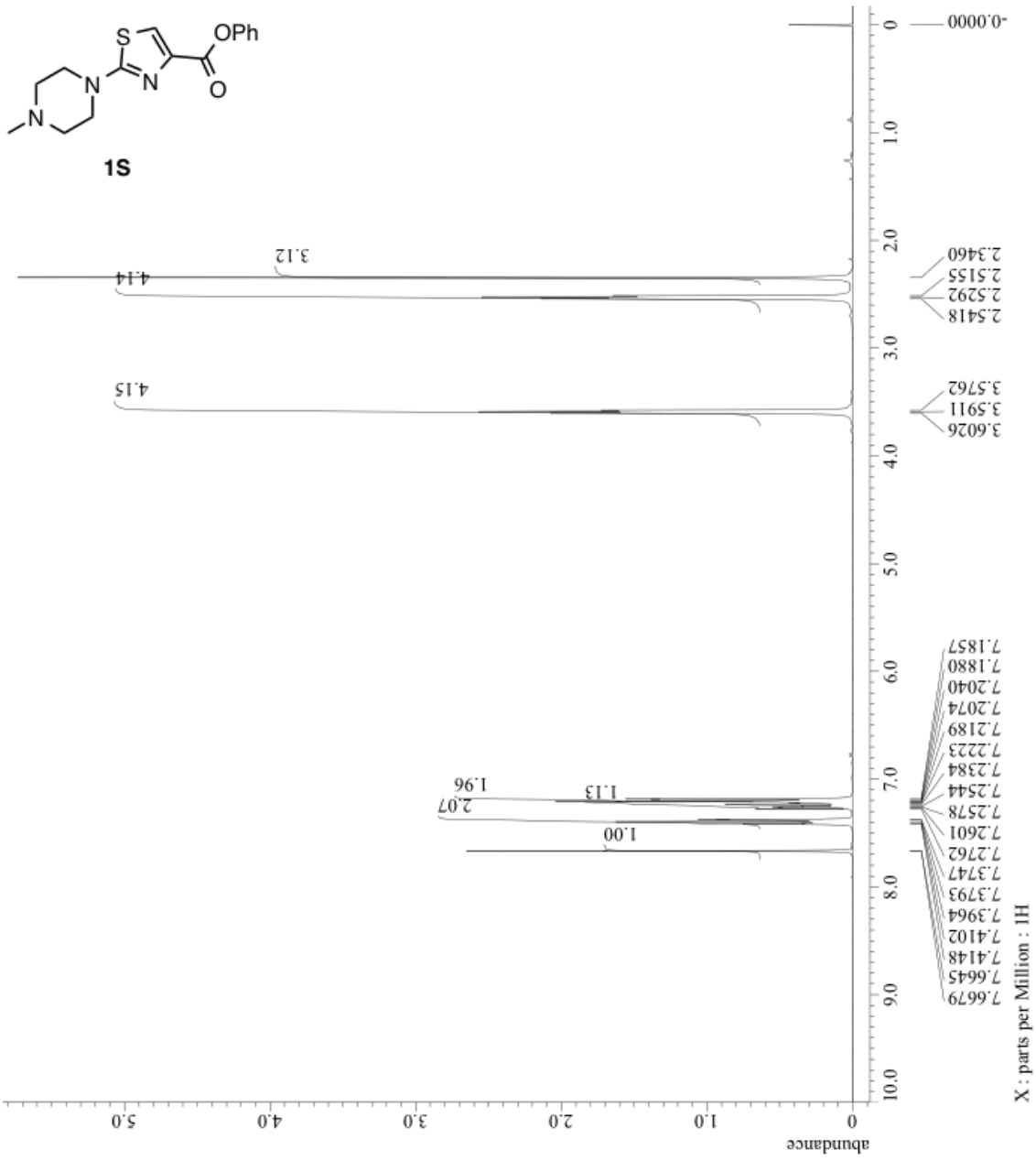
Supplementary Figure 6. ^{13}C NMR (100 MHz, $CDCl_3$) of 1P



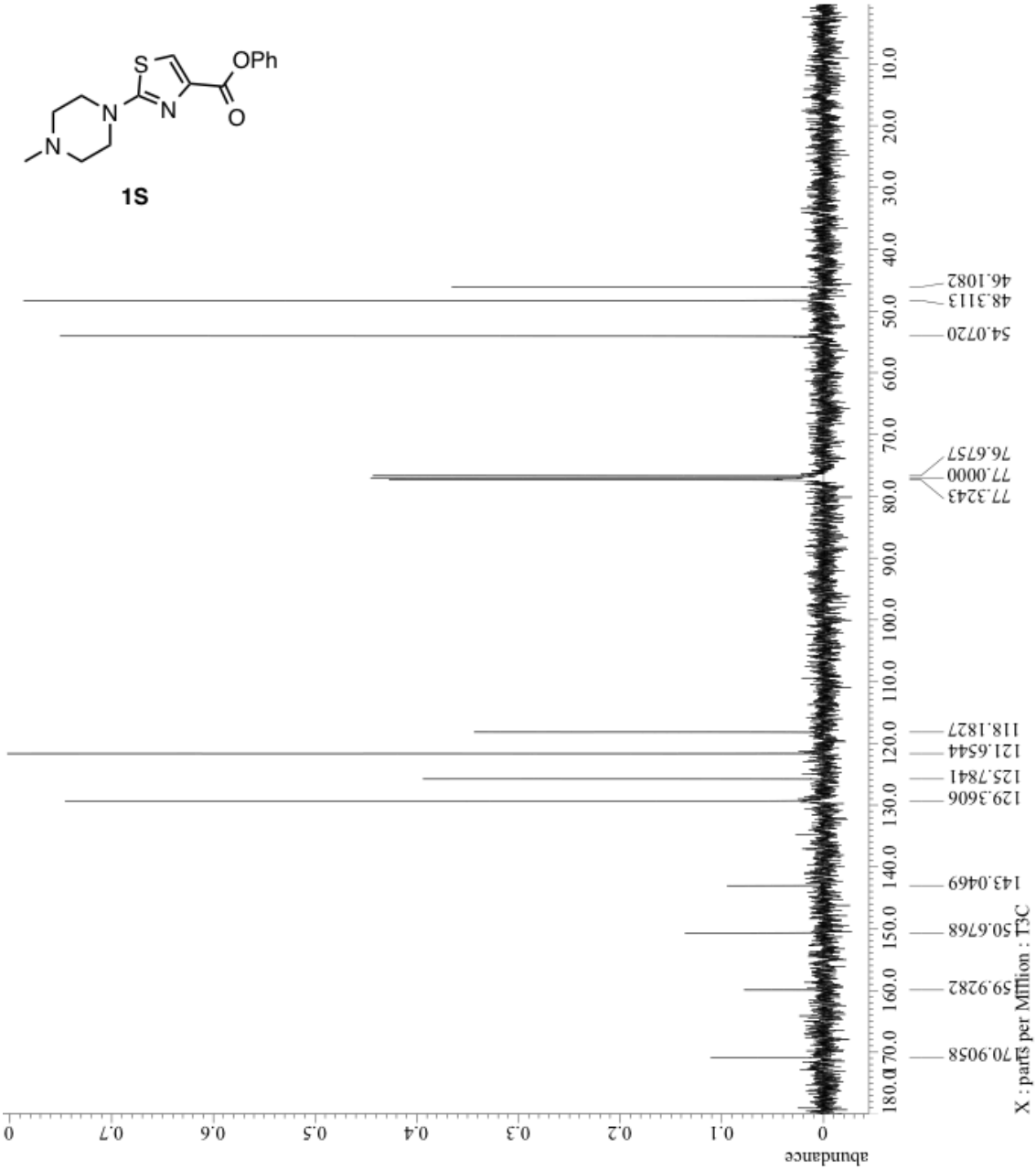
Supplementary Figure 7. ^{1}H NMR (400 MHz, $CDCl_3$) of 1Q



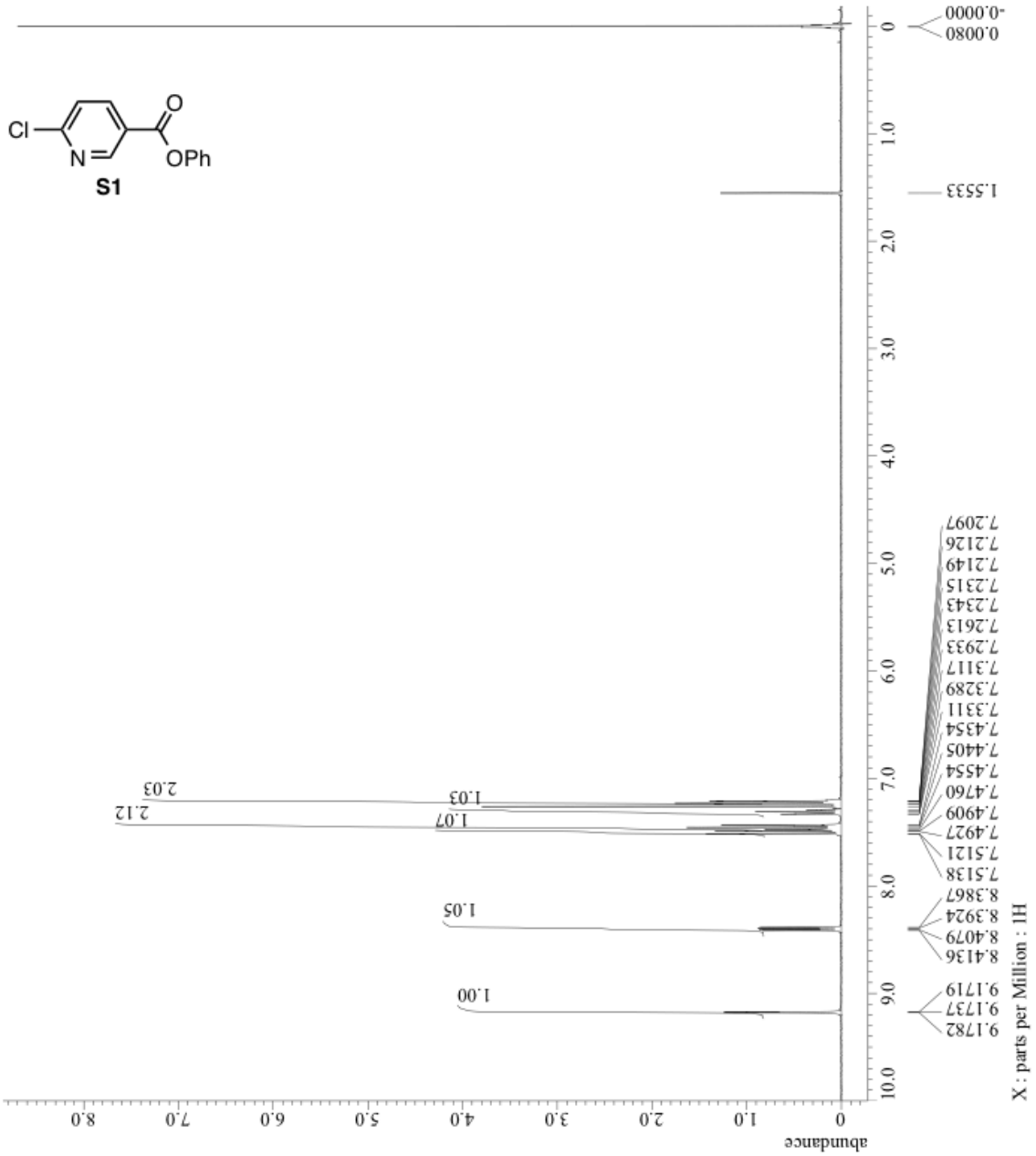
Supplementary Figure 8. ^{13}C NMR (100 MHz, $CDCl_3$) of 1Q



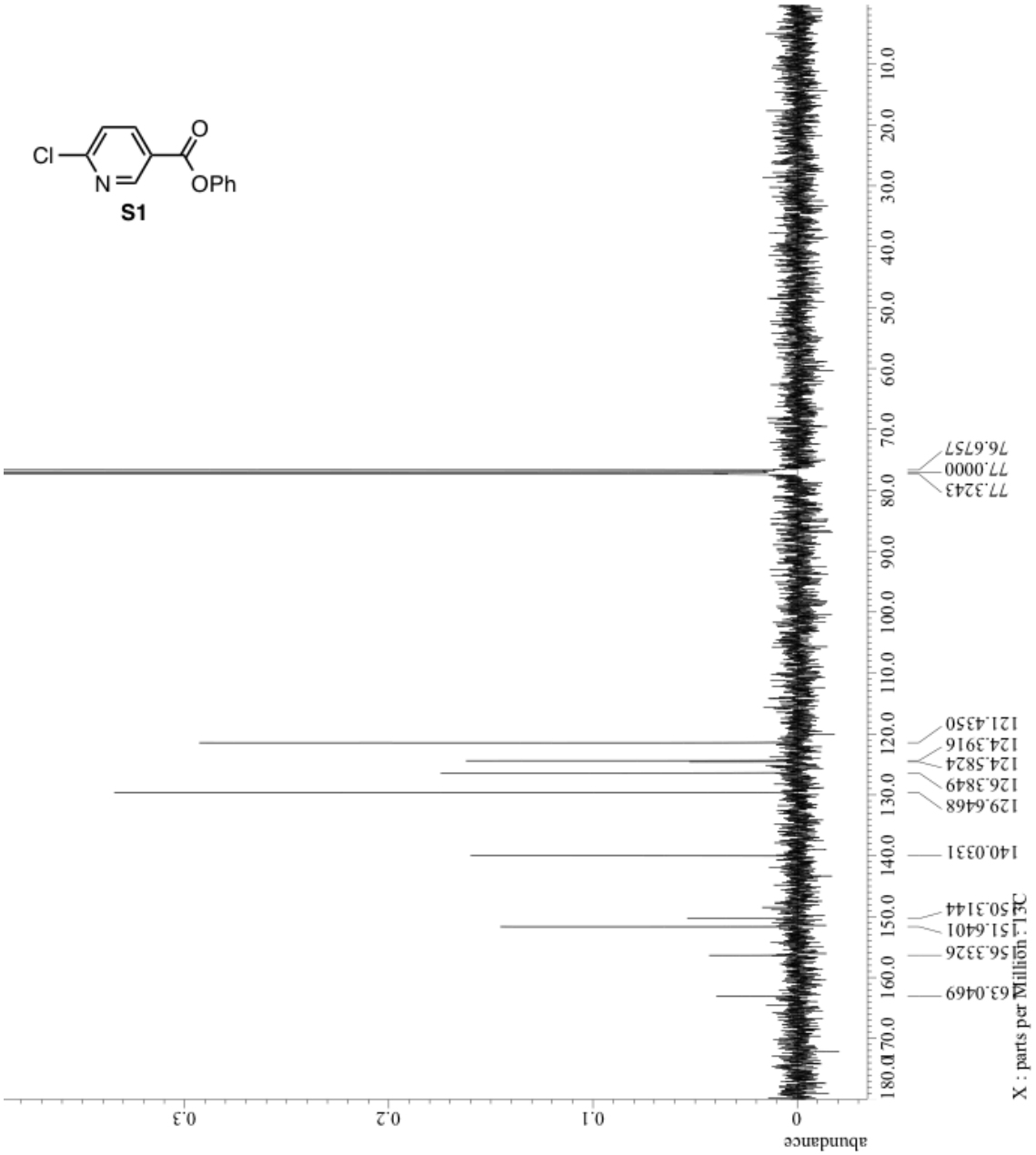
Supplementary Figure 9. ^{1}H NMR (400 MHz, $CDCl_3$) of 1S



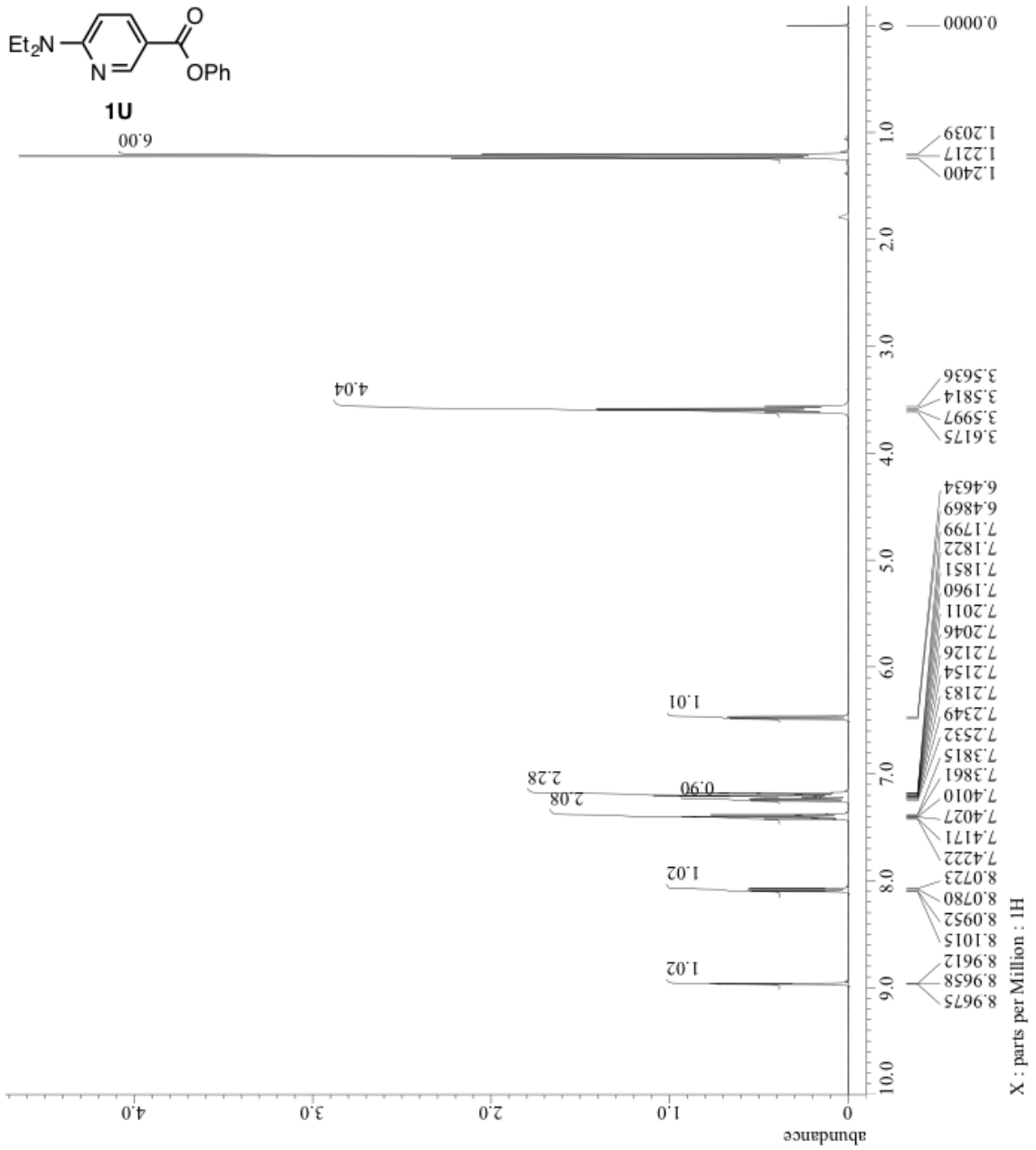
Supplementary Figure 10. ^{13}C NMR (100 MHz, $CDCl_3$) of 1S



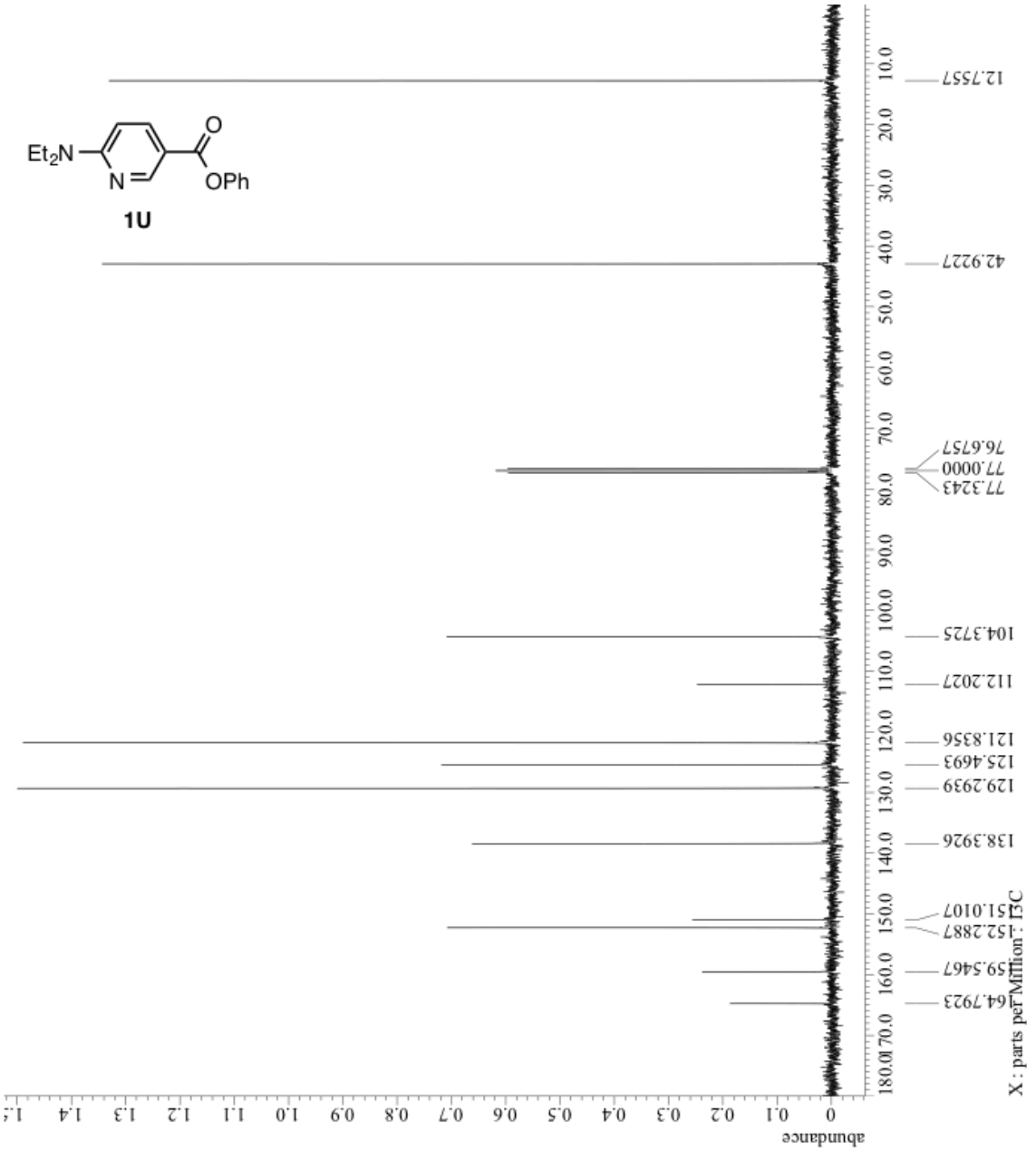
Supplementary Figure 11. ^{1}H NMR (400 MHz, $CDCl_3$) of S1



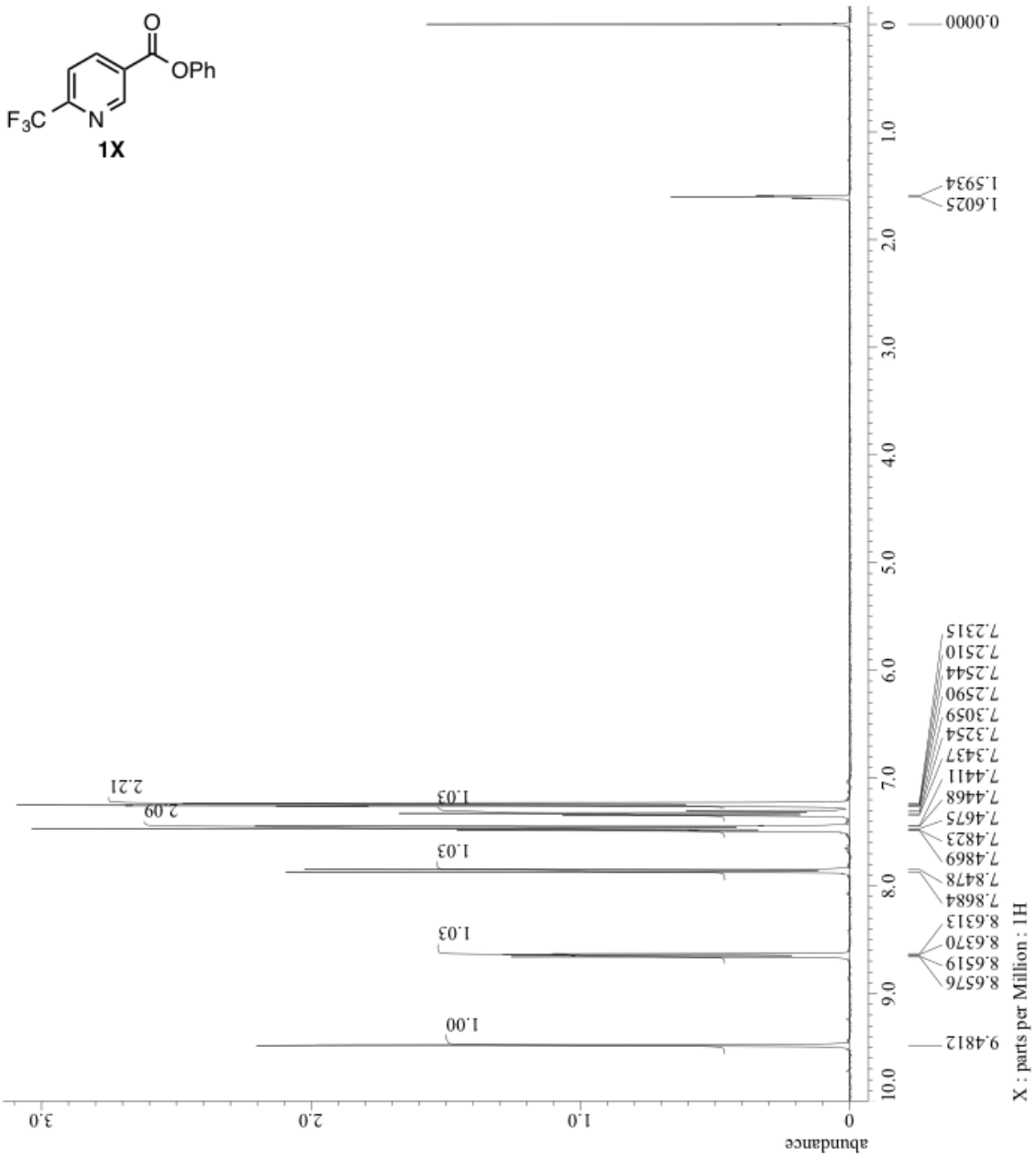
Supplementary Figure 12. ^{1}H NMR (100 MHz, $CDCl_3$) of S1



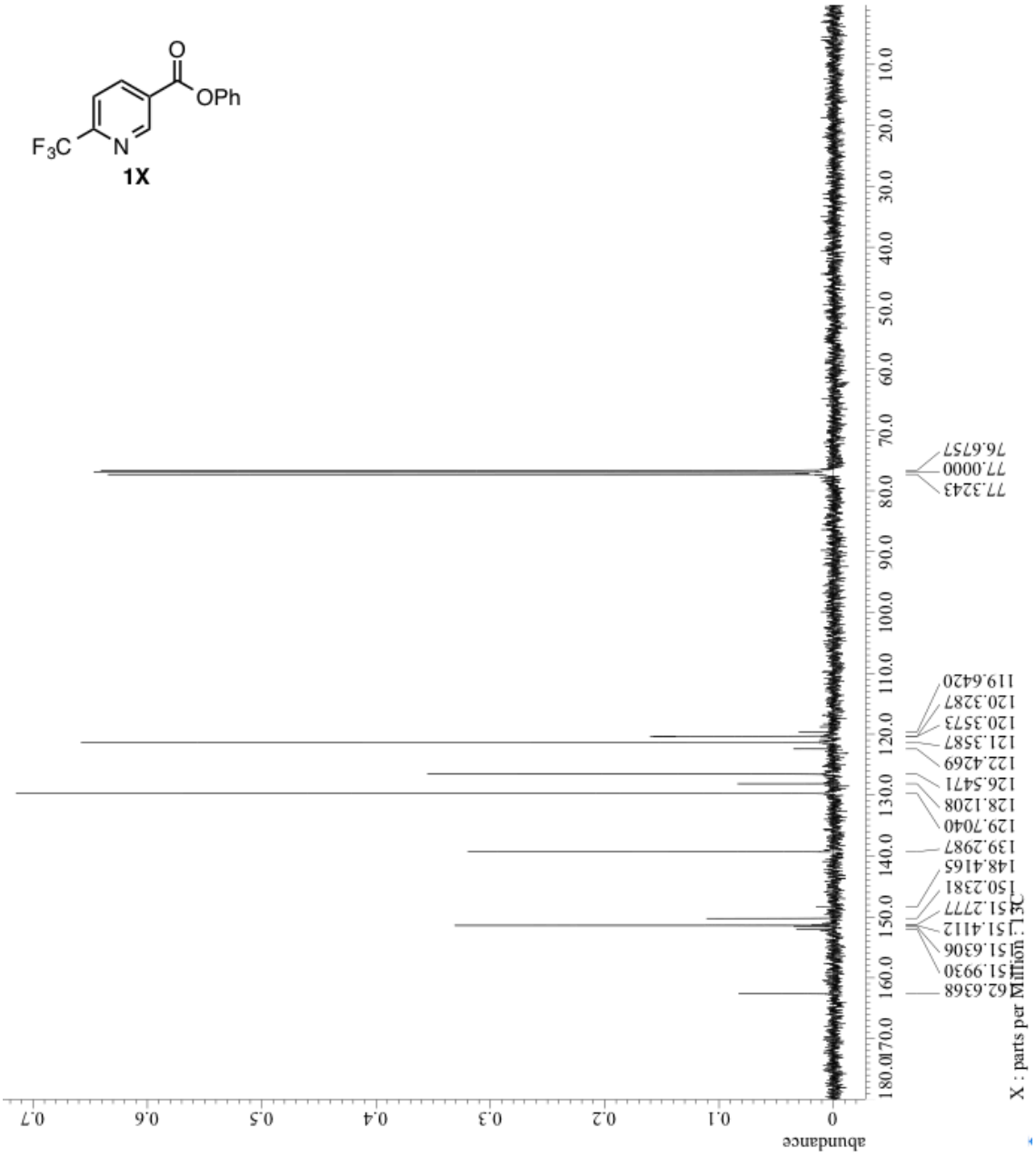
Supplementary Figure 13. ^{1}H NMR (400 MHz, $CDCl_3$) of 1U



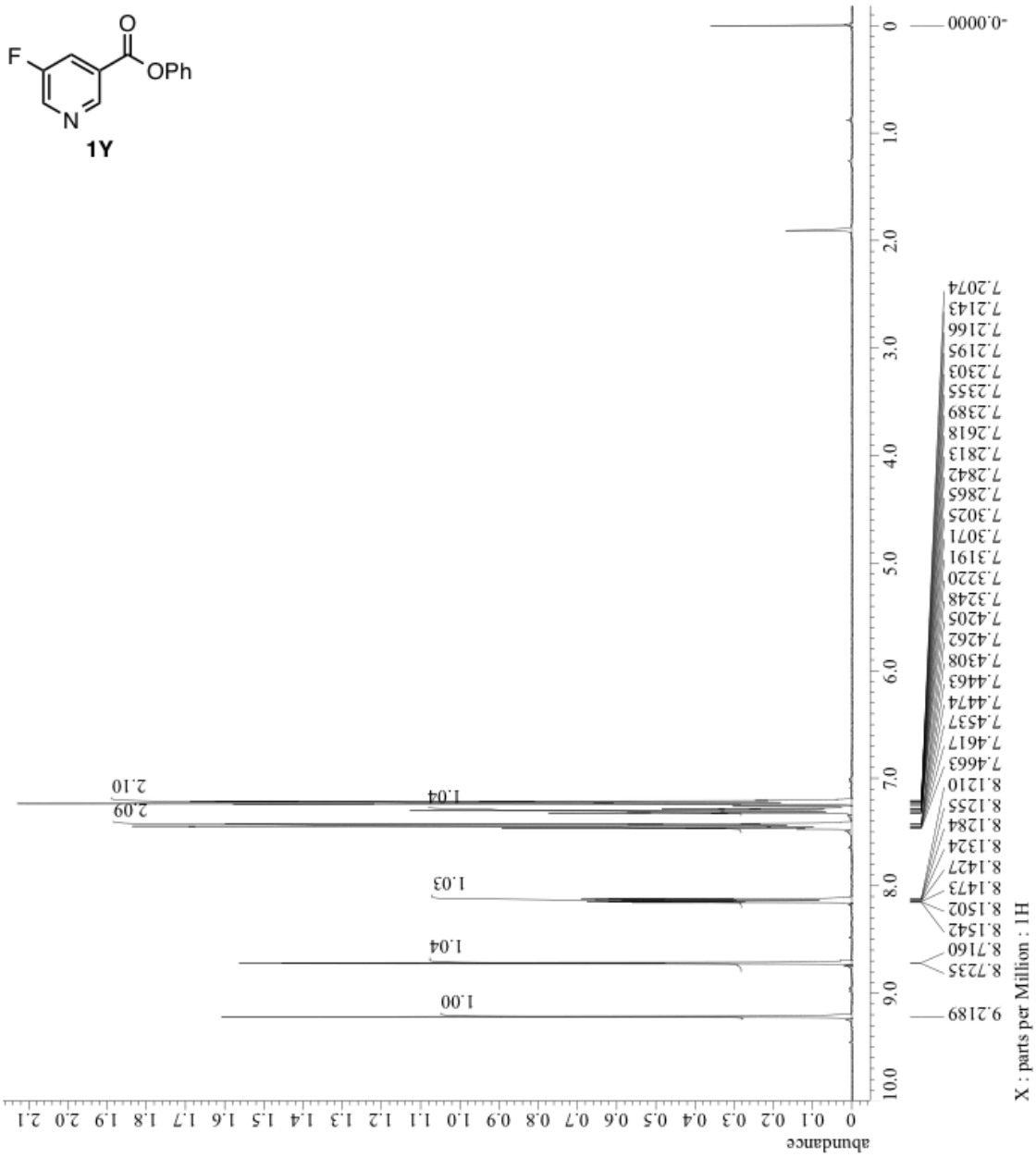
Supplementary Figure 14. ^{13}C NMR (100 MHz, $CDCl_3$) of 1U



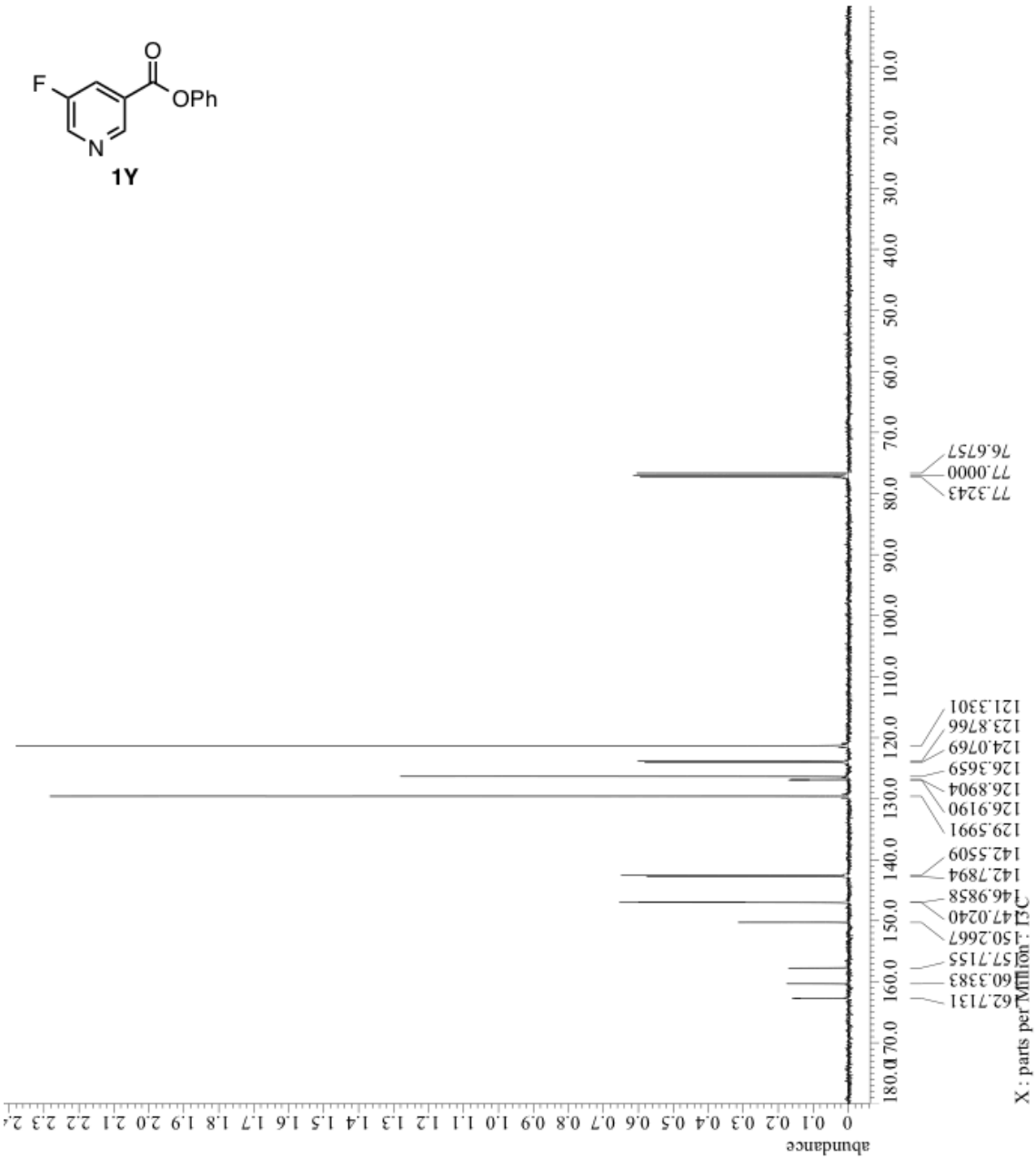
Supplementary Figure 15. ^{1}H NMR (400 MHz, $CDCl_3$) of 1X



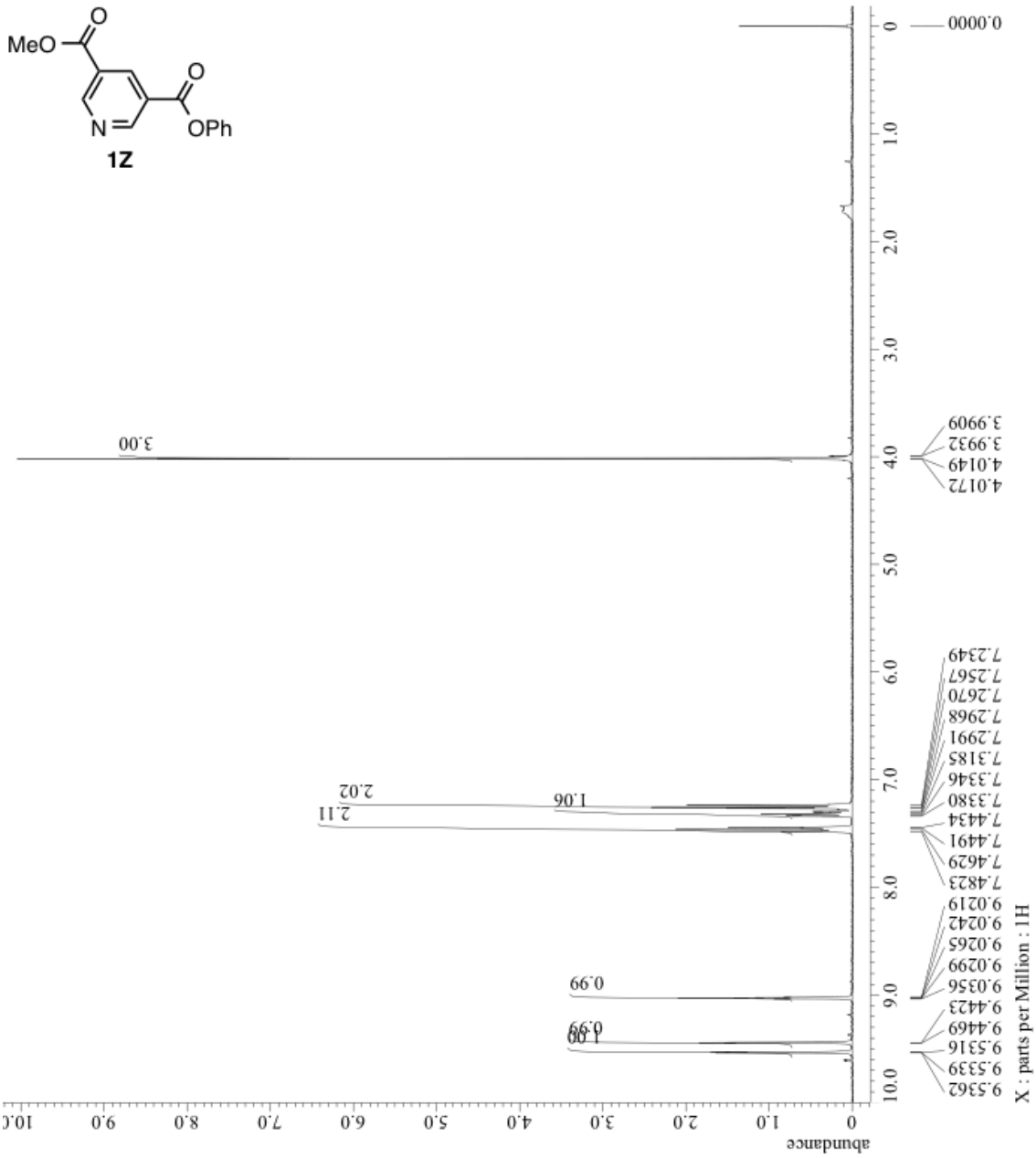
Supplementary Figure 16. ^{13}C NMR (100 MHz, $CDCl_3$) of 1X



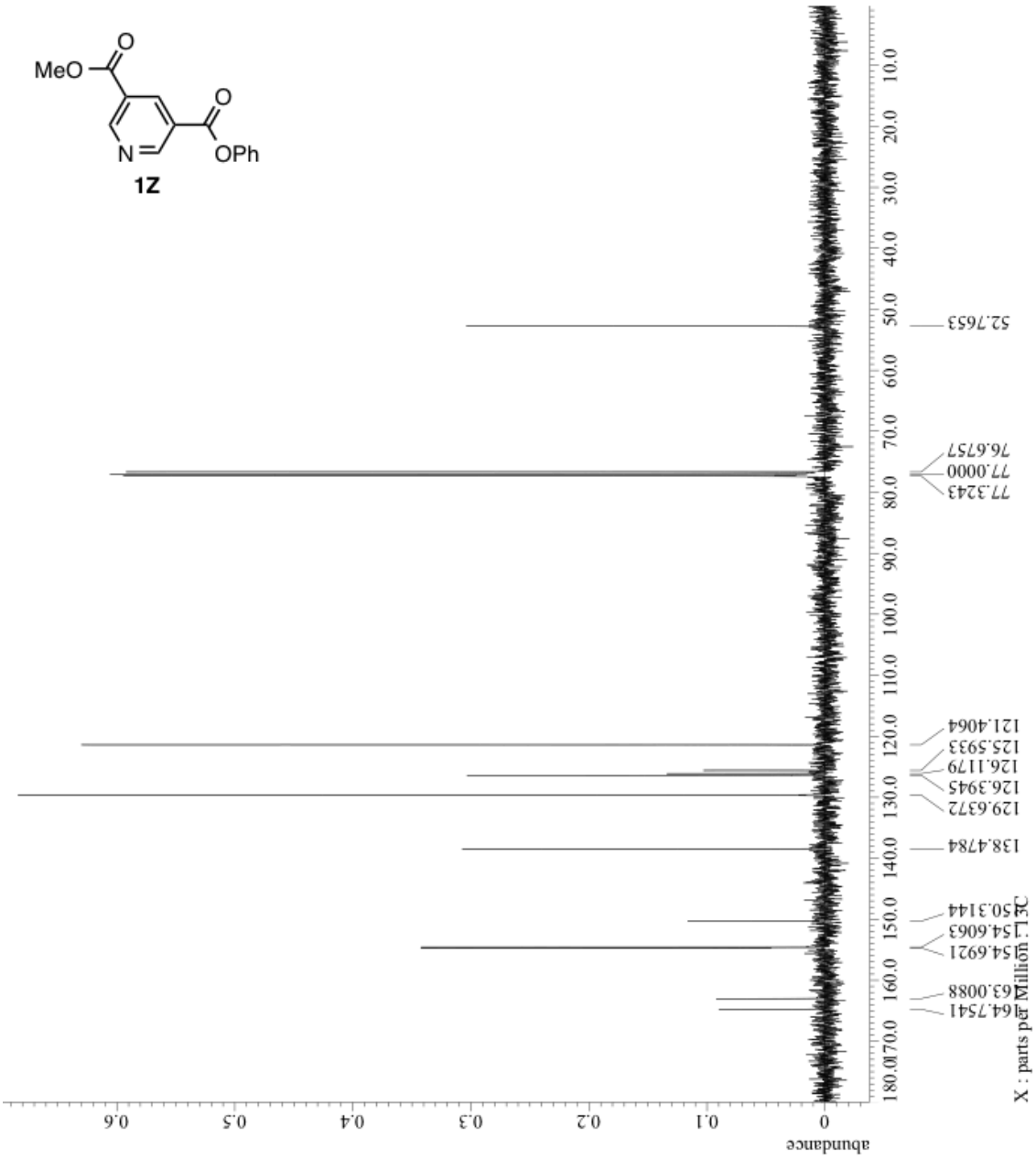
Supplementary Figure 17. ^{1}H NMR (400 MHz, $CDCl_3$) of 1Y



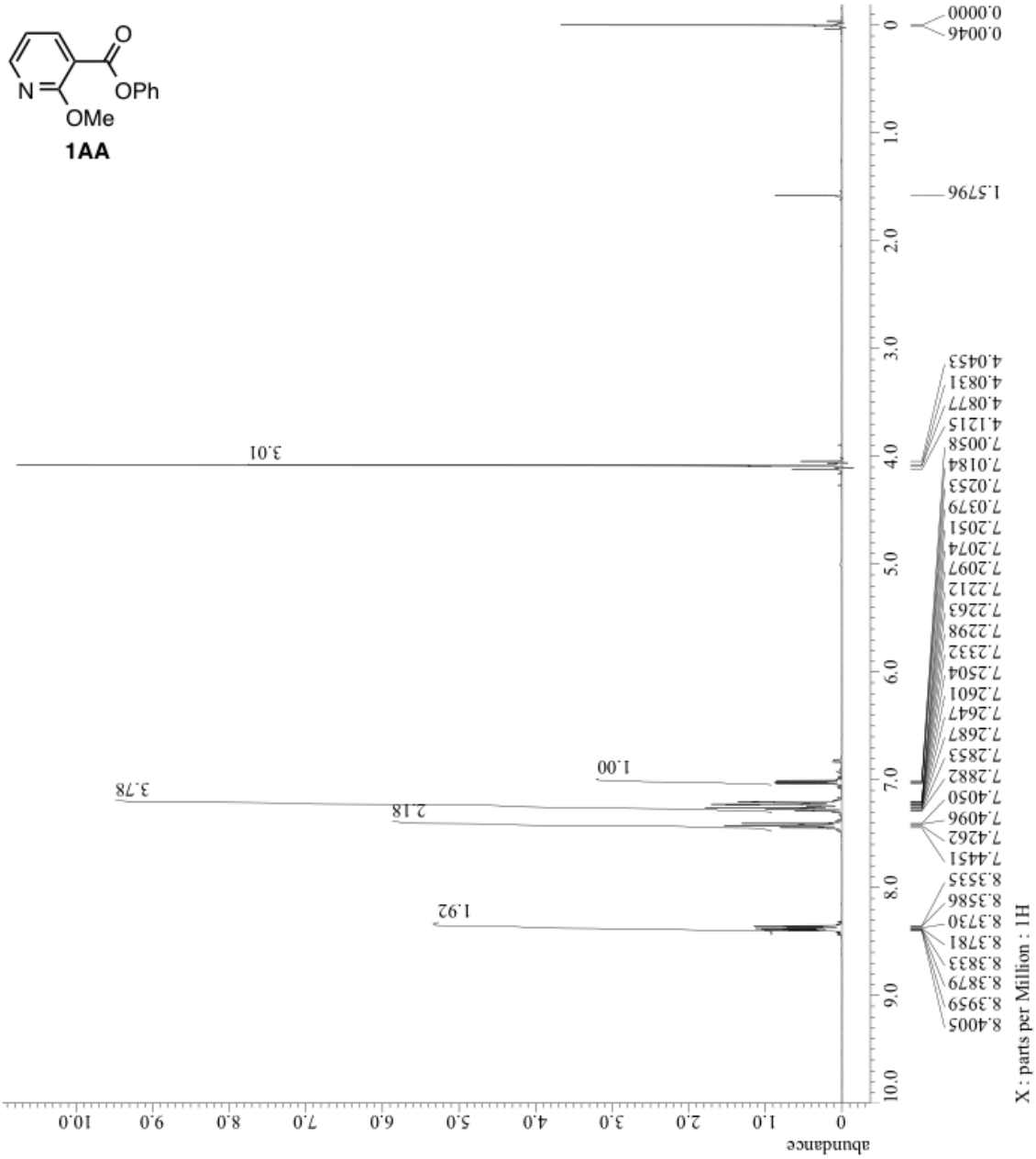
Supplementary Figure 18. ^{13}C NMR (100 MHz, $CDCl_3$) of 1Y



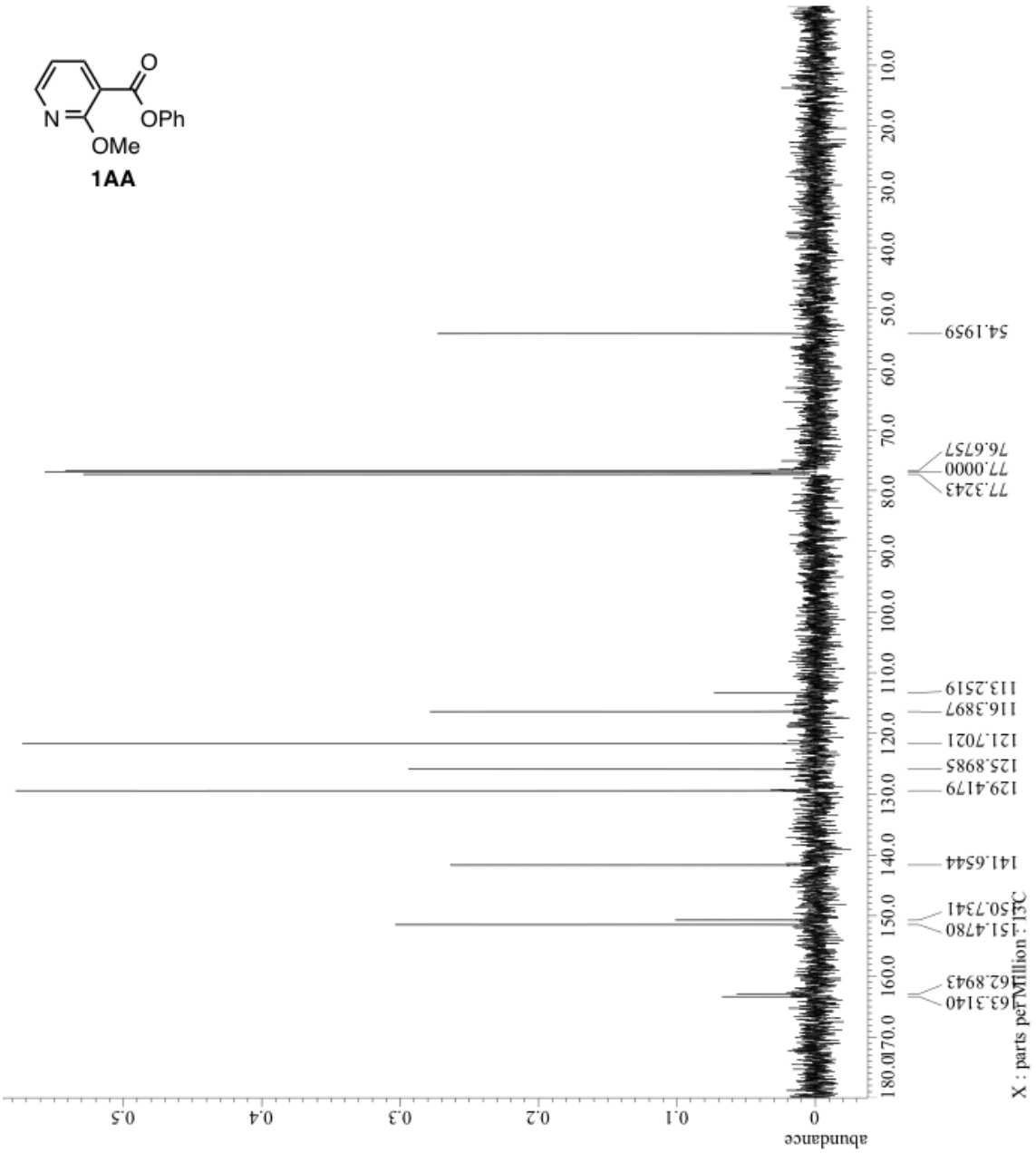
Supplementary Figure 19. ^{1}H NMR (400 MHz, $CDCl_3$) of 1X



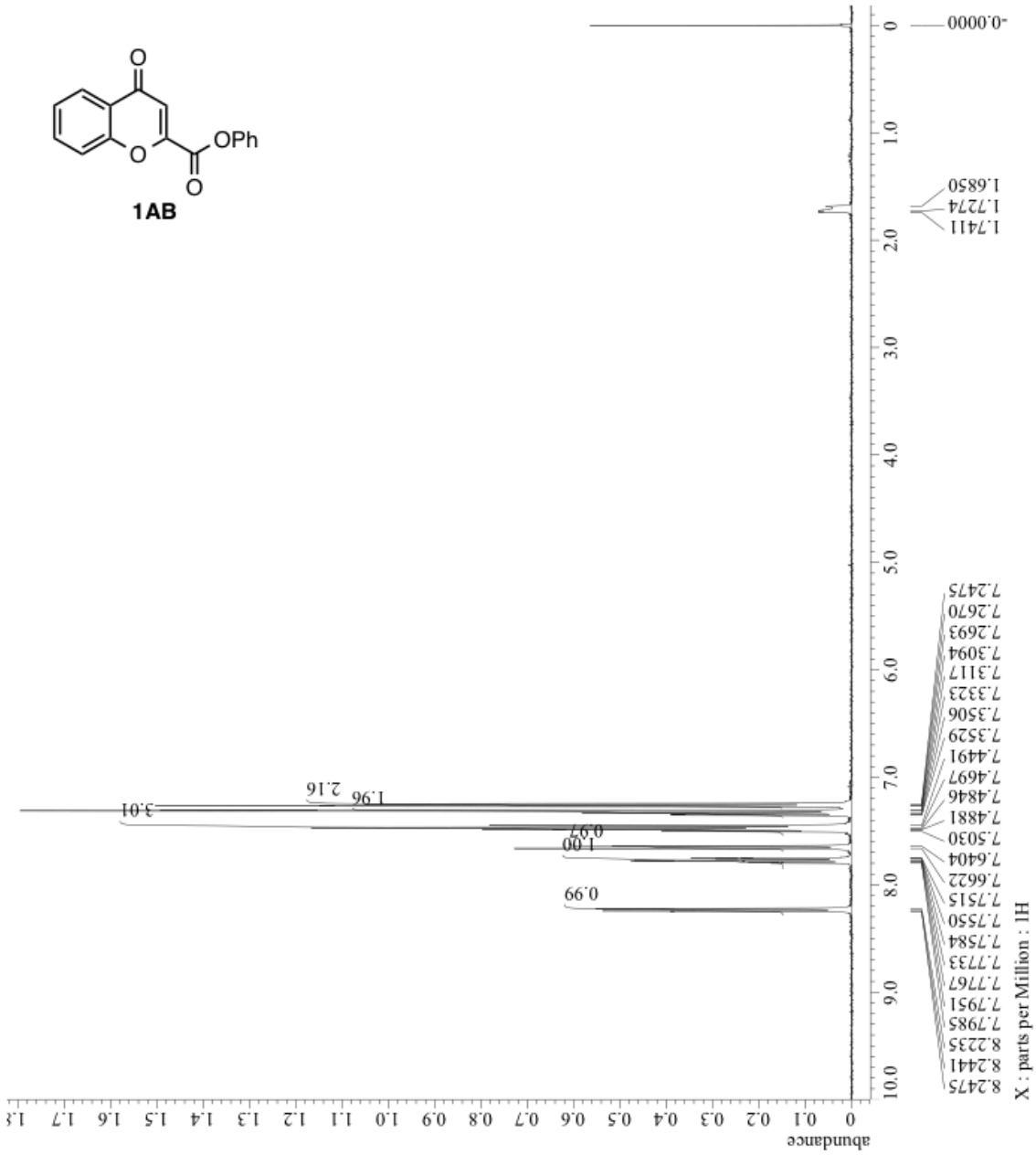
Supplementary Figure 20. ^{13}C NMR (100 MHz, $CDCl_3$) of 1Z



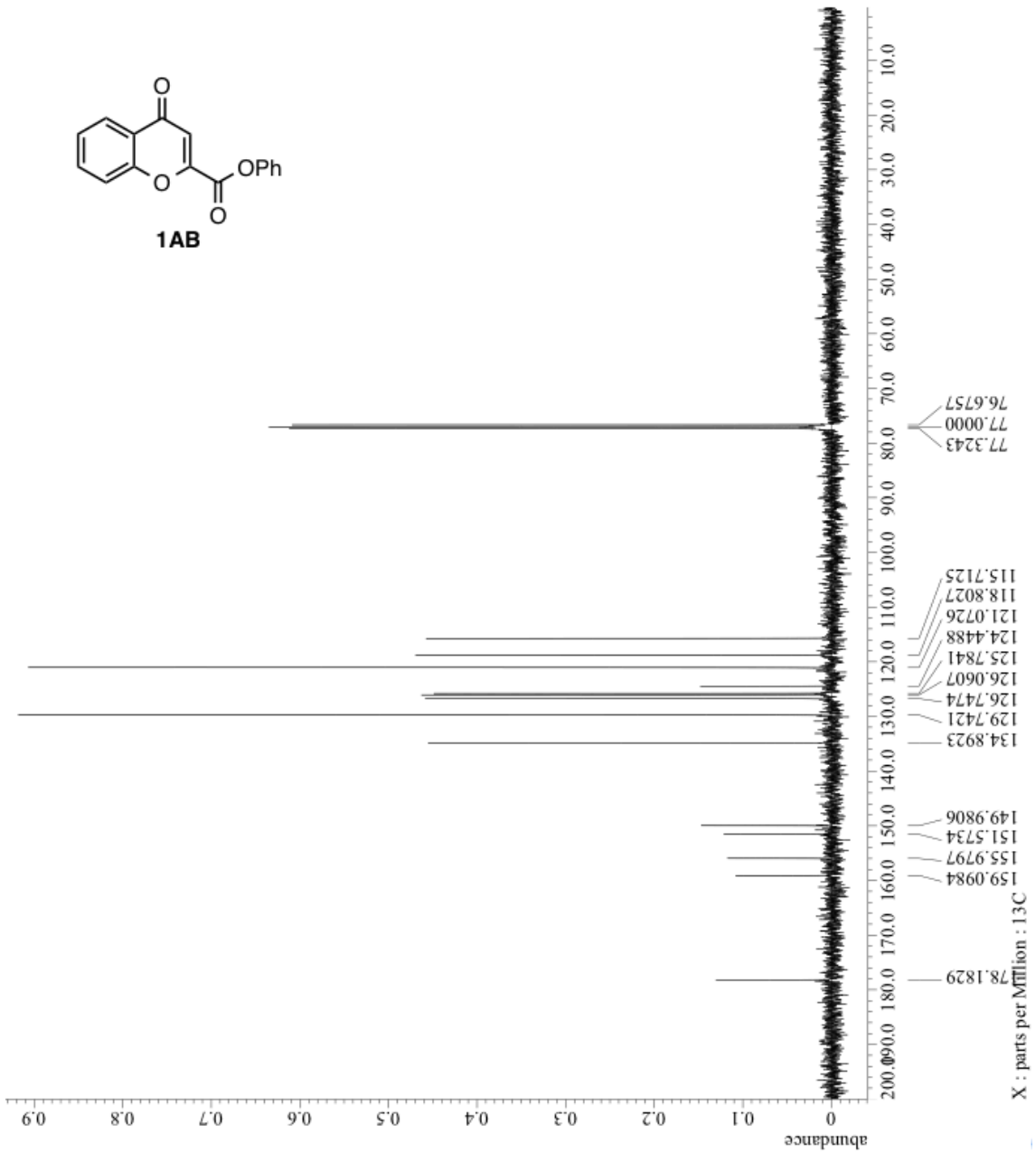
Supplementary Figure 21. ^{1}H NMR (400 MHz, $CDCl_3$) of 1AA



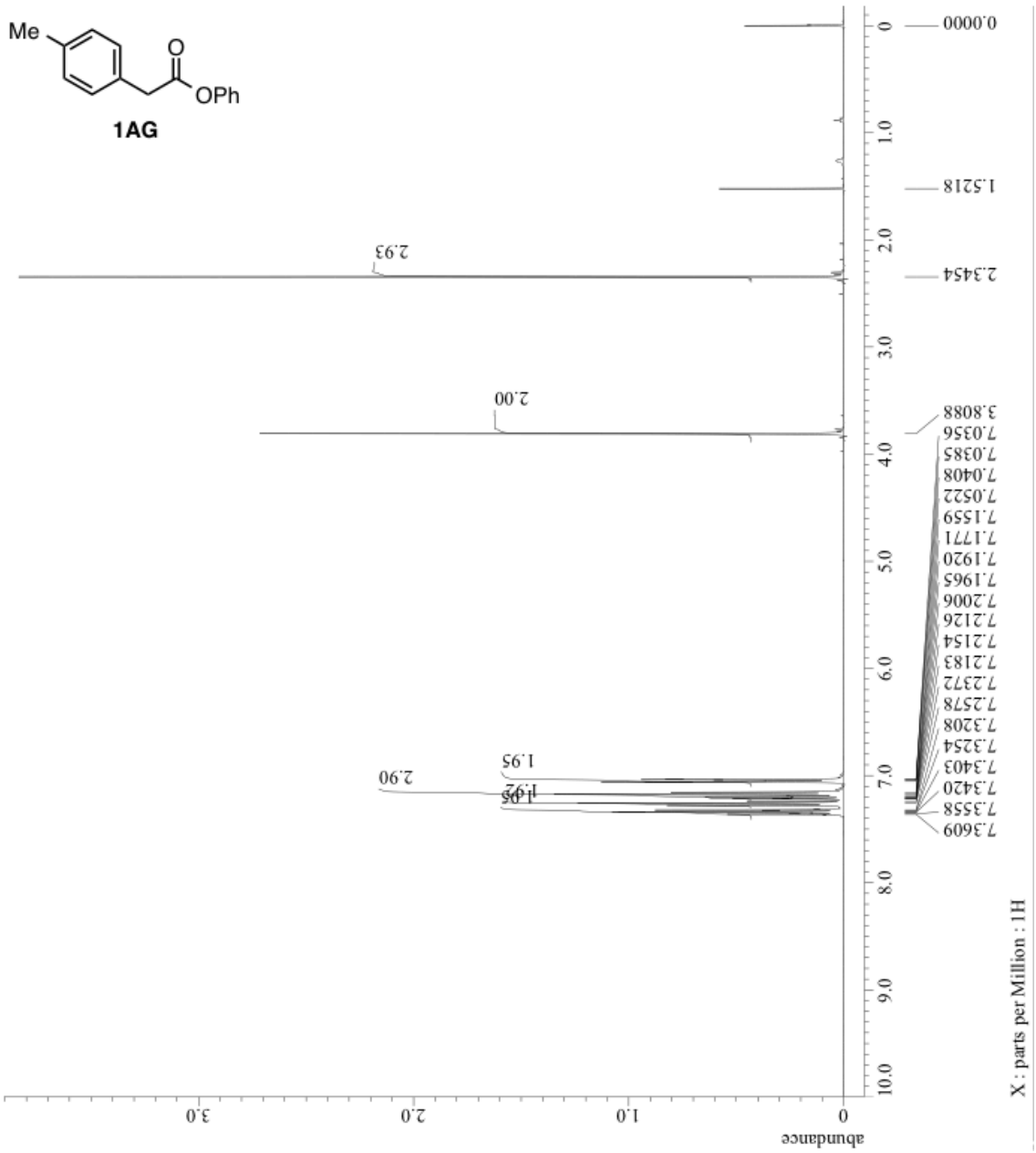
Supplementary Figure 22. ^{13}C NMR (100 MHz, $CDCl_3$) of 1AA



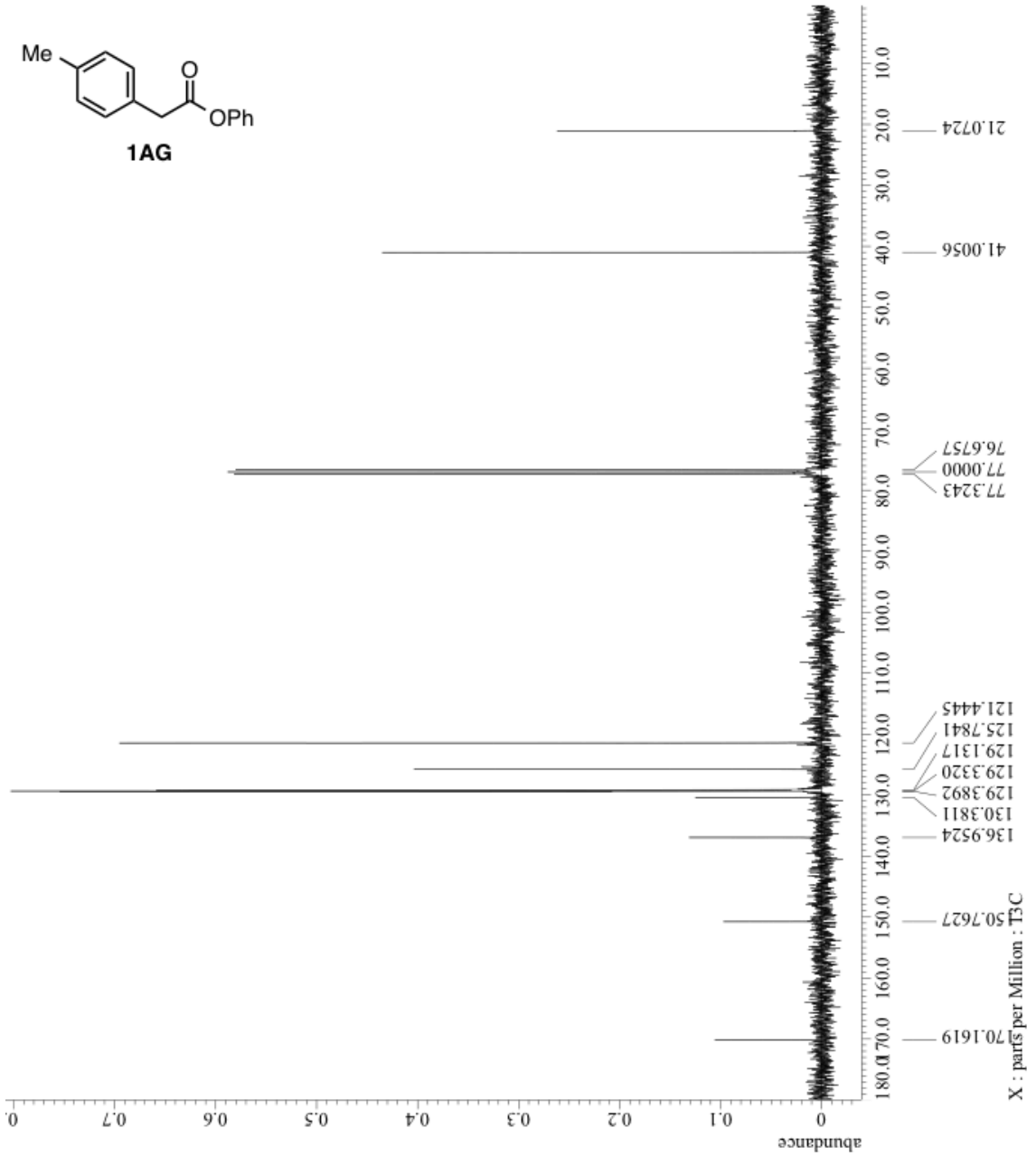
Supplementary Figure 23. ^{1}H NMR (400 MHz, $CDCl_3$) of 1AB



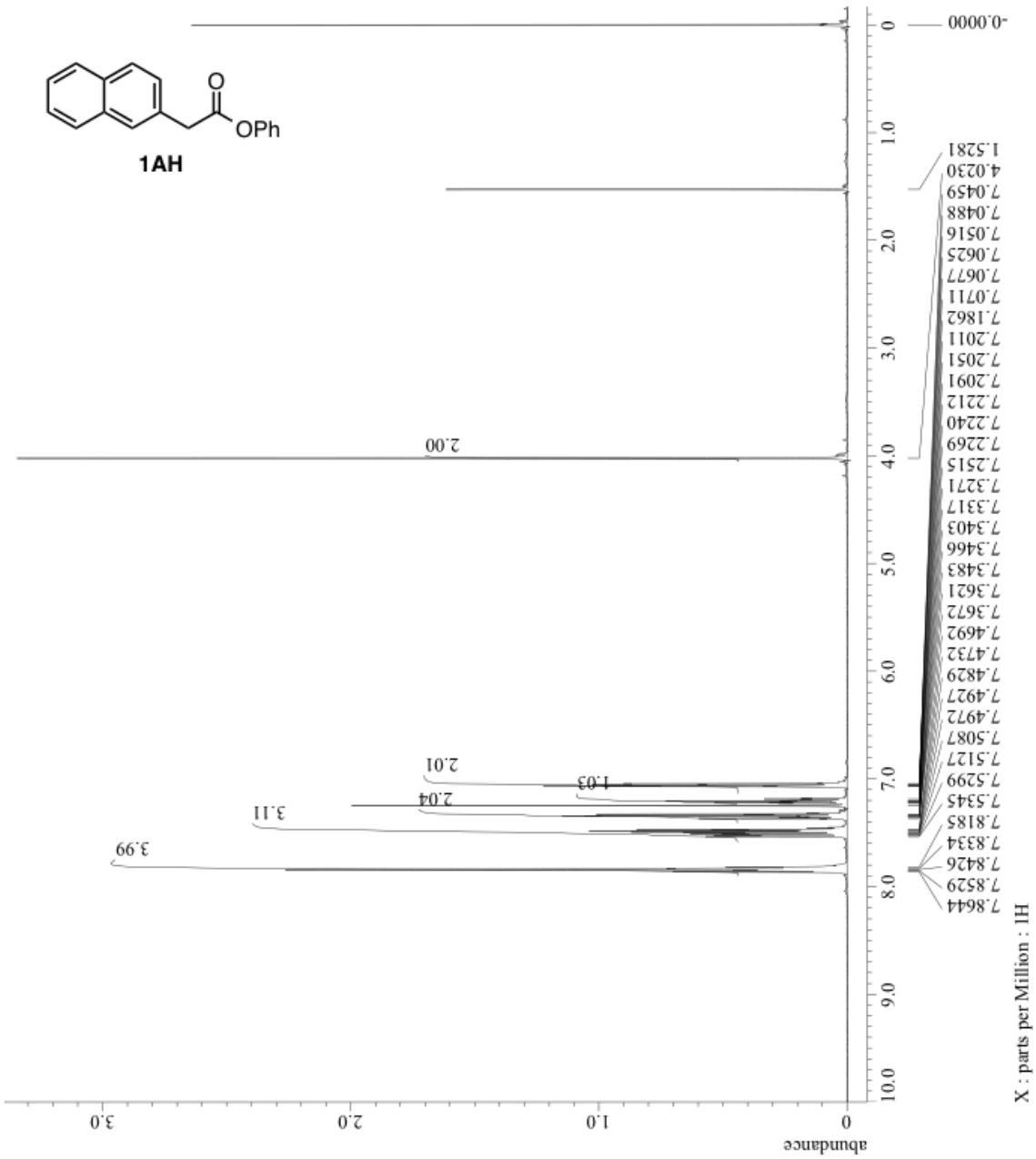
Supplementary Figure 24. ^{13}C NMR (100 MHz, $CDCl_3$) of 1AB



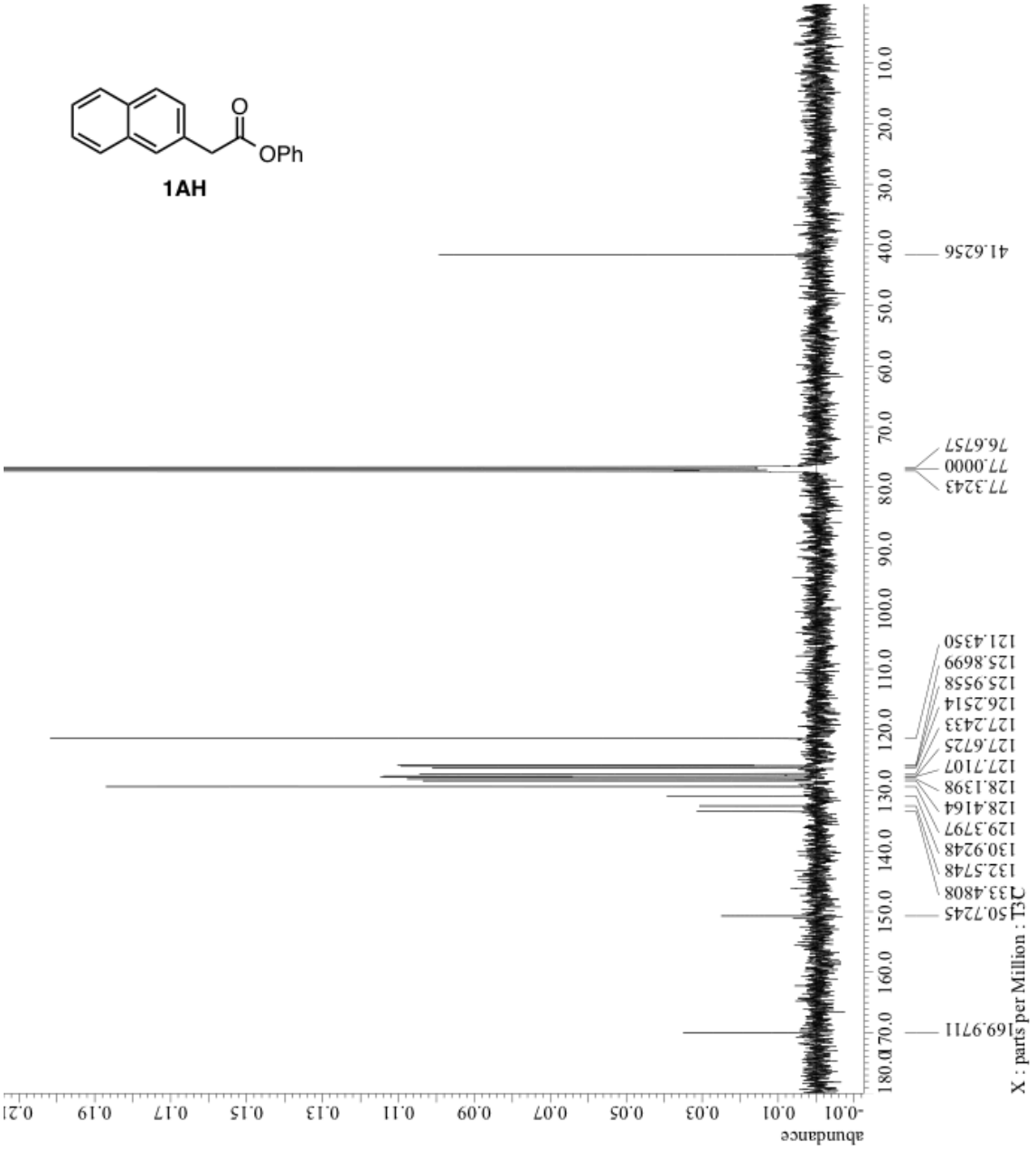
Supplementary Figure 25. ^{1}H NMR (400 MHz, $CDCl_3$) of 1AG



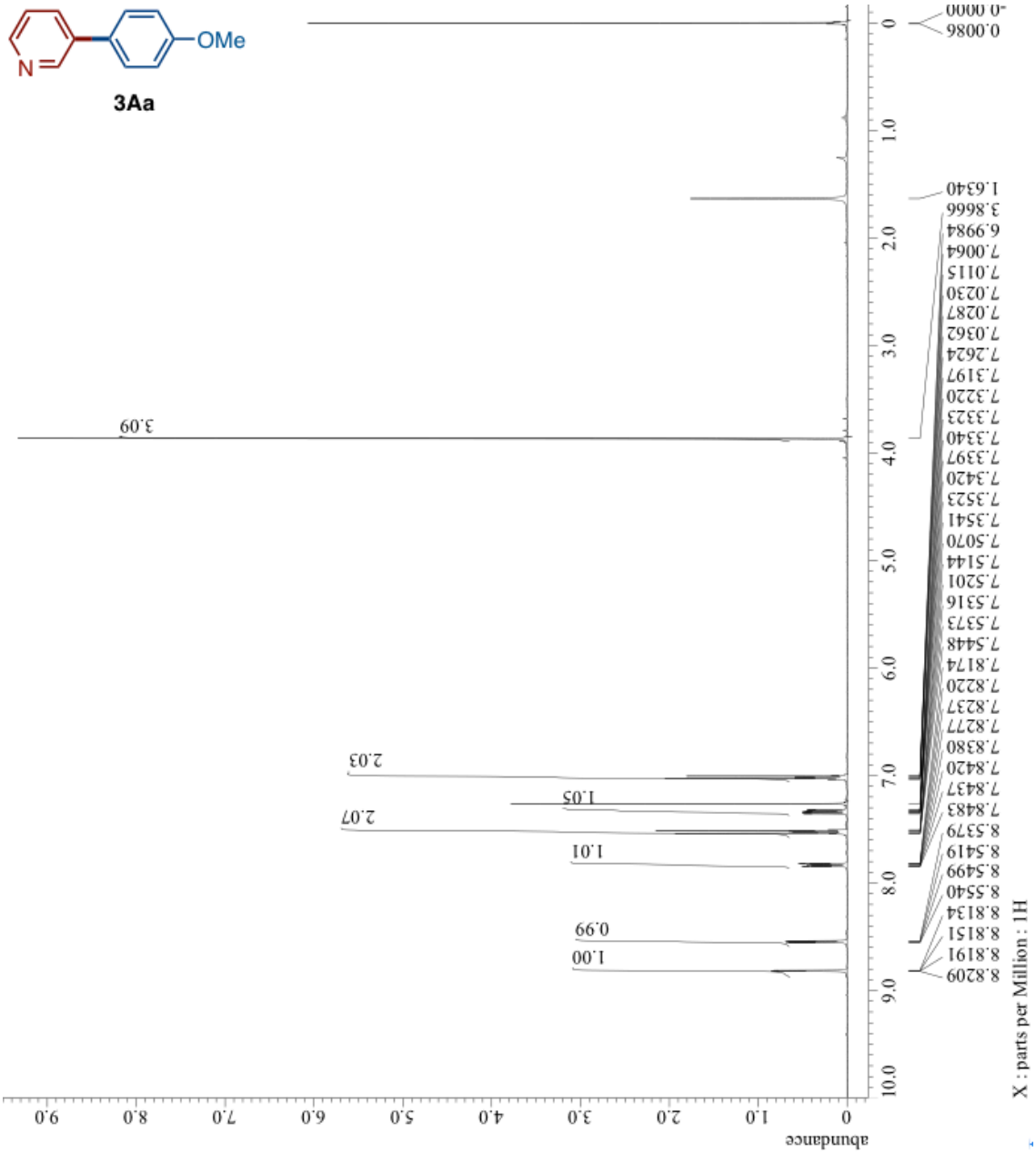
Supplementary Figure 26. ^{13}C NMR (100 MHz, $CDCl_3$) of 1AG



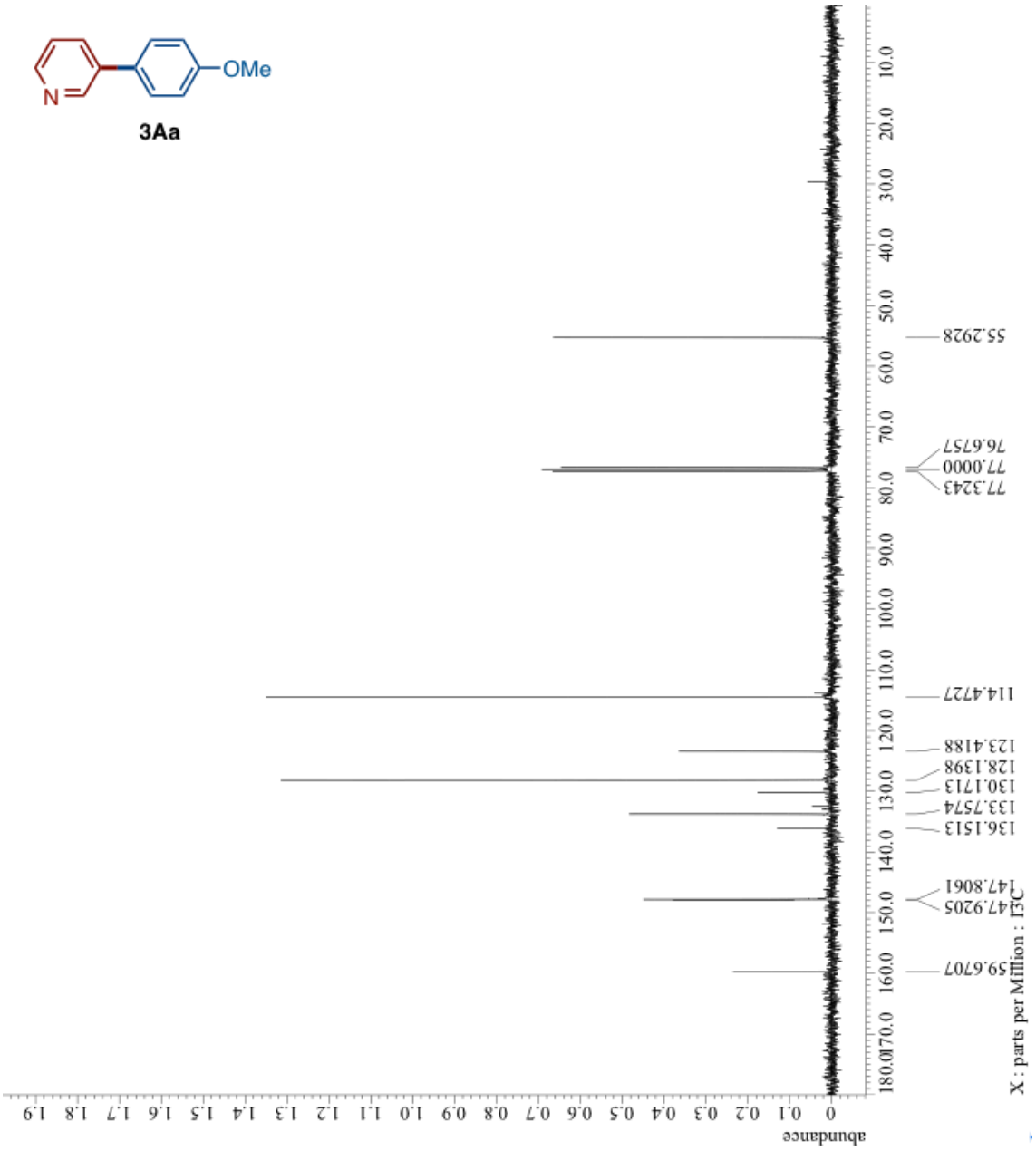
Supplementary Figure 27. ^{1}H NMR (400 MHz, $CDCl_3$) of 1AH



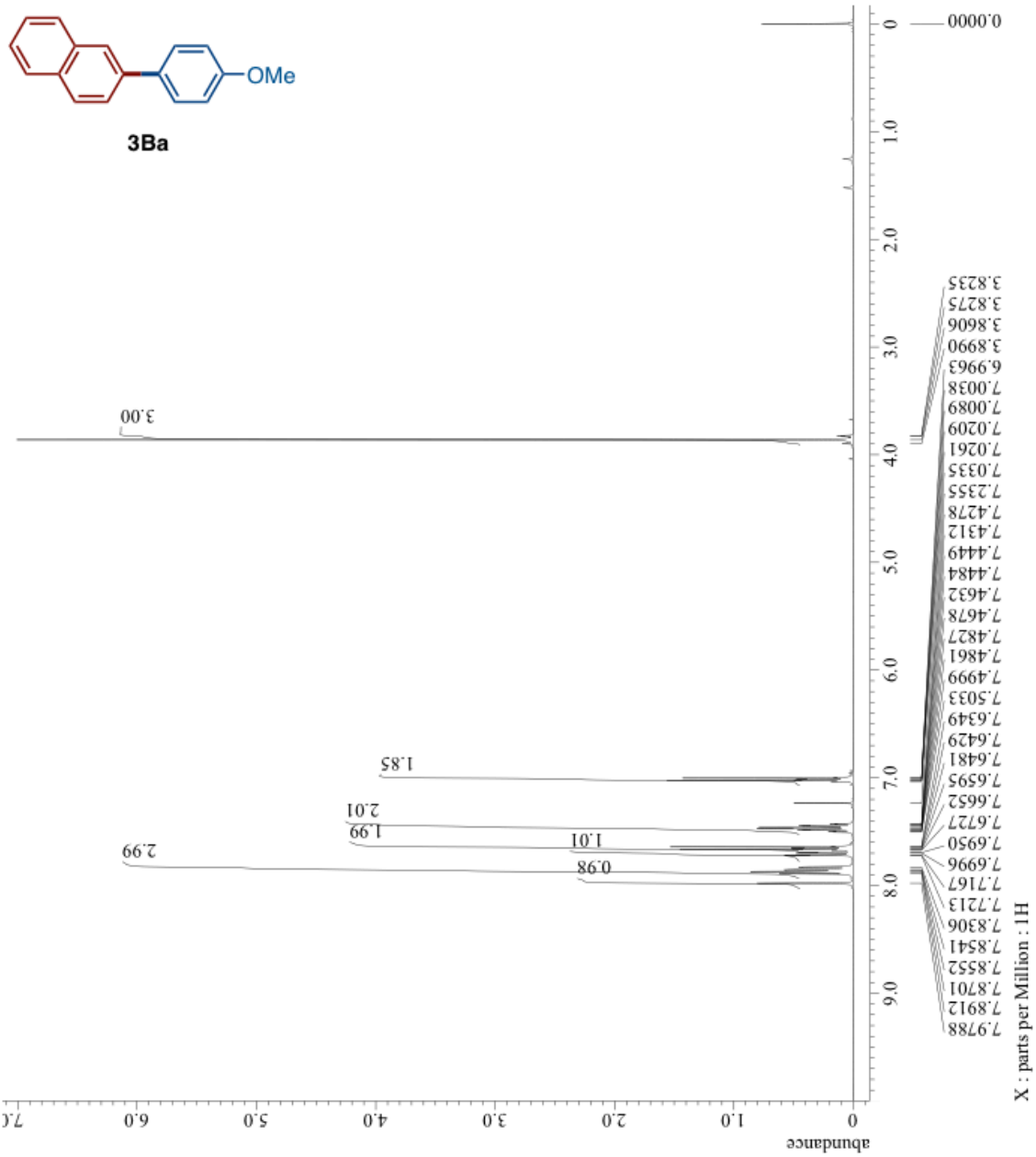
Supplementary Figure 28. ^{13}C NMR (100 MHz, $CDCl_3$) of 1AH



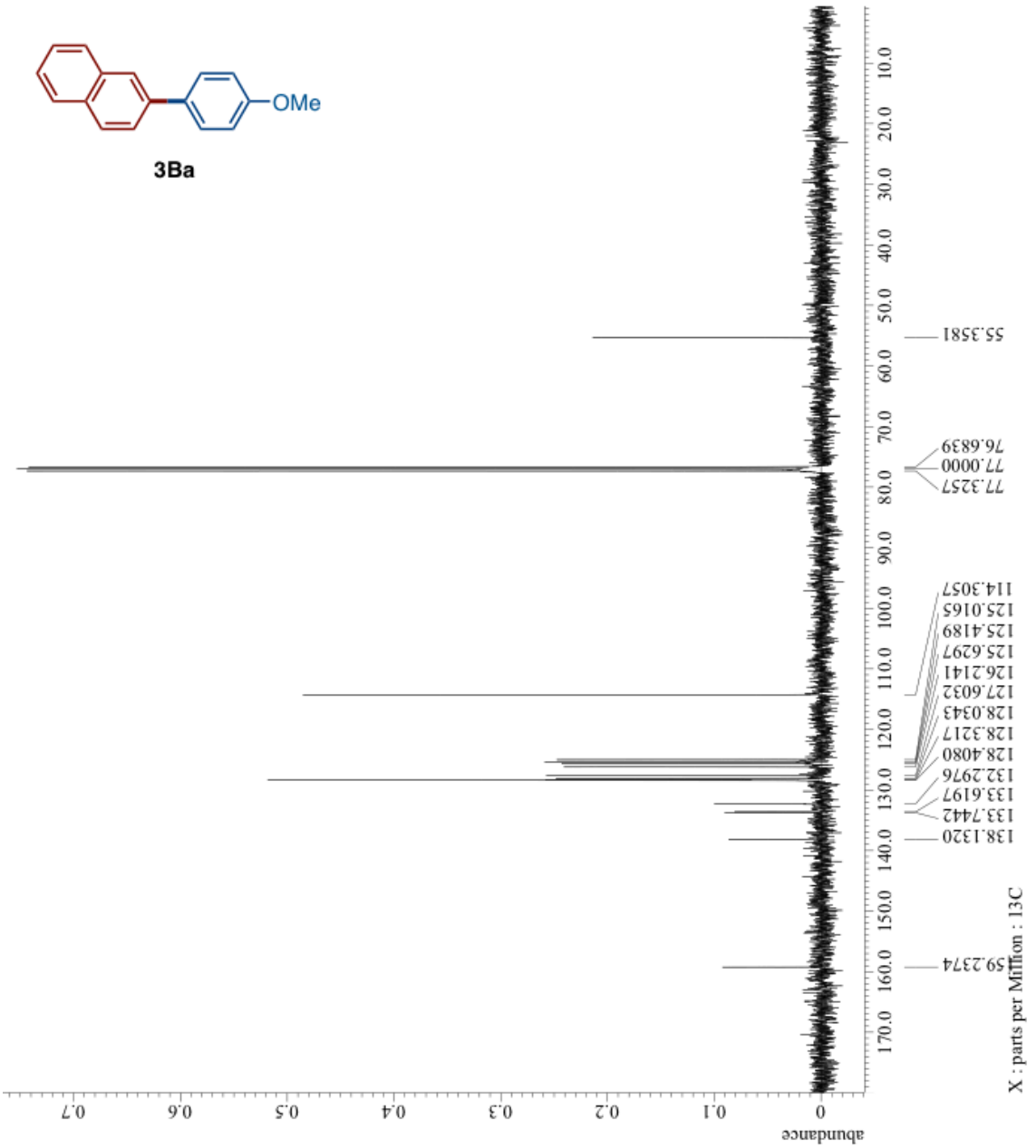
Supplementary Figure 29. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Aa



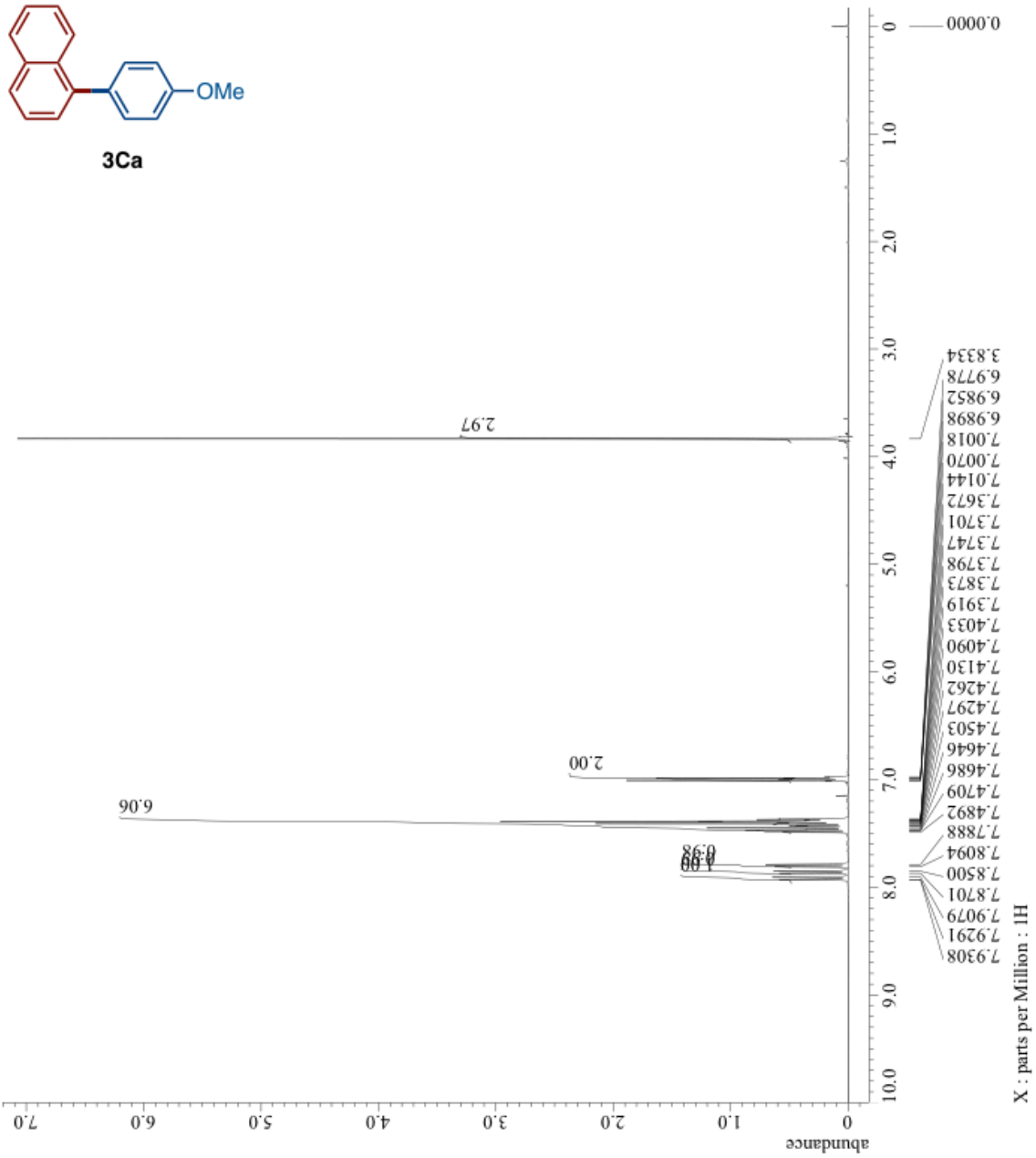
Supplementary Figure 30. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Aa



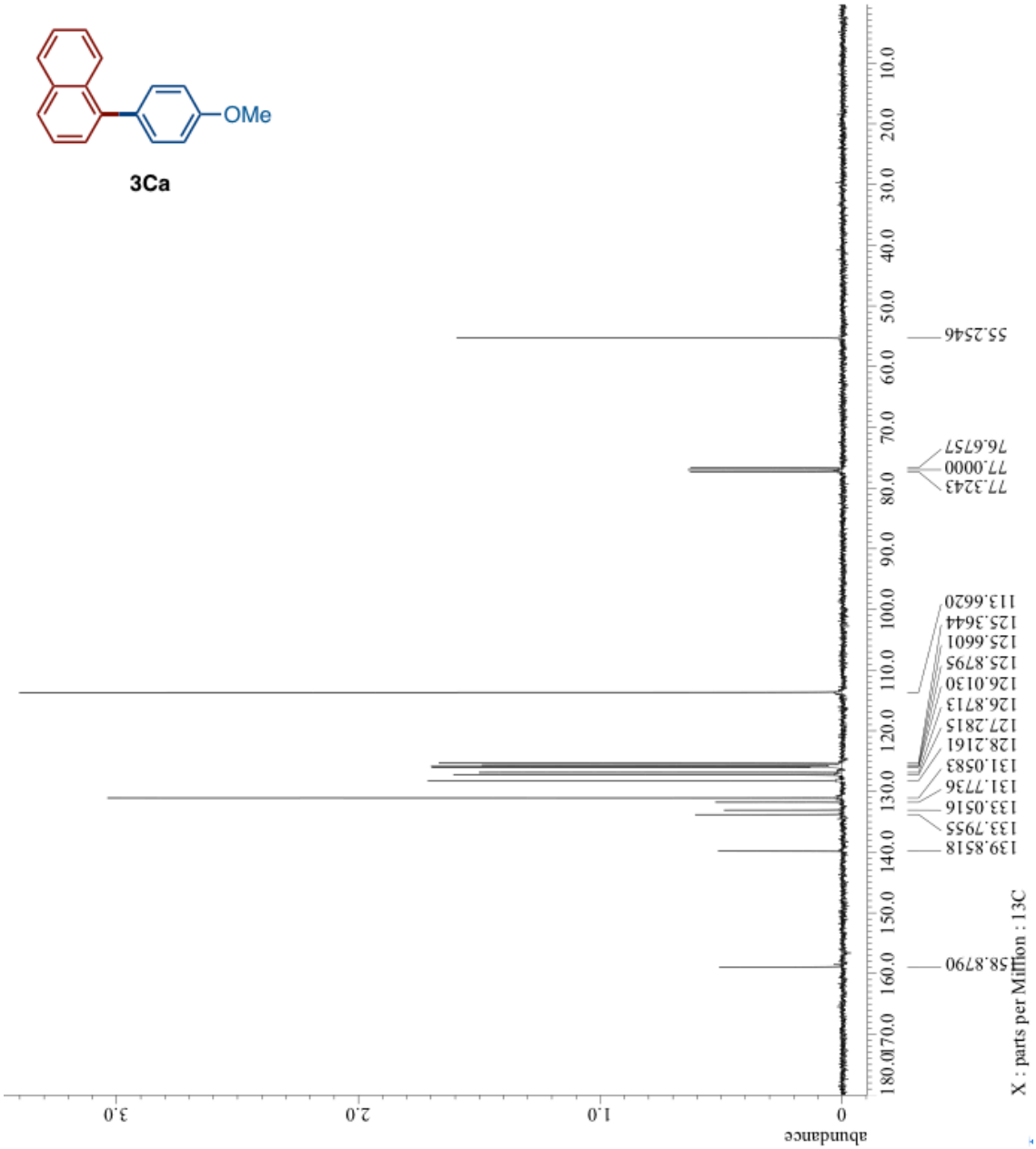
Supplementary Figure 31. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ba



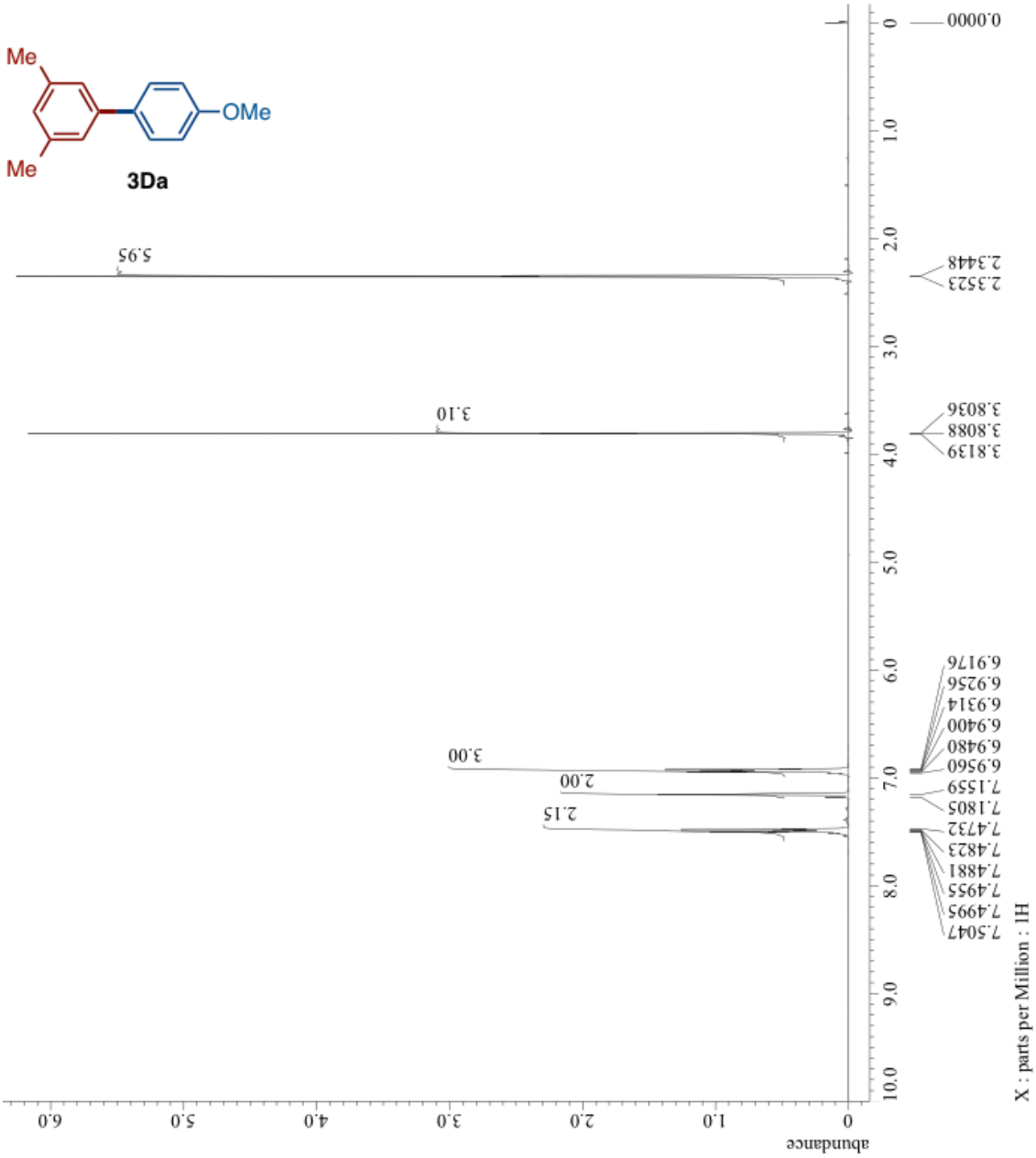
Supplementary Figure 32. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ba



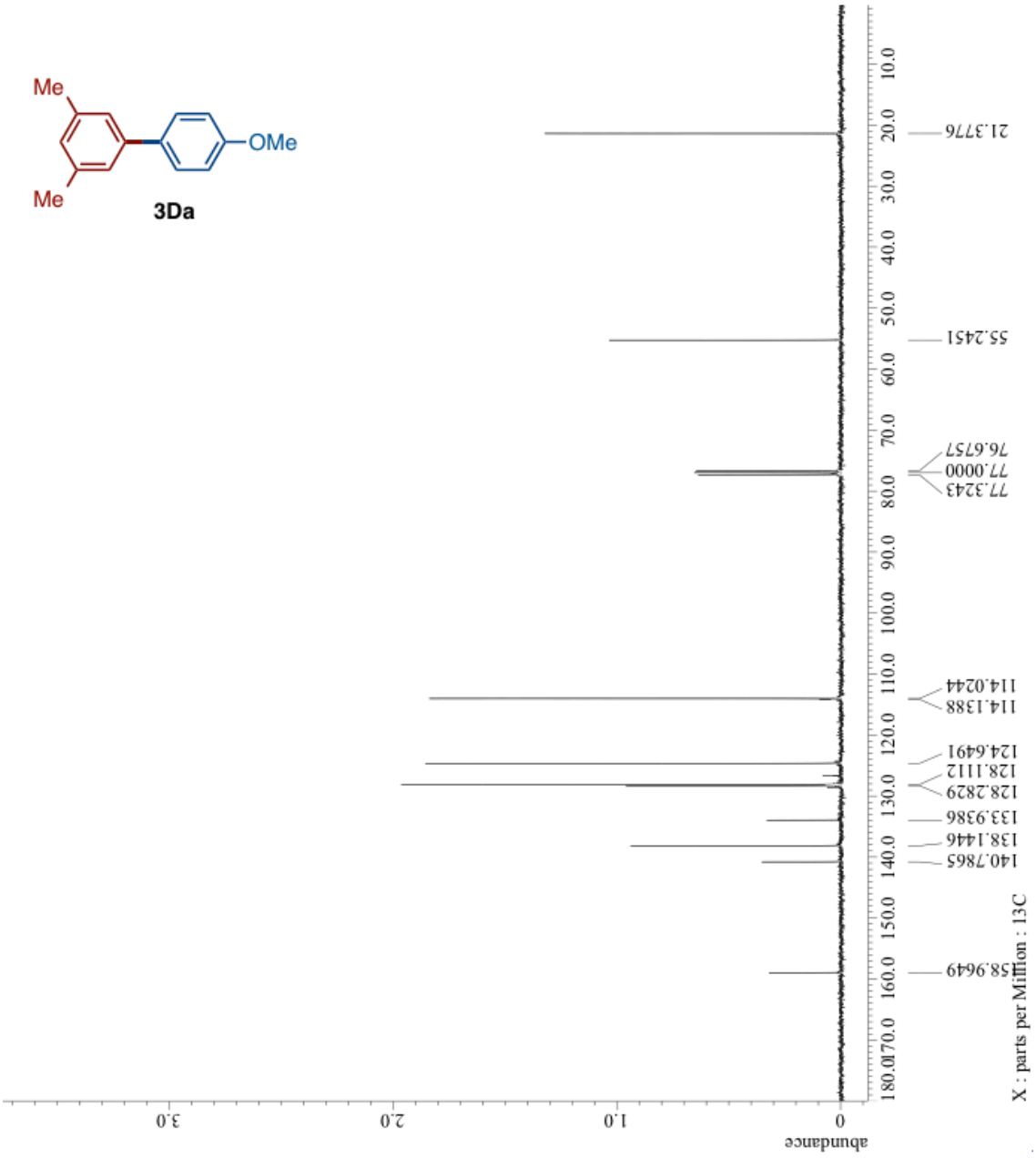
Supplementary Figure 33. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ca



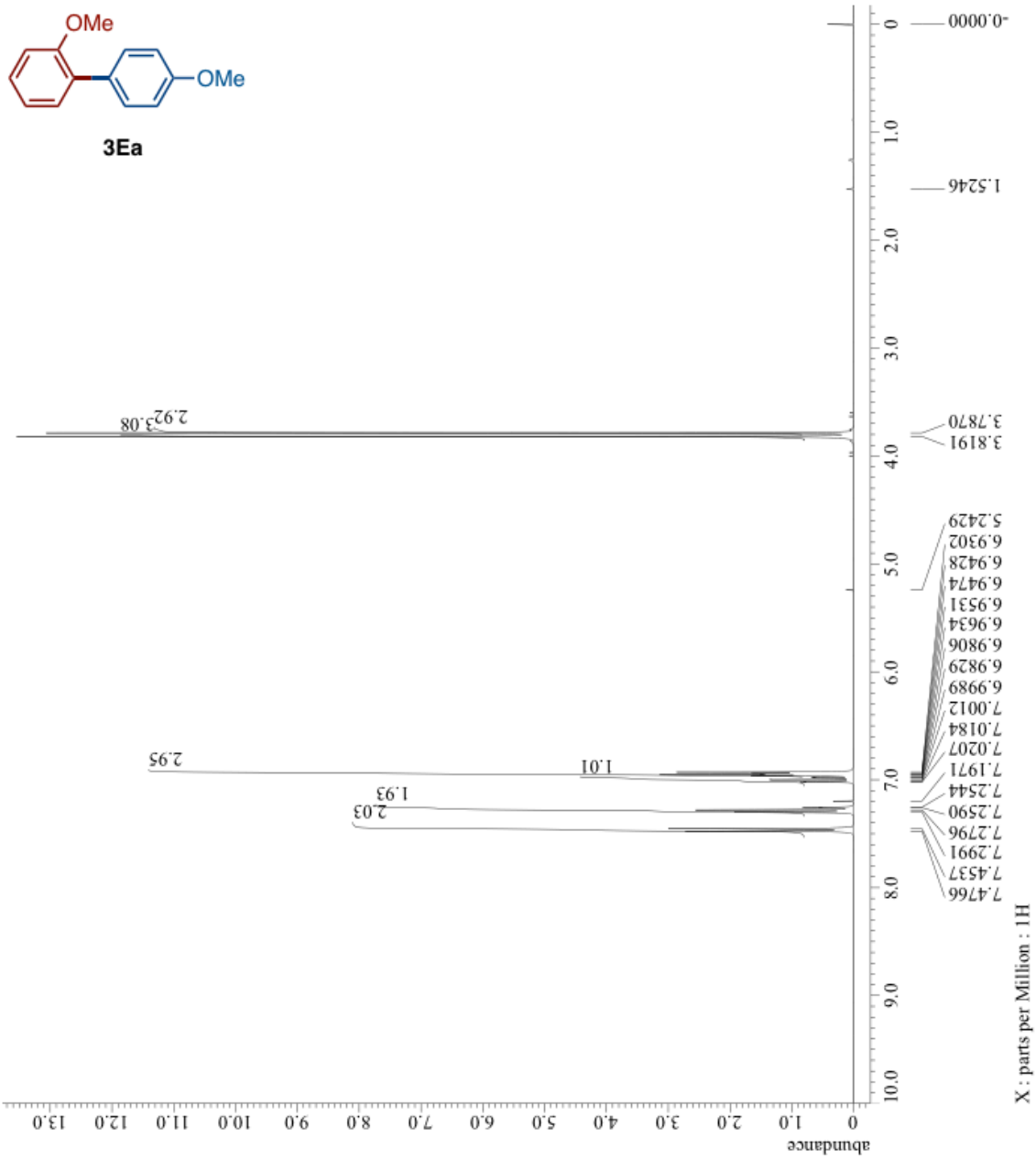
Supplementary Figure 34. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ca



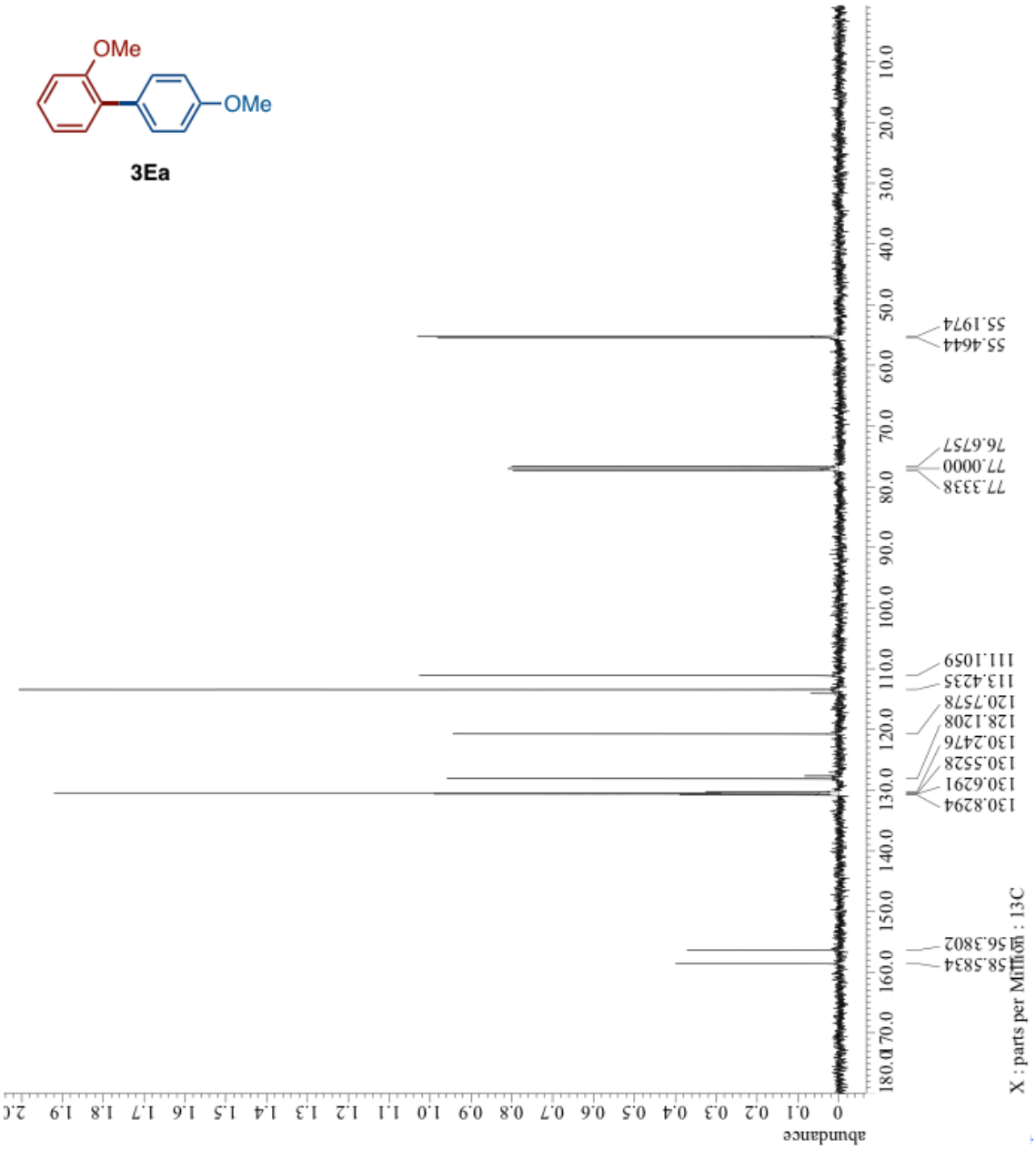
Supplementary Figure 35. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Da



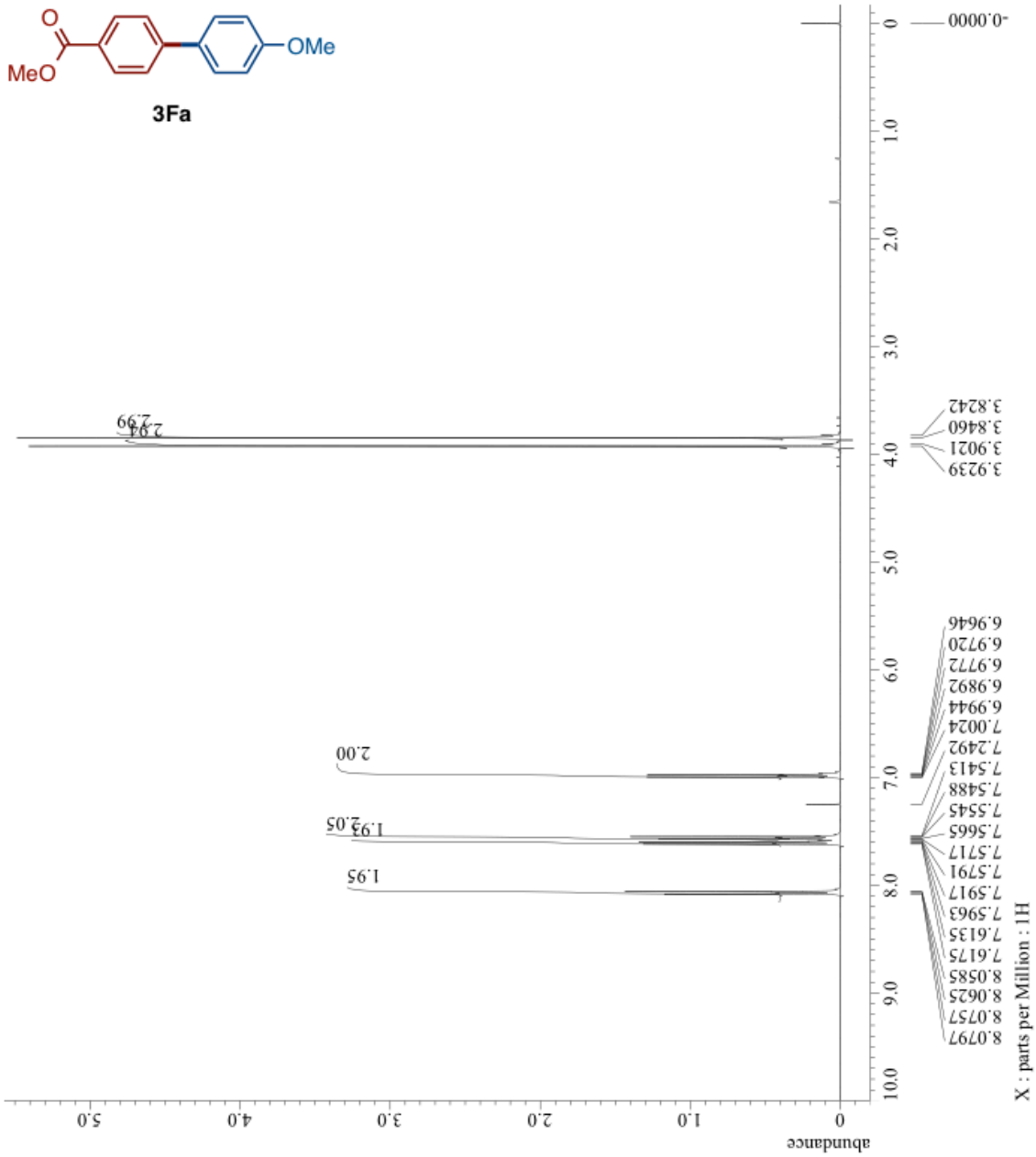
Supplementary Figure 36. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Da



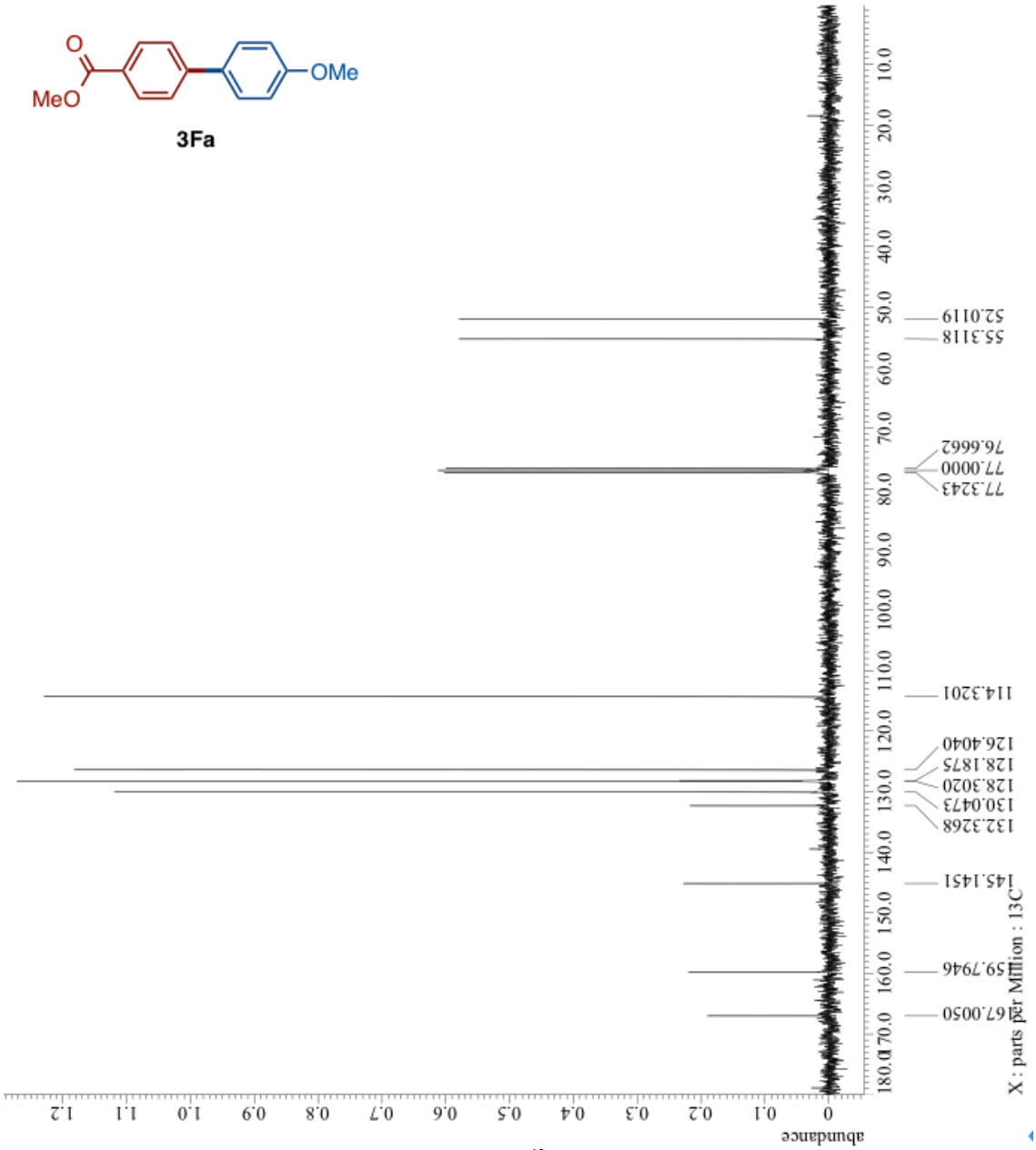
Supplementary Figure 37. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ea



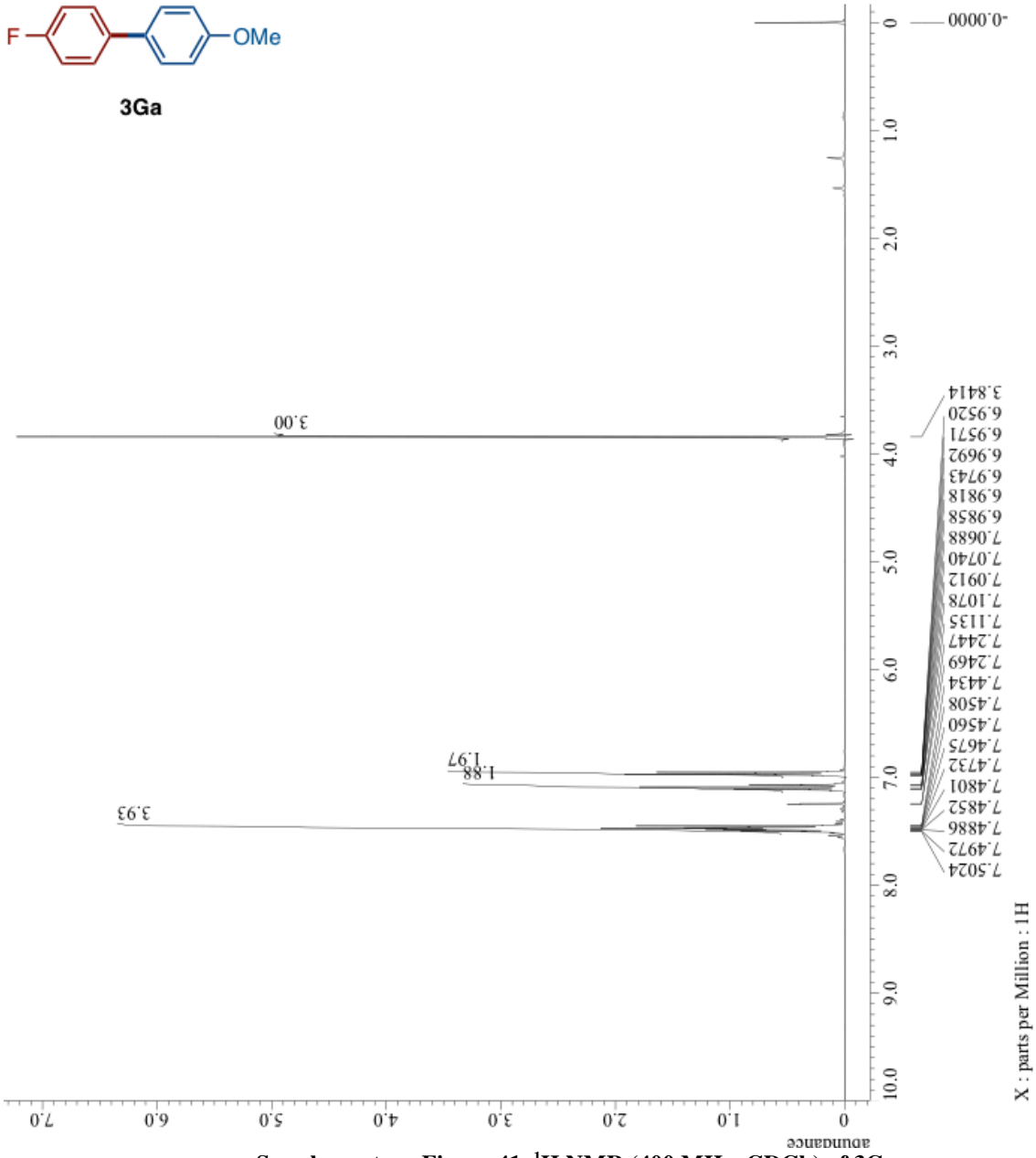
Supplementary Figure 38. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ea



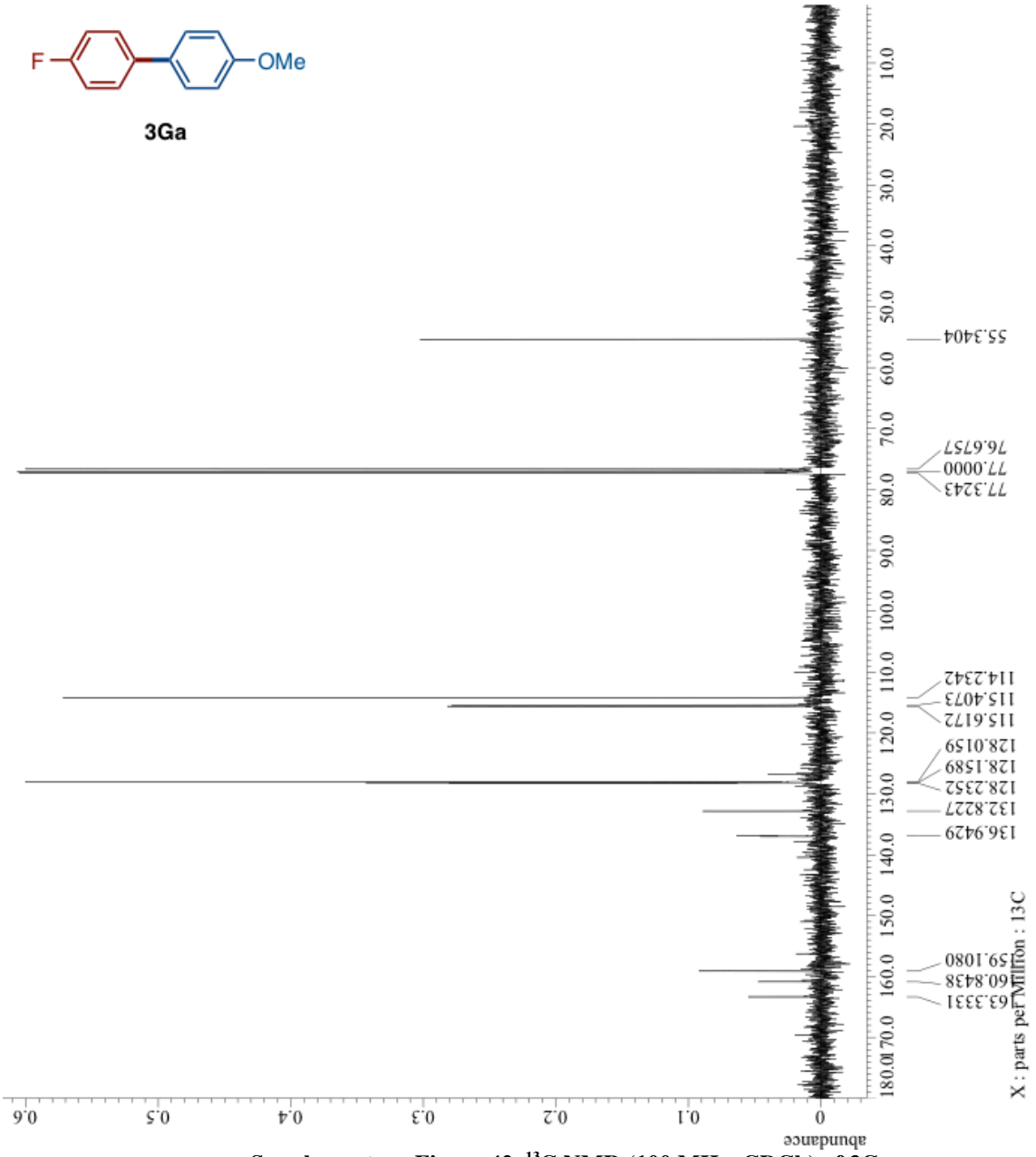
Supplementary Figure 39. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Fa



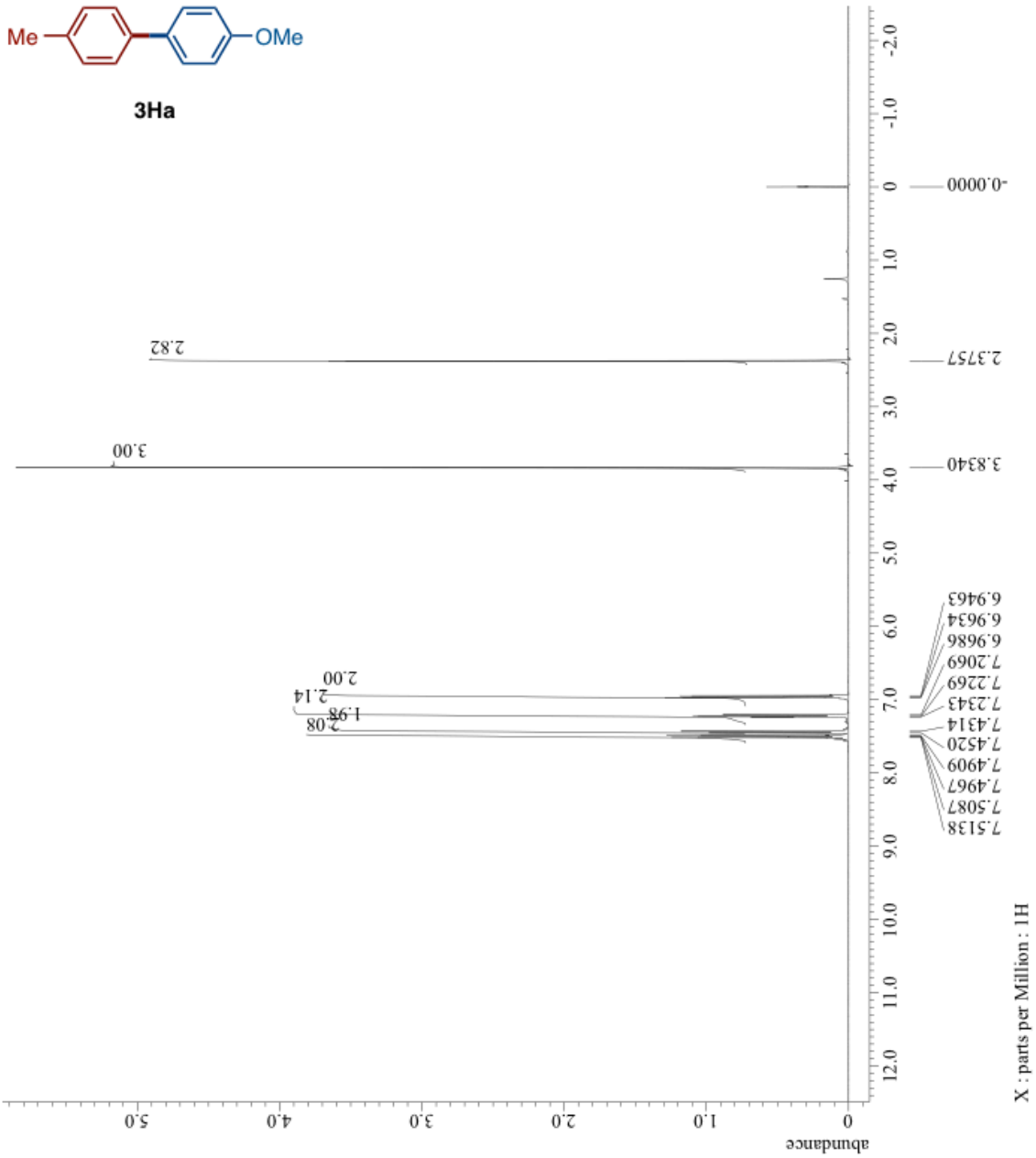
Supplementary Figure 40. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Fa



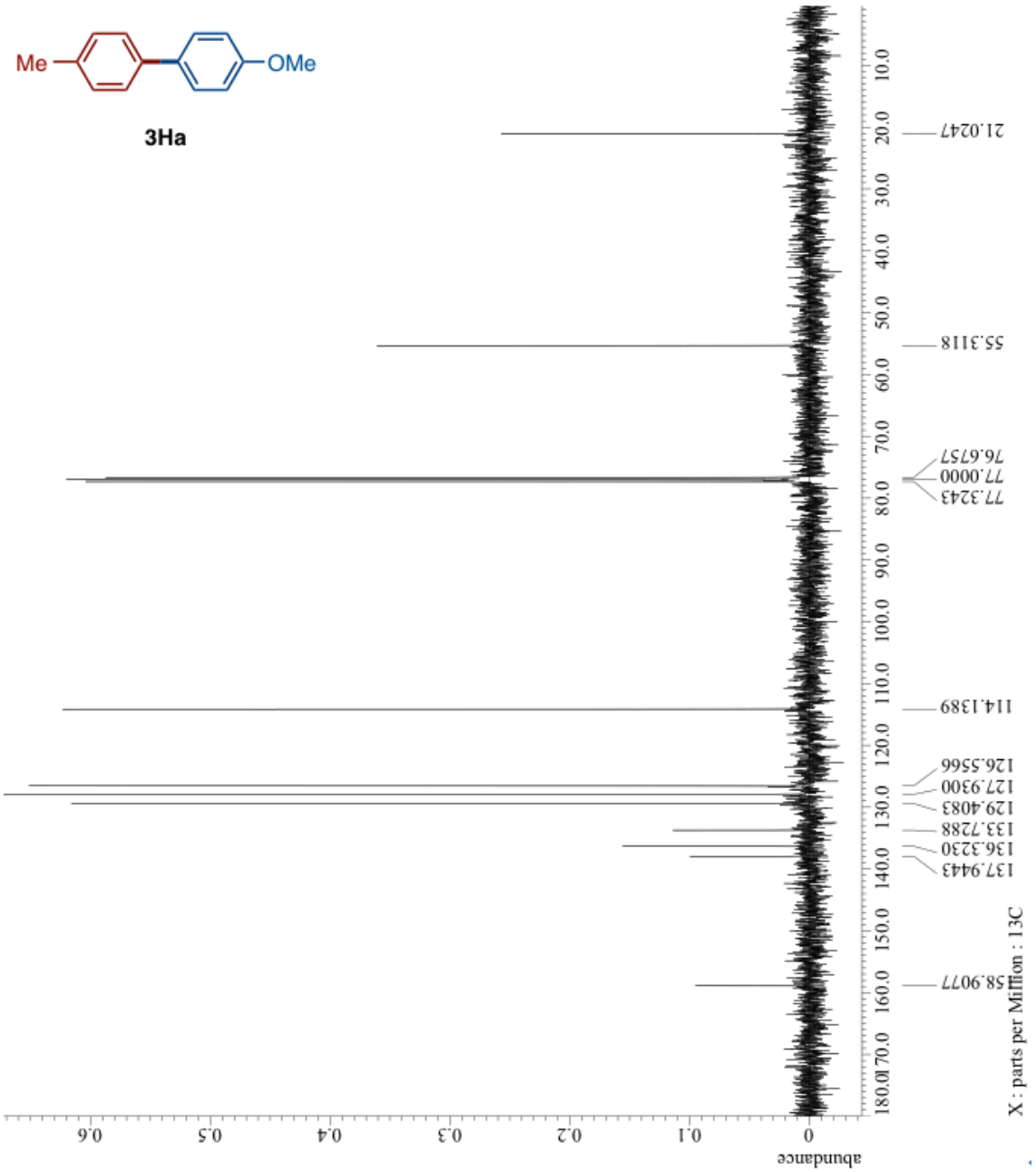
Supplementary Figure 41. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ga



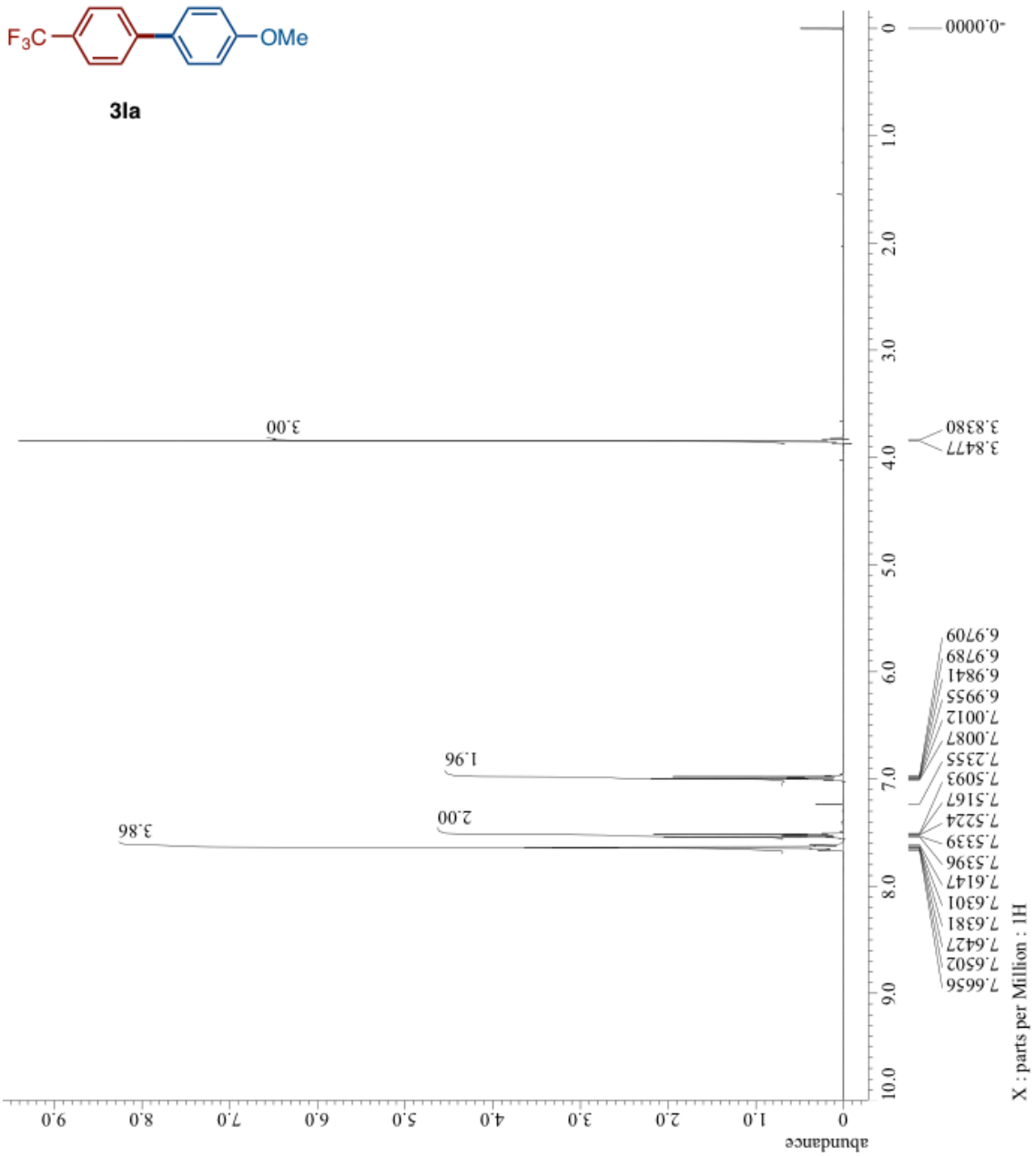
Supplementary Figure 42. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ga



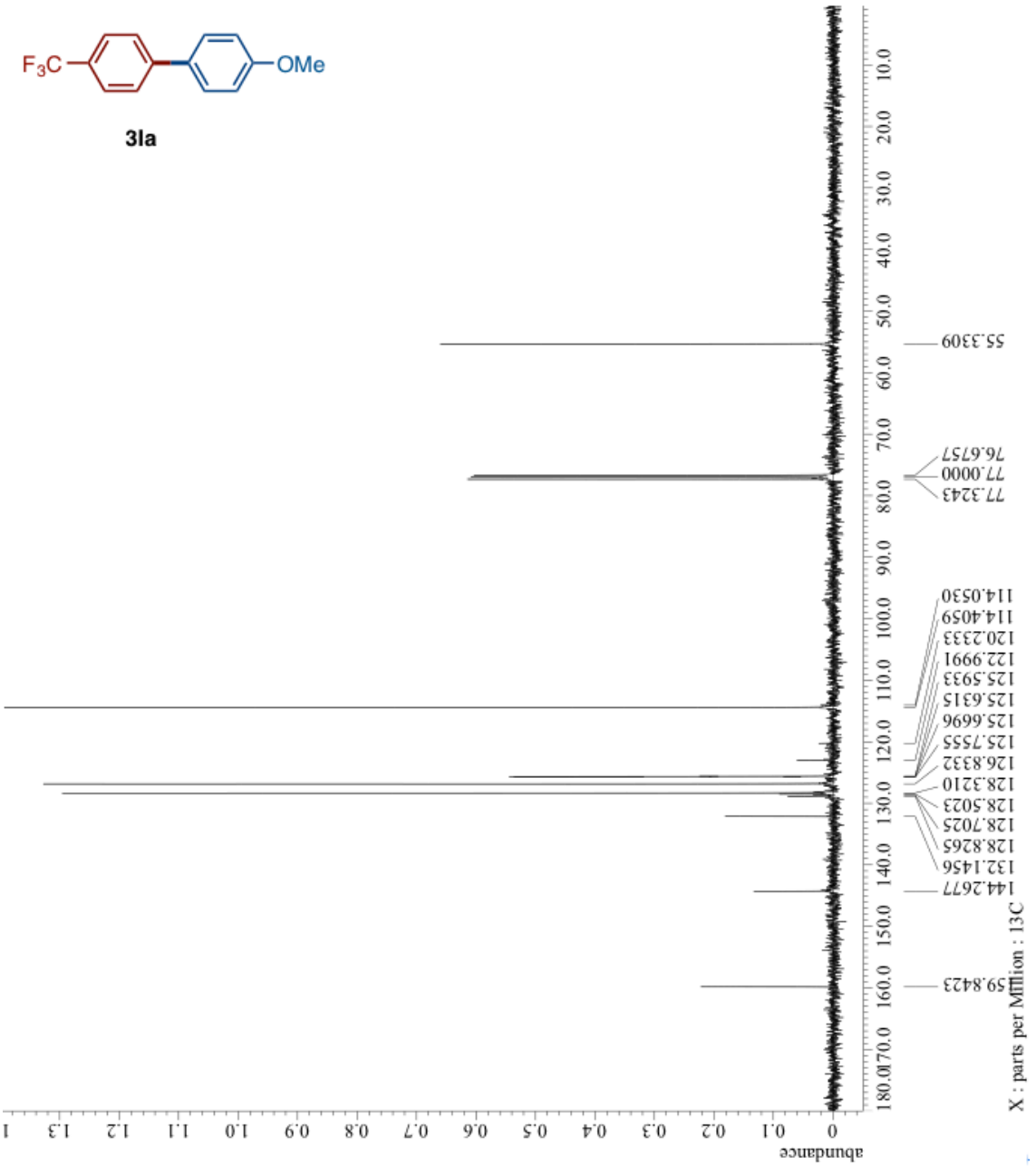
Supplementary Figure 43. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ha



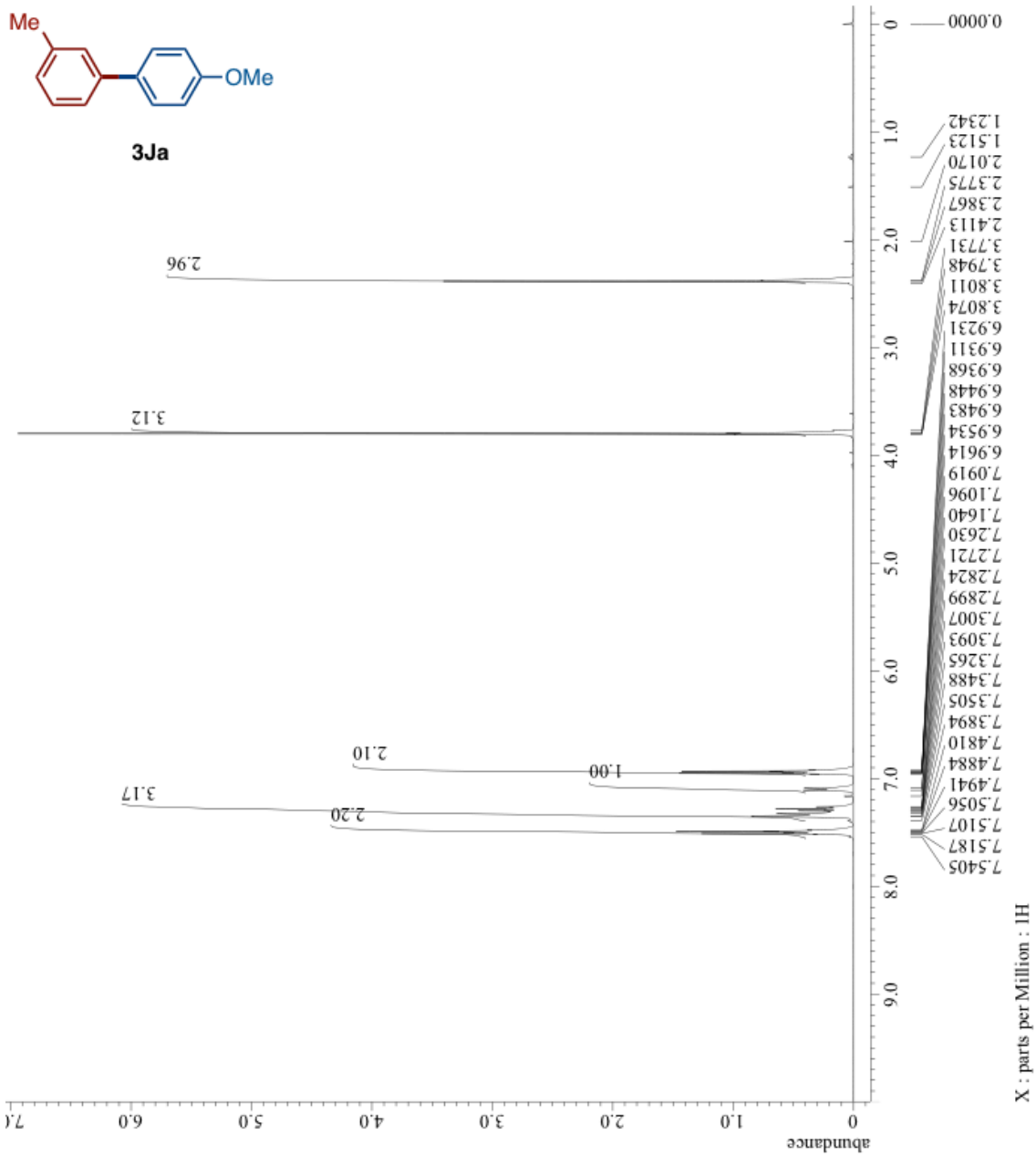
Supplementary Figure 44. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ha



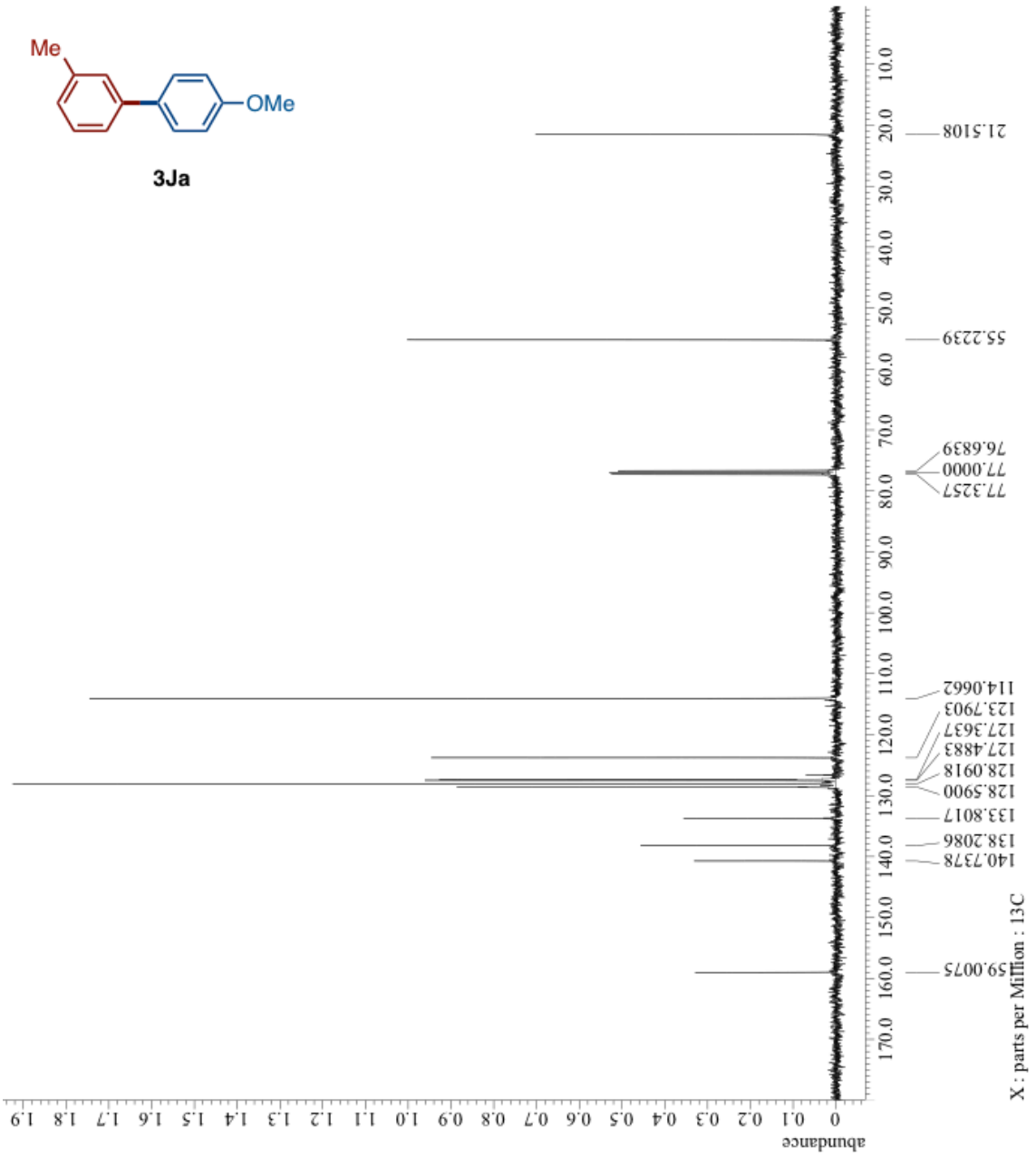
Supplementary Figure 45. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ia



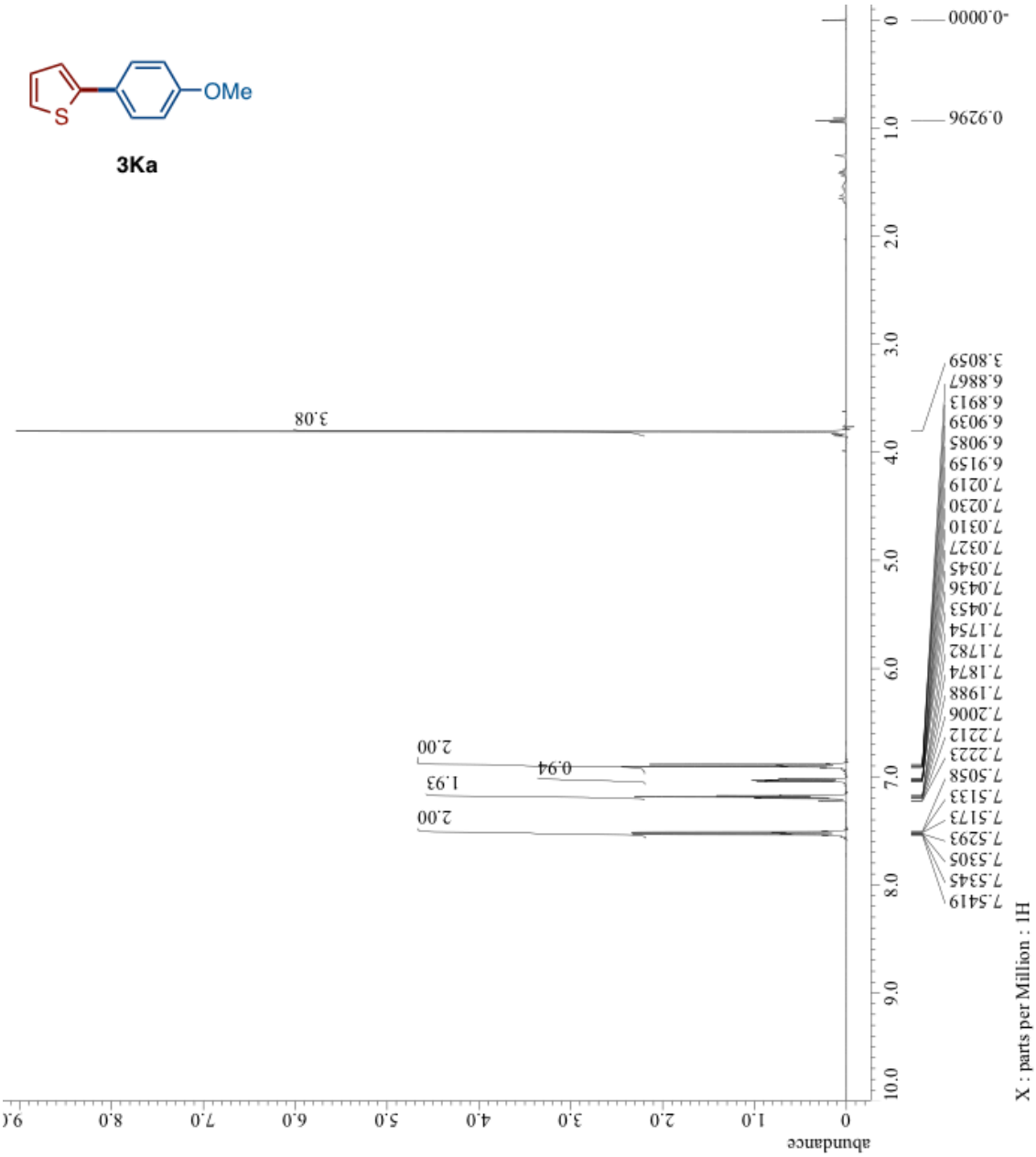
Supplementary Figure 46. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ia



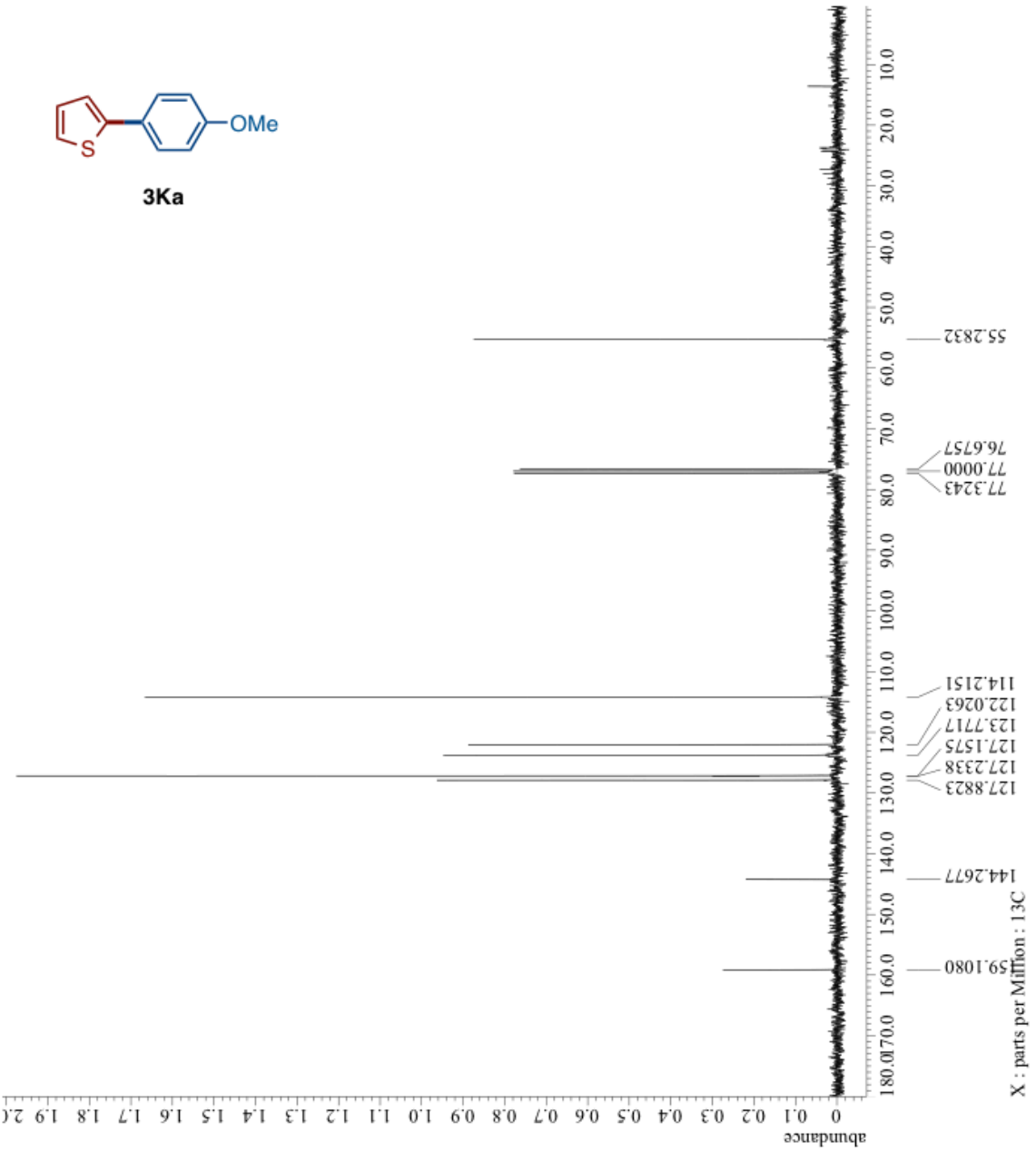
Supplementary Figure 47. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ja



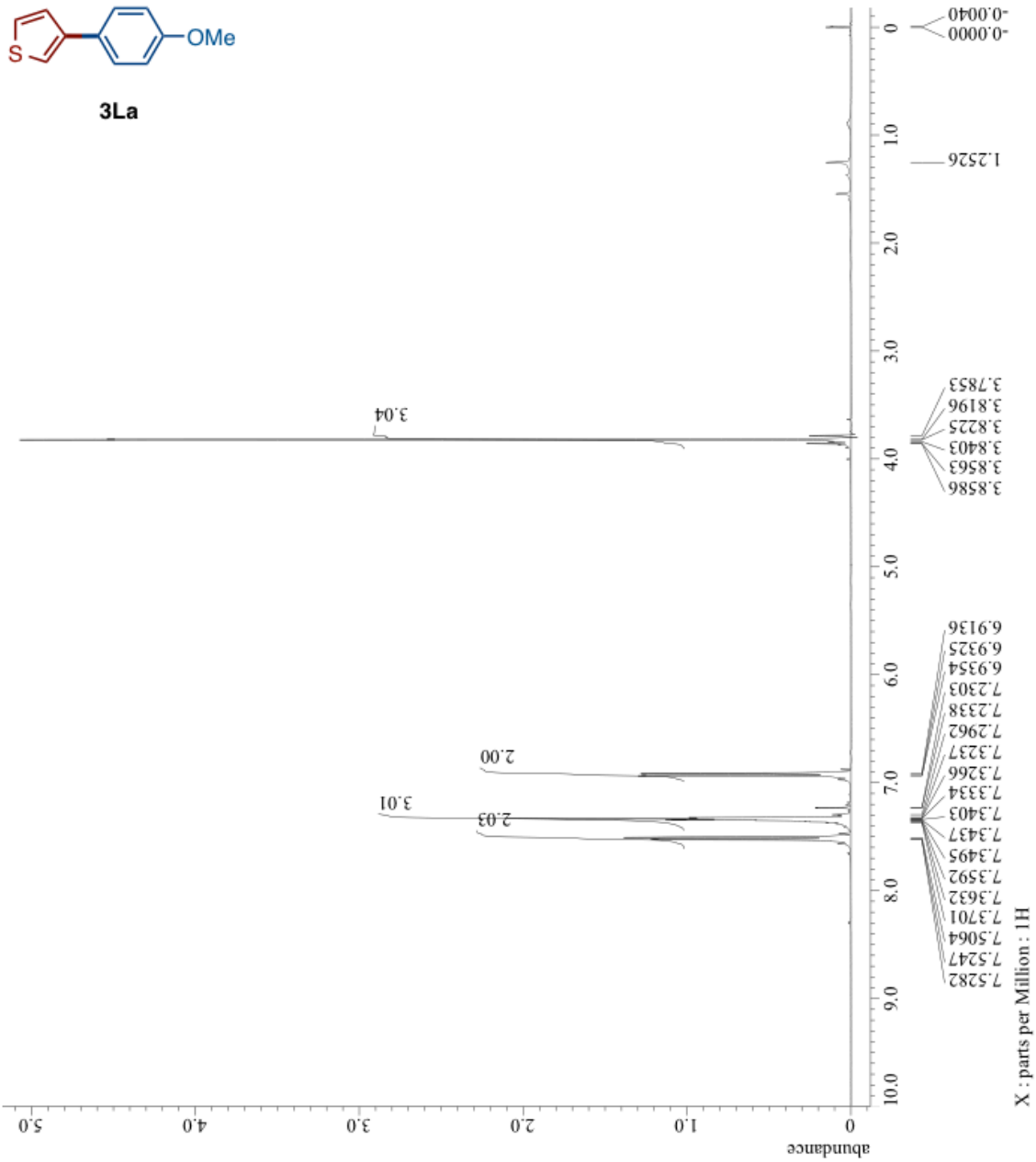
Supplementary Figure 48. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ja



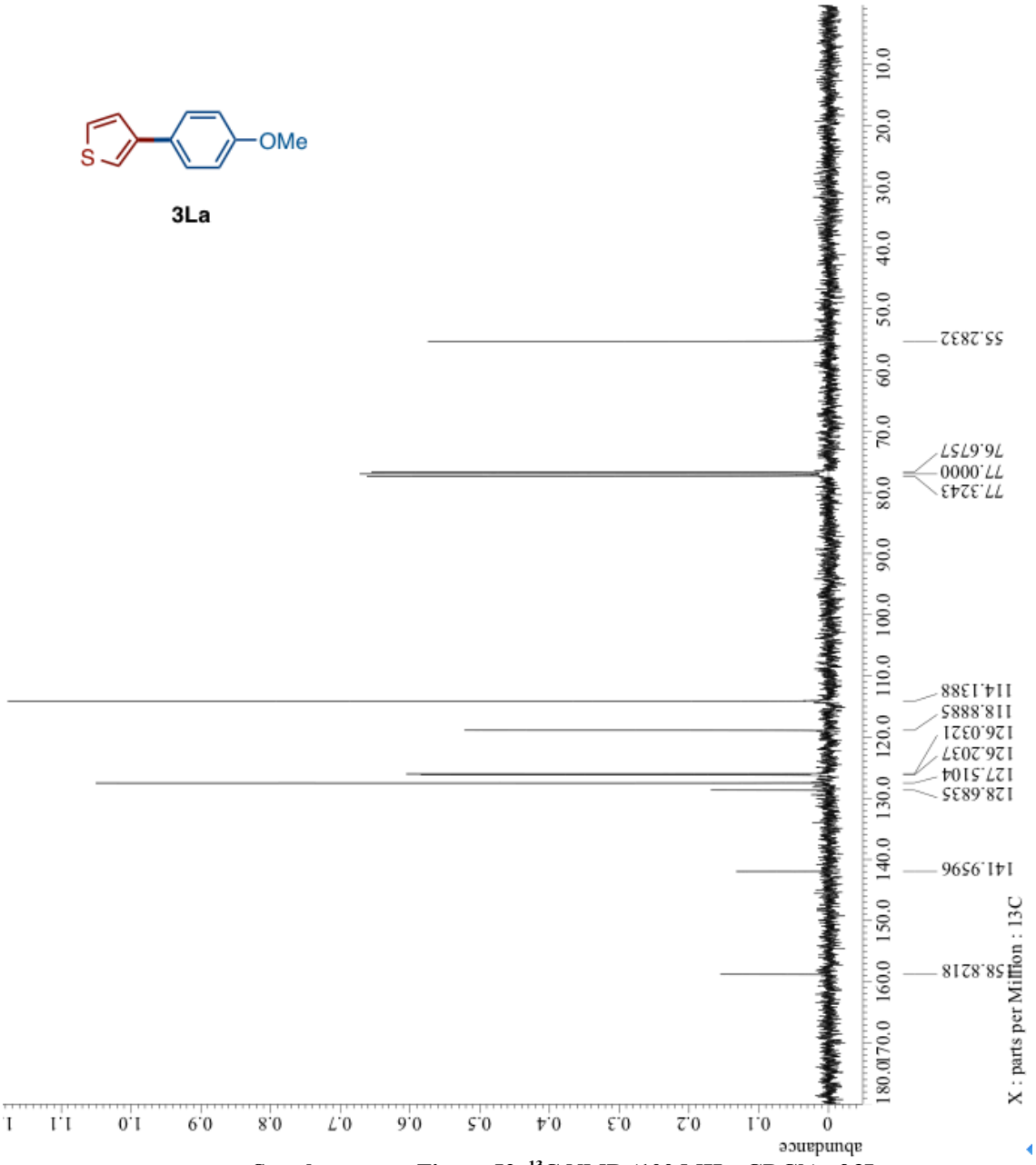
Supplementary Figure 49. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ka



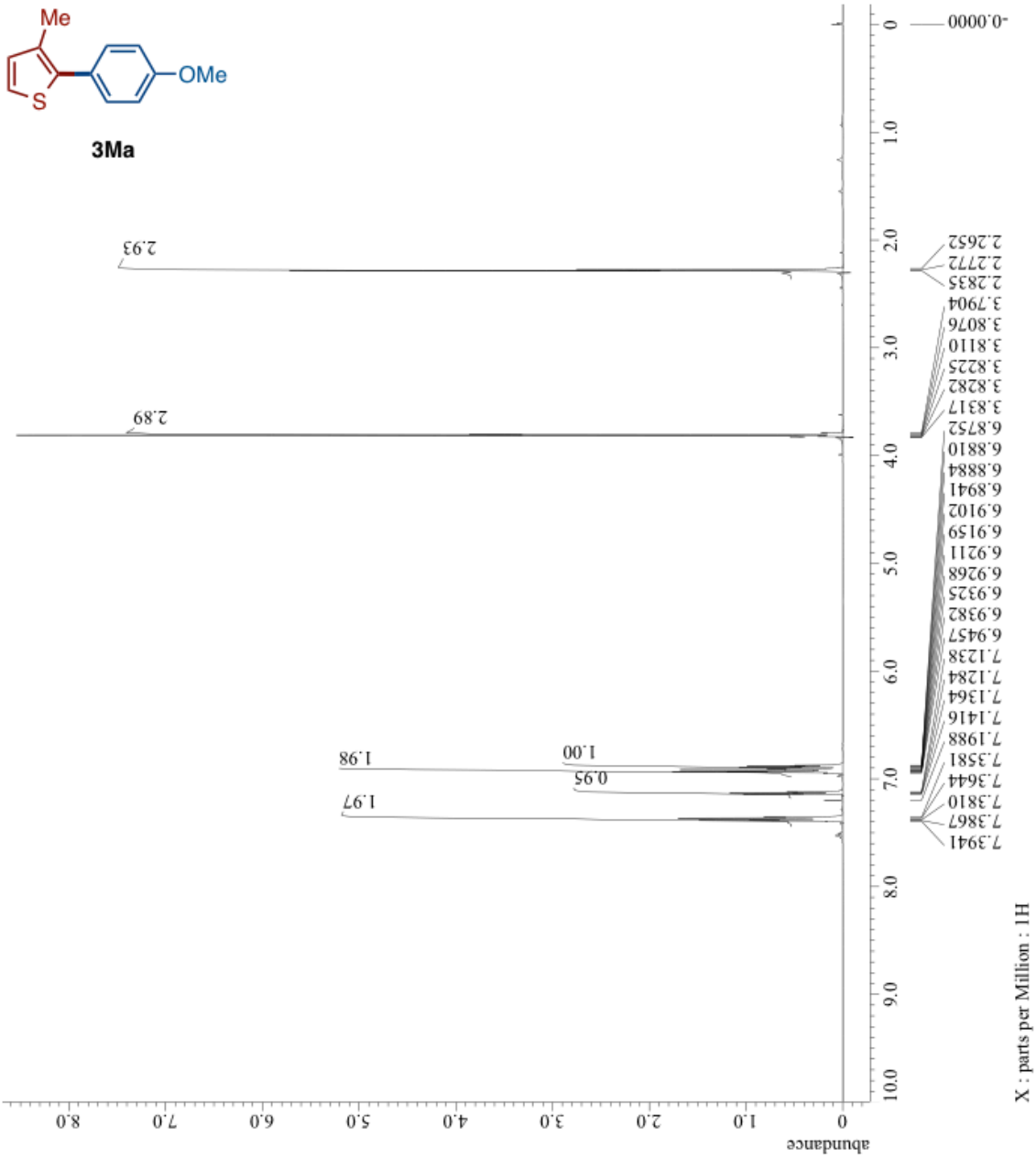
Supplementary Figure 50. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ka



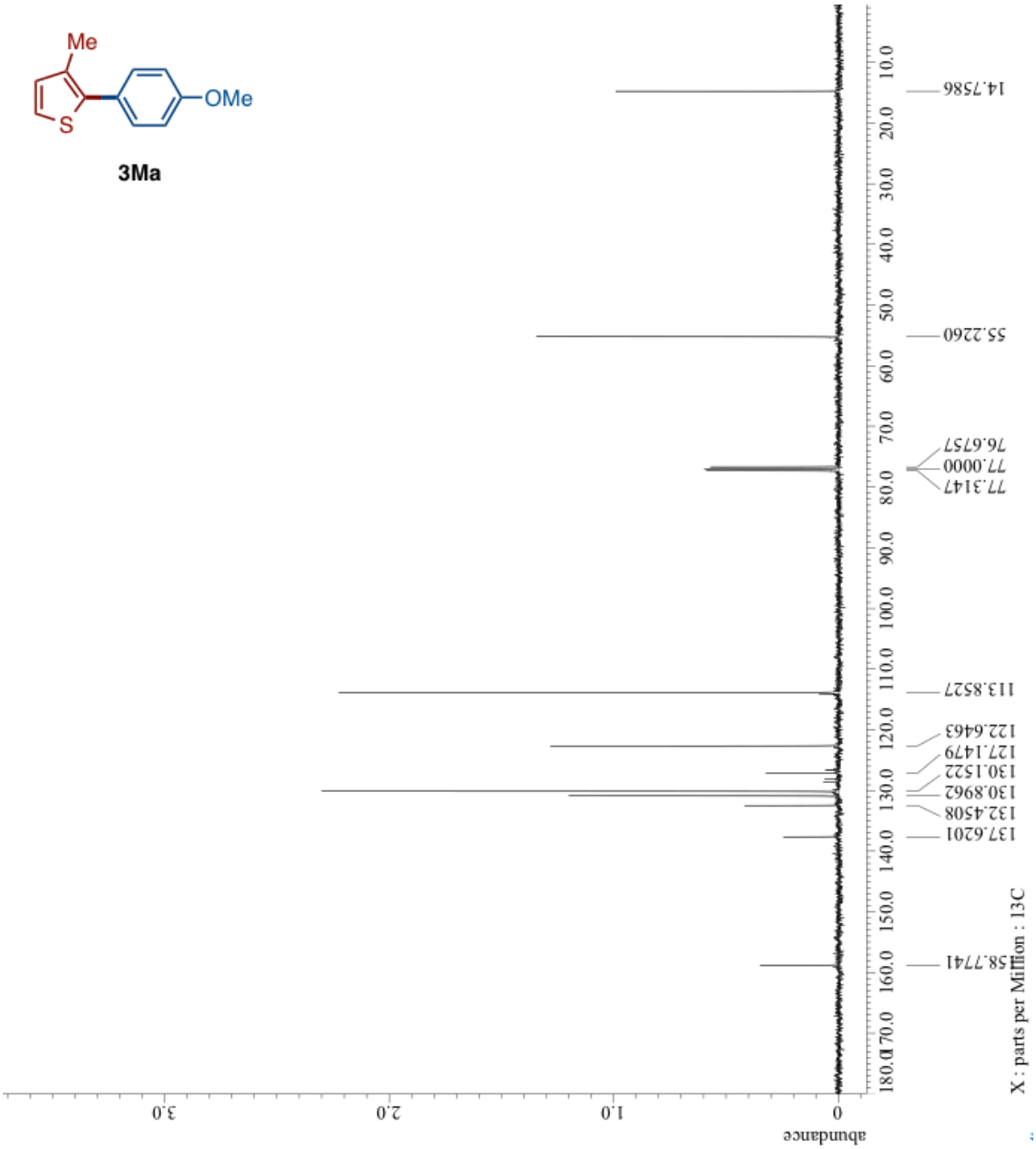
Supplementary Figure 51. ^{1}H NMR (400 MHz, $CDCl_3$) of 3La



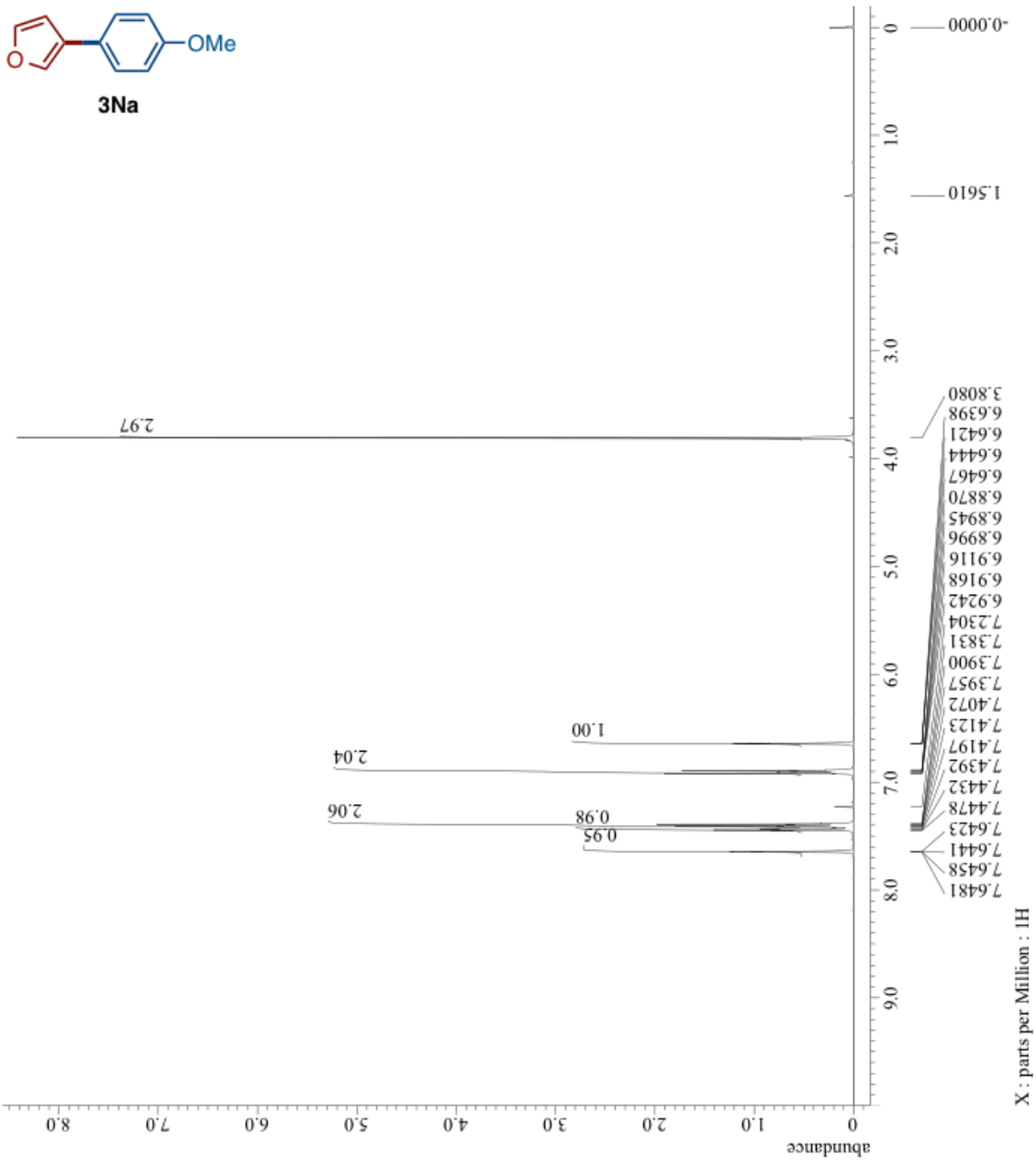
Supplementary Figure 52. ^{13}**C NMR (100 MHz, $CDCl_3$) of 3La**



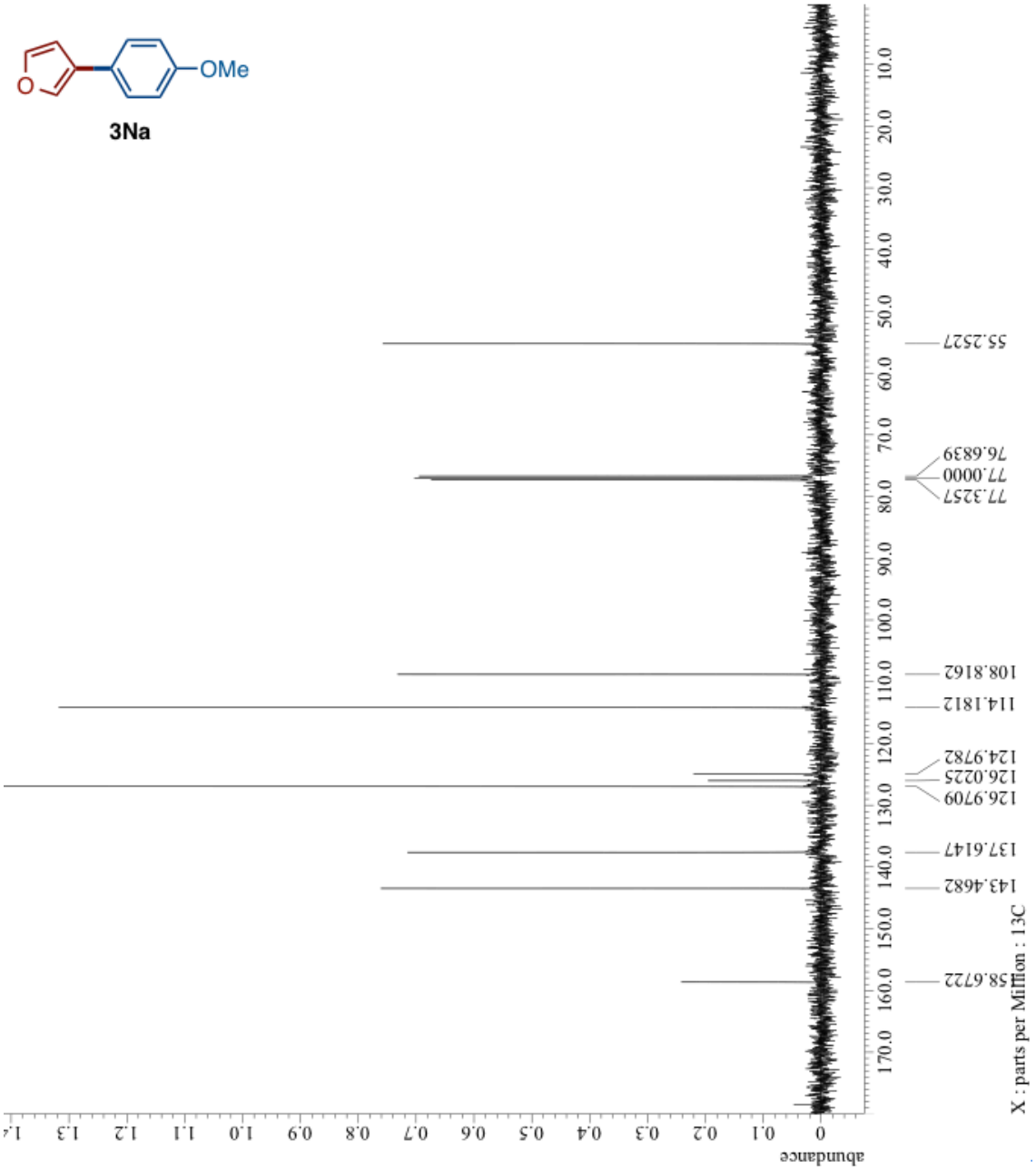
Supplementary Figure 53. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ma



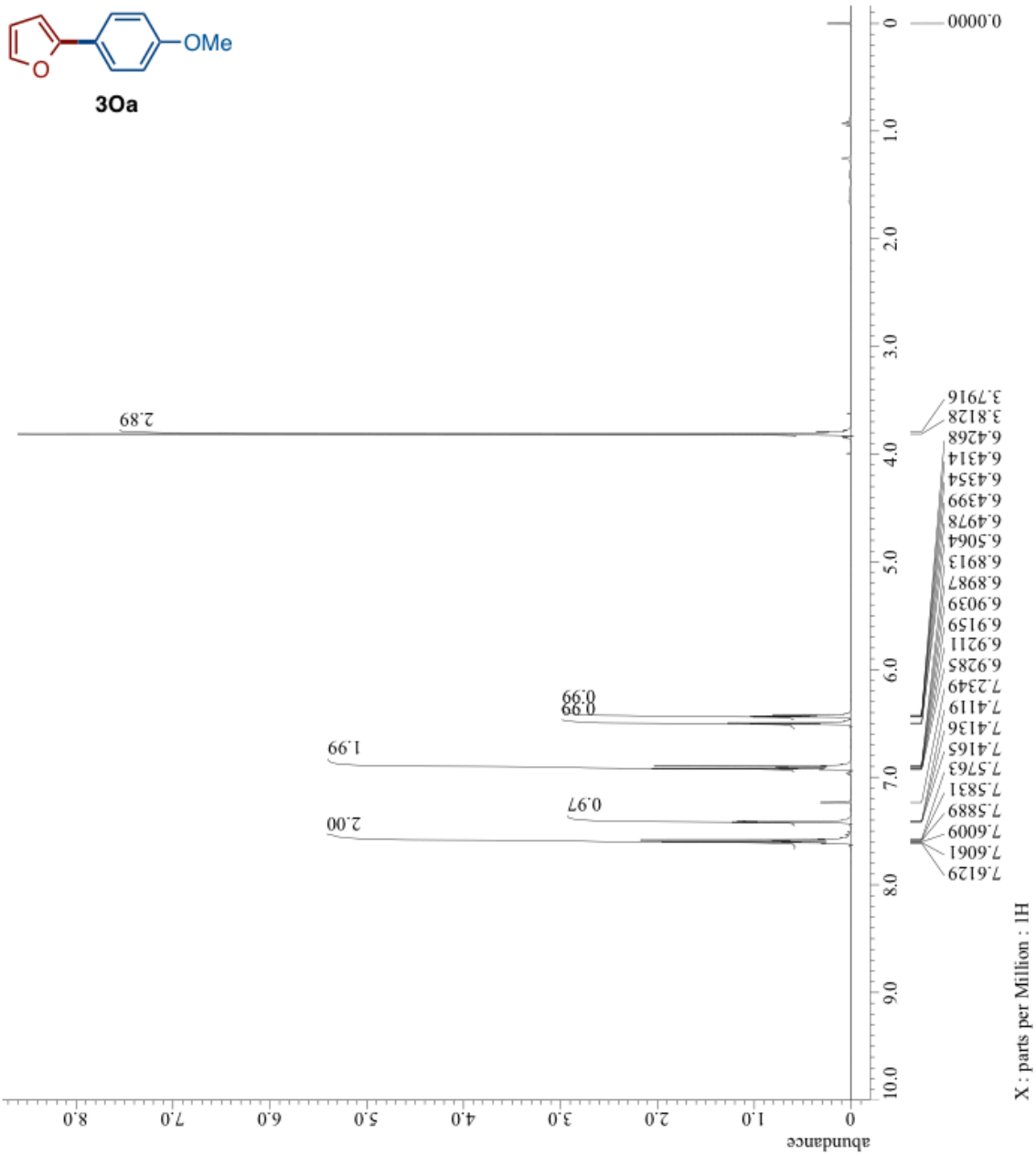
Supplementary Figure 54. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ma



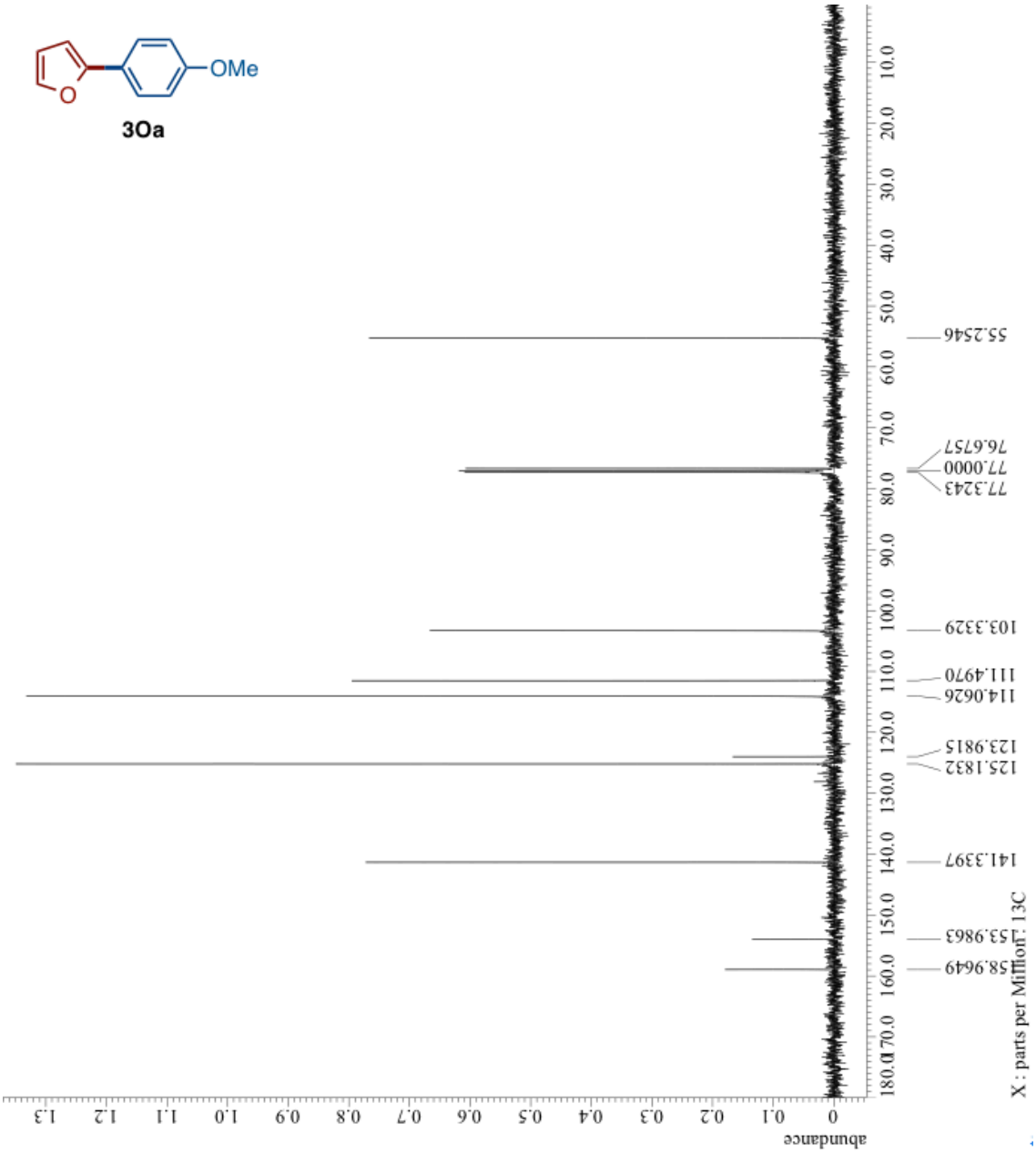
Supplementary Figure 55. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Na



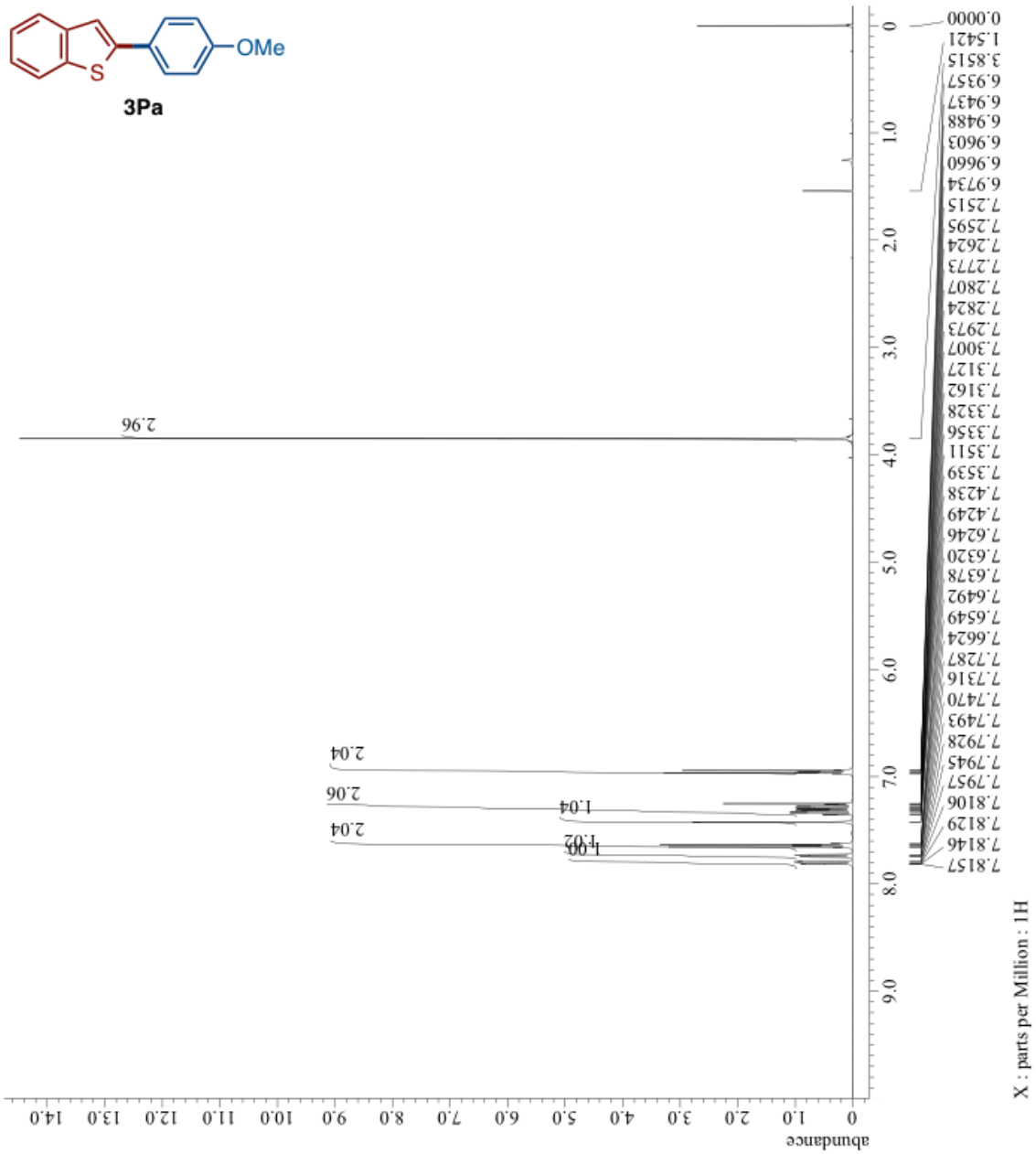
Supplementary Figure 56. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Na



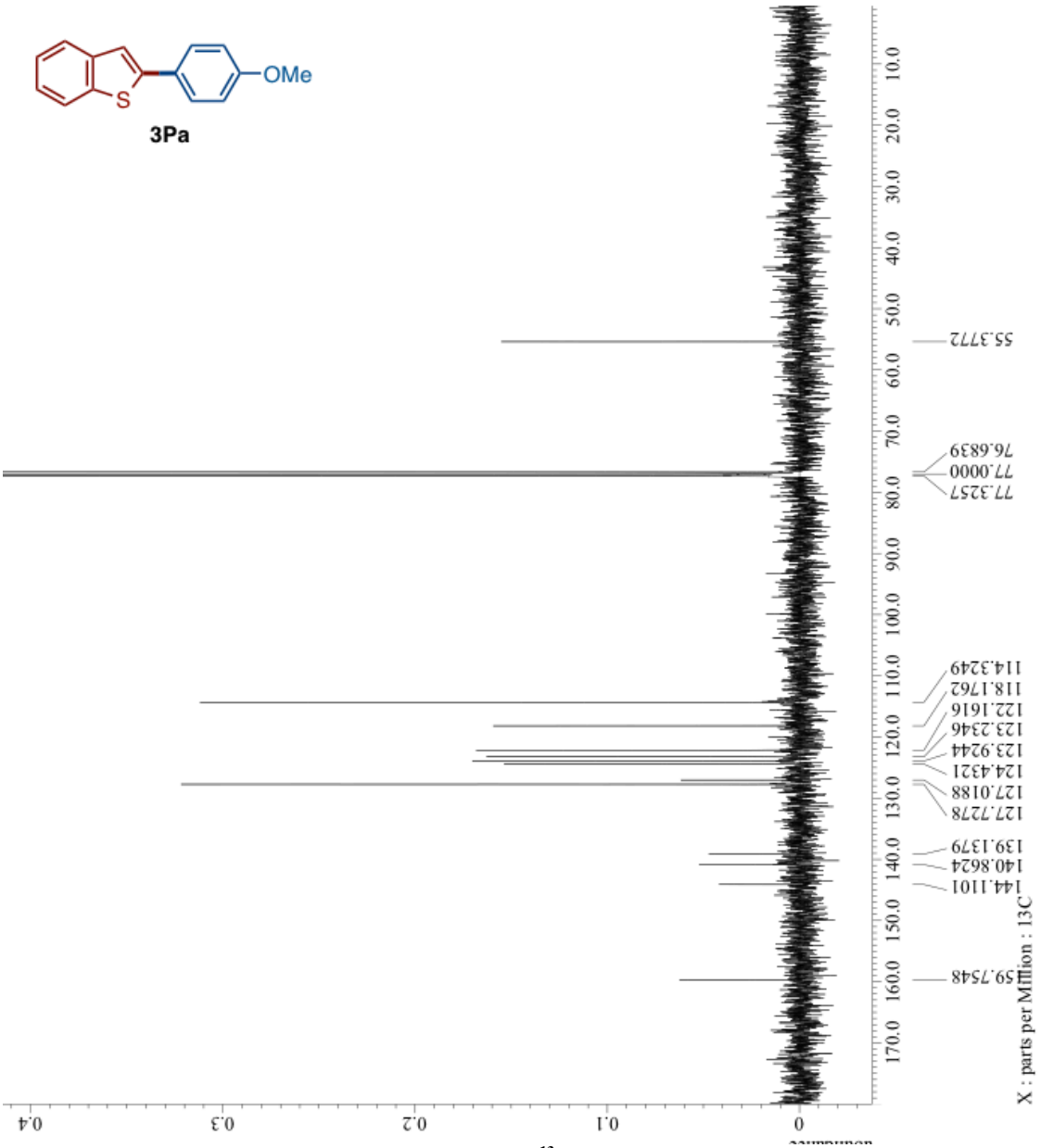
Supplementary Figure 57. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Oa



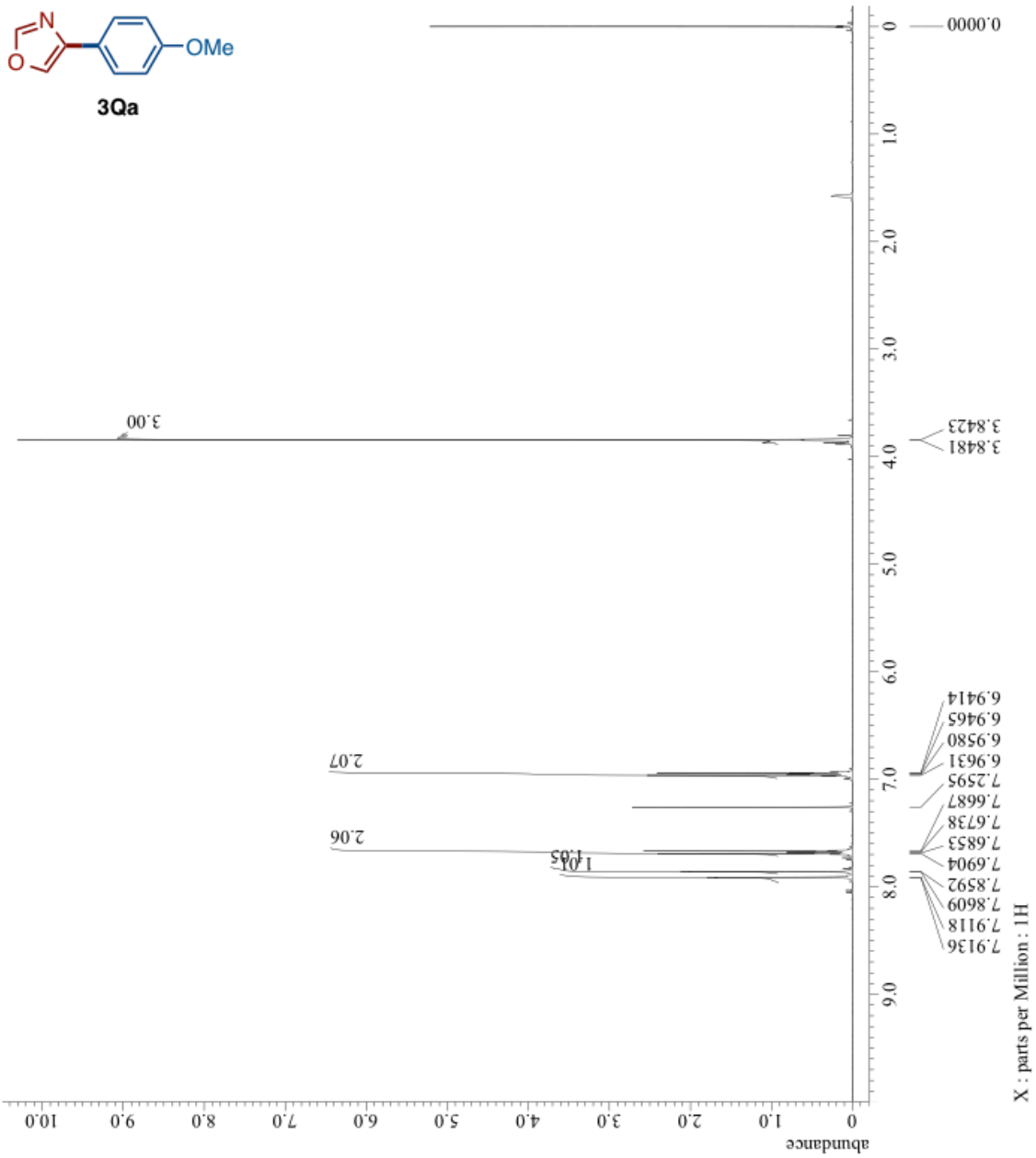
Supplementary Figure 58. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Oa



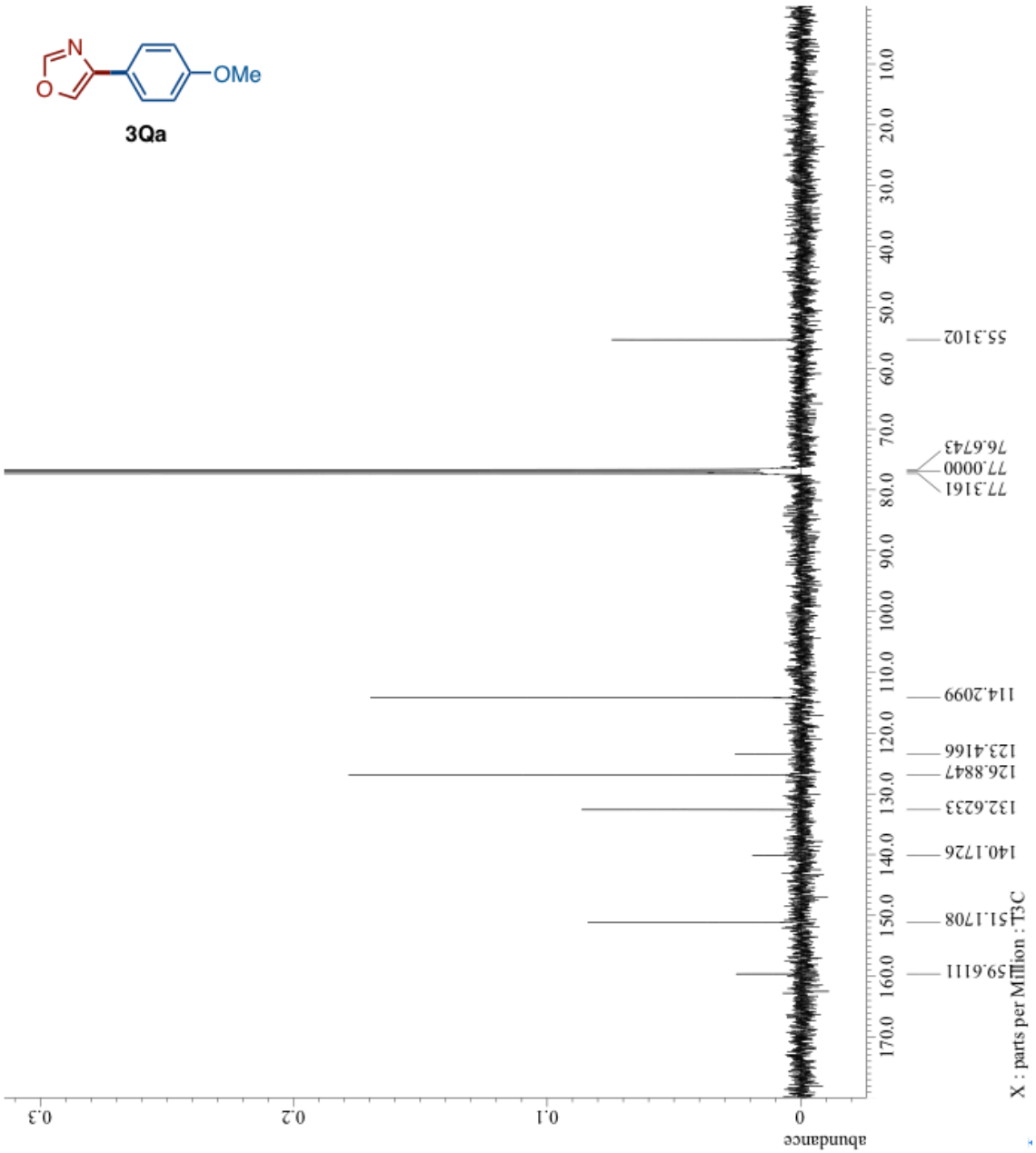
Supplementary Figure 59. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Pa



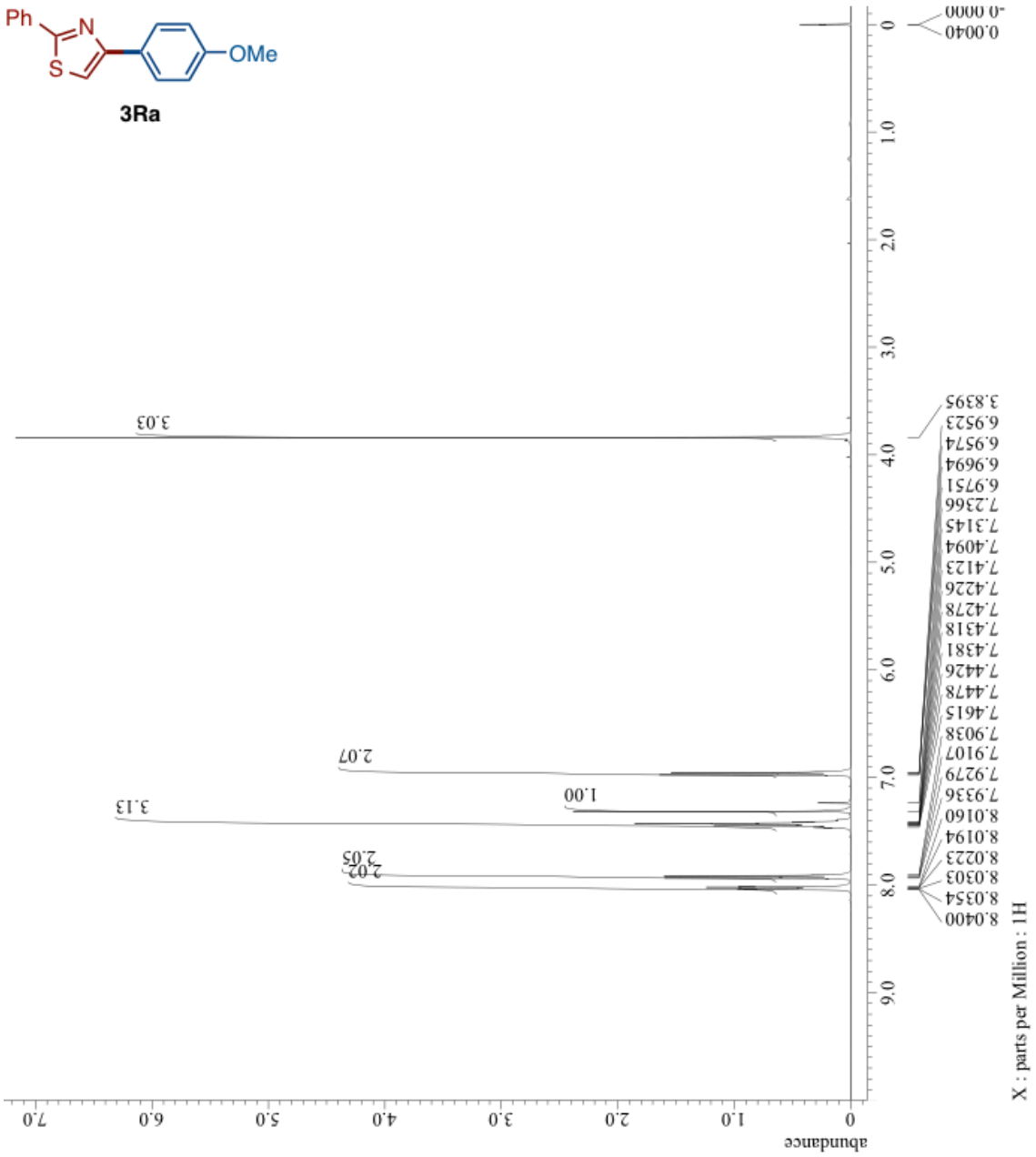
Supplementary Figure 60. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Pa



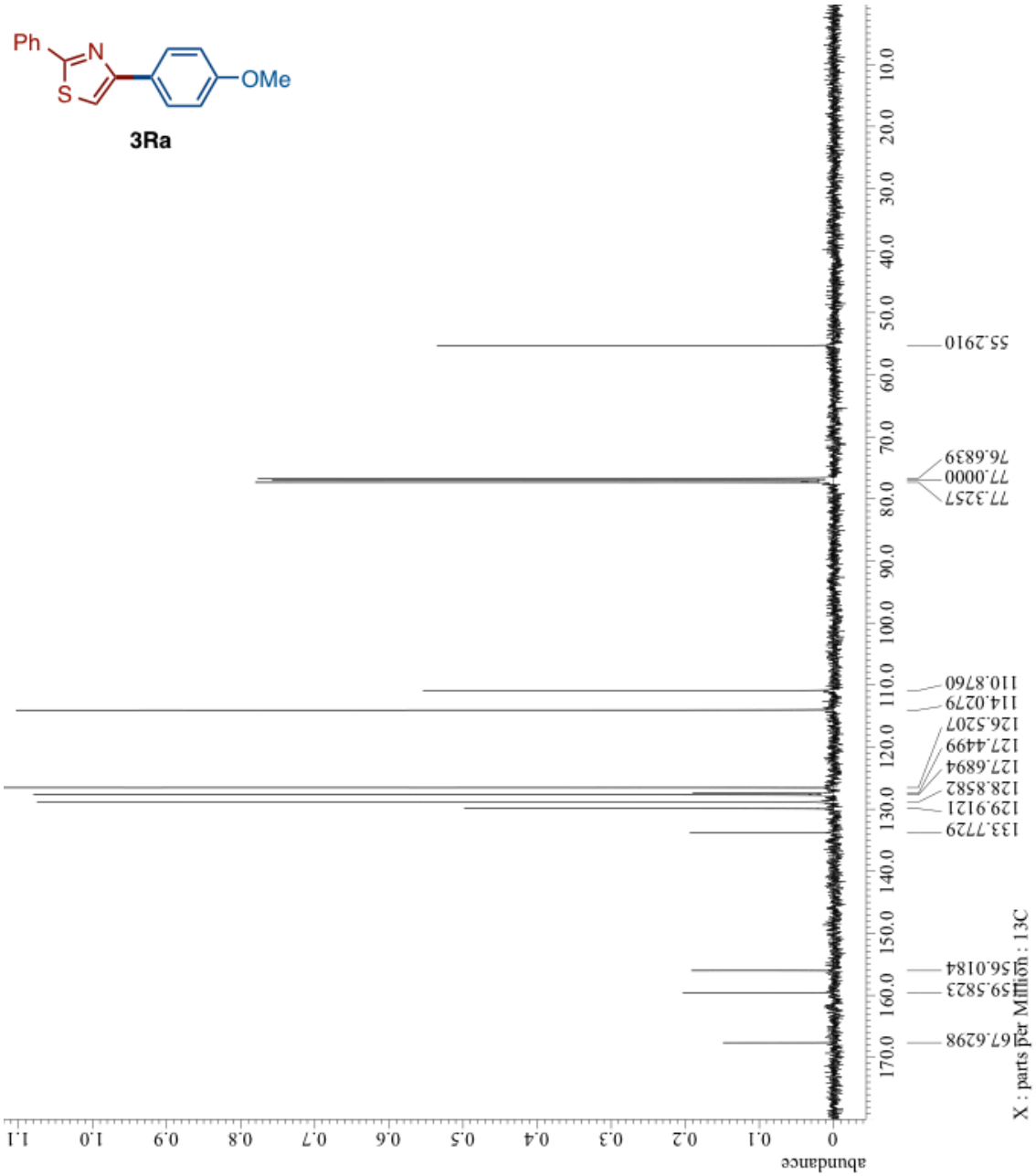
Supplementary Figure 61. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Qa



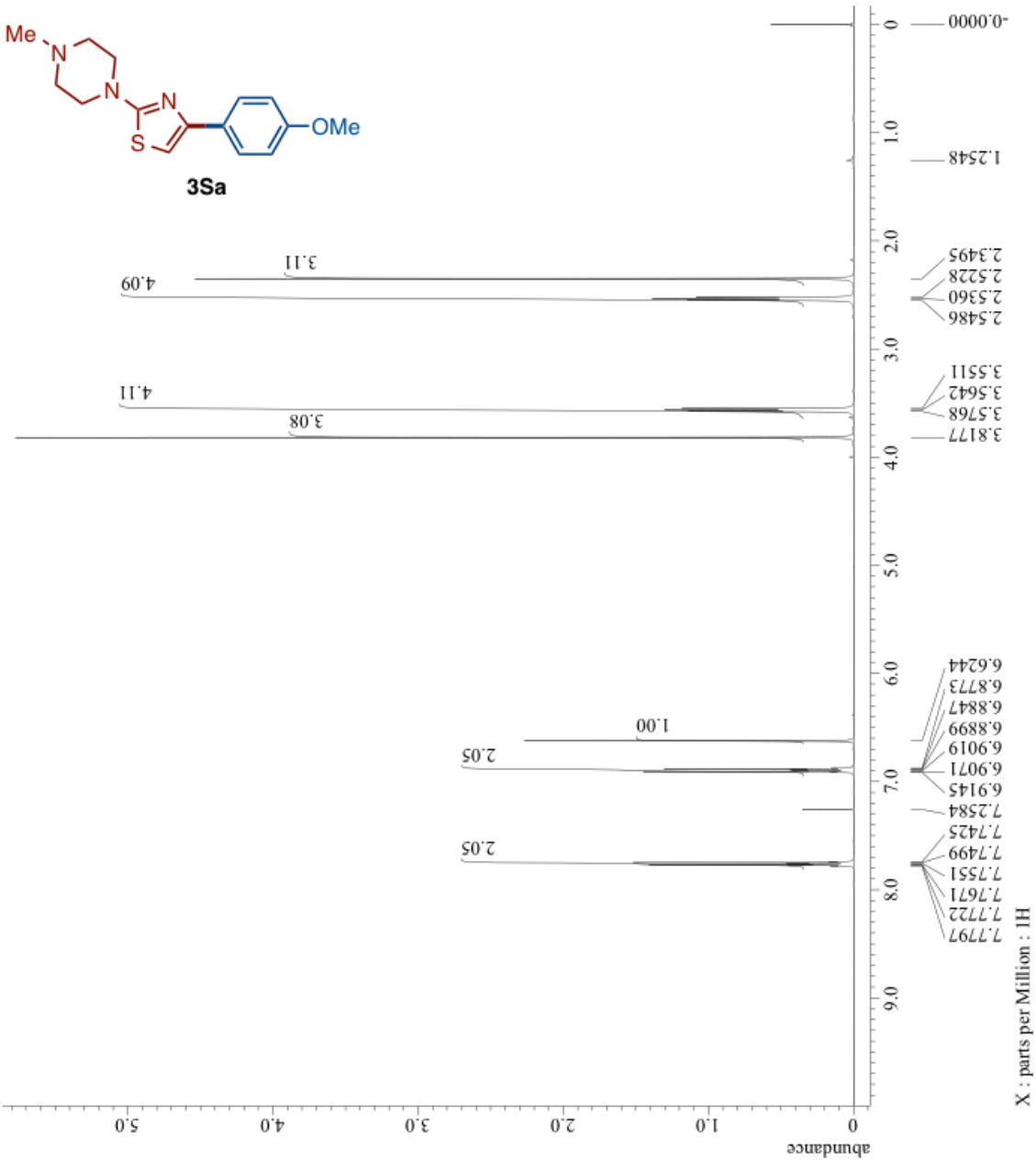
Supplementary Figure 62. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Qa



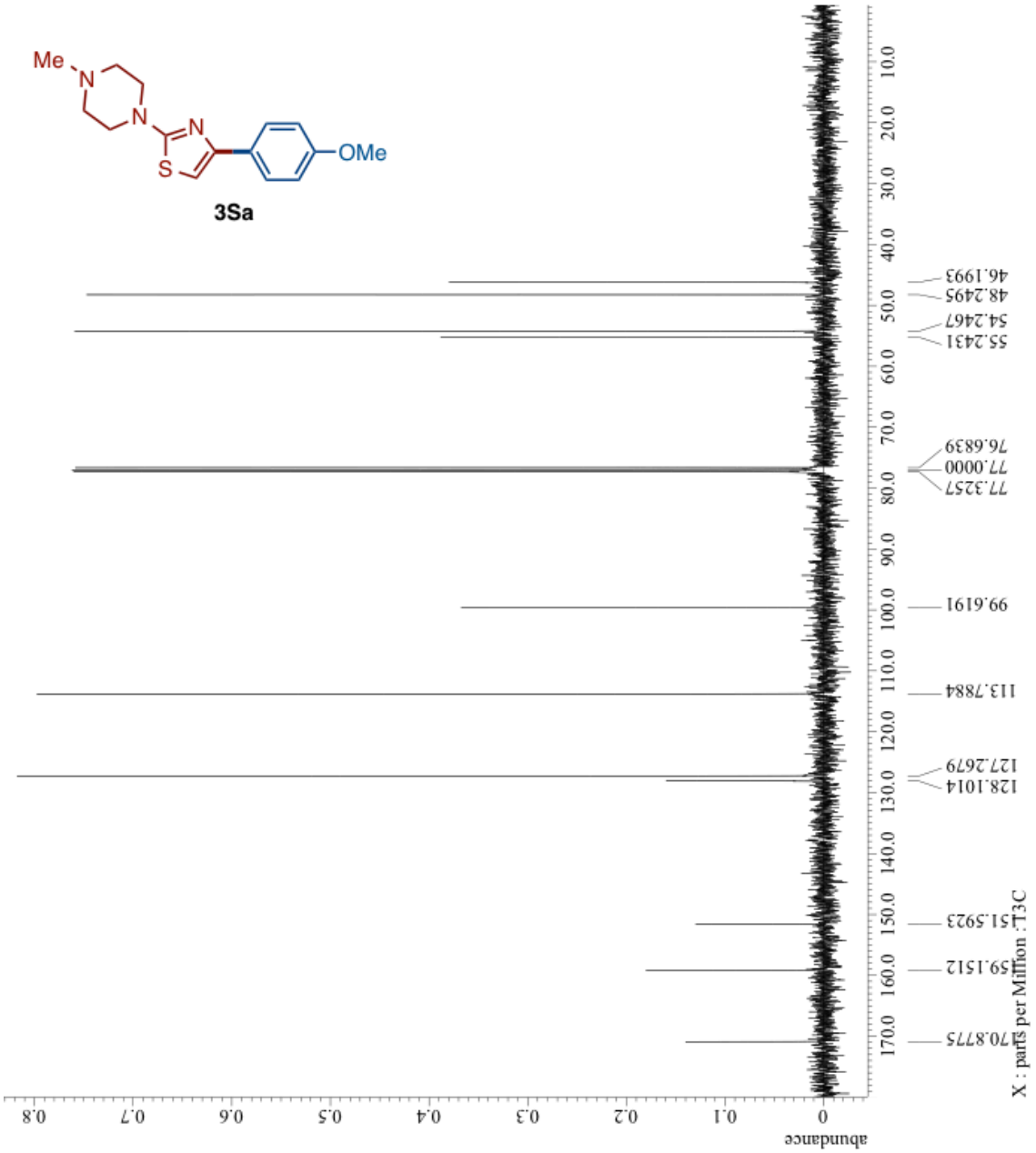
Supplementary Figure 63. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ra



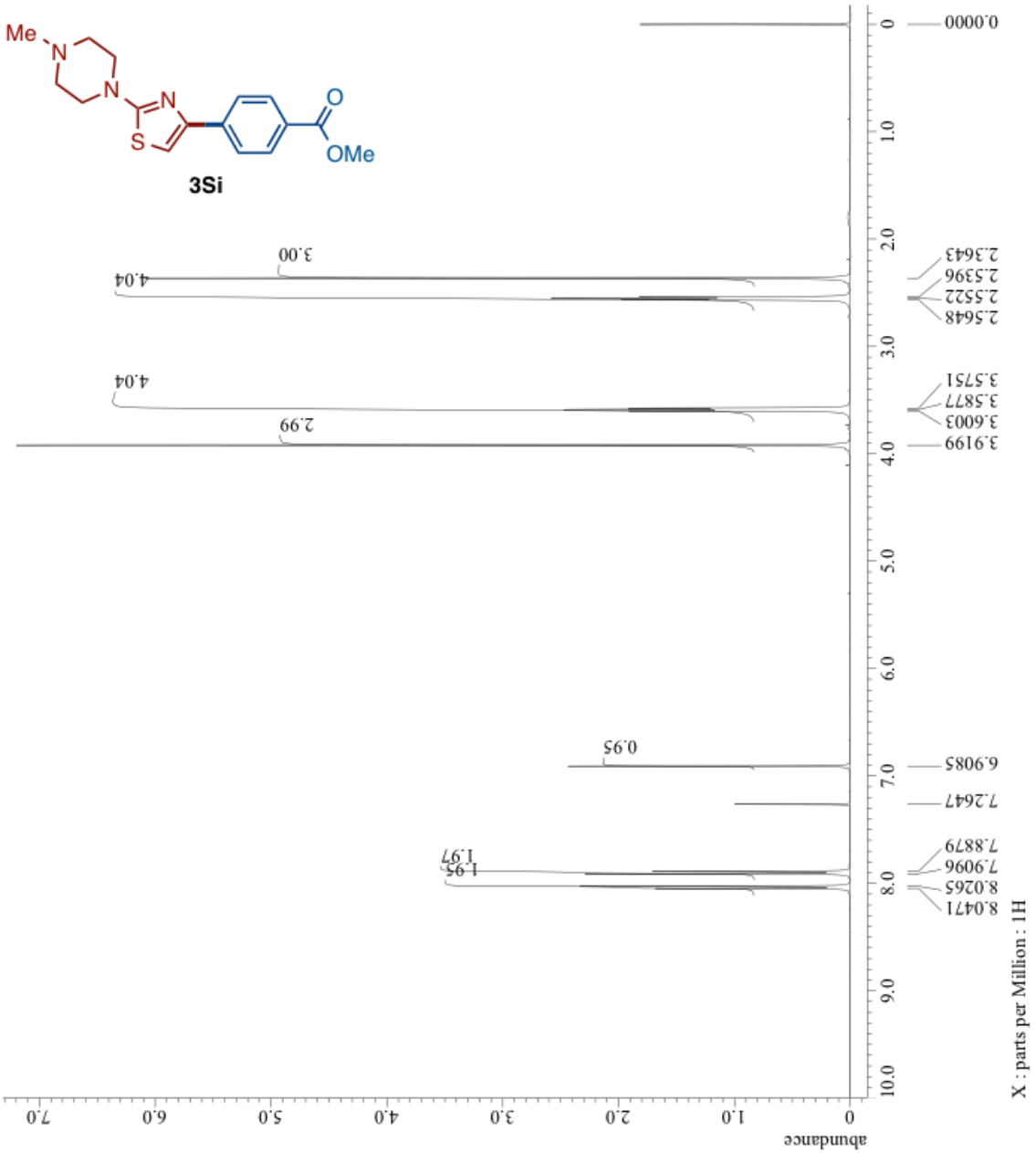
Supplementary Figure 64. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ra



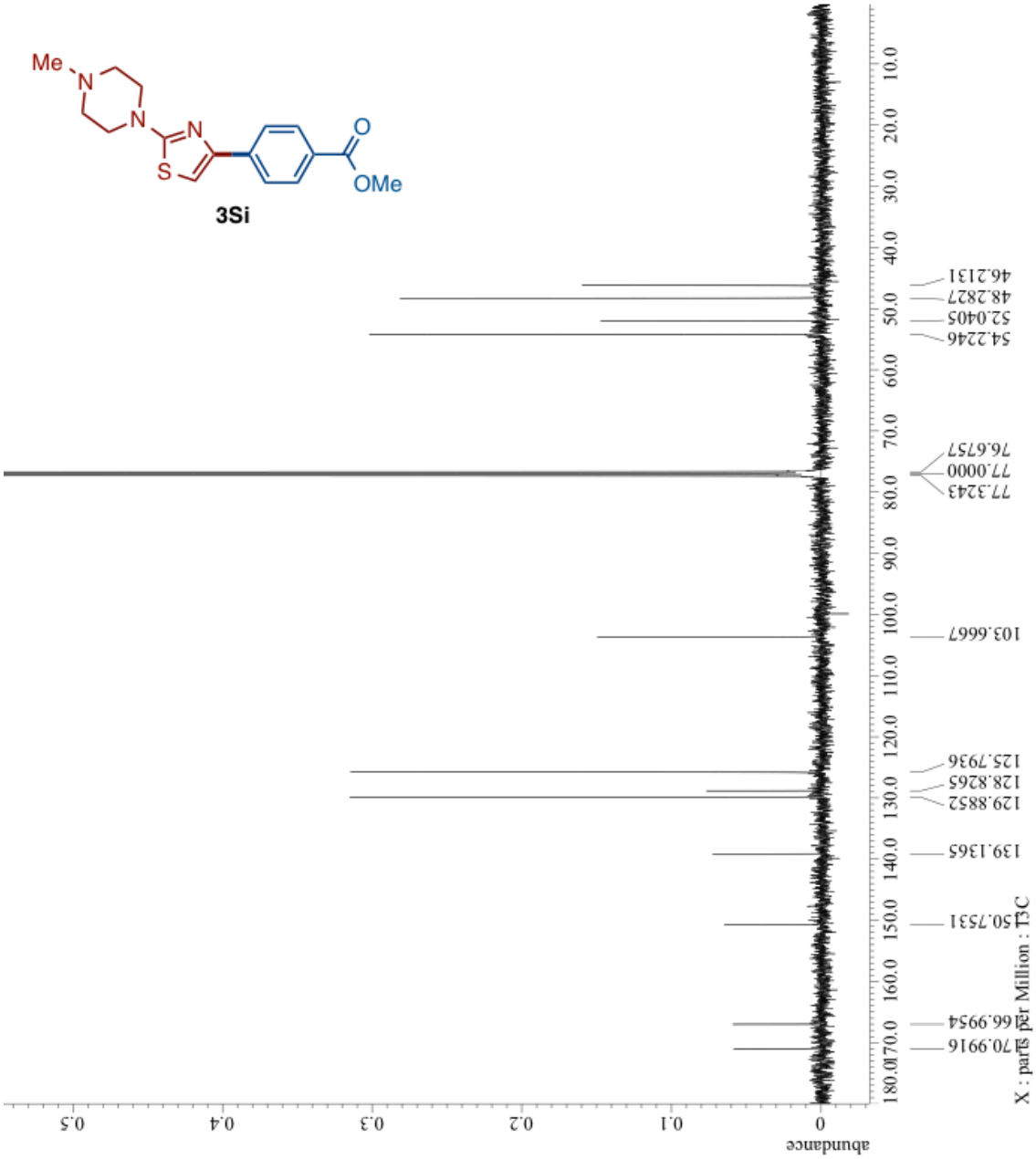
Supplementary Figure 65. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Sa



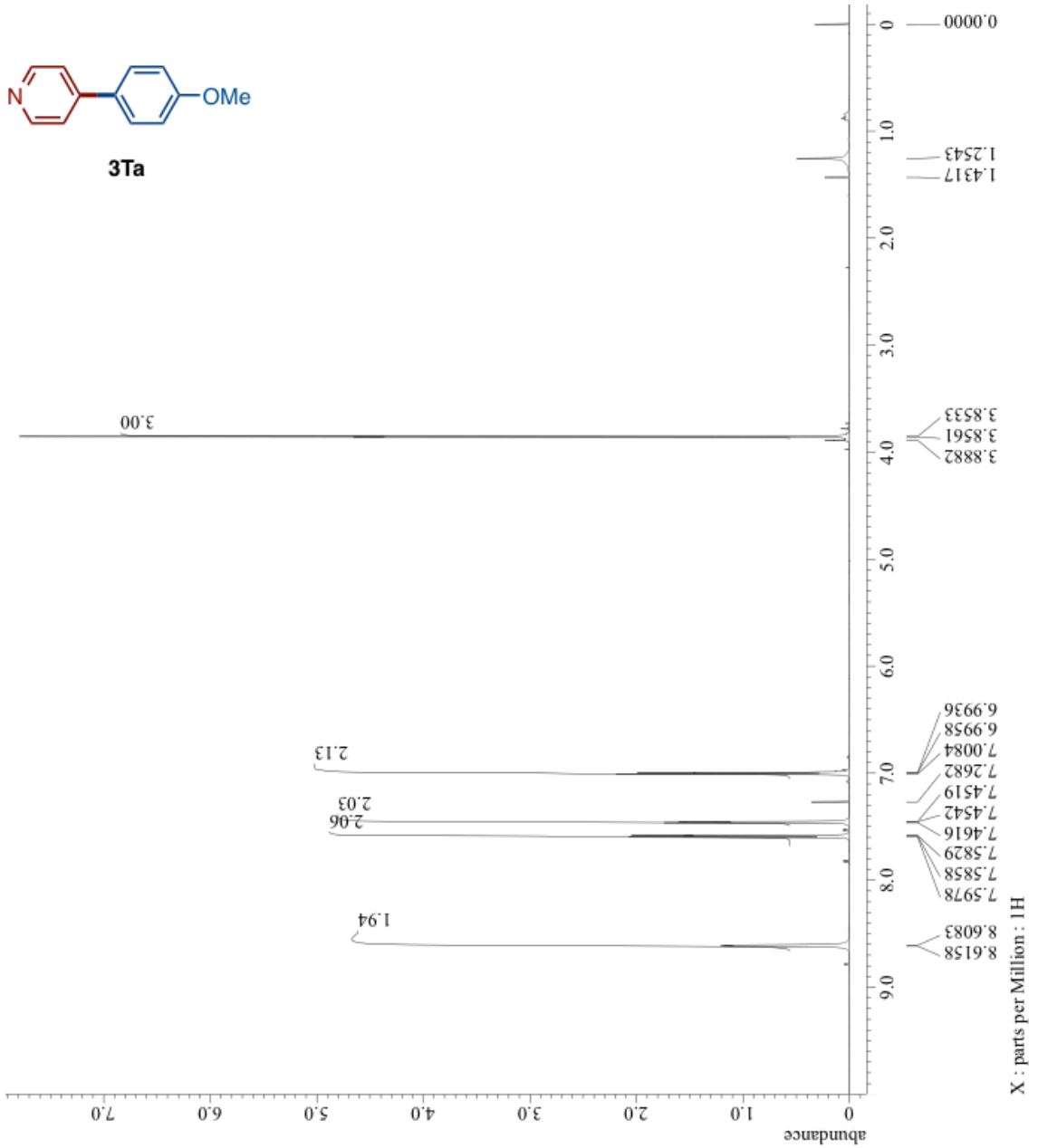
Supplementary Figure 66. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Sa



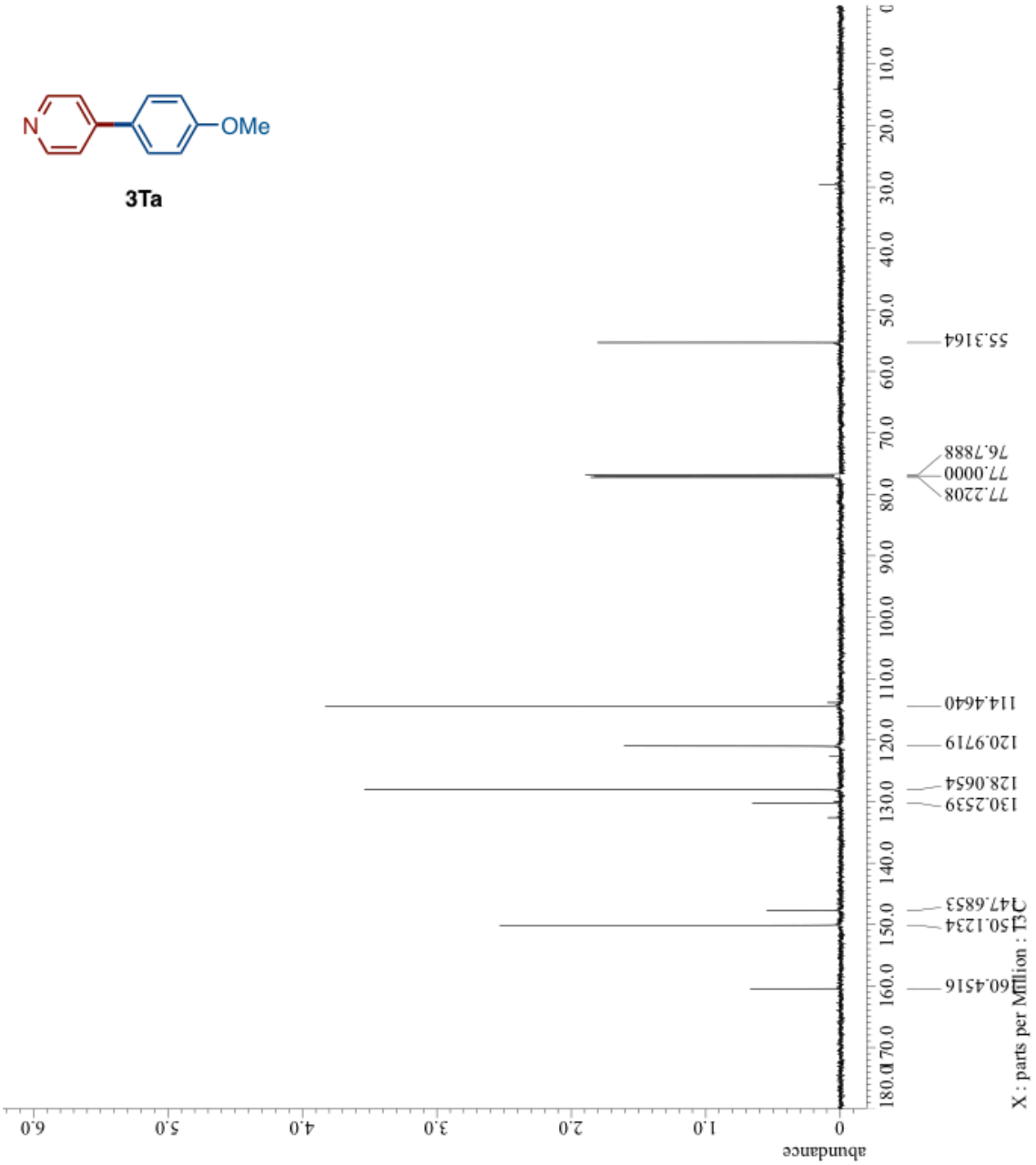
Supplementary Figure 67. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Si



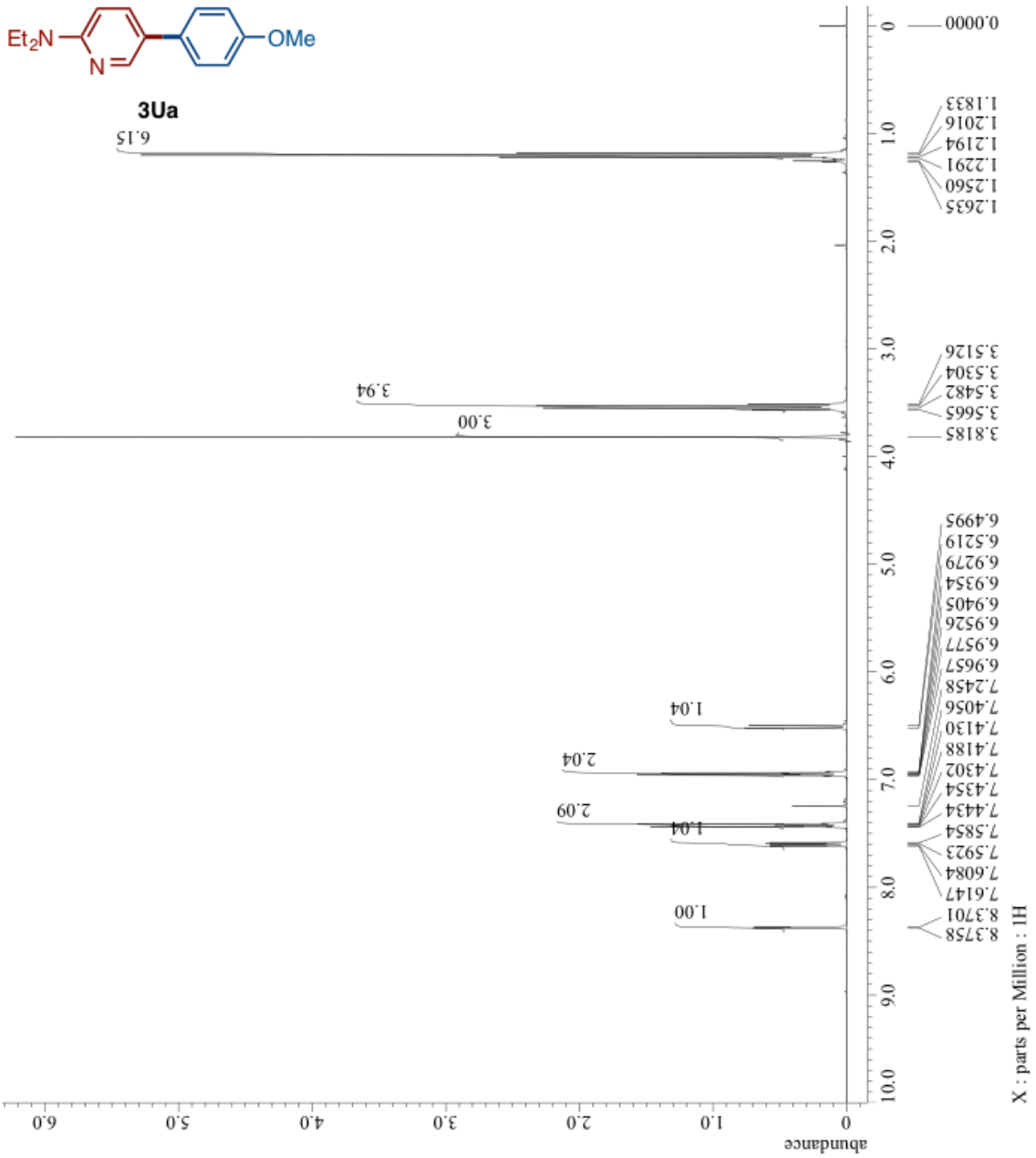
Supplementary Figure 68. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Si



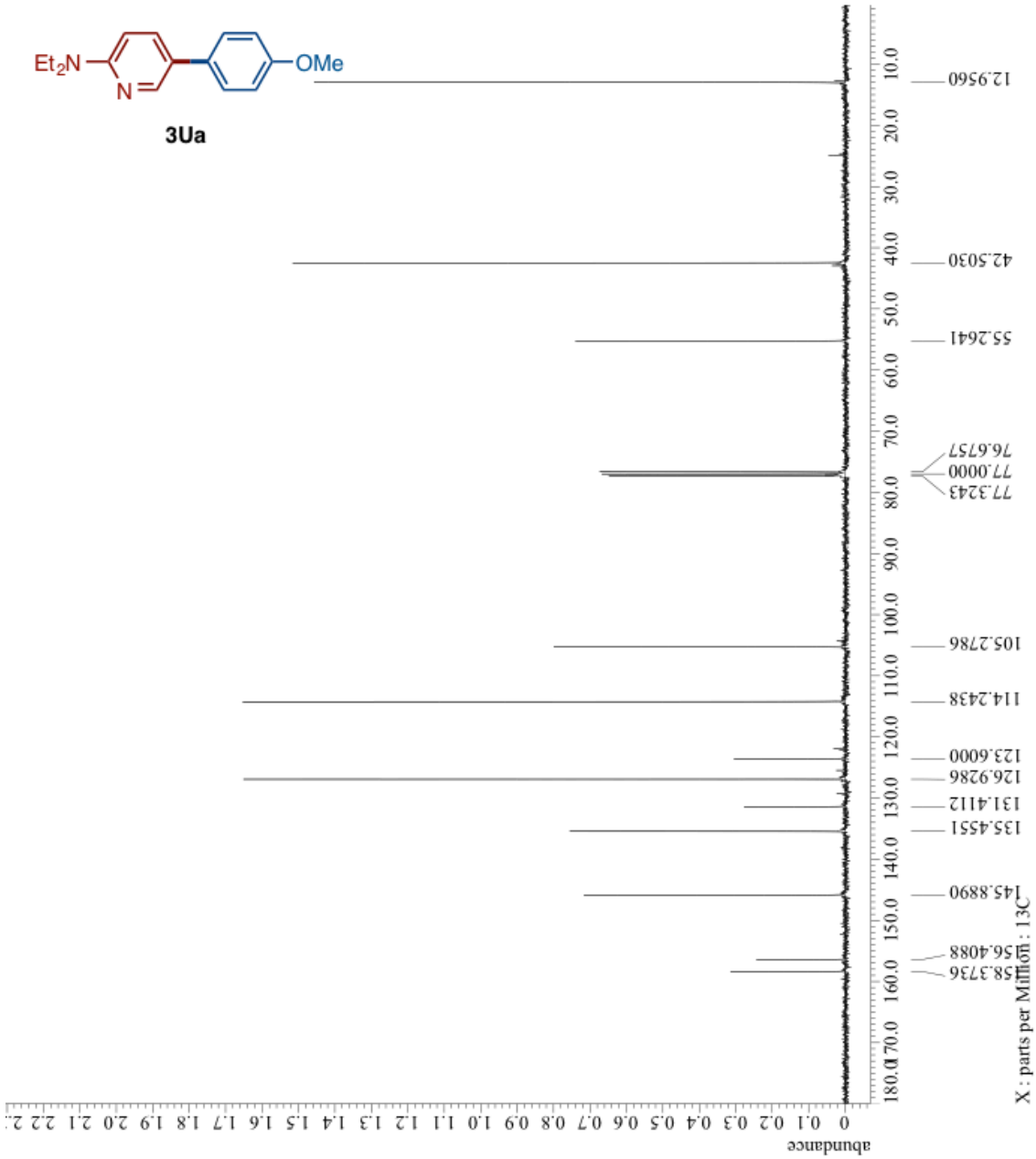
Supplementary Figure 69. ^{1}H NMR (600 MHz, $CDCl_3$) of 3Ta



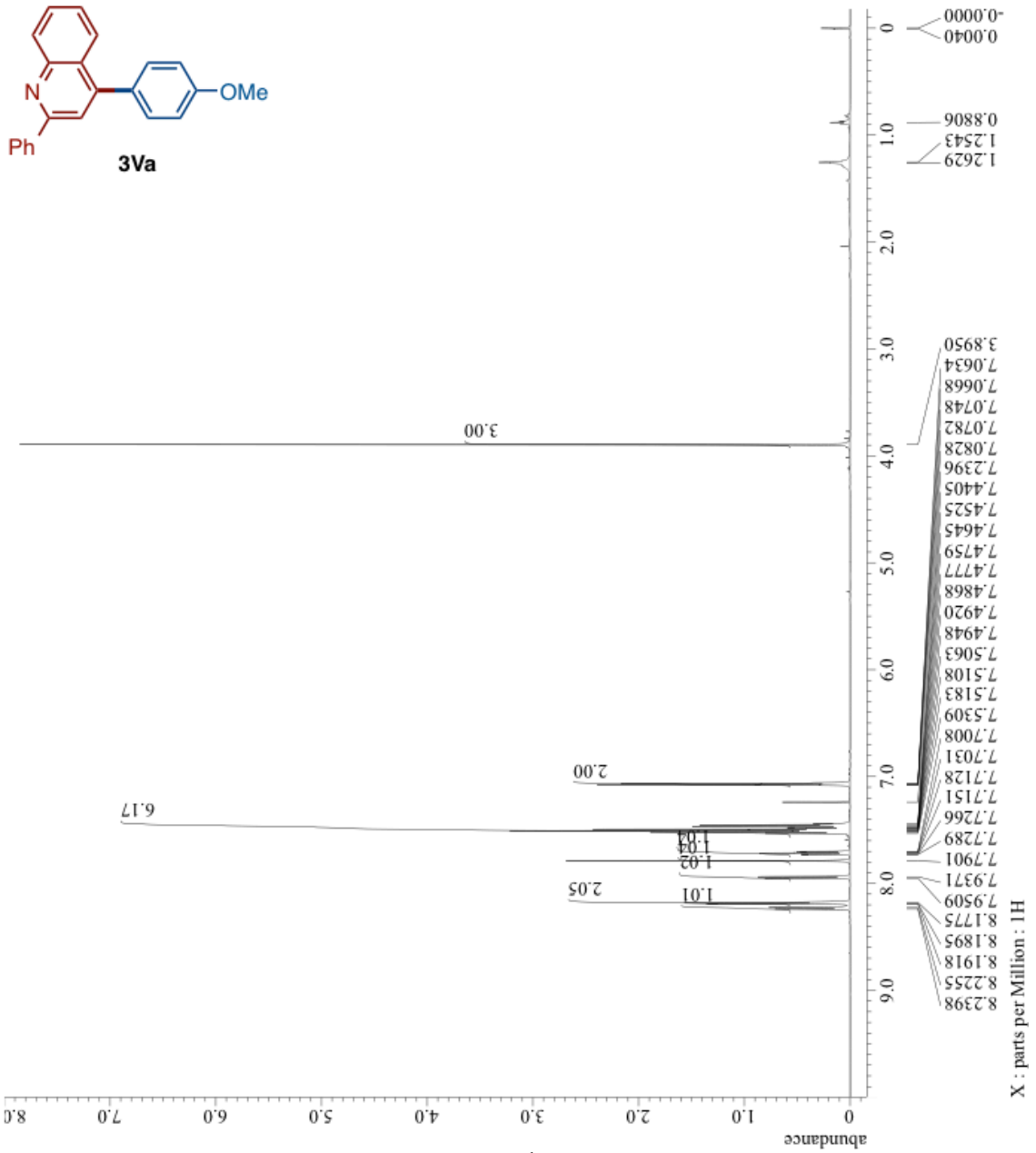
Supplementary Figure 70. ^{13}C NMR (150 MHz, $CDCl_3$) of 3Ta



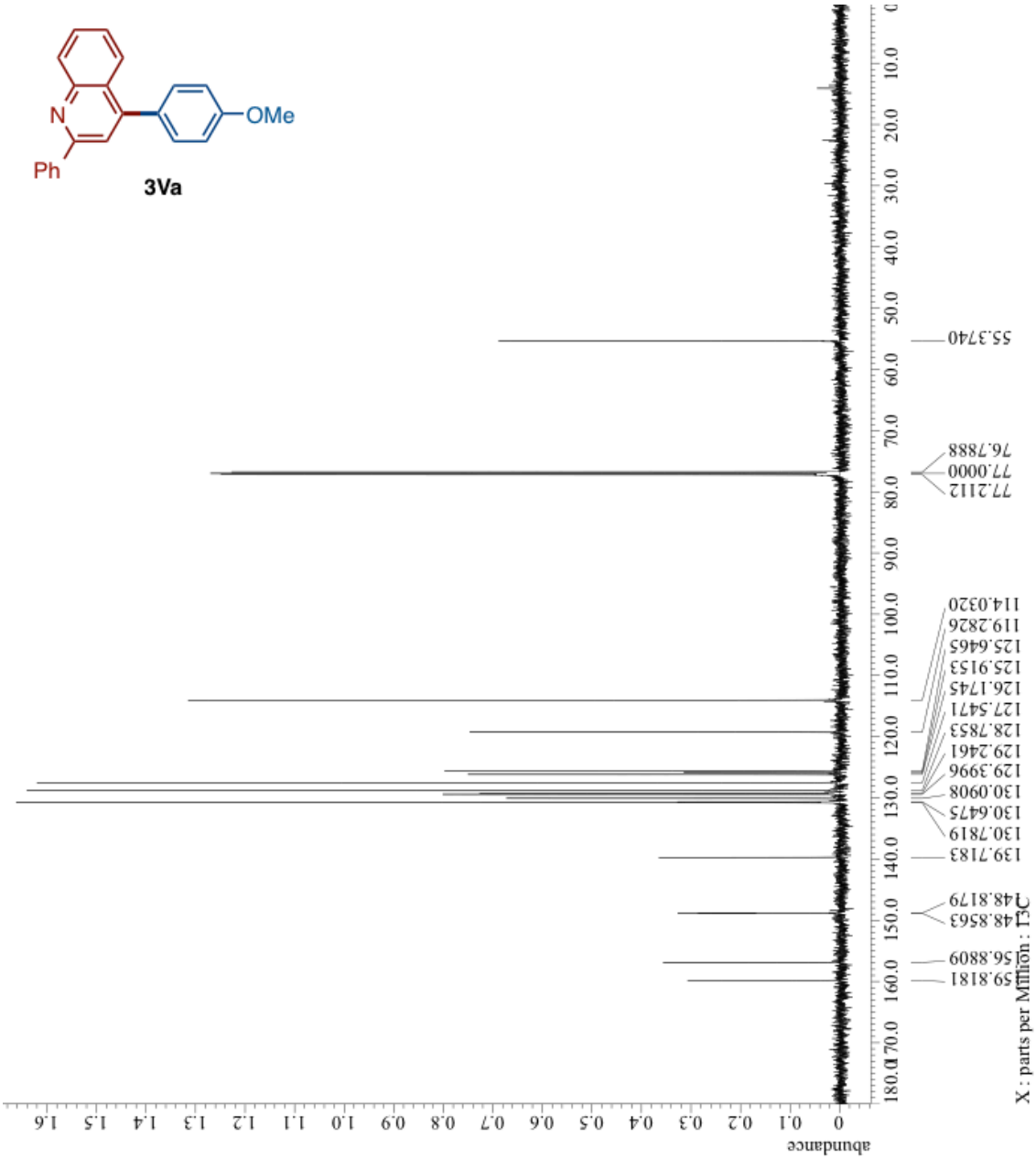
Supplementary Figure 71. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ua



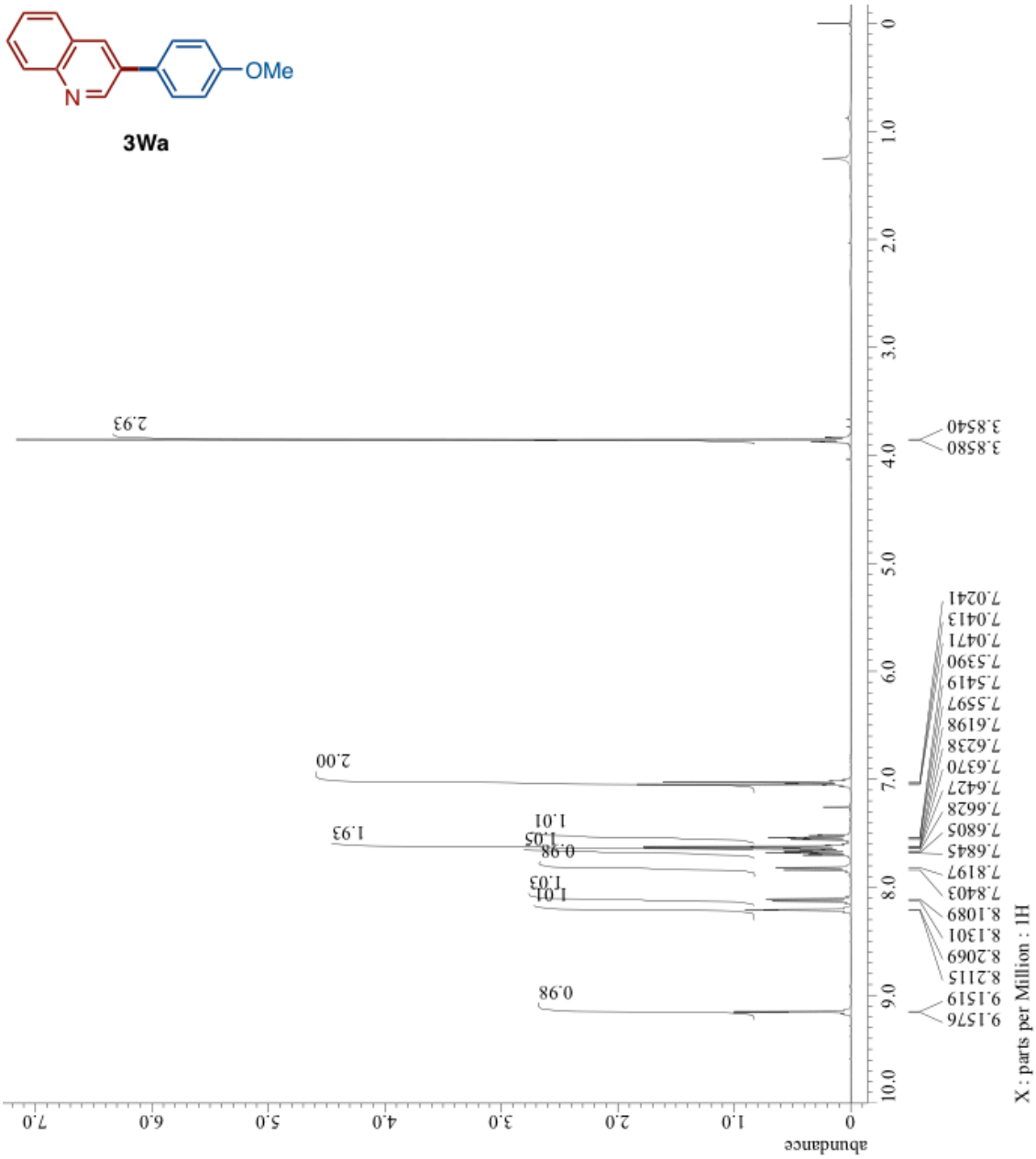
Supplementary Figure 72. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ua



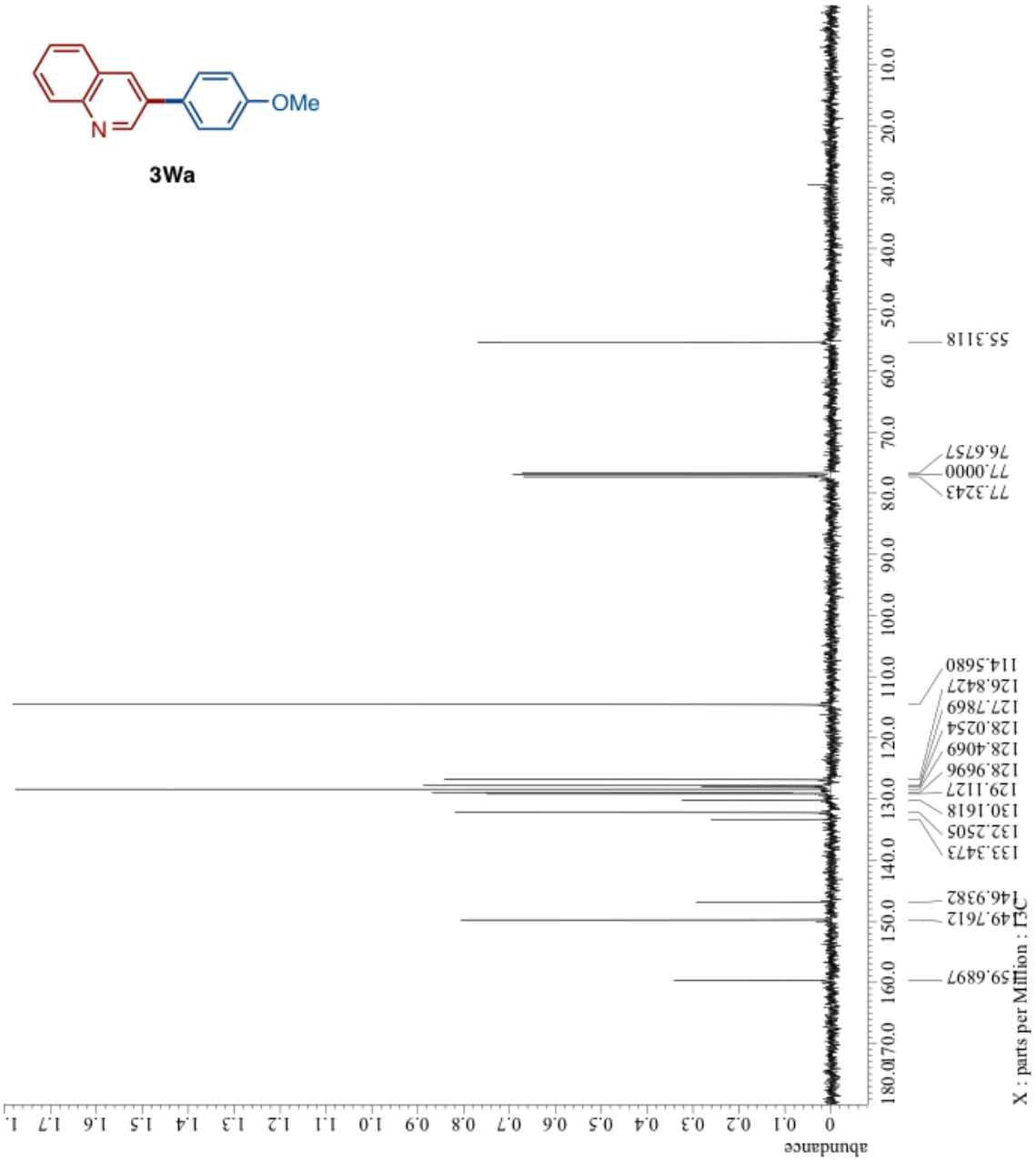
Supplementary Figure 73. ^{1}H NMR (600 MHz, $CDCl_3$) of 3Va



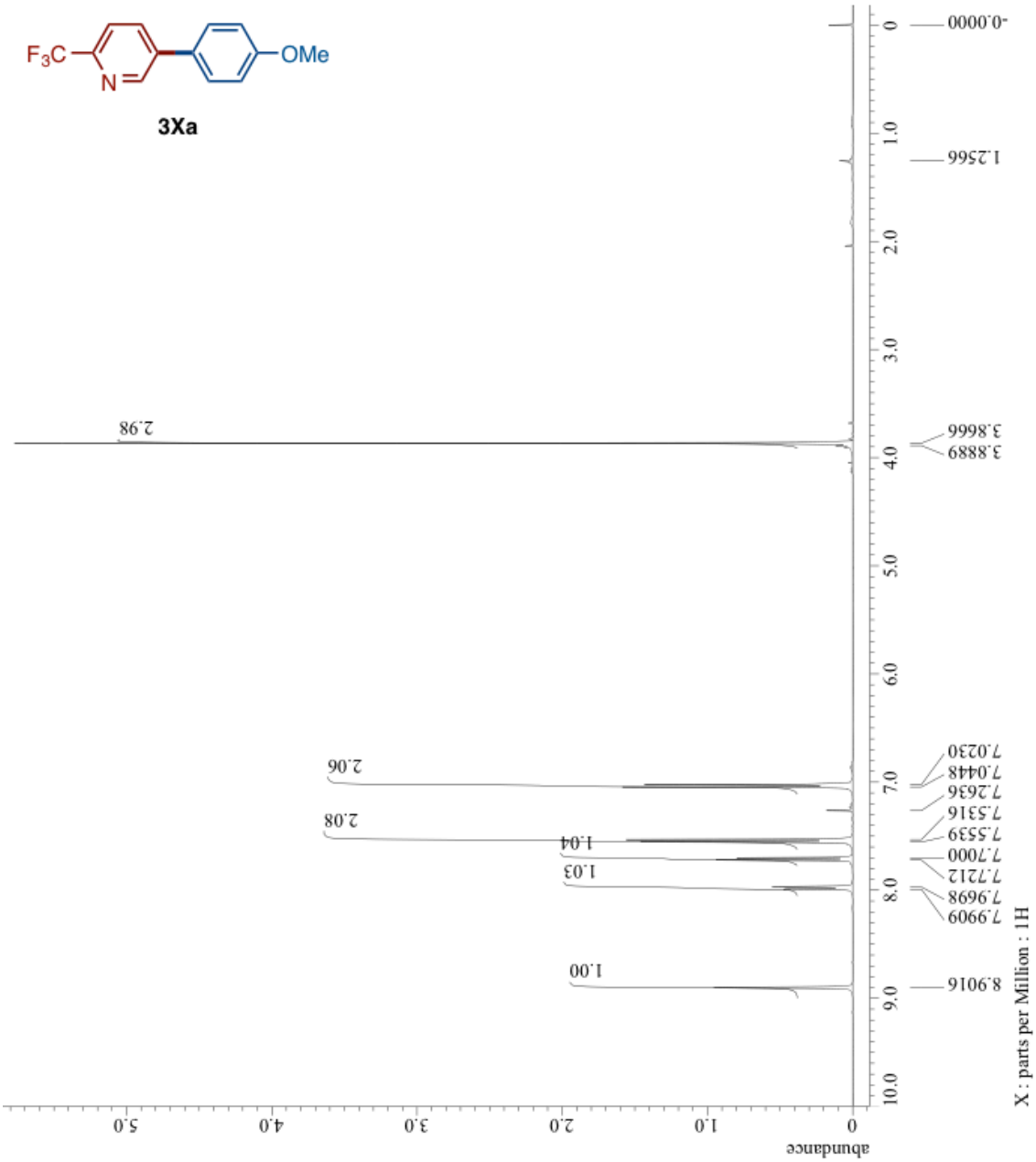
Supplementary Figure 74. ^{13}C NMR (150 MHz, $CDCl_3$) of 3Va



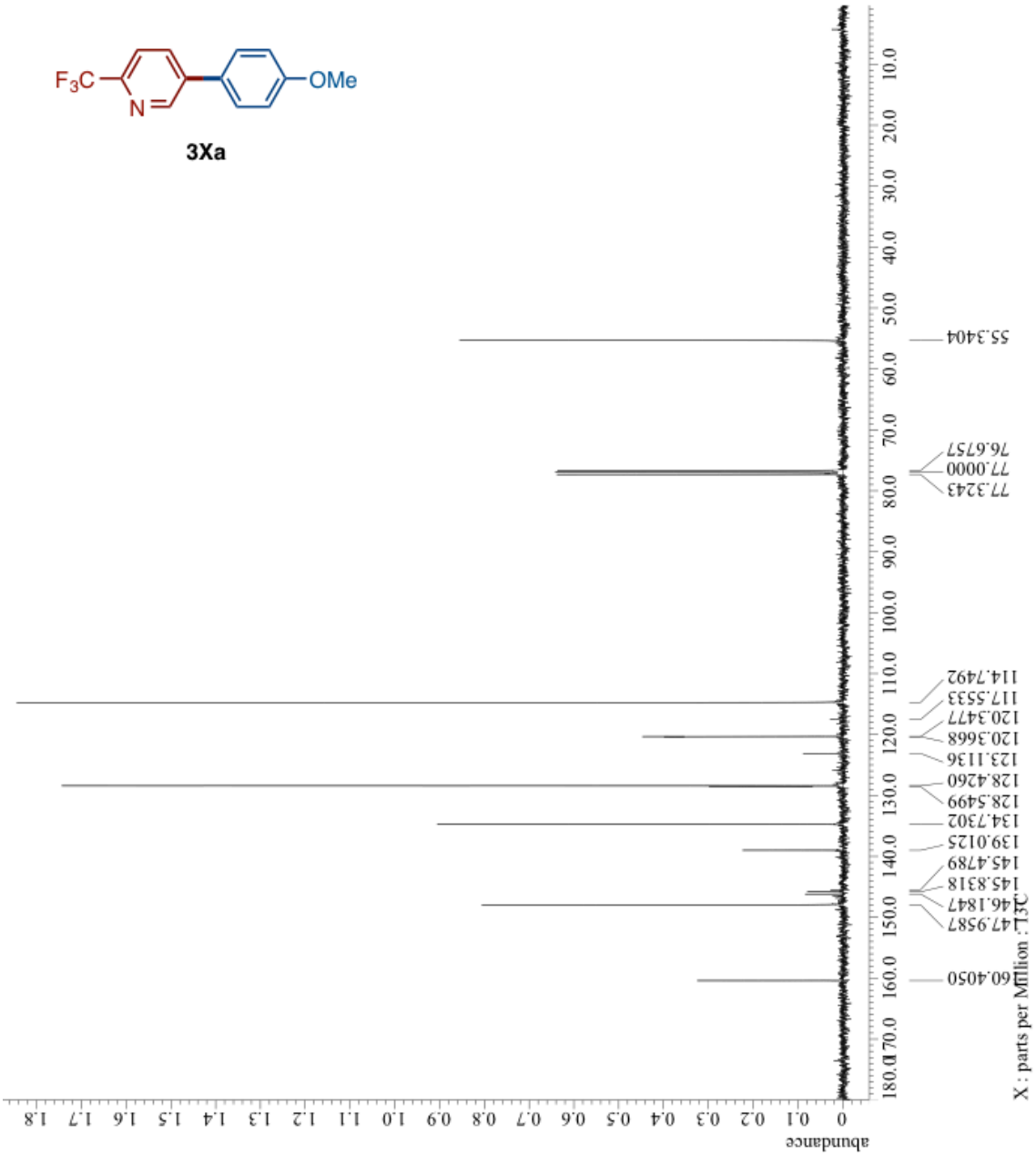
Supplementary Figure 75. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Wa



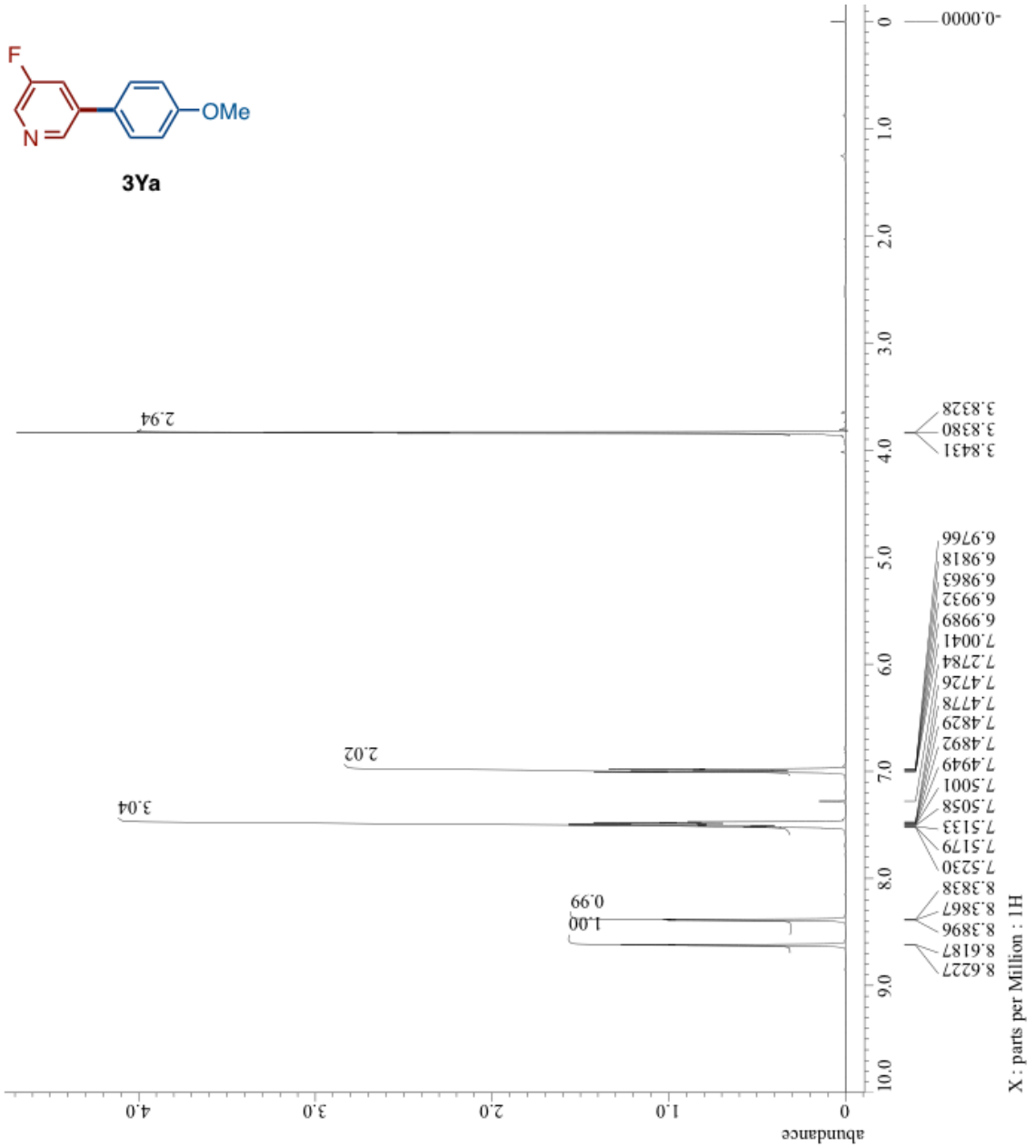
Supplementary Figure 76. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Wa



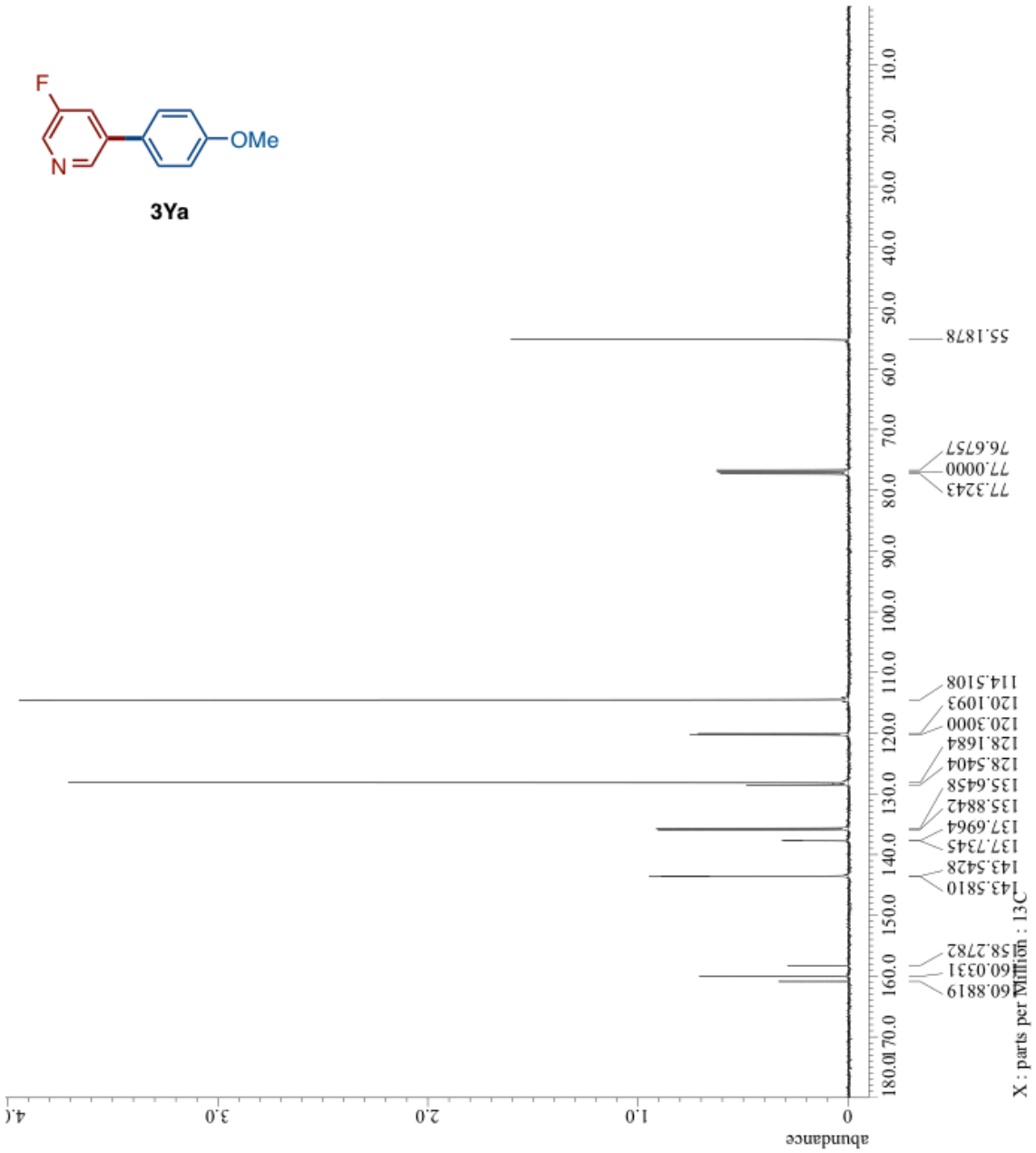
Supplementary Figure 77. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Xa



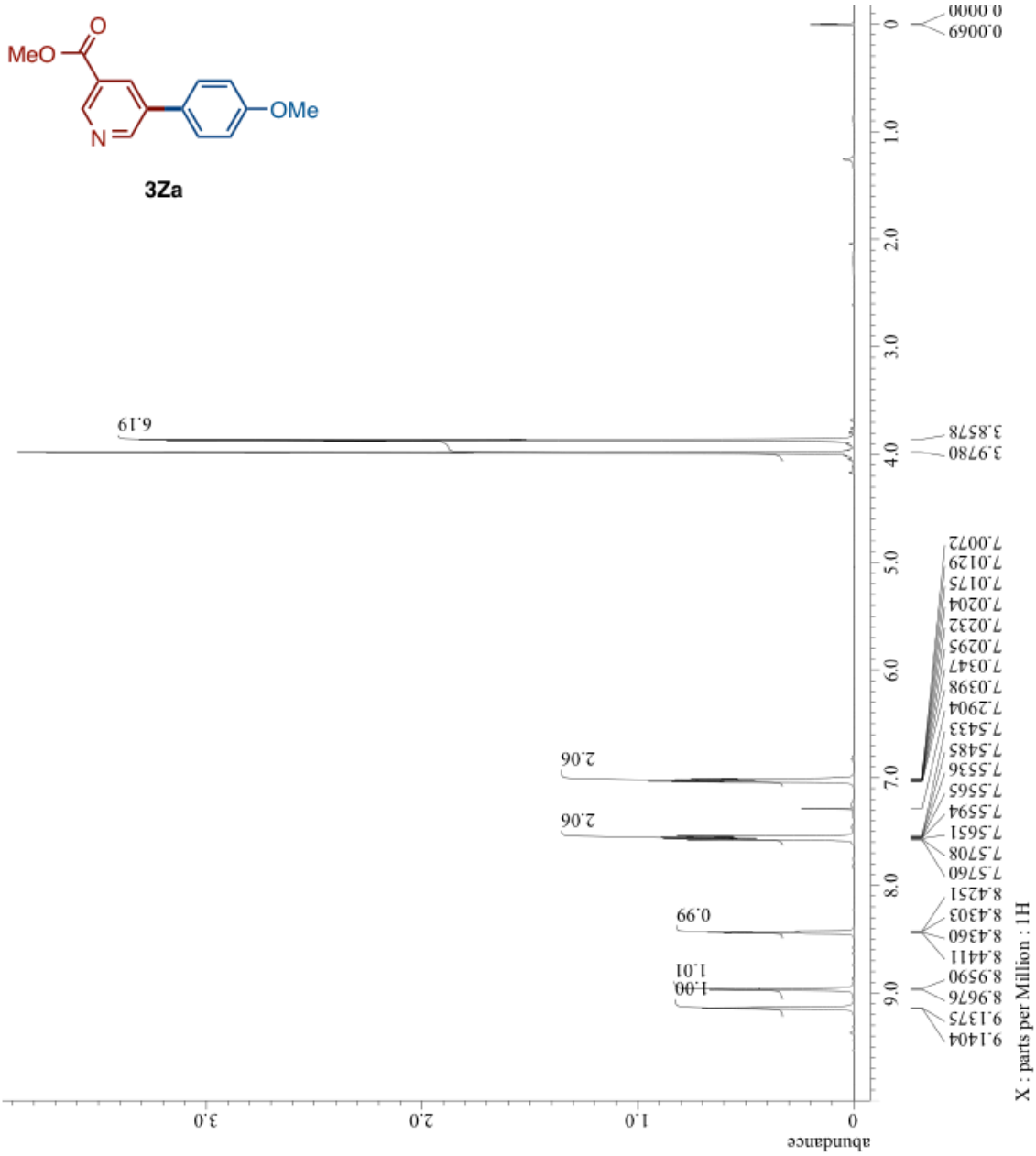
Supplementary Figure 78. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Xa



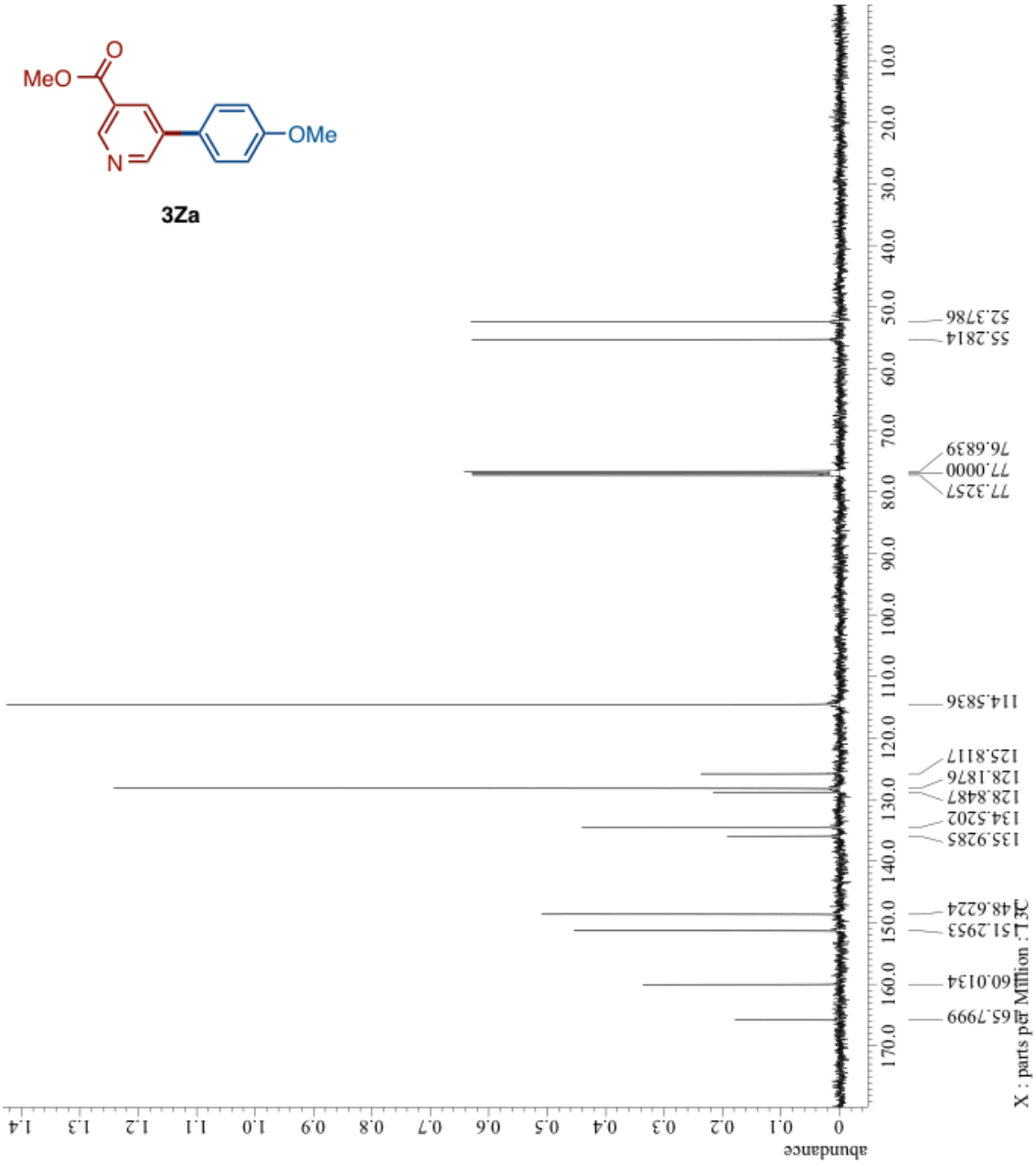
Supplementary Figure 79. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ya



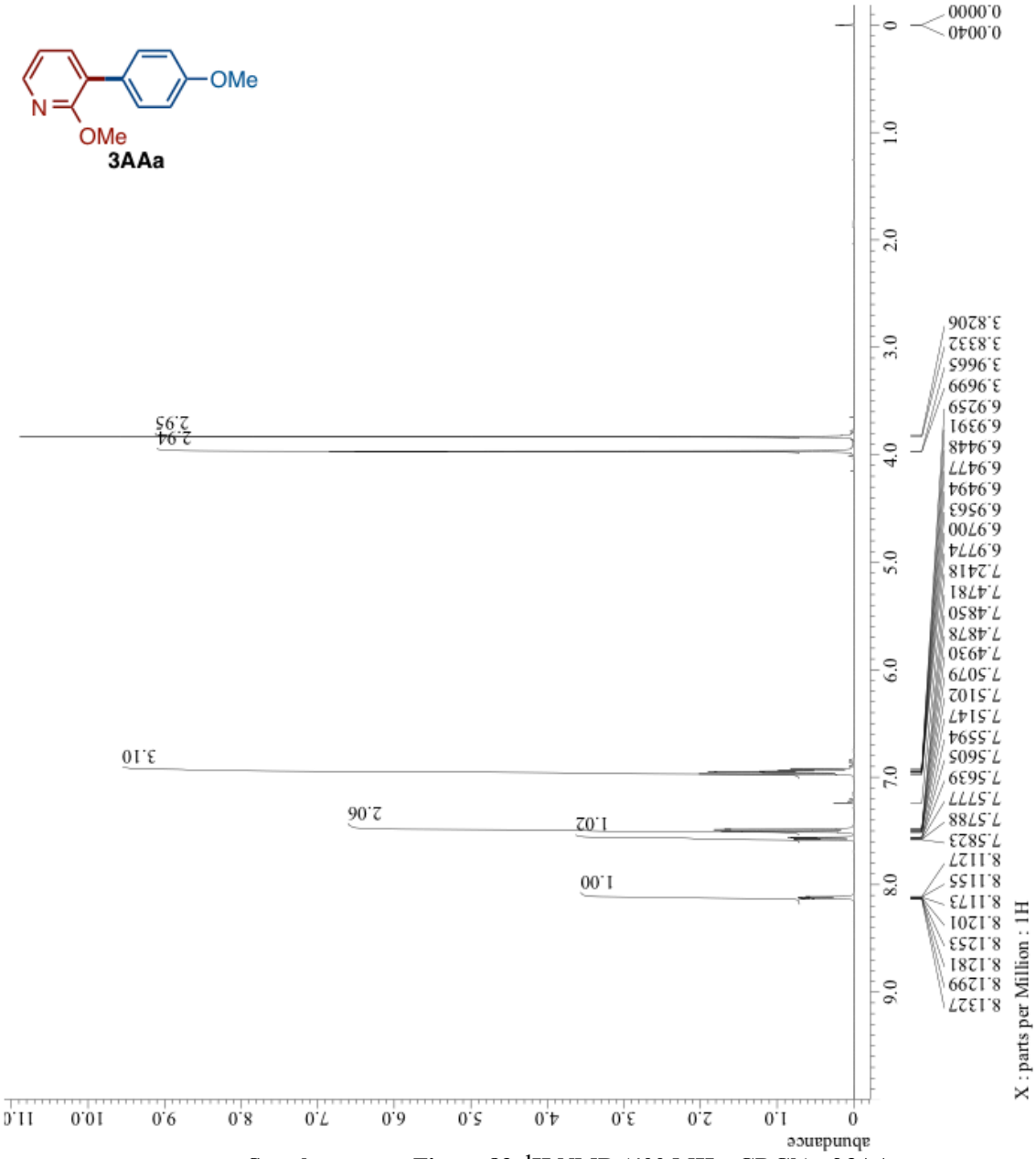
Supplementary Figure 80. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ya



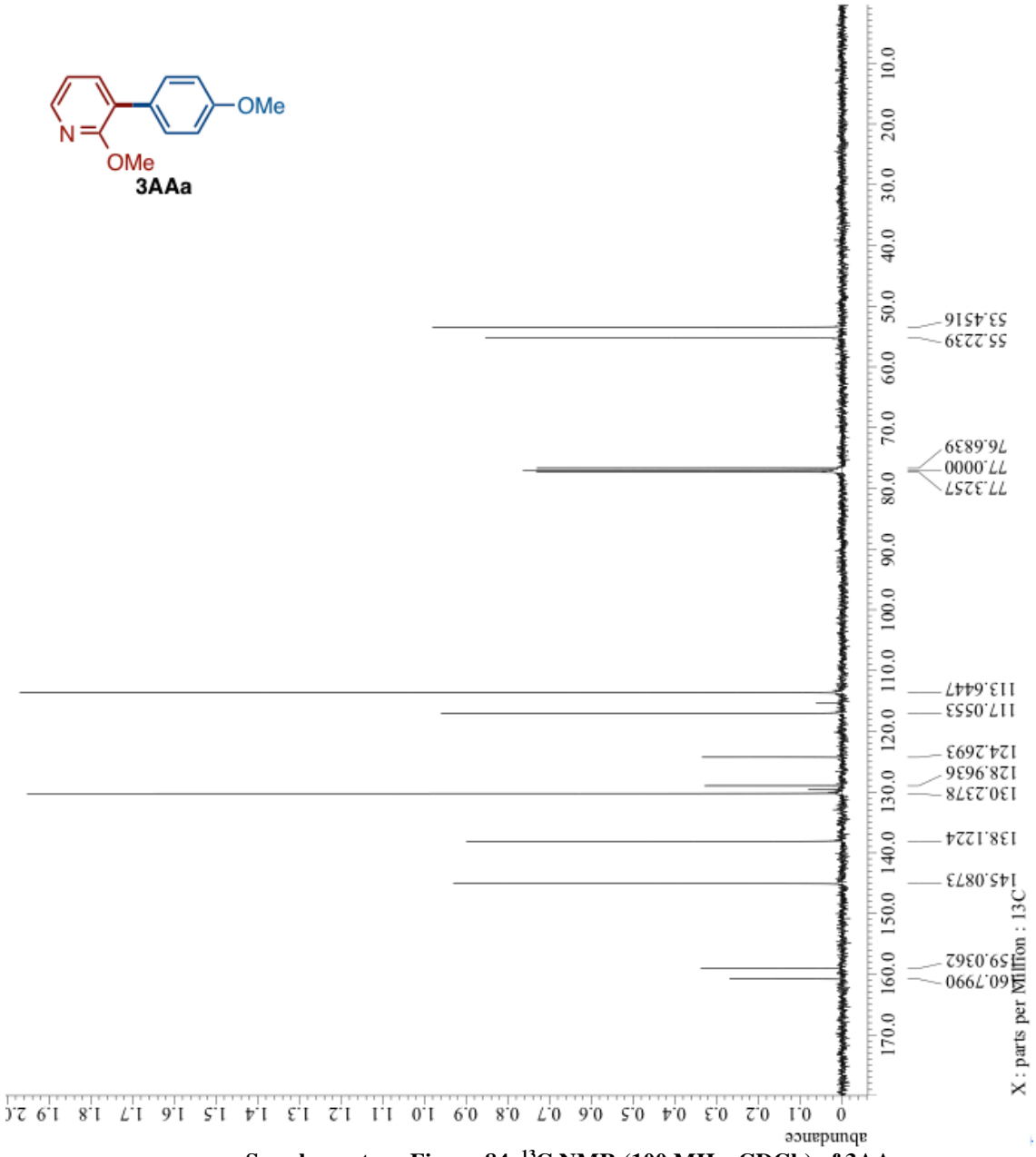
Supplementary Figure 81. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Za



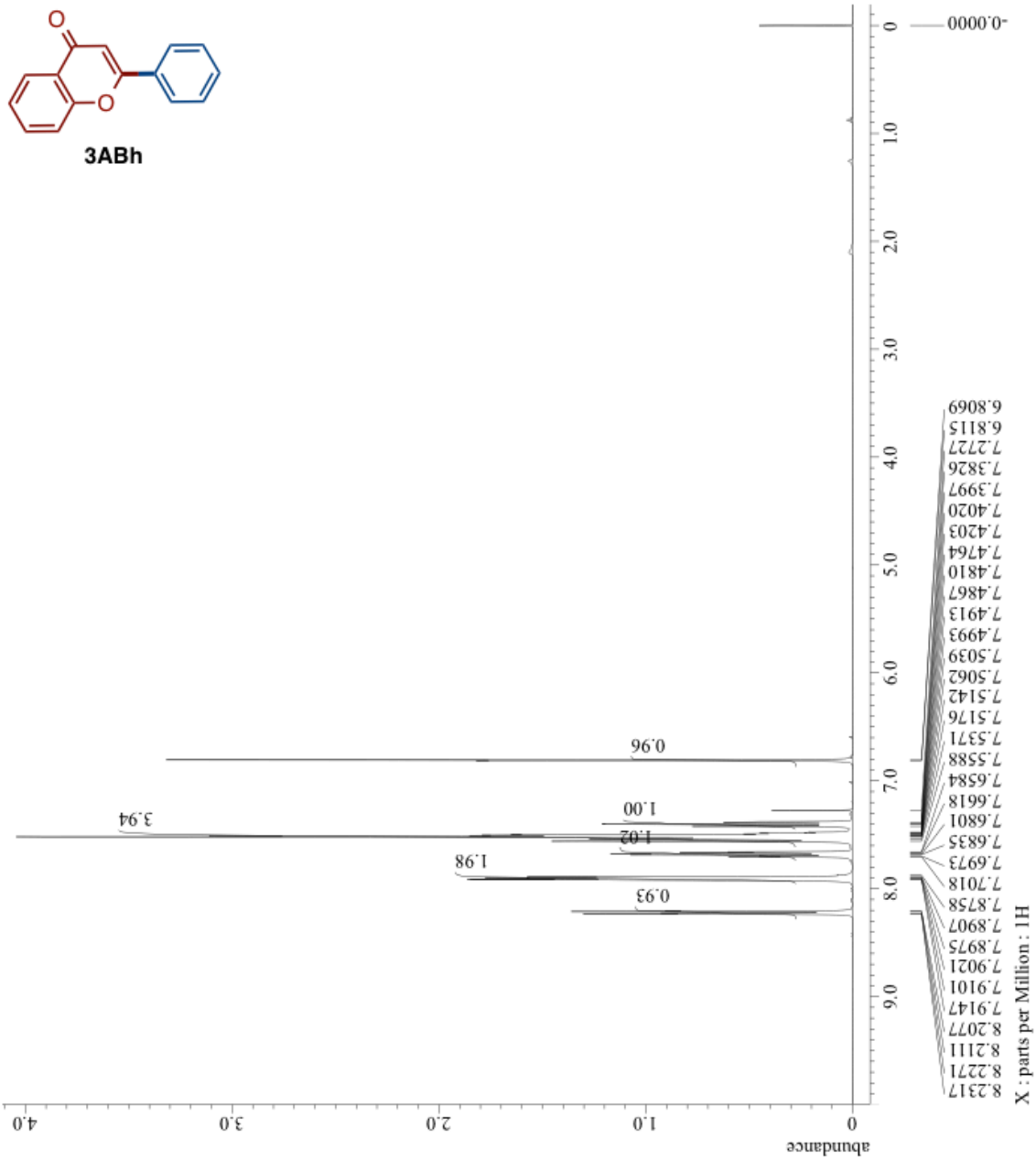
Supplementary Figure 82. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Za



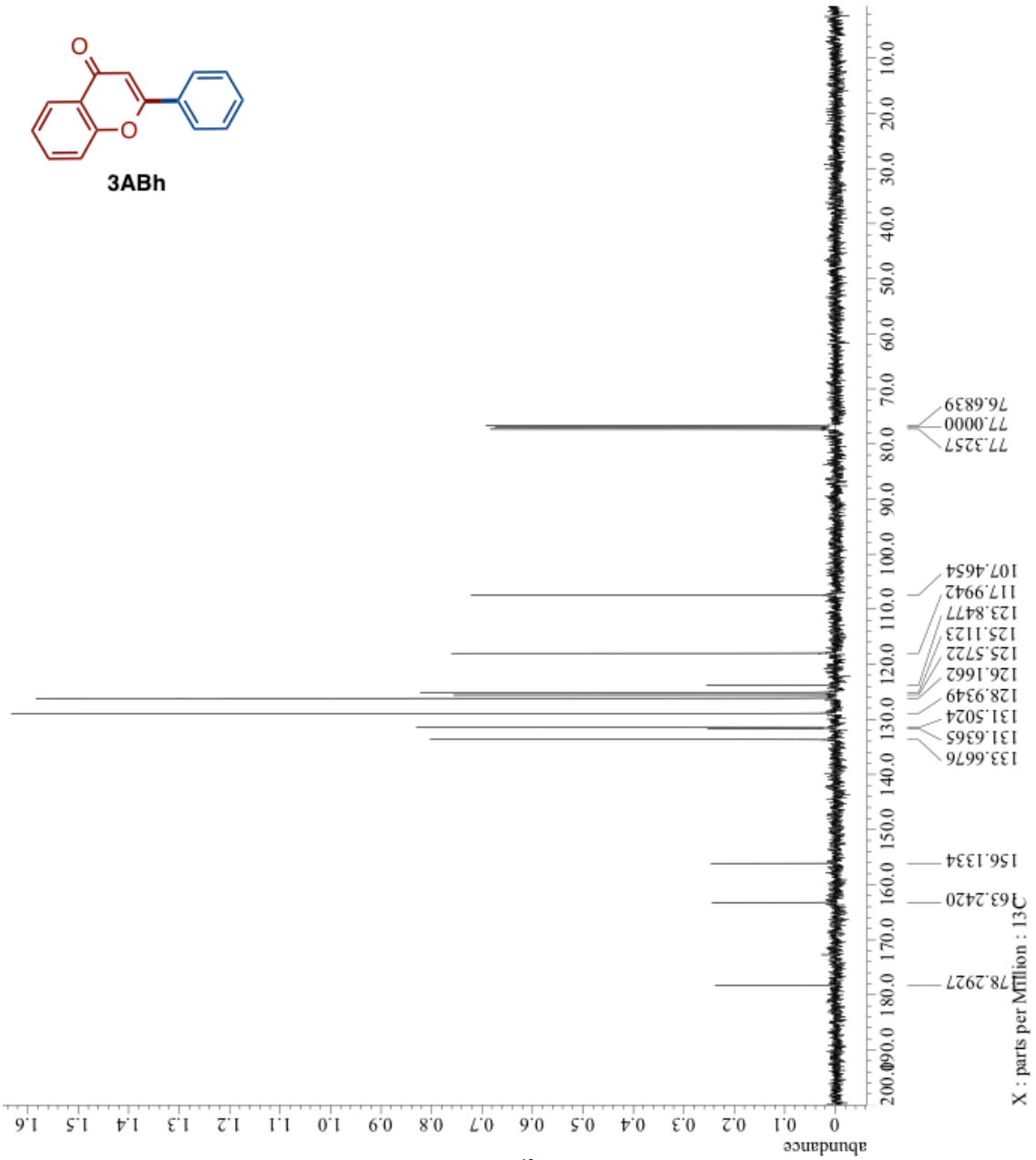
Supplementary Figure 83. ^{1}H NMR (400 MHz, $CDCl_3$) of 3AAa



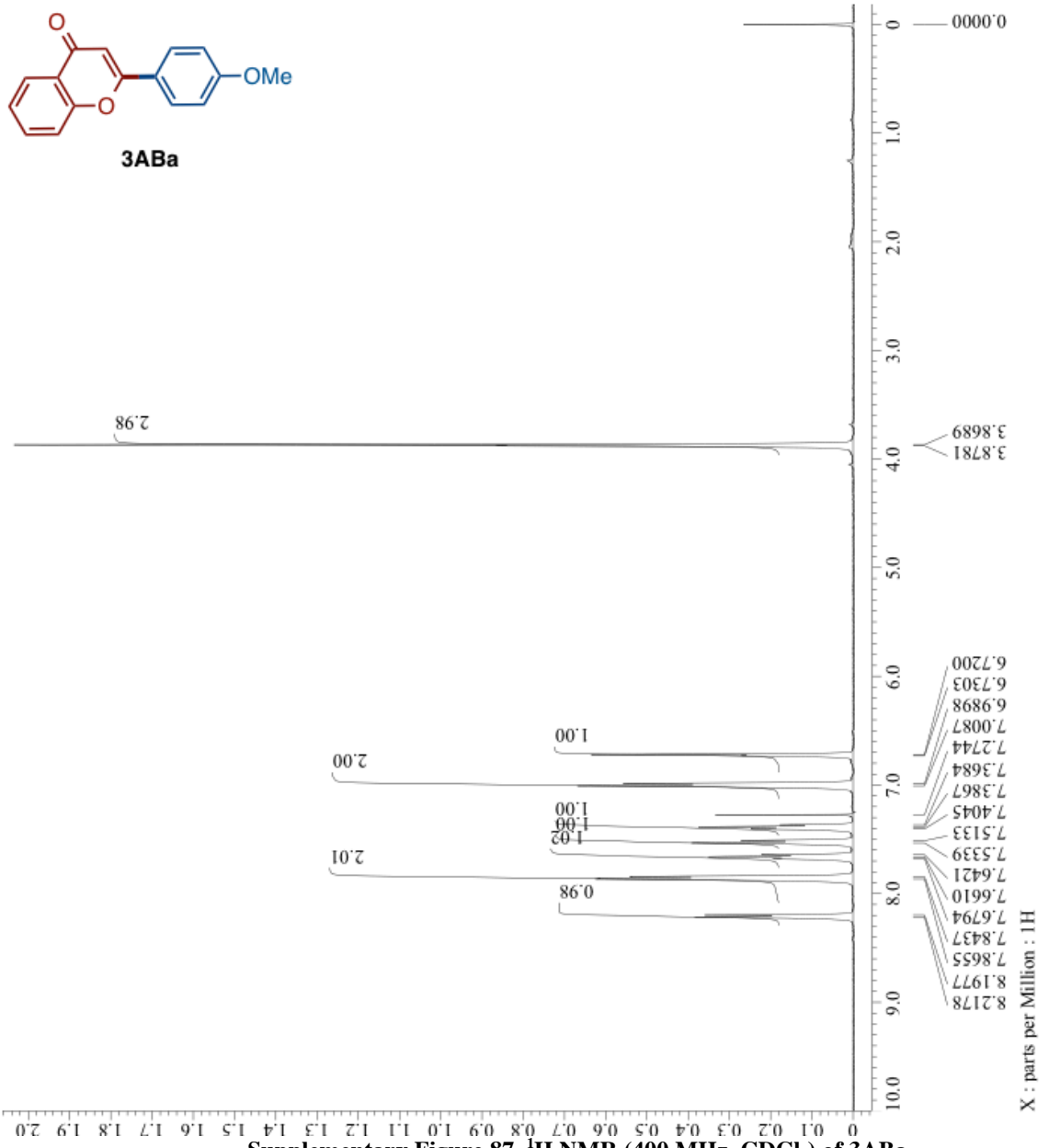
Supplementary Figure 84. ^{13}C **NMR (100 MHz, $CDCl_3$) of 3AAa**



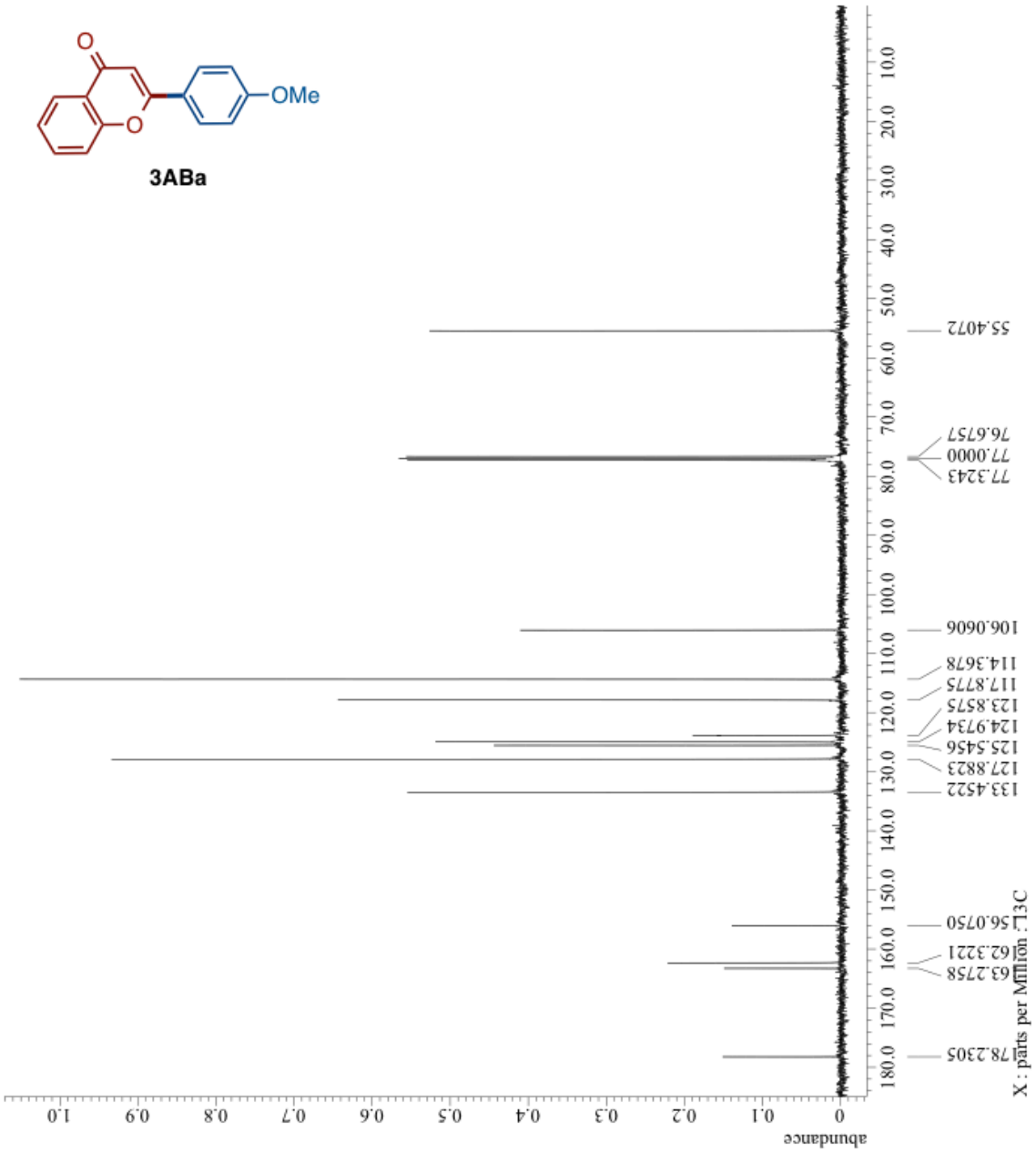
Supplementary Figure 85. ^{1}H NMR (400 MHz, $CDCl_3$) of 3ABh



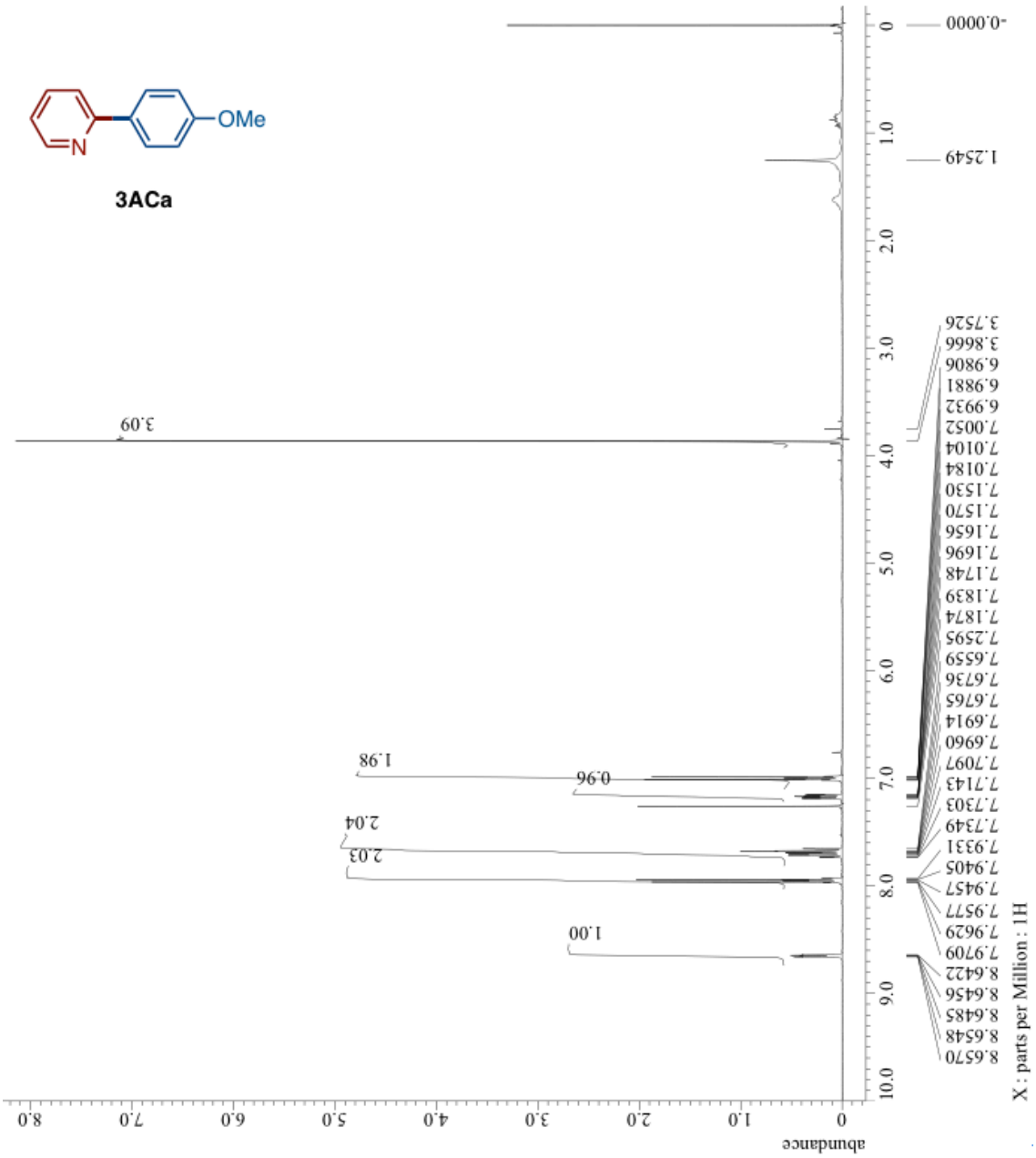
Supplementary Figure 86. ^{13}C NMR (100 MHz, $CDCl_3$) of 3ABh



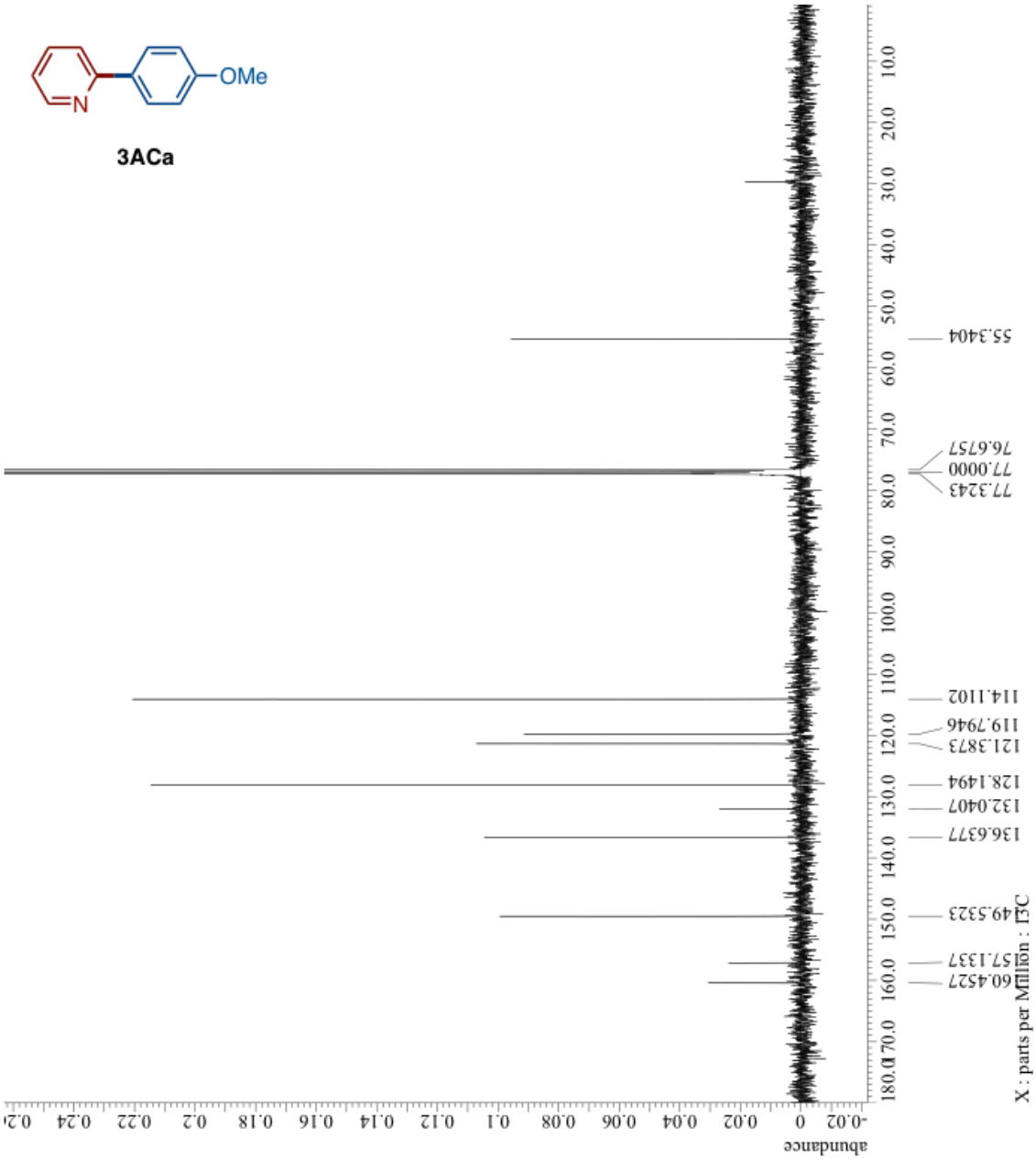
Supplementary Figure 87. ^{1}H NMR (400 MHz, $CDCl_3$) of 3ABa



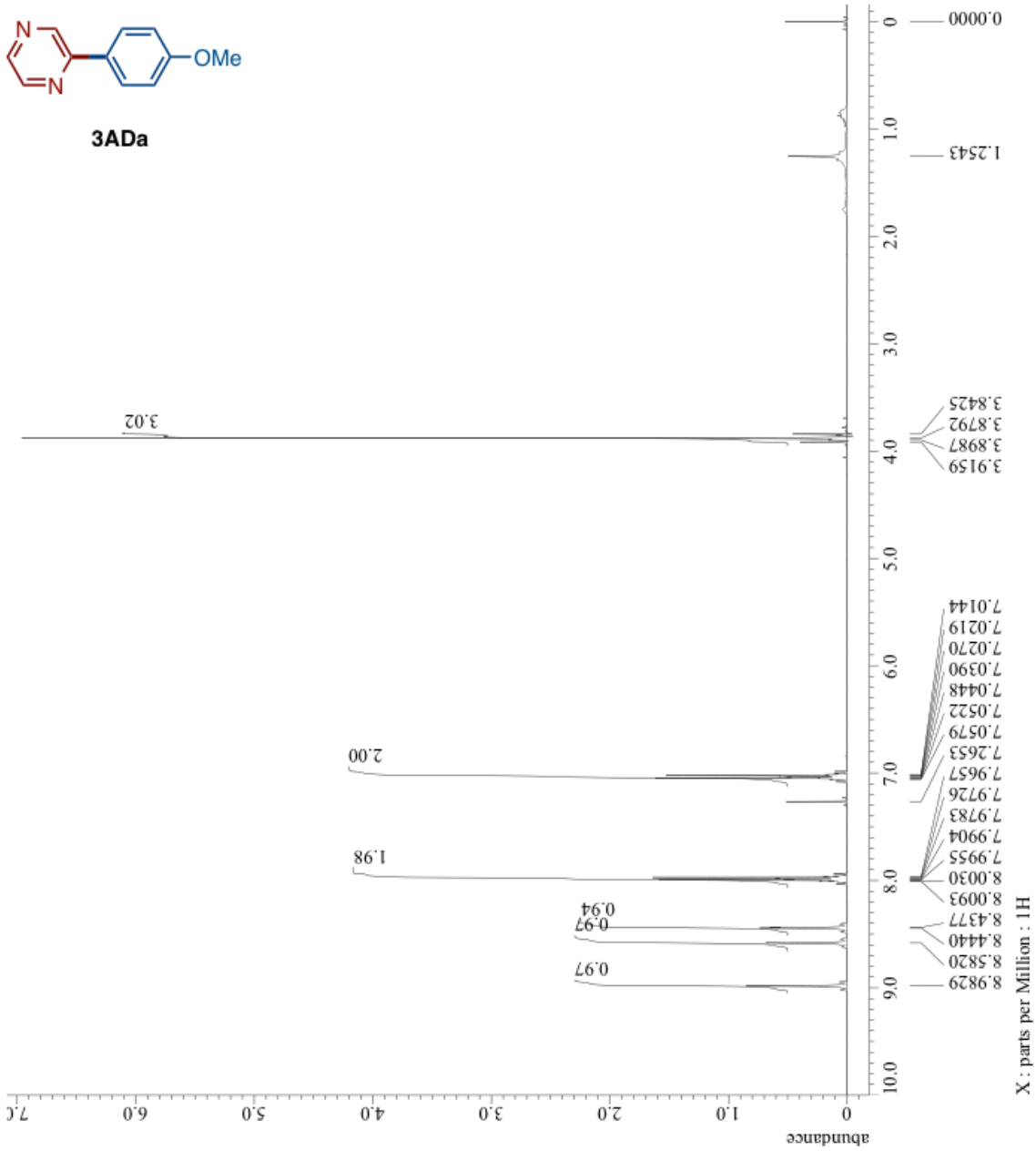
Supplementary Figure 88. ^{13}C NMR (100 MHz, $CDCl_3$) of 3ABa



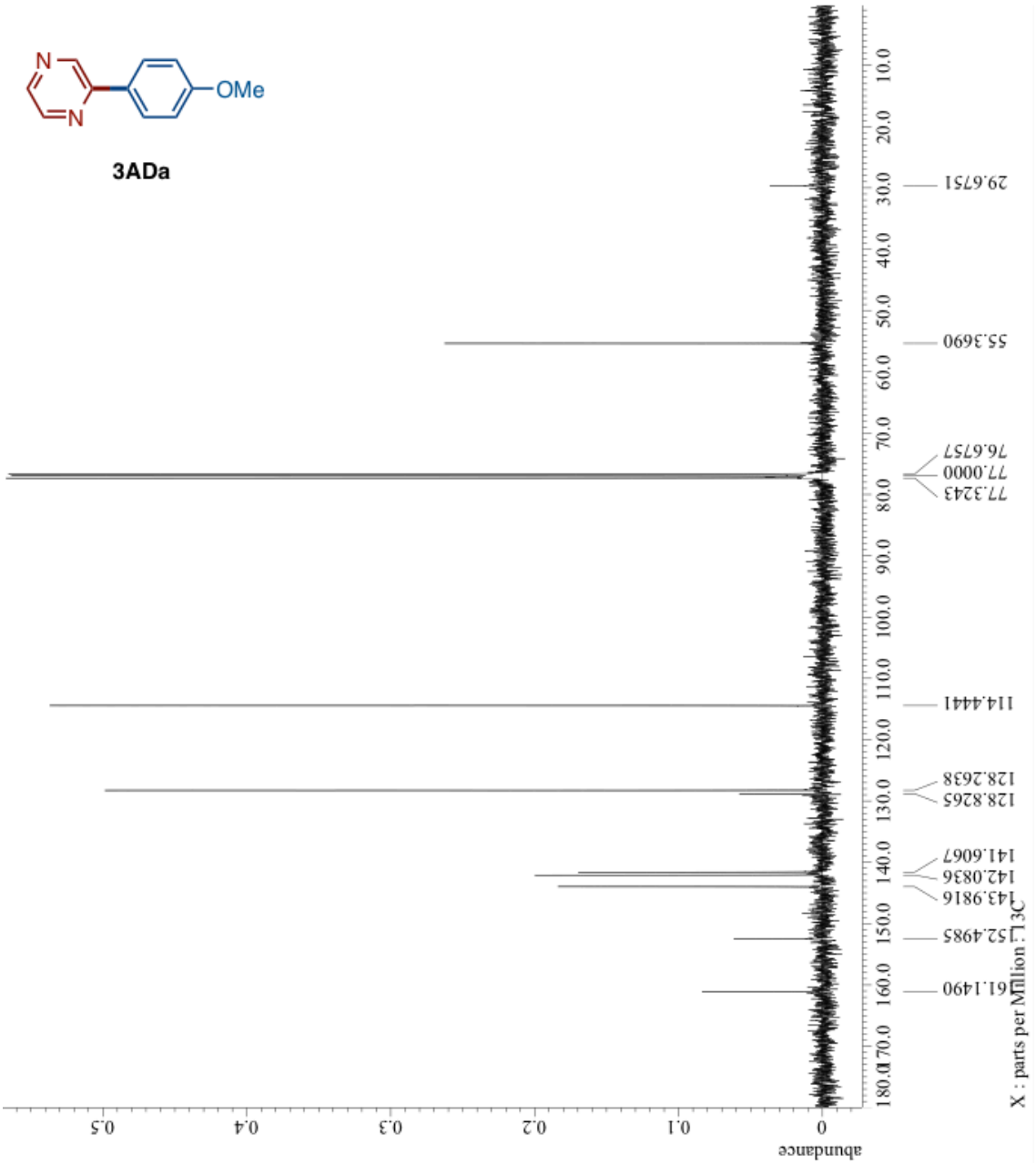
Supplementary Figure 89. ^{1}H NMR (400 MHz, $CDCl_3$) of 3ACa



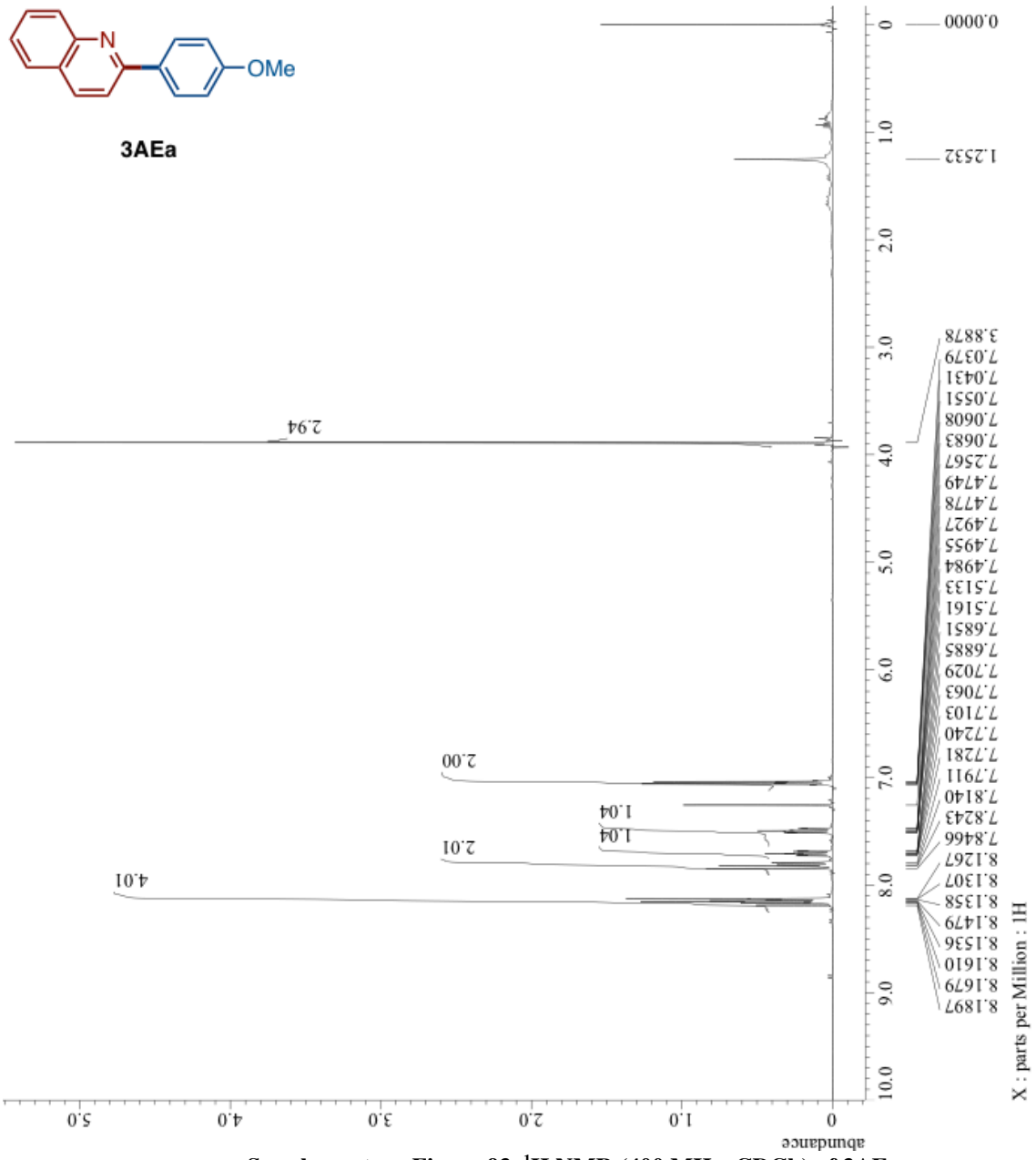
Supplementary Figure 90. ^{13}C NMR (100 MHz, $CDCl_3$) of 3ACa



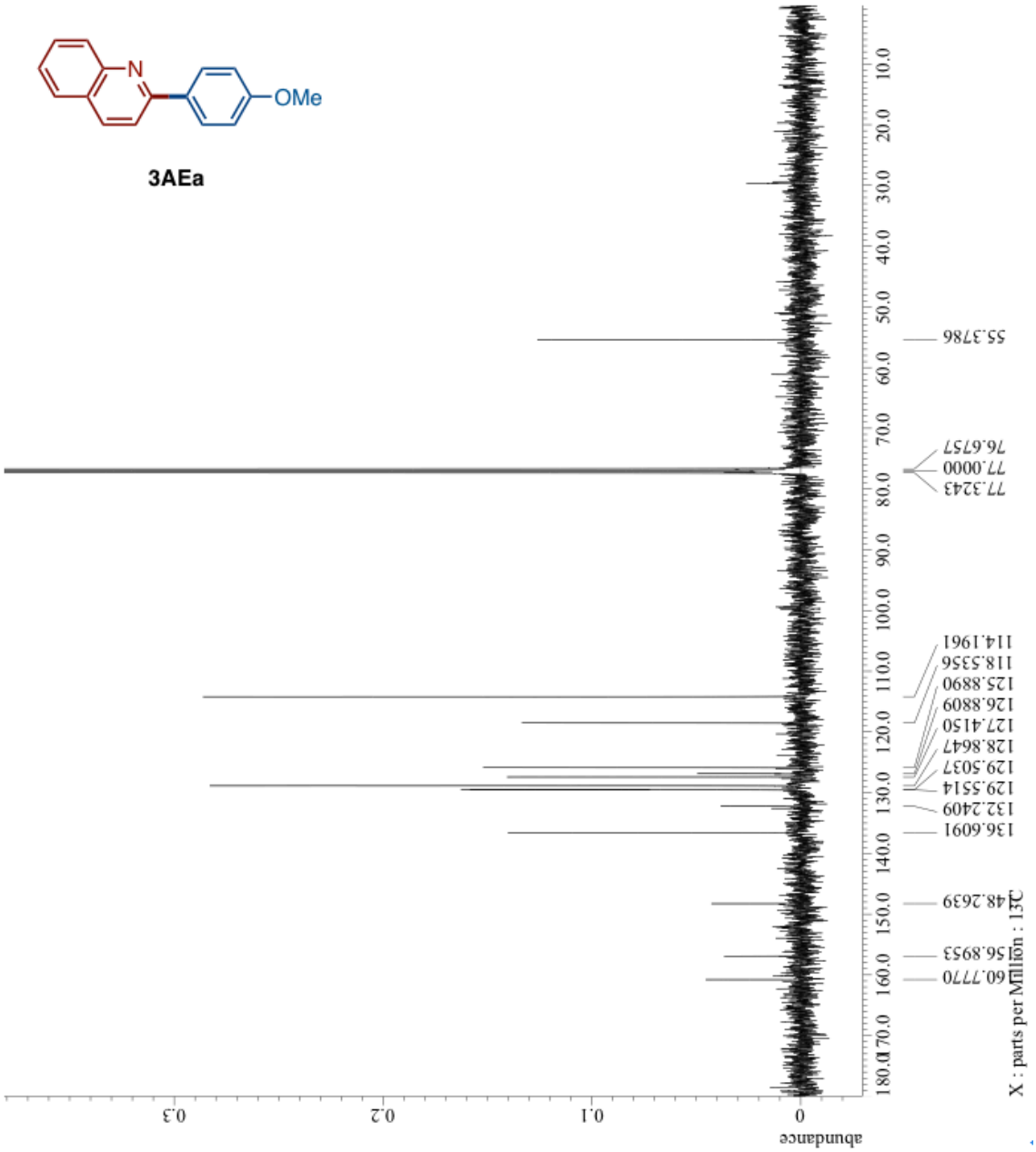
Supplementary Figure 91. ^{1}H NMR (400 MHz, $CDCl_3$) of 3ADa



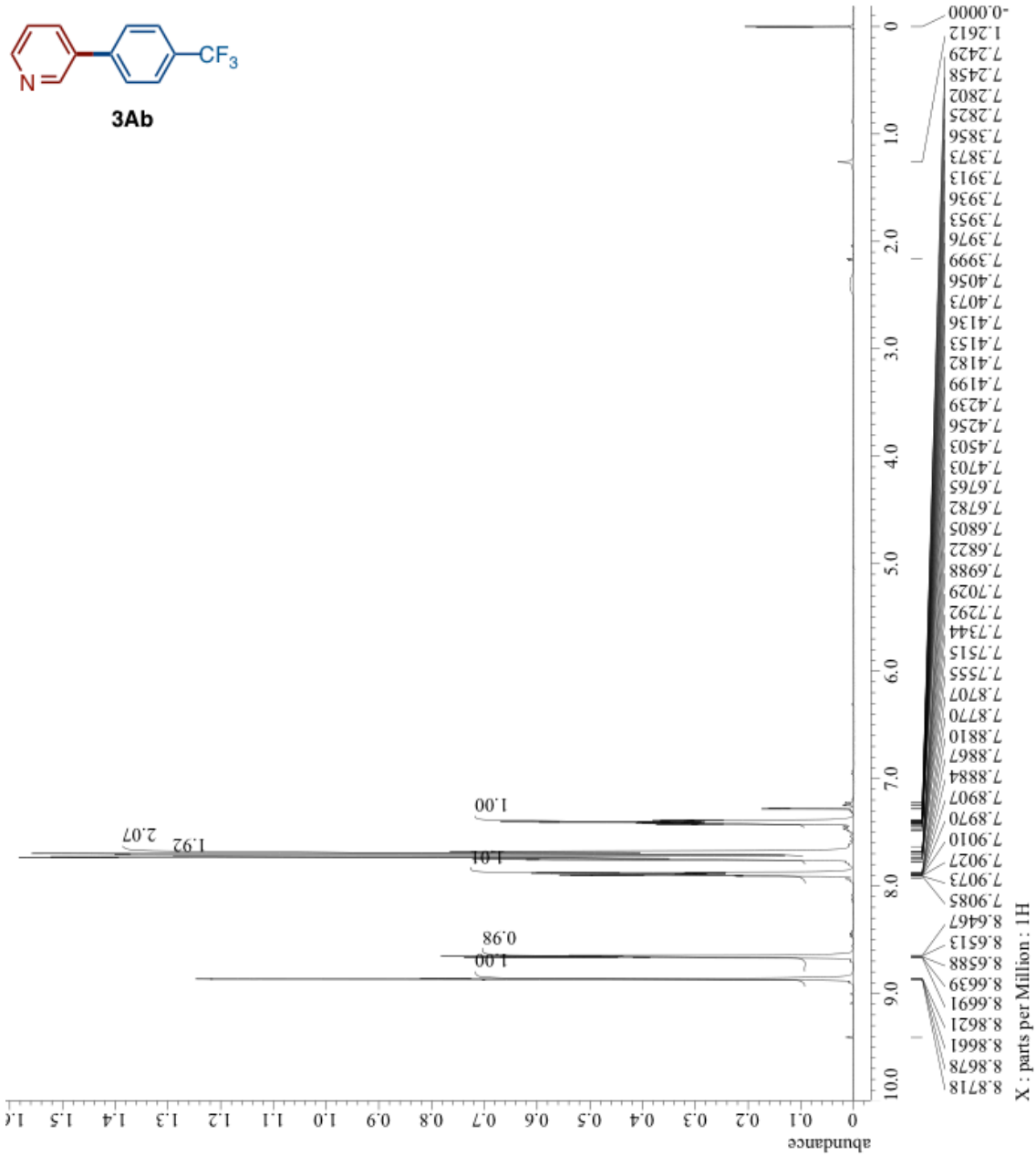
Supplementary Figure 92. ^{13}C NMR (100 MHz, $CDCl_3$) of 3ADa



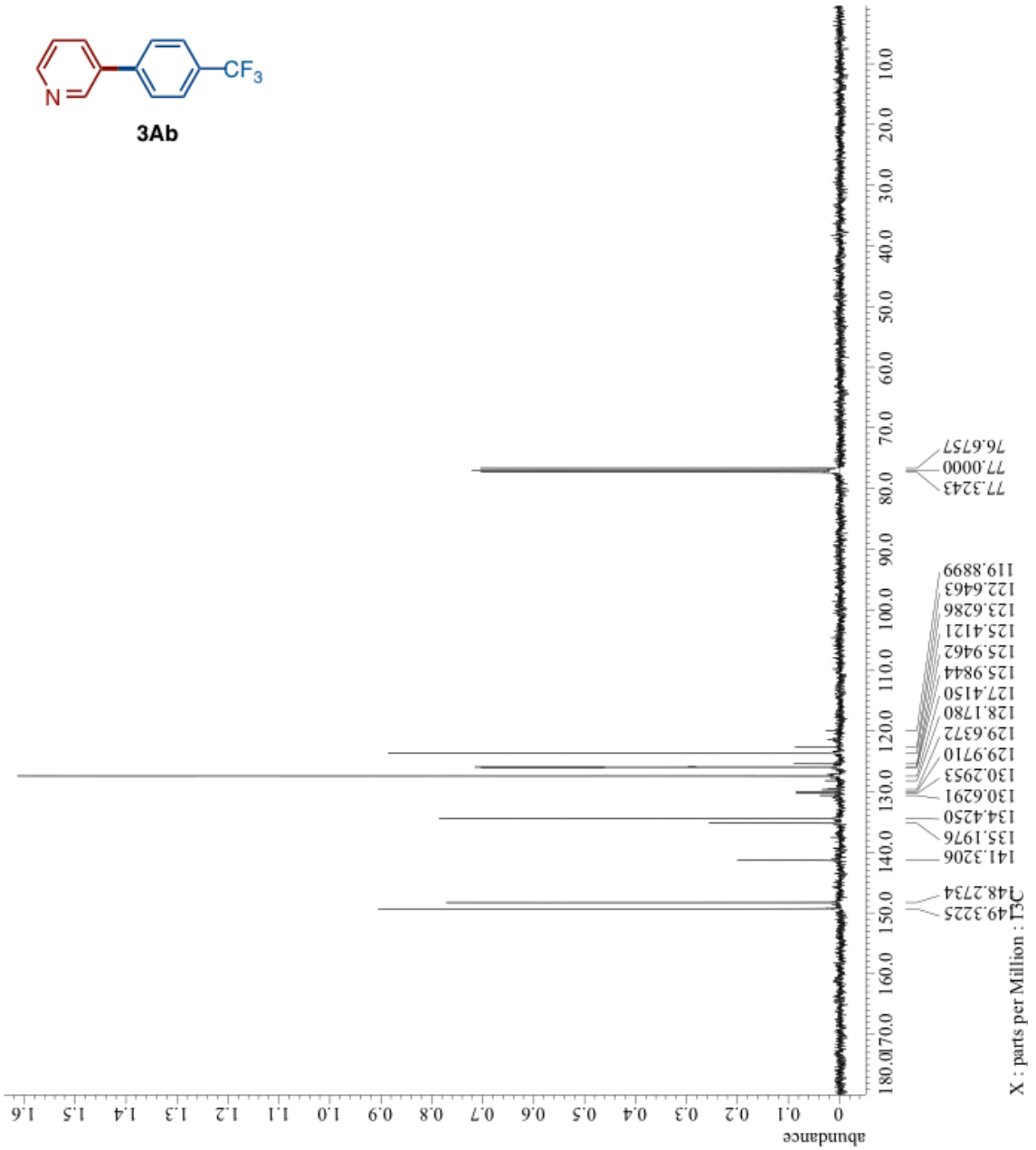
Supplementary Figure 93. ^{1}H NMR (400 MHz, $CDCl_3$) of 3AEa



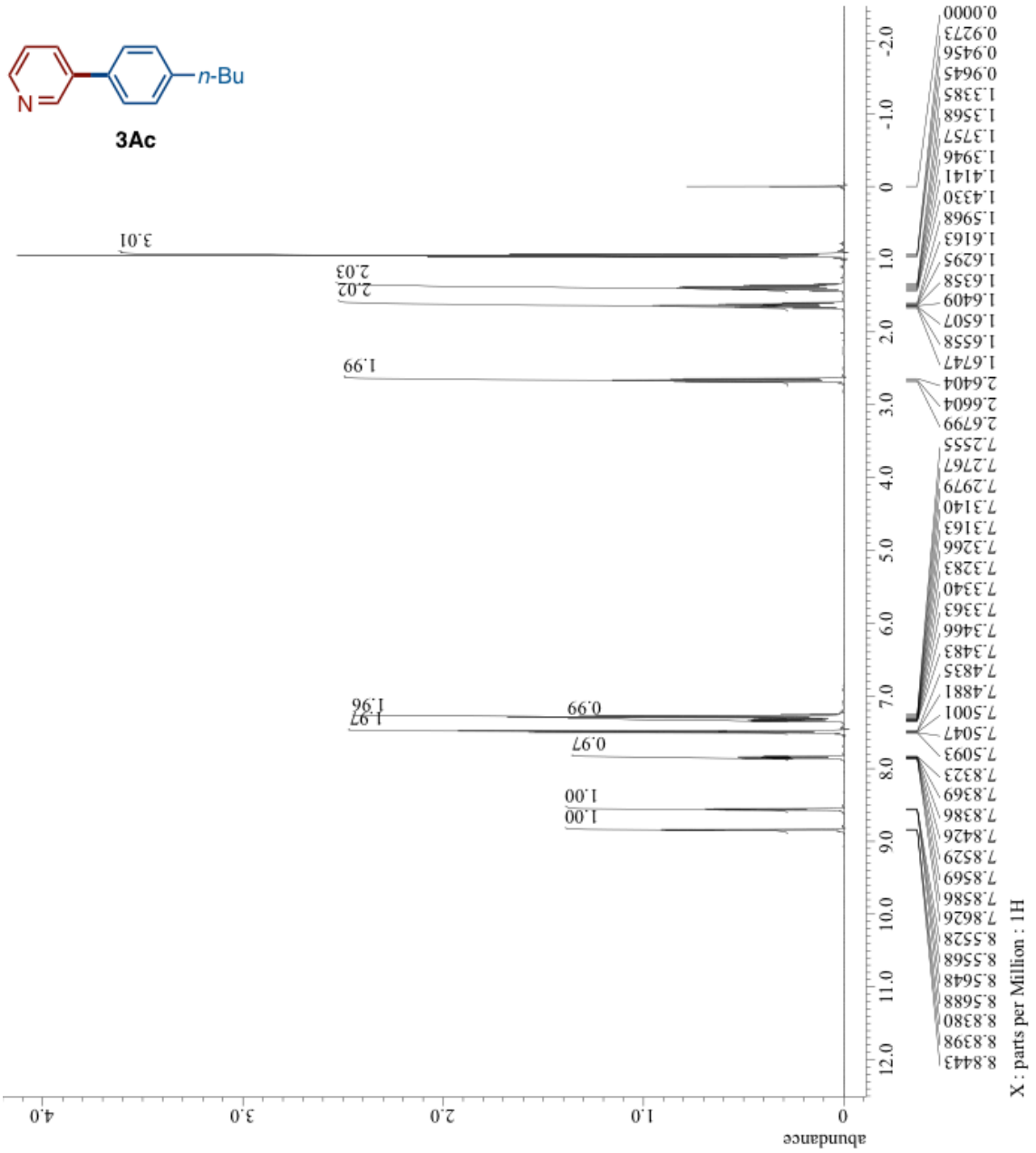
Supplementary Figure 94. ^{13}C NMR (100 MHz, $CDCl_3$) of 3AEa



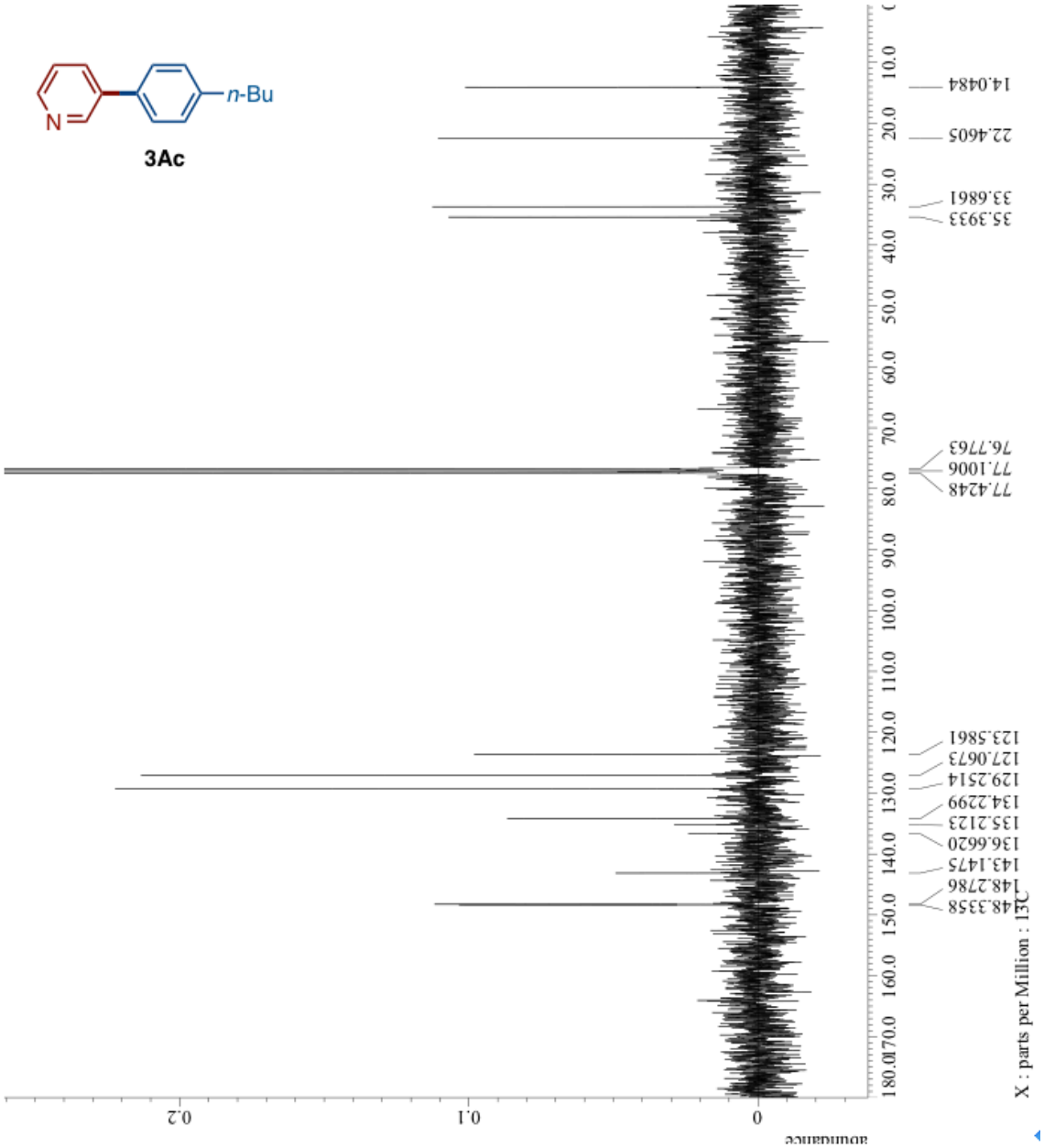
Supplementary Figure 95. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ab



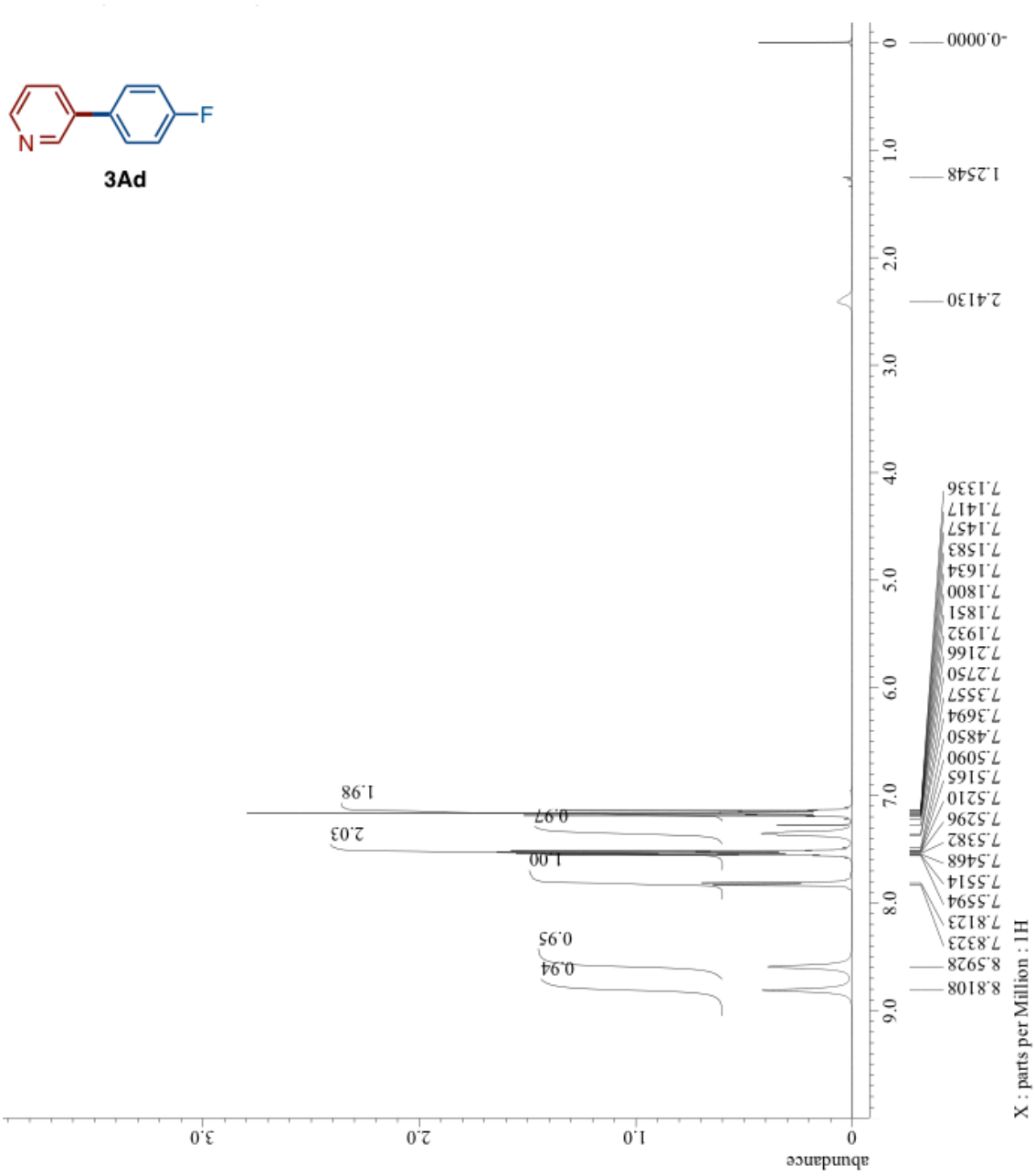
Supplementary Figure 96. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ab



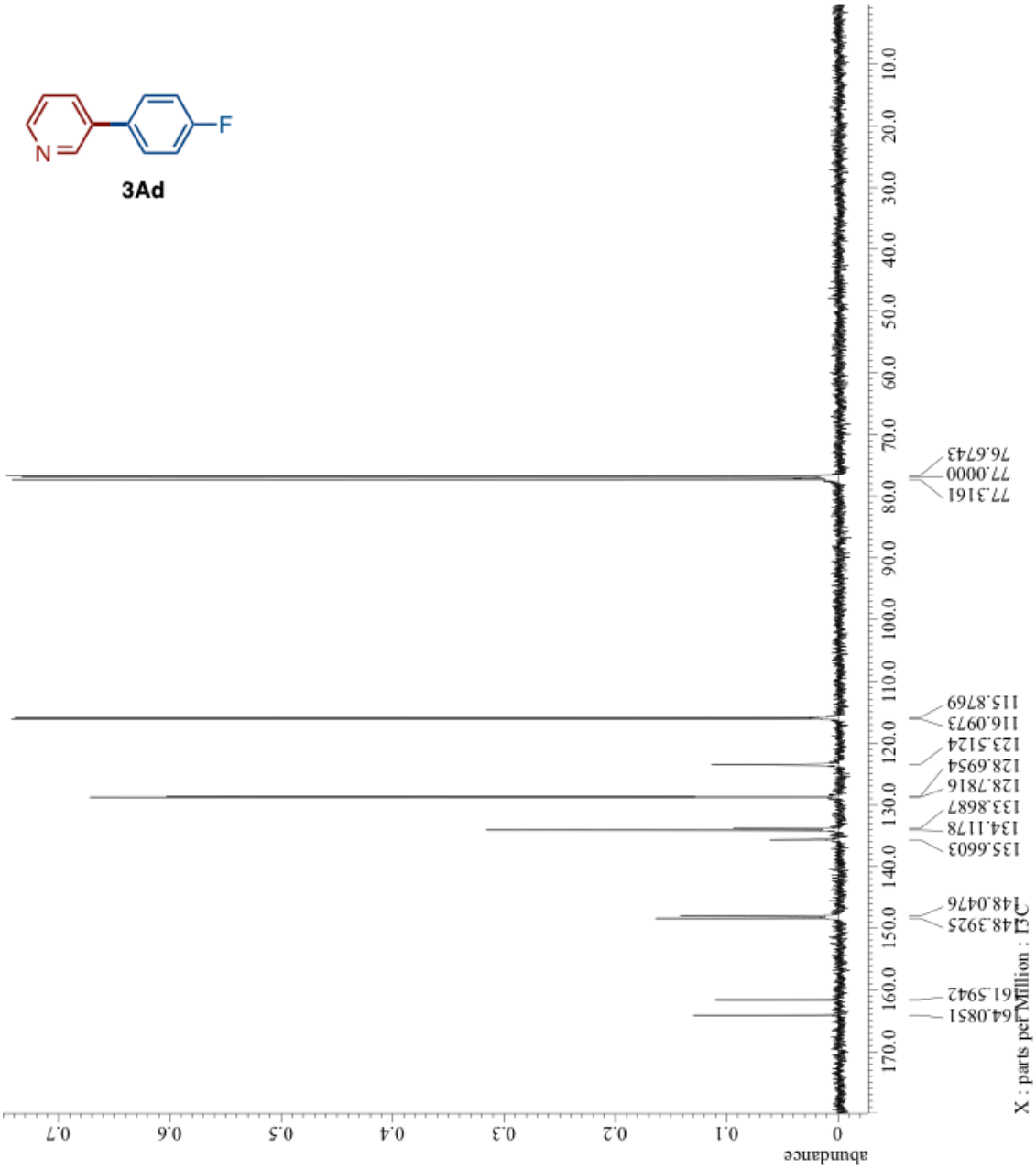
Supplementary Figure 97. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ac



Supplementary Figure 98. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ac



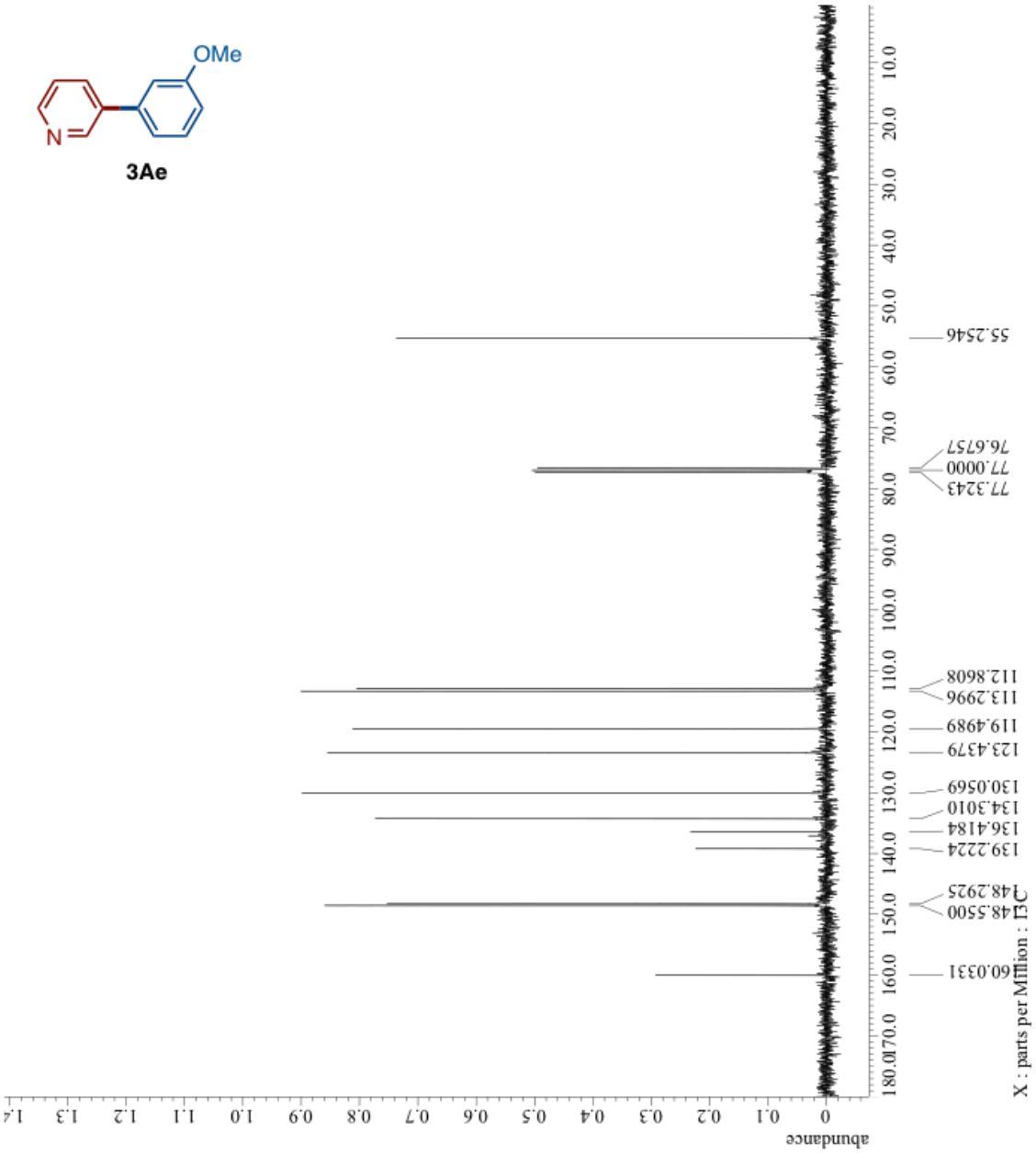
Supplementary Figure 99. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ad



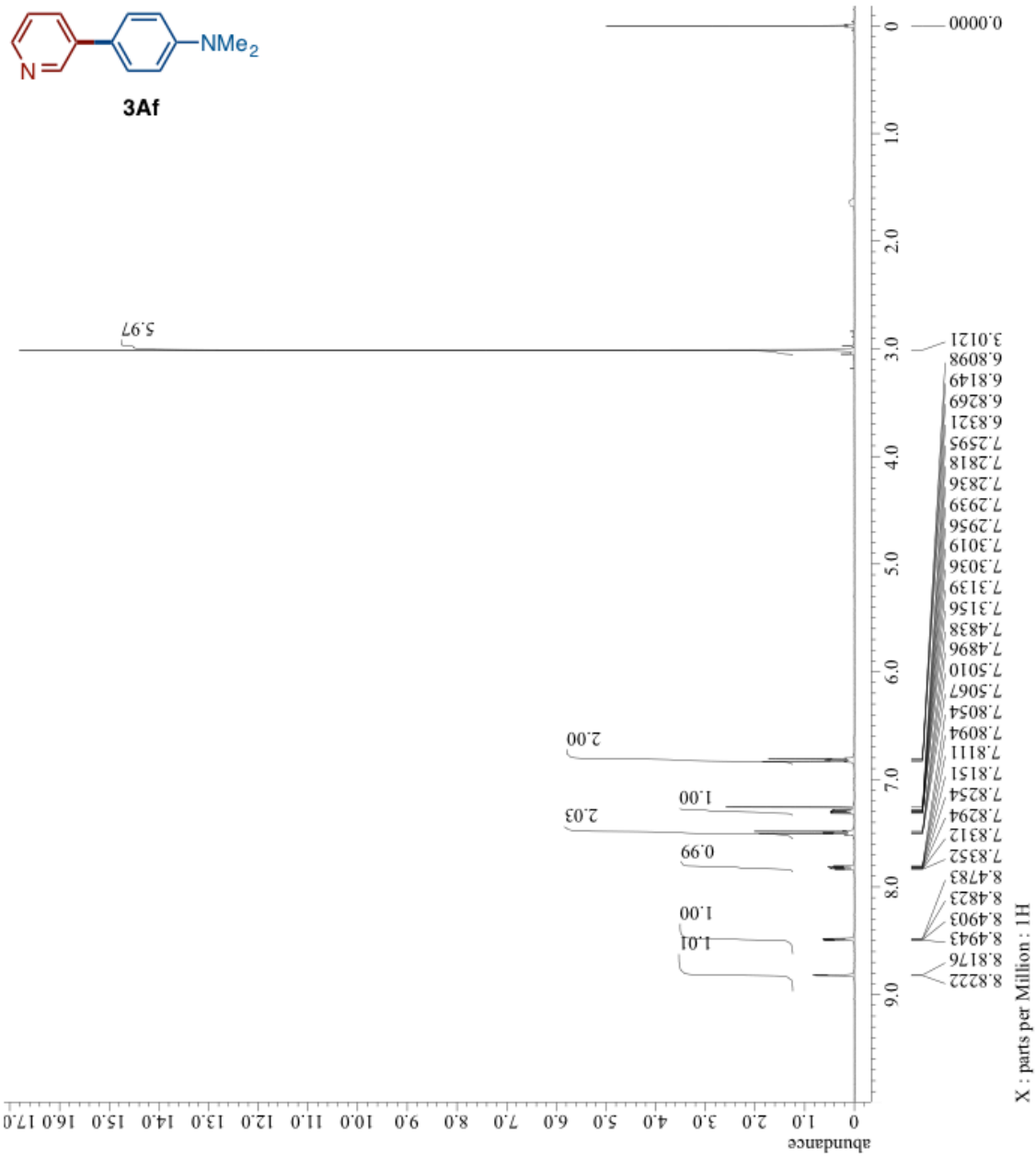
Supplementary Figure 100. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ad



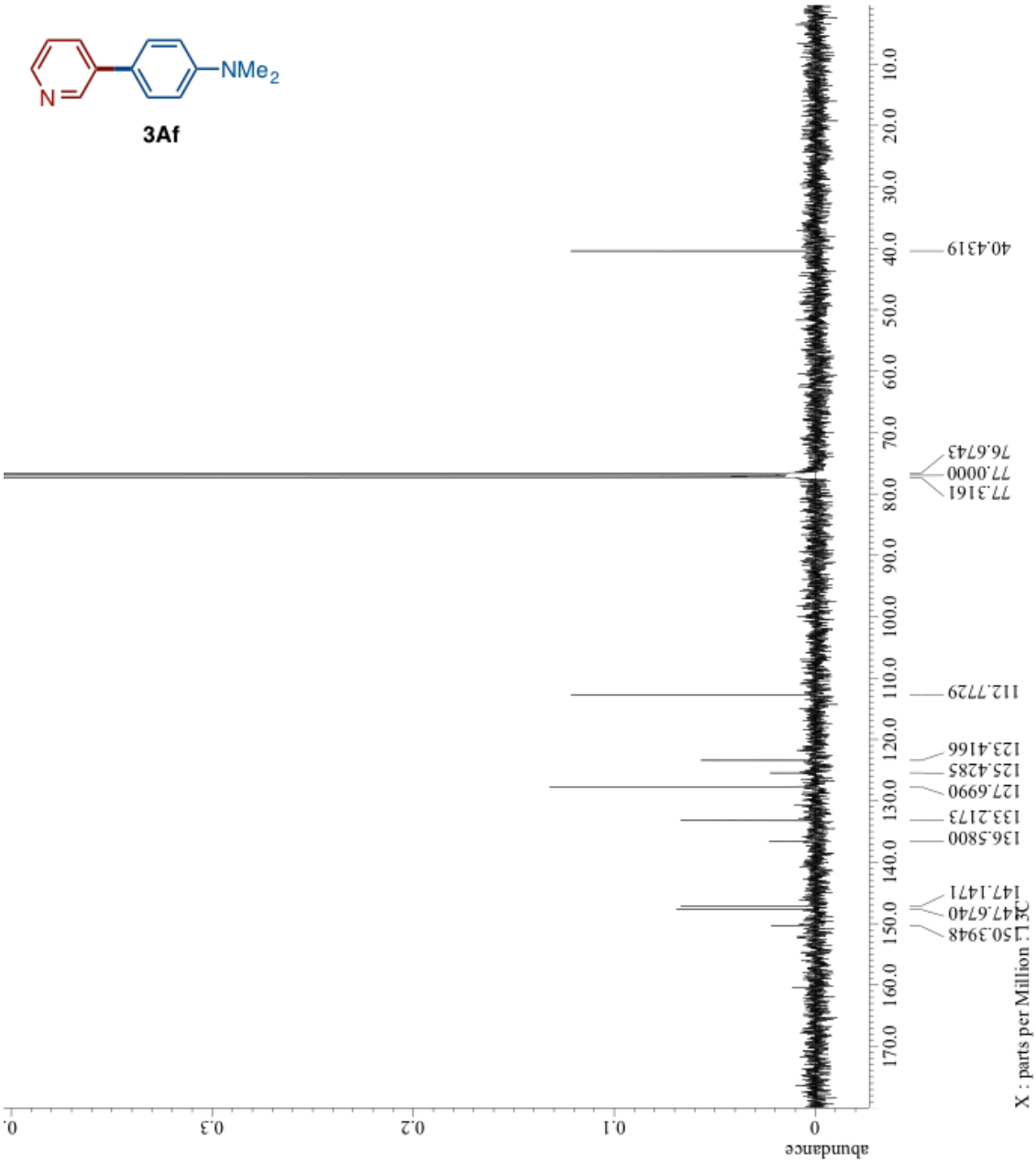
Supplementary Figure 101. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ae



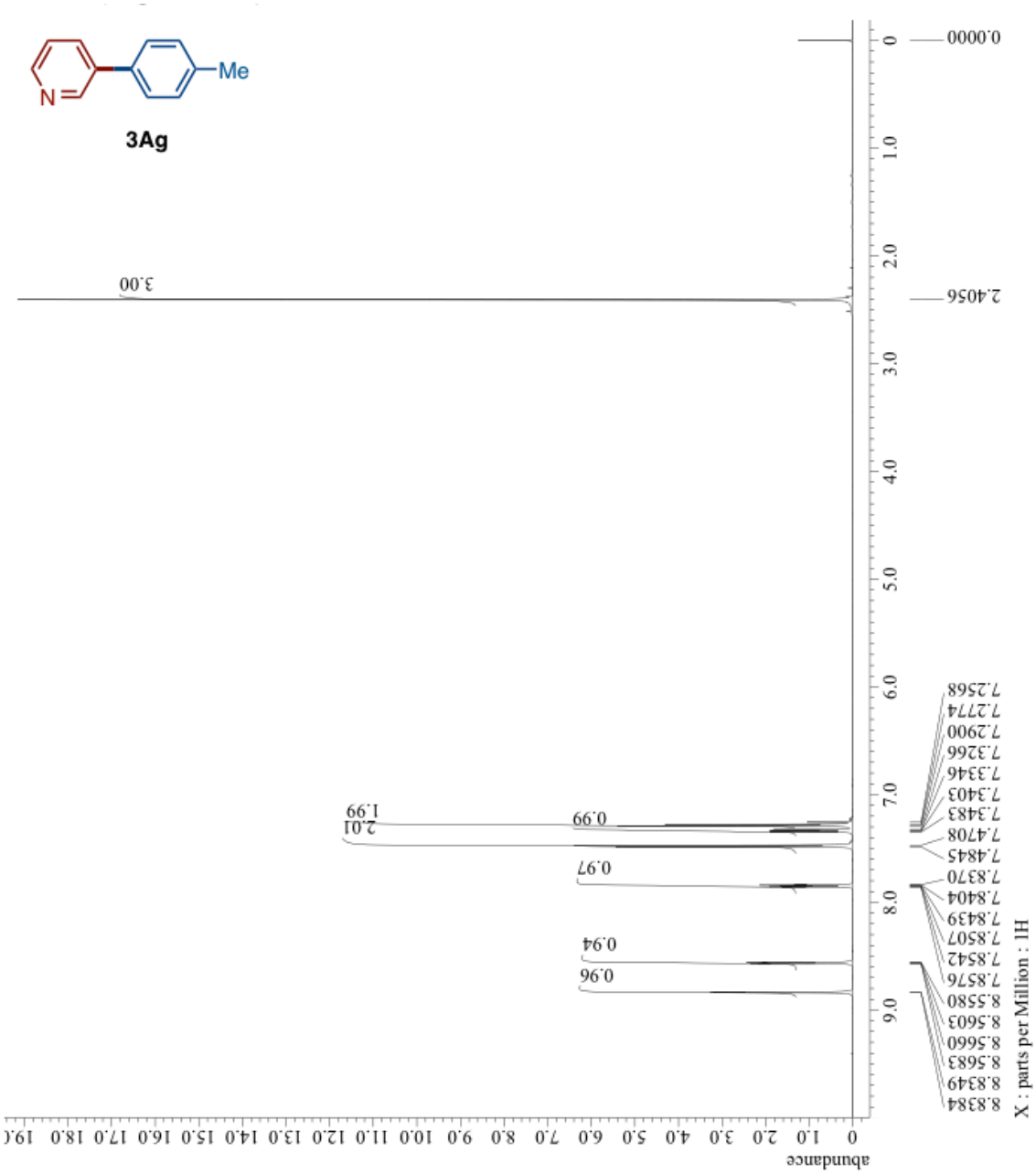
Supplementary Figure 102. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ae



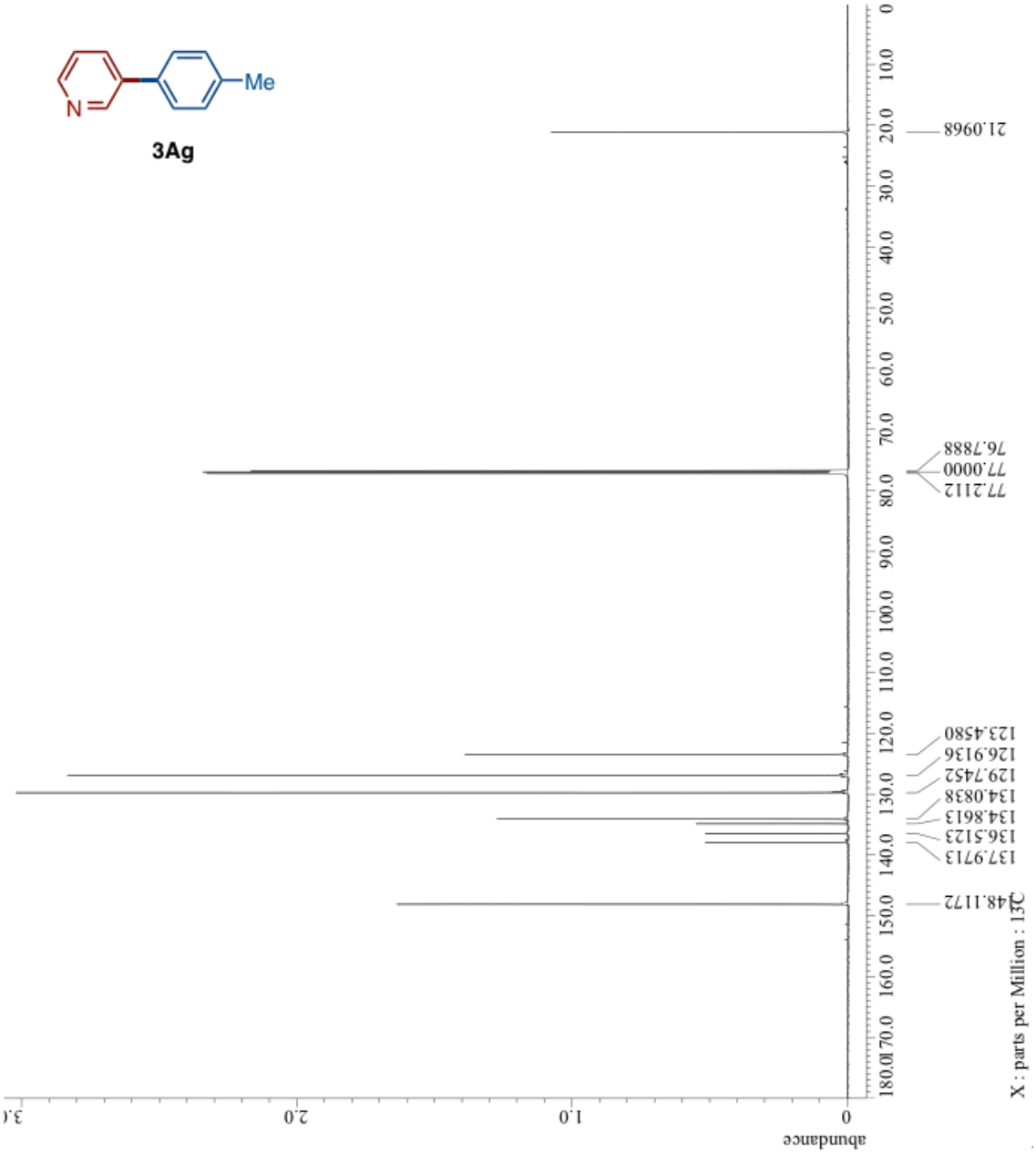
Supplementary Figure 103. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Af



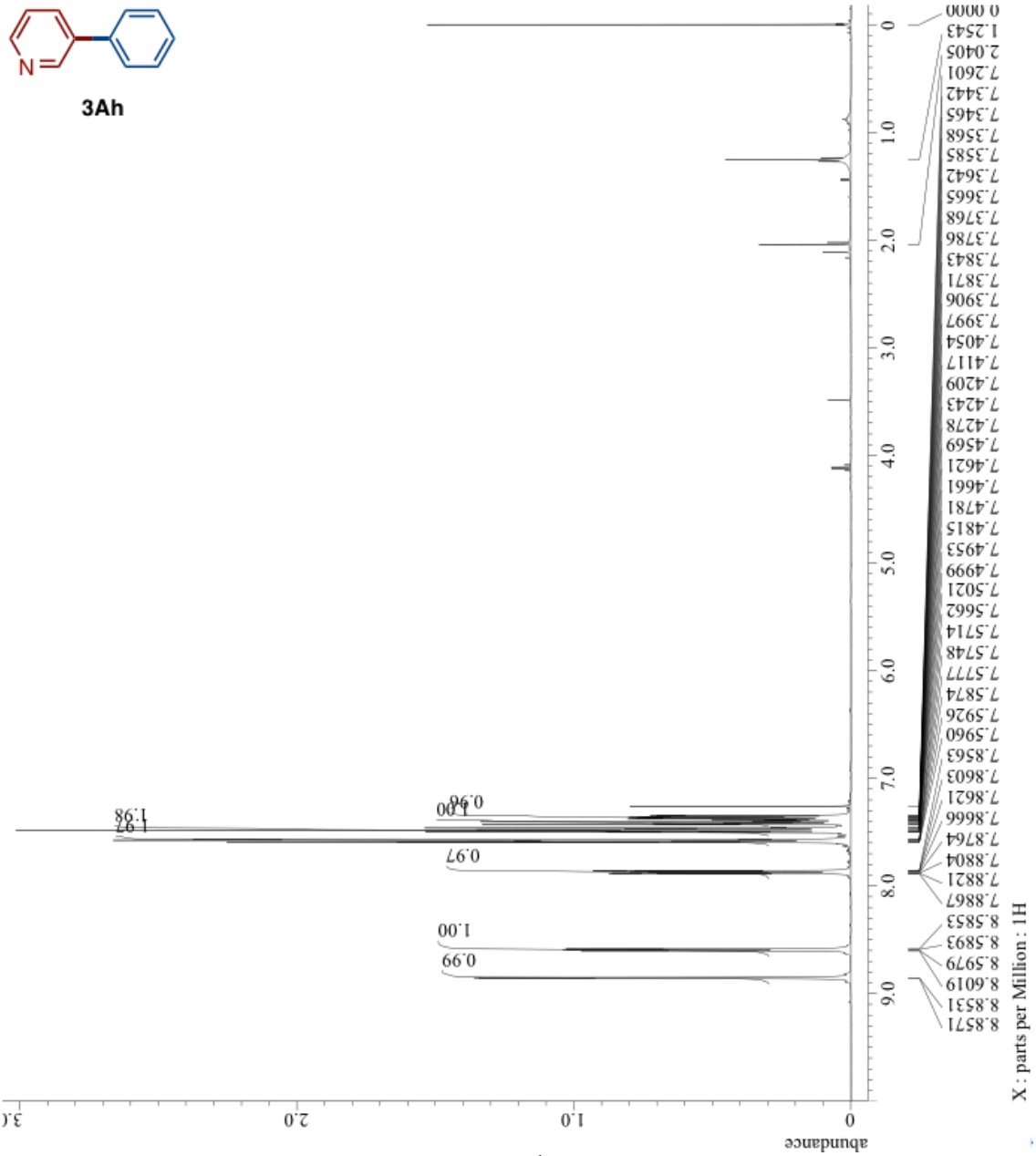
Supplementary Figure 104. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Af



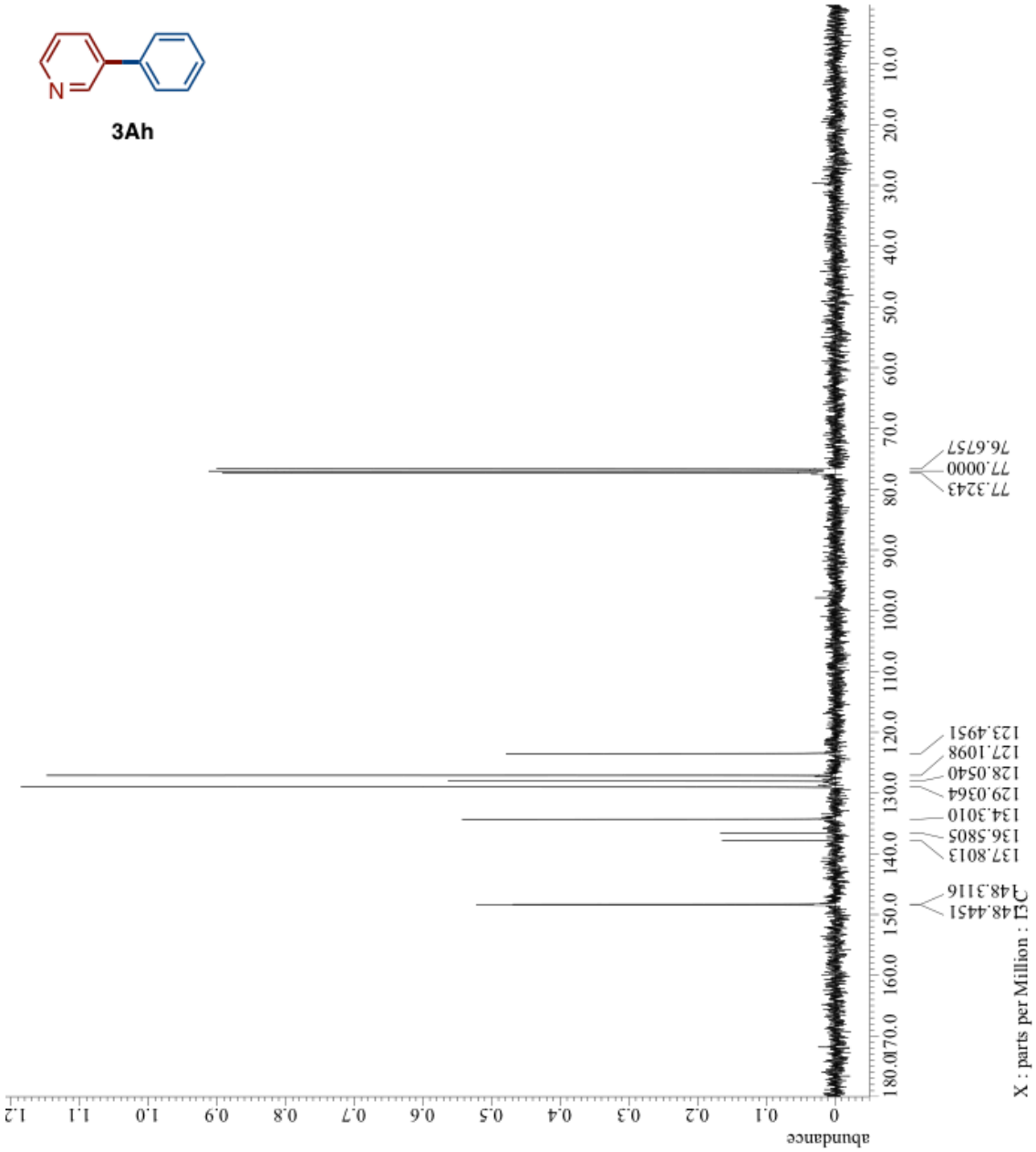
Supplementary Figure 105. ^{1}H NMR (600 MHz, $CDCl_3$) of 3Ag



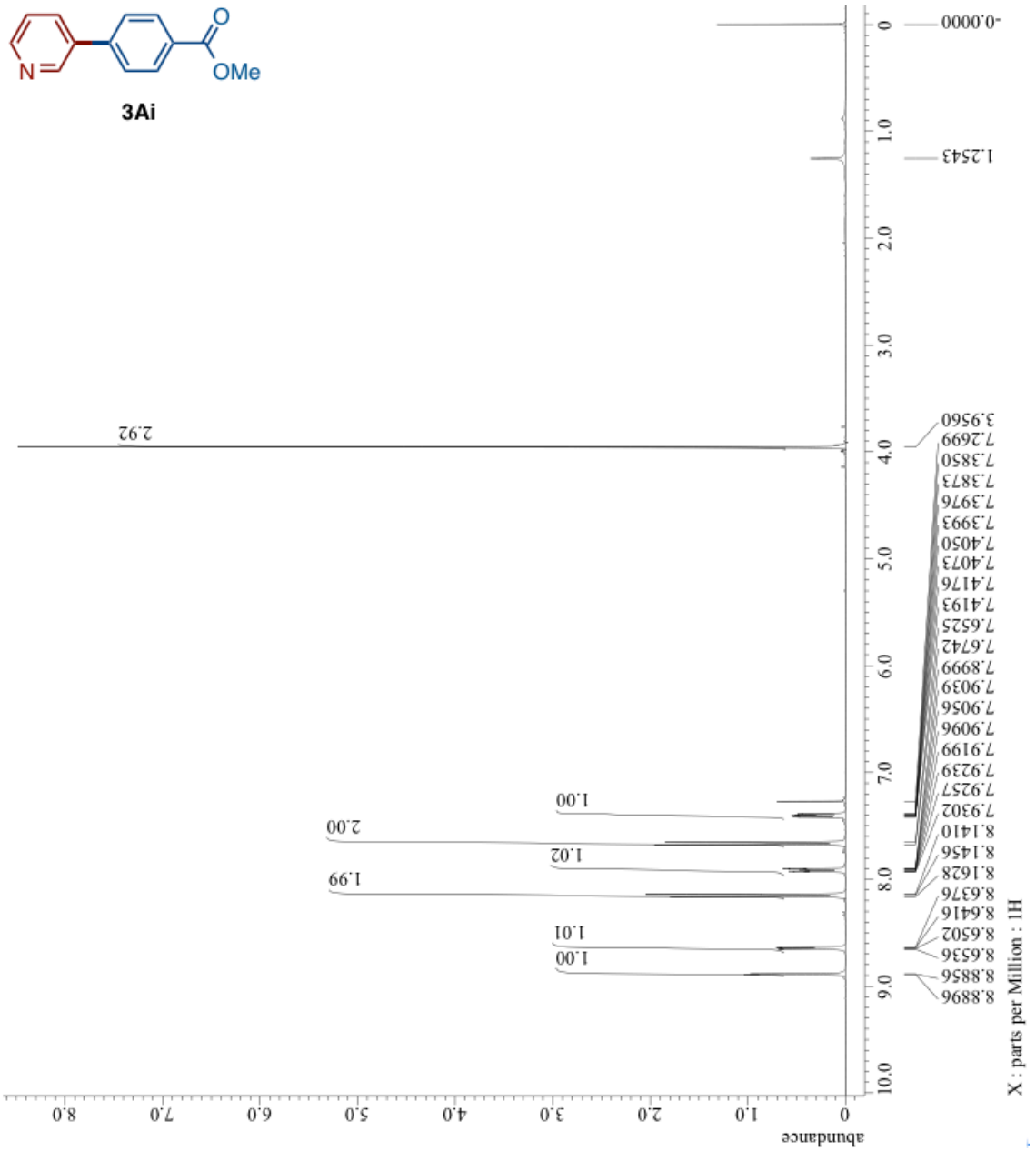
Supplementary Figure 106. ^{13}C NMR (150 MHz, $CDCl_3$) of 3Ag



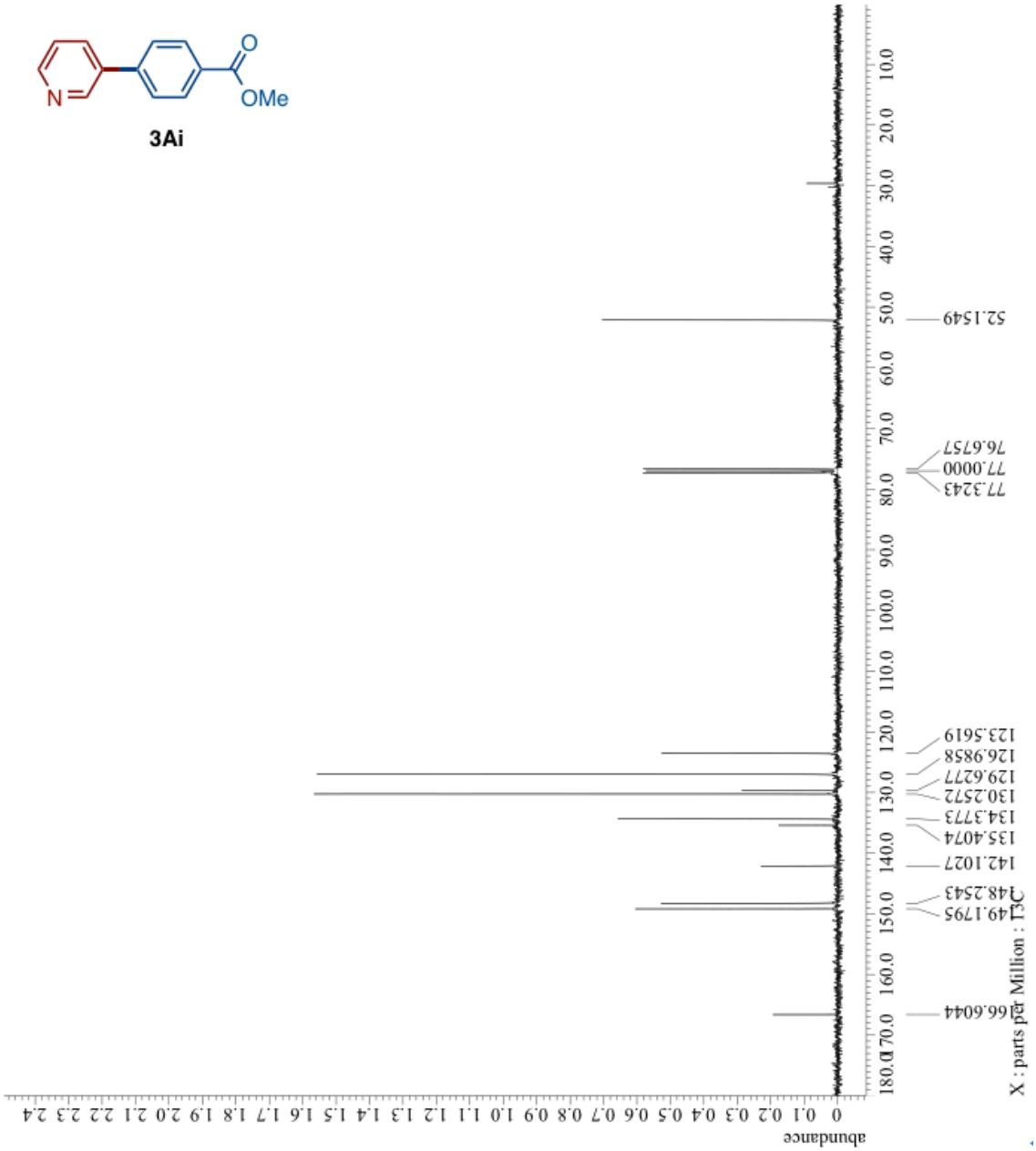
Supplementary Figure 107. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ah



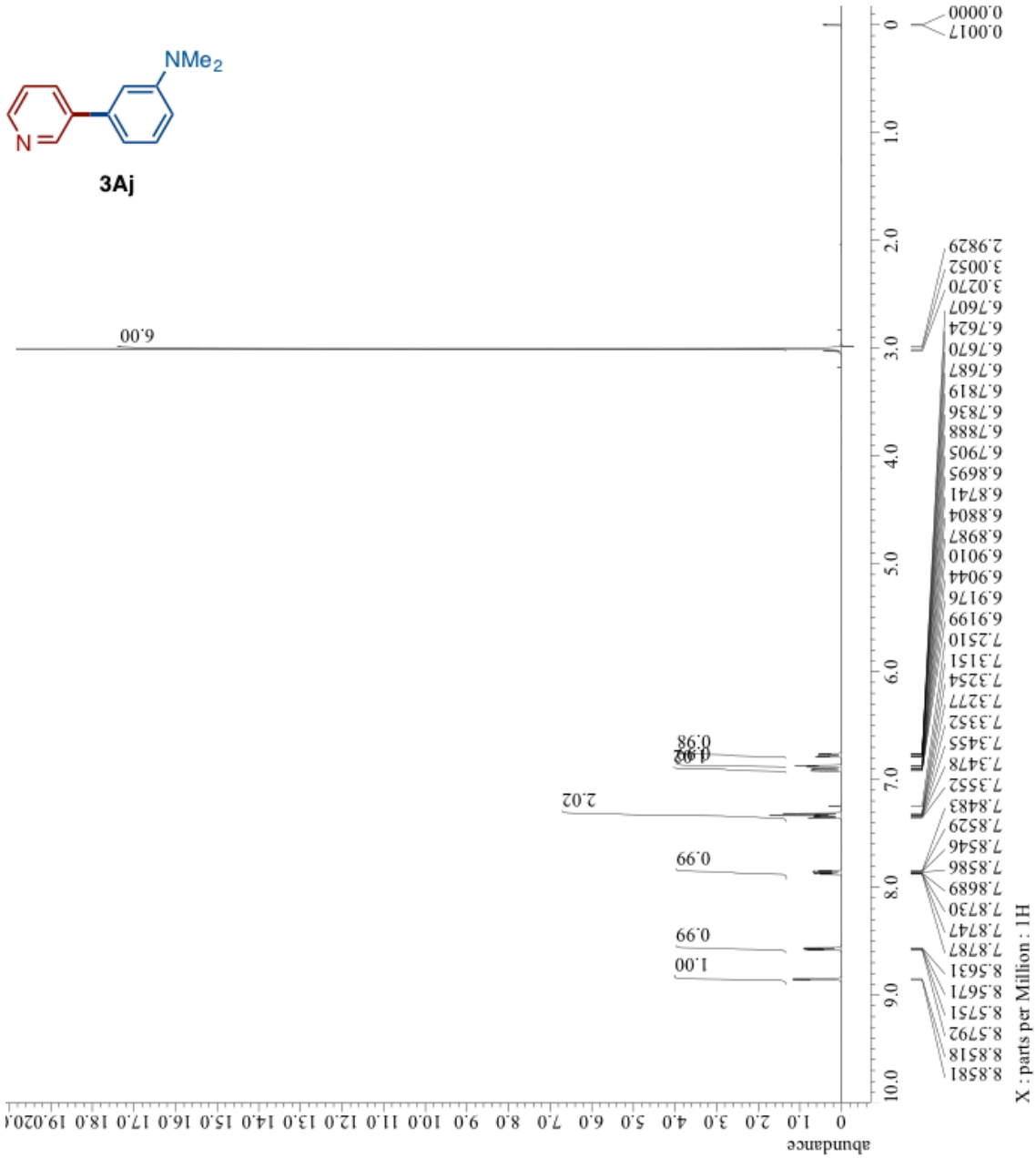
Supplementary Figure 108. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ah



Supplementary Figure 109. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ai

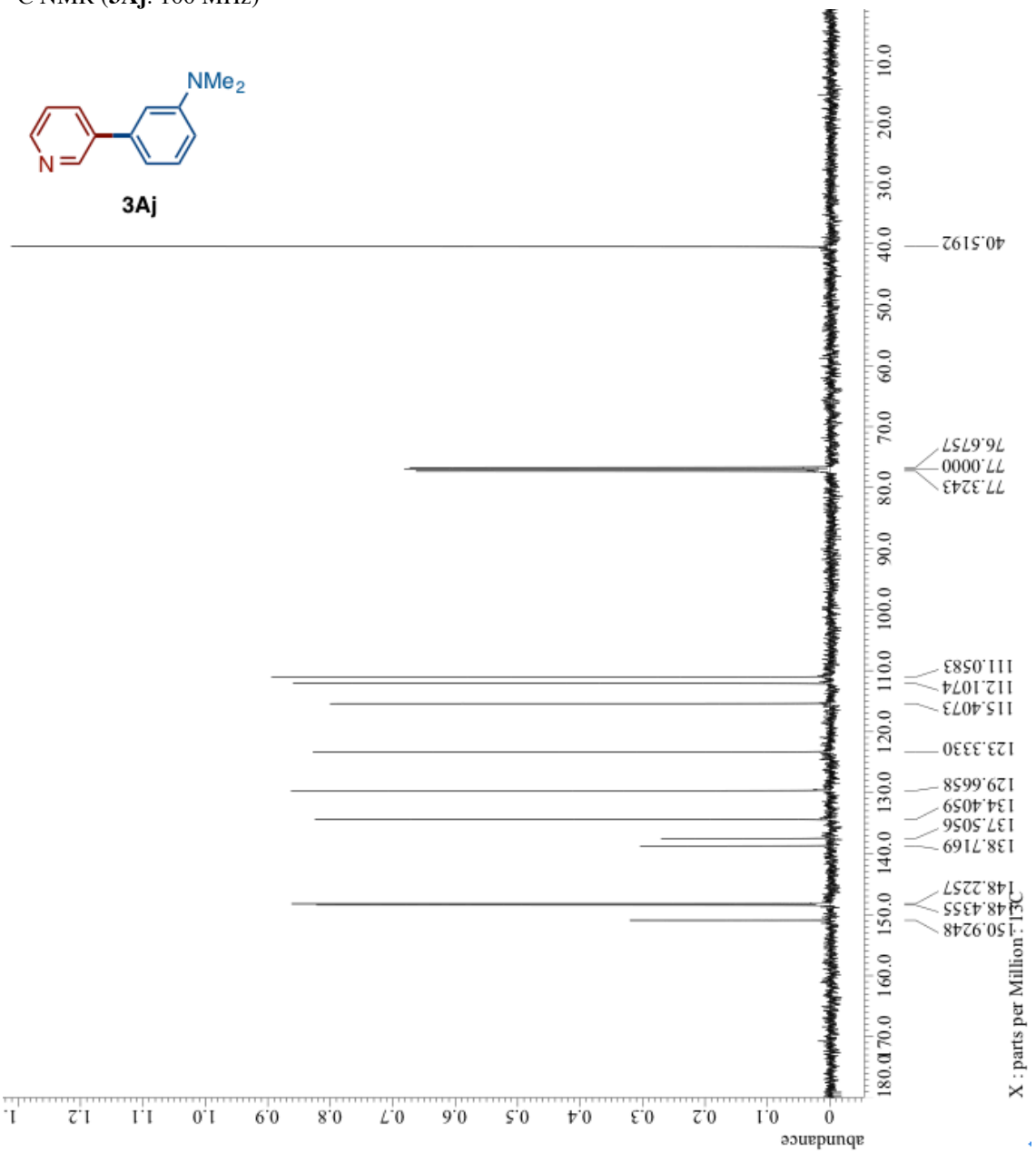


Supplementary Figure 110. ^{13}C **NMR (100 MHz, $CDCl_3$) of 3Ai**

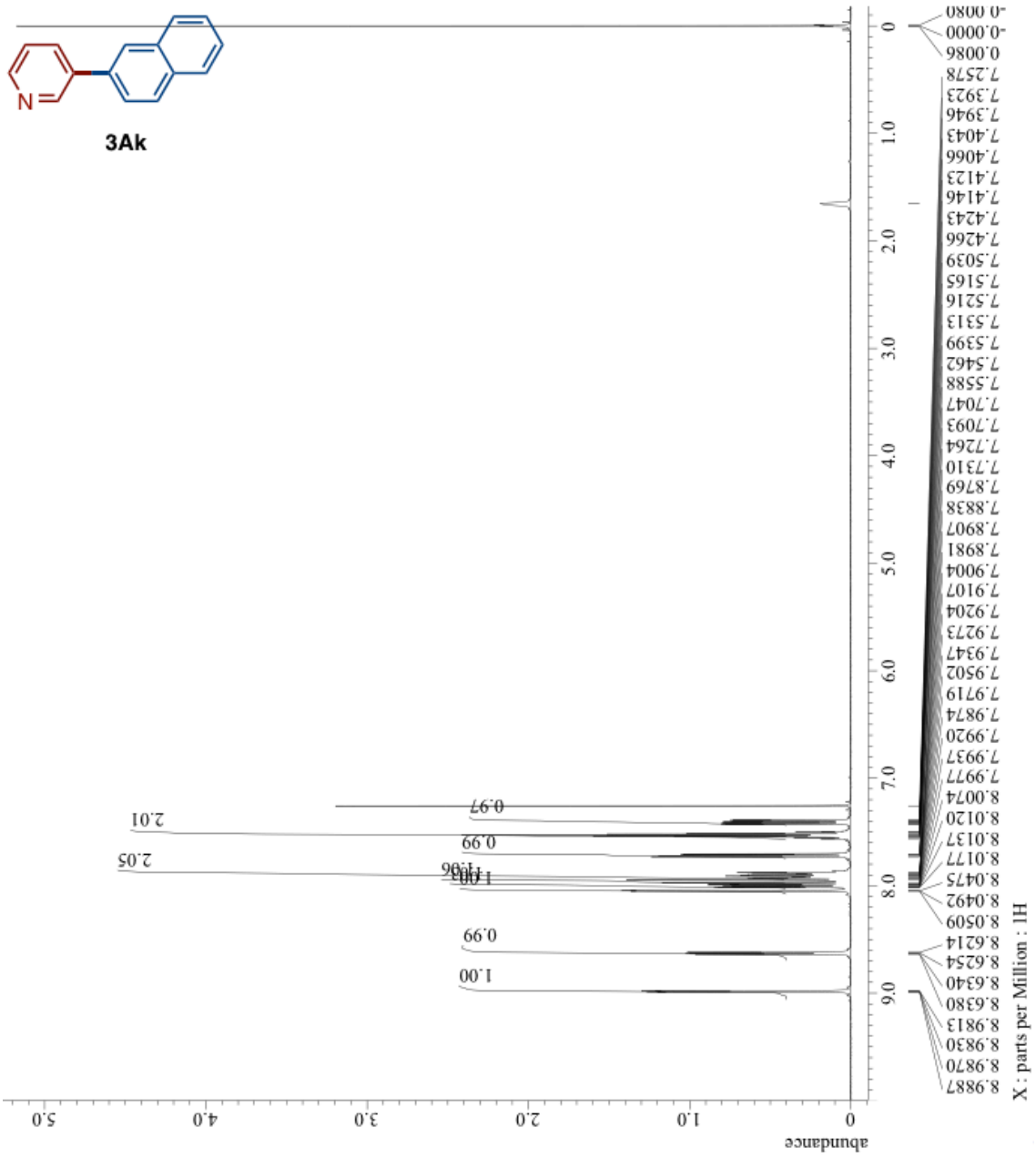


Supplementary Figure 111. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Aj

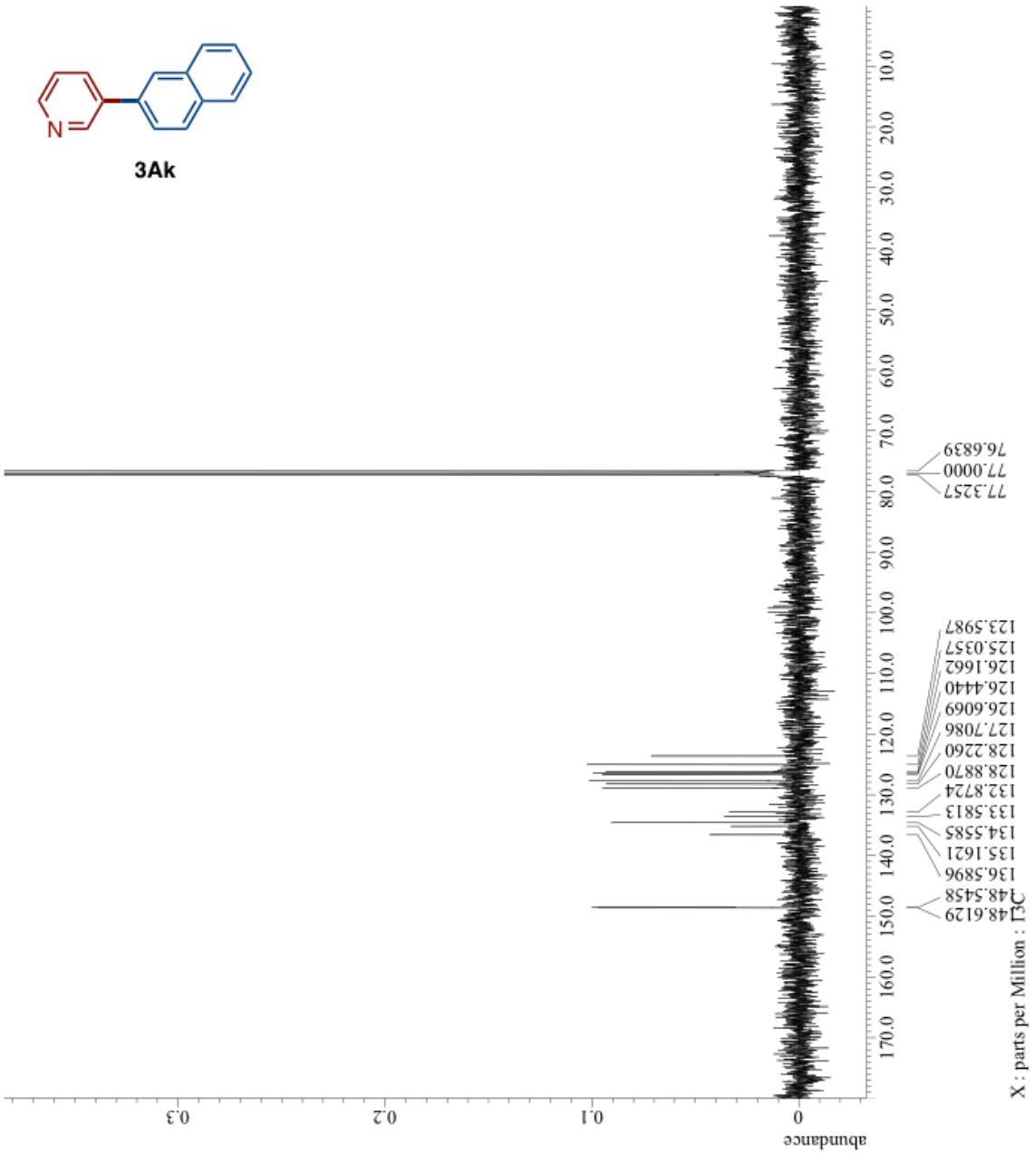
^{13}C NMR (**3Aj**: 100 MHz)



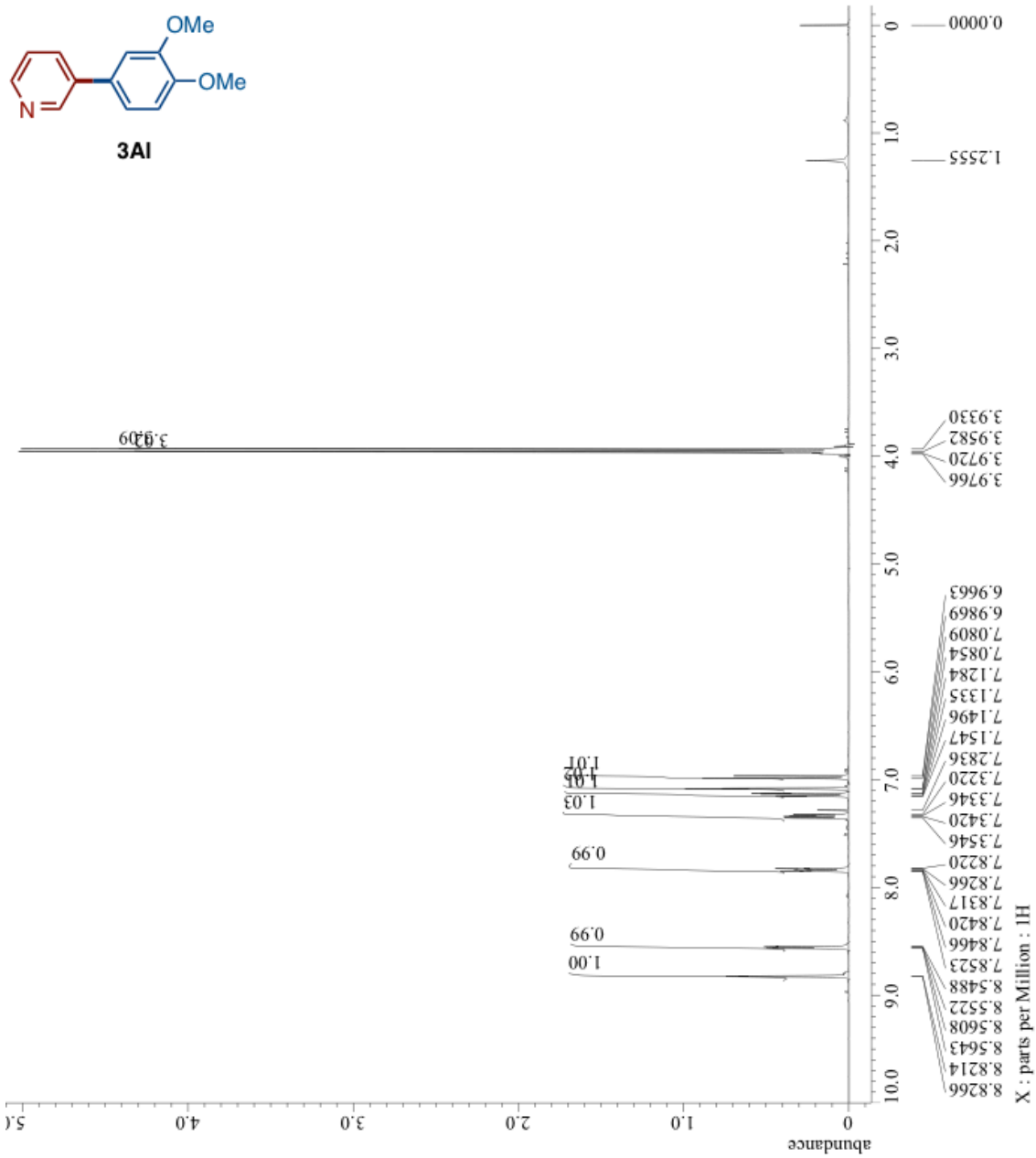
Supplementary Figure 112. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Aj



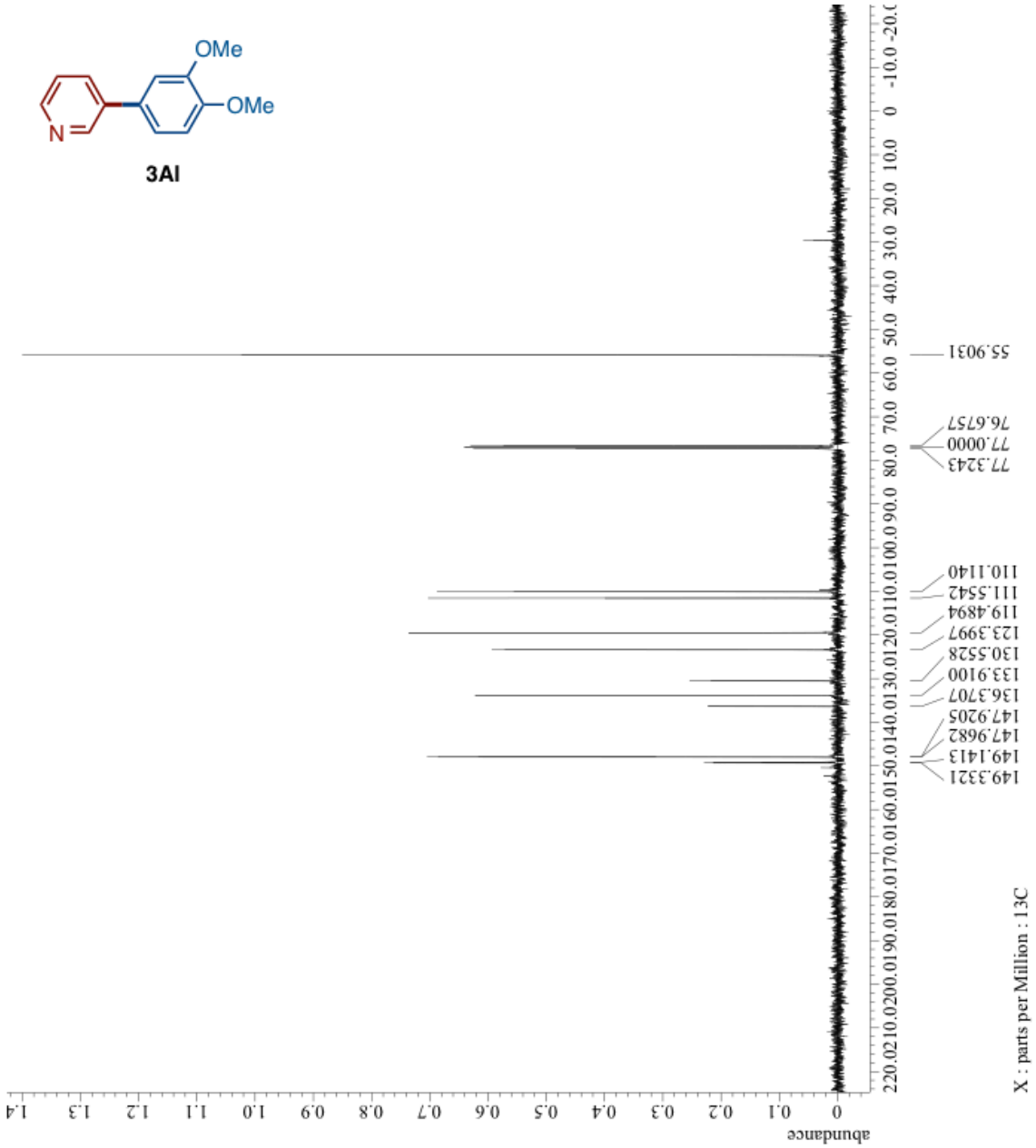
Supplementary Figure 113. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ak



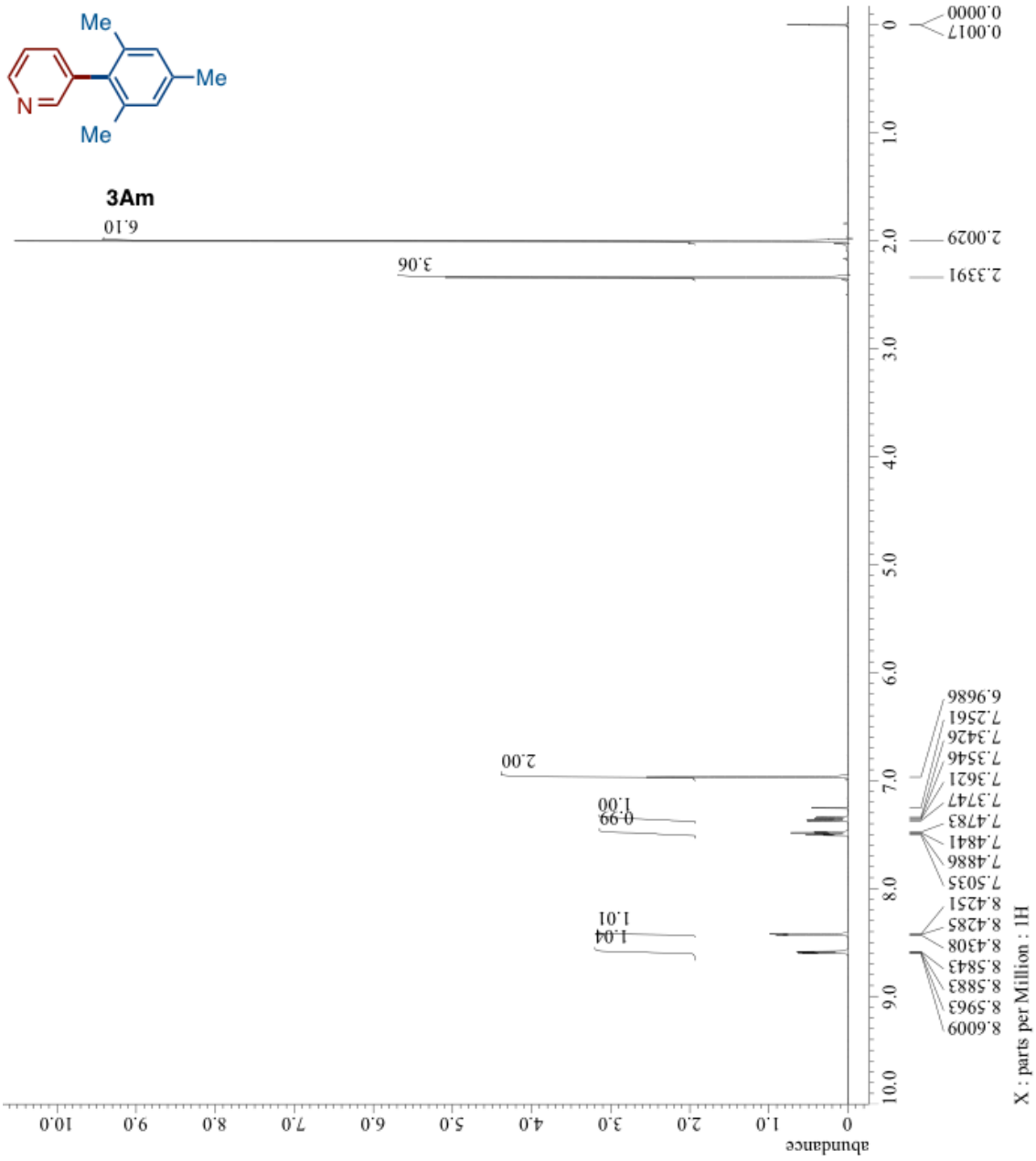
Supplementary Figure 114. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ak



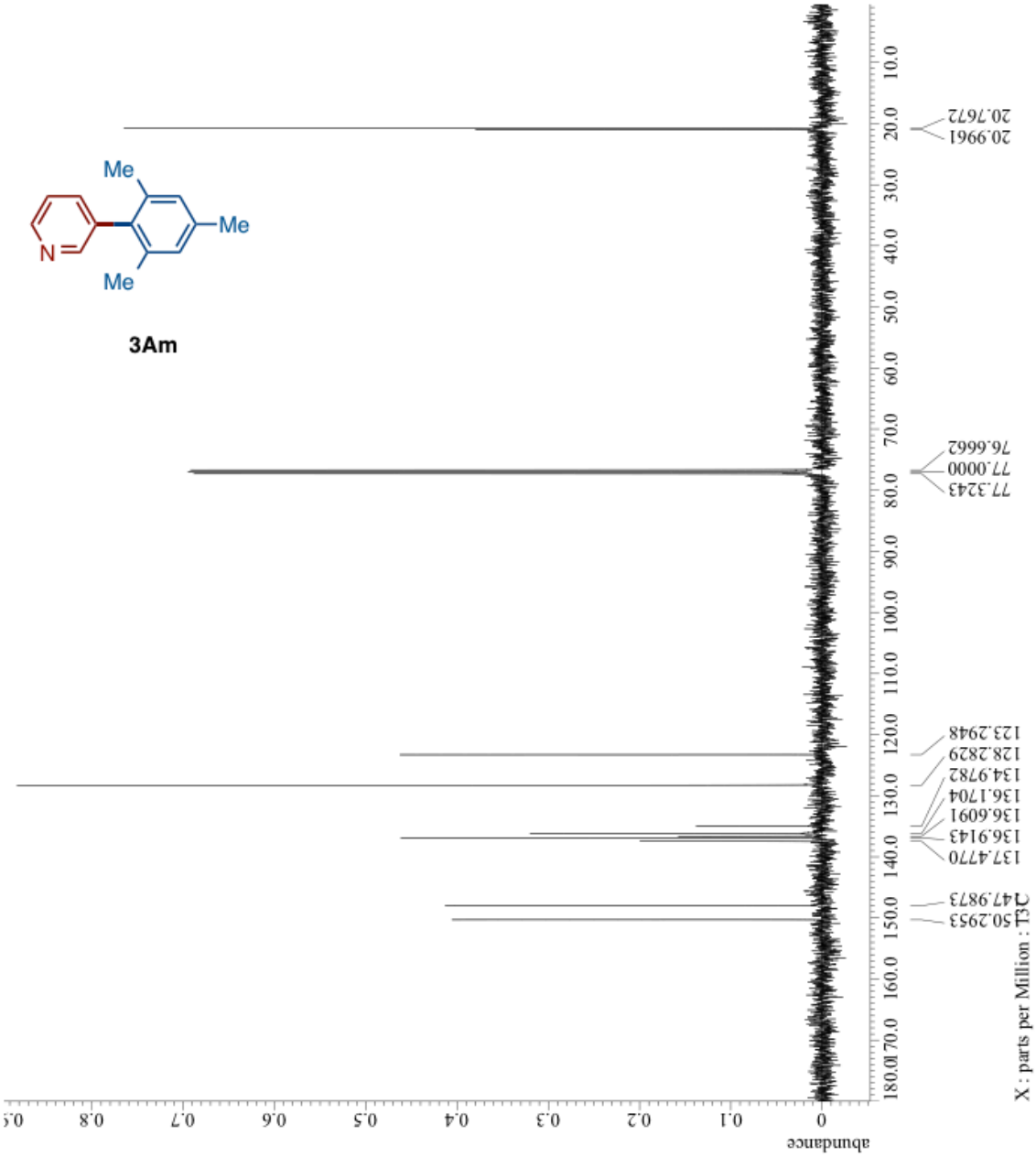
Supplementary Figure 115. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Al



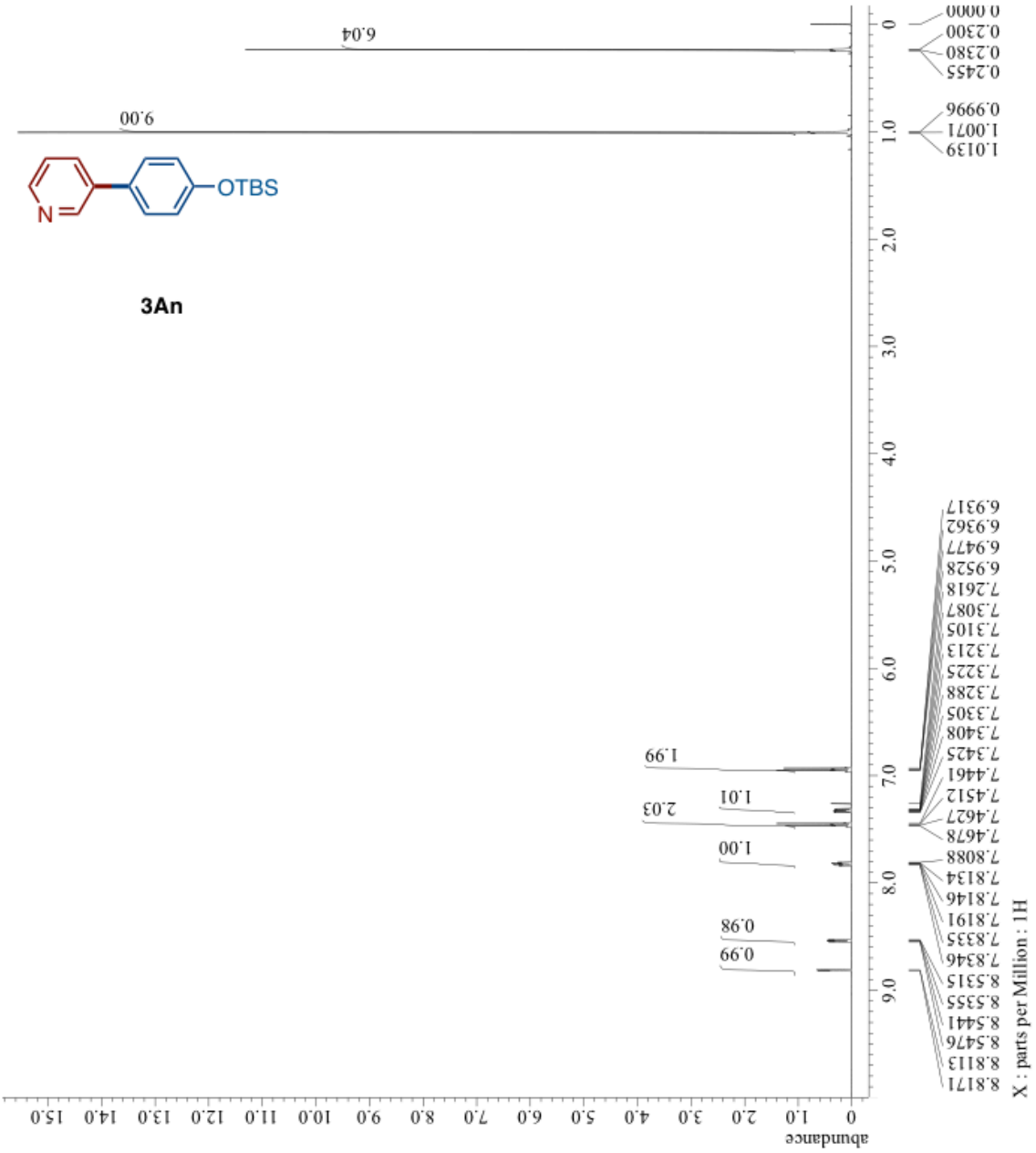
Supplementary Figure 116. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Al



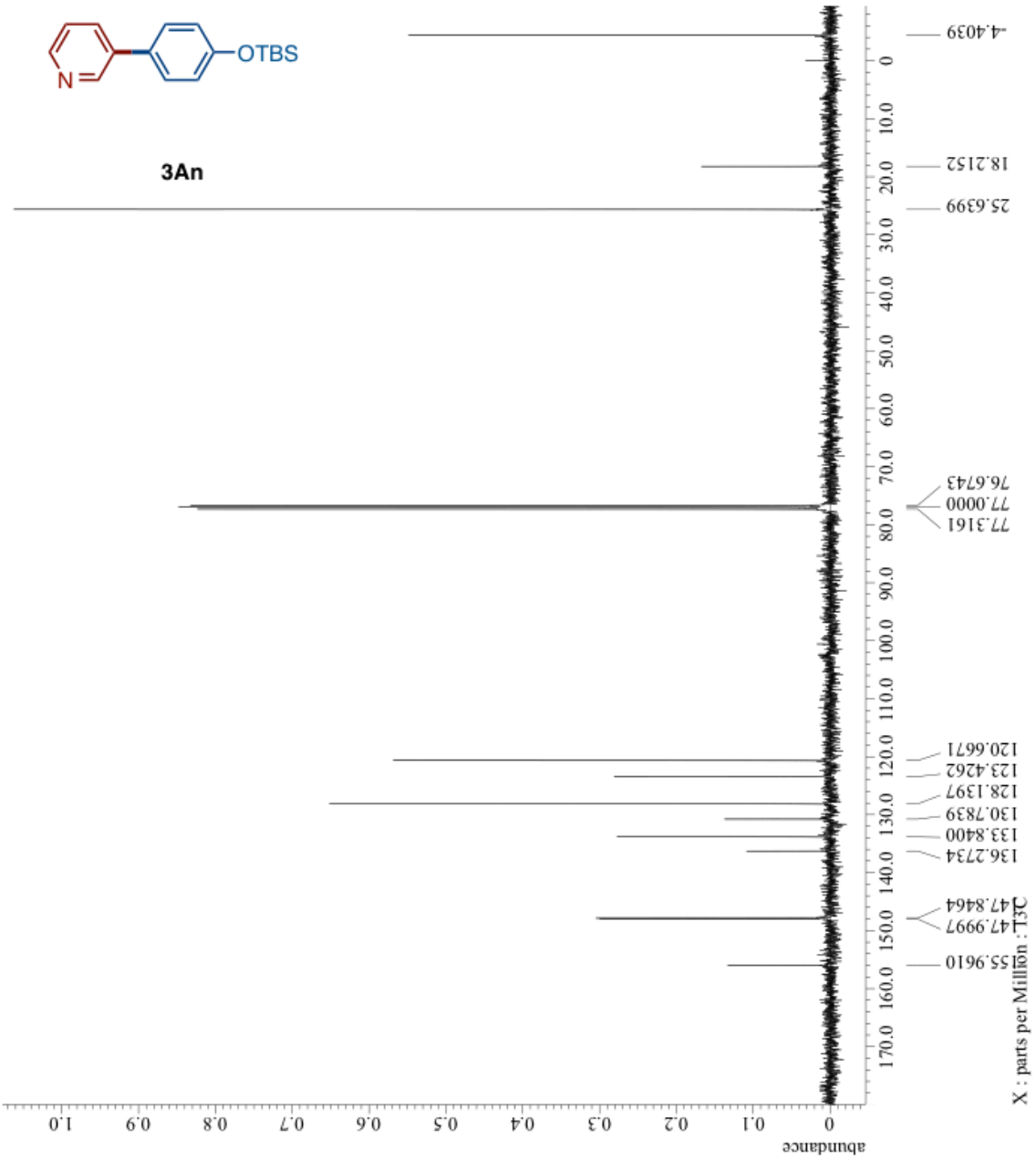
Supplementary Figure 117. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Am



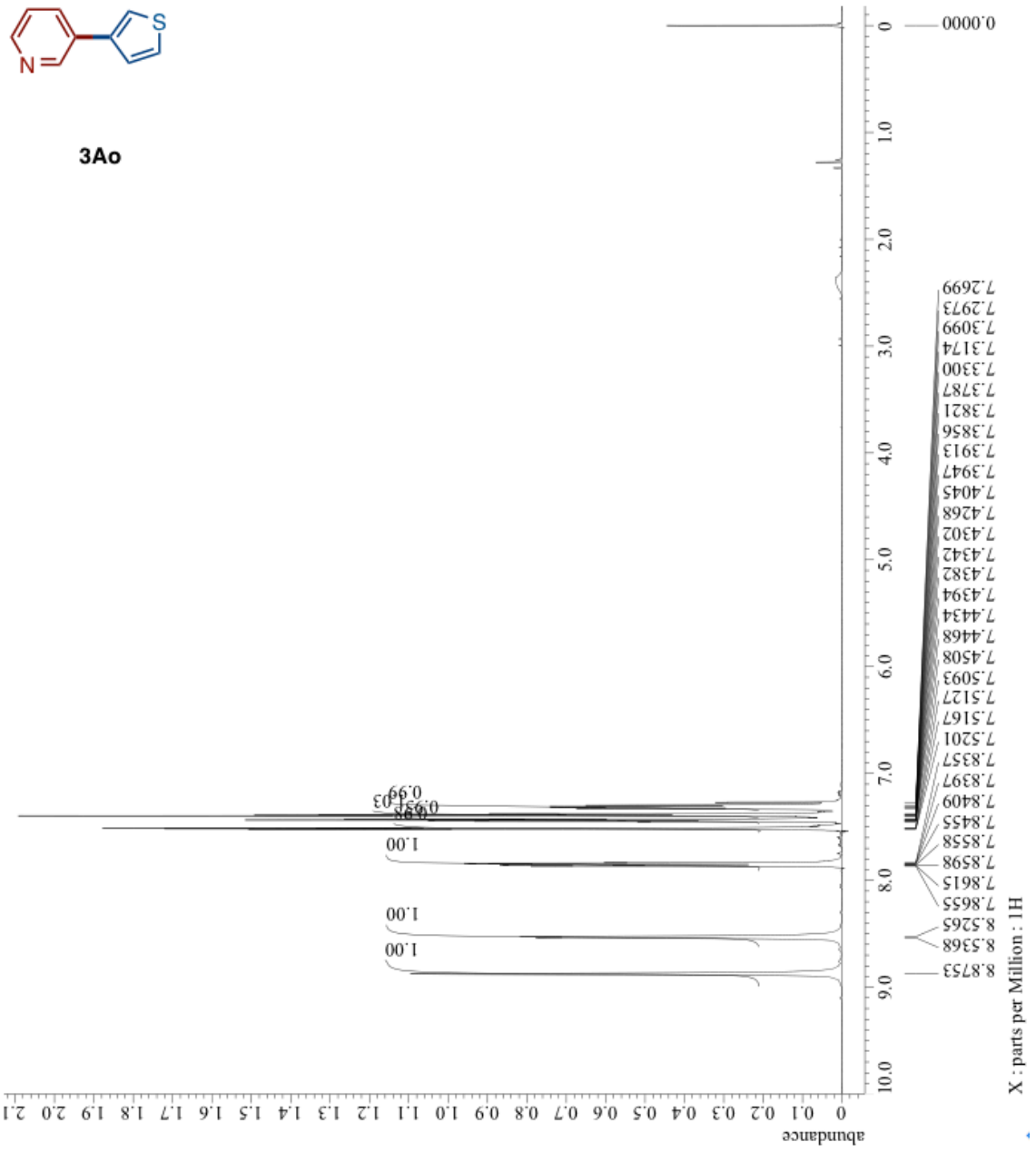
Supplementary Figure 118. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Am



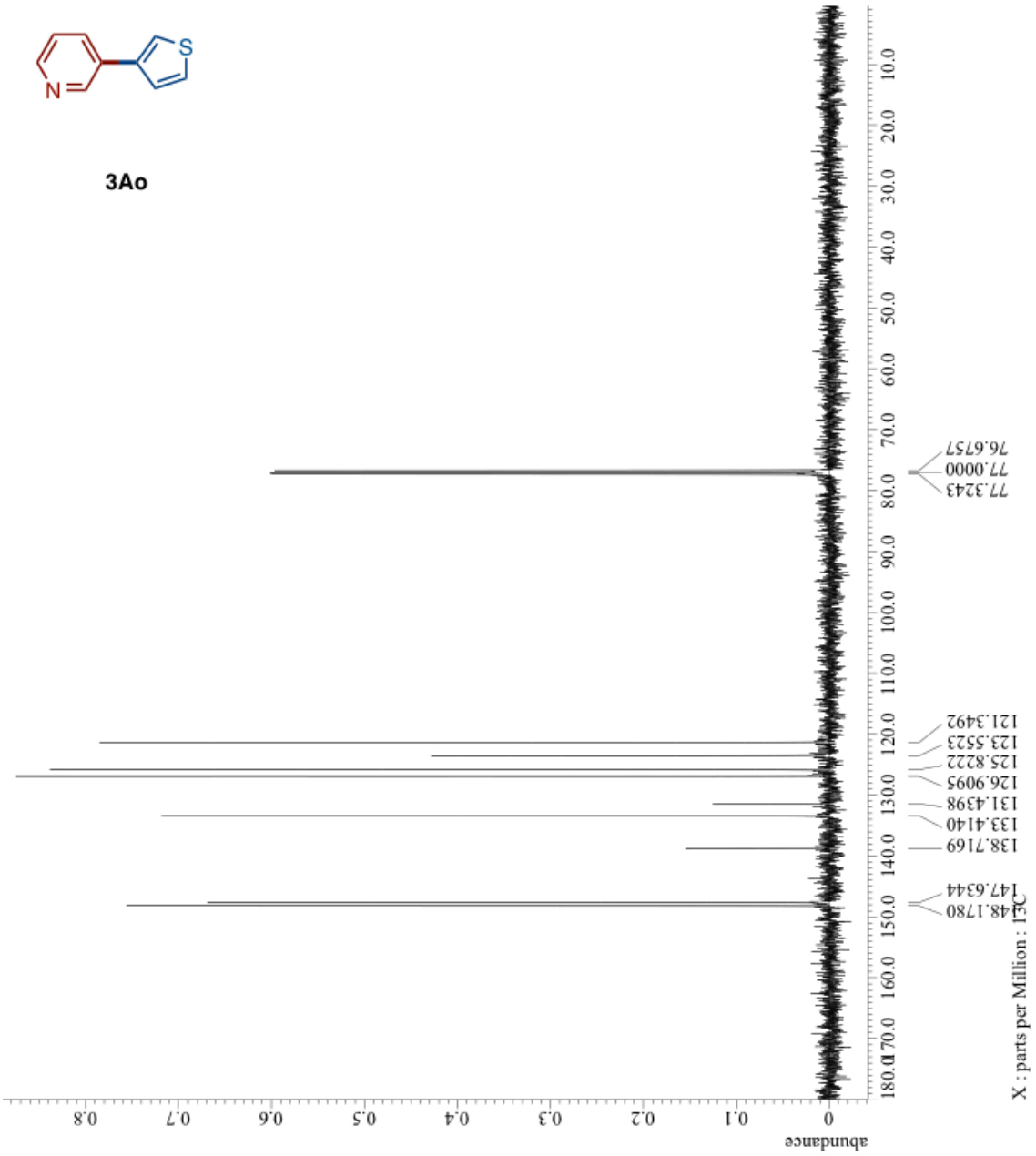
Supplementary Figure 119. ^{1}H NMR (400 MHz, $CDCl_3$) of 3An



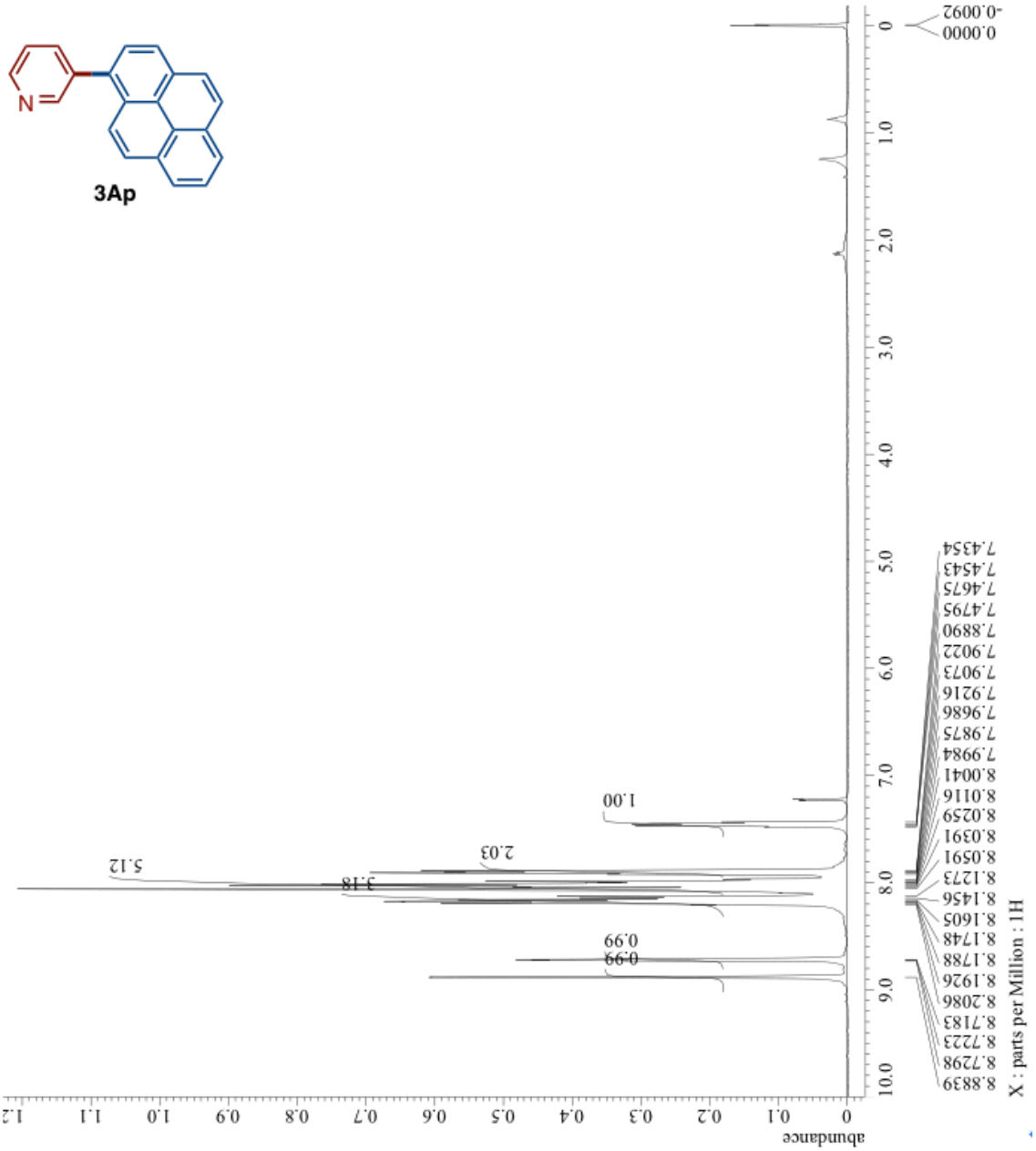
Supplementary Figure 120. ^{13}C NMR (100 MHz, $CDCl_3$) of 3An



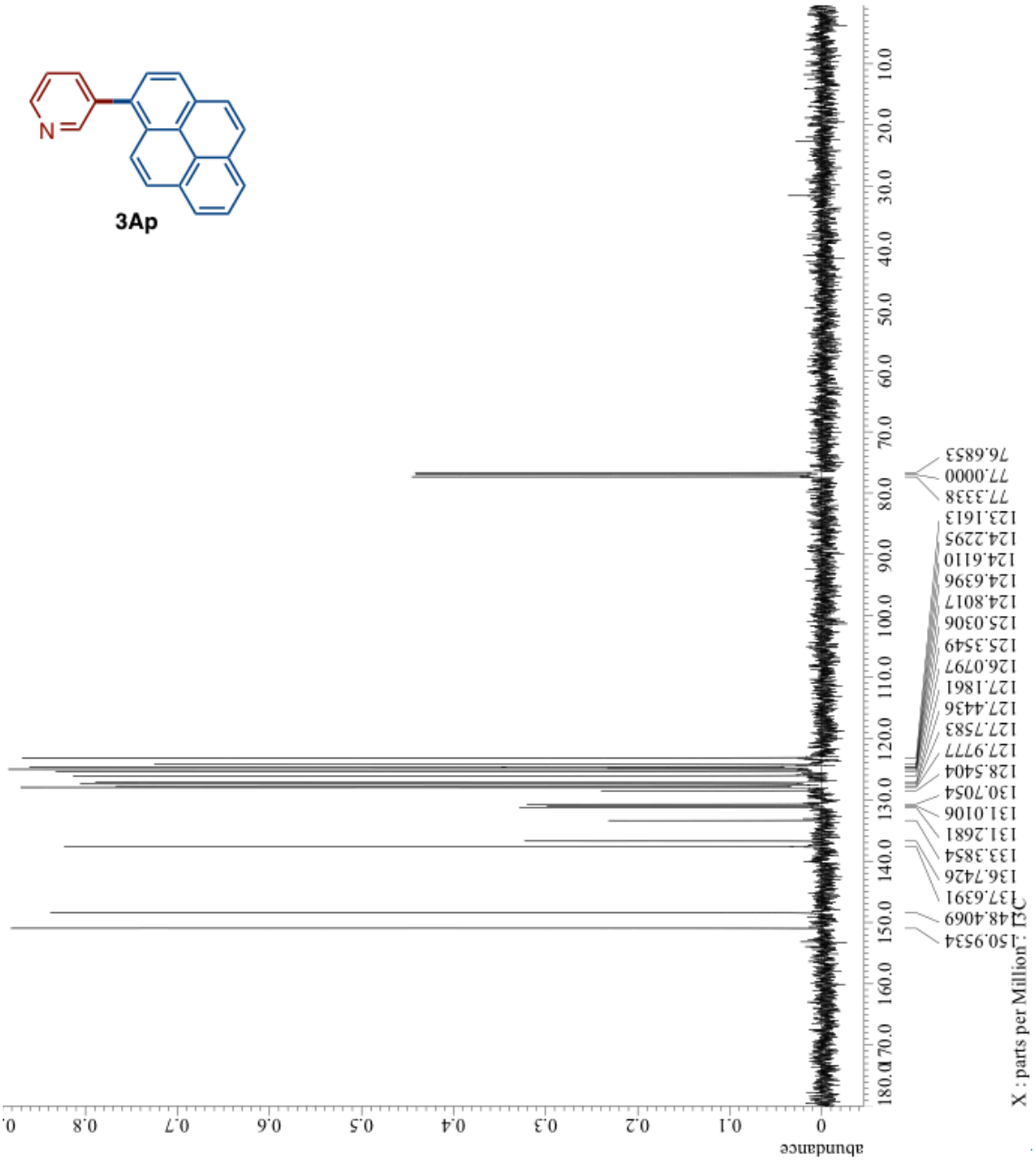
Supplementary Figure 121. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ao



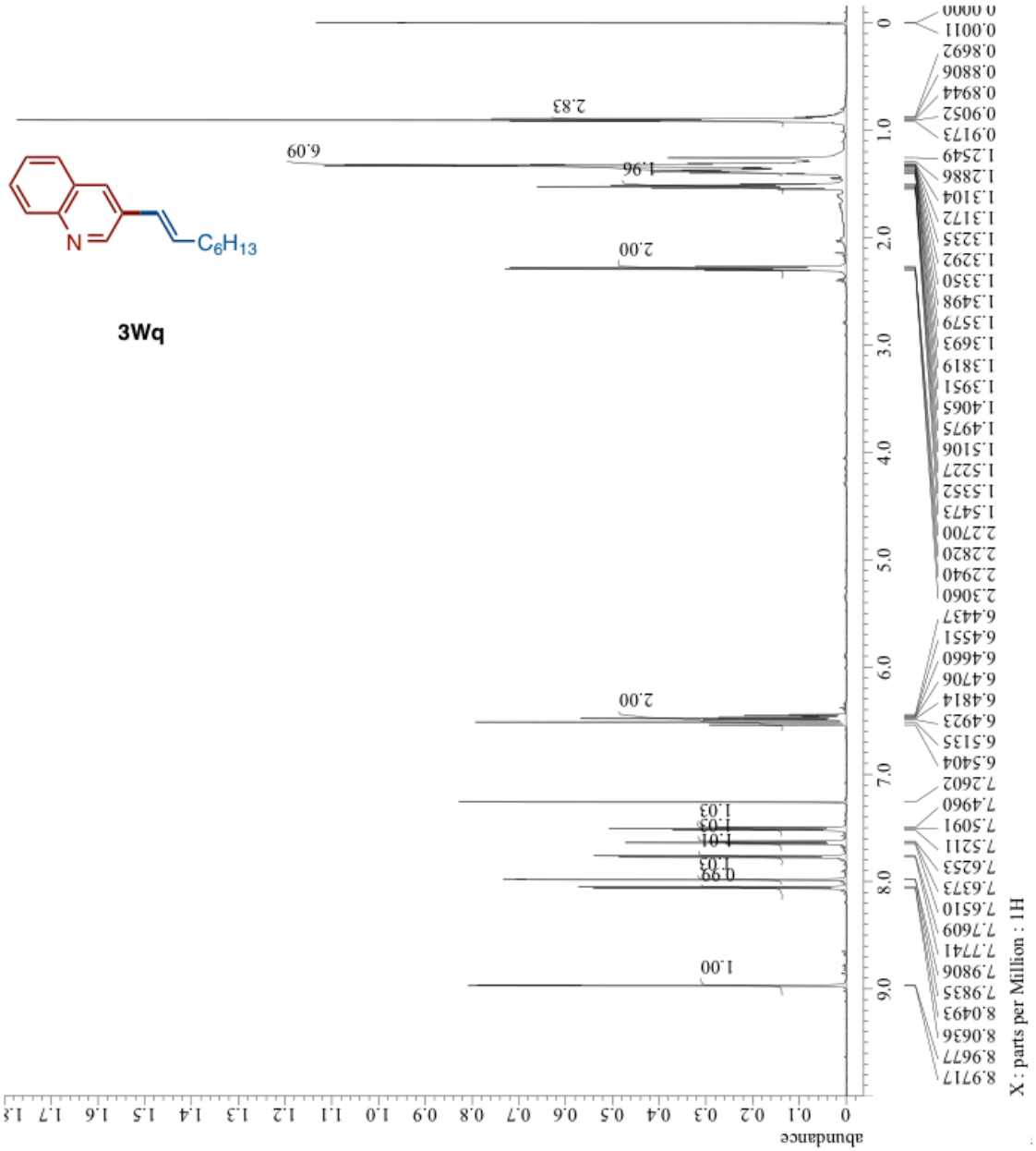
Supplementary Figure 122. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ao



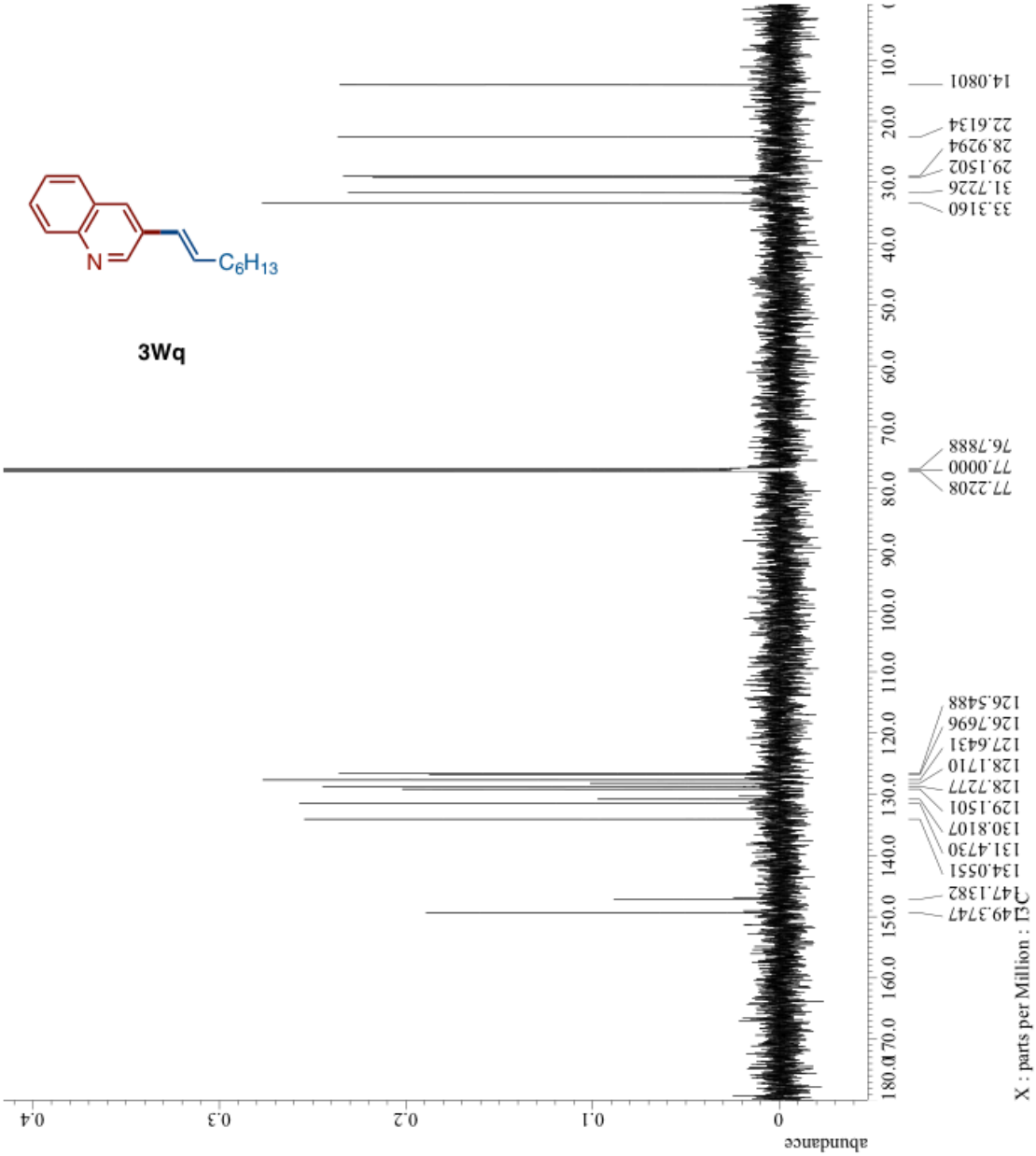
Supplementary Figure 123. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Ap



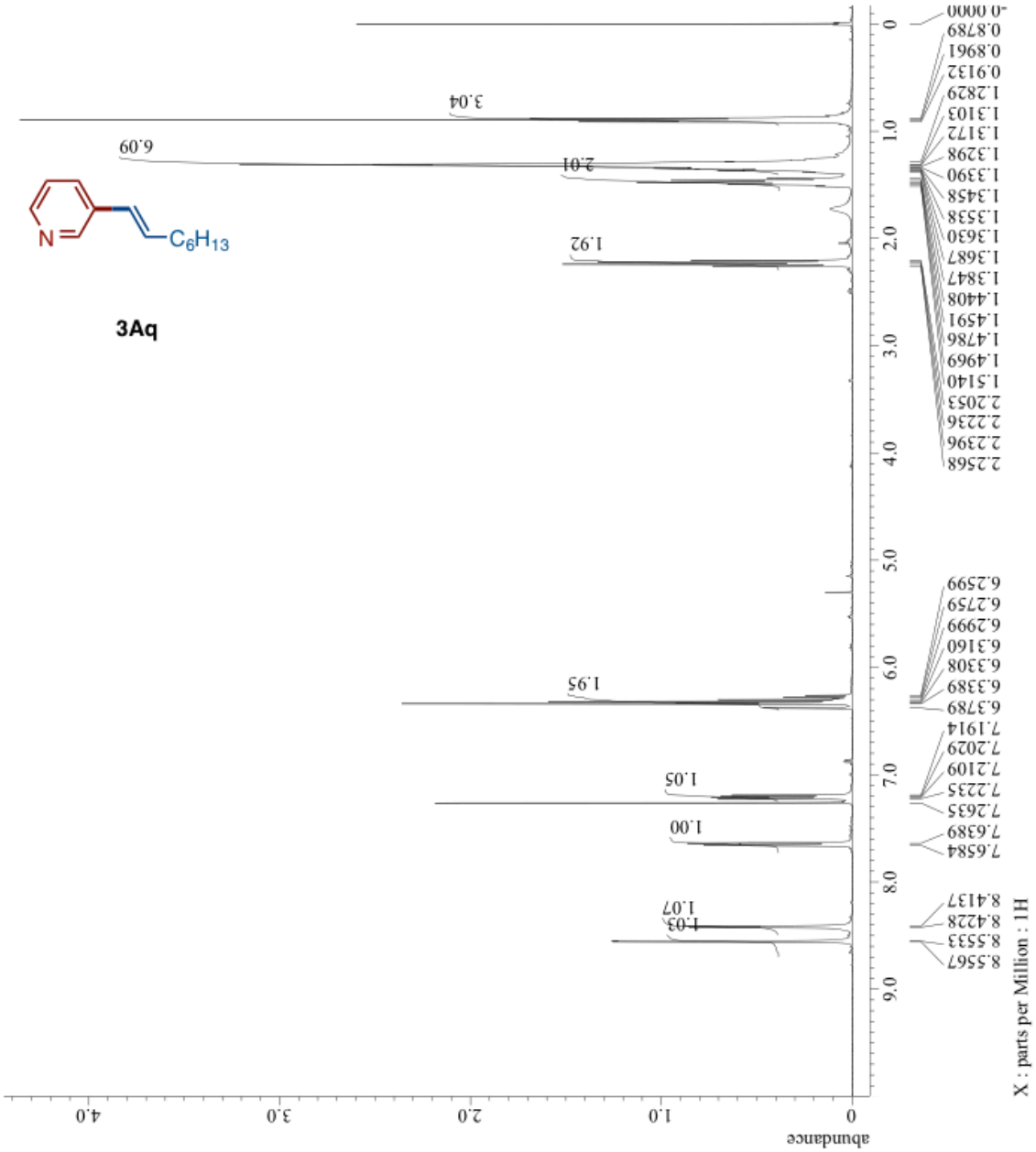
Supplementary Figure 124. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Ap



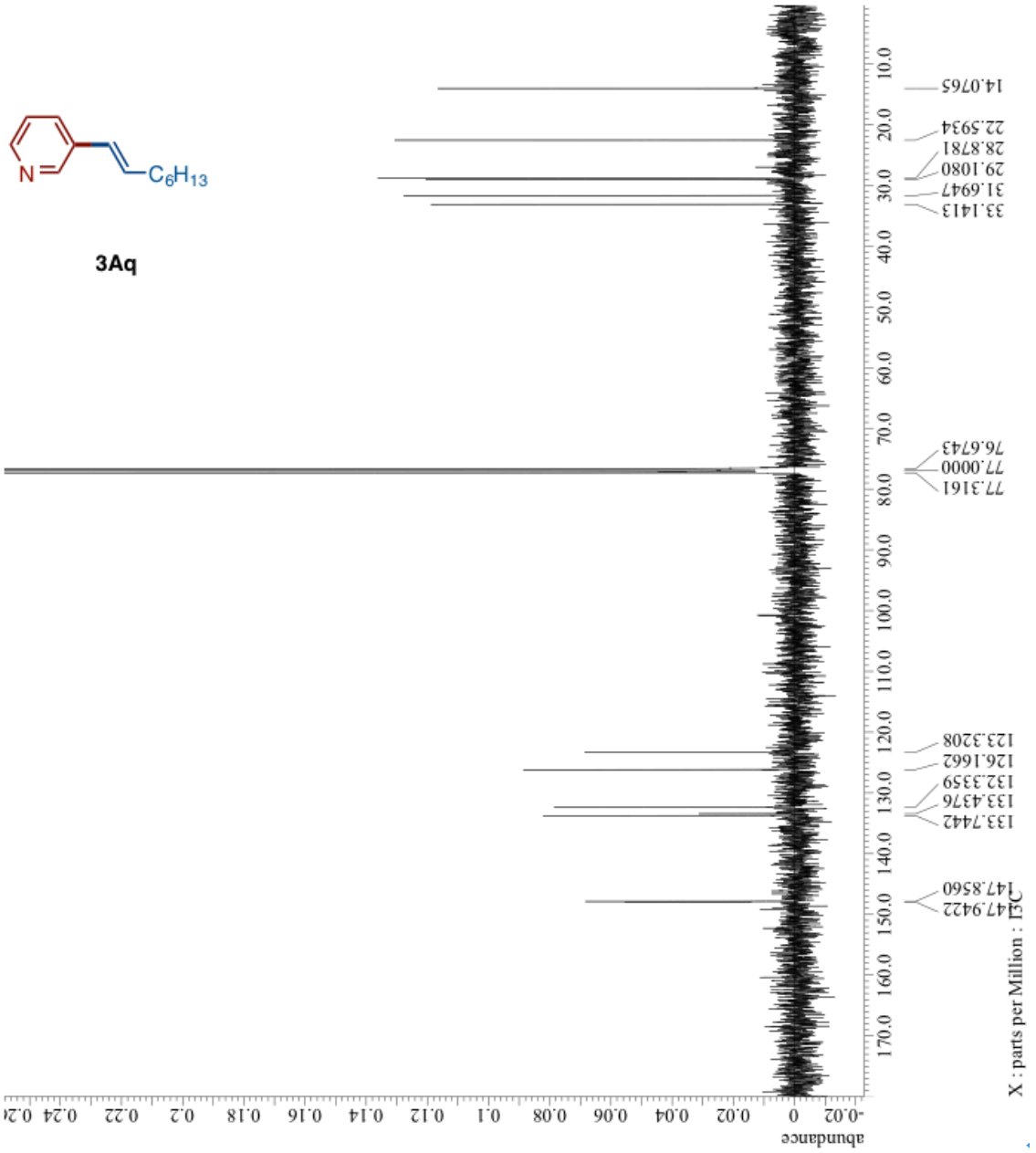
Supplementary Figure 125. ^{1}H NMR (600 MHz, $CDCl_3$) of 3Wq



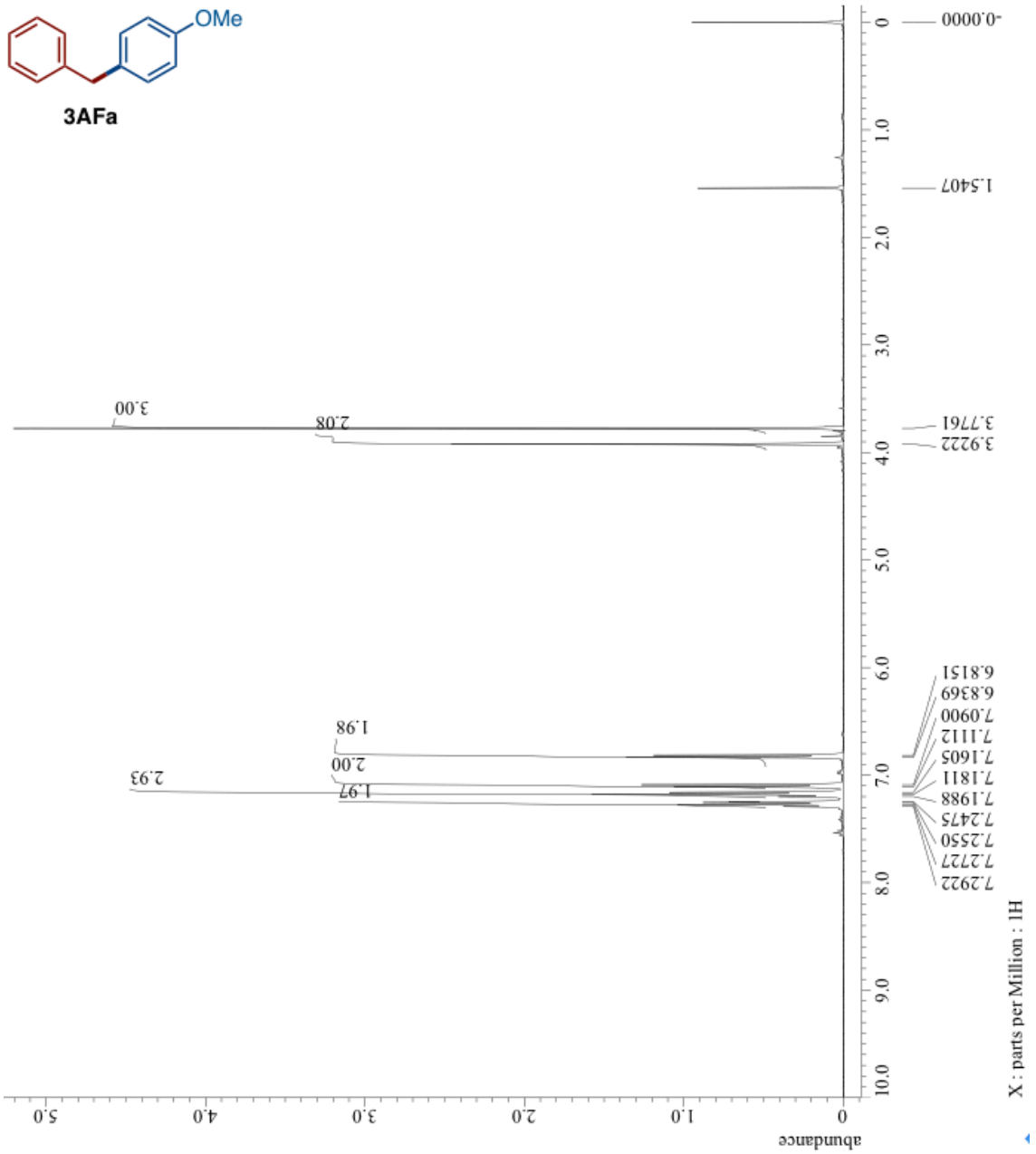
Supplementary Figure 126. ^{13}C NMR (150 MHz, $CDCl_3$) of 3Wq



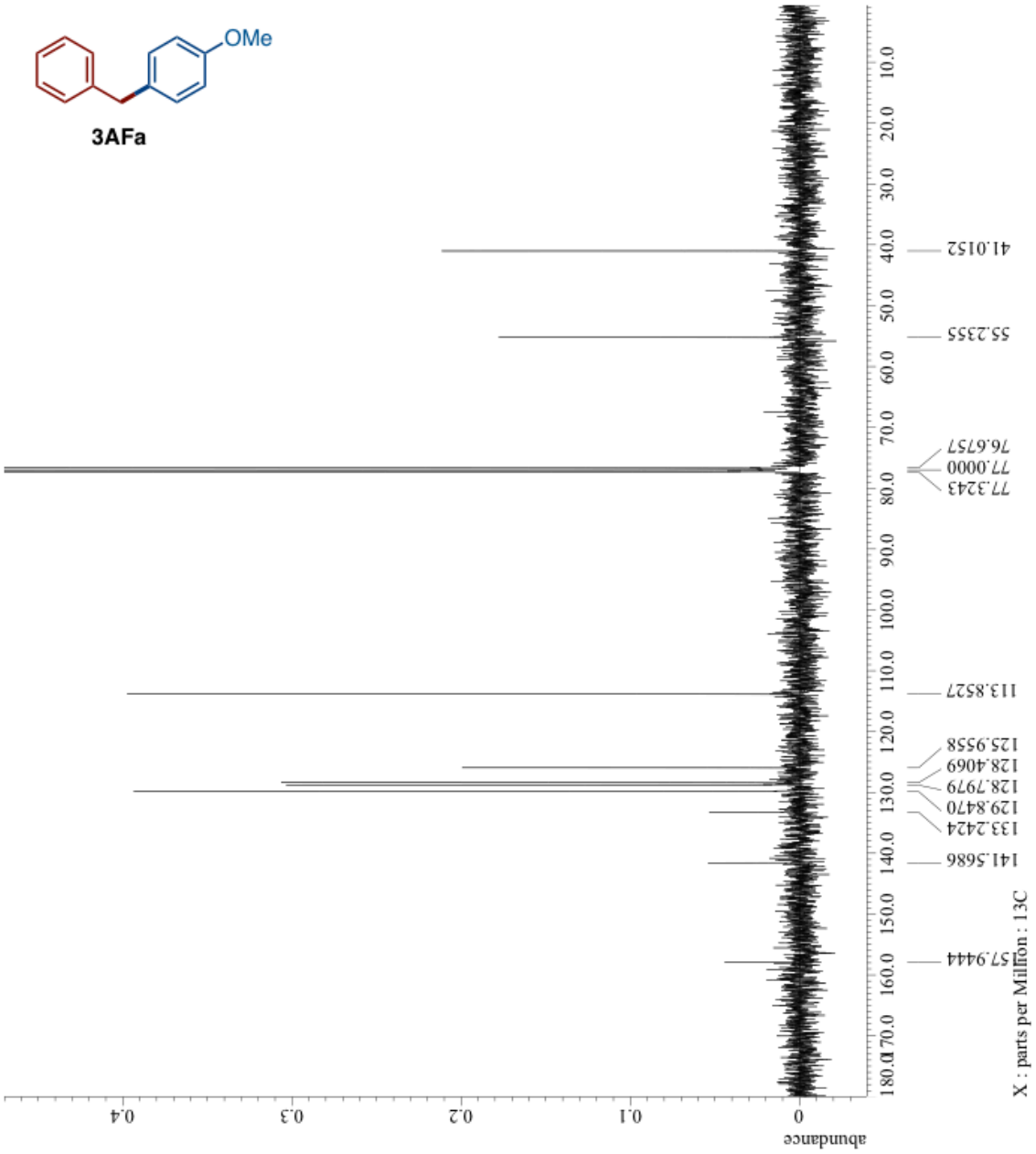
Supplementary Figure 127. ^{1}H NMR (400 MHz, $CDCl_3$) of 3Aq



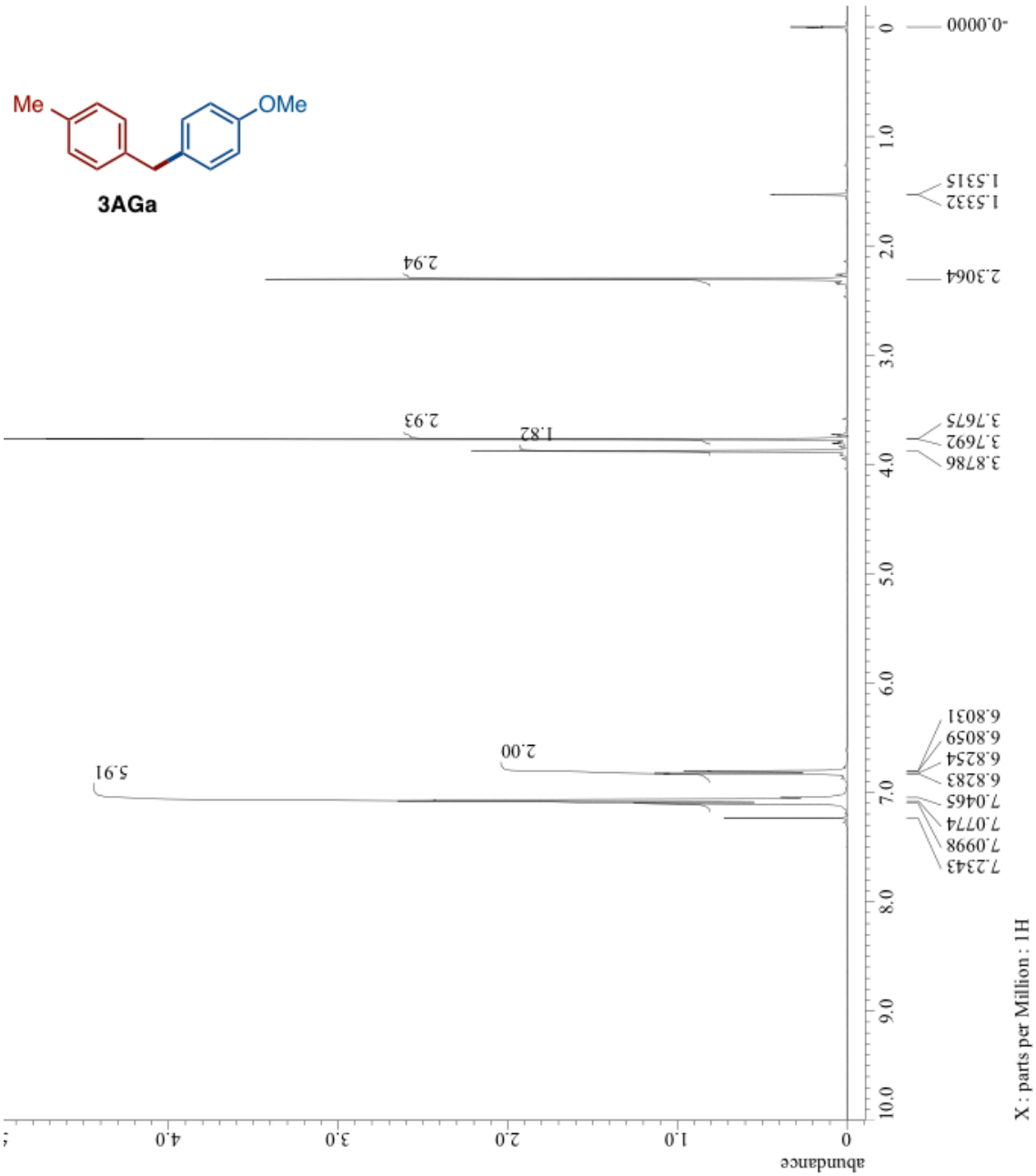
Supplementary Figure 128. ^{13}C NMR (100 MHz, $CDCl_3$) of 3Aq



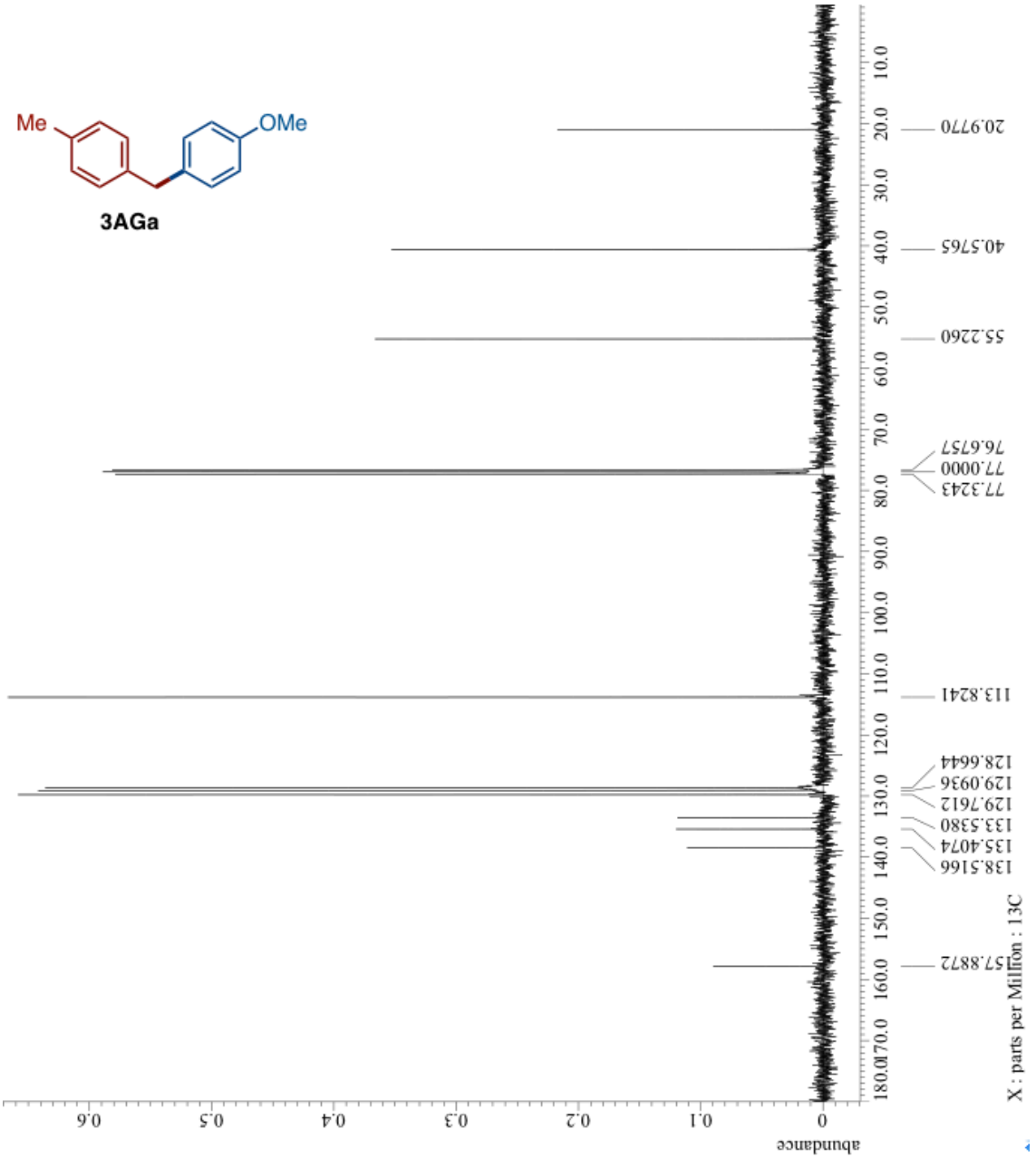
Supplementary Figure 129. ^{1}H NMR (400 MHz, $CDCl_3$) of 3AFa



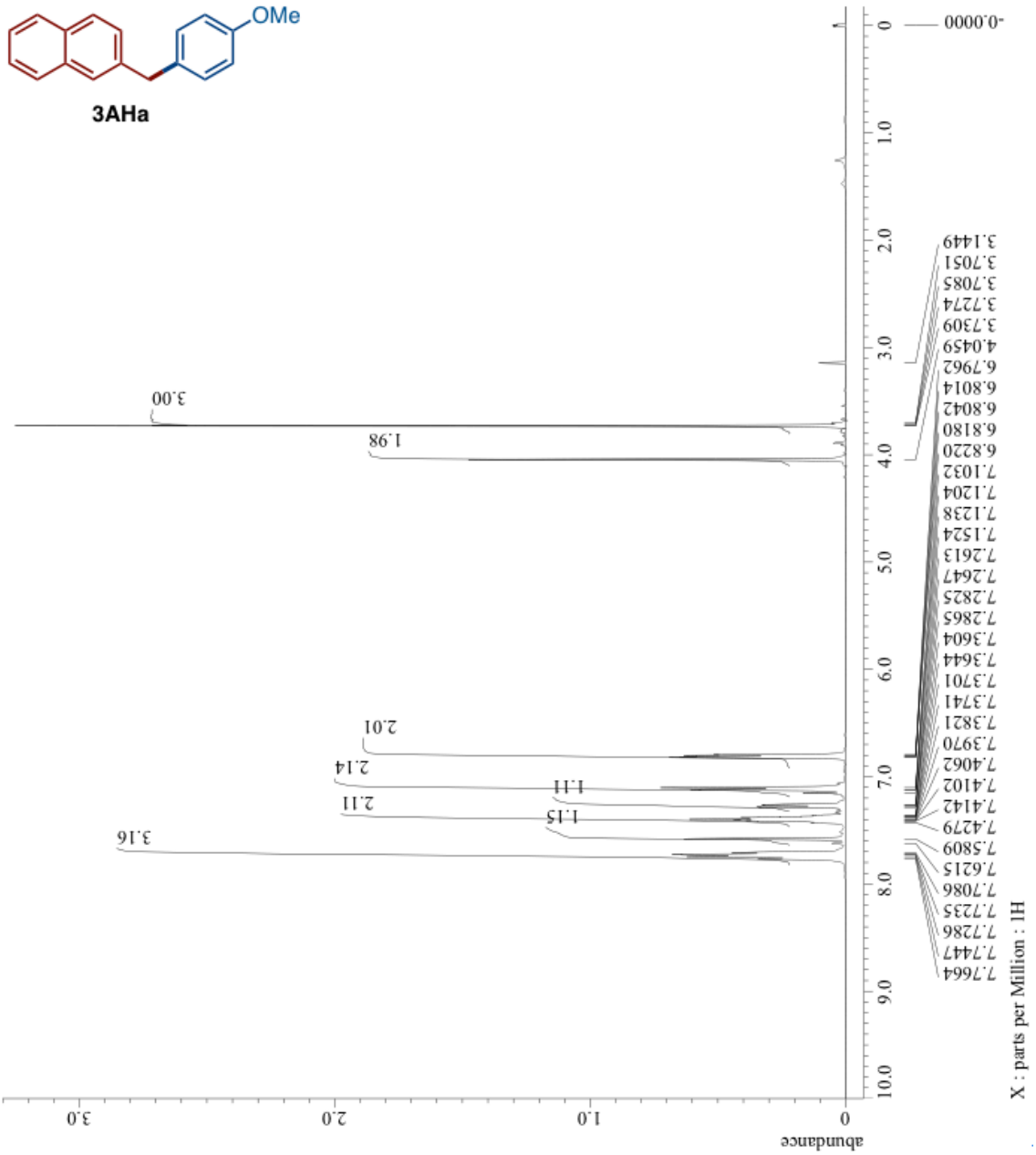
Supplementary Figure 130. ^{13}C NMR (100 MHz, $CDCl_3$) of 3AFa



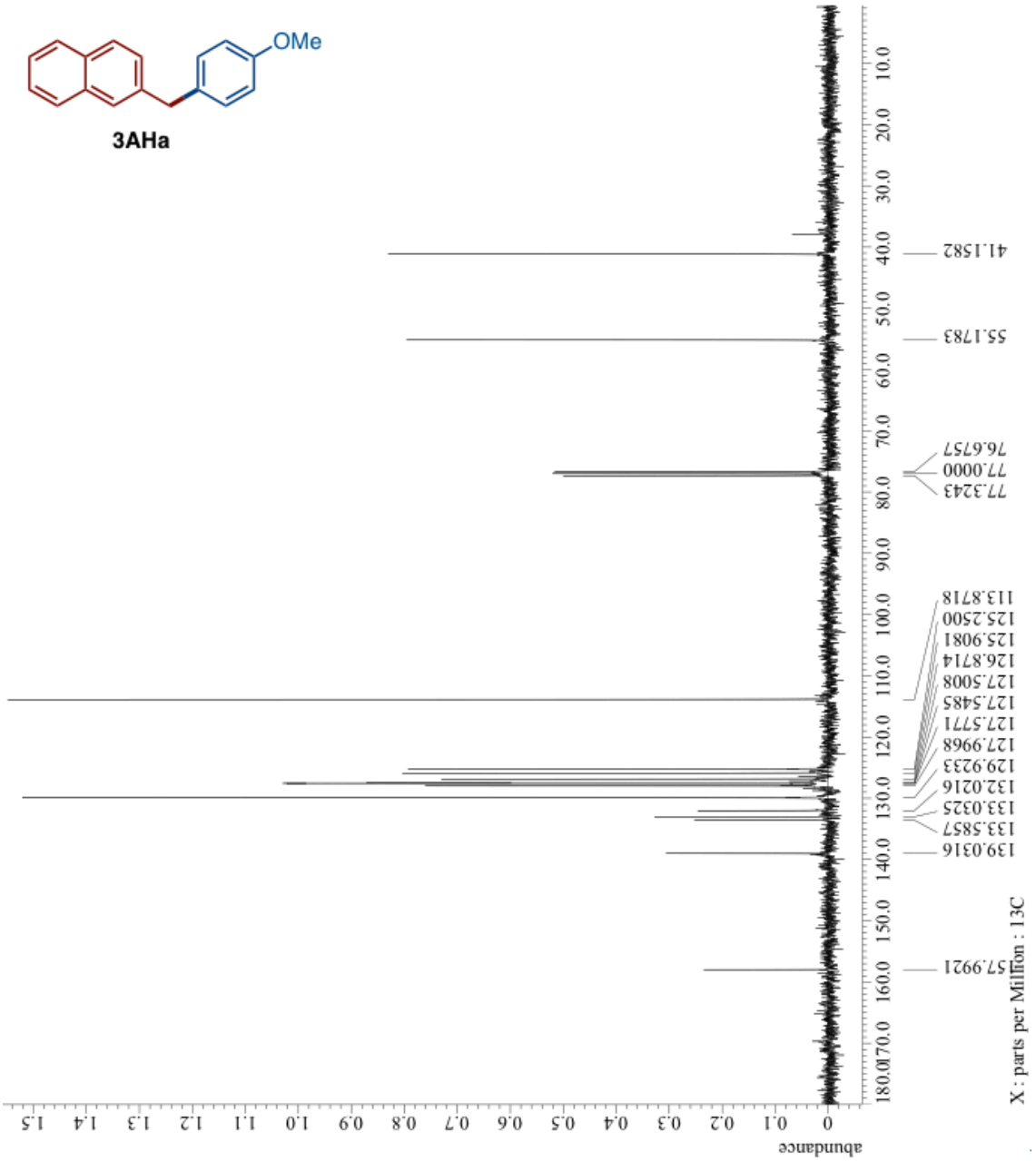
Supplementary Figure 131. ^{1}H NMR (400 MHz, $CDCl_3$) of 3AGa



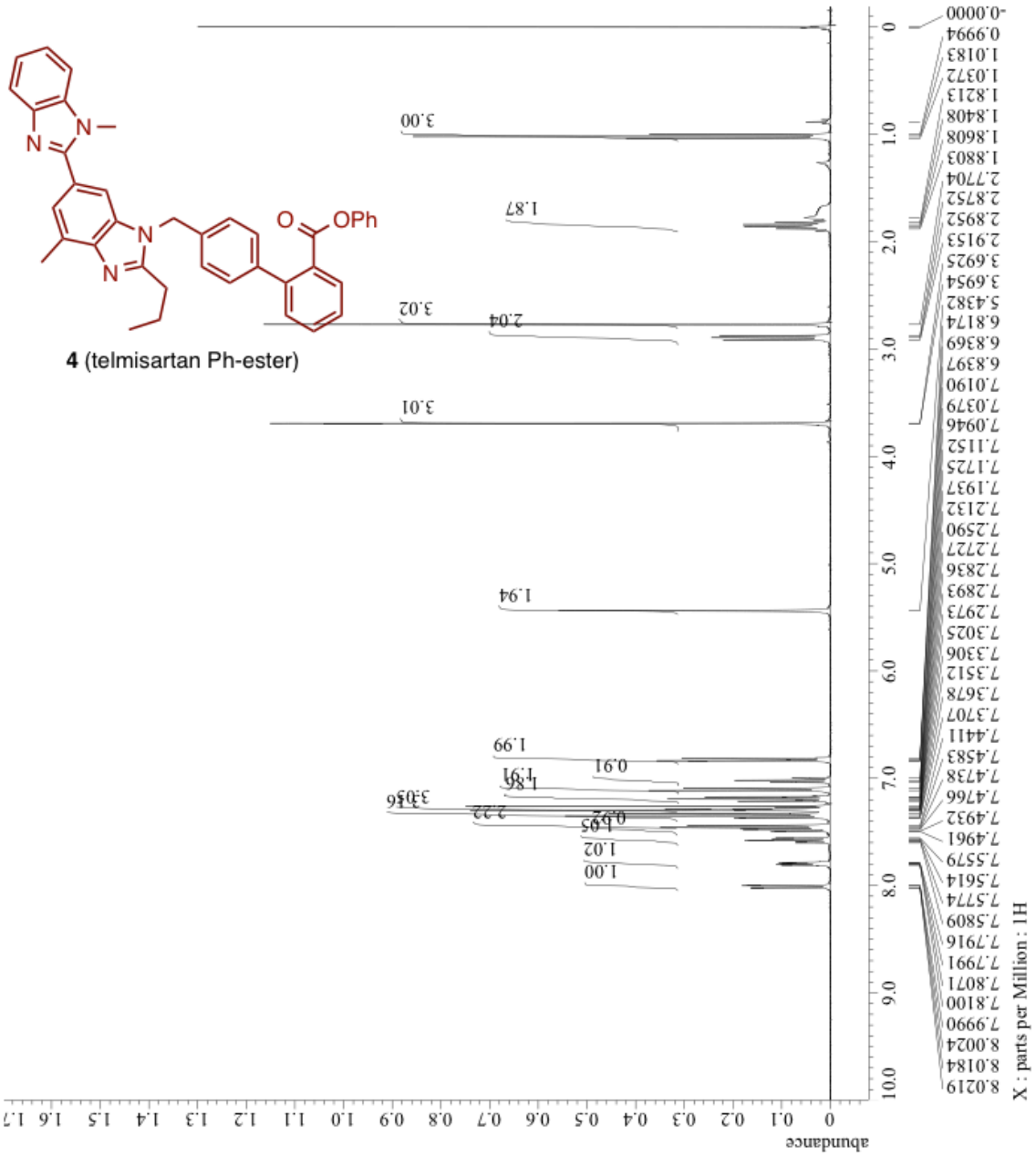
Supplementary Figure 132. ^{13}C NMR (100 MHz, $CDCl_3$) of 3AGa



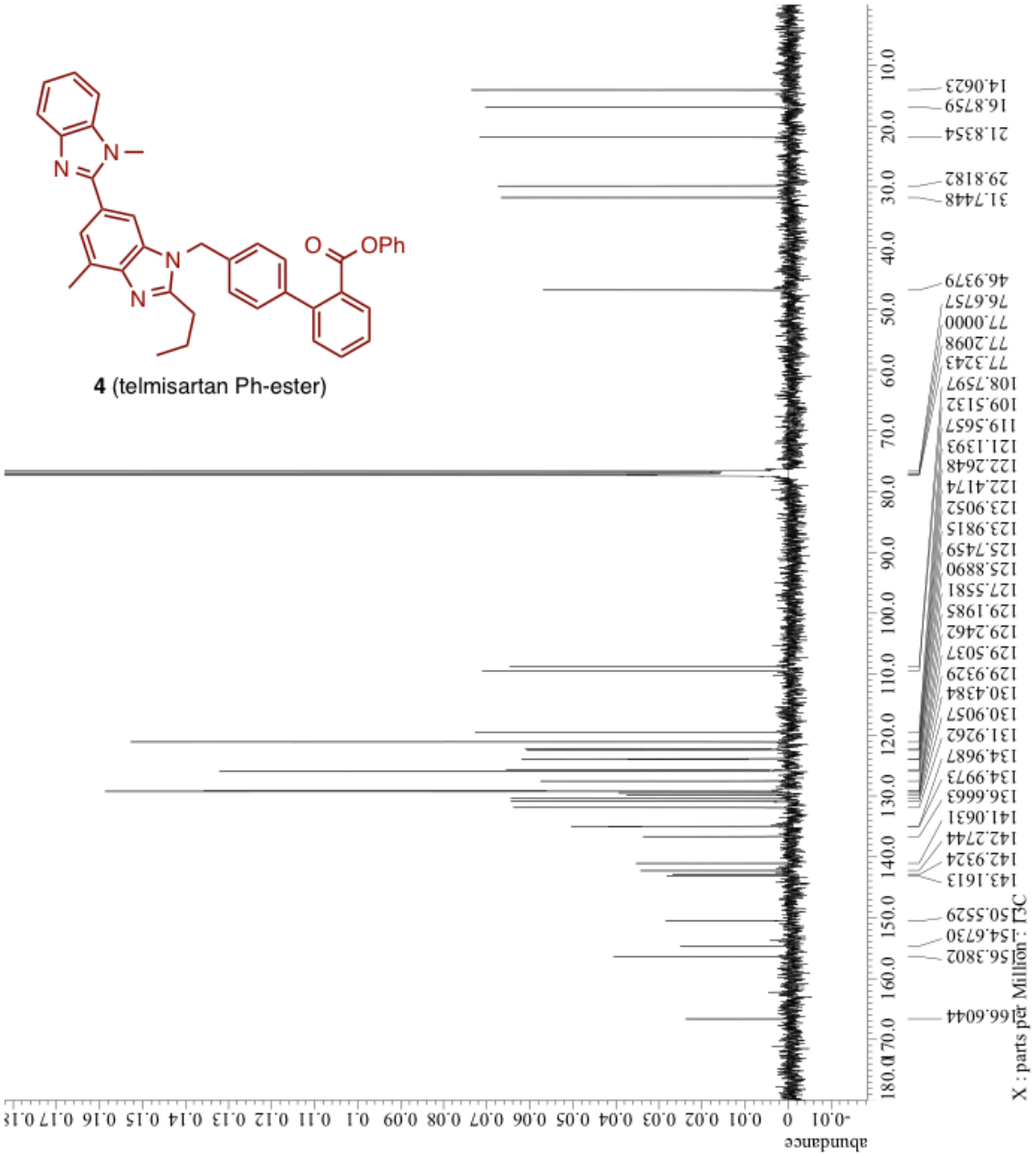
Supplementary Figure 133. ^{1}H NMR (400 MHz, $CDCl_3$) of 3AHa



Supplementary Figure 134. ^{13}C NMR (100 MHz, $CDCl_3$) of 3AHa



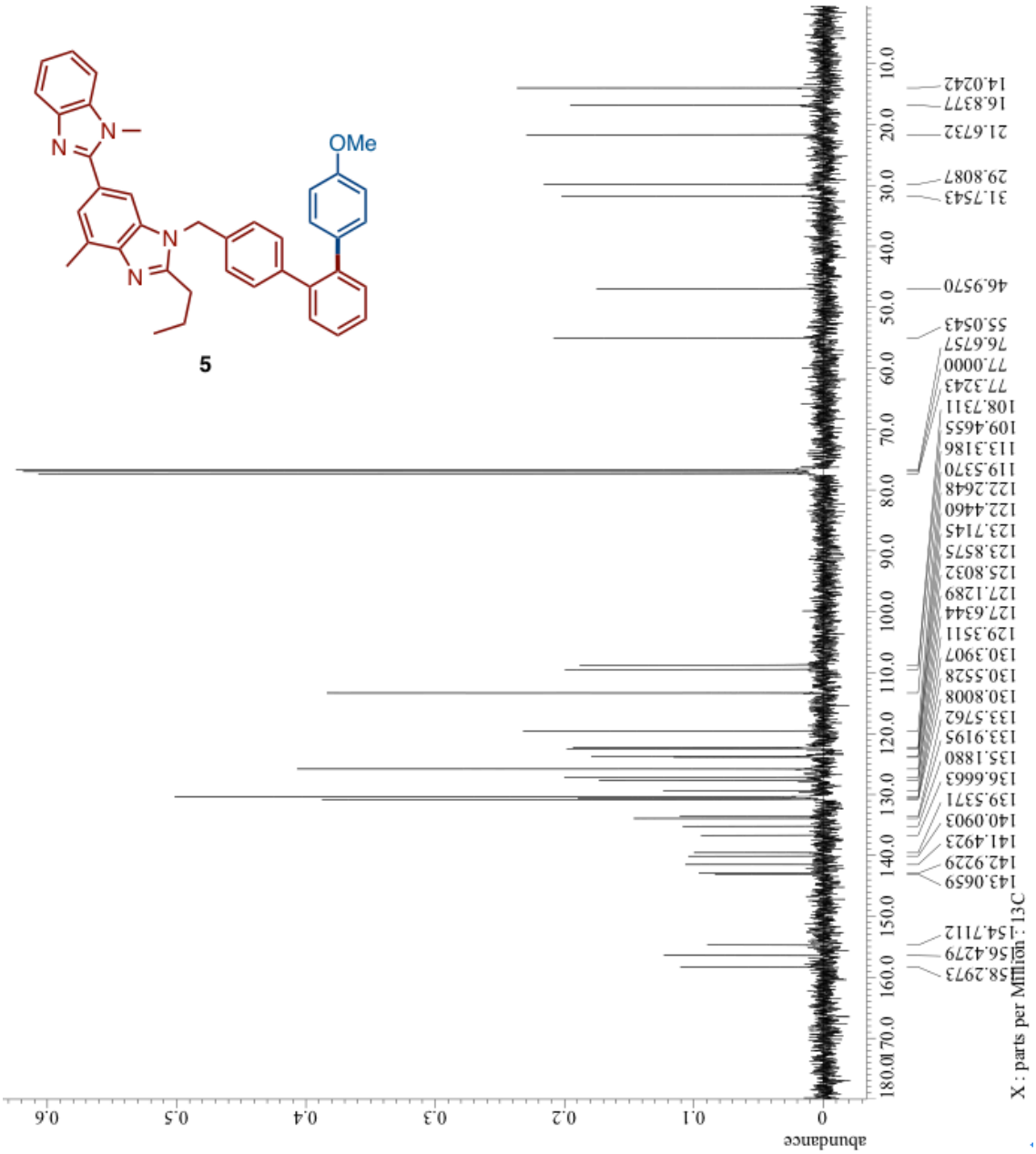
Supplementary Figure 135. ^{1}H NMR (400 MHz, $CDCl_3$) of 4



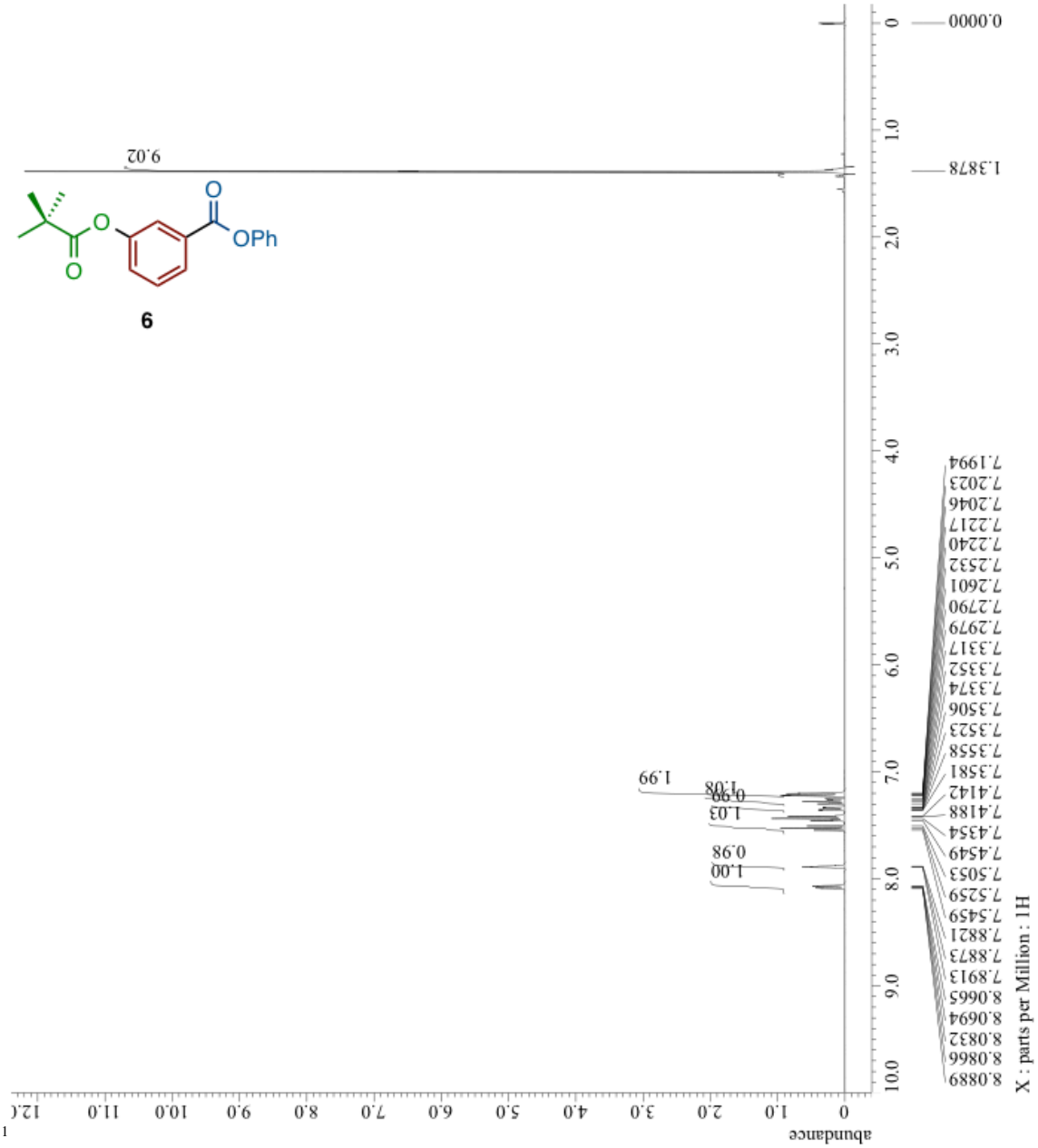
Supplementary Figure 136. ^{13}C NMR (100 MHz, $CDCl_3$) of 4



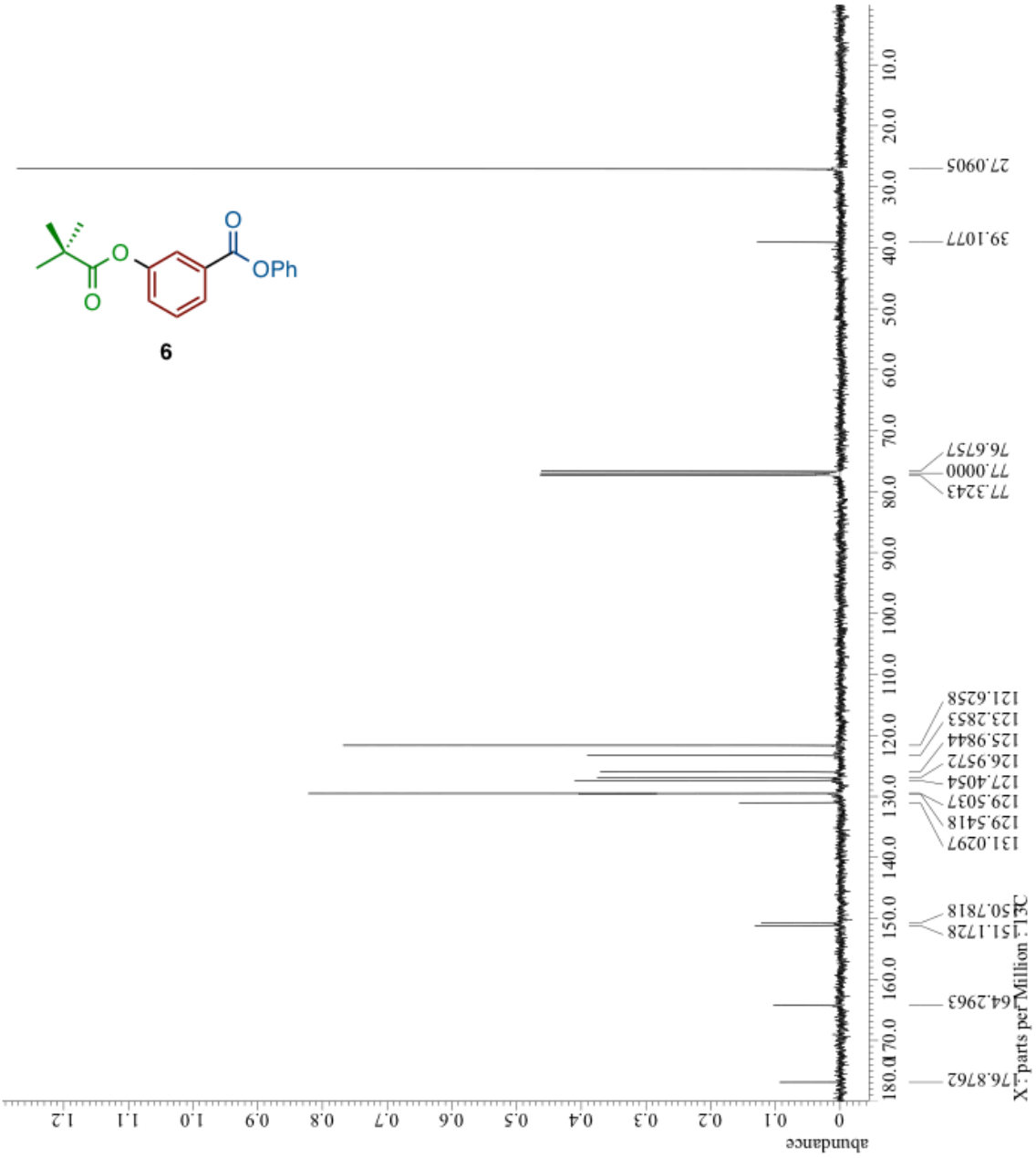
Supplementary Figure 137. ^{1}H NMR (400 MHz, $CDCl_3$) of 5



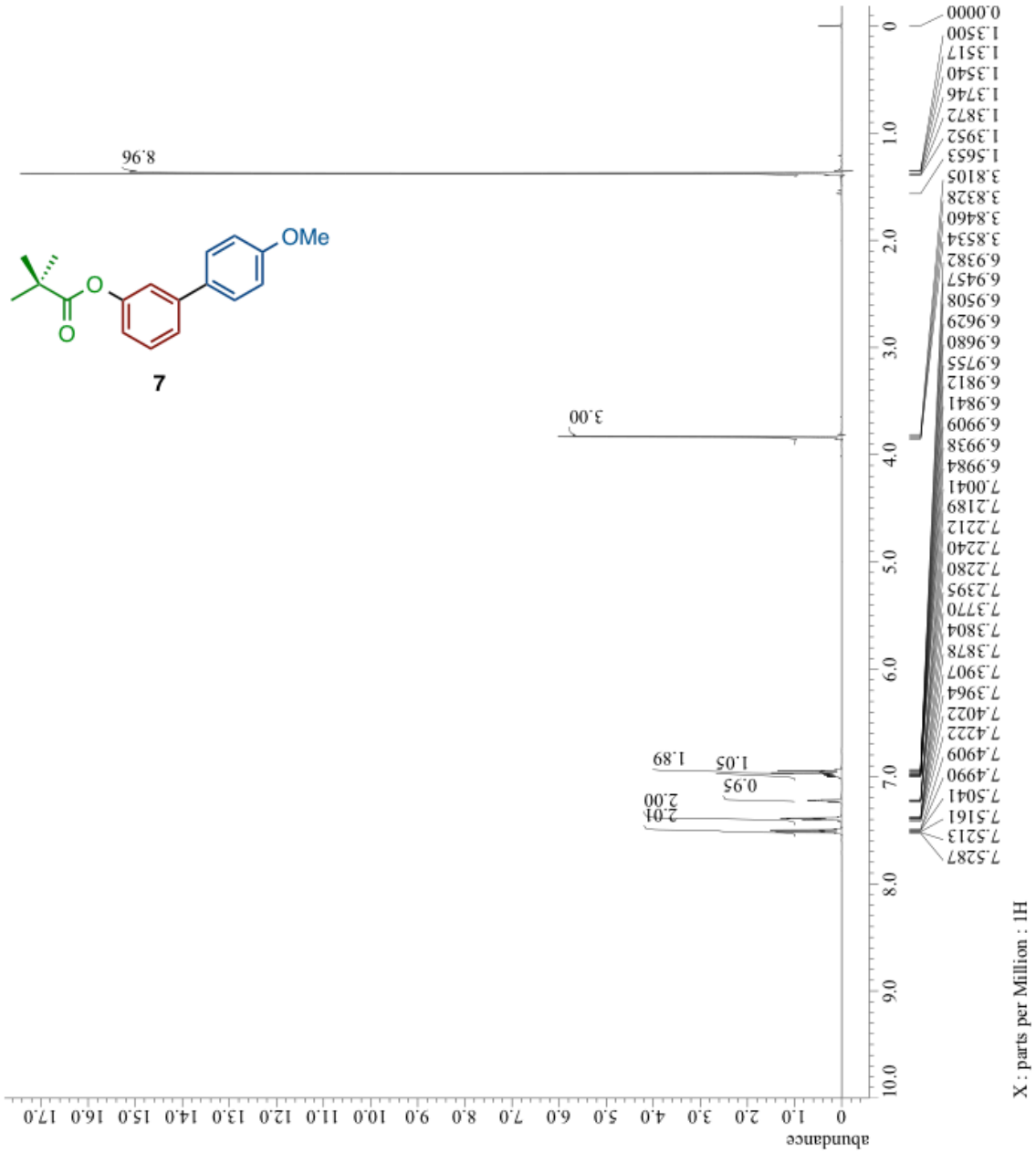
Supplementary Figure 138. ^{13}C NMR (100 MHz, $CDCl_3$) of 5



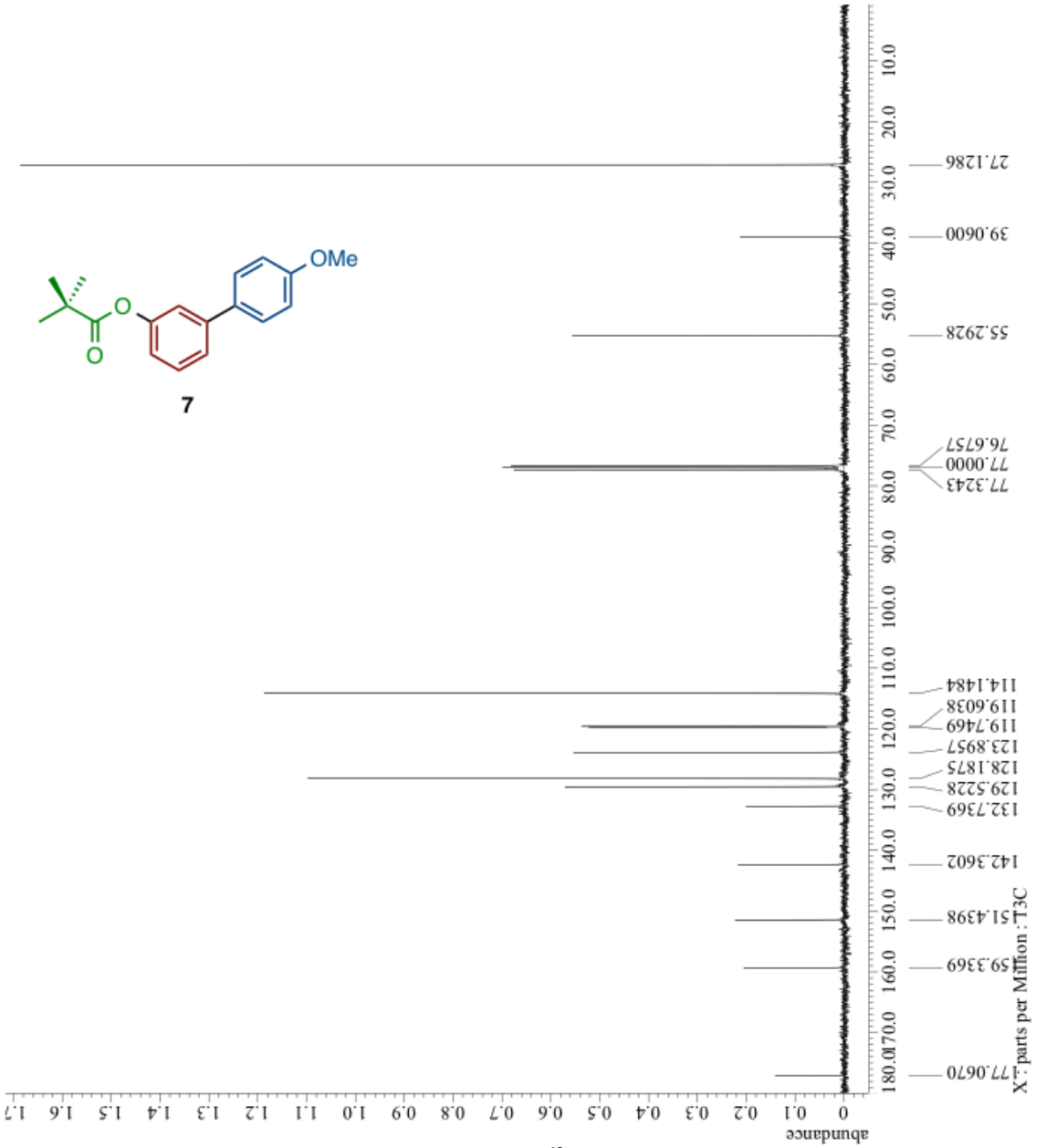
Supplementary Figure 139. ^{1}H NMR (400 MHz, $CDCl_3$) of 6



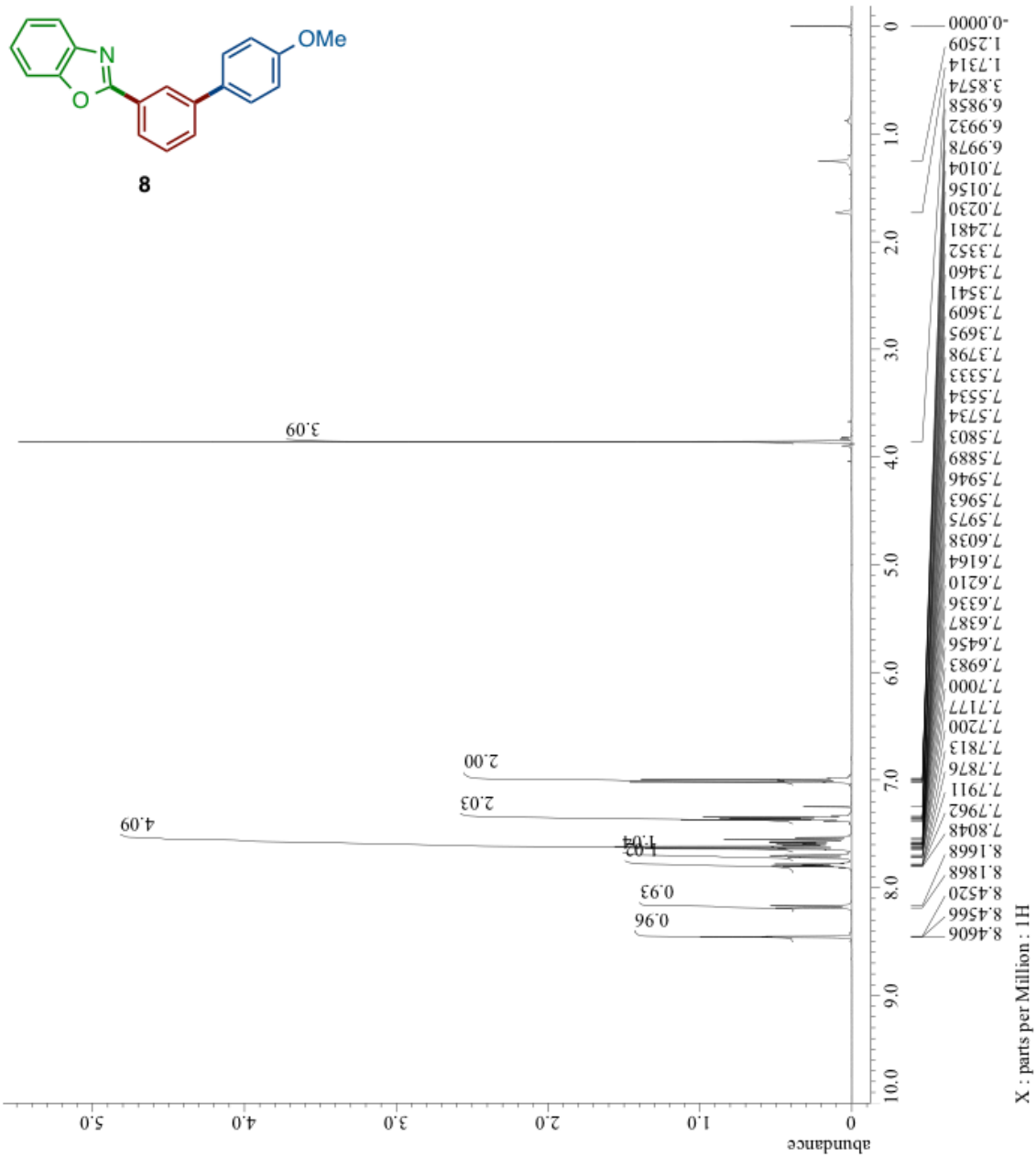
Supplementary Figure 140. ^{13}C NMR (100 MHz, $CDCl_3$) of 6



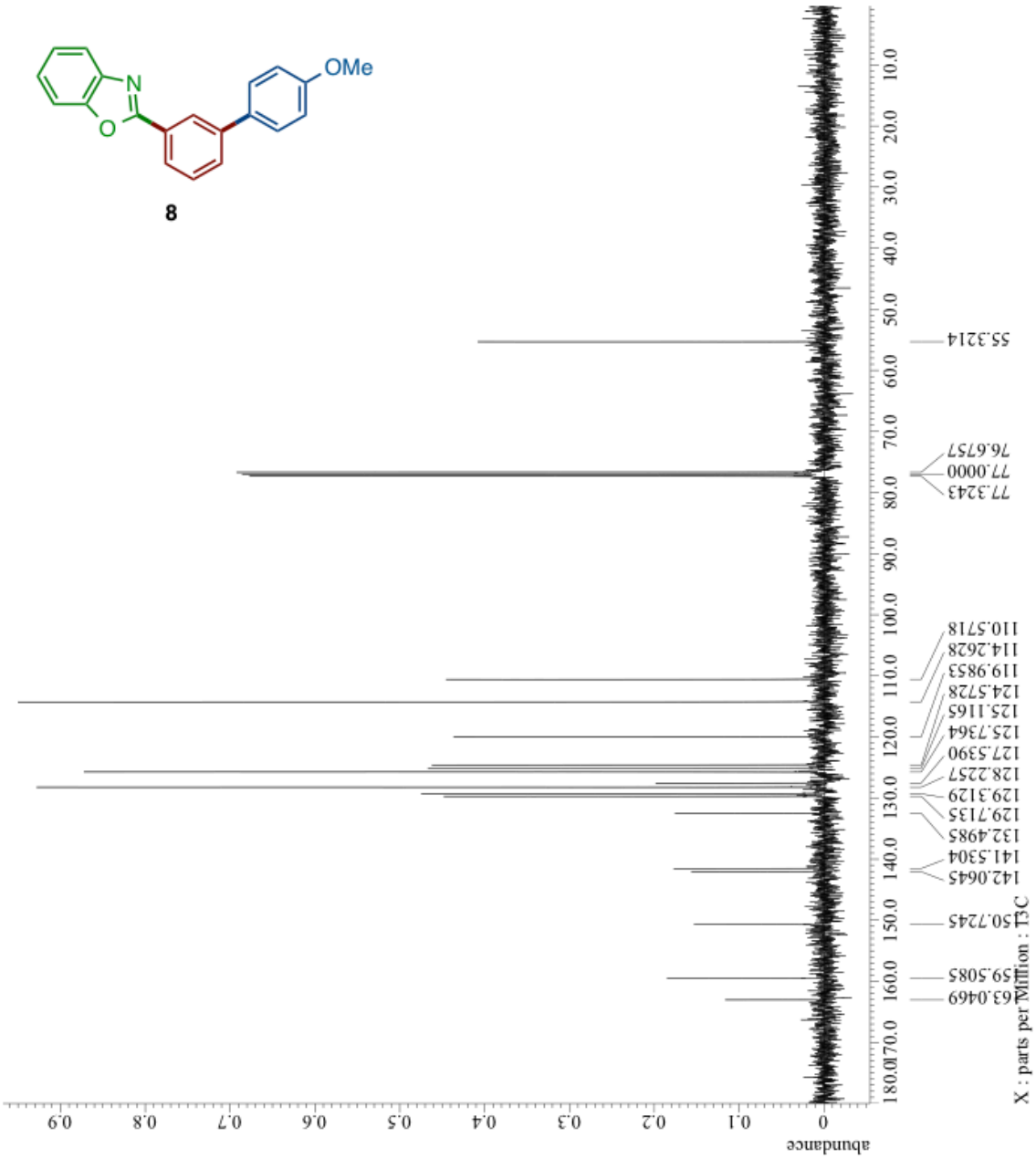
Supplementary Figure 141. ^{1}H NMR (400 MHz, $CDCl_3$) of 7



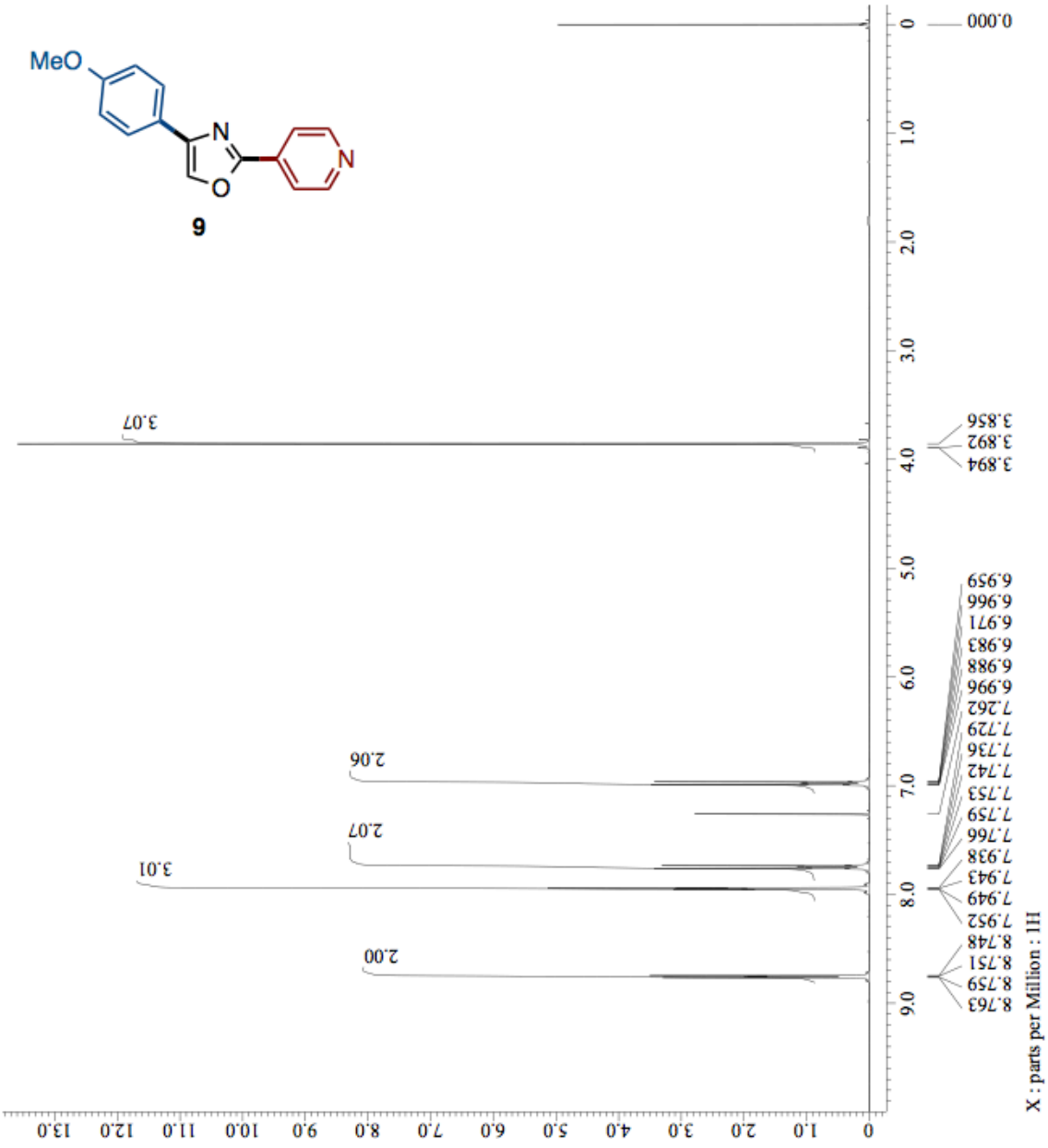
Supplementary Figure 142. ^{13}C NMR (100 MHz, $CDCl_3$) of 7



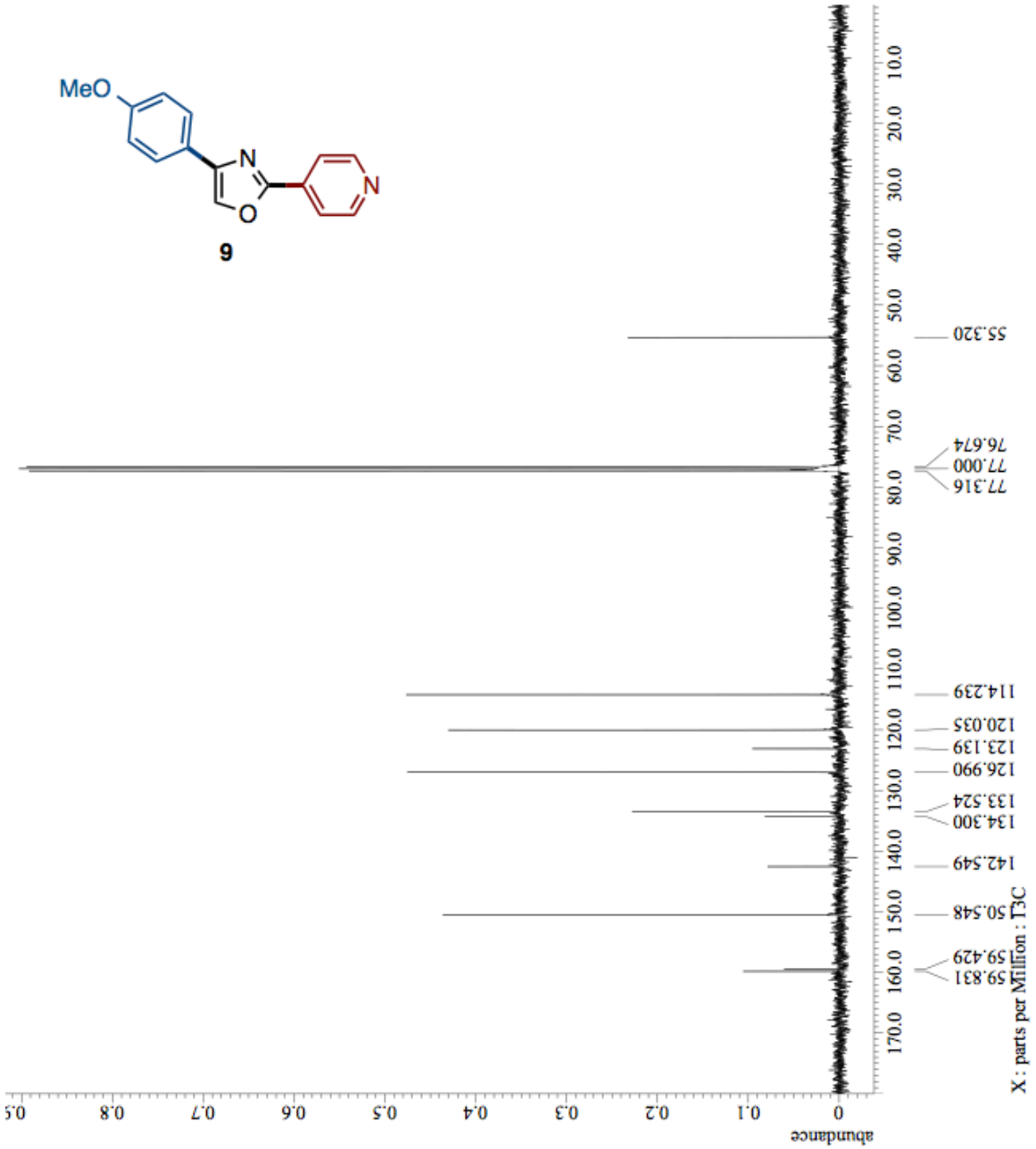
Supplementary Figure 143. ^{1}H NMR (400 MHz, $CDCl_3$) of 8



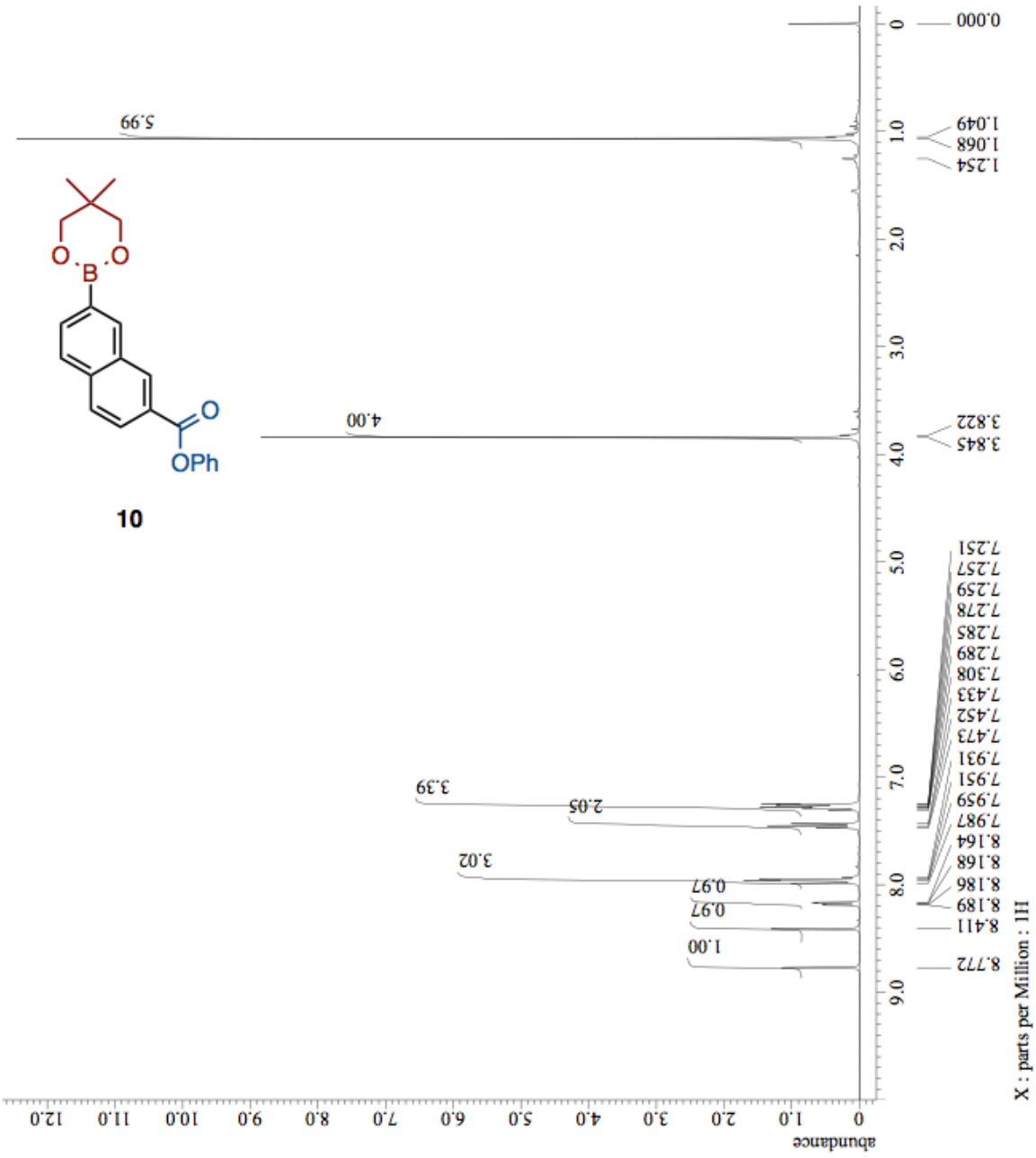
Supplementary Figure 144. ^{13}C NMR (100 MHz, $CDCl_3$) of 8



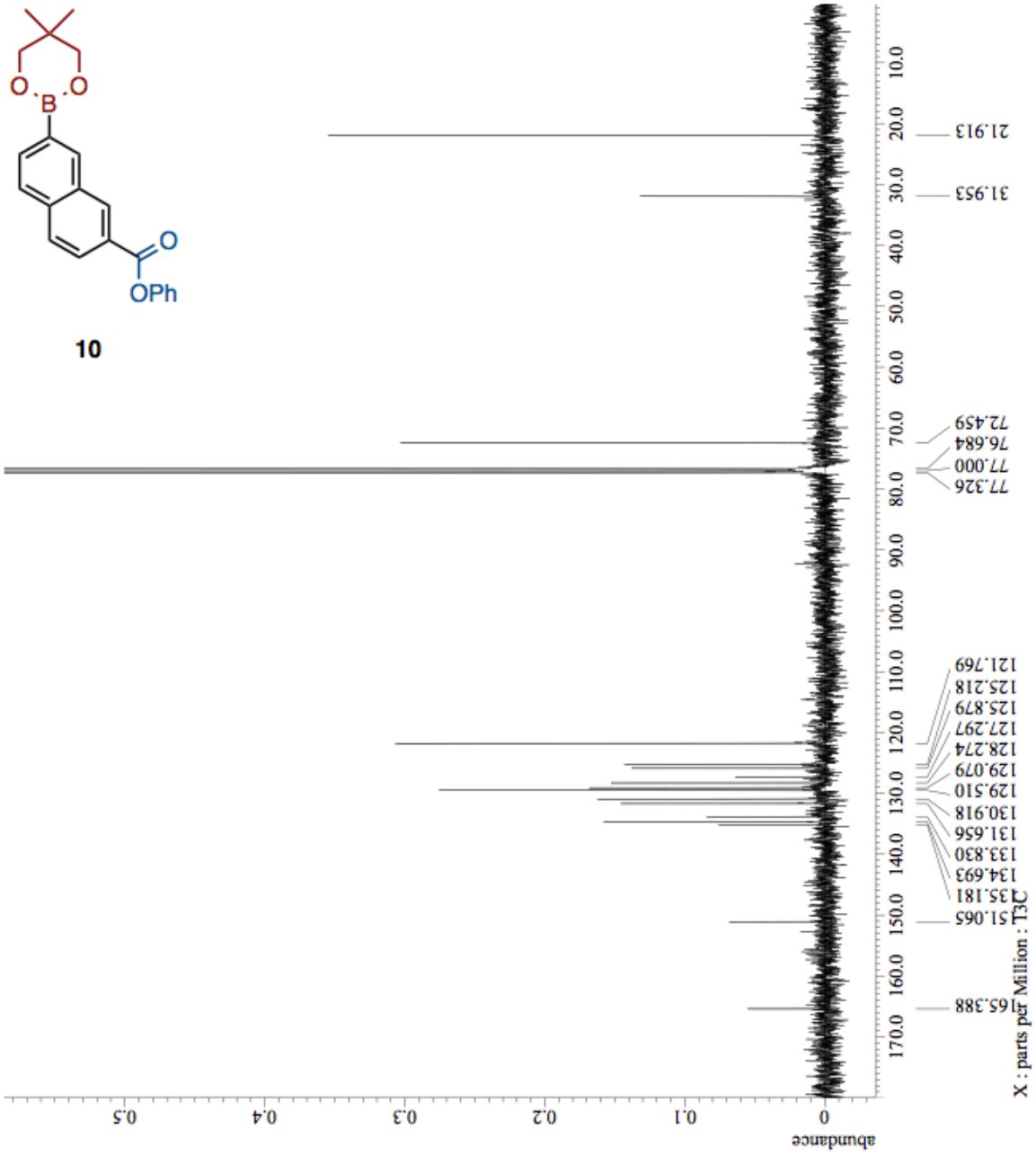
Supplementary Figure 145. ^{1}H NMR (400 MHz, $CDCl_3$) of 9



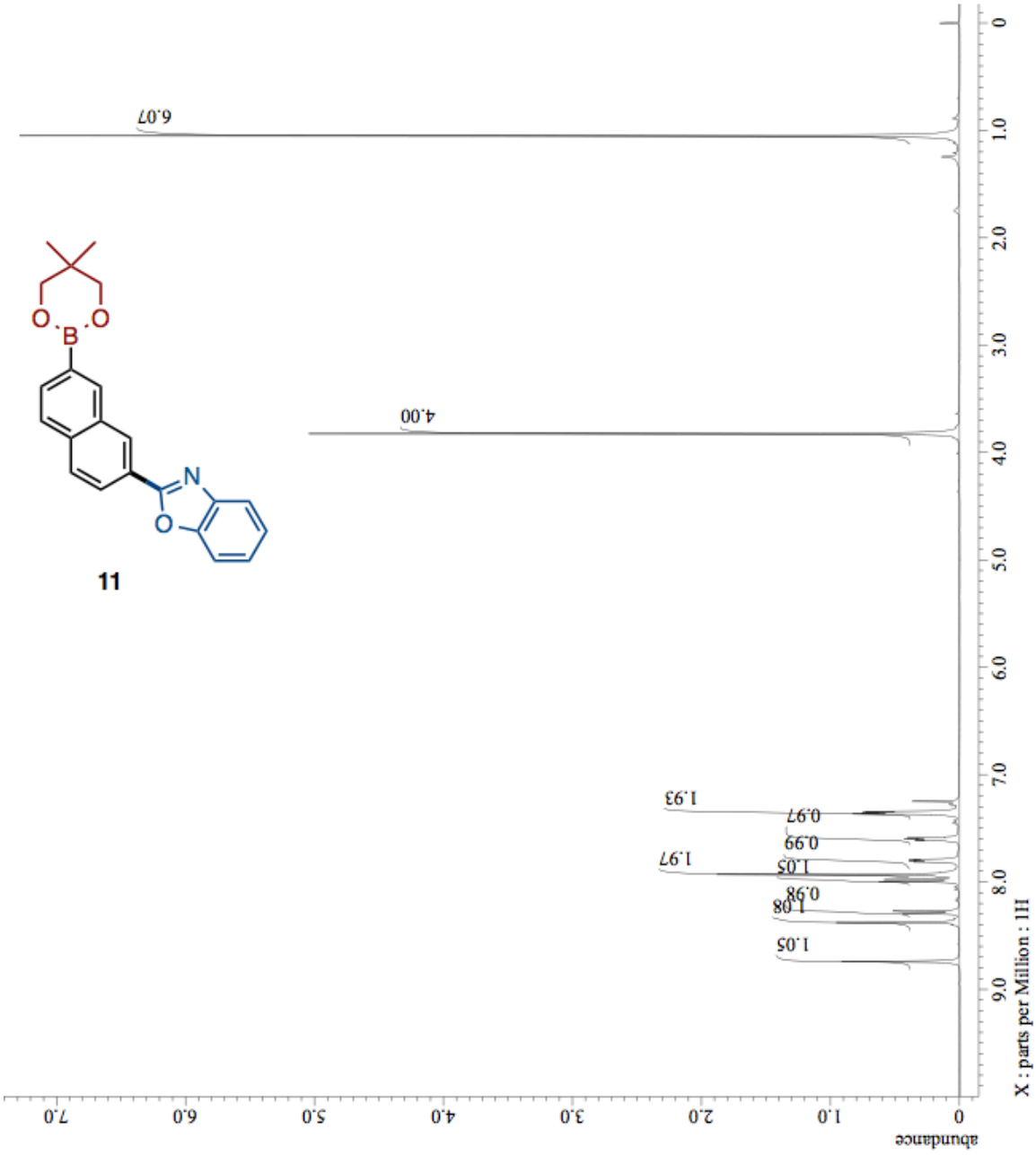
Supplementary Figure 146. ^{13}C NMR (100 MHz, $CDCl_3$) of 9



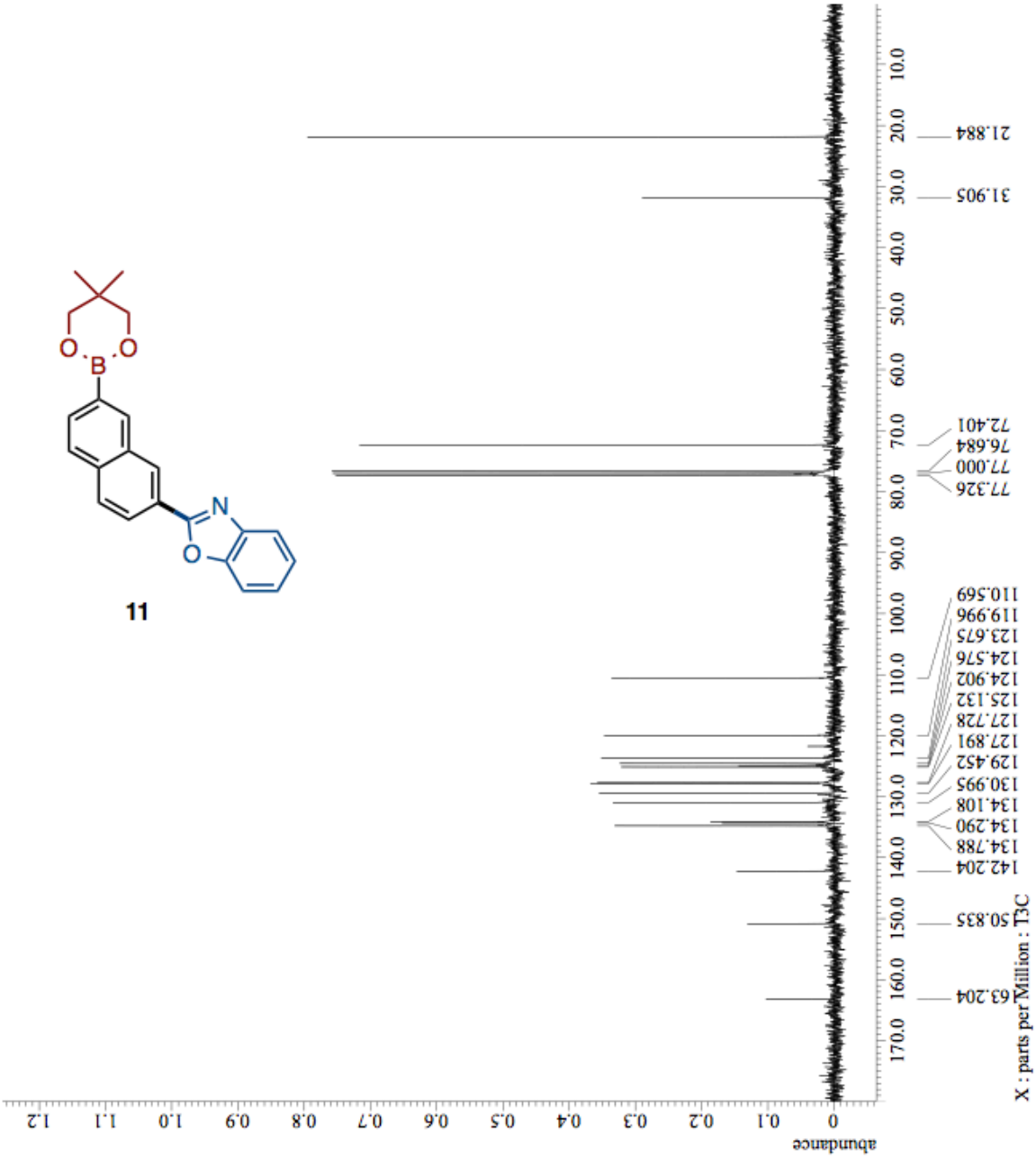
Supplementary Figure 147. ^{1}H NMR (400 MHz, $CDCl_3$) of 10



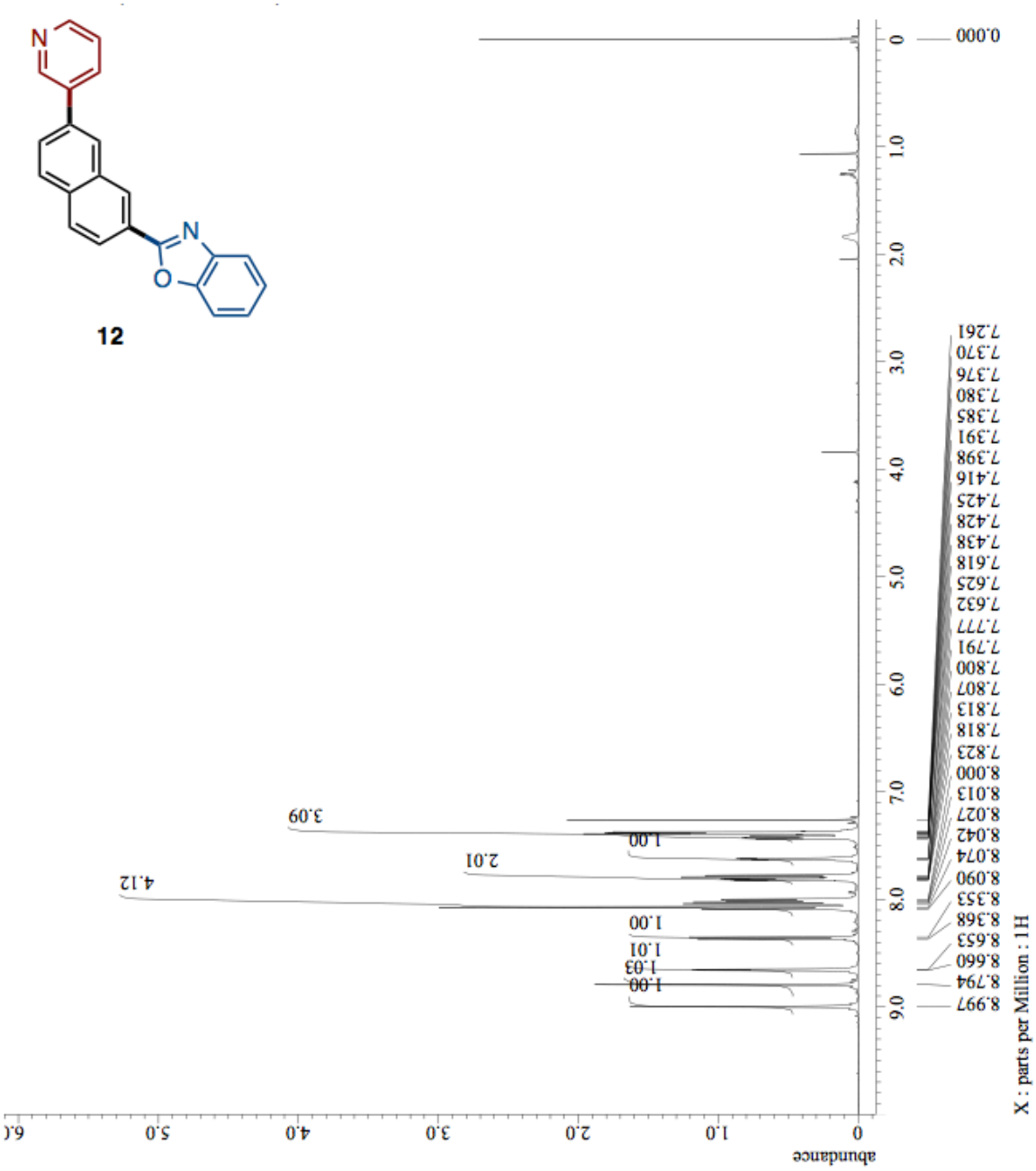
Supplementary Figure 148. ^{13}C NMR (100 MHz, $CDCl_3$) of 10



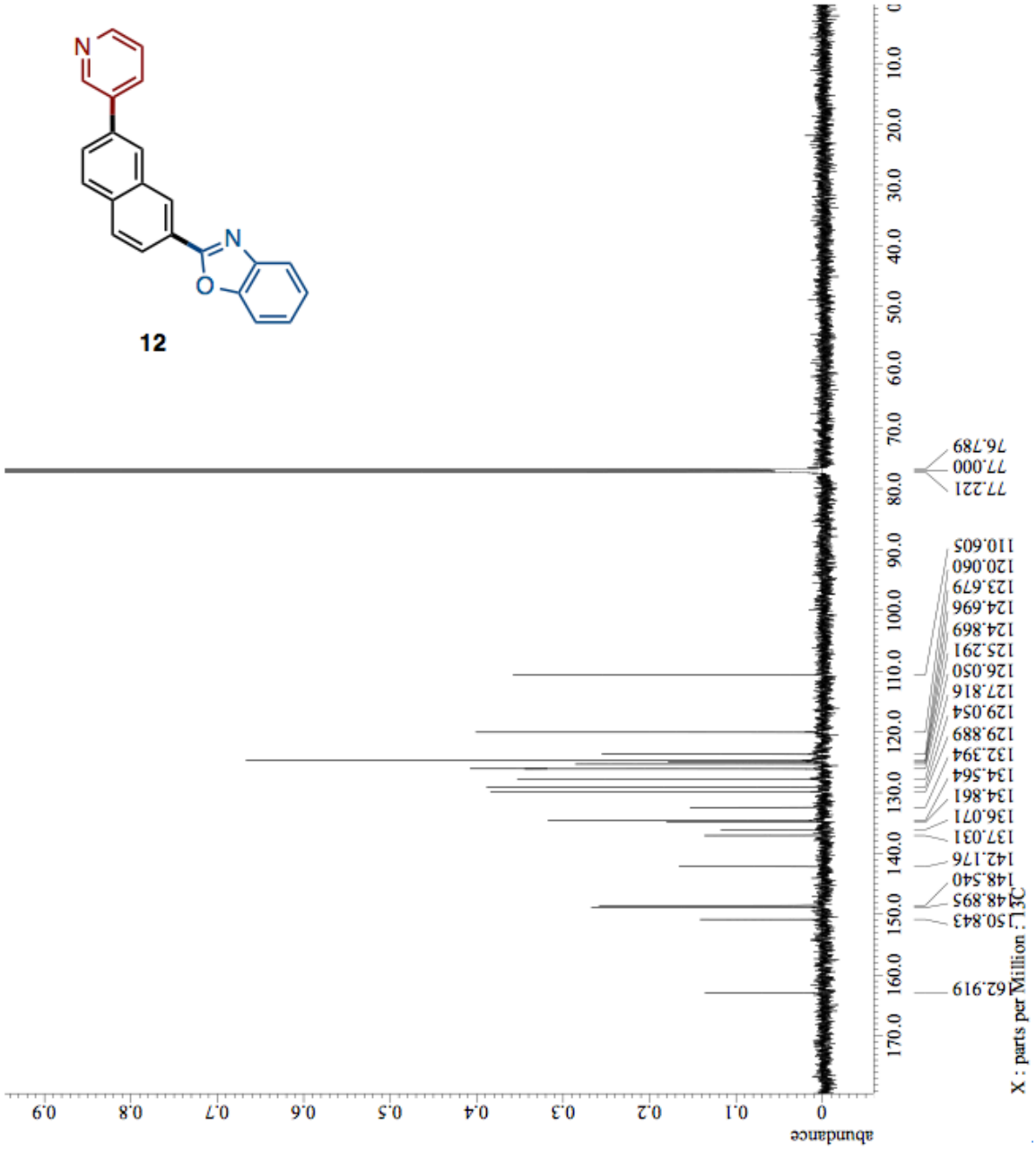
Supplementary Figure 149. ^{1}H NMR (400 MHz, $CDCl_3$) of 11



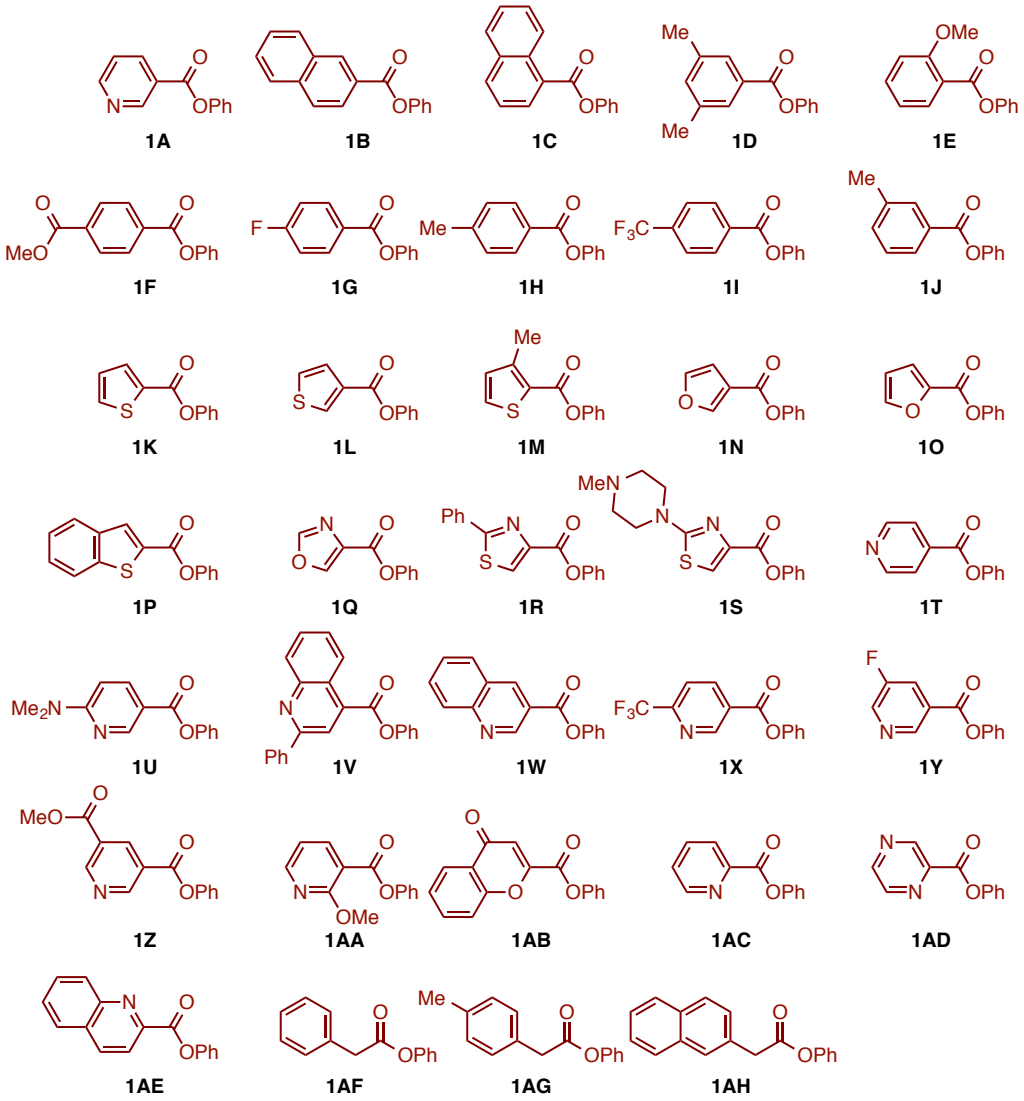
Supplementary Figure 150. ^{13}C NMR (100 MHz, $CDCl_3$) of 11



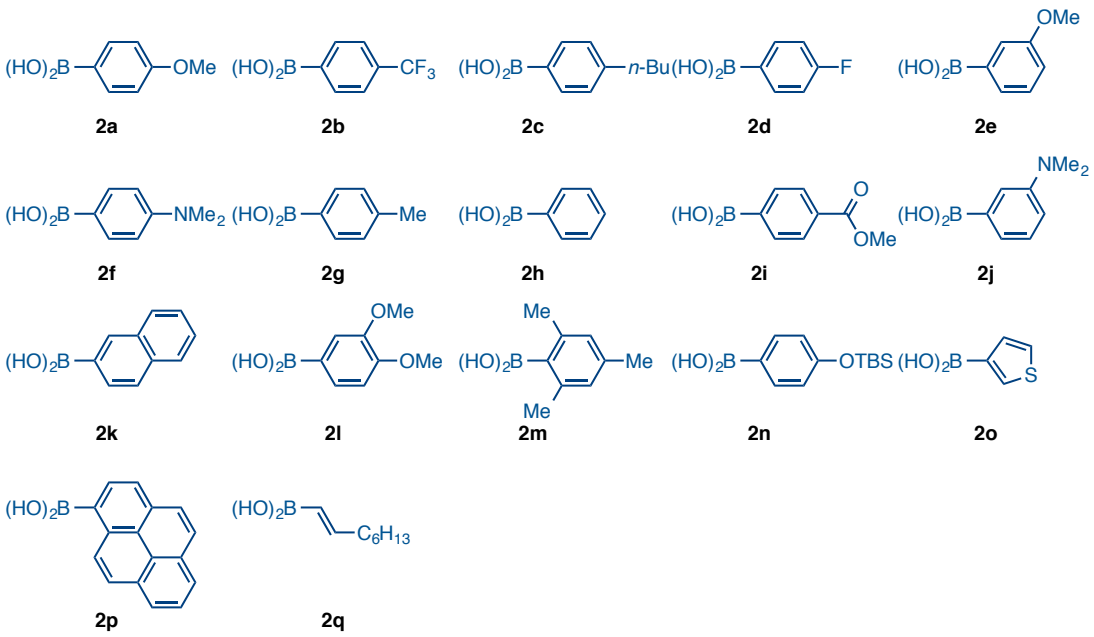
Supplementary Figure 151. ^{1}H NMR (600 MHz, $CDCl_3$) of 12



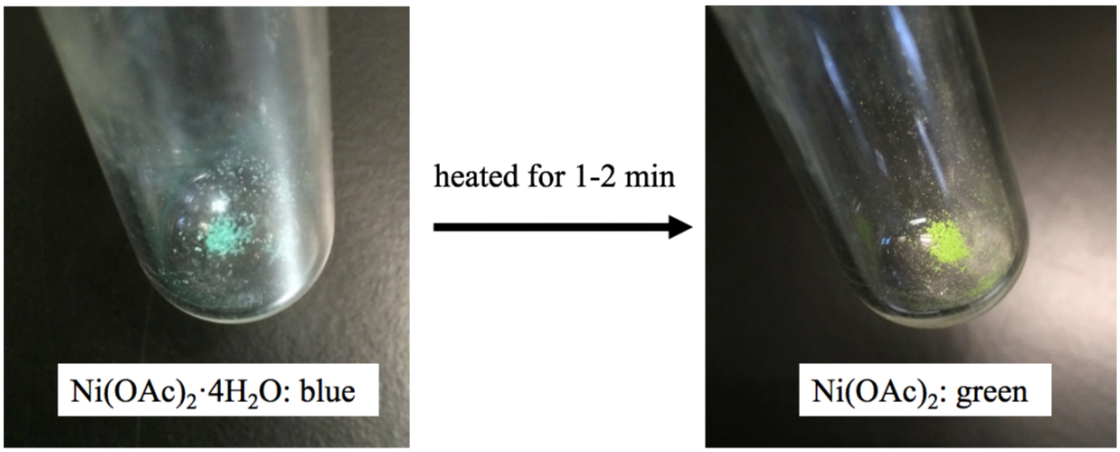
Supplementary Figure 152. ^{13}C NMR (150 MHz, $CDCl_3$) of 12



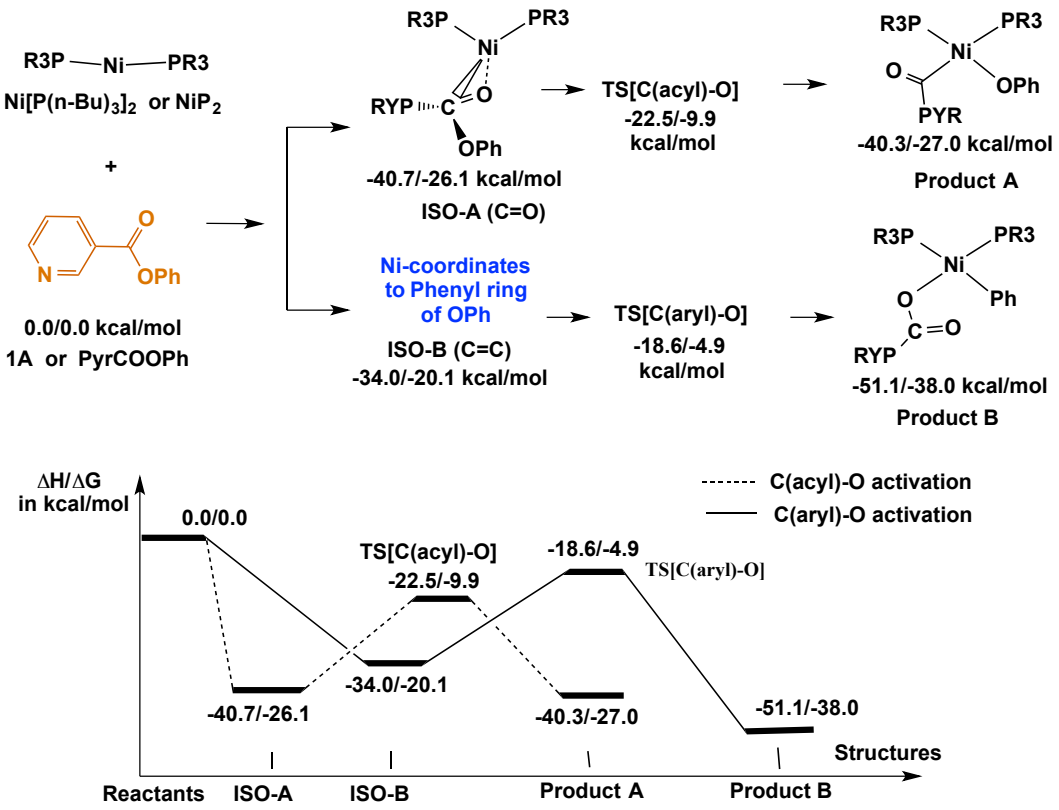
Supplementary Figure 153. Substrate structure of carboxylic acid esters **1**



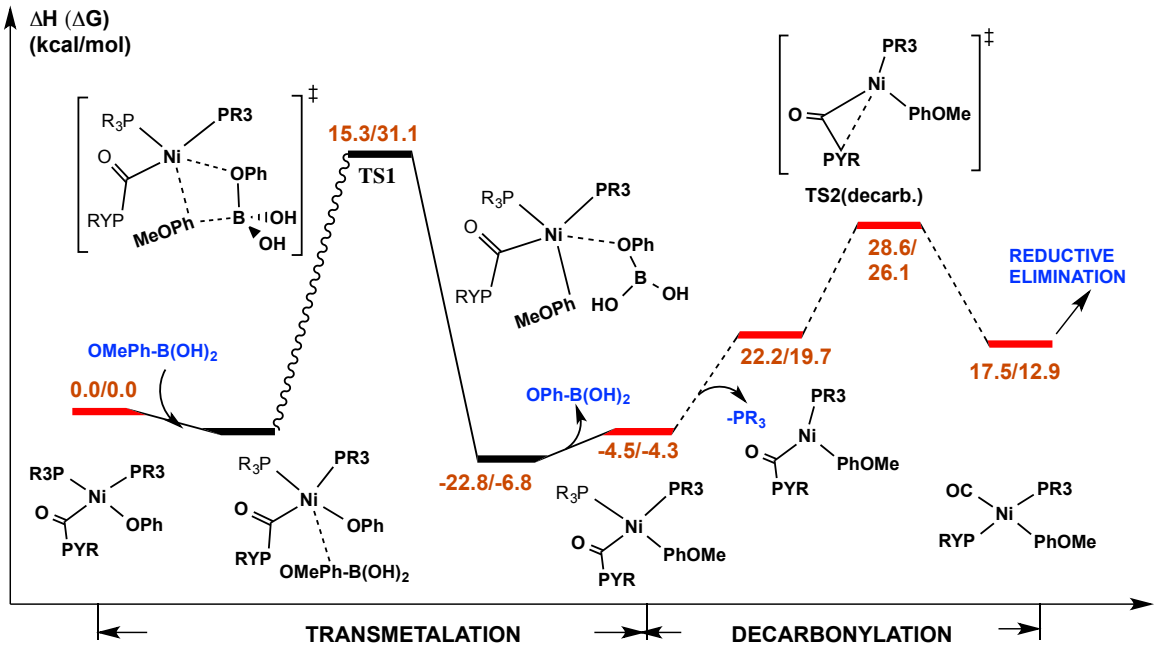
Supplementary Figure 154. Substrate structure of boronic acids **2**



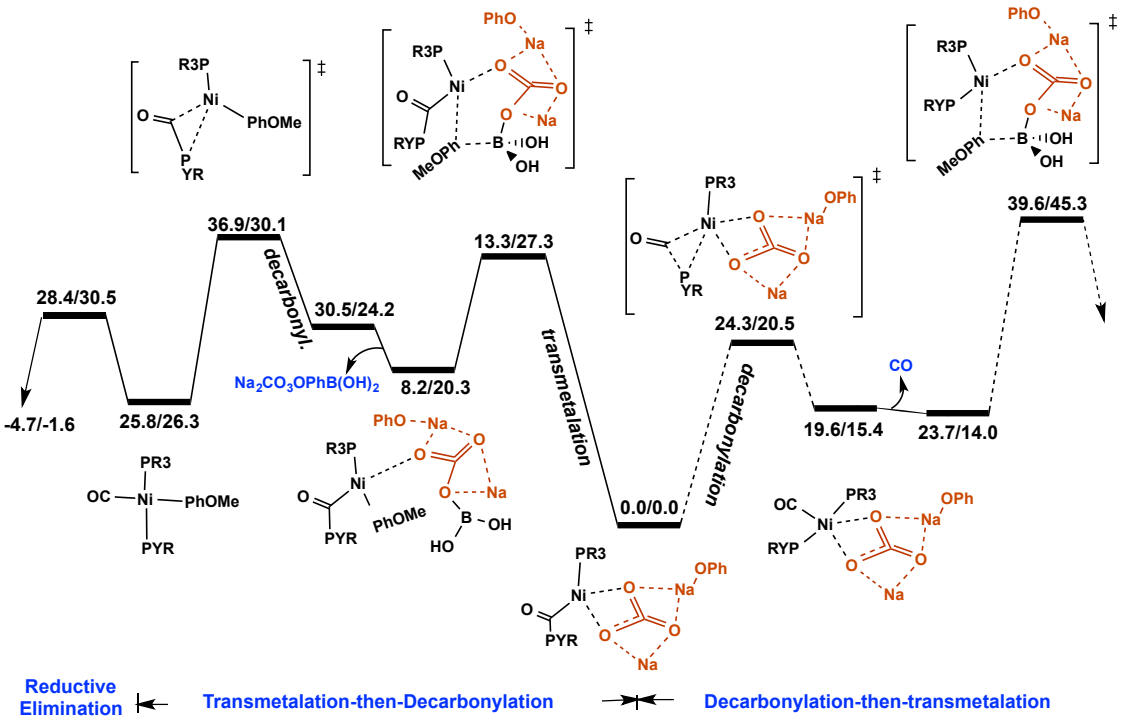
Supplementary Figure 155. How the color of the nickel salt changes



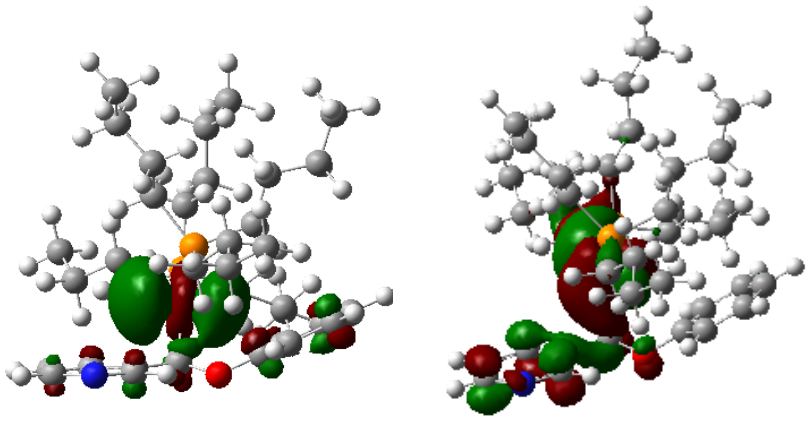
Supplementary Figure 156. Oxidative Addition of Phenyl 3-Pyridinecarboxylate to Ni[P(*n*-Bu)$_3$]$_2$ Catalyst. Schematic presentation of possible reactants, intermediates, transition states and products of the C(acyl)-O and C(aryl)-O oxidative addition of phenyl 3-pyridinecarboxylate to Ni[P(*n*-Bu)$_3$]$_2$ in the no-base condition and at the M06L/BS1 level of theory. For structural parameters, see Cartesian coordinates given in Supplementary Table 13. For total energies, see Supplementary Table 8.



Supplementary Figure 157. Schematic presentation of the favorable transmetalation-then-decarbonylation pathway of the phenyl 3-pyridinecarboxylate and boronic acid cross-coupling catalyzed by Ni[P(*n*-Bu)$_3$]$_2$ complex in the no-base condition. Presented energies are obtained at the M06L/BS1 level of theory.



Supplementary Figure 158. Schematic presentation of the favorable transmetalation-then-decarbonylation pathway of the phenyl 3-pyridinecarboxylate and boronic acid cross-coupling catalyzed by Ni[P(*n*-Bu)$_3$]$_2$ complex in the presence of Na_2CO_3 condition. Presented energies are obtained at the M06L/BS1 level of theory.



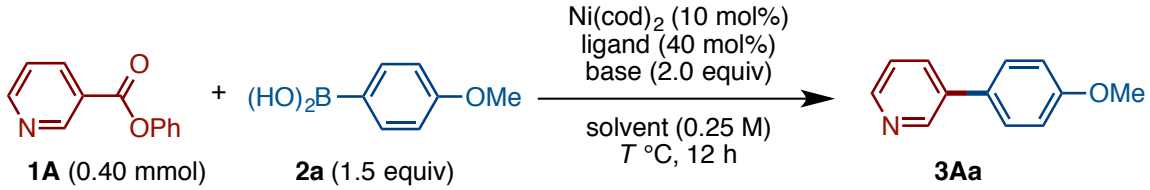
Ni-(C=O) bonding orbital

Pyr ➛Ni$_{LP}$* donor-acceptor bonding orbital

for complex B

Supplementary Figure 159. Important NBO orbitals of the complex B

Supplementary Table 1. Investigation of the reaction parameters

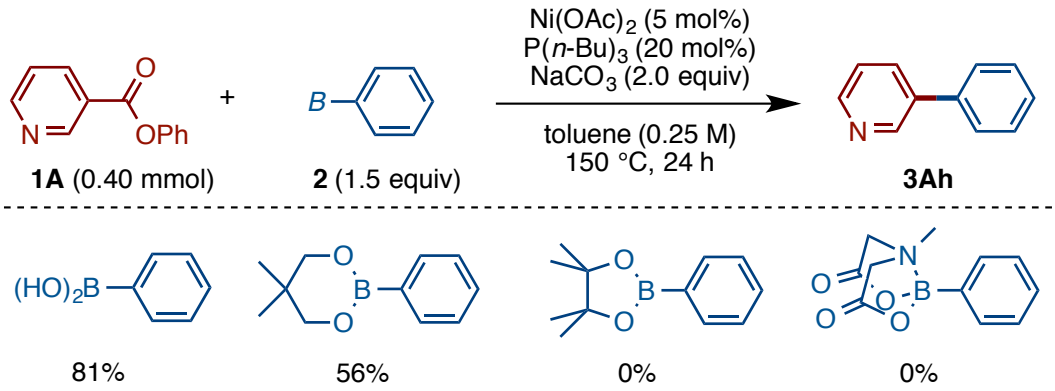


1A (0.40 mmol) **2a** (1.5 equiv) **3Aa**

entry	ligand	base	solvent	*T*	yield of **3Aa** (%)[a]
1	none	Na_2CO_3	1,4-dioxane	150	0
2	PCy_3	Na_2CO_3	1,4-dioxane	150	26
3	dppe	Na_2CO_3	1,4-dioxane	150	0
4	dpph	Na_2CO_3	1,4-dioxane	150	51
5	PPh_2Me	Na_2CO_3	1,4-dioxane	150	47
6	P(*n*-Bu)$_3$	Na_2CO_3	1,4-dioxane	150	65
7	P(*n*-Bu)$_3$	Li_2CO_3	1,4-dioxane	150	64
8	P(*n*-Bu)$_3$	K_2CO_3	1,4-dioxane	150	23
9	P(*n*-Bu)$_3$	Cs_2CO_3	1,4-dioxane	150	15
10	P(*n*-Bu)$_3$	Et_3N	1,4-dioxane	150	68
11	P(*n*-Bu)$_3$	none	1,4-dioxane	150	49
12	P(*n*-Bu)$_3$	Na_2CO_3	toluene	150	95
13	P(*n*-Bu)$_3$	Na_2CO_3	*m*-xylene	150	38
14	P(*n*-Bu)$_3$	Na_2CO_3	DME	150	56
15	P(*n*-Bu)$_3$	Na_2CO_3	*t*-AmylOH	150	53
16	P(*n*-Bu)$_3$	Na_2CO_3	toluene	150	88[b]
17	P(*n*-Bu)$_3$	Na_2CO_3	toluene	140	75
18	P(*n*-Bu)$_3$	Na_2CO_3	toluene	130	60
19	P(*n*-Bu)$_3$	Na_2CO_3	toluene	120	18

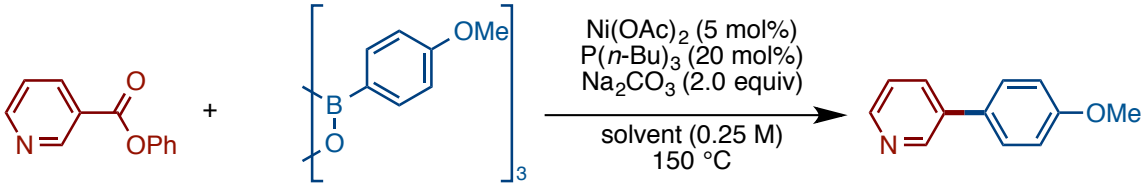
a. GC yield using dodecane as an internal standard. b. The reaction was conducted for 24 h using $Ni(OAc)_2$ (5 mol%) and P(*n*-Bu)$_3$ (20 mol%) as catalyst.

Supplementary Table 2. Investigation of the phenylboronic acids derivatives



1A (0.40 mmol) **2** (1.5 equiv) **3Ah**

Supplementary Table 3. Investigation of alternative protocols

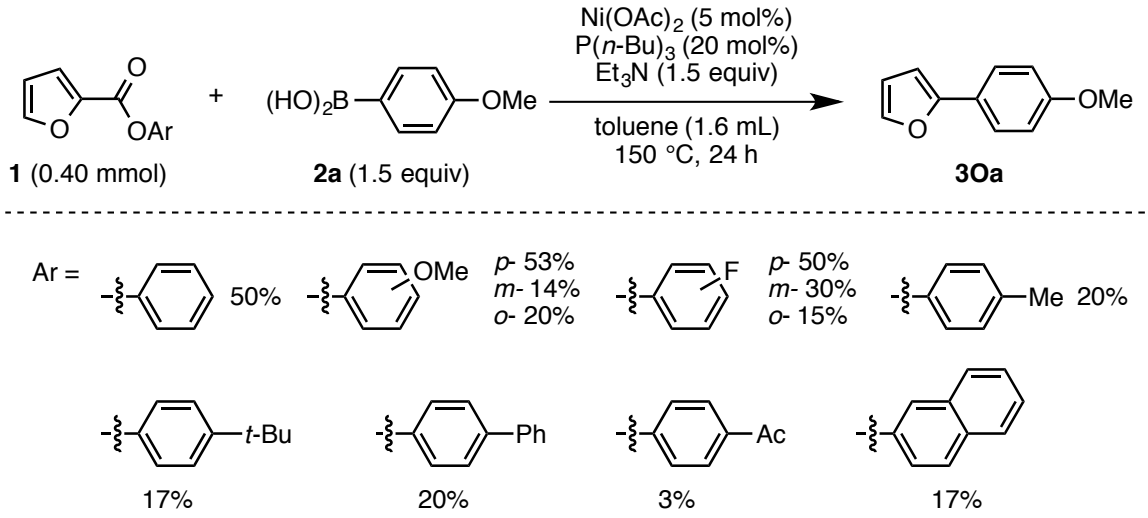


1A (0.40 mmol) **2a** (0.5 equiv) **3Aa**

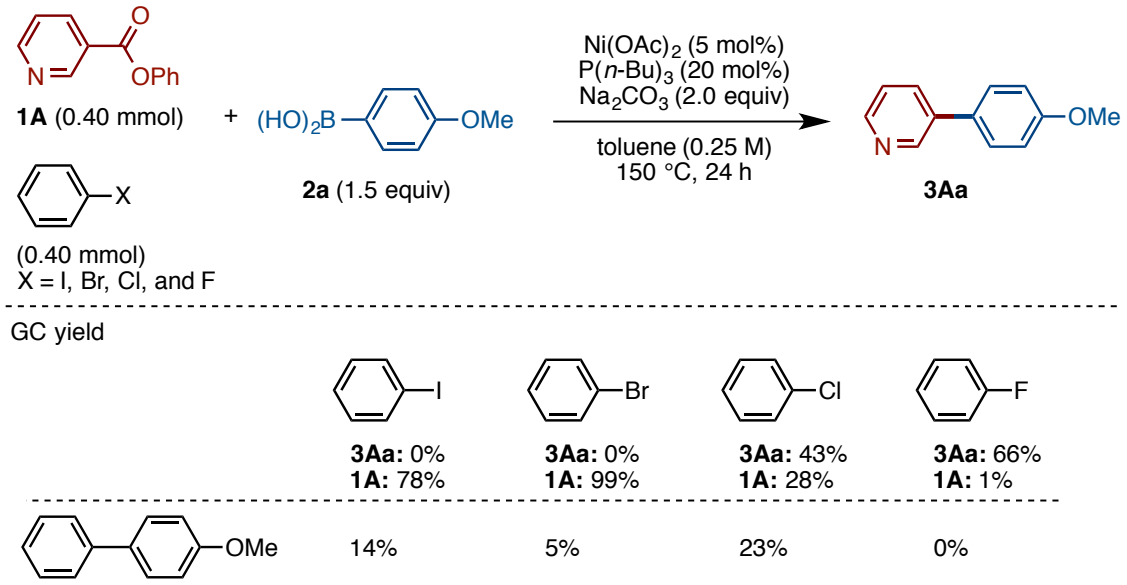
entry	solvent	conditions	GC yield (%)
1	toluene	close system (J-Young)	84
2	*m*-xylene	close system (J-Young)	57
3	anisole	close system (J-Young)	23
4	anisole	open system (Schlenk + condenser)	89 (82)

The number in the parenthesis shows the isolated yield.

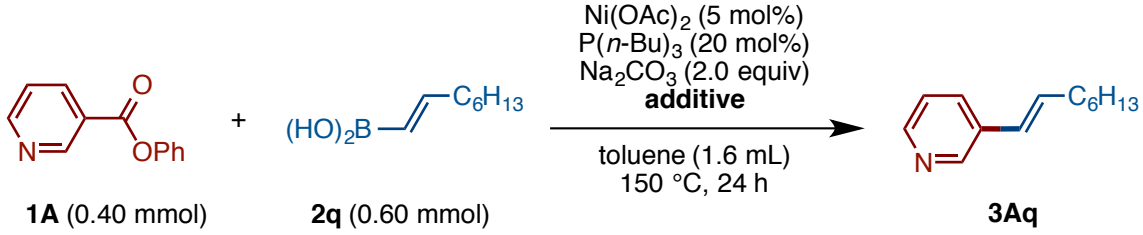
Supplementary Table 4. The effect of the aryl-substituent of carboxylic acids



Supplementary Table 5. Competitive experiments between phenyl esters and haloarenes

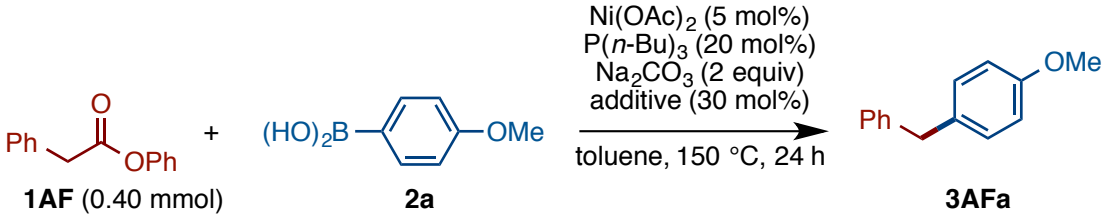


Supplementary Table 6. The effect of salts for the reaction of alkenylboronic acid **2q**



entry	additive	isolated yield of **3Aq**
1	none	24%
2	LiCl: 10 mol%	<20%
3	LiCl: 1 equiv	46%
4	NaCl: 1 equiv	46%
5	LiF: 1 equiv	42%
6	NaF: 1 equiv	46%
7	KF: 1 equiv	38%

Supplementary Table 7. The effect of DMAP for the reaction of **1AF**



1AF (0.40 mmol) **2a** **3AFa**

entry	additive	Isolated yield of **3**
1	none	27%
2	none	43%[a]
3	DMAP (30 mol%)	46%
4	DMAP (1 equiv)	26%

a. The reaction was 48 h.

Supplementary Table 8. Calculated total (in a.u., at the M06L/BS1 level of theory) and relative energies (in kcal/mol) of the reactants, transition states, intermediates and products of the studied C(acyl)-O and C(aryl)-O oxidative addition of phenyl 3-pyridinecarboxylate to $Ni[P(n\text{-}Bu)_3]_2$ complex. For cartesian coordinates of all reported structures see Supplementary Table 13).

Structure	Energies				Relative Energies			
	$-E_{tot}$	-(E +ZPC)	-H	-G	ΔE	Δ(E+ZPC)	ΔH	ΔG
$Ni[P(n\text{-}Bu)_3]_2$ → $Ni[P(n\text{-}Bu)_3]$ + $[P(n\text{-}Bu)_3]$								
$Ni[P(n\text{-}Bu)_3]_2$	1799.047953	1798.302214	1798.262328	1798.375858	-42.1	-41.5	-41.1	-28
$Ni[P(n\text{-}Bu)_3]$	984.149528	983.776269	983.755037	983.826269				
$[P(n\text{-}Bu)_3]$	814.831310	814.459779	814.441825	814.504941				
$Ni[P(n\text{-}Bu)_3]$ + $[P(n\text{-}Bu)_3]$	1798.980838	1798.236048	1798.196862	1798.33121	0.0	0.0	0.0	0.0
Oxidative addition of phenyl 3-pyridinecarboxylate (1A) to $Ni[P(n\text{-}Bu)_3]_2$ catalyst								
$Ni[P(n\text{-}Bu)_3]_2$ + (PyrCOOPh)	2466.886649	2466.956609	2465.904096	2466.070012	0	0	0	0
$Ni[P(n\text{-}Bu)_3]_2$(PyrCOOPh) ISO-A(C=O)	2466.955448	2466.022313	2465.969010	2466.111613	-43.2/0	-41.2/0	-40.7/0	-26.1/0
ISO-B(C=C)	2466.943787	2466.012035	2465.958304	2466.102092	-35.9	-34.8	-34	-20.1
TS[C(acyl)-O]	2466.924214	2465.994081	2465.940003	2466.085737	-23.6/19.6	-23.5/17.7	-22.5/18.2	-9.9/16.2
TS[C(aryl)-O]	2466.918790	2465.987373	2465.933787	2466.077801	-20.2	-19.3	-18.6	-4.9
$Ni[P(n\text{-}Bu)_3]_2$(PyrCO)(OPh), from TS[C(acyl)-O]	2466.954329	2466.022239	2465.968331	2466.112966	-42.5	-41.2	-40.3	-27
$Ni[P(n\text{-}Bu)_3]_2$(PyrCOO)(Ph), from TS[C(aryl)-O]	2466.973059	2466.039236	2465.985560	2466.130675	-54.2	-51.9	-51.1	-38.1
$Ni[P(n\text{-}Bu)_3]_2$ + Na_2CO_3 → $Ni[P(n\text{-}Bu)_3]_2[Na_2CO_3]$								
$NiP_2[Na_2CO_3]$ iso2	2387.576020	2386.809538	2386.761115	2386.894495	-21.0	-19.0	-18.2	-6.4
Iso1	2387.580192	2386.814613	2386.766031	2386.899542	-23.6	-22.2	-21.3	-9.6
Na_2CO_3	588.494676	588.4770470	588.469801	588.508414				
$Ni[P(n\text{-}Bu)_3]_2$	1799.047953	1798.302214	1798.262328	1798.375858				
$Ni[P(n\text{-}Bu)_3]_2$ + Na_2CO_3	2387.542629	2386.779261	2386.732129	2386.884272	0.0	0.0	0.0	0.0
$Ni[P(n\text{-}Bu)_3]_2[Na_2CO_3]$ → $Ni[P(n\text{-}Bu)_3][Na_2CO_3]$ + $[P(n\text{-}Bu)_3]$								
$NiP_2[Na_2CO_3]$, Iso1	2387.580192	2386.814613	2386.766031	2386.899542	0.0	0.0	0.0	0.0
$NiP[Na_2CO_3]$, iso1	1572.707774	1572.316435	1572.287108	1572.380429				
$[P(n\text{-}Bu)_3]$	814.831310	814.459779	814.441825	814.504940				
$NiP[Na_2CO_3]$ + $[P(n\text{-}Bu)_3]$	2387.539084	2386.776214	2386.728933	2386.885369	25.8	24.1	23.2	8.9

Supplementary Table 9. Decarbonylative transmetalation in the absence of Na_2CO_3 base. Calculated total (in a.u., at the M06L/BS1 level of theory) and relative energies (in kcal/mol) of the reactants, transition states, intermediates and products of the studied phenyl 3-pyridinecarboxylate and *p*-anisylboronic acid [*i.e.* MeOPh-B$(OH)_2$] cross-coupling catalyzed by Ni[P(*n*-Bu$)_3]_2$ catalyst in the absence of base (*i.e.* Na_2CO_3). For cartesian coordinates of all reported structure see Supplementary Table 13.

Structure		Energies				Relative Energies			
		$-E_{tot}$	-(E +ZPC)	-H	-G	ΔE	Δ(E+ZPC)	ΔH	ΔG
I. Decarbonylation-then-transmetalation from the oxidative addition product Ni[P(n-Bu$)_3]_2$(PyrCO)(OPh), after one of the ligands [i.*e*. P(n-Bu$)_3$ dissociation].									
I.A.1. P(n-Bu$)_3$ - dissociation									
Ni[P(n-Bu$)_3]_2$(PyrCO)(OPh)		2466.954329	2466.022239	2465.968331	2466.112966	[0.0]	[0.0]	[0.0]	[0.0]
[P(n-Bu$)_3$]		814.831310	814.459779	814.441825	814.504941				
[Ni[P(n-Bu$)_3$](PyrCO)(OPh)+[P(n-Bu$)_3$]		2466.905400	2466.976871	2466.924291	2466.090237	[30.7]	[28.5]	[27.6]	[14.3]
I.A.2. Decarbonylation									
Ni[P(n-Bu$)_3$](PyrCO)(OPh)		1652.074090	1651.517092	1651.482466	1651.585296	0.0	0.0	0.0	0.0
TS [(OC-C(Pyr))		1652.062105	1651.506432	1651.472146	1651.573609	7.5	6.7	6.5	7.3
Ni[P(n-Bu$)_3$](CO)(OPh)(Pyr)		1652.071579	1651.515716	1651.480567	1651.584590	1.6	0.9	1.2	0.4
I.B. Transmetalation from the Ni[P(n-Bu$)_3$](CO)(OPh)(Pyr) complex									
Ni[P(n-Bu$)_3$](CO)(OPh)(Pyr)		1652.071579	1651.515716	1651.480567	1651.584590				
MeOPh_B$(OH)_2$		522.743995	522.585484	522.574127	522.622372				
Ni[P(n-Bu$)_3$](CO)(OPh)(Pyr) +MeOPh_B$(OH)_2$		2174.825574	2174.101200	2174.054694	2174.206962	0.0	0.0	0.0	0.0
Ni[P(n-Bu$)_3$](CO)(Pyr)(OPh)	**iso1**	2174.846852	2174.129090	2174.082738	2174.211641	-13.4	-17.5	-17.6	-2.9
[MeOPh_B$(OH)_2$], B-C, pre-reaction complex	**Iso2**	2174.845932	2174.129063	2174.082710	2174.208173				
TS(B-C act.)	**iso1**	2174.804872	2174.091779	2174.046422	2174.169626				
	iso2	2174.805385	2174.091461	2174.045258	2174.170968	12.7	6.1	5.9	22.6
Ni[P(n-Bu$)_3$](Pyr)(CO)(PhOMe)[(HO$)_2$B-OPh]	**CO-N trans, Iso1**	2174.832348	2174.116384	2174.069275	2174.200053	-4.3	-9.5	-9.2	4.3
	CO-N trans, Iso2	2174.831376	2174.115632	2174.068231	2174.201346				
Ni[P(n-Bu$)_3$](Pyr)(CO)(PhOMe)	**N-CO trans**	1691.334065	1690.750683	1690.71358	1690.822796				
	P-CO trans	1691.334516	1690.750869	1690.71376	1690.823534				
[(HO$)_2$B-OPh], iso2		483.482975	483.352792	483.343067	483.387441				
Ni[P(n-Bu$)_3$](Pyr)(CO)(PhOMe), N-CO trans + [(HO$)_2$B-OPh]		2174.817040	2174.103475	2174.056647	2174.210237	5.4	-1.4	-1.2	-2.1
I.C. Reductive Elimination									
Ni[P(n-Bu$)_3$]	**N-CO trans**	1691.334065	1690.750683	1690.713580	1690.822796	0.0	0.0	0.0	0.0

(Pyr)(CO)(PhOMe)	**TS (RE)**		1691.327295	1690.745196	1690.708668	1690.816121	4.3	3.4	3.1	4.2
	PROD		1691.383292	1690.798020	1690.762157	1690.867216	-30.9	-29.7	-30.5	-27.9
Ni[P(n-Bu)$_3$](CO)			1097.533889	1097.152363	1097.129157	1097.206373				
(PyrPhOMe)			593.806680	593.603521	593.591395	593.641012				
Ni[P(n-Bu)$_3$](CO) + (PyrPhOMe)			1691.340569	1690.755884	1690.720552	1690.847385	-4.1	-3.3	-4.4	-15.4
II. Transmetalation-then-decarbonylation from the complex Ni[P(n-Bu)$_3$](PyrCO)(OPh)										
II.A. Transmetalation										
Ni[P(n-Bu)$_3$](PyrCO)(OPh)			1652.074090	1651.517092	1651.482466	1651.585296				
MeOPh_B(OH)$_2$			522.743995	522.585484	522.574127	522.622372				
Ni[P(n-Bu)$_3$](PyrCO)(OPh)+MeOPh_B(OH)$_2$			2174.818085	2174.102576	2174.056593	2174.207668	0.0	0.0	0.0	0.0
B-OPh product		**Iso1**	2174.837801	2174.120636	2174.074629	2174.199528				
		Iso2	2174.840580	2174.123170	2174.077233	2174.202028				
TS33 (B-C act.)		**iso2**	2174.805385	2174.091461	2174.045258	2174.170968				
CO-N_tr,		**iso1**	2174.811068	2174.095061	2174.049299	2174.174807	4.4	4.7	4.6	20.6
		iso2	2174.815520	2174.098756	2174.053294	2174.177336	1.6	2.4	2.1	19.0
Ni[P(n-Bu)$_3$](PyrCO)(PhOMe)(OPh_B(OH)$_2$		**Iso_1a**	2174.823735	2174.107507	2174.060940	2174.190835				
		Iso-1b	2174.823578	2174.106501	2174.060355	2174.187237				
Ni[P(n-Bu)$_3$](PyrCO)(PhOMe)			1691.327612	1690.742389	1690.706162	1690.811668				
[(HO)$_2$B-OPh], iso2			483.482975	483.352792	483.343067	483.387441				
Ni[P(n-Bu)$_3$](PyrCO)(PhOMe) + PhO-B(OH)$_2$			2174.810587	2174.095182	2174.049229	2174.199109	4.7	4.6	4.6	5.4
II.B. Decarbonylation										
Ni[P(n-Bu)$_3$](PyrCO)(PhOMe)			1691.327612	1690.742389	1690.706162	1690.811668	0.0	0.0	0.0	0.0
TS (decarb.)			1691.315774	1690.731822	1690.695944	1690.801493	7.4	6.6	6.4	6.4
Ni[P(n-Bu)$_3$](Pyr)(CO)(PhOMe)			1691.334534	1690.750651	1690.713580	1690.822512	-4.4	-5.2	-4.7	-6.8
II.C. For reductive elimination see Section I.C										
III. Transmetalation-then-decarbonylation from the oxidative addition product Ni[P(n-Bu)$_3$]$_2$(PyrCO)(OPh), i.e. without the ligand dissociation.										
III.A. Transmetalation										
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(OPh)			2466.954329	2466.022239	2465.968331	2466.112966				
MeOPh_B(OH)$_2$			522.743995	522.585484	522.574127	522.622372				
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(OPh) + MeOPh_B(OH)$_2$			2989.698324	2988.607723	2988.542458	2988.735338	0.0	0.0	0.0	0.0
TS (B-C act.),		**iso-1_up**	2989.673968	2988.582911	2988.518073	2988.685725	15.3	15.7	15.3	31.1
		iso-2_up	2989.675404	2988.585118	2988.520179	2988.685227				
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(PhOMe)[PhO-B(OH)$_2$]			2989.737961	2988.643899	2988.578853	2988.746093	-24.9	-22.7	-22.8	-6.8
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(PhOMe)			2506.221645	2505.262347	2505.206564	2505.354794				

[$(HO)_2$B-OPh], iso2	483.482975	483.352792	483.343067	483.387441				
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(PhOMe) + PhO-B(OH)$_2$	2989.704620	2988.615139	2988.549631	2988.742235	-4.0	-4.7	-4.5	-4.3
III.B. Decarbonylation								
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(PhOMe)	2506.221645	2505.262347	2505.206564	2505.354794	[0.0]	[0.0]	[0.0]	[0.0]
[P(n-Bu)$_3$]	814.831310	814.459779	814.441825	814.504941				
Ni[P(n-Bu)$_3$](PyrCO)(PhOMe)	1691.327612	1690.742389	1690.706162	1690.811668				
Ni[P(n-Bu)$_3$](PyrCO)(PhOMe) + [P(n-Bu)$_3$]	2506.158922	2505.202168	2505.147987	2505.316609	[39.4]	[37.8]	[26.7]	[24.0]
Ni[P(n-Bu)$_3$](PyrCO)(PhOMe)	1691.327612	1690.742389	1690.706162	1690.811668	0.0	0.0	0.0	0.0
TS (decarb.)	1691.315774	1690.731822	1690.695944	1690.801493	7.4	6.6	6.4	6.4
Ni[P(n-Bu)$_3$](Pyr)(CO)(PhOMe)	1691.334534	1690.750651	1690.713580	1690.822512	-4.4	-5.2	-4.7	-6.8
III.C. For reductive elimination see Section I.C								

Supplementary Table 10. Decarbonylative transmetalation in the *presence* of the Na_2CO_3 base. Na_2CO_3 coordination to the C(acyl)-O oxidative addition product Ni[P(n-Bu)$_3$]$_2$(PyrCO)(OPh) and rearrangement. Calculated total (in a.u., at the M06L/BS1 level of theory) and relative energies (in kcal/mol) of the reactants, transition states, intermediates and products of the studied Na_2CO_3 coordination to the phenyl 3-pyridinecarboxylate oxidative addition product Ni[P(*n*-Bu)$_3$]$_2$(PyrCO)(OPh) and following multi-step rearrangement of the resulted intermediates. For cartesian coordinates of all reported structure see Supplementary Table 13.

Structure		Energies				Relative Energies			
		$-E_{tot}$	-(E +ZPC)	-H	-G	ΔE	Δ(E+ZPC)	ΔH	ΔG
A. Reaction Ni[P(n-Bu)$_3$]$_2$(PyrCO)(OPh) + Na_2CO_3 → Ni[P(n-Bu)$_3$]$_2$(PyrCO)(Na_2CO_3)(OPh)									
I.A.1. P(n-Bu)$_3$ - dissociation									
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(OPh)		2466.954329	2466.022239	2465.968331	2466.112966				
Na_2CO_3		588.494676	588.477047	588.469801	588.508414				
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(OPh) + Na_2CO_3		3055.449005	3054.499286	3054.438132	3054.621380	0.0	0.0	0.0	0.0
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(Na_2CO_3)(OPh)	**Iso-1a**	3055.488680	3054.537664	3054.476076	3054.636281	-24.9	-24.1	-23.8	-9.4
	Iso-1b	3055.488591	3054.536383	3054.475062	3054.634673				
B. Ni[P(n-Bu)$_3$]$_2$(PyrCO)(Na_2CO_3)(OPh) → Ni[P(n-Bu)$_3$]$_2$(PyrCO)(Na_2CO_3OPh) isomerization									
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(Na_2CO_3)(OPh)	**Iso-1a**	3055.488680	3054.537664	3054.476076	3054.636281	0.0	0.0	0.0	0.0
	Iso-1b	3055.488591	3054.536383	3054.475062	3054.634673				
Ni[P(n-Bu)$_3$]$_2$(PyrCO)(Na_2CO_3OPh)	**Iso-3a**	3055.505151	3054.555050	3054.492800	3054.656882	-10.3	-10.9	-10.5	-12.9

	Iso-3b	3055.499666	3054.549503	3054.487244	3054.650785				
C. Ligand Exchange: $Ni[P(n\text{-}Bu)_3]_2(PyrCO)(Na_2CO_3OPh) \rightarrow Ni[P(n\text{-}Bu)_3]_2(PyrCO)(NaCO_3) + NaOPh$									
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(Na_2CO_3OPh)$	**Iso-3a**	3055.505151	3054.555050	3054.492800	3054.656882	0.0	0.0	0.0	0.0
	Iso-3b	3055.499666	3054.549503	3054.487244	3054.650785				
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(NaCO_3)$	**Down Iso-3a**	2586.260084	2585.404600	2585.350746	2585.497264				
	UP iso-3b	2586.262707	2585.407175	2585.353485	2585.498639				
Na_OPh		469.175242	469.082344	469.074299	469.114741				
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(NaCO_3)$, iso3b_UP + NaOPh		3055.437949	3054.489519	3054.427784	3054.613380	42.2	41.1	40.8	27.3
D. Reaction: $Ni[P(n\text{-}Bu)_3]_2(PyrCO)(Na_2CO_3OPh) \rightarrow Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh) + [P(n\text{-}Bu)_3]$									
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(Na_2CO_3OPh)$, Iso-3a		3055.505151	3054.555050	3054.492800	3054.656882	0.0	0.0	0.0	0.0
$Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$	**Iso1**	2240.650977	2240.074859	2240.032693	2240.151469				
	Iso2	2240.653829	2240.076958	2240.035154	2240.150825				
$[P(n\text{-}Bu)_3]$		814.831310	814.459779	814.441825	814.504941				
$Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$, iso2 + $[P(n\text{-}Bu)_3]$		3055.485139	3054.536737	3054.476979	3054.655766	12.6	11.5	9.9	0.7

Supplementary Table 11. Calculated total (in a.u., at the M06L/BS1 level of theory) and relative energies (in kcal/mol) of the reactants, transition states, intermediates and products of the studied phenyl 3-pyridinecarboxylate and *p*-anisylboronic acid [*i.e.* MeOPh-$B(OH)_2$] cross-coupling catalyzed by $Ni[P(n\text{-}Bu)_3]_2$ catalyst in the *presence* of base (*i.e.* Na_2CO_3). For cartesian coordinates of all reported structure, see Supplementary Table 13.

Structure		Energies				Relative Energies			
		$-E_{tot}$	-(E +ZPC)	-H	-G	ΔE	Δ(E+ZPC)	ΔH	ΔG
I. Decarbonylation-then-transmetalation from the $Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$ cluster complex									
I.A. Decarbonylation: $Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh) \rightarrow Ni[P(n\text{-}Bu)_3](CO)(Pyr)(Na_2CO_3OPh)$									
$Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$	**Iso-2**	2240.653829	2240.076958	2240.035154	2240.150825	0.0	0.0	0.0	0.0
	TS	2240.612500	2240.039326	2239.996498	2240.118211	25.9	23.6	24.3	20.5
$Ni[P(n\text{-}Bu)_3](CO)(Pyr)(Na_2CO_3OPh)$,Trans-O		2240.621459	2240.047162	2240.003860	2240.126299	20.3	18.7	19.6	15.4
I.A.1. CO-dissociation: $Ni[P(n\text{-}Bu)_3](Pyr)(CO)(Na_2CO_3OPh) \rightarrow Ni[P(n\text{-}Bu)_3](Pyr)(Na_2CO_3OPh) + CO$									
$Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$	**Trans-O**	2240.621459	2240.047162	2240.003860	2240.126299	0.0	0.0	0.0	0.0
	Trans-N	2240.614635	2240.040420	2239.997244	2240.119472				
CO		113.296662	113.291641	113.288337	113.3107850				
$Ni[P(n\text{-}Bu)_3](Pyr)(Na_2CO_3OPh)$,		2127.308317	2126.742004	2126.701406	2126.817765				

$Ni[P(n\text{-}Bu)_3](Pyr)(Na_2CO_3OPh)$ + CO		2240.604979	2240.033645	2239.989743	2240.128550	10.3	8.5	8.9	-1.4
I.B. Transmetalation from the $Ni[P(n\text{-}Bu)_3](Pyr)(Na_2CO_3OPh)$ complex									
$Ni[P(n\text{-}Bu)_3](Pyr)(Na_2CO_3OPh)$,		2127.308317	2126.742004	2126.701406	2126.817765				
$MeOPh\_B(OH)_2$		522.743995	522.585484	522.574127	522.622372				
$Ni[P(n\text{-}Bu)_3](Pyr)(Na_2CO_3OPh)$ + $MeOPh\_B(OH)_2$		2650.052312	2649.327488	2649.275533	2649.440137	0.0	0.0	0.0	0.0
COMPLEX,		2650.054169	2649.328488	2649.276691	2649.413974	-1.2	-0.6	-0.7	16.4
TS1, B-O formation				no barrier was located					
B-O complex		2650.053240	2649.327730	2649.275783	2649.414957	-0.6	-0.2	-0.2	15.8
TS2, B-C active.		2650.025711	2649.302276	2649.250183	2649.390267	16.7	15.8	15.9	31.3
B-C complex: $Ni[P(n\text{-}Bu)_3](Pyr)(MeOPh)(Na_2CO_3(OPh)B(OH)_2)$	**iso1**	2650.040433	2649.315553	2649.263193	2649.403507	7.5	7.5	7.7	23
	iso2	2650.031954	2649.307755	2649.255311	2649.396236				
$Ni[P(n\text{-}Bu)_3](Pyr)(MeOPh)$, O-P trans, Iso-1		1577.980792	1577.406174	1577.371479	1577.476373				
$Na_2CO_3(OPh)B(OH)_2$		1072.020568	1071.872413	1071.854530	1071.919027				
$Ni[P(n\text{-}Bu)_3](Pyr)(MeOPh)$ + $Na_2CO_3(OPh)B(OH)_2$		2650.001360	2649.278587	2649.226009	2649.395400	32.0	30.7	31.1	28.1
I.C. Reductive elimination									
$Ni[P(n\text{-}Bu)_3](Pyr)(MeOPh)(Na_2CO_3(OPh)B(OH)_2)$	**iso1**	2650.040433	2649.315553	2649.263193	2649.403507	0.0	0.0	0.0	0.0
	iso2	2650.031954	2649.307755	2649.255311	2649.396236				
TS, iso2		2650.027094	2649.303384	2649.251479	2649.390739	8.4	7.6	7.4	8.0
COMPLEX_prod,	**iso-1**	2650.065887	2649.340579	2649.288578	2649.427124				
	iso-2	2650.083236	2649.357099	2649.305590	2649.442512	-26.9	-26.1	-26.6	-24.5
$Ni[P(n\text{-}Bu)_3](Na_2CO_3(OPh)B(OH)_2)$		2056.249575	2055.728396	2055.689485	2055.802417				
MeOPh_Pyr		593.806680	593.603521	593.591395	593.641012				
$Ni[P(n\text{-}Bu)_3](Na_2CO_3(OPh)B(OH)_2)$ + MeOPh_Pyr		2650.056255	2649.331917	2649.280880	2649.443429	-9.9	-10.3	-11.1	-25.1
II. Transmetalation-then-decarbonylation from the $Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$ cluster complex									
II.A. Transmetalation from $Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$									
$Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$, Iso-1		2240.653829	2240.076958	2240.035154	2240.150825				
$MeOPh\_B(OH)_2$		522.743995	522.585484	522.574127	522.622372				
$Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh)$ + $MeOPh\_B(OH)_2$		2763.397824	2762.662442	2762.609281	2762.773197	0.0	0.0	0.0	0.0
TS(B-C active.)	**Iso2_down**	2763.364975	2762.630124	2762.576682	2762.718606	20.6	20.3	20.5	34.3
	Iso2_up	2763.375548	2762.641315	2762.588054	2762.729615	14.0	13.3	13.3	27.3
$Ni[P(n\text{-}Bu)_3](PyrCO)(PhOMe)(Na_2CO_3OPhB(OH)_2)$	**Iso2_down**	2763.384351	2762.648868	2762.594958	2762.738319				
	Iso2_up	2763.385586	2762.650096	2762.596291	2762.740707	7.7	7.8	8.2	20.3
II.B. $Ni[P(n\text{-}Bu)_3](PyrCO)(PhOMe)(Na_2CO_3OPhB(OH)_2) \rightarrow Ni[P(n\text{-}Bu)_3](PyrCO)(PhOMe) + (Na_2CO_3OPhB(OH)_2)$									

$Ni[P(n\text{-}Bu)_3](PyrCO)(PhOMe)(Na_2CO_3OPhB(OH)_2]$, Iso2_up	2763.385586	2762.650096	2762.596291	2762.739707	0.0	0.0	0.0	0.0
$Ni[P(n\text{-}Bu)_3](PyrCO)(PhOMe)$	1691.327612	1690.742389	1690.706162	1690.811668				
$Na_2CO_3OPhB(OH)_2$	1072.020568	1071.872413	1071.854530	1071.919027				
$Ni[P(n\text{-}Bu)_3](PyrCO)(PhOMe) + [Na_2CO_3OPhB(OH)_2]$	2763.348180	2762.614802	2762.560692	2762.733495	23.5	22.1	22.3	3.8

II.C. Decarbonylation: $Ni[P(n\text{-}Bu)_3](PyrCO)(PhOMe) \rightarrow Ni[P(n\text{-}Bu)_3](Pyr)(CO)(PhOMe)$
See Supplementary Table 9, section II.B
II.D. Reduction Elimination from the decarbonylated product $Ni[P(n\text{-}Bu)_3](Pyr)(CO)(PhOMe)$
See Supplementary Table 9, section I.C

Supplementary Table 12. Calculated total (in a.u., at the M06/BS1 level of theory) and relative energies (in kcal/mol) of the reactants, important transition states, intermediates and products of the studied phenyl 3-pyridinecarboxylate and *p*-anisylboronic acid [*i.e.* $MeOPh\text{-}B(OH)_2$] cross-coupling catalyzed by $Ni[P(n\text{-}Bu)_3]_2$ catalyst in the absence and presence of base (*i.e.* Na_2CO_3) conditions

Structure	Energies				Relative Energies			
	$-E_{tot}$	-(E +ZPC)	-H	-G	ΔE	Δ(E+ZPC)	ΔH	ΔG
$Ni[P(n\text{-}Bu)_3]_2 \rightarrow Ni[P(n\text{-}Bu)_3] + [P(n\text{-}Bu)_3]$								
$[P(n\text{-}Bu)_3]$	814.490909	814.122914	814.103415	814.170490				
Na_2CO_3	588.394747	588.377485	588.369946	588.409119				
$MeOPh\text{-}B(OH)_2$	522.478119	522.320396	522.308972	522.357204				
$Na_2CO_3(OPh)[B(OH)_2]$	1071.684273	1071.535321	1071.517884	1071.581034				
NaOPh	468.986985	468.894407	468.886389	468.926895				
PyrCOOPh	667.449129	667.265396	667.252733	667.305218				
Transmetalation from the $Ni[P(n\text{-}Bu)_3]_2(OPh)(PyrCO)$ oxidative addition complex (i.e. in the absence of Na_2CO_3)								
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(OPh)$	2465.849470	2464.923877	2464.870386	2465.012720				
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(OPh) + MeOPh\text{-}B(OH)_2$	2988.327589	2987.244273	2987.179358	2987.369924	0.0	0.0	0.0	0.0
TS(TRME, no base)	2988.310009	2987.223803	2987.159129	2987.323873	11.1	12.8	12.7	28.9
Prod., iso1	2988.378488	2987.292071	2987.227559	2987.392273	-31.9	-30.0	-30.2	-14.0
Reaction $Ni[P(n\text{-}Bu)_3]_2(PyrCO)(OPh) + Na_2CO_3 \rightarrow Ni[P(n\text{-}Bu)_3]_2(PyrCO)(Na_2CO_3OPh)$								
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(OPh) + Na_2CO_3$	3054.244217	3053.301362	3053.240332	3053.421839	0.0	0.0	0.0	0.0
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(Na_2CO_3OPh)$	3054.299150	3053.355753	3053.293809	3053.455389	-34.5	-34.1	-33.6	-21.1
Reaction $Ni[P(n\text{-}Bu)_3]_2(PyrCO)(Na_2CO_3OPh) \rightarrow Ni[P(n\text{-}Bu)_3](PyrCO)(Na_2CO_3OPh) + [P(n\text{-}Bu)_3]$								
$Ni[P(n\text{-}Bu)_3]_2(PyrCO)(Na_2CO_3OPh)$	3054.29915	3053.355753	3053.293809	3053.455389	0.0	0.0	0.0	0.0

Ni[P(n-Bu)$_3$](PyrCO)(Na$_2$CO$_3$OPh)	2239.79129	2239.217874	2239.176036	2239.292649				
Ni[P(n-Bu)$_3$](PyrCO)(Na$_2$CO$_3$OPh) + [P(n-Bu)$_3$]	3054.282199	3053.340788	3053.279451	3053.463139	10.6	9.4	9.0	-4.9
Transmetalation from the Ni[P(n-Bu)$_3$](Pyr)(Na$_2$CO$_3$OPh) complex								
Ni[P(n-Bu)$_3$](PyrCO)(Na$_2$CO$_3$OPh) + MeOPh-B(OH)$_2$	2762.269409	2761.538270	2761.485008	2761.649853	0.0	0.0	0.0	0.0
B-O complex	2762.273253	2761.541162	2761.488113	2761.627769	-2.4	-1.8	-2.0	13.9
TS(TRME, Na$_2$CO$_3$OPh)	2762.260184	2761.529096	2761.476239	2761.617153	5.8	5.8	5.5	20.5
Product	2762.270430	2761.537494	2761.484054	2761.626846	-0.7	0.5	0.6	14.4
Ni[P(n-Bu)$_3$](PyrCO)(MeOPh) + Na$_2$CO$_3$(OPh)[B(OH)$_2$]	2762.232157	2761.502610	2761.448586	2761.619122	23.4	22.4	22.9	19.3
Decarbonylation: Ni[P(n-Bu)$_3$](PyrCO)(PhOMe) → Ni[P(n-Bu)$_3$](Pyr)(CO)(PhOMe)								
Ni[P(n-Bu)$_3$](PyrCO)(MeOPh)	1690.547884	1689.967289	1689.930702	1690.038088	0.0	0.0	0.0	0.0
TS (decarbonylation	1690.534837	1689.955043	1689.919302	1690.024305	8.2	7.7	7.2	8.7
Ni[P(n-Bu)$_3$](Pyr)(CO)(MeOPh)	1690.553265	1689.974446	1689.937195	1690.047382	-3.4	-4.5	-4.1	-5.8
Reductive Elimination								
Ni[P(n-Bu)$_3$](Pyr)(CO)(MeOPh)	1690.553265	1689.974446	1689.937195	1690.047382	0.0	0.0	0.0	0.0
TS	1690.546591	1689.968420	1689.932022	1690.038307	4.2	3.8	3.3	5.7

Supplementary Table 13. Cartersian Coordinates (in Å) of all structures reported in Supplementary Tables 8–12.

P(n-Bu)$_3$

P	-0.22309200	0.05246700	-2.07745000
C	1.08468400	-1.12802400	-1.44307700
C	0.35351500	1.63631300	-1.26900500
C	-1.75929200	-0.48077700	-1.14262200
C	0.89197000	1.69646100	0.16815800
C	2.00432600	2.72551600	0.33896600
C	-2.18886600	0.24325000	0.12669600
C	-3.56506300	-0.19756900	0.60942500
C	0.82714700	-1.91461400	-0.15952500
C	2.08879500	-2.55818200	0.40234500
C	2.63777300	2.68819200	1.71951000
C	1.87505800	-3.18757400	1.76718800
C	-3.94158800	0.39784000	1.95477500
H	-0.45215800	2.36704200	-1.40917600
H	1.15001200	1.97381400	-1.94683400
H	0.08175200	1.92818500	0.86248600
H	1.27776100	0.72545600	0.48514700
H	-1.63818200	-1.54601300	-0.91549000
H	-2.58137700	-0.43380100	-1.86699400
H	-1.45701400	0.07075400	0.92173500
H	-2.19594600	1.32802400	-0.03797300
H	1.99115200	-0.51696000	-1.32588400
H	1.31757300	-1.83100600	-2.25091000
H	0.37808300	-1.27261400	0.60810600
H	0.08070200	-2.69729900	-0.35139600
H	1.60519700	3.72932500	0.13822900
H	2.76947300	2.55355000	-0.43104000
H	1.94779800	3.05310400	2.48796100
H	2.91629000	1.66302100	1.99515900
H	2.88259100	-1.79889900	0.46028500
H	2.45510900	-3.31468500	-0.30436500
H	2.79853800	-3.61237500	2.17122800
H	-3.59408400	-1.29454500	0.66332400
H	-4.31440100	0.08060100	-0.14417100
H	-4.92048700	0.05011300	2.29819900
H	-3.20858800	0.13172500	2.72403900
H	-3.97891200	1.49206300	1.90840800
H	1.50807600	-2.44815000	2.48819800
H	1.13378400	-3.99283400	1.72335200
H	3.54288300	3.30039900	1.77311800

Na_2CO_3

C	-0.00000300	0.55668100	0.00051800
O	1.12681600	1.17058900	0.00007500
O	-1.12684800	1.17054400	-0.00032300
O	-0.00000500	-0.77801900	0.00046000
Na	-2.21369100	-0.72022900	-0.0001450
Na	2.21371900	-0.72022600	-0.0002920

PyrCOOPh, phenyl 3-pyridinecarboxylate (**1A**)

C	-0.43246400	0.58772500	-0.20462800
O	0.41039400	-0.44292700	0.08791300
O	-0.07175000	1.69467300	-0.54090700
C	-1.84428700	0.17326800	-0.06762500
C	-2.23591700	-1.10144100	0.35708400
N	-3.50934700	-1.47871600	0.48980300
C	-4.44658200	-0.56961200	0.19245800
C	-2.84071700	1.10423100	-0.37052900
C	-4.16757500	0.72555600	-0.23943000
H	-1.48219700	-1.84690900	0.60029100
H	-5.47898800	-0.89745900	0.30609300
H	-2.55368200	2.09868400	-0.69966700
H	-4.97442700	1.41541400	-0.46430700
C	1.78919900	-0.24072900	0.05683500
C	2.39501800	0.83390700	0.70030200
C	3.78422000	0.91862500	0.69273400
C	4.55241100	-0.05540900	0.05848600
C	2.53816200	-1.22421400	-0.57813100
C	3.92647300	-1.12697700	-0.57406100
H	1.79082200	1.58706700	1.19153900
H	4.26717800	1.75382600	1.19138900
H	5.63554700	0.01966600	0.05960800
H	2.02726900	-2.04985300	-1.06277100
H	4.51710200	-1.89297600	-1.06782100

Ni[P(n-Bu)]

Ni	-3.33216300	-0.00258600	0.01209700
P	-1.31795900	0.00144100	0.00622400
C	-0.54147400	-1.11410200	-1.27370100
C	-0.54130500	1.66573600	-0.32802400
C	-0.52906500	-0.54230400	1.60795800
C	0.86514900	1.76378500	-0.90813600
C	1.29590000	3.20692000	-1.14079900
C	0.88125600	-0.09396700	1.97270600
C	1.32123200	-0.61865100	3.33411700
C	0.86581100	-1.66536200	-1.07449200
C	1.29217500	-2.58763000	-2.21002700
C	2.68633100	3.32092300	-1.74001500
C	2.68111500	-3.16818900	-2.01228000
C	2.71526700	-0.16020000	3.72314300
H	-0.60087000	2.22394400	0.61702300
H	-1.23971700	2.17431900	-1.00401100
H	1.59444500	1.27674200	-0.24830200
H	0.91374500	1.21732800	-1.86108600
H	-0.59323400	-1.63949300	1.61942600
H	-1.21998800	-0.20888300	2.39215400
H	1.60314300	-0.42220700	1.21434200
H	0.93330700	1.00442500	1.97793800
H	-0.60387500	-0.57015200	-2.22685400
H	-1.23911600	-1.95407200	-1.37880300
H	1.59522300	-0.85018000	-0.98524200
H	0.91860600	-2.21771500	-0.12483100
H	1.25347000	3.75110400	-0.18715900
H	0.56386100	3.70000900	-1.79500300
H	3.43758600	2.86172900	-1.08826700
H	2.74315400	2.81144400	-2.70813100
H	1.24982600	-2.03233900	-3.15733400
H	0.55765900	-3.39848900	-2.31036000
H	2.97179100	-3.82512000	-2.83695800
H	1.27698900	-1.71661500	3.32595600
H	0.59557500	-0.29970000	4.09488400

H	3.01572300	-0.54629100	4.70133700
H	3.46054200	-0.49513100	2.99347600
H	2.77468900	0.93272600	3.76783700
H	3.43511300	-2.37677500	-1.94004300
H	2.73751000	-3.75404200	-1.08835700
H	2.98046100	4.36247900	-1.89839300

$B(OH)_2$-PhOMe, iso2: *p*-anisylboronic acid (**2a**)

B	-2.63762800	0.11709300	-0.00125400
O	-3.37722300	-1.03426900	-0.02947300
O	-3.32219500	1.30734700	0.02881900
C	-1.08737600	-0.00629500	-0.00305300
C	-0.47267600	-1.27351500	0.01094900
C	0.90248000	-1.42128600	0.01444000
C	1.72642400	-0.28814400	0.00275300
C	-0.23490400	1.10432700	-0.01629200
C	1.15220100	0.98670900	-0.01403100
H	-1.10170600	-2.16011700	0.01960900
O	3.06279400	-0.52998100	0.00824600
H	-0.64912200	2.11313400	-0.03264200
H	1.77012500	1.87778100	-0.02509700
H	1.37026100	-2.40140500	0.02638000
H	-2.74450800	2.07282200	0.05920700
C	3.92394900	0.59389500	-0.00443700
H	4.93909900	0.19832300	0.00175000
H	3.77826100	1.20385500	-0.90422600
H	3.77600000	1.22583900	0.87970300
H	-4.31786500	-0.83461300	-0.02111800

$(OH)_2$B-OPh, lowest isomer, iso2

B	-2.14015000	0.01066500	0.06296400
O	-3.38394300	-0.46015600	-0.24778400
O	-1.99299900	1.16385000	0.77184500
O	-1.04630900	-0.72513200	-0.34158100
C	0.26011500	-0.33943500	-0.17883900
C	1.17588800	-1.31746500	0.20718400
C	2.52218200	-0.98992100	0.33424200
C	2.95962500	0.30737300	0.07665400
C	0.68932500	0.96004300	-0.44949200
C	2.03807500	1.27554300	-0.31621400
H	0.81772200	-2.32383900	0.40228400
H	3.23115600	-1.75546200	0.63767100
H	4.01083100	0.56081300	0.17646900
H	-0.03198700	1.71091200	-0.75319300
H	2.36911400	2.28921900	-0.52544200
H	-3.33211700	-1.27709100	-0.75031900
H	-2.84922400	1.53680500	0.99665500

NaOPh

O	-1.54748200	0.84553800	-0.58549700
C	-0.34077000	0.43494100	-0.34636700
C	0.70867400	1.32339200	0.03954700
C	1.98737300	0.86925000	0.32565100
C	2.31369000	-0.48911800	0.24737700
C	0.03088400	-0.94363300	-0.42960600
C	1.31764100	-1.38555500	-0.13831600
H	0.47294100	2.38460800	0.10175100
H	2.75227600	1.58800200	0.61840100
H	3.31814900	-0.83526900	0.47364300
H	-0.72039500	-1.65785300	-0.77715700
H	1.54813600	-2.44735200	-0.22159000
Na	-2.82692800	-0.42291900	0.5726560

$NaCO_3$-$B(OH)_2$, lowest isomer, iso3

B	-1.79750000	0.08179800	-0.00029700
C	0.61654000	-0.35804000	0.00142600
O	-0.69394100	-0.78395100	0.00152600
O	0.85343200	0.88950600	0.00400900
Na	3.07154100	0.31507000	-0.00168800
O	1.47507200	-1.26330200	-0.00130000
O	-1.70583300	1.42950800	-0.00210200
O	-3.03033900	-0.50802700	-0.00090500
H	-2.93972200	-1.46380600	0.00175200
H	-0.74611500	1.62741900	-0.00008600

$NaCO_3[B(OH)_2][OPh]$, iso3

C	2.98535300	-0.20026700	0.00783700
O	4.01770300	0.49125600	0.02505000
O	1.73382000	0.37667200	-0.00599400
O	2.92109200	-1.47062200	0.00035600
Na	0.51822900	-1.58152600	-0.0344030
Na	5.22396900	-1.42516800	0.02604400
O	-1.25611500	-0.32818600	-0.04203300
C	-2.56356600	-0.27826100	-0.01758000
C	-3.35791600	-1.45469800	-0.00414000
C	-4.74585100	-1.39882700	0.02251500
C	-5.41627500	-0.17474000	0.03669600
C	-3.26873100	0.95447200	-0.00306200
C	-4.65660600	0.99659700	0.02364600
H	-2.84806700	-2.41821600	-0.01530000
H	-5.31542800	-2.32723700	0.03217700
H	-6.50163200	-0.13447100	0.05759000
H	-2.69181600	1.87727800	-0.01282600
H	-5.15681100	1.96416300	0.03434600
B	1.33742600	1.72964900	-0.00787400
O	0.01391300	1.96209200	-0.02734100
O	2.26139300	2.73341500	0.00884800
H	1.79469200	3.57380900	0.00459300
H	-0.52513400	1.10740000	-0.03580700

$Ni[P(n\text{-}Bu)_3]_2$

Ni	0.00272800	-0.52526600	-1.30802200
P	2.04048600	-0.29380400	-0.73301600
P	-2.02029200	-0.29292600	-0.69795800
C	-1.98730700	0.39185800	1.03606400
C	3.49734100	-0.52871500	-1.87614400
C	2.27740300	1.42600200	-0.05559600
C	2.43055500	-1.40861300	0.70821200
C	-3.07618400	0.92181400	-1.64062000
C	-3.09697500	-1.81108500	-0.56873600
C	-3.17234500	0.21054600	1.97713300
C	-2.93197500	0.85121200	3.33839800
C	-4.09675300	0.66463700	4.29421000
C	-4.18024000	1.70190200	-0.93742600
C	-4.61557900	-1.69548400	-0.50296100
C	-5.29656000	-3.05751000	-0.44544600
C	3.67257100	2.01659600	0.11032500
C	3.63651500	3.44474800	0.63912400
C	3.41896800	-0.96781100	1.78146900
C	3.54633100	-1.98590500	2.90805700
C	4.88085800	-0.85526500	-1.32659600
C	5.92103600	-1.02104900	-2.42782800
C	-6.81115100	-2.96181600	-0.40299500
C	5.01810100	4.05601800	0.78973400

C	7.29631600	-1.37873000	-1.89348800
C	4.50807600	-1.54518400	3.99680900
H	-1.74835000	1.45965500	0.92750100
H	-1.09304600	-0.05020100	1.49507800
H	-4.08551000	0.63378900	1.54052700
H	-3.37685100	-0.86059400	2.11682200
H	-2.73095100	1.92262200	3.19903300
H	-2.01557900	0.43336500	3.77780600
H	-5.01491900	1.10470200	3.88988400
H	-4.29775000	-0.39748300	4.47167800
H	-3.48826200	0.36812500	-2.49599900
H	-2.36737900	1.63502100	-2.08025500
C	-4.89811300	2.66751300	-1.87268200
H	-4.91738100	1.02083200	-0.49361000
H	-3.75487200	2.26845200	-0.09631800
H	-2.72175400	-2.37136400	0.29915000
H	-2.83000300	-2.42674900	-1.43701900
H	-4.92443500	-1.10535900	0.36922000
H	-4.98628300	-1.14763800	-1.38153700
H	1.73849800	1.44162200	0.90316100
H	1.69029500	2.07576400	-0.71717800
H	4.27848200	1.40006700	0.78659500
H	4.19786800	2.00407900	-0.85574000
H	2.74133300	-2.37069100	0.27668600
H	1.45995700	-1.60700200	1.18103700
H	4.41088800	-0.78965000	1.34761700
H	3.10177600	-0.00406600	2.20639700
H	3.54019300	0.37849800	-2.49552200
H	3.19719200	-1.32822000	-2.56569100
H	5.21905200	-0.07636300	-0.63125700
H	4.83533700	-1.78197800	-0.73573100
H	-4.93133400	-3.60370900	0.43548100
H	-4.98317200	-3.65404900	-1.31330600
H	-7.14859300	-2.39925100	0.47436400
H	-7.20054800	-2.44607100	-1.28768800
H	3.11553100	3.45508900	1.60658100
H	3.02454600	4.06249400	-0.03259300
H	5.63677700	3.47138700	1.47946600
H	5.54482500	4.08729400	-0.17047000
H	5.97660200	-0.09118100	-3.01094500
H	5.58050500	-1.79180600	-3.13294300
H	8.03137800	-1.49067800	-2.69538800
H	3.87212600	-2.94787400	2.48848000
H	2.55289800	-2.17305000	3.33862800
H	4.58927400	-2.28695400	4.79626500
H	5.51408200	-1.38254600	3.59485900
H	4.18567400	-0.60281200	4.45319300
H	-3.90843000	1.13087500	5.26549200
H	7.66893100	-0.60818300	-1.20953100
H	7.27127400	-2.32126200	-1.33551300
H	-7.28254300	-3.94790400	-0.36280800
C	-5.97993700	3.47235900	-1.17511300
H	-5.33256900	2.10079800	-2.70798100
H	-4.16122500	3.34444900	-2.32643900
H	-6.48499000	4.15968000	-1.85980400
H	-6.74406700	2.81789600	-0.74173100
H	-5.56301300	4.06943800	-0.35664200
H	4.97349300	5.07889300	1.17441100

Ni[P(n-Bu)$_3$]$_2$-[PyrCOOPh], iso-A

Ni	0.06151300	-1.16131100	0.18964600
P	2.14565600	-0.41510300	-0.07803600
P	-1.27450700	0.38828500	-0.54831000
C	-0.37972200	0.58085000	3.82203400
C	-1.51448900	1.31286100	4.16612400
C	-0.48146900	-0.60373200	3.09424200
C	-2.77064100	0.84435100	3.78053300
C	-2.88682600	-0.33353000	3.04787500
C	-1.74468700	-1.05914200	2.69558100
O	-1.95379700	-2.21028100	1.98741000
C	-1.04744900	-2.56802700	0.93327600
O	0.20657400	-2.79575200	1.18815600
C	-1.75921800	-3.37733800	-0.07561900
H	0.39457600	-1.19433000	2.85773400
H	-3.66749300	1.40111100	4.04065800
H	-3.85774200	-0.70703400	2.73054100
H	0.60513100	0.92569800	4.12982600
H	-1.42299500	2.23463000	4.73346200
C	-3.15792500	-3.45639200	-0.16692400
N	-3.81407300	-4.12051000	-1.12356500
C	-3.07909100	-4.75988000	-2.04056500
C	-1.01777600	-4.07545300	-1.03874000
C	-1.68480600	-4.77450800	-2.03262000
H	-3.77157300	-2.95286600	0.57873000
H	-3.63159200	-5.29046300	-2.81510100
H	0.06792700	-4.05111000	-0.98527500
H	-1.13760600	-5.32520500	-2.79228600
C	-3.07782300	0.00776000	-0.40693300
C	-1.01272400	1.86880700	0.52763200
C	-1.06769100	0.97812600	-2.29285400
C	3.22094100	-1.68619700	-0.88369600
C	2.40433300	1.13634100	-1.05461400
C	2.92922900	-0.07631900	1.56379300
C	-4.06108300	1.12030000	-0.06957900
H	-3.14045800	-0.75807000	0.37404700
H	-3.36865500	-0.50604400	-1.33392900
C	-5.47122800	0.58507000	0.14578500
H	-3.73307300	1.63016900	0.84884900
H	-4.07529500	1.88808400	-0.85469400
C	-2.20947300	1.74279200	-2.95286400
H	-0.83910400	0.08185400	-2.88463400
H	-0.14914600	1.57959400	-2.31787400
C	-1.88491600	2.14102800	-4.38706700
H	-3.12187600	1.13040900	-2.94545600
H	-2.45187100	2.64517900	-2.37635100
C	-1.36179100	3.26569100	0.03346900
H	0.04690400	1.84342500	0.81843300
H	-1.55488900	1.64414600	1.45572300
C	-1.04813300	4.32240500	1.08511100
H	-0.80554000	3.49252400	-0.88912200
H	-2.42449200	3.32457600	-0.23536200
C	3.62753800	2.01613300	-0.82491400
H	1.50815900	1.74326100	-0.86799600
H	2.33358500	0.84671400	-2.11288500
C	3.57571600	3.28210300	-1.67055400
H	3.68706200	2.29681800	0.23642900
H	4.55304200	1.46666100	-1.04314700
C	4.44328100	-0.13296500	1.72710200
H	2.47399200	-0.79950400	2.25343200
H	2.54337800	0.90362200	1.88174900
C	4.87582200	0.19717000	3.15017400
H	4.80337400	-1.13779700	1.46465400
H	4.93840900	0.55466200	1.03000100
C	4.53264400	-1.26557900	-1.53504000

H	2.58488000	-2.17212700	-1.63519600
H	3.39322600	-2.45606700	-0.11859400
C	5.26269900	-2.43934800	-2.17534500
H	4.33541000	-0.50275400	-2.30191600
H	5.19322200	-0.78642600	-0.80109500
C	-6.43824400	1.65048900	0.62846400
H	-5.43118800	-0.23865700	0.87333000
H	-5.83570800	0.13383200	-0.78684100
H	-7.44658500	1.25306100	0.77295000
H	-6.10927100	2.07323700	1.58468500
H	-6.50865100	2.47858200	-0.08523500
C	6.56103000	-2.03123200	-2.84776300
H	4.59746700	-2.92151900	-2.90446500
H	5.46093300	-3.19949900	-1.40754100
H	7.07251400	-2.88524600	-3.30029400
H	6.38386500	-1.29594500	-3.64008300
H	7.25257000	-1.57517400	-2.13122100
C	6.37814000	0.10497100	3.34785900
H	4.36345700	-0.47927000	3.84780300
H	4.52498400	1.20694200	3.40519400
H	6.67050200	0.34806200	4.37306500
H	6.74445500	-0.90427800	3.13111700
H	6.90909700	0.79308300	2.68115400
C	4.76338600	4.19926600	-1.44161700
H	2.63991900	3.81744800	-1.45232500
H	3.51577600	3.00314300	-2.73146000
H	4.70641300	5.10199100	-2.05585800
H	4.82326800	4.51580100	-0.39478500
H	5.70556700	3.69540100	-1.68279500
C	-1.37841500	5.73232700	0.63103200
H	0.01585400	4.25271800	1.35383200
H	-1.60065100	4.08064500	2.00444500
H	-1.14770600	6.47423100	1.40056300
H	-0.81275800	6.00228400	-0.26738700
H	-2.44152100	5.83073600	0.38644700
C	-3.02150000	2.88584900	-5.06377600
H	-1.63115100	1.24032000	-4.96242000
H	-0.97688500	2.75983500	-4.39031800
H	-2.77139100	3.16738200	-6.09029800
H	-3.92900500	2.27399000	-5.10144900
H	-3.27217100	3.80405100	-4.52165200

Ni[P(n-Bu)$_3$]$_2$-[PyrCOOPh], iso-B

Ni	-0.20515700	-1.21877000	-0.31505100
P	-2.21261100	-0.49785800	0.24066600
P	1.02723800	0.58970600	-0.57366800
C	-1.33588500	-3.78347800	-1.08970400
C	-1.24940200	-3.79144800	-2.46070500
C	-0.30490100	-3.23201600	-0.26803000
C	-0.07570000	-3.30338200	-3.09619300
C	0.97736800	-2.83326300	-2.35295900
C	0.89004300	-2.73871900	-0.92837200
O	2.20035200	-2.79807500	-0.31956500
C	2.37953300	-2.23173600	0.88107600
O	1.47251300	-1.84076400	1.60351600
C	3.80809000	-2.03766500	1.20757000
H	-0.27860100	-3.48669700	0.78852300
H	0.00101200	-3.32372600	-4.18004500
H	1.90382100	-2.51453300	-2.82628400
H	-2.20434700	-4.21839300	-0.59658100
H	-2.05806100	-4.20181100	-3.05932500
C	4.84642400	-2.36016100	0.32392900
N	6.13529200	-2.11459500	0.57092000
C	6.43012900	-1.52805500	1.73881400
C	4.14323300	-1.42810000	2.42020100
C	5.47801500	-1.16792900	2.69090800
H	4.61531600	-2.82672000	-0.63227300
H	7.48627700	-1.33245700	1.91966200
H	3.35097800	-1.16402600	3.11552600
H	5.78160100	-0.69281300	3.61838900
C	2.74559700	0.42535800	-1.26930300
C	0.32760300	1.97128700	-1.59581700
C	1.26467100	1.29534800	1.13449800
C	-3.25009000	-1.62647000	1.28463500
C	-2.34752400	1.14724900	1.09663500
C	-3.16846500	-0.32545100	-1.33707100
C	3.86710000	1.27899700	-0.69193700
H	2.65028700	0.59862100	-2.35030300
H	3.01950400	-0.63260700	-1.17845700
C	5.19203200	1.05780800	-1.41087300
H	3.60406200	2.34564400	-0.72706300
H	4.00058400	1.03892700	0.37381300
C	1.24524100	2.80301400	1.35496600
H	2.18865600	0.85827100	1.53345100
H	0.46674300	0.83370100	1.72981800
C	1.07893100	3.16663800	2.82463500
H	2.16384300	3.26200100	0.96257800
H	0.41906300	3.26053200	0.78882800
C	1.22089700	3.12952900	-2.02500400
H	-0.55183200	2.35178500	-1.05571400
H	-0.08412600	1.48401500	-2.49039500
C	0.45693700	4.18741100	-2.81161800
H	1.68960800	3.60256600	-1.15289300
H	2.05140000	2.75119600	-2.63797200
C	-3.52657300	2.07494700	0.83539900
H	-1.42902500	1.68724500	0.83331400
H	-2.24938800	0.94523200	2.17324900
C	-3.32073900	3.44200100	1.47770700
H	-3.66094200	2.20963900	-0.24803200
H	-4.46255600	1.63154100	1.20066800
C	-4.69134200	-0.37230700	-1.33314600
H	-2.78510200	-1.13772100	-1.97191500
H	-2.81375100	0.60119200	-1.81059000
C	-5.27602800	-0.24392400	-2.73433700
H	-5.03089400	-1.31917600	-0.88917200
H	-5.10399900	0.42126100	-0.69615000
C	-4.46462300	-1.07732600	2.02230200
H	-2.55789400	-2.07632000	2.00878500
H	-3.54230000	-2.45333800	0.62182000
C	-5.19671800	-2.15101900	2.81754600
H	-4.15100800	-0.27532100	2.70631600
H	-5.16607300	-0.60864500	1.32006600
C	6.34486500	1.80927400	-0.77025900
H	5.08498300	1.35575700	-2.46329100
H	5.41418400	-0.01825800	-1.42671800
H	7.28679500	1.64156600	-1.30001900
H	6.15968100	2.88908800	-0.75832500
H	6.49080800	1.49358100	0.26911900
C	-6.38367000	-1.60810000	3.59273300
H	-4.48921900	-2.63446200	3.50495200
H	-5.52825100	-2.94190200	2.13049300
H	-6.89948900	-2.39248200	4.15345100
H	-6.07087200	-0.84136400	4.30990800
H	-7.11677000	-1.14548000	2.92303000

C	1.34079400	5.32927000	-3.27973300
H	-0.35824600	4.57611000	-2.18463900
H	-0.03292900	3.71429000	-3.67381800
H	0.77597800	6.08182500	-3.83695800
H	1.81768000	5.83463800	-2.43293100
H	2.14155100	4.96691500	-3.93332200
C	-6.79187900	-0.32272600	-2.75158600
H	-4.85159900	-1.03008500	-3.37365400
H	-4.94462800	0.70649400	-3.17489000
H	-7.19545700	-0.22849100	-3.76359600
H	-7.14314000	-1.27678000	-2.34397000
H	-7.23723100	0.47245300	-2.14373600
C	1.04885100	4.66531500	3.06393200
H	1.88880700	2.70696700	3.40723300
H	0.14979900	2.70959500	3.19525000
H	0.92338800	4.90872400	4.12270200
H	1.97527000	5.14053300	2.72360700
H	0.22370700	5.13586900	2.51737200
C	-4.47574200	4.39581000	1.23325800
H	-2.38628700	3.87595200	1.09035600
H	-3.15968200	3.31420600	2.55750400
H	-4.30467700	5.37235200	1.69452500
H	-4.63322400	4.56024500	0.16177400
H	-5.41120100	3.99790000	1.64077400

TS[C(acyl)-O], iso1

Ni	-0.32032500	-0.97549500	-0.78476800
P	1.83339500	-0.25007600	-0.66633700
P	-1.52711000	0.80101900	-0.44945700
C	1.90022500	-2.58150700	2.70985600
C	1.97762800	-1.76148000	3.83924900
C	0.77073900	-2.59260500	1.89963700
C	0.87980000	-0.95160600	4.14411600
C	-0.25609300	-0.94827900	3.34281900
C	-0.35863500	-1.76519300	2.17719100
O	-1.42015400	-1.73258300	1.42710800
C	-1.41299300	-2.42048600	-0.90517300
O	-0.31705500	-2.93688500	-1.18435700
C	-2.70600900	-3.09084600	-0.96214100
H	0.72756000	-3.24445100	1.03018500
H	0.91186900	-0.30663800	5.02202700
H	-1.10887400	-0.31703000	3.59252600
H	2.74017800	-3.22949200	2.45648400
H	2.86456100	-1.75794700	4.46709100
C	-3.74944200	-2.81550300	-0.06494000
N	-4.95798600	-3.37403500	-0.15187300
C	-5.16696500	-4.24026100	-1.15235900
C	-2.93571400	-4.02841700	-1.97760500
C	-4.19147300	-4.60928100	-2.07521400
H	-3.56033000	-2.15172500	0.77368400
H	-6.16854600	-4.66336500	-1.21534800
H	-2.13987800	-4.27702700	-2.67415300
H	-4.41281200	-5.33527700	-2.85107200
C	-3.27496900	0.51736800	0.02414400
C	-0.73849700	1.67868500	0.96003600
C	-1.58897500	2.00377300	-1.85117900
C	2.88006500	-1.73729300	-0.98392700
C	2.32208100	1.02025800	-1.91482900
C	2.39304400	0.44301700	0.95148600
C	-4.26175800	1.67716000	0.00024700
H	-3.21973400	0.04920400	1.01596400
H	-3.63793400	-0.27024400	-0.64736900
C	-5.63811100	1.24240900	0.48930900
H	-3.90590300	2.51235800	0.61655100
H	-4.34797100	2.07396000	-1.02177200
C	-1.68892800	3.48675300	-1.51003800
H	-2.42780800	1.69660300	-2.48993000
H	-0.68934100	1.82917000	-2.45482400
C	-1.67306100	4.36796600	-2.75206400
H	-2.59998300	3.68625700	-0.93004400
H	-0.85180900	3.77207600	-0.85656500
C	-1.53172400	2.58352800	1.89302000
H	0.11191900	2.22924600	0.53422900
H	-0.29905300	0.87240900	1.56070100
C	-0.64511600	3.08530200	3.02749800
H	-1.96161200	3.43873600	1.35379400
H	-2.38118700	2.02774000	2.31513300
C	3.61652200	1.80081900	-1.71628700
H	1.48410500	1.73115100	-1.95471500
H	2.31786900	0.51815800	-2.89207600
C	3.82906100	2.83857800	-2.81101900
H	3.59869200	2.30469600	-0.73939400
H	4.47808200	1.12203700	-1.68493400
C	3.82982300	0.21111100	1.40051800
H	1.72111200	0.02842000	1.71320000
H	2.17986800	1.52074000	0.91784400
C	4.11072900	0.92101400	2.71826900
H	3.99838800	-0.86838900	1.52636100
H	4.54784700	0.55180500	0.64193100
C	4.29606500	-1.58026400	-1.52061300
H	2.29772500	-2.35982400	-1.67429000
H	2.87853300	-2.28916200	-0.03400600
C	4.97810500	-2.92732900	-1.72656100
H	4.27275400	-1.03845400	-2.47719800
H	4.90484400	-0.96920000	-0.84272600
C	-6.66953900	2.35377800	0.42084900
H	-5.54843300	0.87583400	1.52086100
H	-5.97254800	0.37767700	-0.10063400
H	-7.64703900	2.02447400	0.78347600
H	-6.36611900	3.21434300	1.02687000
H	-6.80161600	2.71105000	-0.60629300
C	6.37785900	-2.79817100	-2.29903100
H	4.35792400	-3.54757700	-2.38782700
H	5.01211000	-3.46069200	-0.76675000
H	6.85331500	-3.77321500	-2.43591800
H	6.36284000	-2.29892300	-3.27406800
H	7.02300400	-2.20599900	-1.64124000
C	-1.39244800	3.93437600	4.03893900
H	0.19131100	3.65656700	2.60017000
H	-0.18513700	2.21809900	3.52384200
H	-0.73584100	4.28658500	4.83930100
H	-1.83855000	4.81643600	3.56649400
H	-2.20622000	3.36886400	4.50519300
C	5.47578900	0.58684900	3.29066800
H	3.32410200	0.64657600	3.43435400
H	4.01760800	2.00585800	2.56619300
H	5.66929500	1.11904100	4.22638900
H	5.56101200	-0.48589800	3.49787200
H	6.27838700	0.84667000	2.59131000
C	-1.73800300	5.84894500	-2.42485000
H	-2.51348200	4.08975000	-3.40217800
H	-0.76489300	4.15109600	-3.33183900
H	-1.72638100	6.46634000	-3.32699000
H	-2.64997100	6.09319000	-1.86979600

H	-0.88891700	6.15512300	-1.80449300
C	5.10212400	3.64380300	-2.62375100
H	2.95995600	3.51075100	-2.84072800
H	3.84562100	2.33327400	-3.78643500
H	5.23775900	4.38303700	-3.41786500
H	5.09450800	4.18189300	-1.66971900
H	5.98442000	2.99509200	-2.62295500

TS[C(aryl)-O], iso1

Ni	-0.04146800	-0.83268100	-1.11912700
P	-2.04552300	-0.42327500	-0.19829800
P	1.08532800	1.00922500	-0.69060500
C	-0.54706000	-3.15657200	-3.44560400
C	0.02248400	-2.76974900	-4.64435800
C	-0.01774300	-2.69345200	-2.21956300
C	1.16147500	-1.93961500	-4.64658400
C	1.71017500	-1.46897700	-3.46690800
C	1.06275100	-1.77161900	-2.25598600
O	2.50680500	-2.23558500	-0.93764300
C	2.00758300	-2.32449100	0.23586500
O	0.81746800	-2.08835500	0.56249000
C	2.96492100	-2.71734600	1.31877900
H	-0.31324700	-3.16654700	-1.28715900
H	1.61025800	-1.64627500	-5.59318200
H	2.58639100	-0.82660600	-3.47840800
H	-1.36989800	-3.86930300	-3.43309100
H	-0.37647000	-3.13876700	-5.58472500
C	4.23881200	-3.21532700	1.02932100
N	5.13066400	-3.57875400	1.95646000
C	4.76376200	-3.43551100	3.23619900
C	2.60751000	-2.58268100	2.66118800
C	3.52463600	-2.94233700	3.63931000
H	4.53873200	-3.32646100	-0.01145600
H	5.50293300	-3.73164300	3.97997200
H	1.62111100	-2.19787000	2.90784600
H	3.28877600	-2.84848700	4.69516100
C	2.69251200	1.29716400	-1.54981200
C	0.10204600	2.56182500	-0.92393700
C	1.56072600	0.94497700	1.10288100
C	-2.92836000	-2.01495700	0.13460700
C	-1.98331000	0.41908400	1.45064500
C	-3.19885700	0.59453900	-1.22555400
C	3.73652100	2.20326700	-0.90613200
H	2.45635800	1.63506500	-2.56841000
H	3.11541500	0.28999700	-1.66168300
C	5.02608900	2.25976400	-1.71606100
H	3.35024400	3.22156000	-0.77459900
H	3.96630100	1.83968800	0.10536700
C	1.55515500	2.22022300	1.93463700
H	2.55048800	0.46821400	1.13799200
H	0.88643500	0.20825700	1.55388100
C	1.70570100	1.92372900	3.42196800
H	2.35497600	2.90034300	1.60792000
H	0.61415000	2.77134100	1.77795300
C	0.78331500	3.92396000	-0.96635100
H	-0.67070800	2.55637300	-0.14018500
H	-0.44946200	2.40624600	-1.86080900
C	-0.22257600	5.05971900	-1.10649500
H	1.38526000	4.08633000	-0.06296100
H	1.48823600	3.95681800	-1.80854700
C	-3.18359500	1.20618100	1.96058700
H	-1.12437700	1.10075300	1.40611900
H	-1.68589600	-0.35390200	2.17457700
C	-2.86949300	1.93719200	3.26030000
H	-3.49082000	1.94305800	1.20374000
H	-4.05027900	0.54833600	2.10770300
C	-4.70502100	0.44554500	-1.04985200
H	-2.93086100	0.37285100	-2.26675100
H	-2.89791000	1.64104700	-1.07242700
C	-5.48826400	1.35953600	-1.98338700
H	-4.99613800	-0.59794200	-1.23634200
H	-4.99606700	0.65551700	-0.01251500
C	-4.02559400	-2.07826600	1.19017500
H	-2.13075700	-2.71965000	0.40530300
H	-3.30304400	-2.36399400	-0.83827000
C	-4.60524400	-3.48001400	1.33396600
H	-3.62144300	-1.75651700	2.16061500
H	-4.83621800	-1.37634200	0.95607100
C	6.08638800	3.13626000	-1.07420100
H	4.79975500	2.62540400	-2.72713000
H	5.41165500	1.23994000	-1.84890800
H	7.00428300	3.16755800	-1.66758900
H	5.73266300	4.16668900	-0.95896300
H	6.35141400	2.77050200	-0.07624200
C	-5.67466000	-3.56883900	2.40764700
H	-3.79194600	-4.18446000	1.55500800
H	-5.01765400	-3.79830200	0.36673800
H	-6.08168600	-4.57990700	2.49566500
H	-5.27579600	-3.28754800	3.38830400
H	-6.51071400	-2.89458600	2.19224300
C	0.43501100	6.42558600	-1.18638500
H	-0.91693200	5.02657900	-0.25495300
H	-0.83969200	4.88700000	-1.99882200
H	-0.30153500	7.22843800	-1.27890200
H	1.03508500	6.62939900	-0.29307400
H	1.10563300	6.49204400	-2.04969800
C	1.70865800	3.17460100	4.28147300
H	2.62925400	1.35098600	3.58419300
H	0.88707900	1.25607400	3.73024800
H	1.80785300	2.93941100	5.34477500
H	2.53671500	3.83888200	4.01219600
H	0.78136700	3.74415700	4.15466200
C	-4.04689900	2.73259300	3.79362300
H	-2.01075000	2.60406200	3.09224600
H	-2.53459200	1.20919000	4.01210400
H	-3.79987900	3.25457800	4.72217700
H	-4.37713200	3.48535400	3.06963500
H	-4.90380500	2.08211800	3.99864400
C	-6.99120400	1.20146800	-1.83899700
H	-5.18743700	1.15883800	-3.02055600
H	-5.20059200	2.40183400	-1.78783500
H	-7.53837200	1.86641800	-2.51286000
H	-7.30458400	0.17575500	-2.06135100
H	-7.31703000	1.42595200	-0.81753800

Ni[P(n-Bu)$_3$]$_2$[PyrCO][OPh], Product A

Ni	0.03695800	-0.83413600	-0.59701200
P	1.81288700	0.25929700	0.06114500
P	-1.60915400	0.82392300	-0.28659100
C	-0.95392600	2.53863300	-0.62088300
C	3.21835300	-0.78957500	0.63838600
C	2.48987500	1.21300500	-1.36402900
C	1.51064100	1.42061200	1.47533600
C	-2.84766000	0.61821200	-1.63309600

C	-2.66285700	0.97558600	1.24352100
C	-1.50831300	3.72706900	0.15034900
C	-0.78332700	5.01913800	-0.20351800
C	-1.23648500	6.20398900	0.62968000
C	-3.77224700	1.80224700	-1.89115400
C	-4.00175400	0.24035500	1.20955800
C	-4.65861000	0.18777900	2.58226300
C	3.94431900	1.66914500	-1.37019100
C	4.29857400	2.40576400	-2.65638100
C	2.22234500	2.76862500	1.45717900
C	1.68478000	3.72379300	2.51480000
C	4.29115000	-0.14462300	1.50875400
C	5.43741600	-1.10170100	1.81099400
C	-6.01707700	-0.48750200	2.54462800
C	5.75087500	2.84493500	-2.70019500
C	6.48810000	-0.49160700	2.72054300
C	2.35538100	5.08477300	2.47657500
H	-1.07281300	2.69950200	-1.70053200
H	0.12882600	2.50905300	-0.46161000
H	-2.58708500	3.83939800	-0.02783800
H	-1.40250900	3.55112900	1.23134000
H	-0.91976000	5.23234200	-1.27226800
H	0.29803400	4.86136700	-0.07026800
H	-2.30290600	6.40729900	0.48604500
H	-1.08304700	6.01773900	1.69888200
H	-3.41924700	-0.28384700	-1.38048600
H	-2.28792400	0.35411800	-2.53830000
C	-4.94803900	1.44061400	-2.78923000
H	-4.15434100	2.20367300	-0.94106400
H	-3.20751800	2.62748600	-2.34798100
H	-2.84078300	2.03412200	1.46650800
H	-2.06001100	0.58182300	2.07289100
H	-4.68260400	0.73626400	0.50405900
H	-3.87833900	-0.78549500	0.84258000
H	1.82380500	2.07154800	-1.52138300
H	2.30796400	0.54669100	-2.21842400
H	4.15370900	2.32375100	-0.51352100
H	4.60947300	0.80136100	-1.25951700
H	1.75400200	0.86602900	2.39042700
H	0.42664600	1.58300900	1.52429400
H	3.30284400	2.62840900	1.59732700
H	2.11087000	3.23764100	0.46725400
H	3.66262300	-1.22376300	-0.26867200
H	2.77427100	-1.63839600	1.17399100
H	4.69270000	0.75770100	1.03075900
H	3.84776800	0.19377800	2.45564200
H	-4.75104300	1.20483300	2.98956500
H	-3.99273000	-0.35485200	3.26787600
H	-6.71288600	0.05464500	1.89459200
H	-5.92745800	-1.50715500	2.15323800
H	3.63900100	3.27789600	-2.76229000
H	4.07491900	1.75823400	-3.51443000
H	5.98846900	3.51566100	-1.86742800
H	6.42651000	1.98595600	-2.62814400
H	5.89749800	-1.41734000	0.86463800
H	5.03291900	-2.01685000	2.26398300
H	7.30587600	-1.18894300	2.92095900
H	1.80199300	3.27134500	3.50844700
H	0.60062600	3.83836400	2.36764000
H	1.94400300	5.76139400	3.23052100
H	3.43254800	5.00348100	2.65621900
H	2.22414400	5.56324700	1.49914800
H	-0.68890300	7.11496500	0.37252500
H	6.92438500	0.40932400	2.27556600
H	6.05790900	-0.20190500	3.68529600
H	-6.47211900	-0.54886500	3.53743600
C	-5.85676000	2.62205800	-3.07598400
H	-5.52024700	0.63244200	-2.31351900
H	-4.56753500	1.02039100	-3.72978500
H	-6.69893300	2.34388000	-3.71551800
H	-6.26919300	3.03741400	-2.14995400
H	-5.31270200	3.42864200	-3.57920600
H	5.98863600	3.37393100	-3.62712300
O	-1.35032100	-2.10333100	-1.08888200
C	-2.09623300	-2.52361900	-0.09024400
C	-3.29915000	-3.22494500	-0.35451600
C	-4.12126900	-3.65510500	0.67829100
C	-3.79006700	-3.41684400	2.01567900
C	-1.77913800	-2.29186200	1.27404400
C	-2.60957600	-2.73176400	2.29920500
H	-3.56389000	-3.40941800	-1.39309700
H	-5.04070500	-4.18557000	0.43730400
H	-4.43999300	-3.75762900	2.81667500
H	-0.87264200	-1.72593700	1.50201400
H	-2.33304500	-2.52853800	3.33241100
C	1.17911400	-2.01812400	-1.52724600
C	1.47220100	-3.39211700	-1.03752100
O	1.54020100	-1.66359600	-2.64357700
C	1.19074600	-3.77238600	0.27648500
N	1.45366300	-4.97910100	0.78382300
C	2.01379300	-5.86866500	-0.04613700
C	2.06399800	-4.33779400	-1.88012100
C	2.33492200	-5.60102600	-1.37705600
H	0.72188500	-3.04897200	0.94643300
H	2.21742900	-6.85130500	0.37781700
H	2.29330700	-4.06182700	-2.90612600
H	2.78726400	-6.37046200	-1.99551300

Ni[P(n-Bu)$_3$]$_2$[PyrCOO][Ph], Product B

Ni	-0.07321600	-1.00421400	-0.81864400
P	-0.95153600	1.15454900	-0.70773900
P	1.99618900	-0.51443500	-0.31690100
C	0.97535100	-4.95548100	0.17400100
C	1.26898800	-5.52870400	-1.06145200
C	0.59278900	-3.61444600	0.25555900
C	1.16645000	-4.75410400	-2.21643500
C	0.79507500	-3.41140500	-2.13110700
C	0.51086600	-2.81960600	-0.89418400
O	-1.76002900	-1.24688400	1.25200200
C	-2.38089300	-1.65434100	0.24758100
O	-1.89605300	-1.71289500	-0.94280800
C	-3.81970500	-2.04592300	0.36891400
H	0.34696700	-3.18741500	1.22750300
H	1.38153700	-5.19557500	-3.18788100
H	0.74113600	-2.81857300	-3.04392400
H	1.03831800	-5.55534800	1.07999000
H	1.56966600	-6.57134000	-1.12490600
C	-4.47008400	-1.95315600	1.60273400
N	-5.76751600	-2.21426600	1.79179700
C	-6.46891800	-2.59115600	0.71481600
C	-4.57299800	-2.44943400	-0.73484300
C	-5.92232600	-2.72790400	-0.55979700
H	-3.89539000	-1.63812700	2.47329100
H	-7.52617000	-2.79528400	0.88239800

H	-4.09178700	-2.52648800	-1.70553200
H	-6.54509700	-3.04034000	-1.39257200
C	3.40235400	-1.61056000	-0.80038500
C	2.63565000	1.16045900	-0.77505200
C	1.88015300	-0.57285700	1.53178800
C	-2.80432400	1.25548400	-0.80189200
C	-0.52551900	1.99980800	0.87902100
C	-0.37138200	2.33178900	-2.02452400
C	4.51649700	-1.80372800	0.22227500
H	3.80672900	-1.19738400	-1.73432500
H	2.98051500	-2.58453400	-1.06172400
C	5.60984200	-2.72825100	-0.29705200
H	4.96024400	-0.84118900	0.50931900
H	4.09819400	-2.22882400	1.14542200
C	2.67900000	0.42756300	2.36017200
H	2.12077000	-1.60165900	1.82541900
H	0.80754900	-0.46732100	1.74735000
C	2.20157600	0.48443200	3.80542700
H	3.74940600	0.18010700	2.33083700
H	2.59651200	1.43665100	1.92681300
C	4.10780200	1.49419600	-0.56681600
H	2.01756400	1.90206800	-0.25328600
H	2.38759000	1.27703500	-1.83827700
C	4.40480700	2.94563000	-0.92563100
H	4.40484600	1.31691700	0.47410400
H	4.73537800	0.82933500	-1.17602900
C	-0.61242500	3.51637700	0.97062000
H	0.49608200	1.69125800	1.12861800
H	-1.15150800	1.51767100	1.64110700
C	-0.07772800	4.03542800	2.29996900
H	-0.03567100	3.97741100	0.15443000
H	-1.64973300	3.85329500	0.83044900
C	-1.27100200	3.49683400	-2.42467000
H	-0.12849000	1.73085900	-2.90929100
H	0.59105000	2.72404900	-1.67270900
C	-0.52386300	4.54704000	-3.23677000
H	-2.12092800	3.12737600	-3.01282700
H	-1.70963600	3.97081700	-1.53560500
C	-3.55749300	1.41209800	0.51726600
H	-3.13169700	0.33769000	-1.30455000
H	-3.07390800	2.08377000	-1.46502300
C	-5.06606300	1.33064100	0.31992200
H	-3.24238800	0.64154800	1.23293800
H	-3.30674300	2.37848600	0.97887300
C	6.71775900	-2.95606400	0.71525600
H	6.02790700	-2.30766400	-1.22214900
H	5.15802700	-3.68777700	-0.58389900
H	7.49344800	-3.62133600	0.32653400
H	7.20078600	-2.01305700	0.99378200
H	6.32823300	-3.40552500	1.63496900
C	-5.83679000	1.47168600	1.62004800
H	-5.31169600	0.37001300	-0.15467500
H	-5.38317900	2.10467100	-0.39307700
H	-6.91652300	1.39562000	1.46210300
H	-5.55584500	0.68669900	2.33045900
H	-5.63904400	2.43720600	2.09908900
C	5.86877800	3.30714700	-0.75522200
H	3.77923600	3.59857600	-0.29934200
H	4.08700600	3.13526700	-1.96014200
H	6.06198300	4.35370500	-1.00539600
H	6.19797800	3.14779300	0.27708700
H	6.50612200	2.69101500	-1.39808200
C	2.97794000	1.48568000	4.64118200
H	2.27117800	-0.51611300	4.25212300
H	1.13189600	0.73893200	3.81181500
H	2.62138800	1.51730100	5.67418300
H	4.04479200	1.23920000	4.66764700
H	2.88817700	2.49757200	4.23006700
C	-0.15871100	5.54597400	2.42208600
H	0.96572300	3.70366500	2.41202800
H	-0.62835000	3.55952300	3.12285600
H	0.24121000	5.90062300	3.37579500
H	0.40577000	6.03900900	1.62326500
H	-1.19468600	5.89348700	2.34925900
C	-1.41786000	5.68708600	-3.68944100
H	-0.05789900	4.06645800	-4.10790700
H	0.30821500	4.93786700	-2.63405000
H	-0.86559600	6.43438100	-4.26573600
H	-2.23564800	5.32213000	-4.31984200
H	-1.87156000	6.19880800	-2.83385900

$Ni[P(n\text{-}Bu)_3]_2[Na_2CO_3]$, lowest isomer, iso1

Ni	0.04713300	-1.37872100	-1.01945400
P	-1.44217100	0.13319900	-0.60644100
P	1.98953400	-0.71812300	-0.55904300
O	-0.94385000	-3.16468200	-1.42273300
C	-1.90103400	-3.31016100	-0.54255500
O	-3.09339500	-2.90939500	-0.75730500
O	-1.60207300	-3.91357500	0.58764800
Na	-3.73013400	-3.69047500	1.2156570
Na	0.56195500	-4.06492600	-0.0386550
C	-2.98401200	0.29028700	-1.63937000
C	-2.08456400	-0.22229400	1.11142700
C	-0.86330700	1.90687500	-0.49263800
C	3.65023700	-1.61488200	-0.58889600
C	2.41163200	0.79511400	-1.59043900
C	1.95465900	-0.08810500	1.20989300
C	-1.45708000	2.86870400	0.52873900
C	-0.70145300	4.19180400	0.57511300
C	-3.84516000	1.54548100	-1.58234200
C	-5.05644500	1.46923900	-2.50452600
C	3.21849600	0.23886100	1.99568800
C	2.90738400	0.72597300	3.40603500
C	3.02834800	2.02247300	-0.92958500
C	3.00412600	3.24790100	-1.83478100
C	4.97057000	-0.85554000	-0.67702900
C	6.18236900	-1.77988600	-0.68268000
C	-5.90598400	2.72729600	-2.47402700
C	7.50017600	-1.03499600	-0.80245100
C	4.15230000	1.04151900	4.21605400
C	-1.26046900	5.16612200	1.59626600
C	3.60338900	4.48084900	-1.18246500
C	-3.47639700	0.23182600	1.52771600
C	-3.84898900	-0.21802900	2.93519200
C	-5.25485400	0.18808200	3.33985800
H	-0.95623500	2.32751600	-1.50515000
H	0.21778200	1.84601700	-0.31498900
H	-2.51834800	3.05864100	0.31720500
H	-1.42948500	2.41333500	1.53033200
H	-3.55992000	-0.61611100	-1.40990600
H	-2.64319500	0.14472300	-2.67346400
H	-4.19220800	1.73777200	-0.55874600
H	-3.24343500	2.42481500	-1.85743800
H	1.38637100	-0.85335700	1.75768400

H	1.28988100	0.78837500	1.20475600
H	3.86808300	-0.64703100	2.05615300
H	3.80923200	1.00663400	1.47957400
H	1.46319300	1.08582700	-2.05883700
H	3.04865600	0.45271900	-2.41802500
H	2.48536500	2.26738500	-0.00339000
H	4.06205600	1.81455700	-0.61861800
H	3.58888400	-2.30113900	-1.44493400
H	3.65257000	-2.26635800	0.29985400
H	4.98305300	-0.24413100	-1.59075300
H	5.07050100	-0.14457800	0.15253700
H	-5.66538400	0.59882000	-2.22290700
H	-4.71736400	1.27037800	-3.53053200
H	-6.77426000	2.65452400	-3.13556700
H	-6.27799800	2.92943600	-1.46327300
H	-5.32721000	3.60380500	-2.78565300
H	6.08356900	-2.50004900	-1.50707600
H	6.17656100	-2.38217600	0.23711200
H	8.35815600	-1.71360100	-0.80220500
H	7.54198400	-0.45140300	-1.72856200
H	7.63507000	-0.33289000	0.02776800
H	2.30352300	-0.03155200	3.92521400
H	2.26745500	1.61774300	3.34007500
H	3.91004400	1.39150300	5.22378700
H	4.79199700	0.15803200	4.31857600
H	4.75187400	1.82001300	3.73191400
H	-0.71119800	4.64892000	-0.42460400
H	0.35758400	3.98550000	0.79288100
H	-0.69980100	6.10509700	1.61838400
H	-2.30566300	5.41152200	1.37881200
H	-1.23146000	4.74103500	2.60571200
H	1.96248800	3.44851400	-2.12569100
H	3.53450000	3.02055200	-2.76987600
H	3.57368300	5.35163900	-1.84374200
H	3.06254700	4.74430600	-0.26637200
H	4.64971300	4.31392900	-0.90364200
H	-1.33126300	0.17100200	1.80958700
H	-2.01788600	-1.31582500	1.20010900
H	-3.55818100	1.32569400	1.47416000
H	-4.21682400	-0.15848200	0.81312700
H	-3.12051300	0.19044900	3.64922300
H	-3.73770700	-1.31131000	3.00914800
H	-5.50596100	-0.14216100	4.35217200
H	-5.37257200	1.27645300	3.31024600
H	-6.00158400	-0.23342700	2.65771400

Decarbonylative transmetalation in the absence of Na_2CO3

For Product-A and $P(n\text{-}Bu)_3$, see above

$Ni[P(n\text{-}Bu)_3][PyrCO][OPh]$

Ni	-1.21202600	0.83229700	-1.12799600
P	0.59344500	-0.19655900	-0.50374500
C	0.63229700	-2.03615000	-0.49643600
C	2.06245800	0.36058700	-1.46750500
C	0.84704800	0.34153800	1.24325700
C	1.58917600	-2.73348100	0.46434100
C	1.50723800	-4.25032500	0.34945100
C	2.44139300	-4.96348100	1.30990100
C	3.36421800	-0.42650300	-1.37815800
C	2.26470200	0.46003300	1.78802500
C	2.27763300	0.98189800	3.21924900
C	3.68009100	1.12859200	3.78059500
H	0.81992900	-2.34821800	-1.53266100
H	-0.39424000	-2.35936800	-0.27900700
H	2.62351900	-2.41372600	0.28577900
H	1.35748900	-2.43506600	1.49663100
H	1.73610600	-4.54337700	-0.68412000
H	0.47105900	-4.56862500	0.52571800
H	3.48483400	-4.68384400	1.12910100
H	2.21179700	-4.70828200	2.34985500
H	2.22034300	1.40723800	-1.17429600
H	1.73068700	0.40206400	-2.51250900
C	4.47669500	0.22239200	-2.19211800
H	3.68931200	-0.51805200	-0.33412000
H	3.20210700	-1.45300400	-1.73569200
H	0.24885800	-0.34202500	1.86180400
H	0.34772100	1.31766500	1.32061800
H	2.77769800	-0.51053600	1.74717900
H	2.85097500	1.13936100	1.15146600
H	1.68797100	0.30570900	3.85283200
H	1.75481000	1.94795900	3.25000600
H	4.20769100	0.16872800	3.78531800
H	4.27690100	1.82429500	3.18108300
H	2.37057100	-6.05017200	1.21403600
H	3.66964200	1.50339700	4.80759300
C	5.78003000	-0.55296900	-2.12965000
H	4.63269300	1.24718200	-1.82793400
H	4.14856600	0.32441600	-3.23522700
H	6.56841800	-0.07042900	-2.71347200
H	6.13990000	-0.64064000	-1.09888000
H	5.65659400	-1.56925800	-2.51858800
O	-2.64422400	2.12467200	-1.19054500
C	-1.73914900	2.82415700	-0.53698700
C	-0.44092600	2.99664500	-1.11708500
C	0.59542200	3.60440700	-0.38958400
C	0.37559200	4.05673800	0.89995200
C	-1.93691100	3.31072900	0.78682400
C	-0.90329000	3.91653100	1.47286000
H	-0.31182000	2.76013200	-2.17371500
H	1.56800200	3.74075200	-0.85808500
H	1.17474600	4.53114100	1.46168600
H	-2.91787800	3.18531200	1.23675000
H	-1.07696600	4.28178000	2.48258700
C	-2.19329700	-0.70247100	-1.48168600
C	-3.03540700	-1.21247900	-0.35736700
O	-2.19786200	-1.24863300	-2.57267400
C	-2.96149300	-0.64743300	0.91921100
N	-3.67725400	-1.06116900	1.96714100
C	-4.52221500	-2.07796400	1.75159300
C	-3.92132300	-2.27615600	-0.55336500
C	-4.68208500	-2.71389400	0.52046200
H	-2.27765000	0.18899300	1.09013200
H	-5.10513700	-2.40214500	2.61259000
H	-3.99263300	-2.72847200	-1.53906900
H	-5.38748300	-3.53259800	0.41573600

TS[(OC-C(Pyr)], Decarbonylation TS

Ni	1.35632800	-0.71440400	0.05261100
P	-0.85115600	-0.63908200	-0.15920300
C	-1.55658700	-2.30126100	-0.53028900
C	-1.54964700	-0.16117300	1.46810900
C	-1.57361500	0.52671000	-1.40131700

C	-2.96111900	-2.38553700	-1.12063000
C	-3.52645700	-3.79747700	-1.04206100
C	-4.89891900	-3.91895700	-1.67879700
C	-3.03084200	-0.41783400	1.71320000
C	-2.05111200	1.87185600	-0.86090600
C	-2.45690300	2.81824900	-1.98211900
C	-2.98403400	4.14082400	-1.45699900
H	-1.51084100	-2.84547100	0.42366000
H	-0.84646400	-2.81571800	-1.18744500
H	-3.64499500	-1.69343800	-0.61199100
H	-2.93865600	-2.06387200	-2.17002900
H	-3.57290200	-4.10322900	0.01237400
H	-2.82591800	-4.49394700	-1.52191200
H	-5.61959700	-3.24867300	-1.19822500
H	-4.86834500	-3.65511700	-2.74114900
H	-1.29809600	0.90070800	1.59311800
H	-0.94571600	-0.68513700	2.21886000
C	-3.49608300	0.13959100	3.05191100
H	-3.63727300	0.02193200	0.90885700
H	-3.23150600	-1.49871500	1.67866600
H	-2.40166200	0.01835200	-1.90964000
H	-0.79961600	0.69436600	-2.15997300
H	-2.90447800	1.72374200	-0.18427100
H	-1.26516100	2.34961700	-0.26382500
H	-3.21027400	2.33504800	-2.62029400
H	-1.58220900	2.99495900	-2.62317600
H	-3.87821400	3.99693000	-0.84044300
H	-2.22987000	4.63446600	-0.83405700
H	-5.29332200	-4.93578500	-1.60313200
H	-3.24871400	4.82563500	-2.26771700
C	-4.96112900	-0.14367300	3.32971300
H	-3.31183900	1.22219700	3.06991000
H	-2.87292300	-0.28115800	3.85235900
H	-5.27837000	0.26329100	4.29353900
H	-5.60334000	0.29596600	2.55898600
H	-5.16124500	-1.22049600	3.34400300
O	1.48096200	0.85347200	1.12714500
C	1.23956200	2.01316800	0.55274600
C	0.82843000	3.12784100	1.32167600
C	0.53493500	4.34350200	0.71605200
C	0.64012300	4.50637700	-0.66787900
C	1.36198400	2.20417600	-0.84603900
C	1.06024200	3.42355700	-1.44074200
H	0.73540500	3.00207300	2.39791700
H	0.21153200	5.17935900	1.33344000
H	0.40383800	5.45948200	-1.13250600
H	1.69853800	1.35966900	-1.45103300
H	1.15665100	3.53061000	-2.51964400
C	3.28759700	-1.29463200	0.03820600
C	1.86239000	-2.17704800	-0.68819300
O	1.98802700	-3.20358300	-1.25322900
C	3.81950400	-1.76865900	1.23994200
C	5.17007100	-1.56705800	1.49471900
C	5.93529200	-0.91102000	0.53264500
C	4.15160900	-0.66780100	-0.86687500
N	5.45134800	-0.46666700	-0.63420600
H	3.18696200	-2.27741100	1.96334800
H	5.62429200	-1.90861600	2.41981200
H	6.99616900	-0.73522500	0.70434200
H	3.77522500	-0.31162200	-1.82613100

$Ni[P(n\text{-}Bu)_3](Pyr)(CO)(OPh)$,

Decarb. Product

Ni	1.35756800	-0.98887000	0.07472000
P	-0.94698200	-0.69069400	-0.13422900
C	-1.90862700	-2.25229100	-0.34407200
C	-1.54666900	0.03709200	1.43900600
C	-1.48948300	0.44502800	-1.49431700
C	-3.31865100	-2.16485800	-0.92062500
C	-4.10336200	-3.45332800	-0.71111900
C	-5.48754400	-3.40587900	-1.33208000
C	-3.04009300	-0.00969800	1.73686200
C	-1.84146200	1.87149700	-1.08147300
C	-2.11448500	2.75840600	-2.28838300
C	-2.50139100	4.17043200	-1.88921000
H	-1.93291400	-2.70622800	0.65630700
H	-1.30908300	-2.93651800	-0.95520100
H	-3.87331500	-1.32747100	-0.47848300
H	-3.26298900	-1.94898000	-1.99557700
H	-4.18137700	-3.65106900	0.36703100
H	-3.53338900	-4.29508800	-1.12673900
H	-6.08334400	-2.58924400	-0.91054600
H	-5.43200700	-3.24347200	-2.41364000
H	-1.17497900	1.06955900	1.44610700
H	-0.98358800	-0.46789000	2.23303800
C	-3.38868300	0.74308800	3.01434000
H	-3.61470800	0.41592500	0.90231700
H	-3.37501200	-1.05328700	1.82631700
H	-2.34542200	-0.01228700	-2.00496400
H	-0.67292300	0.47030900	-2.22605400
H	-2.72422300	1.86481400	-0.42725200
H	-1.02883500	2.31824700	-0.49581000
H	-2.90308100	2.30876100	-2.90805500
H	-1.21290300	2.78306600	-2.91624100
H	-3.41587900	4.17737100	-1.28608600
H	-1.70859100	4.63247900	-1.29027700
H	-6.03864200	-4.33548400	-1.16673800
H	-2.67613900	4.80728900	-2.76086800
C	-4.86927400	0.68738500	3.34357200
H	-3.06463100	1.78745300	2.90958000
H	-2.80203500	0.33180200	3.84663800
H	-5.10386100	1.23996400	4.25730700
H	-5.47136700	1.11621200	2.53526100
H	-5.20600900	-0.34504100	3.48696400
O	1.40919500	0.57446600	1.12683200
C	1.34641500	1.73563300	0.49963500
C	0.99233000	2.89786500	1.22225400
C	0.87502100	4.12427500	0.58043600
C	1.10703800	4.24496600	-0.79180000
C	1.59702800	1.87568900	-0.88431500
C	1.47337100	3.10963300	-1.51407800
H	0.80369000	2.80165100	2.28884800
H	0.59163000	5.00029500	1.15978400
H	1.00781700	5.20682900	-1.28618200
H	1.89124300	0.98948500	-1.44942900
H	1.66598400	3.18357300	-2.58249400
C	3.28859800	-1.11111600	0.23716500
C	1.39429800	-2.54765400	-0.68906200
O	1.42307600	-3.58932800	-1.18734200
C	3.86724000	-0.83386000	1.47565300
C	5.25460400	-0.82436900	1.58749600
C	6.01459800	-1.08061500	0.44869000
C	4.14596700	-1.37126400	-0.83373300
N	5.48465200	-1.34526400	-0.74874900

H	3.24291500	-0.59788300	2.33332300
H	5.73950700	-0.61197800	2.53693000
H	7.10311400	-1.07433800	0.49997000
H	3.74670700	-1.60064400	-1.82352200

Ni[P(n-Bu)$_3$](Pyr)(CO)(OPh)[MeOPh-B(OH)$_2$] Iso-1

Ni	1.23404700	-0.49006600	1.05678100
O	1.39165100	-0.98125800	-0.77641900
B	-1.72558300	-1.52491400	-0.97988500
C	-3.26610000	-1.54502900	-0.79335600
P	0.24496700	1.54455100	0.47139900
C	2.18753400	-2.08020400	1.66716200
C	0.99120600	-0.24724600	2.75122800
C	0.86426900	2.87648300	1.57701100
C	0.81533700	2.07545500	-1.18879400
C	-1.58773200	1.70879200	0.56624000
C	0.39811600	4.29083200	1.25500400
C	1.06550700	5.33764300	2.13733800
C	0.59250600	6.74817400	1.83718500
C	2.32233900	2.31774700	-1.20494000
C	-2.25121100	2.57972000	-0.49479800
C	1.62203200	-3.34541100	1.49503800
N	2.27524000	-4.49012800	1.74560400
C	3.52824300	-4.39863700	2.20127300
C	3.48125500	-2.00948000	2.18197900
C	4.17396100	-3.18981000	2.44113500
C	2.51526900	-1.22603100	-1.45919900
C	2.42295100	-1.83319600	-2.72624700
C	3.56206500	-2.04170600	-3.49440800
C	4.82049100	-1.66349000	-3.02595600
C	3.78788900	-0.85549900	-0.99164300
C	4.92166900	-1.07534400	-1.76658900
C	-4.08755300	-0.55172600	-1.35654600
C	-5.46072400	-0.54593200	-1.17590600
C	-6.06513100	-1.55592700	-0.41518700
C	-3.90090300	-2.54252000	-0.04137600
C	-5.27870200	-2.56305800	0.15370400
O	-7.41548300	-1.47120800	-0.28603600
O	-0.96728300	-2.51093800	-0.39527500
O	-1.14947100	-0.50211200	-1.69550600
C	-8.05462400	-2.47983400	0.47503700
C	-3.72737700	2.80177300	-0.19159700
C	-4.45643000	3.52412000	-1.30958500
C	2.91855600	2.25799900	-2.60379400
C	4.40420100	2.56584000	-2.61265700
H	1.96057500	2.81841100	1.55591300
H	0.57356000	2.60590400	2.60018400
H	0.60096500	4.52560600	0.19998000
H	-0.69300700	4.35639000	1.37162500
H	2.15422100	5.27062200	2.00707100
H	0.87632600	5.09389400	3.19131300
H	0.80129900	7.02411500	0.79815100
H	-0.48776000	6.84519500	1.98850000
H	0.26578100	2.96969800	-1.50616700
H	0.55220400	1.28355300	-1.89509800
H	2.54665400	3.29041500	-0.74266000
H	2.82671800	1.56455100	-0.58075100
H	-1.79878200	2.09437900	1.57327600
H	-2.02300200	0.70425600	0.52405300
H	-1.74665100	3.55260700	-0.57934400
H	-2.13660400	2.09087100	-1.47178500
H	1.08240700	7.48555800	2.47859000
H	0.59965100	-3.45739500	1.13665400
H	4.03692100	-5.34282800	2.39345900
H	3.95887800	-1.04931500	2.36966200
H	5.19018300	-3.17086700	2.82516700
H	1.44172300	-2.12899200	-3.09245000
H	3.46342000	-2.50739400	-4.47198400
H	5.70703300	-1.82976200	-3.63036200
H	3.86582200	-0.38458100	-0.01337700
H	5.89360300	-0.77341000	-1.38251000
H	-3.62706900	0.23588000	-1.95142900
H	-6.09103100	0.22601800	-1.60973100
H	-3.29638300	-3.32856500	0.40613700
H	-5.73023500	-3.35450000	0.74247600
H	-0.17811800	-0.59160800	-1.64095700
H	-0.02452800	-2.34893000	-0.56845000
H	-9.11675400	-2.23762800	0.46890300
H	-7.90671600	-3.47323800	0.03415000
H	-7.69213300	-2.49556000	1.51025400
H	-3.81815900	3.36671500	0.74655700
H	-4.20288800	1.82974200	-0.00428100
H	-5.51045300	3.68669900	-1.06760800
H	-4.00898400	4.50306500	-1.51319600
H	-4.41754300	2.94923300	-2.24160300
H	2.38103800	2.95402300	-3.26227900
H	2.74556800	1.25314400	-3.01375400
H	4.83203000	2.47549600	-3.61491300
H	4.60500300	3.58194000	-2.25525300
H	4.94570800	1.87175500	-1.96046900
O	0.83052000	-0.08862100	3.88412800

Ni[P(n-Bu)$_3$](Pyr)(CO)(OPh)[MeOPh-B(OH)$_2$], Iso-2

Ni	1.37590400	-0.46404400	-0.48582800
O	2.84434600	-1.68624700	0.00873900
B	0.21123100	-2.89505200	0.85980300
C	-1.33753700	-2.87252000	0.71755300
C	0.83241800	-1.54824800	-1.86339800
C	2.24666500	0.86211400	0.59492300
P	-0.36834400	0.89401000	-0.45180000
C	-0.89625500	1.08758100	1.29718400
C	-0.09739300	2.56611700	-1.15980100
C	-1.80500000	0.17350100	-1.35037400
C	-0.98368600	3.69539900	-0.64141200
C	-0.65062300	5.02742200	-1.30087200
C	-2.96374900	1.08270900	-1.74786200
C	-4.08361600	0.29270500	-2.41476200
C	-2.36498300	1.37408500	1.58440100
C	-1.50531000	6.16795000	-0.77870600
C	-5.28017200	1.15609900	-2.77013400
C	2.30854400	0.84731400	1.99046400
N	3.13909600	1.61294100	2.71621800
C	3.95833200	2.43280400	2.04942900
C	3.10538200	1.73891200	-0.07182600
C	3.98365700	2.53382000	0.66213500
C	4.10470900	-1.35381000	-0.27323400
C	5.10610900	-1.48525100	0.70602700
C	6.42426400	-1.14979400	0.41923000
C	6.78080200	-0.66436700	-0.83914500
C	4.47471100	-0.86265200	-1.53998500
C	5.79426500	-0.52273900	-1.81481600
C	-1.96890600	-3.41034400	-0.41994400

C	-3.32040400	-3.22524400	-0.66153600
C	-4.09503200	-2.48882400	0.24513900
C	-2.14657200	-2.17601700	1.62388600
C	-3.50898300	-1.98087400	1.40941700
O	-5.39818400	-2.30404500	-0.09954200
O	0.77888800	-2.06426600	1.80309100
O	0.94731800	-3.65464200	-0.01050300
C	-6.14640700	-1.39245100	0.68498500
C	-2.67029600	1.32157000	3.07548500
C	-4.13730600	1.56683100	3.37849200
H	-0.19648300	2.46226600	-2.24826900
H	0.95278600	2.81674100	-0.97316800
H	-2.04399700	3.46429800	-0.80581400
H	-0.86078000	3.78951700	0.44626000
H	-2.16398100	-0.65331200	-0.72133500
H	-1.40209500	-0.30307700	-2.25256000
H	-3.36852200	1.60611000	-0.87284500
H	-2.60835100	1.86826900	-2.42992200
H	-0.24666600	1.85400600	1.73739200
H	-0.60177100	0.14512800	1.77923200
H	-2.65596700	2.35391200	1.18261200
H	-2.99329200	0.63224300	1.07272200
H	-0.77546100	4.93124600	-2.38782800
H	0.41272900	5.25069200	-1.14165000
H	-2.56974600	5.97858900	-0.95358400
H	-1.37142000	6.30220200	0.29981700
H	-4.39526600	-0.52018300	-1.74492300
H	-3.69178600	-0.20115100	-3.31426400
H	-6.07389400	0.57231000	-3.24398400
H	-5.70582700	1.62763100	-1.87715800
H	-5.00389700	1.95985100	-3.46117200
H	-1.25542100	7.11608900	-1.26212600
H	1.66170500	0.18291900	2.56465000
H	4.62817800	3.03913200	2.65871400
H	3.11603500	1.78821900	-1.16049100
H	4.67262500	3.21425500	0.16880400
H	4.82052000	-1.84567200	1.69151300
H	7.18123400	-1.25871600	1.19243300
H	7.81096900	-0.39695900	-1.05499100
H	3.69700700	-0.74096100	-2.29385700
H	6.05460400	-0.14171200	-2.79998100
H	-1.36876300	-3.95772700	-1.14387000
H	-3.79942800	-3.61447200	-1.55556700
H	-1.69221400	-1.76068400	2.52243700
H	-4.09645300	-1.42719800	2.13574000
H	1.87082100	-3.34629800	-0.02746100
H	1.73865900	-1.99081500	1.66209500
H	-7.11999100	-1.30448000	0.20370200
H	-6.28148000	-1.75104600	1.71265800
H	-5.66482200	-0.40444000	0.71410300
H	-2.04744100	2.05507900	3.60412100
H	-2.36566600	0.33994300	3.46563100
H	-4.34697000	1.51306200	4.44997900
H	-4.45782300	2.55355800	3.02754300
H	-4.77418500	0.82528800	2.88098100
O	0.62841300	-2.11813800	-2.84232300

TS_(B-C act.), transmetalation, Iso1

Ni	0.14438300	0.05056700	-0.78101900
O	0.96100300	2.32049500	-2.36538300
B	2.16401500	1.53431400	-2.49165200
C	2.20195600	0.08988600	-1.03868800
C	0.50901500	0.02752100	1.11286400
P	-1.94501700	-0.41437500	-0.08806300
C	-1.93546500	-2.16659400	0.45582700
C	-2.61478000	0.62018100	1.27972600
C	-3.27806900	-0.34369300	-1.35722300
C	-2.54132700	0.02249500	2.68109500
C	-2.76520600	1.07744700	3.75506700
C	-4.62260100	-0.93025100	-0.93970600
C	-5.74707400	-0.54435500	-1.89230000
C	-1.15404700	-3.03291100	-0.52702100
C	-2.59373500	0.52645100	5.15828600
C	-7.06955300	-1.19558000	-1.52999900
C	0.91898800	-1.15091300	1.75167200
N	1.26486600	-1.24261500	3.04418000
C	1.22577100	-0.11476400	3.76573400
C	0.48091800	1.18375600	1.89607400
C	0.84763500	1.11697500	3.23900300
C	0.58162100	3.03300700	-1.28846000
C	1.46138500	3.72822500	-0.44367300
C	0.95504900	4.49080900	0.60643200
C	-0.41653000	4.57878800	0.84338500
C	-0.79982300	3.11573000	-1.04239800
C	-1.29178000	3.88487400	0.00781300
C	2.40180200	-1.24006000	-1.49193800
C	3.32011900	-2.10879900	-0.91994400
C	4.12101500	-1.66383100	0.14035700
C	3.04264900	0.48052200	0.03182800
C	4.00523800	-0.34011900	0.59529800
O	4.98141700	-2.57398100	0.65434000
O	3.34526600	2.25602600	-2.20891600
O	2.04375700	0.76723100	-3.67018600
H	-3.64832800	0.89096200	1.03086000
H	-2.03885600	1.55361200	1.24696800
H	-3.27866400	-0.78635600	2.78242100
H	-1.55969500	-0.44023200	2.84679900
H	-2.91690900	-0.84335900	-2.26249200
H	-3.38426900	0.71680900	-1.62563100
H	-4.54604100	-2.02505200	-0.89697800
H	-4.88741900	-0.61199700	0.07930900
H	-2.96299900	-2.52639700	0.58925600
H	-1.45845300	-2.19796400	1.44144200
H	-1.66137400	-3.04913100	-1.50359300
H	-0.17604500	-2.55774200	-0.71541000
H	-3.76323800	1.52086500	3.63668300
H	-2.05041900	1.89648800	3.58665600
H	-3.30659800	-0.27990800	5.36175600
H	-1.58710600	0.11397700	5.29146500
H	-5.46176700	-0.81669500	-2.91685800
H	-5.85448900	0.54825600	-1.89458700
H	-7.87195700	-0.88607800	-2.20462200
H	-7.00142200	-2.28737300	-1.57650700
H	-7.37436600	-0.93163100	-0.51160100
H	-2.74114500	1.29672500	5.92013100
H	0.99346200	-2.08271900	1.18351600
H	1.51117100	-0.20530900	4.81388900
H	0.18372000	2.13740400	1.46447200
H	0.83583200	2.00618900	3.86595300
H	2.52676800	3.67316800	-0.63540400
H	1.64908200	5.02927300	1.24764100
H	-0.79804800	5.18208200	1.66190500
H	-1.47146800	2.58832200	-1.71742200
H	-2.36602200	3.94206100	0.17015500

H	1.82090200	-1.59926600	-2.34294800
H	3.44894400	-3.12764400	-1.27616000
H	2.92835500	1.48709500	0.43373100
H	4.62300300	0.02423400	1.41018800
H	4.11989900	1.69131700	-2.23231200
C	5.74165400	-2.18290300	1.78679700
H	6.33086400	-3.05420400	2.06991000
H	6.41593100	-1.35076700	1.55261800
H	5.09170600	-1.89337900	2.62107300
C	-0.93130500	-4.45604800	-0.03846000
C	-0.05982600	-5.25606900	-0.98942400
H	-1.89942800	-4.95473500	0.10344500
H	-0.46334000	-4.42016000	0.95473400
H	0.12666500	-6.26835500	-0.62125000
H	-0.52339200	-5.34243900	-1.97806300
H	0.91193800	-4.76765400	-1.12686800
C	-0.33943700	-0.03435100	-2.54568900
O	-0.80747900	-0.12018600	-3.59442800
H	2.87613700	0.34496500	-3.88722100

TS_(B-C act.), transmetalation, Iso2

Ni	0.19001000	-0.43933200	-0.60971700
O	0.94788800	1.02651200	-2.77361800
B	2.10106500	0.14795700	-2.69645100
C	2.24118700	-0.58834600	-0.84056600
C	0.51938500	0.41179600	1.09262000
P	-1.96703100	-0.25885800	0.01905600
C	-2.32839700	-1.54134300	1.27743500
C	-2.50848400	1.34680900	0.73853200
C	-3.21567500	-0.55245500	-1.30601900
C	-2.53884800	1.43329200	2.26046000
C	-2.65885100	2.87446000	2.73674400
C	-4.64855400	-0.77181500	-0.83357700
C	-5.64234800	-0.79417800	-1.98840000
C	-1.90989600	-2.93537600	0.82630800
C	-2.60083300	2.99550900	4.24792900
C	-7.06663800	-1.05088800	-1.53090100
C	0.71838500	-0.41389400	2.20896900
N	0.96628800	0.02086100	3.45365800
C	1.04465400	1.34579100	3.63060600
C	0.60697000	1.78925600	1.31737500
C	0.87908000	2.26475200	2.59858900
C	0.79022600	2.23049700	-2.18739600
C	1.84135900	3.06405700	-1.77379100
C	1.55577500	4.29051700	-1.17826000
C	0.24204900	4.71662700	-0.98758900
C	-0.53222600	2.66564200	-2.00497100
C	-0.80183100	3.89521500	-1.41345500
C	2.58031100	-1.96727200	-0.83587400
C	3.65161100	-2.48394300	-0.12539900
C	4.46398900	-1.62277200	0.62289400
C	3.08747700	0.22826400	-0.04706800
C	4.18727900	-0.24577700	0.64497900
O	5.49734100	-2.20350000	1.27442100
O	3.34152100	0.79730100	-2.86648800
O	1.87546800	-1.03105300	-3.45976400
H	-3.49449700	1.58974600	0.32148600
H	-1.81607400	2.09847300	0.34146300
H	-3.37209500	0.83563500	2.65587700
H	-1.62477000	0.99887600	2.68602000
H	-2.88860500	-1.40450200	-1.91105900
H	-3.15983600	0.32107500	-1.96999100
H	-4.71380500	-1.72096900	-0.28373900
H	-4.94425300	0.00812000	-0.11646000
H	-3.39480500	-1.50937100	1.53452800
H	-1.78131500	-1.25741600	2.18376400
H	-2.44690100	-3.21278500	-0.09334500
H	-0.84304700	-2.92106000	0.55252900
H	-3.59026700	3.31316100	2.35315600
H	-1.84369100	3.45775800	2.28287600
H	-3.40930100	2.43150200	4.72536100
H	-1.65475000	2.59814000	4.63293800
H	-5.33576400	-1.56222200	-2.71076000
H	-5.58693300	0.16062200	-2.52799500
H	-7.76686400	-1.05851000	-2.37045200
H	-7.15206600	-2.01647400	-1.02131100
H	-7.40251900	-0.28123700	-0.82782600
H	-2.68364700	4.03467400	4.57790000
H	0.68199300	-1.50153900	2.09762900
H	1.24874300	1.68335000	4.64696500
H	0.46816200	2.49774900	0.50363800
H	0.95204200	3.33320700	2.79204400
H	2.86380200	2.73890900	-1.92491100
H	2.38047600	4.92292800	-0.85842700
H	0.03462800	5.67498700	-0.52091100
H	-1.33646300	2.01362800	-2.34129500
H	-1.83517100	4.20678100	-1.27585400
H	2.00807400	-2.65125800	-1.45983600
H	3.89929700	-3.54137800	-0.14830500
H	2.88269600	1.29663200	-0.00168500
H	4.81180000	0.43880000	1.20970800
H	4.01161900	0.13146600	-3.03882500
C	6.35283300	-1.36077200	2.03071800
H	7.11004400	-2.01272000	2.46418100
H	6.83845300	-0.61016900	1.39647100
H	5.80795100	-0.85158000	2.83375200
C	-2.14402900	-3.99660400	1.89153300
C	-1.72173700	-5.38211700	1.43784600
H	-3.20592500	-3.99953800	2.17215100
H	-1.59554800	-3.71449800	2.80045500
H	-1.89092500	-6.13335500	2.21367400
H	-2.27815100	-5.69444100	0.54777200
H	-0.65751500	-5.40648700	1.18094900
C	-0.24128900	-1.61374700	-1.93735900
O	-0.63603800	-2.46022000	-2.61673500
H	1.19451100	-0.84578200	-4.11140700

Ni[P(n-Bu)$_3$](Pyr)(CO)(PhOMe)[OPh-B(OH)$_2$], Iso1

Ni	0.65366500	1.66307100	0.29195800
O	0.54968100	-2.79526600	1.58074400
B	1.61974100	-1.92477300	1.56129800
C	2.61616500	1.73474200	0.18436200
C	0.69503700	0.76901400	-1.41264600
P	-1.61062300	1.32867300	0.23019100
C	-2.33310800	1.57390500	-1.44422200
C	-1.86993300	-0.42854600	0.71481000
C	-2.67345500	2.32353600	1.36339200
C	-2.96007300	-1.23824500	0.02120300
C	-2.77895700	-2.73014300	0.27241400
C	-3.99715700	1.70783100	1.80689800
C	-4.82887100	2.67357100	2.64123100
C	-3.84231500	1.71727500	-1.59452000
C	-3.88079400	-3.58152600	-0.32885900

C	-6.12964600	2.05980600	3.12625100
C	0.71681500	1.50055500	-2.61024500
N	0.64443900	0.97335400	-3.84078000
C	0.55220900	-0.35944100	-3.93136500
C	0.63472200	-0.62143300	-1.55709400
C	0.55387900	-1.19952600	-2.82263100
C	0.50133500	-4.01097600	0.95469200
C	1.05507000	-4.22121000	-0.30989500
C	0.87295300	-5.44861100	-0.94089200
C	0.14663100	-6.46481100	-0.32421400
C	-0.22475200	-5.02425200	1.58059900
C	-0.39944500	-6.24615100	0.93924600
C	3.29373600	2.93670400	0.46422700
C	4.67834700	3.03620400	0.41585200
C	5.45472200	1.91541700	0.10405900
C	3.42207700	0.63852900	-0.14822600
C	4.81953900	0.70490400	-0.17695500
O	6.80474100	2.10479500	0.09547100
O	2.84978000	-2.36170900	1.16147100
O	1.30418200	-0.65990300	1.97689200
H	-2.00679600	-0.43550700	1.80355500
H	-0.90623000	-0.92215700	0.56245200
H	-3.95531600	-0.91352700	0.35732300
H	-2.93454800	-1.06025200	-1.06357000
H	-2.84435200	3.28569600	0.86183100
H	-2.07127000	2.55827300	2.24918900
H	-4.58446600	1.38049200	0.94036300
H	-3.80127700	0.79907800	2.39224900
H	-1.96251300	0.74614400	-2.06132500
H	-1.83570400	2.46535300	-1.84915500
H	-4.35669300	0.83503600	-1.19053200
H	-4.20323900	2.57315400	-1.00648200
H	-2.70702500	-2.91187700	1.35380000
H	-1.80603500	-3.03638900	-0.13712800
H	-4.85822200	-3.33557400	0.10024300
H	-3.95327500	-3.43141800	-1.41151000
H	-5.03745100	3.57264000	2.04508000
H	-4.23261600	3.01664800	3.49735000
H	-6.71539700	2.76589400	3.72091200
H	-6.75408700	1.73838800	2.28587200
H	-5.94407400	1.17835600	3.74912200
H	-3.70187800	-4.64702200	-0.15632000
H	0.78936800	2.58978000	-2.57908100
H	0.48331300	-0.77043200	-4.93836200
H	0.63861600	-1.27186800	-0.68145100
H	0.48905600	-2.27908500	-2.94236400
H	1.62266300	-3.43045500	-0.79043300
H	1.30209900	-5.60590600	-1.92682200
H	0.00657900	-7.41855600	-0.82396400
H	-0.65614200	-4.83101600	2.55822000
H	-0.96839300	-7.03019900	1.43121500
H	2.73247400	3.83234100	0.72617200
H	5.18365000	3.97471900	0.62853300
H	2.96024200	-0.30457100	-0.43904200
H	5.39154500	-0.17736100	-0.44910700
H	2.00673900	-0.01279100	1.82743000
H	3.52406100	-1.67718100	1.20033100
C	7.60392500	0.98305600	-0.22325300
H	8.63865100	1.32175200	-0.17818200
H	7.45997800	0.16489500	0.49428100
H	7.39102400	0.60634600	-1.23181200
C	-4.24543400	1.90630600	-3.05192500
C	-5.74367100	2.07230100	-3.22951700
H	-3.88994300	1.04612500	-3.63503700
H	-3.71853700	2.77878600	-3.46085500
H	-6.01606500	2.20570800	-4.27994500
H	-6.28694100	1.19747000	-2.85631100
H	-6.11400000	2.94399900	-2.67928100
C	0.64778900	2.53162800	1.85007200
O	0.65478300	3.08432100	2.86501200

Ni[P(n-Bu)$_3$](Pyr)(CO)(PhOMe)[OPh-B(OH)$_2$], Iso2

Ni	0.64044100	-1.61990600	-0.35721900
O	0.38083100	2.85149000	-1.71852700
B	1.41869800	2.02307700	-2.09292600
C	2.57186300	-1.75792200	-0.16283100
C	0.74442900	-0.71547600	1.33607400
P	-1.62086800	-1.29075600	-0.26109200
C	-2.30605300	-1.66042500	1.40750200
C	-1.93363200	0.49517900	-0.60694500
C	-2.69986900	-2.21992300	-1.43433200
C	-2.97734400	1.24942600	0.21080200
C	-2.79291700	2.75583600	0.07984800
C	-4.04416400	-1.60019200	-1.80361000
C	-4.90925700	-2.54992600	-2.62214200
C	-3.81094100	-1.81771700	1.58382700
C	-3.85723600	3.55872300	0.80301700
C	-6.23174200	-1.93191400	-3.03769900
C	0.73673000	-1.40282600	2.55955900
N	0.70820500	-0.82914700	3.77037100
C	0.69924400	0.50940300	3.81164700
C	0.77563000	0.68062000	1.42876600
C	0.74179100	1.30760600	2.67275700
C	0.48182100	3.97342900	-0.93337400
C	1.33993900	4.04656100	0.16453400
C	1.30854400	5.17524500	0.97975900
C	0.43579700	6.22608900	0.70852200
C	-0.38935200	5.02438900	-1.21819800
C	-0.41035400	6.14601600	-0.39588100
C	3.16254000	-3.01744600	0.01183100
C	4.53855800	-3.16169700	0.15457400
C	5.37035400	-2.03907800	0.11052700
C	3.41997300	-0.65145700	-0.19153200
C	4.80676400	-0.77410200	-0.06808200
O	6.70802500	-2.28034600	0.25535600
O	2.71634100	2.35558100	-1.85487600
O	1.10342500	0.85457700	-2.72949800
H	-2.15827800	0.57777200	-1.67865600
H	-0.96786700	0.99275500	-0.47117700
H	-3.99088200	0.96030100	-0.10115400
H	-2.89688000	0.97687900	1.27250500
H	-2.84558500	-3.21414200	-0.99048200
H	-2.11339500	-2.39212000	-2.34519000
H	-4.59229600	-1.29737800	-0.90301400
H	-3.88003600	-0.67560400	-2.37410400
H	-1.92051700	-0.88048000	2.07574600
H	-1.79840200	-2.57776100	1.73447500
H	-4.33575700	-0.91662800	1.23992300
H	-4.18303300	-2.64107500	0.95741800
H	-2.76930300	3.03036500	-0.98409400
H	-1.79824800	3.01875500	0.46808700
H	-4.85574400	3.35384000	0.40202300
H	-3.87896300	3.31784700	1.87120200

H	-5.08915000	-3.46148300	-2.03561800
H	-4.34950200	-2.87411200	-3.50970100
H	-6.84175700	-2.62919600	-3.61812800
H	-6.81878900	-1.62762300	-2.16468500
H	-6.07653400	-1.03893800	-3.65243200
H	-3.67917400	4.63435300	0.71219800
H	0.74654700	-2.49547500	2.56729600
H	0.66623700	0.96042800	4.80334200
H	0.81873900	1.29608400	0.52804200
H	0.74807400	2.39290700	2.75284400
H	2.02227500	3.22947500	0.37605200
H	1.97408000	5.22583300	1.83734600
H	0.41549700	7.10048700	1.35161900
H	-1.05160100	4.93832600	-2.07460500
H	-1.09558900	6.95902500	-0.61982900
H	2.54485500	-3.91427400	0.03826100
H	4.99222400	-4.13931600	0.29438300
H	3.00244300	0.34991400	-0.28433900
H	5.42709900	0.11673900	-0.09244700
H	3.30952200	1.67080400	-2.17867200
C	7.56374700	-1.15779400	0.22209100
H	8.57613400	-1.54011500	0.35349100
H	7.50157600	-0.62535800	-0.73627500
H	7.33846500	-0.44905300	1.02972000
C	-4.18118900	-2.08573900	3.03762400
C	-5.67448600	-2.26665900	3.24034100
H	-3.81519500	-1.25563700	3.65681000
H	-3.64265400	-2.97607500	3.38851300
H	-5.92246400	-2.45091900	4.28903300
H	-6.22878200	-1.37739900	2.92160400
H	-6.05460400	-3.11287300	2.65799000
C	0.75478300	-2.39590500	-1.95749600
O	0.88381900	-2.84873900	-3.01355100
H	0.15360500	0.75306500	-2.83490800

Ni[P(n-Bu)$_3$](Pyr)(CO)(PhOMe), CO-N trans

Ni	0.92900900	0.68660700	-0.32255900
C	2.86586000	0.57662000	-0.25761300
C	1.04525700	-1.22989500	-0.19454400
P	-1.34180900	0.48760700	-0.15060300
C	-2.02663100	-0.90022900	-1.14815600
C	-1.72364900	0.11033400	1.61256600
C	-2.35474700	1.97429100	-0.56774300
C	-2.96892900	-0.70875400	1.93299200
C	-3.11225500	-0.96670000	3.42734400
C	-3.72639200	2.12996800	0.07975300
C	-4.42901700	3.40966100	-0.35663800
C	-3.51332200	-0.92469800	-1.47903000
C	-4.33562400	-1.79941700	3.76515300
C	-5.78299300	3.58782600	0.30609500
C	1.02595500	-2.02038300	-1.35424700
N	1.00090200	-3.36039700	-1.38131100
C	1.00912100	-3.99163200	-0.20096900
C	1.09518000	-1.93218200	1.01501300
C	1.06521200	-3.32539300	1.01911600
C	3.65753300	0.38816600	-1.39701400
C	5.04361900	0.32925700	-1.31188500
C	5.67738300	0.45698600	-0.07172600
C	3.51529500	0.70620500	0.96953400
C	4.90820300	0.64750800	1.07711800
O	7.04289500	0.38085400	-0.08824000
H	-1.74854200	1.07492200	2.13683300
H	-0.84336900	-0.41533800	2.00195400
H	-3.87025400	-0.20266300	1.56308500
H	-2.92309800	-1.67108400	1.40337400
H	-2.44036500	1.99396000	-1.66274200
H	-1.73757500	2.84444200	-0.31099800
H	-4.36661900	1.27055700	-0.15424600
H	-3.61904600	2.13430900	1.17366600
H	-1.72834700	-1.81955900	-0.62710900
H	-1.44447000	-0.91159000	-2.07893000
H	-4.11464700	-0.92900500	-0.56089600
H	-3.79420000	-0.00880000	-2.01819100
H	-3.15519900	-0.00422200	3.95518300
H	-2.20482900	-1.46623500	3.79303900
H	-5.25552100	-1.30540500	3.43434300
H	-4.29691400	-2.77728800	3.27356600
H	-4.54397200	3.40180700	-1.44901600
H	-3.78429000	4.26989000	-0.13194400
H	-6.27605600	4.50839000	-0.01742100
H	-6.45272100	2.75410400	0.06981900
H	-5.68799400	3.62961200	1.39635600
H	-4.42413800	-1.97437500	4.84073000
H	1.02041400	-1.54221700	-2.33722600
H	0.98101300	-5.08064900	-0.23715100
H	1.16513000	-1.39764800	1.96310800
H	1.09398100	-3.88574600	1.95050000
H	3.19312100	0.27312200	-2.37525900
H	5.65744300	0.17801300	-2.19610400
H	2.93697400	0.84990400	1.88211600
H	5.37467500	0.75116200	2.05179600
C	7.69899900	0.48570000	1.15718400
H	8.76522200	0.38808400	0.95201200
H	7.51238500	1.45576100	1.63693100
H	7.39047500	-0.30963600	1.84848600
C	-3.88416600	-2.13703300	-2.32420600
C	-5.35812500	-2.17289700	-2.68466100
H	-3.60715100	-3.04993000	-1.78006900
H	-3.27333700	-2.14017900	-3.23667100
H	-5.60774400	-3.04967300	-3.28794100
H	-5.98576100	-2.20051900	-1.78754000
H	-5.64867800	-1.28542200	-3.25703000
C	1.06615000	2.45144800	-0.51141500
O	1.22023800	3.58968000	-0.64584300

Ni[P(n-Bu)$_3$](Pyr)(CO)(PhOMe), CO-P trans

Ni	-0.14755800	-1.97136600	-0.00643800
C	0.15738800	-3.66310600	0.32434600
C	-2.09332500	-2.17030200	0.01197700
P	-0.45801500	0.26234000	-0.19554700
C	-2.03122900	0.80380500	-0.98234500
C	-0.52252700	0.79601200	1.56808500
C	0.85355000	1.26250900	-1.01690600
C	-1.27798300	2.06882000	1.92881500
C	-1.22010300	2.36378600	3.42196200
C	1.16474300	2.64655600	-0.45982600
C	2.34251600	3.28952700	-1.18121500
C	-2.17650600	2.26436000	-1.39241000
C	-1.99857000	3.60967000	3.80396200
C	2.68537500	4.66582900	-0.64094500
C	-2.79159600	-2.41573500	-1.17939700
N	-4.12576800	-2.47910100	-1.30315100
C	-4.84481300	-2.30434500	-0.18771900
C	-2.88535200	-2.02341100	1.15700200

C	-4.27499000	-2.08361500	1.06238400
C	-3.52416000	2.53457200	-2.05038200
C	-3.68467100	3.97835600	-2.49037400
C	1.78614600	-1.65303900	-0.05692200
H	0.52163300	0.85429600	1.90275100
H	-0.95849300	-0.04936700	2.11684200
H	-0.87401200	2.92536900	1.37457200
H	-2.32814400	1.97469900	1.61815400
H	0.56991100	1.32942900	-2.07575300
H	1.76273700	0.65384900	-0.99172600
H	0.28869000	3.30594500	-0.52984000
H	1.40168400	2.56902300	0.61134000
H	-2.84181400	0.50201500	-0.30610600
H	-2.15545000	0.16260800	-1.86502800
H	-2.06030200	2.92691800	-0.52526600
H	-1.37308600	2.54044000	-2.08976000
H	-0.16969900	2.46934800	3.72596000
H	-1.60402300	1.49628600	3.97569800
H	-1.61221700	4.49354900	3.28510400
H	-3.05646800	3.51300000	3.53741100
H	2.11623800	3.35311800	-2.25417400
H	3.21413900	2.62461800	-1.10064800
H	3.53277900	5.11060300	-1.16967600
H	1.83844600	5.35357900	-0.73878500
H	2.94621400	4.62115300	0.42186300
H	-1.94585300	3.80873400	4.87768300
H	-2.23946300	-2.55855800	-2.11201000
H	-5.92791700	-2.35109000	-0.30118200
H	-2.42567500	-1.85341400	2.13176400
H	-4.90557100	-1.96362800	1.94017700
H	-4.32503200	2.26385200	-1.34918400
H	-3.64510400	1.86286300	-2.91063600
H	-4.65836600	4.15569800	-2.95481200
H	-3.59413800	4.66454500	-1.64141100
H	-2.91587200	4.25912500	-3.21828000
O	0.38265900	-4.77255400	0.55679200
C	2.49290500	-1.81716000	-1.25856700
C	3.81690500	-1.41462400	-1.39137600
C	4.48631800	-0.83789100	-0.30635700
C	2.49092300	-1.11505200	1.02267300
C	3.82247000	-0.69710800	0.91355700
H	1.99651600	-2.24845100	-2.12764400
H	4.35403400	-1.53304300	-2.32912800
O	5.77654300	-0.45228000	-0.53724800
H	1.99853400	-0.99006900	1.98764200
H	4.32446900	-0.26981000	1.77643600
C	6.45921500	0.15731300	0.53833000
H	7.45374600	0.40711200	0.16880700
H	5.95622300	1.07563500	0.86997600
H	6.55354600	-0.51882500	1.39792100

TS[Pyr-PhOMe], reductive eliminination

Ni	-1.33141100	-1.35063500	-0.45072000
C	-1.31411400	-3.04354800	-0.99958600
P	0.92800100	-0.92353700	-0.26207200
C	2.19945100	-2.08360200	-0.92698800
C	1.34148400	0.73097300	-0.95015400
C	1.25311400	-0.84067600	1.55680200
C	3.58715600	-2.08631500	-0.29482200
C	4.52008600	-3.09317900	-0.95559100
C	5.89833400	-3.12475600	-0.32026300
C	2.78274300	1.17615800	-1.15083400
C	2.24453600	0.18809800	2.08622700
C	2.23896900	0.26191300	3.60734200
C	3.22689200	1.27849400	4.15024800
C	2.83964600	2.62367600	-1.62659600
C	4.25307700	3.11332800	-1.88219100
C	-1.76759600	0.50777000	-0.09957300
C	-3.16287600	-0.93700700	-0.00482000
C	-3.54520100	-1.28050800	1.30616800
N	-4.80211900	-1.48328900	1.71110400
C	-5.77125100	-1.33503400	0.79876000
C	-4.20632000	-0.78143600	-0.92981800
C	-5.51910500	-0.98664100	-0.52719700
C	-1.52645000	1.16544000	1.12266100
C	-1.26018400	2.52471300	1.17730400
C	-1.25880800	3.29228000	0.00450400
C	-1.83016300	1.31078500	-1.24941300
C	-1.57040700	2.68028000	-1.21248700
O	-0.96240700	4.61492100	0.15528500
C	-0.93345500	5.39765000	-1.02137400
H	2.27003000	-1.87667300	-2.00367100
H	1.76518500	-3.08958900	-0.85502600
H	4.03796800	-1.08689900	-0.34698900
H	3.50554200	-2.31985400	0.77623700
H	4.60540000	-2.85493600	-2.02460600
H	4.06263300	-4.09074000	-0.91011000
H	6.38620300	-2.14608200	-0.38267300
H	5.84018900	-3.39154500	0.74040200
H	0.80456200	1.44626700	-0.31243400
H	0.81536800	0.78138000	-1.91245800
H	3.35920900	1.08094500	-0.22234000
H	3.28137800	0.52596400	-1.88405200
H	1.53888700	-1.85348200	1.86984900
H	0.27654700	-0.65967100	2.02239800
H	3.25944100	-0.03992400	1.73177000
H	1.99809900	1.18137500	1.68324400
H	2.45653100	-0.73218500	4.02088300
H	1.22242500	0.50893900	3.94534400
H	4.25199100	1.03438700	3.85138700
H	3.00894600	2.28310500	3.77202400
H	6.55454100	-3.85141100	-0.80696500
H	3.20447800	1.32569400	5.24232000
H	2.34723800	3.25916400	-0.87539800
H	2.23315900	2.72658900	-2.53770900
H	4.27055700	4.15603800	-2.21073300
H	4.86649400	3.04231100	-0.97769000
H	4.74586900	2.51530700	-2.65631600
H	-2.78000000	-1.40131200	2.07654600
H	-6.79048600	-1.49691000	1.14716000
H	-3.99210500	-0.49710200	-1.95835900
H	-6.33971000	-0.87719400	-1.23172000
H	-1.53793800	0.60349900	2.05501300
H	-1.05143700	3.01787800	2.12313000
H	-2.05692400	0.85643300	-2.21330900
H	-1.60332000	3.25402800	-2.13330300
H	-0.65305200	6.40447400	-0.71289700
H	-0.19456700	5.01984200	-1.74081100
H	-1.91456600	5.43060400	-1.51217100
O	-1.21231600	-4.12591900	-1.40682200

Ni[P(n-Bu)$_3$](CO)[Pyr-PhOMe]

Ni	0.55839900	-1.33451500	1.04696300
P	-1.28584200	-0.20952400	0.43098300

C	1.10577800	-1.01015900	2.68109400
C	-1.07228300	0.75182300	-1.13525300
C	-2.78511600	-1.26456700	0.17483000
C	-1.78786100	1.04427400	1.69352100
C	-3.91199000	-0.77954500	-0.72887300
C	-5.02821800	-1.80959700	-0.84717400
C	-3.22491900	1.54893900	1.72618200
C	-3.44143900	2.60528100	2.80244700
C	-1.93333000	1.97475600	-1.42158800
C	-1.55370900	2.63823700	-2.74036400
C	-6.14848600	-1.36336300	-1.76932900
C	-2.38594100	3.87101700	-3.04254900
C	-4.87991500	3.08463300	2.87585500
C	2.97170800	-0.59382600	-0.70711000
C	1.91285500	-1.61437800	-0.81496300
C	1.01497000	-1.64236100	-1.90604200
N	0.01161300	-2.50556200	-2.07797000
C	-0.17402800	-3.39305000	-1.08293200
C	1.80001000	-2.67560500	0.13904800
C	0.67426200	-3.52391200	0.01266500
C	2.93632200	0.59767600	-1.45860200
C	3.92599600	1.55799300	-1.34534900
C	4.99820800	1.36584600	-0.46612600
C	4.05161200	-0.75717800	0.17033600
C	5.05532300	0.19611400	0.29580800
O	5.91933400	2.36311200	-0.42043200
C	7.00419300	2.19622400	0.47431700
H	-3.16954000	-1.49679000	1.17776000
H	-2.40297900	-2.21569300	-0.21479000
H	-4.33136600	0.16625400	-0.36221700
H	-3.51192000	-0.56521200	-1.73004600
H	-1.08798400	1.88334400	1.57461200
H	-1.53621700	0.60258600	2.66593500
H	-3.51405400	1.96462100	0.75252700
H	-3.90773200	0.70611400	1.90482600
H	-1.15923500	0.01554600	-1.94609600
H	-0.01553100	1.05278400	-1.13443400
H	-2.99727600	1.70586700	-1.44705000
H	-1.82689900	2.70629600	-0.60767900
H	-5.42827700	-2.02118600	0.15401700
H	-4.60414600	-2.75802100	-1.20371200
H	-6.60789700	-0.43446400	-1.41467700
H	-5.77582300	-1.17529800	-2.78196300
H	-1.65925100	1.90595300	-3.55252200
H	-0.48695200	2.90134800	-2.71614600
H	-2.10137200	4.33261100	-3.99216400
H	-2.77251200	3.45497600	2.60829300
H	-3.13013500	2.19986800	3.77464300
H	-5.01748500	3.84811700	3.64634800
H	-5.20318900	3.51641000	1.92247800
H	-5.56150700	2.25824200	3.10471800
H	-3.45143200	3.62437500	-3.10177300
H	-2.27150800	4.62857100	-2.25991200
H	-6.93963800	-2.11456600	-1.84399700
H	1.14221000	-0.91305500	-2.70675600
H	-1.02889900	-4.06068300	-1.18811300
H	2.60411100	-2.92683400	0.82085100
H	0.51262700	-4.32169000	0.73130300
H	2.11055200	0.78714000	-2.14020600
H	3.88586900	2.47437100	-1.92603000
H	4.12717600	-1.65556900	0.77567000
H	5.87258200	0.01876800	0.98624200
H	7.62421800	3.08586800	0.36902300
H	6.66129700	2.11418000	1.51290600
H	7.59894400	1.30867800	0.22615000
O	1.35420600	-0.68651800	3.77655200

Ni[P(n-Bu)$_3$](CO)

Ni	-2.81130600	-0.66271400	-0.04151100
P	-0.61725700	-0.36310300	0.00956800
C	-4.43492500	-0.13641300	-0.13964100
C	-0.09533500	0.36467900	1.63132300
C	0.49831800	-1.82127900	-0.22374700
C	-0.12020600	0.87084000	-1.27732200
C	1.93175100	-1.76742600	0.29364200
C	2.72579300	-3.03339900	-0.05670800
C	1.29055000	0.82775000	-1.85256900
C	1.48894600	1.84704500	-2.96703800
C	1.13294500	1.27265300	1.68647800
C	1.13895200	2.19586500	2.90444800
C	3.65134000	-3.48735700	1.05849800
C	2.07493300	3.38608900	2.73485500
C	2.90247700	1.84512400	-3.52060700
H	0.48584600	-2.05032500	-1.29816200
H	-0.01714600	-2.66576100	0.25032500
H	2.44444200	-0.88425700	-0.10280900
H	1.91905100	-1.63504200	1.38409200
H	-0.31720600	1.85763600	-0.83727000
H	-0.85144400	0.77001600	-2.08783700
H	2.03123500	1.01087500	-1.06219100
H	1.50956700	-0.17805700	-2.23855400
H	0.02829700	-0.49239900	2.30676700
H	-0.97059000	0.90477900	2.01105300
H	2.04421900	0.66100500	1.69769600
H	1.20410100	1.88566400	0.77797400
H	3.30979800	-2.85629000	-0.96835000
H	2.02840000	-3.84252700	-0.31082500
H	4.37971400	-2.70954300	1.31226100
H	3.08719400	-3.71230600	1.96997300
H	1.41865700	1.62267900	3.79725200
H	0.11493300	2.54437200	3.09155000
H	2.42407900	3.77924500	3.69324900
H	1.23633300	2.84649300	-2.58739100
H	0.76937700	1.64531000	-3.77177300
H	3.01310100	2.53805200	-4.35912900
H	3.62984600	2.13530900	-2.75492700
H	3.18677600	0.84900800	-3.87711500
H	2.96335000	3.11036200	2.15603200
H	1.58690000	4.20690100	2.20095400
H	4.21210500	-4.38560400	0.78496900
O	-5.50109500	0.35774100	-0.22359000

[Pyr-PhOMe]

C	1.62785200	0.01649800	0.00511900
C	0.16058600	0.09843500	-0.01321200
C	-0.49470800	1.30814400	-0.30178500
C	-1.87482100	1.39469300	-0.32278300
C	-2.65398900	0.26270500	-0.05225100
C	-0.63679300	-1.02037300	0.25572600
C	-2.02617700	-0.95152500	0.23881400
H	0.09192900	2.19196800	-0.53996700
O	-3.99938500	0.44379300	-0.09692900
H	-0.16475100	-1.96587600	0.51146800
H	-2.60565800	-1.83979300	0.46445400

H	-2.37742000	2.32819400	-0.55664400
C	-4.81097700	-0.68942500	0.15358900
H	-5.84223000	-0.35012600	0.06315500
H	-4.62647600	-1.48712100	-0.57632200
H	-4.64829600	-1.08780900	1.16256400
C	2.43135800	1.10816400	0.35866300
C	3.81259900	0.97327700	0.35410100
C	4.36269700	-0.25620900	0.00357300
C	2.30114100	-1.16599600	-0.34243100
N	3.62607700	-1.31841900	-0.34373600
H	1.97281800	2.04807200	0.65714700
H	4.45424200	1.80436300	0.63069500
H	5.44254000	-0.39775200	-0.00046600
H	1.72323000	-2.03585400	-0.65724900

Ni[P(n-Bu)$_3$](PyrCO)[PhO-B(OH)$_2$-PhOMe], iso1

Ni	-0.61661200	-0.63880600	-0.40421400
O	-2.19286600	-1.78989600	-0.00661800
B	-1.47091600	-2.22276500	1.32900400
C	0.02149300	-2.54510700	0.73547400
C	-1.53932800	0.61502600	-1.41415000
P	1.10781200	0.69108700	-0.25539200
C	2.64119500	-0.03068300	-0.97493900
C	0.96366000	2.37613300	-0.98628400
C	1.40859400	0.92221600	1.54963600
C	2.24200900	3.16542300	-1.24485000
C	1.95232400	4.54424500	-1.82480300
C	2.13673600	2.17211500	2.02580600
C	2.25569400	2.21357300	3.54400700
C	3.97164600	0.29670400	-0.30589000
C	3.21466000	5.33297900	-2.12203600
C	2.95500100	3.46430600	4.04455600
C	-3.50370300	-1.45126800	-0.13374400
C	-4.02422700	-1.35011000	-1.42907800
C	-5.34454600	-0.96210200	-1.62424500
C	-6.16583300	-0.67540100	-0.53463800
C	-4.32958500	-1.18298400	0.96208400
C	-5.65012500	-0.79531400	0.75377500
C	1.16523000	-2.48359500	1.56400300
C	2.40367300	-2.95118100	1.16064300
C	2.55855100	-3.49874000	-0.12358500
C	0.22324500	-3.09055300	-0.54878900
C	1.46493700	-3.55818900	-0.98873400
O	3.81329500	-3.91721100	-0.43773800
O	-2.24151500	-3.32731900	1.82413100
O	-1.32285500	-1.10043100	2.24566400
C	4.02634500	-4.37492400	-1.76213500
C	5.12881900	-0.46805700	-0.93622500
C	6.46447600	-0.14524900	-0.29097700
H	0.28423300	2.93983900	-0.33197700
H	0.42184600	2.25122400	-1.93167900
H	2.82574400	3.27907600	-0.32305900
H	2.88541200	2.60820800	-1.94026200
H	1.93622500	0.01697000	1.87392700
H	0.42211700	0.84877300	2.02497900
H	3.14069200	2.22497700	1.58312100
H	1.60635300	3.07106400	1.68059500
H	2.65244800	0.25909800	-2.03376300
H	2.48790500	-1.11604200	-0.96905700
H	4.17332400	1.37543800	-0.35251100
H	3.92088400	0.04509600	0.76304100
H	1.31837500	5.10122200	-1.12156700
H	1.35428900	4.43233800	-2.73903600
H	3.81352900	5.47870700	-1.21662600
H	3.84625700	4.81112600	-2.84894200
H	2.79449400	1.31917300	3.88504400
H	1.25246800	2.14191600	3.98470400
H	3.03612500	3.47584500	5.13477500
H	3.96879400	3.54342100	3.63733900
H	2.41301500	4.36765700	3.74488700
H	2.98970900	6.32164700	-2.53105200
H	-3.37096100	-1.56835400	-2.26952700
H	-5.73338100	-0.88409500	-2.63643800
H	-7.19644700	-0.36891300	-0.68782700
H	-3.94261600	-1.29265700	1.96809600
H	-6.27983800	-0.58169400	1.61364300
H	1.05403900	-2.06220600	2.56172800
H	3.27410400	-2.90463800	1.81032100
H	-0.63339900	-3.18376900	-1.21446000
H	1.56447200	-3.96913900	-1.98781000
H	-2.10094000	-1.02922300	2.80553500
H	-1.81706700	-3.68095300	2.60811100
H	5.08506500	-4.62272300	-1.83022200
H	3.42897400	-5.26712200	-1.98306000
H	3.78704600	-3.59465500	-2.49632600
H	5.16644100	-0.24486200	-2.01143100
H	4.92524200	-1.54449300	-0.85768800
H	7.28432800	-0.70251000	-0.75220200
H	6.70102500	0.92083800	-0.37633200
H	6.45762200	-0.39234700	0.77601200
C	-2.43410200	1.55544700	-0.68692300
O	-1.49154300	0.57321400	-2.63192400
C	-2.39816000	1.65736500	0.70704900
N	-3.18207100	2.47673500	1.41411900
C	-4.05308100	3.22163500	0.72152200
C	-3.35650800	2.33896000	-1.38701400
C	-4.18352600	3.18714200	-0.66713200
H	-1.71371300	1.01680600	1.27050400
H	-4.68823000	3.88140500	1.31144000
H	-3.40878800	2.25727800	-2.46958100
H	-4.91970200	3.81245800	-1.16279400

Ni[P(n-Bu)$_3$](PyrCO)[PhO-B(OH)$_2$-PhOMe], iso2

Ni	-0.61384500	-0.65440100	-0.42672000
O	-2.17956100	-1.79389900	-0.01739500
B	-1.44001200	-2.24148900	1.36879700
C	0.03275300	-2.55432200	0.73487300
C	-1.54719000	0.60024700	-1.42530700
P	1.10342700	0.68648200	-0.26477500
C	2.65337200	-0.01790900	-0.96641700
C	0.95232400	2.37112800	-0.99553800
C	1.38048500	0.91683600	1.54426900
C	2.22735800	3.17028100	-1.23918000
C	1.93506700	4.54654600	-1.82376400
C	2.09422300	2.17079800	2.03149400
C	2.19713400	2.20881000	3.55097200
C	3.97235300	0.32002000	-0.28013200
C	3.19568600	5.34246600	-2.10897100
C	2.87998900	3.46430600	4.06216900
C	-3.48809900	-1.44996900	-0.13811200
C	-4.03208300	-1.37748600	-1.42668600
C	-5.35630700	-0.99513200	-1.60758500

C	-6.15940300	-0.68711300	-0.51008600
C	-4.29579700	-1.15596700	0.96576700
C	-5.62087400	-0.77637900	0.77159400
C	1.17700000	-2.50013700	1.56446000
C	2.41713400	-2.95386600	1.15400900
C	2.57453800	-3.48432900	-0.13779700
C	0.23711900	-3.08006300	-0.55752500
C	1.48180200	-3.53716600	-1.00340500
O	3.83100100	-3.89238100	-0.45686600
O	-2.16465000	-3.31902500	1.95455100
O	-1.34747500	-1.12584100	2.27263300
C	4.04763200	-4.32906300	-1.78782800
C	5.14363900	-0.43611200	-0.89478900
C	6.46842200	-0.10151000	-0.23330700
H	0.26163800	2.92897900	-0.34814900
H	0.42130800	2.24262200	-1.94666000
H	2.79831300	3.28854800	-0.30992300
H	2.88368500	2.61758100	-1.92606200
H	1.90935900	0.01418300	1.87409900
H	0.38864800	0.83649300	2.00724400
H	3.10222200	2.23287100	1.59926100
H	1.56024600	3.06642300	1.68320900
H	2.67542100	0.27381100	-2.02455700
H	2.51028800	-1.10448300	-0.96456400
H	4.16662300	1.40018500	-0.32474000
H	3.90957200	0.06845900	0.78818800
H	1.29045400	5.10053400	-1.12795100
H	1.34737300	4.42982800	-2.74412300
H	3.78462000	5.49236400	-1.19773100
H	3.83756100	4.82365200	-2.82904200
H	2.74049900	1.31828600	3.89485200
H	1.19016200	2.12654900	3.98100800
H	2.95124100	3.47270500	5.15310500
H	3.89660600	3.55436100	3.66432800
H	2.33228000	4.36362100	3.76080700
H	2.96918500	6.32949500	-2.52108400
H	-3.39200800	-1.60918300	-2.27396800
H	-5.76237300	-0.93672800	-2.61443300
H	-7.19312100	-0.38545700	-0.65229300
H	-3.87843700	-1.21449700	1.96326300
H	-6.23554200	-0.54100900	1.63676600
H	1.06042100	-2.09593800	2.56849600
H	3.28742500	-2.91208900	1.80410300
H	-0.61631800	-3.16683600	-1.22845900
H	1.58299800	-3.93316500	-2.00833200
H	-1.99591200	-1.23006300	2.97385000
H	5.10760100	-4.57054100	-1.85851500
H	3.45485100	-5.22081100	-2.02260400
H	3.80517500	-3.53887200	-2.51027700
H	5.19302400	-0.21410300	-1.96981600
H	4.94808300	-1.51410200	-0.81737600
H	7.29842500	-0.65317500	-0.68302000
H	6.69755300	0.96625900	-0.31773100
H	6.44997500	-0.34667200	0.83399300
C	-2.43326800	1.54732500	-0.69789000
O	-1.50163800	0.55599200	-2.64328100
C	-2.41908500	1.62811400	0.69820800
N	-3.19525700	2.45767900	1.40232300
C	-4.03811100	3.23026500	0.70555700
C	-3.32687900	2.35965300	-1.40257200
C	-4.14867300	3.21473300	-0.68514700
H	-1.76786100	0.95751400	1.26661900
H	-4.66656000	3.89815400	1.29366000
H	-3.36109100	2.29407700	-2.48703800
H	-4.86339500	3.86194700	-1.18409200
H	-2.19209200	-4.07091600	1.36010100

TS[transmet], iso2

Ni	-0.60129700	-0.54824000	-0.39043700
O	-2.11974500	-1.90525500	-0.16258300
B	-1.58167100	-2.52808500	1.02048300
C	0.63179100	-2.05608000	0.14249500
C	-1.73137800	0.76629900	-1.15883000
P	1.03120600	0.87883500	-0.30003200
C	2.64886300	0.24164100	-0.92364500
C	0.79699900	2.47654400	-1.18812800
C	1.27144800	1.30585600	1.48135000
C	2.01430700	3.34367800	-1.49033300
C	1.63643800	4.60285100	-2.26038900
C	1.93224600	2.62739600	1.85327600
C	2.03404500	2.80250700	3.36336500
C	3.92698900	0.71896000	-0.24428000
C	2.83749000	5.46746000	-2.59889500
C	2.66678300	4.12348600	3.76156500
C	-3.47609400	-1.66821200	-0.32577100
C	-3.92771900	-1.45975400	-1.62693200
C	-5.27397400	-1.18743500	-1.84423500
C	-6.16614200	-1.13310900	-0.77452000
C	-4.35323200	-1.61806300	0.75548100
C	-5.70024200	-1.35263800	0.51922700
C	1.47748400	-2.15369000	1.26559900
C	2.63256500	-2.92567900	1.28116800
C	2.99112700	-3.66076000	0.14545500
C	1.00633900	-2.85019000	-0.95588300
C	2.15767800	-3.64337000	-0.97643200
O	4.16406900	-4.35483400	0.22905000
O	-1.46379900	-3.88744700	1.08295500
O	-1.59506500	-1.78145000	2.17091200
C	4.58104000	-5.04229700	-0.93300300
C	5.15388300	-0.00592800	-0.78459500
C	6.44123200	0.43407200	-0.11149900
H	0.04437400	3.04130000	-0.61933200
H	0.30023900	2.20934800	-2.12842700
H	2.53773400	3.62994500	-0.56948500
H	2.74105800	2.76656800	-2.07924000
H	1.82653000	0.46633900	1.91699400
H	0.27327100	1.25982400	1.93557400
H	2.93647500	2.69187000	1.41488700
H	1.36124700	3.46570800	1.42997700
H	2.67336100	0.47227800	-1.99712800
H	2.59750200	-0.84875000	-0.85331200
H	4.05813700	1.80287400	-0.36646900
H	3.86016900	0.54119100	0.83888800
H	0.91304600	5.18100800	-1.66953300
H	1.10750300	4.31746700	-3.17958200
H	3.36175100	5.79094000	-1.69314900
H	3.55958400	4.91913900	-3.21356400
H	2.61287900	1.96780600	3.78187500
H	1.03139800	2.71875800	3.80385200
H	2.73601100	4.23003400	4.84748300
H	3.67982900	4.21745300	3.35561000
H	2.08557900	4.97136400	3.38352000
H	2.54990600	6.36604800	-3.15147000
H	-3.21506100	-1.49192600	-2.44493800

H	-5.62528300	-1.01763200	-2.85820400
H	-7.21645600	-0.91998600	-0.94894700
H	-3.97951600	-1.75559800	1.76457100
H	-6.38516700	-1.30742600	1.36134600
H	1.22598400	-1.59858100	2.17114700
H	3.28047100	-2.97174400	2.15350500
H	0.39134200	-2.83663300	-1.85898200
H	2.40421000	-4.22411700	-1.86055500
H	-1.26782400	-2.29921200	2.91241000
H	5.54453100	-5.49239400	-0.69370800
H	3.87495300	-5.83352100	-1.21599500
H	4.70170700	-4.35958600	-1.78460600
H	5.22174500	0.15820100	-1.86874100
H	5.01195900	-1.08871600	-0.65536500
H	7.31064400	-0.09728100	-0.50842800
H	6.61710300	1.50607400	-0.25216900
H	6.40661400	0.24935300	0.96756600
C	-2.70265900	1.48533000	-0.27178000
O	-1.78530700	0.94319200	-2.37527000
C	-2.62879100	1.35290100	1.11723700
N	-3.47062400	1.93351300	1.97765500
C	-4.44566200	2.68080100	1.44474000
C	-3.73259700	2.26922500	-0.79958600
C	-4.62125800	2.87728100	0.07415800
H	-1.85007300	0.71639000	1.54660500
H	-5.13014300	3.14572900	2.15369700
H	-3.81366000	2.37154300	-1.87940900
H	-5.44072100	3.49190000	-0.28702900
H	-1.41921600	-4.27746300	0.20616500

TS[transmet], iso1

Ni	-0.63525800	-0.37612200	-0.36597600
O	-2.23503900	-1.62436000	-0.23493300
B	-1.78550800	-2.39241400	0.89022200
C	0.46333400	-2.00508500	0.15457800
C	-1.70819400	1.06105600	-0.99610100
P	1.12494300	0.89613000	-0.32338000
C	2.66480900	0.07930000	-0.93537600
C	1.04154800	2.47791600	-1.26065800
C	1.40938200	1.37565500	1.43699200
C	2.34373300	3.18794500	-1.61471100
C	2.09476500	4.49170800	-2.36306500
C	2.26424400	2.59615200	1.75715700
C	2.38832200	2.82319500	3.25851700
C	3.98114200	0.36979600	-0.22427200
C	3.37915200	5.19680200	-2.75987700
C	3.21806300	4.04744000	3.60077800
C	-3.56629300	-1.37322100	-0.49861400
C	-3.90234600	-1.05172600	-1.81128100
C	-5.22311600	-0.74660800	-2.12059800
C	-6.20365100	-0.76868700	-1.12964800
C	-4.53301900	-1.40200800	0.50426500
C	-5.85265300	-1.10009800	0.17683800
C	1.29946100	-2.11710100	1.28364000
C	2.42354300	-2.93465200	1.32053300
C	2.75216900	-3.70791100	0.20161600
C	0.80432000	-2.84141500	-0.92324800
C	1.91930700	-3.68300500	-0.92159700
O	3.89622200	-4.44727300	0.30194600
O	-1.86753800	-3.74664600	0.71492500
O	-1.75089700	-1.71969200	2.09280300
C	4.27617700	-5.19092700	-0.83845400
C	5.09491000	-0.54743000	-0.71488800
C	6.41845100	-0.29330300	-0.01653900
H	0.37778400	3.14056500	-0.68705500
H	0.48262500	2.24794700	-2.17547100
H	2.94060400	3.39876700	-0.71813100
H	2.96728600	2.53190700	-2.23800800
H	1.80989300	0.48304000	1.93291900
H	0.40818300	1.51826100	1.86404800
H	3.26736900	2.48991000	1.32568500
H	1.82692700	3.49030600	1.29126700
H	2.73901800	0.32815200	-2.00211700
H	2.47725500	-0.99688700	-0.89321400
H	4.27992600	1.41857600	-0.35993000
H	3.85678300	0.22432300	0.85885600
H	1.48225900	5.15326900	-1.73544300
H	1.48808300	4.28428200	-3.25462000
H	3.98514200	5.44284700	-1.88123100
H	3.99337200	4.56549100	-3.41089700
H	2.83074600	1.92962700	3.71993600
H	1.38409400	2.91596300	3.69353200
H	3.30183300	4.19314900	4.68115300
H	4.23365800	3.96268600	3.19951000
H	2.77676700	4.95657800	3.17847700
H	3.18299400	6.12956000	-3.29577200
H	-3.11826300	-1.02195900	-2.56177000
H	-5.48463700	-0.48877500	-3.14301700
H	-7.23362700	-0.52709600	-1.37401500
H	-4.24774300	-1.62422700	1.52795600
H	-6.60745000	-1.11106500	0.95865900
H	1.07011300	-1.52839400	2.17447300
H	3.06962600	-2.98586100	2.19421300
H	0.18342600	-2.83109000	-1.82129700
H	2.13972200	-4.29757200	-1.78959200
H	-1.45691400	-2.26121300	2.82871500
H	-1.56967000	-4.25252000	1.47353700
H	5.21930600	-5.67632600	-0.58724700
H	3.53325000	-5.95776600	-1.09194900
H	4.42393800	-4.54369900	-1.71290700
H	5.21279700	-0.42540800	-1.80028000
H	4.78342600	-1.59112000	-0.56278500
H	7.20323400	-0.96524800	-0.37479000
H	6.76375500	0.73359300	-0.17873200
H	6.32827800	-0.43916100	1.06533500
C	-2.72077700	1.56134800	-0.00710200
O	-1.76049800	1.45419000	-2.15895200
C	-2.55682000	1.32789600	1.36056200
N	-3.44006300	1.67883900	2.29975800
C	-4.55821500	2.27826400	1.87109300
C	-3.89389500	2.19741800	-0.42391200
C	-4.83173200	2.55770100	0.53169100
H	-1.66355000	0.80154800	1.70391400
H	-5.28034200	2.54602200	2.64214200
H	-4.04899500	2.37255700	-1.48601100
H	-5.76593100	3.03788400	0.25434700

Ni[P(n-Bu)$_3$](PyrCO)[PhOB(OH)$_2$][PhOMe], iso1a

Ni	0.45916600	0.02253300	-0.43359100
O	2.24592400	-0.69100400	-1.33503700
B	2.22146600	-0.77140900	-2.72185000
C	-0.15968700	-1.79925400	-0.05615300
C	1.16060400	1.78552400	-0.76564200

P	-1.39849400	0.93791700	0.09012300
C	-2.67085600	0.02619400	1.06485400
C	-1.27434500	2.58380300	0.92707600
C	-2.21004200	1.29140800	-1.51843900
C	-2.47037600	3.11566900	1.70860100
C	-2.27651500	4.56728200	2.12711100
C	-3.49531400	2.10994200	-1.48576900
C	-4.18414500	2.16676800	-2.84335800
C	-3.37784900	-1.10867700	0.33136500
C	-3.43167200	5.10212800	2.95413300
C	-5.44437600	3.01262000	-2.82909800
C	2.19904300	2.19388600	0.24783300
O	0.98797700	2.50347300	-1.75274300
C	3.37169700	-0.91090900	-0.54967000
C	3.27912100	-1.85585100	0.46566800
C	4.36848400	-2.04021700	1.31240700
C	5.52907000	-1.28828700	1.14392900
C	4.51865100	-0.14583900	-0.73183800
C	5.60000700	-0.34382100	0.12211300
C	-0.44359000	-2.72465300	-1.08080100
C	-0.93460600	-4.00245800	-0.82861200
C	-1.16163600	-4.41475700	0.48841900
C	-0.36677400	-2.27017300	1.24874700
C	-0.85416500	-3.54904100	1.53962700
O	-1.69197400	-5.66920100	0.64236700
O	3.35983900	-1.13840600	-3.36697200
O	1.00252200	-0.46853200	-3.24637500
C	-2.02711600	-6.05446300	1.95767400
C	-4.16832800	-2.00024600	1.28025500
C	-4.78934000	-3.19416600	0.57799700
H	-0.99219900	3.28531300	0.12966400
H	-0.39941700	2.53767300	1.58727200
H	-3.39297800	3.03175200	1.11871100
H	-2.63230400	2.49922900	2.60305500
H	-2.38635700	0.31261500	-1.98556000
H	-1.44296400	1.78574800	-2.12904900
H	-4.19717200	1.69544300	-0.74573000
H	-3.27359300	3.13246700	-1.14808700
H	-3.41021800	0.74841400	1.43216100
H	-2.15844500	-0.36898000	1.95083900
H	-4.05037700	-0.69352700	-0.43438200
H	-2.64816600	-1.72629100	-0.20326100
H	-2.14283000	5.18270300	1.22679400
H	-1.33769100	4.65799600	2.68985100
H	-4.37538200	5.04567300	2.40082200
H	-3.56053600	4.52435100	3.87572100
H	-4.42211000	1.14309600	-3.16400800
H	-3.47745600	2.55545400	-3.58864800
H	-5.93040600	3.03701000	-3.80842800
H	-6.17314400	2.62560000	-2.10882900
H	-5.22421100	4.04698500	-2.54425800
H	-3.27881500	6.14679100	3.23879800
H	2.35453500	-2.41382800	0.58313300
H	4.30457300	-2.77487900	2.10989000
H	6.37417300	-1.43338800	1.81029800
H	4.55264000	0.59617800	-1.52380300
H	6.49895700	0.25218100	-0.00985400
H	-0.30595400	-2.42860600	-2.12206100
H	-1.17043300	-4.69493300	-1.63419800
H	-0.16107700	-1.61090900	2.09648600
H	-1.00619300	-3.84978600	2.57269800
H	0.94927100	-0.49443500	-4.20330300
H	3.27398300	-1.20637200	-4.31948400
H	-2.47764800	-7.04466300	1.88363800
H	-1.14388200	-6.11038600	2.60788100
H	-2.74899300	-5.36084800	2.41125800
H	-4.94359800	-1.41085400	1.79018500
H	-3.48682000	-2.35320100	2.06742800
H	-5.34440600	-3.83319000	1.27153300
H	-5.48458400	-2.88051800	-0.20876300
H	-4.01568600	-3.81041200	0.10510700
C	2.28917500	1.52010000	1.47083100
N	3.21758000	1.75203900	2.40151800
C	4.11839200	2.70230600	2.11866300
C	3.14205000	3.19252800	-0.00917100
C	4.12129200	3.44955700	0.94035200
H	1.55350100	0.73885000	1.69538700
H	4.88136600	2.87587000	2.87680000
H	3.08784300	3.73345400	-0.95156200
H	4.88014800	4.21019700	0.78063900

Ni[P(n-Bu)$_3$](PyrCO)[PhOB(OH)$_2$][PhOMe], iso1b

Ni	-0.25456300	-0.80161600	-0.13188000
O	-1.95642000	-2.16037000	-0.07251000
B	-2.63937300	-1.76795500	-1.23086800
C	-1.46177100	0.71850100	-0.49781000
C	0.84491800	-2.35572500	0.01438700
P	1.37773700	0.46704000	0.44611700
C	0.90520600	2.05872000	1.25554900
C	2.51443200	-0.35169200	1.65089700
C	2.46288800	0.99038500	-0.94480000
C	3.29771400	0.50487900	2.63841500
C	4.34629100	-0.30683500	3.38800800
C	3.72257300	1.76825100	-0.58073000
C	4.41367600	2.35676800	-1.80366100
C	0.56627400	3.20848900	0.31163200
C	5.10968000	0.51698200	4.40911500
C	5.69265400	3.09762100	-1.45862900
O	1.00260000	-3.03774200	1.02597000
C	1.39104600	-2.87369500	-1.28882900
C	-2.55872600	-2.29909900	1.16579200
C	-1.92524400	-1.73074800	2.26712600
C	-2.47858800	-1.89501100	3.53314500
C	-3.65378500	-2.62435900	3.69854300
C	-3.72658600	-3.04120800	1.31610300
C	-4.27065300	-3.19593400	2.58798400
C	-1.54348000	1.21777800	-1.81478900
C	-2.35437800	2.29064800	-2.17292900
C	-3.12575700	2.93008400	-1.19680400
C	-2.26633400	1.38054900	0.44144500
C	-3.08921800	2.46484700	0.11905100
O	-3.86713000	3.99974200	-1.62197700
O	-3.94111300	-1.39515200	-1.14392800
O	-1.85697700	-1.88623200	-2.34276900
C	-4.60934600	4.68630400	-0.63616000
C	-0.11152800	4.36617500	1.03198700
C	-0.50484200	5.48501300	0.08440700
H	3.19971000	-0.95125300	1.03436100
H	1.91056200	-1.09169200	2.18855600
H	3.78912800	1.34554700	2.13031300
H	2.60715300	0.95819400	3.36231200
H	1.82370700	1.57901400	-1.61741300
H	2.72734500	0.08404300	-1.50389300

H	3.48318100	2.57893000	0.12331200
H	4.42136100	1.10767100	-0.04836900
H	1.71283500	2.36222500	1.93264700
H	0.03624600	1.83030700	1.88590200
H	1.48202500	3.56730200	-0.18150200
H	-0.09472900	2.86267900	-0.49004500
H	5.04462900	-0.74474000	2.66148900
H	3.85853200	-1.15882800	3.88024400
H	5.63016900	1.35538200	3.93351700
H	4.43568500	0.93881300	5.16240700
H	3.71446800	3.03213000	-2.31572900
H	4.62695900	1.55155700	-2.51946200
H	6.17252200	3.51615200	-2.34761100
H	5.49808500	3.92543400	-0.76819400
H	6.41703300	2.43412200	-0.97426400
H	5.85963100	-0.07985300	4.93554800
H	-0.99803100	-1.17737500	2.11285300
H	-1.98442700	-1.45067700	4.39251400
H	-4.08393400	-2.75081600	4.68737800
H	-4.20148600	-3.48354100	0.44689900
H	-5.18390500	-3.77202300	2.70742400
H	-0.93233700	0.76317200	-2.59924300
H	-2.39098100	2.66731100	-3.19298500
H	-2.25643500	1.05577800	1.48446900
H	-3.68262000	2.94314400	0.89336500
H	-2.21645500	-1.47216900	-3.12985200
H	-4.31745300	-1.09483000	-1.97378500
H	-5.11352200	5.50699800	-1.14666200
H	-5.36016700	4.03832700	-0.16519100
H	-3.96048200	5.09428200	0.15116300
H	0.54598300	4.75053500	1.82435200
H	-1.00721500	3.97971200	1.53856100
H	-1.00947500	6.30455900	0.60456100
H	0.37015600	5.90590500	-0.42325000
H	-1.18511900	5.11433500	-0.69142800
C	1.32775400	-2.10385000	-2.45421400
N	1.78774100	-2.49329200	-3.64647400
C	2.34304300	-3.71140700	-3.70300800
C	1.97665400	-4.13934100	-1.38059400
C	2.46071600	-4.56721000	-2.60814700
H	0.86732000	-1.11208900	-2.40567000
H	2.71314300	-4.02087900	-4.67998100
H	2.03443200	-4.75413200	-0.48539400
H	2.92177800	-5.54341400	-2.72686700

Ni[P(n-Bu)$_3$](PyrCO)[PhOMe]

Ni	1.17131900	-0.47180400	-0.00722600
P	-1.07237500	-0.76154900	0.02052200
C	-1.81966500	-0.44843100	-1.63964800
C	-1.69855200	-2.41788800	0.54698800
C	-1.85962100	0.45801500	1.16379100
C	-3.22522700	0.13441900	-1.72367600
C	-3.62523100	0.45808800	-3.15736800
C	-5.01929800	1.05019800	-3.25956200
C	-3.10202100	-2.82919600	0.11756800
C	-3.25652100	0.21443700	1.71956800
C	-3.70699900	1.36550300	2.61106800
C	-5.08231200	1.14548400	3.21394100
C	-3.48500300	-4.21113100	0.63241100
C	-4.87491700	-4.63436500	0.19320000
C	3.06246700	-0.39012700	0.10053100
C	1.18238100	0.97179700	-1.11057100
C	0.61948000	2.17002600	-0.42334700
O	1.39380200	0.93577600	-2.31026300
C	0.83093600	2.40528500	0.93996600
N	0.22673600	3.37332700	1.63304300
C	-0.64143200	4.14460000	0.96285300
C	-0.25331300	3.01780500	-1.11097400
C	-0.90654700	4.01723300	-0.39965400
H	-1.76322400	-1.39811100	-2.18827300
H	-1.12150400	0.21773300	-2.16175000
H	-3.95781100	-0.55790200	-1.28757400
H	-3.28501600	1.05324300	-1.12183200
H	-3.55838700	-0.45363600	-3.76594500
H	-2.88915500	1.15363600	-3.58379200
H	-5.77369400	0.35835400	-2.87001500
H	-5.09897900	1.97676600	-2.68086500
H	-1.60653300	-2.44659500	1.64119100
H	-0.97461200	-3.15352600	0.17546100
H	-3.84100900	-2.09702500	0.46611000
H	-3.16954400	-2.82123000	-0.97938400
H	-1.82753200	1.42078400	0.63531800
H	-1.15611700	0.57625200	1.99809200
H	-3.98240100	0.08270800	0.90711000
H	-3.27446400	-0.72287800	2.29409300
H	-3.69718700	2.29383000	2.02218400
H	-2.96536000	1.51550000	3.40744400
H	-5.84258200	1.02339200	2.43509900
H	-5.10396900	0.24248500	3.83325600
H	-5.28828500	1.28305100	-4.29330000
H	-5.38875900	1.98434300	3.84455000
H	-3.42063300	-4.21621800	1.72902000
H	-2.74247900	-4.94349700	0.28811300
H	-5.13743300	-5.62563900	0.57258000
H	-5.63452600	-3.93174700	0.55216700
H	-4.95297400	-4.66733200	-0.89869400
H	1.52593300	1.76200100	1.48380900
H	-1.15204000	4.90716200	1.54959400
H	-0.42273500	2.86295300	-2.17430700
H	-1.61243800	4.68428200	-0.88507100
C	3.66586200	-0.43810600	1.37386600
C	5.03249900	-0.64131600	1.52977500
C	5.85050000	-0.77992200	0.40349700
C	3.91414300	-0.49839900	-1.00494400
C	5.28823900	-0.70346300	-0.87387400
H	3.05912500	-0.33131600	2.27388000
H	5.49111400	-0.69206900	2.51425700
O	7.17913800	-0.97472100	0.65338900
H	3.49381000	-0.41713300	-2.00718200
H	5.90787400	-0.79387000	-1.76100600
C	8.02525100	-1.11570500	-0.46913100
H	9.03089200	-1.26813800	-0.07698000
H	7.74330400	-1.97924200	-1.08547000
H	8.01676200	-0.21839400	-1.10134700

TS(decarb.), Ni[P(n-Bu)$_3$](PyrCO)[PhOMe]

Ni	0.62804400	-1.37460200	0.01360600
P	-1.30664100	-0.42834700	-0.13666500
C	-2.65799900	-1.55302100	-0.70035200
C	-1.82926600	0.15235900	1.52605100
C	-1.40317800	1.07756200	-1.19926900
C	-3.90115300	-0.95004900	-1.34563000
C	-5.00943900	-1.98055300	-1.51970300
C	-6.24037700	-1.41172600	-2.20194600

C	-3.25241200	0.68397700	1.65501400
C	-0.97573500	2.37870000	-0.52229200
C	-0.73631700	3.49917300	-1.52469700
C	-0.28639900	4.78453400	-0.85432200
C	-3.50225200	1.34921500	3.00199800
C	-4.92603200	1.85230100	3.15546800
C	1.62028700	0.30233500	0.07947500
C	1.98317200	-2.95417800	0.15642500
C	0.34499700	-3.11326200	-0.04785000
O	-0.17202400	-4.18707800	-0.16995400
C	2.55477500	-3.07297200	1.42823500
C	3.92999700	-3.23338200	1.52962600
C	4.68261100	-3.26134500	0.35665200
C	2.83811800	-3.00199400	-0.95329400
N	4.16213200	-3.15057300	-0.87335700
H	-2.93100200	-2.13459100	0.19172400
H	-2.20216700	-2.28050700	-1.38087400
H	-4.28247700	-0.10701500	-0.75445300
H	-3.64037700	-0.53129600	-2.32689200
H	-5.27915100	-2.38353100	-0.53371500
H	-4.62185200	-2.83361500	-2.09242200
H	-6.66043000	-0.57716500	-1.63023200
H	-6.00086500	-1.03280300	-3.20131800
H	-1.09747300	0.92019700	1.81080200
H	-1.66973400	-0.68192900	2.21986500
H	-3.46436600	1.40496900	0.85150100
H	-3.96846800	-0.13810300	1.51413900
H	-2.42277500	1.17659100	-1.59124100
H	-0.75406700	0.88520100	-2.06295200
H	-1.74349300	2.68971200	0.20120200
H	-0.05656800	2.22810200	0.05544200
H	-1.64648000	3.67526300	-2.11515200
H	0.03051900	3.16639100	-2.23852800
H	-1.04358800	5.15798700	-0.15607000
H	0.63407600	4.62226400	-0.28111500
H	-7.02675600	-2.16291500	-2.31457600
H	-0.08991000	5.57786300	-1.58164800
H	-2.79441500	2.18056000	3.12349100
H	-3.26568600	0.63761800	3.80440900
H	-5.08570700	2.33035900	4.12559200
H	-5.17212300	2.58688300	2.38121600
H	-5.64818300	1.03355200	3.06805800
H	1.92822200	-3.03638400	2.31670200
H	4.41672300	-3.32712000	2.49538100
H	5.76415200	-3.37719400	0.40530500
H	2.42398300	-2.91098300	-1.95808100
C	1.91313000	0.98982100	1.27423400
C	2.52034600	2.24201300	1.29465000
C	2.86896400	2.86614400	0.09276000
C	2.01582600	0.95286500	-1.09940200
C	2.63148500	2.20855500	-1.11554200
H	1.63628300	0.54698300	2.23405700
H	2.72309500	2.76429600	2.22698000
O	3.42254300	4.11484300	0.20331700
H	1.81889300	0.48367500	-2.06671000
H	2.90311400	2.66634200	-2.06269200
C	3.75400600	4.76885600	-1.00300800
H	4.15977600	5.74156600	-0.72378700
H	4.50923700	4.21383000	-1.57495000
H	2.87238600	4.91534300	-1.64251600

TS(B-C), Ni[P(n-Bu)$_3$]$_2$(PyrCO)[PhOB(OH)$_2$-PhOMe], Iso-1_up

Ni	0.03529900	-0.30574000	-0.60445800
O	-2.47597100	-1.06978700	-0.94030700
B	-1.91682300	-2.32953300	-0.49853800
C	0.19537000	-2.32789200	-0.26855100
P	-0.89519000	0.75999300	1.37480100
C	0.08623200	-0.38282600	-2.46586500
P	1.95956000	0.81630700	-0.76211400
C	-0.59622500	2.60172200	1.22220300
C	3.24676700	-0.30606500	-1.45493900
C	2.14526400	2.40288200	-1.69813300
C	2.56360100	1.20116800	0.93629500
C	-2.72959900	0.71168700	1.49090200
C	-0.39966200	0.33654900	3.11484200
C	-0.16192400	3.38059800	2.45683200
C	0.27541100	4.79931200	2.11894500
C	0.66159400	5.60545500	3.34581000
C	-3.39197900	1.61656700	2.51908100
C	-1.15528500	-0.88192100	3.65729900
C	3.51983100	2.77971300	-2.24777400
C	3.59385200	4.25351400	-2.62452100
C	3.84446000	2.00966000	1.09198200
C	4.18857400	2.24141100	2.55814000
C	3.82972800	-1.29176900	-0.45073700
C	4.93268900	4.64352800	-3.22358400
C	5.50402000	2.97402000	2.74861600
O	0.70920800	-1.04669800	-3.27550200
C	-3.81018300	-0.97088200	-1.16421500
C	-4.72158600	-2.01141300	-0.93238700
C	-6.07814000	-1.80977700	-1.17026000
C	-6.55722000	-0.58787600	-1.63787200
C	-4.29441800	0.25935000	-1.62692800
C	-5.65090400	0.44626600	-1.86400300
C	0.59157700	-2.54905800	1.07345400
C	1.49793500	-3.52877400	1.45881100
C	2.06276100	-4.36806800	0.49247200
C	0.81887800	-3.17917600	-1.20120900
C	1.72056900	-4.18421800	-0.85031600
O	2.92006700	-5.32652500	0.95255200
O	-2.01585600	-3.30238100	-1.50739000
O	-2.27226100	-2.59840000	0.84267300
H	-1.51861500	3.03350100	0.81038100
H	0.15648000	2.74143100	0.43523100
H	-0.97405400	3.40365700	3.19736800
H	0.67239600	2.86638500	2.95730500
H	-0.52690600	5.30711400	1.56728100
H	1.12626100	4.74640900	1.42294700
H	-0.18193400	5.70358700	4.03710400
H	1.47709900	5.12206000	3.89550100
H	-3.00513700	-0.33829000	1.65255800
H	-3.10697600	0.94267000	0.48817200
H	-3.00171800	1.41314700	3.52762600
H	-3.14810600	2.66979400	2.31486600
H	-0.54116600	1.19557800	3.77977700
H	0.68007900	0.13421300	3.09949900
H	-2.09548200	-0.55309200	4.12085200
H	-1.46533400	-1.53667300	2.83425300
H	1.78041300	3.18939800	-1.02016500
H	1.42274900	2.37902600	-2.52229100
H	4.31495900	2.55071000	-1.52634800
H	3.73737100	2.16543900	-3.13130600

H	2.65467000	0.22638100	1.43540900
H	1.75009800	1.71627400	1.45780600
H	4.68196900	1.50444200	0.58873100
H	3.73738400	2.98298400	0.59213600
H	4.05042600	0.28888300	-1.90550700
H	2.75732900	-0.85580600	-2.26888800
H	4.37285700	-0.75140300	0.33830000
H	3.02091800	-1.83839800	0.05176000
H	3.39212500	4.85871500	-1.72897000
H	2.78379900	4.48777500	-3.32809600
H	5.75211200	4.45100400	-2.52268900
H	5.14231400	4.07126000	-4.13345500
H	4.21502500	1.27404700	3.07800500
H	3.37163400	2.80894100	3.02754300
H	5.72231100	3.14970000	3.80544200
H	6.33915400	2.40359000	2.32896300
H	5.49103000	3.94821100	2.24838700
H	0.99324600	6.61392600	3.08417700
H	4.96619600	5.70406800	-3.48662100
H	-4.36147000	-2.96693100	-0.56925600
H	-6.77092500	-2.62746400	-0.98534400
H	-7.61814700	-0.44434200	-1.82069000
H	-3.59427100	1.06451300	-1.78563200
H	-5.99732600	1.41226600	-2.22514300
H	0.14911400	-1.94110500	1.85560200
H	1.76482600	-3.67593700	2.50351200
H	0.56843600	-3.07755100	-2.25350300
H	2.14515200	-4.81722500	-1.62441300
H	-1.89015700	-3.42543000	1.14686900
H	-1.59126200	-4.12387800	-1.25156200
C	3.47107700	-6.20491800	-0.00994700
H	4.11785100	-6.89045300	0.53757500
H	2.69105100	-6.77646000	-0.52844500
H	4.06779400	-5.66592300	-0.75778500
C	-0.33725300	-1.69017500	4.65533300
C	-1.02027400	-2.98519900	5.05532600
H	-0.12051700	-1.08031600	5.54282400
H	0.64145600	-1.91488600	4.20599900
H	-0.41575200	-3.56952900	5.75462800
H	-1.98912800	-2.79797500	5.53034700
H	-1.20655000	-3.61221600	4.17496800
C	-4.90632700	1.44331700	2.51902800
C	-5.61284200	2.38191100	3.47988000
H	-5.14418900	0.39990800	2.76769600
H	-5.28178500	1.59209500	1.49704400
H	-6.69758000	2.24499400	3.46041400
H	-5.27917000	2.22104600	4.51104400
H	-5.40846700	3.42950200	3.23270900
C	4.77549700	-2.29219000	-1.10125100
C	5.49010900	-3.15722600	-0.07828800
H	5.51173900	-1.75622300	-1.71688500
H	4.20058000	-2.92136000	-1.79532100
H	6.13455800	-3.90436800	-0.55164400
H	6.12145300	-2.54880300	0.57871100
H	4.77561200	-3.68816500	0.56021000
C	-0.95299900	0.59074700	-2.95062200
C	-1.18121000	1.83322000	-2.34882700
C	-1.69872100	0.27718800	-4.09161200
N	-2.04859300	2.74333600	-2.80312900
H	-0.60912900	2.10817900	-1.46182900
C	-2.61546300	1.20313000	-4.56752000
H	-1.54891300	-0.68145300	-4.58060300
C	-2.74938100	2.41798100	-3.89714200
H	-3.21828400	0.99248000	-5.44540100
H	-3.45992800	3.16436700	-4.24933200

TS(B-C), Ni[P(n-Bu)$_3$]$_2$(PyrCO)[PhOB(OH)$_2$-PhOMe], Iso-2_up

Ni	0.04365700	-0.28828400	-0.59523800
O	-2.46671000	-1.12606500	-1.04805300
B	-1.98024100	-2.37672300	-0.48868700
C	0.15126700	-2.32184800	-0.34563100
P	-0.89533800	0.72562500	1.39330100
C	0.11593700	-0.27756300	-2.45900600
P	1.97062100	0.83279200	-0.69867600
C	-0.58619500	2.57042600	1.27390500
C	3.26247700	-0.28281600	-1.39256800
C	2.16683900	2.43348700	-1.61008000
C	2.57355500	1.18850200	1.00584700
C	-2.73219600	0.69071300	1.45956200
C	-0.42303500	0.28767700	3.13419000
C	-0.18360500	3.33698200	2.52745200
C	0.28233800	4.75225600	2.21282600
C	0.68485400	5.53048500	3.45233300
C	-3.41211400	1.55335100	2.51253400
C	-1.16118400	-0.94849100	3.66282600
C	3.53797500	2.80392400	-2.16956500
C	3.59391500	4.26024700	-2.61167400
C	3.87732000	1.96106000	1.15875400
C	4.28730100	2.09379200	2.61974300
C	3.82193600	-1.29352800	-0.39942300
C	4.93014600	4.64006300	-3.22330600
C	5.57359000	2.87762400	2.80496300
O	0.74586700	-0.90409900	-3.29557100
C	-3.80842400	-0.97189200	-1.22108700
C	-4.75580600	-1.97322900	-0.96167600
C	-6.10942100	-1.71340500	-1.16102000
C	-6.54957300	-0.47300200	-1.61738100
C	-4.25346000	0.27575300	-1.67516900
C	-5.60656200	0.52064700	-1.87374000
C	0.52714400	-2.61191700	0.98867300
C	1.42582300	-3.61316500	1.33565400
C	2.00524300	-4.39936200	0.33473700
C	0.79545900	-3.11818700	-1.31183000
C	1.69082200	-4.13991200	-1.00267600
O	2.85253800	-5.38463400	0.75549700
O	-2.10166300	-3.52050800	-1.29018500
O	-2.33441900	-2.54664500	0.85585700
H	-1.49424000	3.01009200	0.83874900
H	0.19000100	2.71546300	0.51188600
H	-1.01938500	3.36649600	3.24071100
H	0.62799900	2.81207600	3.05305100
H	-0.50891000	5.28623400	1.67010500
H	1.13260400	4.69431500	1.51570000
H	-0.15384700	5.62662800	4.14988700
H	1.49708900	5.02739800	3.98863000
H	-3.03188000	-0.35945400	1.55832400
H	-3.06716200	0.99091400	0.45952500
H	-3.06611400	1.27919000	3.52045600
H	-3.13411200	2.60954400	2.38027800
H	-0.58708200	1.14212000	3.79948300
H	0.66043500	0.10661000	3.13166200
H	-2.07099800	-0.63310400	4.19117900
H	-1.51980800	-1.56892000	2.83253200

H	1.81913000	3.21271800	-0.91507400
H	1.43578800	2.43200800	-2.42717400
H	4.32973600	2.61909900	-1.43213400
H	3.77005800	2.15415800	-3.02352300
H	2.63961000	0.20783800	1.49743500
H	1.77611000	1.72165900	1.53326400
H	4.68315800	1.47164000	0.59225800
H	3.76694500	2.96434700	0.72142800
H	4.07800200	0.31885500	-1.81209000
H	2.78676200	-0.81114000	-2.22867300
H	4.36667300	-0.77285900	0.40203200
H	3.00212900	-1.83708100	0.08884500
H	3.38114200	4.90265000	-1.74542100
H	2.78394600	4.45168300	-3.32819700
H	5.74980400	4.48506800	-2.51346400
H	5.14811100	4.03361900	-4.10874700
H	4.39096400	1.08991200	3.05375100
H	3.46957600	2.57518700	3.17578300
H	5.85198500	2.95881100	3.85904100
H	6.40713200	2.39976600	2.27943700
H	5.47892200	3.89426700	2.40879000
H	1.02695100	6.53959500	3.20717400
H	4.95301600	5.68943600	-3.52894700
H	-4.42971300	-2.94466100	-0.60948500
H	-6.83039100	-2.50092700	-0.95462600
H	-7.60831100	-0.28436400	-1.76925700
H	-3.51699300	1.05078500	-1.85098900
H	-5.92152000	1.50038700	-2.22686700
H	0.06881700	-2.04706300	1.79482400
H	1.67539100	-3.81822900	2.37486900
H	0.58271300	-2.95353600	-2.36572400
H	2.13256800	-4.72788100	-1.80205500
H	-2.09359100	-3.43318400	1.13850700
C	3.43730600	-6.19355600	-0.24697900
H	4.07284100	-6.91128000	0.27197600
H	2.67729300	-6.73297100	-0.82575500
H	4.05226600	-5.60154000	-0.93829800
C	-0.29916500	-1.80173000	4.58379800
C	-0.97491800	-3.10222800	4.97766900
H	-0.02336900	-1.22529100	5.47727400
H	0.64878900	-2.02176100	4.07101800
H	-0.34859600	-3.70657300	5.63964100
H	-1.92417800	-2.92116100	5.49326200
H	-1.19781400	-3.70704600	4.09042500
C	-4.92947100	1.42379400	2.44489900
C	-5.64526900	2.27563200	3.47711700
H	-5.20274000	0.36711900	2.57163700
H	-5.26511400	1.69196900	1.43357400
H	-6.73159300	2.16871200	3.41209200
H	-5.34745100	2.00048200	4.49494500
H	-5.41042000	3.33780500	3.34676600
C	4.76161300	-2.29332300	-1.05954800
C	5.44945100	-3.19360700	-0.04870700
H	5.51403000	-1.75326100	-1.65177400
H	4.18769800	-2.89672000	-1.77695800
H	6.09118700	-3.93644000	-0.53266100
H	6.07934100	-2.61128500	0.63293000
H	4.71865700	-3.73309600	0.56370300
C	-0.91225500	0.71974500	-2.92205100
C	-1.16448800	1.93072100	-2.26852900
C	-1.62342100	0.45995000	-4.09817800
N	-2.02995900	2.85449600	-2.69896200
H	-0.61418700	2.16850200	-1.35769800
C	-2.53743900	1.39946600	-4.55165300
H	-1.44647100	-0.46888200	-4.63391200
C	-2.70189500	2.57718000	-3.82387000
H	-3.11410800	1.22922000	-5.45566300
H	-3.41159000	3.33364000	-4.15564300
H	-1.91380100	-3.30915800	-2.20772600

$Ni[P(n\text{-}Bu)_3]_2(PyrCO)[PhOB(OH)_2](PhOMe)$

Ni	0.57958700	-0.96023400	-0.02835200
O	-1.23583200	2.17547100	3.57364500
B	-0.59409600	0.97305500	3.34357100
C	2.51706800	-1.04739400	0.31595900
P	0.74051100	1.08549000	-1.07224000
C	0.63963500	-2.31158600	1.27235600
P	-1.62714700	-1.26571700	-0.33506300
C	-0.68766700	2.25670400	-0.85286800
C	-2.22306600	-3.01347500	-0.37917800
C	-2.46260100	-0.55244200	1.14742700
C	-2.38055100	-0.51838300	-1.85642900
C	2.15676300	2.09196000	-0.46952800
C	1.02382400	1.00936700	-2.89745200
C	-1.12095900	3.07286100	-2.06546500
C	-2.36928300	3.90173100	-1.79455800
C	-2.90175100	4.59455100	-3.03539800
C	2.24995300	3.53033600	-0.95585200
C	2.05477200	-0.05644900	-3.23754500
C	-3.89558800	-0.90694800	1.52450600
C	-4.30898800	-0.20881400	2.81558000
C	-3.74964600	0.14241500	-1.75282900
C	-4.14423300	0.84820000	-3.04406500
C	-3.61917300	-3.29620300	-0.92303300
C	-5.72510600	-0.54946800	3.24157300
C	-5.45306300	1.60789100	-2.92984500
O	0.42895600	-2.01581000	2.46658100
C	-0.98839000	3.28760600	2.81878700
C	0.30827800	3.75860400	2.59508000
C	0.49787600	4.92391500	1.85859500
C	-0.59110200	5.62636500	1.34441700
C	-2.08414600	3.98963800	2.31511600
C	-1.88117700	5.15663000	1.58458600
C	3.36098600	-1.68880000	-0.61019900
C	4.74681700	-1.65612500	-0.50539300
C	5.35262100	-0.99568200	0.56799600
C	3.15758200	-0.42994200	1.39702400
C	4.54893600	-0.38640800	1.53177300
O	6.72023100	-1.01254900	0.58926300
O	-0.90648200	-0.03768900	4.20554600
O	0.25650300	0.85338000	2.28021900
H	-0.42529700	2.91739200	-0.01490100
H	-1.54598500	1.67543300	-0.49366600
H	-0.30362200	3.72803200	-2.39931500
H	-1.32511500	2.40456600	-2.91556700
H	-2.14943900	4.63638300	-1.00993200
H	-3.14454200	3.24380300	-1.37046100
H	-2.16042900	5.28118400	-3.45797300
H	-3.15369600	3.86852900	-3.81763400
H	3.07224800	1.53406800	-0.70646900
H	2.07728700	2.06515400	0.62602700
H	2.33656800	3.56459000	-2.05191600
H	1.32438000	4.07111200	-0.70860700
H	1.32548900	1.99346900	-3.28154700

H	0.07211200	0.76813600	-3.38819100
H	2.97639600	0.11526300	-2.66324400
H	1.67895300	-1.02852600	-2.88270700
H	-2.33960300	0.53864300	1.09204700
H	-1.80669500	-0.86514700	1.96949900
H	-4.59749100	-0.64023100	0.72404800
H	-3.98662700	-1.99375900	1.66018900
H	-2.39009300	-1.30924100	-2.61801100
H	-1.66358900	0.22156800	-2.22853900
H	-4.51666600	-0.59785100	-1.48857800
H	-3.74529500	0.87602700	-0.93124300
H	-2.12476900	-3.38981300	0.64959500
H	-1.48948800	-3.58486600	-0.96196800
H	-4.37310700	-2.68582700	-0.41043600
H	-3.67193600	-3.00491700	-1.98133800
H	-4.20524300	0.87759900	2.68351700
H	-3.59702100	-0.47321100	3.60829400
H	-6.45243000	-0.26234300	2.47413800
H	-5.84030000	-1.62560600	3.41103100
H	-4.20234400	0.11131600	-3.85633300
H	-3.33786200	1.53995900	-3.32896900
H	-5.71389300	2.11052900	-3.86556400
H	-6.28138300	0.94038600	-2.66986100
H	-5.39605700	2.37551300	-2.14959000
H	-3.80499800	5.17390400	-2.82317600
H	-6.00454600	-0.03935000	4.16744400
H	1.15456000	3.20601200	2.99158300
H	1.50885200	5.28745900	1.68892300
H	-0.43470500	6.53482100	0.76905400
H	-3.08310200	3.60882700	2.50783200
H	-2.73940800	5.69895900	1.19610500
H	2.93699600	-2.21837900	-1.46280700
H	5.37952800	-2.14178200	-1.24475600
H	2.57244200	0.06690500	2.17018100
H	4.98793200	0.12027500	2.38610700
H	0.53508400	-0.07767400	2.19677900
H	-0.47982800	-0.85873800	3.92345300
C	7.34552900	-0.35809400	1.67254100
H	8.41923400	-0.47423800	1.52366300
H	7.09933500	0.71166900	1.70035100
H	7.06516000	-0.80402400	2.63590200
C	2.39911500	-0.14939800	-4.71515900
C	3.41056600	-1.24833600	-4.99223800
H	2.79022000	0.81772900	-5.05932900
H	1.48323300	-0.32433600	-5.29657600
H	3.68224400	-1.30260800	-6.04995100
H	4.33139200	-1.08847800	-4.41956700
H	3.01743400	-2.22842100	-4.69996500
C	3.42621000	4.27455800	-0.33665600
C	3.47538800	5.73636300	-0.74282500
H	4.36251900	3.77207500	-0.61386200
H	3.36161000	4.19004200	0.75793700
H	4.31711500	6.26226300	-0.28380800
H	3.57127700	5.84365600	-1.82859900
H	2.55783400	6.25956700	-0.44741800
C	-3.99446600	-4.76725500	-0.79401600
C	-5.36304300	-5.07882300	-1.37182200
H	-3.96122700	-5.05189500	0.26643600
H	-3.22838200	-5.37899600	-1.28932000
H	-5.61695800	-6.13736500	-1.26937700
H	-6.14670200	-4.50167100	-0.86934300
H	-5.40955400	-4.83031900	-2.43755100
C	0.92653800	-3.72959300	0.92333700
C	1.04673700	-4.10543900	-0.41732700
C	1.06008900	-4.72599300	1.89225300
N	1.27824700	-5.34950100	-0.83881300
H	0.93294000	-3.33102200	-1.18338600
C	1.31151400	-6.02754200	1.47940300
H	0.96745100	-4.45881300	2.94203100
C	1.41108600	-6.28489900	0.11270400
H	1.42882000	-6.83481200	2.19603300
H	1.60633900	-7.29702400	-0.23961600

Ni[P(n-Bu)$_3$]$_2$(PyrCO)[PhOMe]

Ni	-0.35145900	-0.59068200	-0.24451800
P	1.86563300	-0.38961600	-0.14251500
P	-0.89755100	1.59155600	0.17782600
C	0.16418700	2.96417700	-0.49548500
C	2.84308500	-1.88693500	0.31752200
C	2.27534200	-0.08498600	-1.91665500
C	2.63299200	0.95842500	0.87228800
C	-2.58616900	2.10637500	-0.34821700
C	-0.93466100	1.85266800	2.00681200
C	0.53609300	4.11407600	0.43324500
C	1.51462700	5.08206200	-0.21949700
C	1.98555100	6.17795400	0.71869000
C	-3.02121500	3.52383200	-0.01034900
C	-1.73479800	0.74014100	2.67145000
C	-1.67492900	0.73948900	4.19017300
C	3.66975600	-0.36649200	-2.46468400
C	3.75067800	-0.09596700	-3.96191600
C	3.79359300	1.76269900	0.29950700
C	4.18952400	2.91281300	1.21732400
C	4.32721900	-1.72091700	0.62161900
C	5.01431500	-3.05234100	0.89799100
C	-2.40350900	-0.45384200	4.78371200
C	5.12258600	-0.38915700	-4.54178300
C	6.48462800	-2.89475100	1.24079800
C	5.24028800	3.82609900	0.61309700
C	-4.43824700	3.83210500	-0.47956900
C	-4.87653500	5.24487500	-0.13934000
C	-2.20116500	-1.05882900	-0.64405700
C	-0.12569000	-2.39536800	-0.75777000
C	-0.29808800	-3.46204400	0.28208400
O	0.18301600	-2.71986900	-1.90508000
C	-0.44873100	-3.12946000	1.62948800
N	-0.59473800	-4.01272600	2.62038800
C	-0.60441400	-5.30587900	2.26651100
C	-0.29663600	-4.81651300	-0.05394100
C	-0.45933300	-5.75601800	0.95514500
H	-0.34958100	3.34779500	-1.38715800
H	1.08752200	2.50577600	-0.87393900
H	-0.36450500	4.65176200	0.76160200
H	0.99092600	3.71960500	1.35490000
H	1.05123400	5.52142200	-1.11314400
H	2.37984700	4.51011500	-0.58776500
H	1.14741300	6.78652700	1.07420900
H	2.47873400	5.75705000	1.60294200
H	-3.28127000	1.36818600	0.07275900
H	-2.62890800	1.93624800	-1.43223800
H	-2.96079400	3.69079500	1.07512900
H	-2.32929500	4.25026600	-0.46199700
H	-1.32506100	2.84527700	2.26778800
H	0.10055300	1.82150400	2.37105300

H	-2.78348200	0.77972000	2.34224400
H	-1.35580100	-0.22203400	2.29370600
H	1.98080000	0.95168900	-2.13169900
H	1.54720800	-0.71472100	-2.44782100
H	4.42730200	0.23765000	-1.94765800
H	3.93724900	-1.41573000	-2.27529900
H	2.91657200	0.50226700	1.83034700
H	1.82543400	1.65567600	1.12114100
H	4.66357600	1.11741500	0.11926800
H	3.51175600	2.16847900	-0.68488900
H	2.68963800	-2.60436500	-0.50045700
H	2.33838300	-2.33172300	1.18563600
H	4.83954800	-1.21764300	-0.20827000
H	4.45866100	-1.06295200	1.49251900
H	-2.09676100	1.67638300	4.57899300
H	-0.62303500	0.73103900	4.50751100
H	-3.46135600	-0.45267400	4.49909800
H	-1.97328100	-1.39513200	4.42194000
H	3.47926900	0.95159200	-4.15175800
H	2.98891800	-0.69741000	-4.47555700
H	5.89508300	0.22310700	-4.06382600
H	5.40014600	-1.43788500	-4.39075500
H	4.90086700	-3.70215100	0.01960700
H	4.49075900	-3.56561000	1.71575200
H	6.96365500	-3.85845200	1.43398300
H	4.54539500	2.50532700	2.17301000
H	3.28814300	3.49394200	1.46323300
H	5.50212900	4.64642900	1.28747600
H	6.16070100	3.27895500	0.38318300
H	4.88463000	4.27119500	-0.32339000
H	2.70002200	6.84898000	0.23355100
H	7.03273800	-2.41162400	0.42474300
H	6.61889400	-2.27462200	2.13371800
H	-2.35499600	-0.46470300	5.87597500
H	-5.13001800	3.10557800	-0.03278700
H	-4.50047400	3.67055600	-1.56415500
H	-5.89344200	5.45107400	-0.48447900
H	-4.85429200	5.41713000	0.94224700
H	-4.21511100	5.98711300	-0.59940400
H	5.16227200	-0.18970000	-5.61616600
H	-0.43787300	-2.06921300	1.90560400
H	-0.73357300	-6.02080300	3.07839400
H	-0.17162100	-5.09813400	-1.09696300
H	-0.47322100	-6.82057700	0.74026400
C	-3.17199100	-1.43957300	0.29889400
C	-4.51318200	-1.59487900	-0.04152800
C	-4.92994800	-1.38898400	-1.35960500
C	-2.64732800	-0.89676600	-1.96120800
C	-3.98705000	-1.04533400	-2.33041700
H	-2.88892100	-1.61604300	1.33820600
H	-5.25578800	-1.88212700	0.69937300
O	-6.26822900	-1.55920200	-1.59979900
H	-1.92795700	-0.64379100	-2.74184600
H	-4.27950600	-0.90016700	-3.36629400
C	-6.70218400	-1.36074300	-2.92725400
H	-7.78021800	-1.52435600	-2.92691600
H	-6.49233700	-0.34102000	-3.27746600
H	-6.23102300	-2.06868000	-3.62230300

Decarbonylative transmetalation in the presence of Na_2CO3

$Ni[P(n\text{-}Bu)_3]_2(PyrCO)[Na_2CO_3](OPh)$, iso_1a

Ni	-0.33021400	-0.86931300	0.26652500
P	-2.34631400	-0.08344800	-0.02581400
P	0.85526400	1.13108800	0.06313000
C	0.07056100	2.63915200	0.81492600
C	-3.59382400	-1.22159500	-0.77055900
C	-2.91218300	0.19348400	1.70600000
C	-2.55936600	1.47730700	-0.99604800
C	2.56028700	1.13340100	0.74872100
C	1.09294700	1.43319000	-1.74379000
C	0.14840000	3.95328100	0.04876100
C	-0.69583300	5.04688700	0.69065200
C	-0.72292400	6.33013500	-0.11942700
C	3.22798300	2.47923200	1.00921500
C	2.28776000	2.25265200	-2.21381000
C	2.42140300	2.20303600	-3.72907700
C	-4.39911800	0.27437000	2.03293800
C	-3.54792500	2.52030700	-0.48884500
C	-4.91505800	-0.62872700	-1.24813600
C	3.64430100	2.95286200	-4.22491700
O	1.31467100	-1.91474200	0.56856400
C	-1.15442600	-2.55471400	0.54129300
C	-0.95633200	-3.54992400	-0.55702500
O	-1.68682700	-2.88661800	1.59274000
C	1.82922200	-1.88192800	1.78679100
C	3.11703800	-2.41694100	2.02834500
C	3.69983600	-2.32571100	3.28787700
C	3.03042000	-1.71569900	4.35187800
C	1.15098100	-1.29718000	2.88029300
C	1.74850900	-1.21160500	4.13356600
Na	2.41615400	-2.61850200	-1.3483710
O	4.52762200	-1.99760000	-0.97598700
C	4.24817700	-0.85051300	-1.57020400
O	4.98720000	0.17660200	-1.30531300
O	3.22029900	-0.77975300	-2.33796700
Na	5.66313500	-0.86053800	0.55141100
C	4.69190100	2.30036900	1.39211000
C	5.38758500	3.60706000	1.72703700
H	0.51218700	2.75026800	1.81395200
H	-0.98603100	2.40430400	1.00073300
H	1.19186000	4.28513500	-0.03335700
H	-0.19107700	3.79941500	-0.98796600
H	-0.32229600	5.24618700	1.70408200
H	-1.72158600	4.66949500	0.82427800
H	0.28285900	6.74549100	-0.24137900
H	-1.12410600	6.15418200	-1.12451400
H	3.15985000	0.56581700	0.02466400
H	2.53722700	0.55078700	1.67676700
H	3.17259400	3.11838100	0.11984400
H	2.70262200	3.02303800	1.80807100
H	0.15261300	1.82380200	-2.15616200
H	1.22569300	0.42482800	-2.15590400
H	2.21185400	3.29756900	-1.87741100
H	3.20335700	1.82015200	-1.78729600
H	-2.38445400	1.08511800	2.07149600
H	-2.47209500	-0.65484300	2.24935700
H	-4.88074700	1.09631100	1.48722600
H	-4.89959300	-0.64642400	1.70172300
H	-2.81518200	1.16691600	-2.01727300
H	-1.57475700	1.94602400	-1.08237100
H	-4.56669600	2.11174400	-0.46606600
H	-3.30685200	2.78232200	0.55356800

H	-3.77089600	-2.00822600	-0.02527300
H	-3.09395400	-1.72405900	-1.60952100
H	-5.40920400	-0.07995200	-0.43651800
H	-4.73070800	0.11194700	-2.03881500
H	1.51138400	2.60105400	-4.20270700
H	2.49446800	1.14616200	-4.01350800
H	3.60987500	4.01185500	-3.94317000
H	4.55562600	2.52773800	-3.79058800
H	-1.34336600	7.09769800	0.35205600
H	3.74226300	2.90528000	-5.31366500
H	3.65385100	-2.86359100	1.19325300
H	4.69161400	-2.74792200	3.44486400
H	3.49151500	-1.65129200	5.33294600
H	0.14861300	-0.89986200	2.71051700
H	1.20310000	-0.74505500	4.95107900
H	5.19344200	1.80477900	0.54946100
H	4.75412100	1.61237900	2.25119700
H	6.43835000	3.45629200	1.99153700
H	5.35999900	4.29566200	0.87582400
H	4.90462900	4.11277900	2.57045300
C	-0.52521300	-3.13362400	-1.81894900
N	-0.27537500	-3.95606700	-2.84197700
C	-0.48133900	-5.26303600	-2.62317500
C	-1.17850900	-4.91520400	-0.36051600
C	-0.93899500	-5.78672400	-1.41383700
H	-0.36657300	-2.06223000	-1.99467800
H	-0.26769800	-5.92422900	-3.46110300
H	-1.52308900	-5.25980600	0.61128500
H	-1.09067300	-6.85645700	-1.30710100
C	-5.86205500	-1.69890100	-1.77610500
C	-7.17599300	-1.12710700	-2.27665300
H	-6.05134700	-2.43208700	-0.98030000
H	-5.36319900	-2.25582100	-2.58042800
H	-7.84402600	-1.90903900	-2.64749100
H	-7.70453600	-0.59229700	-1.48043800
H	-7.01465500	-0.41643400	-3.09419700
C	-4.63903000	0.45852700	3.52654300
C	-6.11385400	0.51057100	3.88151200
H	-4.14016500	1.37901100	3.85914000
H	-4.14941000	-0.35919800	4.07180900
H	-6.26886700	0.64334400	4.95557600
H	-6.61654000	1.33874700	3.37055900
H	-6.62491000	-0.41192500	3.58596200
C	-3.51877800	3.78235300	-1.34222800
C	-4.39221200	4.89365600	-0.79033900
H	-3.82495200	3.53194300	-2.36671000
H	-2.47848200	4.13092700	-1.42249900
H	-4.35011000	5.79011600	-1.41501500
H	-5.44051000	4.58351800	-0.72595100
H	-4.07481000	5.18102200	0.21885100

Ni[P(n-Bu)$_3$]$_2$(PyrCO)[Na$_2$CO$_3$](OPh), iso_1b

Ni	-0.27639100	-0.80158400	-0.31134200
P	-2.16763600	0.30987100	-0.28733500
P	1.13250200	0.98458900	0.25442800
C	0.55468200	2.43891600	1.25097000
C	-3.63022200	-0.42000800	-1.14848100
C	-2.64369400	0.38925300	1.49797000
C	-2.10059500	2.04644600	-0.92175000
C	2.75201500	0.51994000	0.98555100
C	1.56298700	1.59173400	-1.43582700
C	0.94732100	3.83922700	0.79577000
C	0.21157500	4.92093600	1.57650900
C	0.46560200	6.31805200	1.04107500
C	3.62893800	1.62519800	1.56001700
C	2.89655200	2.29303100	-1.66234900
C	3.09727600	2.61433500	-3.13640900
C	-4.09151400	0.66177400	1.89136700
C	-2.90754800	3.13301900	-0.22084800
C	-4.80950000	0.49373600	-1.46225600
C	4.46783400	3.20368000	-3.41584100
O	1.19485700	-2.07722100	-0.13255600
C	-0.99088700	-2.21540300	-1.32653200
O	-0.54767800	-2.31211300	-2.47126600
C	-1.91543900	-3.24845300	-0.79093300
C	1.53904700	-2.49092500	1.07136400
C	2.66240700	-3.33934300	1.22440800
C	3.07250600	-3.75435600	2.48633000
C	2.38842300	-3.35354800	3.63759800
C	0.84752700	-2.10774100	2.24351600
C	1.27130800	-2.53095400	3.49944700
Na	1.97924000	-2.41319300	-2.2681830
O	4.15607500	-2.42819000	-1.62186900
C	4.17317000	-1.13938000	-1.90487100
O	5.02798100	-0.38225400	-1.29302100
O	3.31329700	-0.67102500	-2.73637200
Na	5.35264100	-1.99887000	0.19533700
C	5.00654500	1.08860700	1.92926800
C	5.89405600	2.12223700	2.59813600
H	0.87872500	2.26121900	2.28494600
H	-0.54139700	2.39156100	1.28517600
H	2.03181200	3.98456000	0.88472200
H	0.72199100	3.95483900	-0.27592800
H	0.49442100	4.86294500	2.63608100
H	-0.86727700	4.70268500	1.54838000
H	1.52836900	6.57709300	1.08972500
H	0.16118300	6.39869400	-0.00915300
H	3.29213600	0.00823800	0.17566900
H	2.55465300	-0.23001800	1.75999300
H	3.75068700	2.44089100	0.83741700
H	3.15341800	2.07085700	2.44663400
H	0.72484400	2.19749100	-1.80661500
H	1.58729300	0.67979400	-2.04816600
H	2.97116900	3.21388600	-1.06596700
H	3.70408000	1.61469400	-1.35257300
H	-1.97172000	1.11866500	1.96850700
H	-2.33807400	-0.57924800	1.91536500
H	-4.43477800	1.61910000	1.47833200
H	-4.74516200	-0.10836800	1.45789200
H	-2.36790400	1.99172100	-1.98489400
H	-1.04624800	2.33932200	-0.91187500
H	-3.98365300	2.92903800	-0.29323100
H	-2.67415600	3.13780700	0.85585700
H	-3.96140600	-1.27390300	-0.54189000
H	-3.24946600	-0.85788900	-2.08130000
H	-5.19454200	0.95358300	-0.54373900
H	-4.47852300	1.32740100	-2.09714900
H	2.30877000	3.29925200	-3.48338600
H	2.97956500	1.67617900	-3.69142800
H	4.63355400	4.12916100	-2.85132900
H	5.25276000	2.49711300	-3.12531900
H	-0.08654600	7.07694700	1.60283900
H	4.60692500	3.43585100	-4.47623200
H	3.19324800	-3.63469800	0.32073900

H	3.93413800	-4.41468200	2.57381900
H	2.71153100	-3.68834300	4.61866300
H	-0.01277500	-1.44253200	2.13735200
H	0.71928300	-2.21335000	4.38145400
H	5.47658300	0.72237100	1.00611500
H	4.88464700	0.21409700	2.58839400
H	6.88236400	1.71976500	2.83887100
H	6.04347300	2.99086400	1.94806800
H	5.45010500	2.48649600	3.53124500
C	-2.23592900	-3.28668900	0.56815000
N	-3.08892900	-4.15545300	1.11629000
C	-3.66080900	-5.03713300	0.28578200
C	-2.51290400	-4.19108300	-1.63286600
C	-3.40448900	-5.10080000	-1.08437700
H	-1.75300800	-2.57566300	1.24264200
H	-4.36537400	-5.73138400	0.74121000
H	-2.27239300	-4.18234600	-2.69294300
H	-3.90099900	-5.84616300	-1.69799300
C	-5.94050900	-0.25032300	-2.16053700
C	-7.11531900	0.65039300	-2.49604700
H	-6.27332800	-1.07835100	-1.51990900
H	-5.55254400	-0.71932900	-3.07471500
H	-7.91931900	0.10158400	-2.99333300
H	-7.53608500	1.10564300	-1.59308400
H	-6.81261000	1.46634800	-3.16091100
C	-2.60514000	4.51054100	-0.79894700
C	-3.31354400	5.63263600	-0.06280300
H	-2.87796800	4.52327500	-1.86241700
H	-1.51726200	4.67433600	-0.77161600
H	-3.07051600	6.61118000	-0.48607300
H	-4.40133600	5.51410300	-0.10533200
H	-3.02976000	5.65262500	0.99574500
C	-4.27143300	0.67561200	3.40421000
C	-5.70883700	0.92626600	3.82226900
H	-3.61567100	1.44430800	3.83540000
H	-3.92142600	-0.28026100	3.81648300
H	-5.81929000	0.93306800	4.90984900
H	-6.06930200	1.89046000	3.44810200
H	-6.37715300	0.15359000	3.42773100

Ni[P(n-Bu)$_3$]$_2$(PyrCO)[Na$_2$CO$_3$OPh], iso_3a

Ni	0.12947700	-0.24948100	-0.89960100
P	-1.94533500	-1.22011500	-0.27805300
P	-0.47075400	1.83002000	-0.50002300
C	1.93194700	0.27945800	-1.10777600
O	0.67561900	-1.91924300	-1.70089300
C	1.03128500	-2.85419700	-0.82513400
O	0.78347200	-2.68886200	0.41691400
O	1.67797000	-3.85388600	-1.29189600
Na	2.91907100	-3.64118000	0.64181900
Na	2.89857900	-2.14750000	-2.4835090
O	4.16307600	-2.26386400	-0.61466200
C	5.18413400	-1.55927400	-0.22257500
C	5.62202400	-1.54627100	1.13155100
C	6.70102700	-0.78018000	1.54974500
C	7.41360500	0.01407300	0.64743600
C	5.93139100	-0.74219200	-1.11733300
C	7.01287600	0.01882200	-0.68984400
C	-2.14234900	-2.87679200	-1.05871500
C	-1.87905800	-1.49720800	1.54873800
C	-3.57554000	-0.37945600	-0.56699100
C	0.79155300	3.17564400	-0.53475200
C	-1.70441600	2.31891900	-1.78972700
C	-1.28085700	1.99974700	1.15042700
C	-4.75370900	-0.67526200	0.35372100
C	-5.94627500	0.22393000	0.05123700
C	-3.51598800	-3.53322900	-1.10916700
C	-3.47686900	-4.86769700	-1.84322800
C	-1.49765300	3.36937000	1.78115200
C	-2.84941300	3.24439000	-1.39172600
C	0.33525300	4.59887200	-0.83482600
C	-4.83572300	-5.54009800	-1.92112600
C	-7.13937400	-0.05022600	0.94835100
O	2.53015000	0.32763800	-2.18208000
C	2.64104300	0.61924800	0.15940900
C	-2.55068600	-2.73985200	2.11734100
C	-2.32225700	-2.88142500	3.61653200
C	-2.97543400	-4.12229200	4.19811900
H	5.06674300	-2.14156900	1.85902200
H	6.99063000	-0.79689300	2.59980900
H	8.26070400	0.60905200	0.97713600
H	5.62273100	-0.71876500	-2.16279600
H	7.55215300	0.62970300	-1.41302500
H	-3.84754600	-0.57677500	-1.61371700
H	-3.38564700	0.69948500	-0.52743100
H	-5.05343700	-1.72821600	0.27668000
H	-4.45346800	-0.52508800	1.40100300
H	-1.42095700	-3.52309600	-0.54592100
H	-1.74260900	-2.76252500	-2.07338500
H	-3.90870200	-3.69428200	-0.09625500
H	-4.23712500	-2.86885300	-1.60763300
H	-0.66863300	1.38423000	1.82422700
H	-2.24039800	1.47045300	1.07668000
H	-0.52806800	3.85155200	1.96741300
H	-2.04028300	4.03356300	1.09678900
H	-2.10959200	1.38021500	-2.18585000
H	-1.12837100	2.75163500	-2.61770000
H	-3.32764800	2.87935200	-0.46971700
H	-2.46274300	4.24305000	-1.14731000
H	1.54071600	2.87488000	-1.27863900
H	1.31272800	3.13768600	0.43186900
H	-0.13609700	4.64056500	-1.82664700
H	-0.43431800	4.92375000	-0.12339900
H	-2.75863200	-5.52983300	-1.34119100
H	-3.07621500	-4.71063200	-2.85374400
H	-4.78861500	-6.49601000	-2.45027700
H	-5.23940000	-5.73638100	-0.92181100
H	-5.56157500	-4.90871900	-2.44540900
H	-6.23247600	0.10423000	-1.00318400
H	-5.63174500	1.27352400	0.15493800
H	-7.98125800	0.60965100	0.72169700
H	-7.48980300	-1.08184300	0.83689200
H	-6.88252300	0.09288700	2.00350700
H	-2.27545300	-0.59420100	2.03272600
H	-0.80807500	-1.53527200	1.77529600
H	-3.63066700	-2.72392400	1.91562500
H	-2.15961700	-3.63112700	1.60672800
H	-2.70250200	-1.98456800	4.12537400
H	-1.24176600	-2.89831200	3.81312900
H	-2.80123900	-4.20957000	5.27424700
H	-4.05933400	-4.11184100	4.03941700
H	-2.58767800	-5.03161200	3.72626700
C	2.10301300	0.25526200	1.39775300
N	2.63930800	0.58905900	2.57596000

C	3.75956200	1.32684000	2.53575000
C	3.82898900	1.35632900	0.14767500
C	4.39224600	1.72650400	1.36085600
H	1.20234100	-0.36629500	1.41454900
H	4.17624300	1.60948600	3.50219500
H	4.27274800	1.63401400	-0.80440000
H	5.31289500	2.30021900	1.40130600
C	1.49765700	5.58375700	-0.79569100
C	1.07715600	7.00334400	-1.12961400
H	2.27623100	5.24766500	-1.49371500
H	1.95902400	5.55213500	0.20072400
H	1.92212800	7.69639100	-1.09610500
H	0.64211600	7.06226100	-2.13310500
H	0.32200100	7.36999200	-0.42608100
C	-3.90868200	3.35178700	-2.48069900
C	-5.06284100	4.25702300	-2.09025800
H	-4.28444000	2.34370400	-2.70880100
H	-3.44219500	3.71193200	-3.40726400
H	-5.81567200	4.32048200	-2.88041400
H	-5.56298700	3.89166600	-1.18648100
H	-4.71637200	5.27470400	-1.88112400
C	-2.27296500	3.25968400	3.08836600
C	-2.47930000	4.60081600	3.76804100
H	-1.74610600	2.57162100	3.76332800
H	-3.24509400	2.78766800	2.88260700
H	-3.04427800	4.50280300	4.69892200
H	-1.52119100	5.07209000	4.01162300
H	-3.02743900	5.29358400	3.12047300

Ni[P(n-Bu)$_3$]$_2$(PyrCO)[Na$_2$CO$_3$OPh], iso_3b

Ni	0.21266300	-0.18031800	-0.18821400
P	-1.88689100	-1.25411400	-0.21119300
P	-0.52739000	1.85044600	0.09639700
C	1.96737700	0.42178100	0.15304100
O	1.10846600	-1.77381200	-0.92068800
C	1.15808800	-2.71084900	0.01911200
O	0.61471700	-2.49274700	1.15356800
O	1.82167000	-3.77234100	-0.25181200
Na	2.70698900	-3.43005800	1.87038900
Na	3.39594200	-2.46645700	-1.3002090
O	4.37393100	-2.47889000	0.72944600
C	5.31462000	-1.59602900	0.91078700
C	5.36085900	-0.75528900	2.05808400
C	6.33337700	0.22375600	2.20806000
C	7.32386900	0.41465000	1.23893700
C	6.35133700	-1.39766400	-0.04400500
C	7.32276000	-0.41616900	0.11759400
C	-1.78306500	-2.89063400	-1.05477400
C	-2.37922900	-1.59956800	1.53689600
C	-3.37772100	-0.44124600	-0.96364200
C	0.66192800	3.20628400	0.48606000
C	-1.34128000	2.39652000	-1.47444200
C	-1.79111200	1.93225100	1.44126900
C	-4.77101700	-0.79085800	-0.45446200
C	-5.84021900	0.10487600	-1.06803600
C	-3.05384500	-3.58155500	-1.53306200
C	-2.75325100	-4.89484900	-2.24465600
C	-2.22694300	3.25657600	2.05451500
C	-2.58628300	3.27432900	-1.39382400
C	0.25476000	4.63913500	0.16137700
C	-4.00363200	-5.59258400	-2.74888800
C	-7.24093000	-0.22475300	-0.58552300
C	2.85534100	0.69933300	-1.01792100
O	2.39168100	0.50230200	1.29586100
C	-3.17432100	-2.86357800	1.83553300
C	-3.45235500	-3.02673600	3.32433700
C	-4.23064000	-4.29014100	3.64505500
H	4.57765300	-0.86980800	2.80554200
H	6.31864200	0.85606800	3.09457100
H	8.08289100	1.18158900	1.36307000
H	6.36325000	-2.03893000	-0.92689700
H	8.08992900	-0.29472300	-0.64635000
H	-3.31264500	-0.60874600	-2.04833500
H	-3.23842400	0.64016800	-0.84158700
H	-5.00444000	-1.84374200	-0.65844300
H	-4.80599000	-0.68316400	0.63952600
H	-1.22335100	-3.53878900	-0.36920200
H	-1.10552900	-2.73113800	-1.90246400
H	-3.73370200	-3.77810100	-0.69318400
H	-3.60714800	-2.92289000	-2.21816700
H	-1.38805500	1.28465200	2.23133200
H	-2.67129200	1.39707500	1.06076300
H	-1.36486800	3.75747200	2.51613900
H	-2.60018800	3.94219100	1.28324700
H	-1.57708200	1.47591200	-2.02255700
H	-0.55860300	2.88846200	-2.06723300
H	-3.30144100	2.85164900	-0.67072600
H	-2.32871300	4.26978500	-1.00654900
H	1.58679500	2.96775700	-0.05448900
H	0.91783600	3.10030600	1.54874100
H	0.09877200	4.74264900	-0.92176000
H	-0.70719900	4.89076500	0.62438000
H	-2.20460500	-5.55566100	-1.56010800
H	-2.06761300	-4.70174000	-3.08078200
H	-3.76971800	-6.53132600	-3.25887900
H	-4.68735000	-5.82696400	-1.92558800
H	-4.55278300	-4.96117700	-3.45612600
H	-5.79154500	0.03068500	-2.16342300
H	-5.59977300	1.15249200	-0.83179900
H	-7.99110100	0.43630500	-1.02801600
H	-7.51634500	-1.25361700	-0.84024900
H	-7.31747200	-0.12871200	0.50286200
H	-2.92556100	-0.71826300	1.90009600
H	-1.43030500	-1.62705200	2.08292900
H	-4.12720000	-2.85955400	1.28898200
H	-2.62123000	-3.74189800	1.47323800
H	-4.00261800	-2.14639200	3.68530800
H	-2.49841500	-3.02393700	3.86863000
H	-4.42284100	-4.39100500	4.71696100
H	-5.19947600	-4.29923700	3.13383300
H	-3.68529100	-5.18342100	3.32209500
C	2.33800800	0.66320000	-2.31809100
N	3.04853300	0.91476100	-3.42013500
C	4.34498900	1.21781700	-3.23847300
C	4.20836600	1.01622200	-0.85653900
C	4.96474700	1.27828400	-1.99303600
H	1.28301800	0.40603700	-2.45011400
H	4.91517900	1.42193100	-4.14408000
H	4.64258700	1.03913100	0.14144900
H	6.02145100	1.51668000	-1.91370800
C	1.30437300	5.64792700	0.61076800
C	0.93729200	7.07672200	0.25307400
H	2.27188200	5.38501500	0.16252300
H	1.44605300	5.55680800	1.69622800

H	1.69709000	7.78836900	0.58722400
H	0.82526200	7.19795000	-0.82969500
H	-0.01307000	7.36896800	0.71275200
C	-3.28084700	3.40985900	-2.74252500
C	-4.53367800	4.26399500	-2.67600000
H	-3.53092200	2.40493400	-3.11265000
H	-2.57591800	3.82824100	-3.47318900
H	-5.02316000	4.34544600	-3.65019100
H	-5.26226600	3.84275700	-1.97452200
H	-4.30491700	5.27959400	-2.33582600
C	-3.31542100	3.04695100	3.10052400
C	-3.76811800	4.34082100	3.75185400
H	-2.95061400	2.34713700	3.86457000
H	-4.17053300	2.54550100	2.62357900
H	-4.55284600	4.17081600	4.49382800
H	-2.93657800	4.84041000	4.25998100
H	-4.16270900	5.04170800	3.00856000

Ni[P(n-Bu)$_3$]$_2$(PyrCO)[NaCO$_3$], iso_3a

Ni	-0.36589100	-1.12021800	-0.50636400
P	1.72393200	-0.13950000	-0.01017900
P	-1.54814800	0.70059400	-0.36872100
C	-1.88325600	-2.10241400	-1.01789100
O	0.34560300	-2.93653400	-0.30909200
C	1.15754200	-3.13454800	-1.38175700
O	1.37739400	-2.14358400	-2.13275000
O	1.62226600	-4.31153700	-1.50606000
Na	0.25874000	-5.13038500	0.04560300
C	2.91563700	-1.43383700	0.54196300
C	2.47518300	0.64160400	-1.50933300
C	1.82683900	1.16881300	1.30632500
C	-3.28026000	0.71821300	-1.00875300
C	-1.72011800	1.13436900	1.42558200
C	-0.72302000	2.13158000	-1.19919100
C	2.94828600	2.20134800	1.28430700
C	2.73630500	3.28490900	2.33408000
C	4.13789500	-1.03458400	1.35583300
C	-1.46896200	3.42303100	-1.50935300
C	-0.52968200	4.47124200	-2.09433400
C	-1.70938300	2.60302500	1.83427000
C	-1.60702100	2.77979800	3.34373200
C	-4.24887200	1.75573700	-0.45243800
C	-5.63189700	1.64248700	-1.08189400
C	-6.61844400	2.64930100	-0.51854400
C	-1.23134500	5.77292100	-2.43578400
C	3.84701000	4.31917000	2.35952100
C	-1.56669200	4.23745300	3.76465200
C	-2.60748600	-2.84662200	0.06792700
O	-2.25545100	-2.20997400	-2.17738200
C	3.99115800	0.61238700	-1.65590900
H	1.81032700	0.64374200	2.27261000
H	0.87386100	1.71160300	1.27402000
H	3.92336400	1.72050000	1.43765900
H	3.00112200	2.67383700	0.29236900
H	3.20928700	-1.96214200	-0.37292000
H	2.30927000	-2.15869100	1.09955900
H	4.75659800	-0.31831400	0.79951000
H	3.83074200	-0.51368500	2.27433200
H	-0.32108100	1.71268500	-2.13096700
H	0.16226700	2.35947100	-0.59046200
H	-2.28657900	3.22534600	-2.21644600
H	-1.94005100	3.83082500	-0.60603200
H	-0.90459500	0.60758300	1.93629600
H	-2.63795800	0.64240800	1.77530500
H	-0.85945100	3.11972900	1.36194800
H	-2.60822000	3.11209300	1.46001000
H	-3.68800500	-0.28315900	-0.82328800
H	-3.20570700	0.79660200	-2.10145300
H	-4.33967800	1.63083800	0.63589500
H	-3.86774100	2.77302100	-0.60378800
H	-6.01101500	0.62196600	-0.93543900
H	-5.54246400	1.77210900	-2.16884900
H	-7.60567800	2.55402100	-0.97870100
H	-6.74409000	2.51974000	0.56182000
H	-6.27518000	3.67621400	-0.68435300
H	-0.04128200	4.05992700	-2.98829200
H	0.28077400	4.65718700	-1.37391100
H	-0.53950500	6.51261500	-2.84740700
H	-2.02266700	5.61390400	-3.17590600
H	-1.69928700	6.21518600	-1.54961000
H	2.63611800	2.81580500	3.32299100
H	1.77063400	3.77697600	2.14239100
H	3.66870600	5.09225100	3.11201600
H	4.81389800	3.85650800	2.58469500
H	3.94557700	4.81900300	1.38984500
H	-0.70405300	2.26181400	3.69829200
H	-2.45052300	2.26936800	3.82766400
H	-1.48627700	4.34616900	4.84952100
H	-0.71072800	4.75450900	3.31681200
H	-2.46977300	4.76861700	3.44551200
H	2.11202100	1.67716700	-1.56020800
H	2.01911200	0.10116400	-2.34559400
H	4.47208000	1.16804000	-0.83829500
H	4.34804900	-0.42359200	-1.56826900
C	-2.10673500	-2.90773600	1.37301500
N	-2.71610900	-3.53464200	2.38467300
C	-3.89826100	-4.10927300	2.11278300
C	-3.83621100	-3.46003700	-0.18695100
C	-4.49921400	-4.09516600	0.85615300
H	-1.14843500	-2.42773200	1.58679800
H	-4.39020400	-4.60439800	2.94918800
H	-4.24361800	-3.42126000	-1.19492400
H	-5.46274900	-4.57332500	0.70607500
C	4.99246500	-2.23923700	1.73101000
C	6.21137700	-1.86457600	2.55463800
H	5.30344100	-2.75607700	0.81308600
H	4.37385800	-2.96139200	2.28173200
H	6.81473000	-2.73889800	2.81439200
H	6.85795700	-1.16840000	2.00948900
H	5.92260900	-1.37312300	3.49038000
C	4.45210700	1.18749900	-2.98885600
C	5.96015200	1.14420400	-3.15841300
H	4.09456000	2.22307400	-3.07768700
H	3.96652400	0.63413100	-3.80337100
H	6.27650700	1.56140200	-4.11859400
H	6.46516600	1.71236400	-2.36940500
H	6.33317900	0.11574900	-3.10675000

Ni[P(n-Bu)$_3$]$_2$(PyrCO)[NaCO$_3$], iso_3b

Ni	0.17409100	-1.18831800	-0.76989600
P	-1.79507600	-0.01571500	-0.23039600
P	1.55042800	0.49554000	-0.45988000
C	1.58793300	-2.43762600	-0.90032600
O	-0.88963000	-2.62144100	-1.46579300

C	-1.29146600	-3.44052300	-0.45253900
O	-1.41560600	-2.94179000	0.70001500
O	-1.47673400	-4.65118100	-0.79477600
Na	-0.07445500	-4.38780400	-2.5481600
C	-3.26247800	-0.87757300	-0.93173200
C	-1.97993300	-0.03899500	1.60778000
C	-2.03776600	1.76671500	-0.69232000
C	3.37213600	0.18606800	-0.46588800
C	1.27947500	1.69196500	-1.84643200
C	1.24208900	1.39594900	1.12376700
C	-2.97487100	2.64842500	0.12460200
C	-2.93427300	4.09829500	-0.34321700
C	-4.58788600	-0.13960600	-1.05363500
C	2.27480900	2.36427900	1.68640900
C	1.78577600	3.01171500	2.97624800
C	1.40479900	3.18545100	-1.56452600
C	0.92088600	4.03158600	-2.73472700
C	4.30420400	1.32597900	-0.86188500
C	5.76851800	0.91041700	-0.79693000
C	6.71486800	2.02342500	-1.20899600
C	2.79267000	3.97911700	3.57115000
C	-3.85450800	5.00640900	0.45188300
C	1.00878800	5.52160400	-2.45958700
O	1.92444400	-3.05416500	-1.91506800
C	2.27735000	-2.75004500	0.39198700
C	-3.38445500	-0.15487300	2.18399300
H	-2.32978000	1.77919600	-1.75238100
H	-1.04412200	2.23155500	-0.67269100
H	-4.00516800	2.27389600	0.07605800
H	-2.69176200	2.60825100	1.18647700
H	-3.36365200	-1.78802400	-0.33001800
H	-2.93604200	-1.23300900	-1.91571500
H	-4.93946500	0.19796000	-0.06972100
H	-4.46361900	0.77200800	-1.65686800
H	1.04945500	0.60561800	1.86238100
H	0.27872100	1.90964900	1.00151400
H	3.21837900	1.83471100	1.87889600
H	2.51039200	3.14934700	0.95646200
H	0.27751300	1.47605200	-2.23600900
H	1.96732300	1.39217400	-2.64764800
H	0.82019500	3.45321100	-0.67064500
H	2.44547800	3.44250800	-1.32426500
H	3.53676600	-0.66196800	-1.14362300
H	3.62967500	-0.18900500	0.53474500
H	4.06911700	1.66276100	-1.88141600
H	4.15148100	2.20034200	-0.21731000
H	5.92147300	0.03026700	-1.43593400
H	6.00032000	0.57907700	0.22457700
H	7.76070500	1.70927800	-1.15612100
H	6.52000600	2.34950600	-2.23633300
H	6.60087400	2.90032500	-0.56268200
H	1.54295400	2.22557800	3.70372700
H	0.83834400	3.53192000	2.77439800
H	2.42250400	4.43415100	4.49375200
H	3.73536900	3.47438400	3.80791400
H	3.02386900	4.79042900	2.87252700
H	-3.19406000	4.14027900	-1.41036400
H	-1.89804900	4.46329700	-0.27809500
H	-3.80902600	6.04163200	0.10255500
H	-4.89653700	4.67809100	0.37597600
H	-3.59082100	5.00459400	1.51489300
H	-0.11808800	3.75454800	-2.96518400
H	1.50200700	3.77690300	-3.63113900
H	0.65985400	6.11354200	-3.30987000
H	0.39995800	5.79925000	-1.59204500
H	2.03869100	5.82637100	-2.24538300
H	-1.48381000	0.86009800	1.99859100
H	-1.38723200	-0.90210100	1.92872800
H	-4.00246400	0.69899000	1.87236000
H	-3.87268300	-1.05039100	1.77553000
C	1.72476800	-2.36400100	1.61910500
N	2.33440400	-2.52717100	2.79739800
C	3.54431500	-3.10292500	2.77604800
C	3.52395100	-3.38038200	0.40335900
C	4.17275700	-3.55740900	1.61732500
H	0.72047200	-1.93176200	1.63137600
H	4.03772000	-3.20785600	3.74165400
H	3.96261500	-3.69749000	-0.54010400
H	5.15014600	-4.02731800	1.67452200
C	-5.66280600	-1.01165900	-1.69137800
C	-6.98953200	-0.29200500	-1.85341900
H	-5.79671100	-1.91532600	-1.08209500
H	-5.30550900	-1.36491400	-2.66831400
H	-7.74836000	-0.93230500	-2.31198700
H	-7.38087500	0.04178600	-0.88627600
H	-6.88359400	0.59744200	-2.48436500
C	-3.37780900	-0.23968600	3.70467600
C	-4.77143500	-0.37149600	4.29218400
H	-2.88172900	0.65204900	4.11336600
H	-2.75857700	-1.09274600	4.01169700
H	-4.75087200	-0.43061800	5.38399000
H	-5.39996300	0.48348800	4.01962500
H	-5.27148500	-1.27305900	3.92259700

Ni[P(n-Bu)$_3$](PyrCO)[Na$_2$CO$_3$OPh], iso1

Ni	0.66633900	1.31838800	-0.39284600
P	-0.76788200	-0.31610900	-0.27301300
C	-0.09934400	2.31323400	0.97255800
O	2.17745800	2.48078500	-0.81008800
C	2.60887600	1.61456600	-1.70376400
O	1.80179300	0.60371600	-1.90695300
O	3.74589200	1.70608100	-2.23161700
Na	3.79365100	-0.67343000	-1.8780490
Na	4.36031900	2.21667000	0.08056200
O	4.32872900	-0.02897600	0.20815000
C	3.51836500	-0.69784800	0.98469200
C	3.56320900	-2.11800100	1.08093900
C	2.68862700	-2.82655500	1.90092300
C	1.72093500	-2.16753900	2.66089900
C	2.51871400	-0.05463600	1.76847300
C	1.65399400	-0.77277400	2.58380300
C	-1.66381400	-0.59323300	1.31086700
C	-2.05621000	-0.21861600	-1.59255500
C	0.19031900	-1.84821700	-0.62430100
C	-0.34867600	-3.18721900	-0.13971000
C	0.56419500	-4.33705900	-0.54619600
C	-2.66156800	-1.51334300	-2.12358800
C	-3.69184500	-1.25748600	-3.21630600
C	-2.94779900	-1.41291700	1.30396800
C	-3.54905100	-1.54333000	2.69764600
C	-4.83529000	-2.34915300	2.70865100
C	0.18314400	-5.65159600	0.10910600
C	-4.28213300	-2.53834000	-3.77791800
C	-1.37558300	3.04841900	0.68244400

O	0.41752700	2.42646200	2.07915800
H	4.32696000	-2.64680800	0.50913500
H	2.76518600	-3.91244900	1.94741700
H	1.04150100	-2.72488900	3.30139300
H	2.41604700	1.02885700	1.71983400
H	0.91050300	-0.22532000	3.16187600
H	1.18052200	-1.67955100	-0.18009600
H	0.34720800	-1.85340900	-1.71179300
H	-0.43174000	-3.16345700	0.95649000
H	-1.36075700	-3.37258300	-0.52351200
H	-1.58183900	0.32270800	-2.42182600
H	-2.84092700	0.45346100	-1.21787100
H	-1.86444100	-2.15727100	-2.52181100
H	-3.12939700	-2.08519700	-1.31241400
H	-1.87327400	0.40342300	1.72141700
H	-0.92479100	-1.03802500	1.99088200
H	-3.68581600	-0.94900800	0.63393600
H	-2.76149300	-2.41592500	0.89931800
H	-3.72991900	-0.54054000	3.10787200
H	-2.80845800	-2.00716000	3.36365600
H	-5.25264600	-2.43786400	3.71533600
H	-5.59891100	-1.88570000	2.07466600
H	-4.67069300	-3.36337900	2.32900500
H	1.59679500	-4.07340700	-0.27999200
H	0.54889300	-4.43871200	-1.64059700
H	0.83373900	-6.47179500	-0.20742400
H	0.25295600	-5.57652200	1.20041400
H	-0.84714900	-5.93607600	-0.13133300
H	-3.22558100	-0.67384800	-4.02140800
H	-4.49085500	-0.62080800	-2.81309100
H	-5.02084200	-2.33851200	-4.55878400
H	-3.50469500	-3.17482400	-4.21412500
H	-4.77862300	-3.12234200	-2.99551200
C	-1.90414000	3.10602600	-0.60945800
N	-3.04476600	3.72264400	-0.93254600
C	-3.70784300	4.31773100	0.06751800
C	-2.08159400	3.69148100	1.70343900
C	-3.27075200	4.33433000	1.39206600
H	-1.35720400	2.62221200	-1.42305600
H	-4.64064600	4.80959700	-0.20611500
H	-1.68240800	3.66575300	2.71466400
H	-3.85635600	4.83987200	2.15416300

Ni[P(n-Bu)$_3$](PyrCO)[Na$_2$CO$_3$OPh], iso2

Ni	0.90631000	0.79214700	-1.43494800
P	-1.12153200	0.62069400	-0.69538700
C	1.13545600	2.38280800	-0.50070300
O	2.78659500	0.51835600	-1.91131900
C	2.46771900	-0.62058300	-2.48403600
O	1.18172500	-0.81641400	-2.62392500
O	3.33441800	-1.49282500	-2.75954000
Na	1.78117800	-3.05146600	-2.0953900
Na	4.05824300	-1.01263400	-0.4656480
O	2.29463100	-2.32799900	-0.00231900
C	1.37563800	-2.47404200	0.91261600
C	0.15759000	-3.16891400	0.66103500
C	-0.81230400	-3.34518200	1.64272400
C	-0.63702300	-2.82522900	2.92543900
C	1.52262400	-1.95512400	2.23109800
C	0.54315700	-2.12754300	3.20016000
C	-1.13554100	0.45537800	1.13660000
C	-2.23098700	2.02998200	-1.10992800
C	-1.91166900	-0.91017100	-1.34645100
C	-3.00376600	-1.57543100	-0.51877000
C	-3.40597400	-2.92920300	-1.08834000
C	-3.73269900	1.77263700	-1.14896400
C	-4.52155300	3.02687400	-1.50239200
C	-2.40931800	0.79884800	1.90041300
C	-2.24224600	0.59146600	3.40000000
C	-3.48289700	0.96833100	4.18887200
C	-4.49760100	-3.60609100	-0.27929200
C	-6.01738600	2.77887100	-1.57555300
O	0.62115200	3.45949600	-0.77900100
C	2.19636200	2.30579700	0.55673600
H	-0.01708400	-3.59403000	-0.32927900
H	-1.71843100	-3.89909500	1.39821700
H	-1.39435600	-2.96402100	3.69150600
H	2.43636900	-1.41125900	2.46742300
H	0.70000900	-1.70724400	4.19263200
H	-1.07748700	-1.61125100	-1.47674700
H	-2.26177800	-0.68174700	-2.36211700
H	-2.64368800	-1.72384400	0.50883000
H	-3.88735300	-0.92707000	-0.44594700
H	-1.89240400	2.40657600	-2.08268700
H	-1.98575800	2.82962700	-0.40005700
H	-3.95652700	0.98672100	-1.88441600
H	-4.08520300	1.38583200	-0.18383600
H	-0.31502300	1.08639400	1.50374700
H	-0.81797300	-0.57607300	1.34668200
H	-2.69284300	1.84316100	1.70358300
H	-3.24960000	0.18864500	1.54437900
H	-1.38007700	1.17629300	3.74981800
H	-1.97778600	-0.45920800	3.58048900
H	-3.34741600	0.81037900	5.26246900
H	-3.74355100	2.02212300	4.04101100
H	-4.34803600	0.37391700	3.87536900
H	-2.51358800	-3.57158300	-1.12519100
H	-3.72995100	-2.80884600	-2.13128100
H	-4.75873700	-4.58742700	-0.68512000
H	-4.18651500	-3.75027300	0.76158900
H	-5.41080400	-3.00182700	-0.26232400
H	-4.15875000	3.42226100	-2.46056700
H	-4.30587500	3.80646900	-0.75936800
H	-6.56976000	3.68802200	-1.82826700
H	-6.25754600	2.02580700	-2.33392400
H	-6.40599000	2.41175300	-0.61956500
C	2.61107900	1.06925400	1.05561100
N	3.63059100	0.89956500	1.90356200
C	4.26064800	2.01122800	2.31511200
C	2.84947900	3.44800400	1.02278900
C	3.89595300	3.29790200	1.92414900
H	2.08430400	0.16406900	0.73477300
H	5.09881600	1.86071300	2.99363600
H	2.53450200	4.42246200	0.65781600
H	4.43781900	4.15708200	2.30785800

TS(decarb.)
Ni[P(n-Bu)$_3$](PyrCO)[Na$_2$CO$_3$OPh],

Ni	-0.06053300	0.93686500	-0.21398500
P	-2.19790500	0.39364300	-0.03003500
C	0.07131100	2.44183700	0.56074900
C	1.67421600	1.94271700	-0.12243900
O	0.43762000	-0.26168700	-1.76915300
C	0.56815900	-1.35512800	-1.05700100

O	0.28886400	-1.26005300	0.21159900
O	1.02974100	-2.41763600	-1.57609200
Na	1.94030600	-2.87838000	0.47121200
Na	2.82653300	-0.89331800	-2.1952120
O	3.71238600	-1.76272300	-0.32820100
C	4.77831600	-1.30221900	0.26282800
C	4.89858600	-1.25458600	1.67973200
C	6.00631300	-0.69498800	2.30438000
C	7.06142800	-0.16272200	1.55884700
C	5.88381000	-0.78484100	-0.46762700
C	6.98559500	-0.22427500	0.16524200
C	-2.63732400	-0.93105100	-1.22243500
C	-2.45371100	-0.28180900	1.66023100
C	-3.42163300	1.75156500	-0.24468300
C	-4.79373700	1.60238000	0.40490500
C	-5.70166700	2.79029000	0.11417700
C	-4.10409400	-1.17806800	-1.55056700
C	-4.27860200	-2.29879800	-2.56798700
C	-5.73362100	-2.55261100	-2.91824700
C	-7.06040100	2.66661500	0.77974100
C	2.06425800	2.49409100	-1.34919000
N	3.33919000	2.65083400	-1.72220100
C	4.27862800	2.29465100	-0.83221800
C	2.67250700	1.57839900	0.78508400
C	4.00232800	1.77028000	0.42811400
C	-3.57693700	-1.28748800	1.88602400
C	-3.63679100	-1.75848900	3.33349700
C	-4.72473100	-2.78959600	3.57347200
H	4.07021200	-1.63821400	2.27751400
H	6.04565000	-0.66454500	3.39223700
H	7.92372300	0.27795900	2.05051600
H	5.83522500	-0.81271800	-1.55720600
H	7.79924900	0.17654700	-0.43790000
H	-3.52173400	1.90813700	-1.32727600
H	-2.93561500	2.65837400	0.13713400
H	-5.28473700	0.68120300	0.06580900
H	-4.67663800	1.49605700	1.49264300
H	-2.15850100	-1.83885600	-0.83221300
H	-2.08122600	-0.68996400	-2.13621400
H	-4.67040200	-1.42599800	-0.64303800
H	-4.55850400	-0.25823200	-1.94634700
H	-3.82235700	-3.21600700	-2.17174000
H	-3.70992700	-2.05310900	-3.47458000
H	-5.84199500	-3.35877900	-3.64885300
H	-6.31247900	-2.83152300	-2.03119700
H	-6.20146500	-1.65768000	-3.34272000
H	-5.82411300	2.89005400	-0.97288600
H	-5.20453500	3.71272700	0.44310200
H	-7.70083700	3.52487000	0.55971900
H	-7.58669600	1.76710200	0.44259900
H	-6.96363600	2.59756600	1.86849400
H	1.30849800	2.80182800	-2.07153600
H	5.31205100	2.42774600	-1.14976500
H	2.41531100	1.14182000	1.74799500
H	4.81487200	1.48231200	1.09036100
H	-2.56687300	0.58442200	2.32625300
H	-1.49295700	-0.74222500	1.91633100
H	-4.54849800	-0.85992300	1.60534300
H	-3.42925800	-2.15582500	1.22827200
H	-3.79341000	-0.88924400	3.98671600
H	-2.65912800	-2.17059600	3.61803700
H	-4.75609400	-3.11259700	4.61754500
H	-5.71286500	-2.38946900	3.32199600
H	-4.56875400	-3.68109600	2.95661600
O	-0.09621600	3.48421400	1.09584200

Ni[P(n-Bu)$_3$](Pyr)(CO)[Na$_2$CO$_3$OPh], trans O

Ni	-0.00149000	1.17534000	-0.15513800
P	-2.19324400	0.44198300	-0.00451900
C	-0.22265200	2.45048700	0.98328900
C	1.82632100	1.79891400	-0.31209900
O	0.38099500	0.02841800	-1.67203900
C	0.51767300	-1.15638900	-1.09400200
O	0.26454600	-1.23584300	0.16583100
O	0.95868400	-2.12324400	-1.78845600
Na	1.90084000	-2.90358800	0.15991300
Na	2.79122600	-0.62035100	-2.2344360
O	3.69596300	-1.74134100	-0.52301900
C	4.70107800	-1.36322200	0.21787200
C	4.61417500	-1.30595000	1.63693800
C	5.66711200	-0.85016800	2.42057300
C	6.86879900	-0.43722500	1.84007000
C	5.94382500	-0.95860500	-0.34126600
C	6.99120000	-0.50509700	0.44992800
C	-2.57307500	-0.83454400	-1.26755200
C	-2.40350300	-0.33218100	1.64868300
C	-3.50118600	1.73425200	-0.14143200
C	-4.86049400	1.46876300	0.49782900
C	-5.83575800	2.61662100	0.27265300
C	-4.02832200	-1.10452200	-1.62750100
C	-4.15563800	-2.16858600	-2.71056300
C	-5.59769700	-2.44280900	-3.09716500
C	-7.18364100	2.37855400	0.92946300
C	2.22261400	2.43518500	-1.49227400
N	3.49680500	2.73951400	-1.78925600
C	4.42929400	2.42395500	-0.87796200
C	2.81490200	1.48897300	0.61894400
C	4.14393800	1.80201900	0.33236600
C	-3.46457400	-1.41507900	1.80665500
C	-3.48063100	-2.00467800	3.21121400
C	-4.51620500	-3.10245300	3.37488200
H	3.67049700	-1.59208000	2.10602500
H	5.54768600	-0.80884400	3.50233800
H	7.69057900	-0.08173400	2.45492000
H	6.05144500	-0.99556600	-1.42537700
H	7.92062200	-0.19372700	-0.02510900
H	-3.61470600	1.94538800	-1.21344400
H	-3.07642000	2.65038200	0.28865100
H	-5.29815100	0.54177700	0.10664200
H	-4.73360400	1.30692300	1.57766500
H	-2.08033100	-1.74829300	-0.91278100
H	-2.00955100	-0.53587100	-2.15987100
H	-4.59321900	-1.42275800	-0.74108000
H	-4.50933400	-0.17857600	-1.97399600
H	-3.67774400	-3.09379200	-2.36145800
H	-3.58233400	-1.85398800	-3.59256800
H	-5.67215500	-3.21020500	-3.87228600
H	-6.18097800	-2.78603100	-2.23595000
H	-6.08460400	-1.53919200	-3.47975500
H	-5.96679600	2.76791100	-0.80748200
H	-5.39200100	3.54716800	0.65132100
H	-7.87405300	3.20791200	0.75421900
H	-7.65643400	1.46855100	0.54475700
H	-7.08085500	2.25794200	2.01315400

H	1.48644000	2.69101400	-2.25483200
H	5.45768300	2.67135200	-1.13954100
H	2.57118300	0.97746000	1.54876800
H	4.94321700	1.53348700	1.01995400
H	-2.57444600	0.48861800	2.35929200
H	-1.41683900	-0.74650400	1.88261600
H	-4.46151400	-1.02127200	1.56791800
H	-3.27729700	-2.21955400	1.08137200
H	-3.66714600	-1.20137800	3.93681200
H	-2.48082500	-2.39246400	3.44881700
H	-4.51514100	-3.51597900	4.38707700
H	-5.52570600	-2.72893100	3.17219400
H	-4.33071900	-3.92886800	2.68037900
O	-0.38290700	3.33324700	1.71637700

Ni[P(n-Bu)$_3$](Pyr)(CO)[Na$_2$CO$_3$OPh], trans N

Ni	-0.16850300	-1.50174900	-0.42224200
C	-0.82495600	-3.13044700	0.11892300
P	-1.95913200	-0.29571300	0.05977600
C	0.63481500	0.12298700	-1.04079000
O	1.41175900	-2.36923100	-1.14419400
C	2.12544200	-2.84296400	-0.12348800
O	1.65975900	-2.74631300	1.06288000
O	3.28648000	-3.28719100	-0.40057900
Na	3.93960500	-2.42019900	1.62395000
Na	3.52226200	-1.18555700	-1.5578500
O	4.47382200	-0.63306800	0.40724400
C	4.71245200	0.62015700	0.67255500
C	4.26560100	1.23934700	1.87322500
C	4.46656000	2.59184000	2.11883700
C	5.13183300	3.40122000	1.19411400
C	5.40855300	1.46352600	-0.23763700
C	5.60501100	2.81470600	0.01789800
C	-1.70827400	1.21708500	1.07350600
C	-2.69196500	0.22869900	-1.54473500
C	-3.24425000	-1.27125300	0.95234700
C	-4.38447900	-0.53473400	1.64717900
C	-5.36386200	-1.49695600	2.30763400
C	-4.18681300	0.51608000	-1.62326600
C	-4.60883600	0.92826600	-3.02791300
C	-2.68083700	2.37595100	0.87620200
C	-2.31759000	3.57267300	1.74608500
C	-3.25677000	4.74799200	1.54530500
C	-6.48976600	-0.77981700	3.03040200
C	-6.09832300	1.19947600	-3.13640700
C	0.62247700	0.47155000	-2.39722800
N	1.30895000	1.49701100	-2.92907600
C	2.04601800	2.23770400	-2.09037000
C	1.43652500	0.90322000	-0.20132900
C	2.14476600	1.98554600	-0.72477200
H	3.72380400	0.62432600	2.59319000
H	4.09369000	3.02583300	3.04563200
H	5.28720400	4.45814400	1.39034000
H	5.77738500	1.02054500	-1.16342700
H	6.13366200	3.42383300	-0.71410400
H	-2.69799900	-1.86517400	1.69601600
H	-3.63513200	-2.00044300	0.22908500
H	-3.97631100	0.14284500	2.40986700
H	-4.92841600	0.10223100	0.93900500
H	-2.43586900	-0.56671600	-2.25648600
H	-2.10906900	1.10032700	-1.86983600
H	-4.75466400	-0.37547300	-1.32260700
H	-4.46738300	1.30672400	-0.91549600
H	-0.69208500	1.56633000	0.86260600
H	-1.70234800	0.88853500	2.12098400
H	-2.67844200	2.68419100	-0.17853800
H	-3.71003100	2.06545200	1.09718100
H	-1.28492700	3.87480100	1.52681600
H	-2.32041200	3.26494600	2.80039000
H	-2.98301300	5.59855700	2.17500400
H	-3.24539500	5.09077900	0.50527600
H	-4.28997300	4.47697400	1.78708700
H	-4.81832300	-2.14275300	3.00857700
H	-5.77656500	-2.16927600	1.54335400
H	-7.18719600	-1.48263400	3.49358700
H	-6.10266800	-0.12921900	3.82190800
H	-7.06422500	-0.14948600	2.34331800
H	-4.31730300	0.14164400	-3.73670100
H	-4.04177600	1.82071200	-3.32449100
H	-6.38374000	1.49417100	-4.14965800
H	-6.68375600	0.31202100	-2.87364200
H	-6.40555200	2.00417700	-2.45989200
H	0.03589700	-0.11285000	-3.10881700
H	2.59350200	3.06754900	-2.53718000
H	1.52605700	0.67025300	0.86050200
H	2.77877200	2.59971300	-0.08940800
O	-1.18875900	-4.17092000	0.44908200

Ni[P(nBu)$_3$](Pyr)(CO)[Na$_2$CO$_3$OPhB(OH)$_2$] (PhOMe), CO-P trans, iso2

Ni	0.55085900	1.43910200	-1.04966200
P	0.00481200	0.51913200	0.97292500
C	-1.36786500	1.78174600	-1.34584100
O	-0.30207900	-2.24520600	-2.13575400
C	0.45394500	-3.02018300	-1.50320700
O	1.80976700	-2.76824300	-1.73374400
O	0.12639800	-3.93767300	-0.72006900
Na	-2.17891400	-3.31405900	-1.0308070
C	-1.02301200	-0.99319200	1.06526000
C	1.40551900	0.14982700	2.10688500
C	-0.95711500	1.80128000	1.86363900
C	-0.26253100	3.15750900	1.82435900
C	-1.45905700	-1.39077900	2.47380600
C	-1.80364100	3.10974700	-1.21940400
N	-3.08021000	3.51519100	-1.28163700
C	-4.00147900	2.57269200	-1.51771600
C	-2.35885100	0.83378600	-1.62150500
C	-3.69258600	1.23023400	-1.71137800
C	2.07975700	-1.19509800	1.85426200
B	2.84685000	-3.47226300	-1.09591300
C	2.48764400	1.37254300	-0.65187600
O	4.08722200	-3.03292200	-1.45974900
O	2.65084300	-4.47213100	-0.21269000
C	3.02321000	2.53437500	-0.06722100
C	4.34204600	2.60312600	0.36573900
C	5.19187400	1.50245800	0.20366500
C	3.36963800	0.30423700	-0.82918200
C	4.70484000	0.34814400	-0.40976000
O	6.46368800	1.65435900	0.67464300
C	7.32236500	0.53884000	0.55537900
O	-3.81925100	-2.15023700	-0.43876800
H	-1.13660700	1.47824500	2.89671000
H	-1.93587600	1.85863600	1.36800700
H	0.65458900	3.12778400	2.43067600

H	0.07368700	3.35754700	0.79434000
H	-0.42622600	-1.80124400	0.62320100
H	-1.90700800	-0.87468300	0.42295200
H	-0.60165800	-1.39918400	3.16271300
H	-2.15406600	-0.63840000	2.87121300
H	-1.07855600	3.90932600	-1.04178800
H	-5.03784200	2.90841200	-1.55369000
H	-2.11320600	-0.22165100	-1.73885400
H	-4.48195400	0.50562500	-1.89191700
H	1.04822000	0.21349200	3.14326900
H	2.13684800	0.95572900	1.97172500
H	1.41490200	-2.01885700	2.15554900
H	2.24926200	-1.32791100	0.77553300
H	2.39206900	3.41278600	0.07600700
H	4.73845800	3.50173400	0.83148400
H	3.03520300	-0.63951500	-1.26002700
H	5.33182700	-0.52721300	-0.55266500
H	4.77092100	-3.54478900	-1.01831400
H	8.27453000	0.83674300	0.99388400
H	6.93216500	-0.33327300	1.09764800
H	7.48032400	0.25594800	-0.49339100
H	1.68503000	-4.59740900	-0.12073900
C	-4.84642300	-1.42448500	-0.13067300
C	-6.03334400	-1.41419100	-0.91958000
C	-7.10793900	-0.58637200	-0.61871200
C	-7.07671600	0.26624700	0.48754200
C	-4.85616400	-0.56293500	1.00503500
C	-5.93777500	0.25782400	1.29634100
H	-6.06823800	-2.06618900	-1.79174200
H	-7.98831800	-0.60382600	-1.26036300
H	-7.91915800	0.91241700	0.71756500
H	-3.96985300	-0.54661300	1.63944600
H	-5.89178400	0.90892800	2.16891600
Na	1.23943100	-0.87999000	-3.1233190
C	3.41199400	-1.31082300	2.58426000
C	4.17085700	-2.57993600	2.24663800
H	3.23779200	-1.24727200	3.66695000
H	4.02515400	-0.43561300	2.32633400
H	5.11289700	-2.64744900	2.79848200
H	3.58541600	-3.47731700	2.47079700
H	4.40700000	-2.61263400	1.17708300
C	-1.15357900	4.30236500	2.28020100
C	-0.45719700	5.64824100	2.19767800
H	-1.49435900	4.11311800	3.30701800
H	-2.05887100	4.31019300	1.65799200
H	-1.10788300	6.46507500	2.52077800
H	0.44112700	5.67251300	2.82416100
H	-0.14348200	5.86488800	1.17000100
C	-2.13542400	-2.75590900	2.48264000
C	-2.70187400	-3.12253900	3.84167900
H	-1.40350600	-3.51248400	2.15977500
H	-2.93132500	-2.74956500	1.72479900
H	-3.16197100	-4.11461700	3.83605200
H	-1.92642500	-3.12209600	4.61612800
H	-3.47175300	-2.40602900	4.14898600
C	0.92548400	2.23180900	-2.56280500
O	1.18443200	2.77216000	-3.55343200

$[Na_2CO_3OPhB(OH)_2]$

O	-2.39246100	-0.26204400	0.67775600
C	-1.50997100	-1.21952500	0.20138700
O	-1.34593900	-2.20660200	0.92593600
O	-0.93315600	-0.99255000	-0.91648900
Na	0.26086000	0.99965300	-1.13482800
B	-2.82692500	0.83189700	-0.05429600
O	-3.57903800	1.73216500	0.63445800
O	-2.51886700	1.02642500	-1.37788500
H	-3.87965900	2.43850800	0.05738200
H	-2.05400000	0.21377500	-1.66198200
Na	0.49484300	-2.90842300	-0.2528160
O	2.35641900	-1.74787300	-0.09430900
C	2.27510700	-0.49286300	0.15148300
C	2.96643000	0.49355800	-0.63193300
C	1.45452300	0.04282700	1.20437600
C	2.85161700	1.85744200	-0.37640800
H	3.61247600	0.13835800	-1.43266900
C	1.34431200	1.40811800	1.44084400
H	0.90683400	-0.66160900	1.82905900
C	2.02965400	2.34210300	0.64996700
H	3.41063900	2.56068600	-0.99253500
H	0.70707500	1.75462000	2.25333000
H	1.95283000	3.40650900	0.84894600

TS (Transm.), iso2_down
Ni[P(n-Bu)$_3$](PyrCO)[Na_2CO_3OPh][$B(OH)_2PhOMe$]

Ni	0.87095300	0.24394800	0.16107100
P	-1.23162800	1.02954900	0.13752200
C	0.96252600	0.75765500	1.92545100
O	1.77860800	-2.29031100	-0.65470400
C	1.29364100	-1.72858800	-1.80976900
O	0.73449300	-0.60155500	-1.72433200
O	1.39886500	-2.41276000	-2.85709200
Na	3.15657500	-3.70461600	-2.1894910
C	-2.51525300	0.29169600	1.22578900
C	-1.13206600	2.81699400	0.58245200
C	-1.93792400	0.92163500	-1.55487100
C	-3.43141500	1.13664900	-1.77899700
C	-3.81532400	0.82825200	-3.22097800
C	-2.13847800	3.77809300	-0.03373800
C	-1.92016400	5.21310500	0.42743900
C	-3.69792600	1.15467800	1.65238700
C	-4.70721700	0.35746100	2.46908800
C	-5.88364800	1.19613800	2.93393000
C	-5.30263300	0.98767900	-3.47902100
C	-2.89738500	6.18920400	-0.20258400
O	1.13837800	1.86415700	2.41569200
C	0.89120400	-0.45062400	2.81766800
B	2.97930500	-1.80494600	-0.04778400
C	2.88323300	0.42222600	0.00816100
O	3.20795200	-2.16747000	1.26315200
O	4.06678400	-1.91451500	-0.94449200
C	3.82493800	0.69141100	1.03047700
C	4.96589300	1.45132100	0.83210700
C	5.21024900	2.02760600	-0.42136400
C	3.16818600	1.03787600	-1.23012700
C	4.29837000	1.82265400	-1.46038400
O	6.35525300	2.75759200	-0.52761000
C	6.60944600	3.37625800	-1.77354900
Na	-0.47407200	-1.29426400	-3.7637860
O	-2.19781000	-2.18617700	-2.82918900
C	-2.66285800	-2.45922700	-1.65263300
C	-1.83678900	-2.93523600	-0.58763600
C	-4.04428300	-2.30221800	-1.32539900

C	-2.35291800	-3.26481500	0.66164900
C	-4.54605500	-2.62539400	-0.07038700
C	-3.71321000	-3.11465800	0.94114300
H	-1.70219400	-0.10071700	-1.87032800
H	-1.33822700	1.58978000	-2.18987700
H	-3.99327900	0.45689000	-1.12393400
H	-3.73986700	2.15779600	-1.51744300
H	-0.11082100	3.13170500	0.33368500
H	-1.17059500	2.86305500	1.67758500
H	-2.07087500	3.73695700	-1.13033700
H	-3.16292800	3.47072700	0.21284600
H	-2.00204800	-0.08222200	2.12139800
H	-2.86143900	-0.60528000	0.69367900
H	-3.34533600	2.01488400	2.24021800
H	-4.20518400	1.57939800	0.77630200
H	-4.19818900	-0.09172800	3.33340700
H	-5.05670900	-0.48956600	1.86305000
H	-6.59982500	0.60783600	3.51451500
H	-5.55433800	2.03004300	3.56362900
H	-6.42392000	1.62645400	2.08346700
H	-3.49734600	-0.20143900	-3.43853600
H	-3.24588000	1.48458000	-3.89647000
H	-5.56595600	0.75675600	-4.51541000
H	-5.88510800	0.31891000	-2.83526100
H	-5.63916800	2.01016600	-3.27282500
H	-0.88877900	5.51262600	0.19696800
H	-2.00205500	5.25407100	1.52205200
H	-2.72972500	7.21380300	0.14098900
H	-2.80942600	6.18905800	-1.29451700
H	-3.93281200	5.92577100	0.03883700
H	3.67488300	0.24931500	2.01525300
H	5.68321600	1.62407500	1.63055900
H	2.48739400	0.88449200	-2.06597400
H	4.46055100	2.26491000	-2.43892500
H	7.54500000	3.92332900	-1.65724100
H	6.72009900	2.63862300	-2.57876300
H	5.81145700	4.07757200	-2.04772600
H	4.87027200	-1.55264300	-0.56160000
H	-0.77429200	-3.07293500	-0.78846200
H	-4.70935400	-1.93528400	-2.10730600
H	-1.67825300	-3.63118600	1.43620100
H	-5.61076300	-2.49521800	0.12516000
H	-4.11308100	-3.36167100	1.92109500
H	2.38949300	-2.15869100	1.76886300
C	0.22593800	-1.62561600	2.44072000
N	0.20660800	-2.74238400	3.17869700
C	0.87236000	-2.71436400	4.34198900
C	1.55462700	-0.44153000	4.04831800
C	1.55321800	-1.59594400	4.82022400
H	-0.31638100	-1.66299800	1.49035700
H	0.86134500	-3.63768100	4.91927900
H	2.06640300	0.46489200	4.36263700
H	2.07155900	-1.63787600	5.77343900

TS (Transm.), iso2_up

Ni[P(n-Bu)$_3$](PyrCO)[Na$_2$CO$_3$OPh][B(OH)$_2$PhOMe]

Ni	1.04268400	0.05328600	0.09432500
P	-0.97856400	1.01551200	-0.07978200
C	1.57587300	1.51289300	1.07525500
O	0.62133600	-2.35803700	1.21763300
C	0.47196800	-2.62558400	-0.11042800
O	0.40322100	-1.63249900	-0.89496800
O	0.35641000	-3.82673400	-0.45336200
Na	1.31170200	-4.71884100	1.45639700
C	-1.82917100	0.55229200	1.47889900
C	-0.96671400	2.85782800	-0.14724900
C	-2.00464600	0.43289500	-1.48551400
C	-3.52109800	0.60252900	-1.42939200
C	-4.15926600	0.27054100	-2.77196500
C	-2.20197800	3.63190400	-0.58836200
C	-1.96625500	5.13609600	-0.52304000
C	-3.06978300	1.31526500	1.93179300
C	-3.62364500	0.75648600	3.23605700
C	-4.92257400	1.41945800	3.65650000
C	-5.66011800	0.49531300	-2.77484300
C	-3.16265900	5.94256500	-0.99404800
C	2.24465800	2.64862700	0.37588800
O	1.36822700	1.58480800	2.29319600
B	1.88344700	-1.88595000	1.76486100
C	2.92263100	-0.68079000	0.26309400
O	1.85141400	-1.10054900	2.89120000
O	2.78288900	-2.98830500	1.78012800
C	3.97438900	-0.13758700	1.04291900
C	5.30792000	-0.22272800	0.68194000
C	5.66612200	-0.84324300	-0.52259900
C	3.33324200	-1.28493200	-0.94438200
C	4.66730800	-1.37498600	-1.34220600
O	6.99660400	-0.87900300	-0.80080600
C	7.38411700	-1.48113700	-2.02172800
Na	-0.73971300	-3.14747100	-2.4683440
O	-2.87880300	-2.95806700	-2.22274200
C	-3.62697700	-2.77544100	-1.18338200
C	-3.10396300	-2.73656500	0.14532200
C	-5.03811800	-2.58059100	-1.28200000
C	-3.90512300	-2.47684300	1.25103200
C	-5.82534100	-2.30927400	-0.17065900
C	-5.27440300	-2.24042300	1.11364600
H	-1.77673300	-0.63326900	-1.60825700
H	-1.59443600	0.93727400	-2.37292100
H	-3.93155100	-0.06673900	-0.66119400
H	-3.79859900	1.62253300	-1.13718700
H	-0.13044400	3.12960200	-0.80465700
H	-0.65416200	3.18053800	0.85680500
H	-2.46828100	3.35165200	-1.61702700
H	-3.07175500	3.37315700	0.02911900
H	-1.05200500	0.61616500	2.25352100
H	-2.06166600	-0.51543600	1.36499000
H	-2.83111800	2.38063700	2.06335500
H	-3.85076500	1.26993500	1.16240700
H	-2.86737000	0.86269200	4.02561100
H	-3.78327600	-0.32297500	3.11362800
H	-5.29700000	1.02039300	4.60341500
H	-4.79978800	2.50123800	3.77985600
H	-5.70172300	1.26335800	2.90204700
H	-3.92520300	-0.77451600	-3.01643000
H	-3.68844000	0.88692300	-3.55297100
H	-6.11203900	0.21741300	-3.73205900
H	-6.14059900	-0.10426400	-1.99442200
H	-5.90647300	1.54665500	-2.58547000
H	-1.08149300	5.38747400	-1.12487100
H	-1.70893000	5.41230600	0.50892400
H	-2.97627200	7.01866600	-0.93949600
H	-3.41733000	5.70378900	-2.03206100

H	-4.04810500	5.72956600	-0.38577300
H	3.72975400	0.33992400	1.99060900
H	6.09504400	0.19123400	1.30707700
H	2.58499900	-1.70790400	-1.61130400
H	4.91722300	-1.85205200	-2.28515800
H	8.46981000	-1.40295100	-2.06847300
H	7.09576000	-2.53894000	-2.06079200
H	6.94581200	-0.96385600	-2.88386000
H	3.62652600	-2.72767800	2.15844000
H	-2.03763300	-2.91366000	0.28092400
H	-5.48470800	-2.61559900	-2.27529200
H	-3.44769300	-2.45155300	2.24139200
H	-6.89423300	-2.14455700	-0.30725700
H	-5.89420100	-2.02522000	1.98022300
H	1.43126200	-0.23233600	2.76256700
C	2.73520200	2.51049000	-0.92647700
N	3.30005600	3.49966300	-1.62412200
C	3.38610000	4.69152200	-1.01729100
C	2.36317600	3.89798300	0.99066900
C	2.93984000	4.94035000	0.27952400
H	2.66665200	1.53534900	-1.41471500
H	3.83720200	5.49179000	-1.60262300
H	1.98988700	4.02738300	2.00378400
H	3.04322500	5.93034000	0.71308500

Ni[P(n-Bu)$_3$](PyrCO)[Na$_2$CO$_3$OPhB(OH)$_2$](PhOMe) Iso2_down

Ni	0.62675000	0.84033800	0.00795800
P	-1.61231000	1.01360700	-0.16747300
C	0.55781000	1.81692500	1.56533800
O	1.91197800	-1.77665400	-0.03748300
C	1.66177800	-1.44952400	-1.34687800
O	0.77604500	-0.57121900	-1.52030600
O	2.26281500	-2.06441000	-2.26118700
Na	4.37058600	-1.21257400	-2.2542050
C	-2.67803800	0.25410700	1.12685300
C	-2.03004500	2.81123600	-0.18504800
C	-2.20748800	0.28728400	-1.74733100
C	-3.69408200	0.02473800	-1.95272800
C	-3.94356500	-0.74186700	-3.24507900
C	-3.24104700	3.28896800	-0.97469800
C	-3.40407100	4.80224800	-0.90680200
C	-4.05693800	0.85296800	1.38063700
C	-4.81387300	0.09346200	2.46226500
C	-6.18137500	0.68481600	2.75210800
C	-5.40504100	-1.10295200	-3.43878800
C	-4.59431800	5.30558500	-1.70316200
O	0.42809800	3.01607700	1.77671300
C	0.78229000	0.86553500	2.71426600
B	3.08747100	-2.25206100	0.50641500
C	2.57205600	1.13126900	-0.10403400
O	3.12816700	-2.66195700	1.79159500
O	4.25233800	-2.28734800	-0.24017300
C	3.56021500	0.92272900	0.87989900
C	4.92282800	1.06642700	0.63498500
C	5.37109100	1.45694900	-0.63103400
C	3.06593400	1.50456900	-1.36636000
C	4.43333800	1.67698800	-1.64473000
O	6.72732800	1.59307000	-0.77918900
C	7.18268800	2.08692800	-2.02027100
Na	-0.02224800	-2.01992000	-3.3053000
O	-1.46348600	-3.01217400	-2.08026300
C	-2.00270300	-3.10640600	-0.90609000
C	-1.23356200	-3.12829500	0.29766600
C	-3.41579300	-3.19711200	-0.72485500
C	-1.82351200	-3.25225800	1.55086300
C	-3.99391200	-3.30914700	0.53414100
C	-3.21028200	-3.34242800	1.69177300
H	-1.68969600	-0.67812400	-1.80024100
H	-1.79601700	0.90710700	-2.55763400
H	-4.06497000	-0.58569500	-1.11866000
H	-4.27474000	0.95640300	-1.94657900
H	-1.12742400	3.32040800	-0.54553600
H	-2.10995400	3.11579200	0.86615200
H	-3.14676500	2.98202700	-2.02653300
H	-4.15928300	2.81186500	-0.60645500
H	-2.09953700	0.27177200	2.06104800
H	-2.75898800	-0.80844400	0.85681300
H	-3.96077600	1.90944300	1.67194300
H	-4.65424900	0.85197900	0.45906300
H	-4.20919000	0.07495900	3.37977200
H	-4.90879000	-0.95605400	2.15237000
H	-6.71228800	0.12609200	3.52809300
H	-6.10267500	1.72418800	3.09017200
H	-6.81171000	0.68322100	1.85606000
H	-3.32633000	-1.65207100	-3.21833100
H	-3.58696700	-0.14671400	-4.09923900
H	-5.57053200	-1.66956100	-4.35995100
H	-5.76765100	-1.71537000	-2.60494600
H	-6.03732700	-0.20902800	-3.48254300
H	-2.48218700	5.27972900	-1.26599700
H	-3.50169900	5.10375400	0.14505300
H	-4.69711600	6.39257100	-1.64147300
H	-4.50259800	5.04250800	-2.76273300
H	-5.52918400	4.86495000	-1.34013500
H	3.26547400	0.62059800	1.88687600
H	5.66052800	0.89579400	1.41593700
H	2.36589200	1.67919400	-2.18500300
H	4.74692000	2.01034400	-2.63157600
H	8.26567100	2.17690200	-1.93839600
H	6.94308600	1.40380300	-2.84820500
H	6.75318600	3.07042400	-2.24990000
H	4.98240700	-2.54562200	0.33074000
H	-0.14990900	-3.06591400	0.21641900
H	-4.04137900	-3.18898900	-1.61693700
H	-1.18614800	-3.26712600	2.43493200
H	-5.07910900	-3.37521000	0.61614300
H	-3.66930200	-3.43138800	2.67277900
H	2.29841700	-2.52048200	2.28720500
C	0.67537400	-0.51740100	2.53221400
N	1.09568600	-1.42479500	3.42077100
C	1.59334200	-0.96043300	4.57930100
C	1.26921300	1.32179100	3.94050700
C	1.66628400	0.39245300	4.89627300
H	0.26217000	-0.91304800	1.60100900
H	1.95630900	-1.71220100	5.27760600
H	1.35578700	2.39324300	4.10449400
H	2.06158700	0.70572700	5.85782400

Ni[P(n-Bu)$_3$](PyrCO)[Na$_2$CO$_3$OPhB(OH)$_2$](PhOMe) Iso2_up

Ni	1.07310700	0.47920500	-0.13383800

P	-1.14399100	0.95227000	-0.12638900
C	1.38513000	1.91761600	0.94016700
O	0.92025000	-1.85867500	1.13606900
C	0.97200800	-2.27446600	-0.18330400
O	0.69329200	-1.38148600	-1.02652600
O	1.20570600	-3.47614900	-0.43503400
Na	2.23023400	-4.65530800	1.16021900
C	-1.85356500	0.44558000	1.49166700
C	-1.51211100	2.75463900	-0.29086200
C	-2.09543400	0.08885400	-1.44154800
C	-3.61283900	-0.04514100	-1.35206500
C	-4.18411900	-0.62747600	-2.63892500
C	-2.87445100	3.23009100	-0.77696600
C	-2.95245400	4.75099300	-0.82532600
C	-3.21028700	0.99046400	1.92255400
C	-3.63086200	0.46411100	3.28925600
C	-5.02655900	0.91110100	3.68357000
C	-5.69567600	-0.75510400	-2.60305700
C	-4.27684300	5.25858300	-1.36608300
C	1.68695500	3.25285400	0.35251800
O	1.29437100	1.80885200	2.17632000
B	2.02594500	-1.67412100	1.95453300
C	3.01487700	0.13558300	-0.18064500
O	2.05854000	-0.73083500	2.91224600
O	3.03896900	-2.62082900	1.86865800
C	3.98718000	0.46148700	0.78809300
C	5.31707700	0.06731400	0.68836000
C	5.74923800	-0.66238600	-0.42279600
C	3.49854800	-0.58091300	-1.29008100
C	4.83272900	-0.98075200	-1.42581700
O	7.07370700	-1.00948400	-0.43787000
C	7.53436400	-1.70433400	-1.57633200
Na	-0.11250000	-3.10936100	-2.4990230
O	-2.13359600	-3.50094100	-1.90710800
C	-2.92088300	-3.39624100	-0.88659100
C	-2.44321600	-3.10786200	0.42739100
C	-4.33628200	-3.54693200	-0.99614800
C	-3.30203000	-2.94102000	1.50777600
C	-5.18376500	-3.36769900	0.08889300
C	-4.68596500	-3.05247100	1.35760000
H	-1.66456500	-0.91906100	-1.49692600
H	-1.81125500	0.59074800	-2.37876300
H	-3.87039900	-0.70559200	-0.51246900
H	-4.09158100	0.92061800	-1.14860900
H	-0.74225200	3.15875000	-0.96112600
H	-1.28430300	3.19143900	0.69307500
H	-3.06926500	2.82536200	-1.78015100
H	-3.67796700	2.84358100	-0.13660800
H	-1.08793300	0.71485900	2.23316500
H	-1.87708200	-0.65199700	1.46529700
H	-3.18477500	2.08956800	1.94935500
H	-3.98061300	0.72223600	1.18795500
H	-2.89974500	0.78514200	4.04372400
H	-3.58515000	-0.63302500	3.27288500
H	-5.31140600	0.54093000	4.67261600
H	-5.10605500	2.00370600	3.70416000
H	-5.76983800	0.54387700	2.96704800
H	-3.72076700	-1.60856400	-2.81054800
H	-3.88286200	0.01067700	-3.48370400
H	-6.08958800	-1.20281100	-3.52076300
H	-6.00775500	-1.38671500	-1.76459300
H	-6.17540000	0.22286500	-2.47997900
H	-2.12396100	5.13321500	-1.43835900
H	-2.78011600	5.15012400	0.18387500
H	-4.31638500	6.35108700	-1.39146000
H	-4.45126700	4.89800900	-2.38551200
H	-5.11511700	4.91197700	-0.75215800
H	3.69697600	1.02157900	1.67566100
H	6.04370200	0.32370600	1.45636700
H	2.80977500	-0.86112000	-2.08613000
H	5.14317200	-1.53152200	-2.30948800
H	8.59973800	-1.87727300	-1.42162100
H	7.02742700	-2.67131300	-1.69975500
H	7.39360100	-1.12082100	-2.49551400
H	3.81106600	-2.31664700	2.35593500
H	-1.36832800	-3.00400500	0.56882200
H	-4.74556800	-3.77546500	-1.97984500
H	-2.88069400	-2.71234700	2.48802800
H	-6.25905100	-3.47246100	-0.05634000
H	-5.35353300	-2.90976600	2.20351500
H	1.56929700	0.09252100	2.69023500
C	1.97429700	3.38477700	-1.00922300
N	2.17020200	4.55210000	-1.62785300
C	2.08182000	5.65405800	-0.86979800
C	1.61957300	4.41680000	1.12219800
C	1.81815200	5.64085100	0.49920300
H	2.03849300	2.47714000	-1.61465200
H	2.22893400	6.60118800	-1.38781400
H	1.39703000	4.33685000	2.18352400
H	1.76446600	6.57285900	1.05396500

Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh]

Ni	0.88220700	0.41811300	-1.22760500
P	-1.10985800	0.00757500	-0.50359400
C	0.74940900	2.21005500	-0.68162900
O	2.70628800	0.43298300	-1.93024000
C	2.60666400	-0.85082800	-2.18436400
O	1.41795400	-1.35006300	-1.94052400
O	3.58931400	-1.55441200	-2.52959500
Na	2.71485000	-3.10809300	-0.9528450
Na	4.70127000	-0.20645400	-0.8462050
O	3.69358800	-1.71911100	0.50985300
C	3.05244300	-1.14403900	1.48884100
C	1.77769200	-1.59403600	1.93867300
C	1.10326200	-0.97083800	2.98231400
C	1.64505600	0.14073600	3.63139200
C	3.58470600	-0.02122000	2.18407900
C	2.89718500	0.60010700	3.22031600
C	-1.54382600	0.74158200	1.12268300
C	-2.42029700	0.56329400	-1.67701000
C	-1.29168400	-1.82005200	-0.34138800
C	-2.31387300	-2.39433500	0.63035800
C	-2.23444500	-3.91381000	0.70721400
C	-3.74883900	-0.18485000	-1.68189300
C	-4.71925100	0.37593400	-2.71360800
C	-3.00684700	0.84938900	1.53307600
C	-3.15181200	1.40909200	2.94282100
C	-4.59967300	1.54197600	3.37829600
C	-3.23922700	-4.50931000	1.67667600
C	-6.03882600	-0.37358400	-2.74744800
H	1.33769200	-2.46848400	1.45530400
H	0.13619800	-1.36330900	3.29869600
H	1.11017500	0.62705100	4.44169200
H	4.57502900	0.34050700	1.90188400

H	3.34683600	1.45886100	3.71655400
H	-0.29026700	-2.16935400	-0.06161500
H	-1.45361400	-2.20407500	-1.35750000
H	-2.14586500	-1.97898600	1.63441600
H	-3.33242900	-2.09661300	0.34688000
H	-1.97189300	0.51659300	-2.67726300
H	-2.57690300	1.63205200	-1.47706900
H	-3.57268200	-1.24916800	-1.89297700
H	-4.21654000	-0.15071000	-0.68946700
H	-1.09127800	1.74053200	1.11929100
H	-0.96978400	0.17395300	1.86606200
H	-3.54458600	1.49732600	0.82626000
H	-3.50441300	-0.12742500	1.48401900
H	-2.65040400	2.38453600	2.99644100
H	-2.60672500	0.75714300	3.64052400
H	-4.68585900	1.94090500	4.39267800
H	-5.15384000	2.21199400	2.71222900
H	-5.10916100	0.57229800	3.36035700
H	-1.21467000	-4.20177400	1.00053100
H	-2.38606800	-4.33453400	-0.29632900
H	-3.16562400	-5.59922800	1.72200800
H	-3.08609000	-4.12542700	2.69091000
H	-4.26529900	-4.25963500	1.38650500
H	-4.24623300	0.34824600	-3.70442900
H	-4.89659200	1.43839400	-2.49896900
H	-6.72377200	0.04097900	-3.49196500
H	-5.88786700	-1.43101200	-2.99025800
H	-6.54310300	-0.33204800	-1.77602000
C	0.01844800	3.19197200	-1.36470200
N	-0.03624600	4.49042900	-1.02405300
C	0.66035100	4.86428500	0.05514300
C	1.46821200	2.64251800	0.44141800
C	1.42663300	3.98369600	0.81549200
H	-0.56444000	2.92340200	-2.24904400
H	0.59966900	5.91894900	0.32475900
H	2.05279100	1.93228800	1.02761300
H	1.97414900	4.34043000	1.68561700

Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh-B(OH)$_2$PhOMe]

Ni	0.70458300	-0.72390700	0.48636300
P	-1.02108900	0.54014100	0.31179500
C	0.90710600	-0.14603500	2.25387200
O	2.38656500	-1.83128400	0.23874800
C	1.80685300	-2.41747800	-0.84732500
O	0.73145300	-1.82738300	-1.21791300
O	2.29713800	-3.45077400	-1.34284400
Na	4.16088800	-3.48275700	0.29734300
C	-2.26339500	0.59248700	1.65824900
C	-0.41182400	2.26968400	0.15108600
C	-1.89176800	0.05399900	-1.22870400
C	-3.31577500	0.54199000	-1.47041200
C	-3.86020000	0.03569400	-2.79960600
C	-1.19255600	3.24198300	-0.72449300
C	-0.63179300	4.65539600	-0.62742000
C	-3.16170800	1.82130700	1.75842500
C	-4.16580200	1.68079600	2.89566300
C	-5.06640400	2.89379700	3.04202500
C	-5.30531900	0.43793200	-3.03140900
C	-1.32815700	5.63577700	-1.55408000
H	-1.88700600	-1.04547300	-1.20783300
H	-1.22435400	0.34060200	-2.05460800
H	-3.96080900	0.17599900	-0.65851200
H	-3.37204700	1.63866900	-1.44751000
H	0.62614800	2.20587200	-0.20059500
H	-0.34597000	2.65179800	1.17867500
H	-1.16569000	2.90135700	-1.77097400
H	-2.25332800	3.25729600	-0.44251900
H	-1.70413300	0.46623900	2.59375100
H	-2.86828100	-0.31329900	1.53703300
H	-2.55693400	2.72582100	1.91718900
H	-3.70575900	1.98209300	0.81864300
H	-3.62340600	1.49985100	3.83344100
H	-4.77196000	0.78061900	2.72425500
H	-5.78110000	2.77392500	3.86091800
H	-4.48289200	3.79866300	3.24314800
H	-5.64093300	3.07396200	2.12696400
H	-3.76556600	-1.05820500	-2.81957400
H	-3.22848600	0.41429300	-3.61574400
H	-5.68188800	0.07348300	-3.99131400
H	-5.95545200	0.03382900	-2.24758000
H	-5.42395600	1.52724800	-3.02239200
H	0.44576800	4.63447700	-0.83735800
H	-0.72123500	4.99808000	0.41271900
H	-0.89715900	6.63844800	-1.48104500
H	-1.25014700	5.32002700	-2.60090600
H	-2.39534500	5.71639800	-1.32078800
C	1.46921000	1.05878700	2.69358500
N	1.71126900	1.36303600	3.97876800
C	1.38292400	0.44753800	4.89708900
C	0.56347700	-1.07644000	3.24417300
C	0.81206300	-0.78330900	4.58299500
H	1.75752600	1.82433700	1.97228100
H	1.58253300	0.71457300	5.93468000
H	0.10481900	-2.02825200	2.97404400
H	0.56197000	-1.49184400	5.36899900
B	3.76475700	-0.91065500	-0.01034900
C	3.33214700	0.54701400	-0.50696600
O	4.34843700	-1.09303300	1.28991600
O	4.55849600	-1.64714000	-0.98214200
C	3.68538900	1.71222400	0.19313000
C	3.43077400	2.98532500	-0.30158900
C	2.80565500	3.13912800	-1.54330200
C	2.68807000	0.74258400	-1.73901600
C	2.41675100	2.00640700	-2.26383700
H	4.16911600	1.61928900	1.16461900
H	3.71256800	3.87625800	0.25269900
O	2.61276300	4.42456300	-1.96121200
H	2.37141600	-0.12234800	-2.32263200
H	1.91460900	2.09794400	-3.22185900
C	1.93089000	4.60382100	-3.18722500
H	1.83617400	5.68071700	-3.32890400
H	2.48771500	4.17280400	-4.02845200
H	0.92772300	4.15645400	-3.16110000
H	5.18097700	-0.61787400	1.33516400
H	4.32762400	-1.42306000	-1.88635400
Na	0.30345900	-3.77456300	-2.6310620
O	-1.48699600	-4.59118100	-1.80387600
C	-2.24597800	-3.91665500	-1.00821600
C	-1.84761300	-3.55581300	0.31801100
C	-3.55071800	-3.47581100	-1.39190700
C	-2.68534900	-2.85085100	1.17145000
H	-0.85293700	-3.85758500	0.65036300
C	-4.37523600	-2.76567800	-0.52954500
H	-3.89196500	-3.72656400	-2.39584900

C	-3.96275300	-2.44652700	0.76672200
H	-2.33733700	-2.60462800	2.17614100
H	-5.36239400	-2.45446800	-0.87330800
H	-4.61730700	-1.90256000	1.44421200

TS(transmet), from Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh-B(OH)$_2$PhOMe]

Ni	1.07784100	0.35904900	0.01774300
P	-1.06131700	1.00375300	-0.27367000
C	1.42442500	2.09056600	0.67420500
O	1.31062100	-2.04647100	1.36772000
C	1.05335600	-2.40233900	0.07618300
O	0.68231200	-1.48251300	-0.71286800
O	1.15445500	-3.61414300	-0.22332300
Na	2.49357300	-4.20045600	1.56022800
C	-2.02324400	0.85824500	1.28679300
C	-1.20115400	2.75219300	-0.84618600
C	-1.97469000	-0.02557100	-1.49486900
C	-3.50151400	-0.02891700	-1.47392000
C	-4.07181700	-0.82153700	-2.64315700
C	-2.46015000	3.21445900	-1.56707500
C	-2.36899600	4.67622500	-1.98692700
C	-3.27031000	1.71332500	1.48299000
C	-3.99602000	1.35013400	2.77217600
C	-5.22369600	2.20710000	3.02119800
C	-5.58910500	-0.85193400	-2.63989000
C	-3.60682700	5.15382900	-2.72444700
H	-1.62921300	-1.05455700	-1.33353100
H	-1.60036300	0.27438800	-2.48483900
H	-3.84755700	-0.47953300	-0.53173400
H	-3.90513500	0.99082200	-1.49959100
H	-0.33024800	2.91629600	-1.49450700
H	-1.01089900	3.37882500	0.03573900
H	-2.63085800	2.59357400	-2.45801700
H	-3.34406600	3.07661000	-0.93104700
H	-1.32538700	1.04759300	2.11184000
H	-2.28132000	-0.20728400	1.35140500
H	-2.99637800	2.77867000	1.49507100
H	-3.96199300	1.58753900	0.64062300
H	-3.29852500	1.43661400	3.61720900
H	-4.27898200	0.28897500	2.72430300
H	-5.73512100	1.92775800	3.94668300
H	-4.96043800	3.26791300	3.09634500
H	-5.94634400	2.10914800	2.20387800
H	-3.66727300	-1.84166300	-2.60129300
H	-3.70863400	-0.37906000	-3.58337100
H	-5.98665300	-1.44632800	-3.46842000
H	-5.96314800	-1.29105700	-1.70862500
H	-6.01094000	0.15640000	-2.72492700
H	-1.47933100	4.81568800	-2.61594300
H	-2.20068700	5.29577400	-1.09558600
H	-3.52701100	6.20400700	-3.01858900
H	-3.77697000	4.56813900	-3.63444800
H	-4.50260100	5.05275300	-2.10216900
C	2.08699900	3.02334400	-0.14600200
N	2.37847400	4.28478400	0.19138400
C	2.02605500	4.68656500	1.42094000
C	1.06853300	2.55720400	1.94572100
C	1.37924900	3.86180900	2.33273900
H	2.41005700	2.72318100	-1.14522200
H	2.27593400	5.71443500	1.68228400
H	0.52811100	1.92270700	2.65088600
H	1.11301400	4.23099900	3.32013300
B	2.48938600	-1.29833900	1.73655900
C	3.06402900	-0.05199900	0.03141000
O	2.38481100	-0.40765100	2.78717100
O	3.60118700	-2.17298800	1.74357100
C	4.07637200	0.72020700	0.65656100
C	5.38928000	0.74749700	0.22125100
C	5.76307200	0.01706600	-0.91563000
C	3.48737100	-0.75119400	-1.11851300
C	4.79983100	-0.73164600	-1.59483200
H	3.82202300	1.29468800	1.54498700
H	6.14791000	1.33395000	0.73344600
O	7.07240600	0.10268700	-1.27407300
H	2.76936400	-1.35038800	-1.67484700
H	5.05964600	-1.29151600	-2.48829000
C	7.47131200	-0.60894100	-2.43010100
H	8.53762000	-0.42024800	-2.55152300
H	7.30496600	-1.68794500	-2.31894000
H	6.93795900	-0.26141900	-3.32348300
H	4.40933200	-1.70339400	1.96636200
Na	-0.25169900	-3.24654300	-2.1410050
O	-2.24343000	-3.49334900	-1.40946300
C	-3.02093900	-3.24154600	-0.40781600
C	-2.53404300	-2.76614600	0.84723100
C	-4.43703300	-3.40439300	-0.48793800
C	-3.38648900	-2.47029800	1.90610400
H	-1.45886300	-2.62123800	0.95782200
C	-5.27715500	-3.09685100	0.57313600
H	-4.85016000	-3.76478400	-1.42942800
C	-4.76970100	-2.62087600	1.78659100
H	-2.96333900	-2.10219600	2.84183100
H	-6.35251000	-3.22824000	0.45347800
H	-5.43008600	-2.38401000	2.61638100
H	1.66754400	0.21491800	2.62456400

Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh-B(OH)$_2$](PhOMe), Iso1

Ni	0.98799400	0.77124400	-0.37735000
P	-1.27097800	1.00140700	-0.37547300
C	1.17700000	2.57440800	0.07080600
O	1.28169700	-1.45003400	1.36469900
C	1.35322400	-1.94954800	0.07916700
O	0.78066300	-1.24040500	-0.79032200
O	1.90529100	-3.05266300	-0.12120900
Na	4.16021700	-2.83410300	-0.0260130
C	-1.88291300	0.65235600	1.32640200
C	-1.88248800	2.69069400	-0.79425900
C	-2.13321700	-0.16665800	-1.50769800
C	-3.60862500	-0.50873800	-1.32117900
C	-4.12386700	-1.35446700	-2.47916800
C	-3.31603300	2.88135900	-1.27085200
C	-3.64117300	4.34582600	-1.53489100
C	-3.28609900	1.08499400	1.73307400
C	-3.61247900	0.69297500	3.16927100
C	-5.04002200	1.02981600	3.55876600
C	-5.60094700	-1.67930400	-2.35385300
C	-5.05828000	4.55347000	-2.03807800
H	-1.55690000	-1.09963800	-1.45729600
H	-1.96374400	0.23853500	-2.51687700
H	-3.73752900	-1.06816000	-0.38397600
H	-4.22421100	0.39510400	-1.23395600

H	-1.19333800	3.07493100	-1.55771500
H	-1.68142900	3.31114300	0.09116400
H	-3.47893500	2.30353000	-2.19187000
H	-4.02723000	2.47904600	-0.53805700
H	-1.14658200	1.11493300	2.00028800
H	-1.77363900	-0.43314100	1.45441100
H	-3.39361600	2.17327900	1.61937200
H	-4.03029100	0.63368200	1.06471700
H	-2.90598500	1.18710300	3.85092400
H	-3.44140200	-0.38569700	3.28601800
H	-5.25549600	0.76145100	4.59686800
H	-5.24361200	2.10040100	3.44499100
H	-5.75386900	0.49282100	2.92425100
H	-3.53098000	-2.27814200	-2.52445400
H	-3.93837800	-0.81889000	-3.42287300
H	-5.95113600	-2.31363900	-3.17419200
H	-5.79907200	-2.20923400	-1.41605000
H	-6.21075300	-0.76839700	-2.35650200
H	-2.92174000	4.75005100	-2.25988100
H	-3.48317900	4.91971700	-0.61137100
H	-5.27644700	5.60939400	-2.22065800
H	-5.22887100	4.01458100	-2.97652400
H	-5.79382700	4.18467500	-1.31508100
C	1.32841200	3.60541000	-0.87180800
N	1.38789600	4.91453800	-0.58672400
C	1.30748700	5.26379200	0.70342600
C	1.12036700	2.98544700	1.41082800
C	1.18107100	4.33923700	1.73575100
H	1.39704800	3.36049200	-1.93418700
H	1.35281700	6.33158800	0.91789200
H	1.02428600	2.24831800	2.20992100
H	1.13068800	4.67170500	2.77011200
B	2.34192400	-1.31003900	2.22623200
C	2.92706500	0.57408400	-0.37181400
O	2.17353200	-0.61733200	3.38262500
O	3.57655900	-1.86171600	1.95707300
C	3.83159800	1.10176000	0.57319400
C	5.19820300	0.84727800	0.54288000
C	5.74615400	0.07005400	-0.48396300
C	3.51543600	-0.21086900	-1.37917800
C	4.89744300	-0.45995000	-1.46087000
H	3.45379800	1.73887600	1.37380800
H	5.87011100	1.26404800	1.28995400
O	7.10340400	-0.10817800	-0.45048400
H	2.88163500	-0.65059800	-2.15084800
H	5.29684900	-1.02705300	-2.29950800
C	7.67870700	-0.81087000	-1.53083500
H	8.75400200	-0.82243100	-1.35413400
H	7.31470000	-1.84724500	-1.58705400
H	7.47378900	-0.32082500	-2.49128700
H	4.21946000	-1.53842800	2.59617700
Na	0.31586200	-3.24785500	-2.0453350
O	-1.66196500	-3.78960700	-1.41282900
C	-2.43575300	-3.62473700	-0.38931400
C	-1.97146700	-3.08258400	0.84657900
C	-3.82273100	-3.96097200	-0.41859800
C	-2.82081000	-2.85907000	1.92380600
H	-0.91516500	-2.83002100	0.92991200
C	-4.66353300	-3.72030500	0.66006900
H	-4.22091100	-4.38630100	-1.33926300
C	-4.18325500	-3.15594000	1.84628300
H	-2.40972300	-2.43979600	2.84344500
H	-5.71977400	-3.97633800	0.57524800
H	-4.84495700	-2.96912800	2.68828700
H	1.27830000	-0.27647400	3.46442700

Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh-B(OH)$_2$](PhOMe), Iso2

Ni	1.06935300	0.78177900	-0.39560700
P	-1.19814700	1.00611600	-0.36044500
C	1.26487300	2.57881200	0.07382300
O	1.25913000	-1.57365600	1.25719300
C	1.24537300	-2.02898300	-0.05223900
O	0.85367900	-1.20049100	-0.91342600
O	1.54929300	-3.22200500	-0.26924100
Na	3.11345800	-3.99949900	1.11678300
C	-1.79272800	0.65627200	1.34846600
C	-1.77939200	2.70924300	-0.77061700
C	-2.11960900	-0.14015700	-1.46877500
C	-3.60488400	-0.41499200	-1.24717200
C	-4.19704200	-1.20784800	-2.40532900
C	-3.21533200	2.95144000	-1.21467400
C	-3.48380800	4.42527900	-1.49064500
C	-3.15654200	1.17125100	1.79140900
C	-3.48099100	0.77659600	3.22703600
C	-4.85775100	1.24055800	3.66624500
C	-5.68163100	-1.47194400	-2.23440300
C	-4.90188200	4.68871400	-1.96352700
H	-1.58601500	-1.09785000	-1.41352200
H	-1.95133300	0.24333700	-2.48656500
H	-3.73359800	-0.98695500	-0.31721400
H	-4.17126300	0.51563500	-1.12152900
H	-1.09712400	3.06834000	-1.55245400
H	-1.53392900	3.32686700	0.10536300
H	-3.42507600	2.37028900	-2.12420000
H	-3.92531800	2.58921500	-0.45988100
H	-1.01516100	1.04916300	2.01922900
H	-1.75077400	-0.43730500	1.44815500
H	-3.19332100	2.26647800	1.69898500
H	-3.94180300	0.78345300	1.12982700
H	-2.71206100	1.18438200	3.89780200
H	-3.41005100	-0.31583100	3.31673300
H	-5.07186300	0.96392800	4.70249700
H	-4.95555900	2.32898300	3.58792900
H	-5.63927200	0.79801000	3.03869200
H	-3.64820300	-2.15530500	-2.49434400
H	-4.02124300	-0.65612800	-3.34151300
H	-6.08877600	-2.06719400	-3.05787200
H	-5.86940500	-2.01950200	-1.30457200
H	-6.25052800	-0.53594800	-2.19041600
H	-2.76477600	4.78867000	-2.23743800
H	-3.27858500	5.00348200	-0.57916800
H	-5.07823900	5.75103300	-2.15414600
H	-5.11822400	4.14696500	-2.89088700
H	-5.63578300	4.36083000	-1.21925400
C	1.41705600	3.61305000	-0.86444800
N	1.47167600	4.92132000	-0.57328400
C	1.38547300	5.26328700	0.71854800
C	1.20353200	2.97980800	1.41667900
C	1.25948300	4.33298600	1.74605000
H	1.49051000	3.37294300	-1.92760600
H	1.42647700	6.33035000	0.93832600
H	1.11429000	2.23219900	2.20545800
H	1.20522300	4.66177300	2.78167500

B	2.41300800	-1.10333800	1.84518000
C	3.00895800	0.59028500	-0.42612700
O	2.24944200	-0.17127500	2.82005600
O	3.59746200	-1.76344500	1.54054300
C	3.92419200	1.14999400	0.48965300
C	5.28491300	0.84575700	0.48729100
C	5.80949900	-0.00434100	-0.49502900
C	3.58379600	-0.24783500	-1.39855000
C	4.94997200	-0.54515100	-1.45365900
H	3.55777500	1.83690800	1.25303300
H	5.96852100	1.28615400	1.21024700
O	7.15728700	-0.23253000	-0.43695600
H	2.94261600	-0.71390500	-2.14620300
H	5.33079400	-1.19030700	-2.24100500
C	7.71011100	-1.03198500	-1.46139700
H	8.78199600	-1.08008900	-1.26910900
H	7.29711400	-2.05005000	-1.45398000
H	7.54007800	-0.59630900	-2.45425400
H	3.07038600	0.08068000	3.24898400
H	4.36727300	-1.17823200	1.52610500
Na	0.11446900	-3.10672900	-2.2461250
O	-1.79013600	-3.72913900	-1.47543200
C	-2.54010200	-3.58492100	-0.43137600
C	-2.04680500	-3.07486700	0.80733400
C	-3.92977200	-3.91093800	-0.43964100
C	-2.87398900	-2.86374500	1.90463400
H	-0.98724300	-2.83583600	0.87700600
C	-4.74702700	-3.68704300	0.66028000
H	-4.34944000	-4.31190800	-1.36174300
C	-4.23941300	-3.15010200	1.84787000
H	-2.44247300	-2.46164800	2.82249700
H	-5.80687200	-3.93260100	0.59066200
H	-4.88384400	-2.97331000	2.70501800

Ni[P(n-Bu)$_3$](Pyr)(PhOMe), iso-1

Ni	-1.06092300	-0.45259900	-0.00481300
P	1.20203400	-0.53735000	0.01130500
C	1.89692200	0.69774000	-1.17001400
C	1.90218100	-0.08339500	1.65757800
C	1.95620000	-2.16335200	-0.44055000
C	3.30461800	0.50744300	1.74791300
C	3.69217500	0.85084100	3.18069400
C	3.37853800	-2.49114900	-0.00012200
C	3.81238700	-3.87714800	-0.45962400
C	3.31060000	0.51155900	-1.70497900
C	3.71567400	1.62724800	-2.65967100
C	5.07730200	1.46374800	3.28380100
C	5.10989100	1.43789000	-3.22918000
C	5.21830200	-4.23402300	-0.01185600
C	-2.93686600	-0.46065900	-0.07090200
C	-1.14142100	1.39756400	0.03502700
H	1.82082800	-0.98057300	2.28631400
H	1.18618700	0.63492400	2.07981800
H	4.04625200	-0.18557600	1.33010200
H	3.36273800	1.41711000	1.13365600
H	1.86646400	-2.24265300	-1.53262000
H	1.27603300	-2.92779000	-0.04306300
H	4.08487600	-1.74492400	-0.38511800
H	3.44870300	-2.43424000	1.09523000
H	1.79073200	1.67372500	-0.67503600
H	1.19005900	0.73660000	-2.00913300
H	4.03285300	0.46277100	-0.88000900
H	3.38688200	-0.45410900	-2.22569300
H	3.63732100	-0.05778400	3.79563600
H	2.94559900	1.53866700	3.60019400
H	5.84250400	0.78115600	2.89885300
H	5.14475500	2.38883400	2.70146400
H	3.65192800	2.58898300	-2.13286000
H	2.98206300	1.68830300	-3.47478200
H	5.38477500	2.24800800	-3.91006800
H	3.74326100	-3.92887700	-1.55475000
H	3.09799100	-4.62136400	-0.08232500
H	5.51342300	-5.23056700	-0.35159400
H	5.95211300	-3.52154400	-0.40337900
H	5.30245700	-4.21949500	1.08006200
H	5.86304700	1.40559500	-2.43442200
H	5.18637800	0.49831600	-3.78713200
H	5.34054100	1.70492400	4.31715300
C	-1.17903700	2.14137600	-1.15493500
N	-1.04955500	3.47286400	-1.22367800
C	-0.90098100	4.13542800	-0.06974100
C	-1.02497500	2.12391500	1.22651900
C	-0.89129400	3.51050200	1.17381100
H	-1.30795600	1.63352200	-2.11280600
H	-0.79696000	5.21735900	-0.14639000
H	-1.03134200	1.61567300	2.19019100
H	-0.78841200	4.09697500	2.08384300
C	-3.60967300	-0.45629500	-1.30753900
C	-4.97332500	-0.69869800	-1.40275700
C	-5.72437800	-0.92420900	-0.24313300
C	-3.72264100	-0.64869100	1.07456400
C	-5.09679100	-0.89377200	1.00451800
H	-3.05516300	-0.26560800	-2.22635700
H	-5.48454000	-0.71089900	-2.36217800
O	-7.05748100	-1.15040600	-0.43321600
H	-3.26170600	-0.61290800	2.06196200
H	-5.66307800	-1.05088800	1.91760700
C	-7.84241300	-1.35448200	0.72358500
H	-8.86368200	-1.51184900	0.37664100
H	-7.51381000	-2.23651300	1.28863100
H	-7.81803300	-0.48335900	1.39099000

TS(decarb.) from Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh-B(OH)$_2$](PhOMe), Iso1

Ni	1.43738900	0.22085600	-0.12995200
P	-0.65948400	1.00338300	-0.11021700
C	2.40429100	1.82090200	0.04778700
O	0.51029000	-2.31278700	1.51514700
C	0.50610800	-2.65399000	0.18385500
O	0.93464100	-1.79241000	-0.63417000
O	0.00338600	-3.75851000	-0.12119100
Na	-1.93964500	-4.83388300	-0.0302980
C	-1.38198000	0.84903100	1.58548100
C	-0.64954800	2.81982200	-0.45424900
C	-1.87691300	0.27328400	-1.29506900
C	-3.36881400	0.61069000	-1.28428300
C	-4.01577100	0.31804300	-2.63215100
C	-1.86295000	3.59142300	-0.95380900
C	-1.52593500	5.06273300	-1.16780500
C	-2.72361400	1.47418200	1.94403300
C	-3.03777200	1.34365000	3.42913500
C	-4.42749000	1.84138700	3.78203000
C	-5.50257800	0.61927200	-2.65049700

C	-2.69351500	5.86756100	-1.70883500
H	-1.76967700	-0.81318500	-1.18090800
H	-1.45078100	0.51833200	-2.28086200
H	-3.87262100	0.01760000	-0.51132200
H	-3.53896300	1.66070200	-1.02327300
H	0.16138500	2.95563700	-1.18076600
H	-0.25974000	3.27885500	0.46564300
H	-2.21659800	3.16357600	-1.90310700
H	-2.70849000	3.51075600	-0.25731800
H	-0.60155800	1.27692600	2.23574800
H	-1.40204400	-0.22955400	1.80389800
H	-2.73401700	2.53675500	1.66541600
H	-3.52339600	0.99527500	1.36629900
H	-2.28019200	1.88694600	4.01070100
H	-2.93504300	0.28953000	3.72533100
H	-4.63712200	1.75150800	4.85162300
H	-4.55338200	2.89453600	3.50830000
H	-5.19459300	1.27284900	3.24407900
H	-3.84420100	-0.73833800	-2.88512400
H	-3.50405000	0.90371500	-3.41089000
H	-5.95426400	0.40124900	-3.62290300
H	-6.02651900	0.02180800	-1.89643600
H	-5.69460700	1.67439200	-2.42556900
H	-0.66721700	5.13688000	-1.84963800
H	-1.18008700	5.49218100	-0.21722700
H	-2.43109300	6.91862200	-1.85888800
H	-3.03478800	5.47267400	-2.67216700
H	-3.54908200	5.83586200	-1.02519100
C	2.64425200	2.68236800	-1.05587000
N	2.74841300	4.01031200	-0.99906200
C	2.64559900	4.58889800	0.20846800
C	2.35484500	2.47397200	1.30709400
C	2.46400000	3.85437600	1.38176500
H	2.75486400	2.24410700	-2.05074000
H	2.72478400	5.67483900	0.23435600
H	2.20341700	1.88735800	2.21323000
H	2.39604200	4.36470600	2.34043700
B	1.70139700	-1.80426300	2.04187100
C	3.38020800	0.23021400	-0.06467100
O	1.66085100	-0.77704900	2.94336900
O	2.84599600	-2.46111200	1.72436800
C	4.25850000	0.10799700	1.03438800
C	5.49786200	-0.50370800	0.92728600
C	5.92613800	-1.01490400	-0.30558400
C	3.86705500	-0.24361900	-1.29948900
C	5.10186800	-0.87844800	-1.42565200
H	3.95980500	0.50894600	2.00180500
H	6.16353500	-0.58437800	1.78317100
O	7.15757600	-1.60176800	-0.31409700
H	3.25298300	-0.13644800	-2.19344700
H	5.41428900	-1.25573200	-2.39462600
C	7.61328700	-2.10867200	-1.55170400
H	8.59992400	-2.53233500	-1.36487700
H	6.95060600	-2.89407700	-1.93766400
H	7.69671300	-1.31801400	-2.30859400
H	3.63301800	-1.95200100	1.94925400
Na	-0.59754200	-2.73273900	-2.2241330
O	-2.66735900	-3.27261900	-1.53243100
C	-3.52084900	-2.75117500	-0.68745200
C	-3.12727200	-2.34242000	0.62203100
C	-4.89840600	-2.58540900	-0.99920200
C	-4.03726600	-1.80975900	1.53182400
H	-2.07206200	-2.41416500	0.89387000
C	-5.79394400	-2.04983700	-0.08253600
H	-5.23460700	-2.87685700	-1.99292600
C	-5.38019100	-1.65237700	1.19299600
H	-3.68471600	-1.49935700	2.51553300
H	-6.83881200	-1.93637600	-0.36804000
H	-6.08779900	-1.23400900	1.90259400
H	0.78100500	-0.38791100	2.97209700

TS(reductive elimination) from Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh-B(OH)$_2$](PhOMe), Iso2

Ni	1.58572600	0.01223600	-0.66138900
P	-0.31954300	0.32636600	0.43022400
C	1.62963900	2.70119600	-1.14121500
O	1.70515000	-3.07413800	0.75144600
C	1.28774300	-2.94202100	-0.55777000
O	1.78926400	-2.01427200	-1.24931400
O	0.41782900	-3.76335500	-0.92307000
Na	-0.33665300	-4.41440000	1.0950690
C	-1.15133400	-1.14915300	1.18009600
C	-0.00300500	1.41271300	1.90844200
C	-1.61750600	1.17299300	-0.57616400
C	-3.04359800	1.35118800	-0.06049600
C	-3.82390700	2.35667100	-0.89627500
C	-0.97746700	2.52073500	2.28620000
C	-0.38503200	3.48525200	3.30496000
C	-2.27795800	-0.98185900	2.19336700
C	-2.69429600	-2.30603700	2.82177400
C	-3.85601000	-2.16819200	3.78903100
C	-5.23671600	2.56505200	-0.38246900
C	-1.32854000	4.61936000	3.66280700
H	-1.65062500	0.61480800	-1.52195000
H	-1.17970100	2.15002000	-0.82329400
H	-3.56753200	0.38707000	-0.09013900
H	-3.05201900	1.67755200	0.98605600
H	0.97814400	1.86517400	1.71606000
H	0.16136400	0.73527400	2.75779900
H	-1.26526300	3.08727400	1.38826500
H	-1.90970800	2.09801000	2.68520000
H	-0.32032800	-1.69711500	1.65109400
H	-1.49741900	-1.74441800	0.32165300
H	-1.97498300	-0.28504200	2.98899900
H	-3.15675300	-0.53887400	1.71378900
H	-1.82913300	-2.75495700	3.33692500
H	-2.97551900	-2.99888300	2.01297900
H	-4.14616800	-3.12828500	4.22585300
H	-3.60831500	-1.49061100	4.61319600
H	-4.73452000	-1.75670800	3.28086000
H	-3.85204800	2.00603800	-1.93743300
H	-3.27968800	3.31346300	-0.91226300
H	-5.80537000	3.26058600	-1.00731800
H	-5.78026700	1.61386500	-0.35970500
H	-5.23197500	2.96522400	0.63809300
H	0.55359000	3.89444700	2.90181700
H	-0.09923100	2.93126400	4.20996200
H	-0.88749700	5.30745900	4.38941200
H	-1.59624200	5.20300100	2.77483400
H	-2.26169900	4.23904000	4.09218100
C	1.05408600	2.61342600	-2.42903500
N	0.10477700	3.41580400	-2.90683800
C	-0.35246800	4.38670500	-2.09987500

C	1.14387900	3.75003100	-0.33985100
C	0.13942700	4.58530900	-0.81463300
H	1.38161700	1.82702500	-3.10867200
H	-1.13772300	5.02325200	-2.50450500
H	1.53876400	3.91502500	0.65881100
H	-0.25048400	5.38588700	-0.19016100
B	2.75018300	-2.20186000	1.16251900
C	2.63865500	1.73408800	-0.66891100
O	2.36314500	-1.13598100	1.91700900
O	4.00806600	-2.60921300	0.87477400
C	3.31002500	1.91870200	0.58899200
C	4.40609200	1.17439600	0.96366200
C	4.93558400	0.19565100	0.08580200
C	3.21361600	0.72888100	-1.55050200
C	4.37279500	0.00180400	-1.15301900
H	2.96514900	2.68899400	1.27431800
H	4.90369100	1.35029200	1.91418300
O	5.98142800	-0.55315000	0.60302200
H	2.98788200	0.74001000	-2.61664000
H	4.77536500	-0.73669600	-1.83921400
C	6.72112500	-1.31659000	-0.33851000
H	7.57570600	-1.72477700	0.20136500
H	6.12458900	-2.14186100	-0.74752900
H	7.07075800	-0.68764100	-1.16547600
H	3.03863800	-0.44786300	1.99615800
H	4.69992300	-1.98368500	1.13651000
Na	-0.08371200	-2.14685000	-2.7205270
O	-2.12430800	-1.82496400	-2.33697600
C	-3.31965600	-1.72629500	-1.86365200
C	-3.76448300	-2.49723100	-0.74643400
C	-4.28986500	-0.83559900	-2.41255300
C	-5.02806700	-2.33750400	-0.19029400
H	-3.06498000	-3.22338300	-0.32695600
C	-5.55317700	-0.69307700	-1.85593400
H	-3.99829600	-0.24124900	-3.27757600
C	-5.94022800	-1.42683800	-0.72931700
H	-5.30974000	-2.93834700	0.67551900
H	-6.25170700	0.01533900	-2.30115100
H	-6.92847200	-1.30264000	-0.29556700

Prod: (reductive elimination) from Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh-B(OH)$_2$](PhOMe), Iso1

Ni	1.58572600	0.01223600	-0.66138900
P	-0.31954300	0.32636600	0.43022400
C	1.62963900	2.70119600	-1.14121500
O	1.70515000	-3.07413800	0.75144600
C	1.28774300	-2.94202100	-0.55777000
O	1.78926400	-2.01427200	-1.24931400
O	0.41782900	-3.76335500	-0.92307000
Na	-0.33665300	-4.41440000	1.0950690
C	-1.15133400	-1.14915300	1.18009600
C	-0.00300500	1.41271300	1.90844200
C	-1.61750600	1.17299300	-0.57616400
C	-3.04359800	1.35118800	-0.06049600
C	-3.82390700	2.35667100	-0.89627500
C	-0.97746700	2.52073500	2.28620000
C	-0.38503200	3.48525200	3.30496000
C	-2.27795800	-0.98185900	2.19336700
C	-2.69429600	-2.30603700	2.82177400
C	-3.85601000	-2.16819200	3.78903100
C	-5.23671600	2.56505200	-0.38246900
C	-1.32854000	4.61936000	3.66280700
H	-1.65062500	0.61480800	-1.52195000
H	-1.17970100	2.15002000	-0.82329400
H	-3.56753200	0.38707000	-0.09013900
H	-3.05201900	1.67755200	0.98605600
H	0.97814400	1.86517400	1.71606000
H	0.16136400	0.73527400	2.75779900
H	-1.26526300	3.08727400	1.38826500
H	-1.90970800	2.09801000	2.68520000
H	-0.32032800	-1.69711500	1.65109400
H	-1.49741900	-1.74441800	0.32165300
H	-1.97498300	-0.28504200	2.98899900
H	-3.15675300	-0.53887400	1.71378900
H	-1.82913300	-2.75495700	3.33692500
H	-2.97551900	-2.99888300	2.01297900
H	-4.14616800	-3.12828500	4.22585300
H	-3.60831500	-1.49061100	4.61319600
H	-4.73452000	-1.75670800	3.28086000
H	-3.85204800	2.00603800	-1.93743300
H	-3.27968800	3.31346300	-0.91226300
H	-5.80537000	3.26058600	-1.00731800
H	-5.78026700	1.61386500	-0.35970500
H	-5.23197500	2.96522400	0.63809300
H	0.55359000	3.89444700	2.90181700
H	-0.09923100	2.93126400	4.20996200
H	-0.88749700	5.30745900	4.38941200
H	-1.59624200	5.20300100	2.77483400
H	-2.26169900	4.23904000	4.09218100
C	1.05408600	2.61342600	-2.42903500
N	0.10477700	3.41580400	-2.90683800
C	-0.35246800	4.38670500	-2.09987500
C	1.14387900	3.75003100	-0.33985100
C	0.13942700	4.58530900	-0.81463300
H	1.38161700	1.82702500	-3.10867200
H	-1.13772300	5.02325200	-2.50450500
H	1.53876400	3.91502500	0.65881100
H	-0.25048400	5.38588700	-0.19016100
B	2.75018300	-2.20186000	1.16251900
C	2.63865500	1.73408800	-0.66891100
O	2.36314500	-1.13598100	1.91700900
O	4.00806600	-2.60921300	0.87477400
C	3.31002500	1.91870200	0.58899200
C	4.40609200	1.17439600	0.96366200
C	4.93558400	0.19565100	0.08580200
C	3.21361600	0.72888100	-1.55050200
C	4.37279500	0.00180400	-1.15301900
H	2.96514900	2.68899400	1.27431800
H	4.90369100	1.35029200	1.91418300
O	5.98142800	-0.55315000	0.60302200
H	2.98788200	0.74001000	-2.61664000
H	4.77536500	-0.73669600	-1.83921400
C	6.72112500	-1.31659000	-0.33851000
H	7.57570600	-1.72477700	0.20136500
H	6.12458900	-2.14186100	-0.74752900
H	7.07075800	-0.68764100	-1.16547600
H	3.03863800	-0.44786300	1.99615800
H	4.69992300	-1.98368500	1.13651000
Na	-0.08371200	-2.14685000	-2.7205270
O	-2.12430800	-1.82496400	-2.33697600
C	-3.31965600	-1.72629500	-1.86365200
C	-3.76448300	-2.49723100	-0.74643400
C	-4.28986500	-0.83559900	-2.41255300

C	-5.02806700	-2.33750400	-0.19029400
H	-3.06498000	-3.22338300	-0.32695600
C	-5.55317700	-0.69307700	-1.85593400
H	-3.99829600	-0.24124900	-3.27757600
C	-5.94022800	-1.42683800	-0.72931700
H	-5.30974000	-2.93834700	0.67551900
H	-6.25170700	0.01533900	-2.30115100
H	-6.92847200	-1.30264000	-0.29556700

Prod: (reductive elimination) from Ni[P(n-Bu)$_3$](Pyr)[Na$_2$CO$_3$OPh-B(OH)$_2$](PhOMe), Iso2

Ni	1.54535300	0.01447500	-0.53247000
P	-0.29849200	0.34547000	0.59689200
C	1.49842600	2.66733400	-1.27736000
O	2.31135500	-3.21823800	0.81029000
C	1.58702800	-3.01945100	-0.31842100
O	1.86362400	-2.00985500	-1.03799600
O	0.70515000	-3.86797000	-0.57918200
Na	-1.33958500	-4.42646200	0.0887130
C	-1.13578100	-1.07067000	1.45371800
C	-0.03240900	1.58942700	1.95738700
C	-1.57451000	1.09762400	-0.51265700
C	-3.03713500	1.25740500	-0.10891300
C	-3.75055000	2.22746300	-1.04319300
C	-1.07165400	2.67426400	2.21377200
C	-0.55682900	3.76832100	3.13975600
C	-2.27136100	-0.82697100	2.44060400
C	-2.64120300	-2.09711400	3.19782800
C	-3.89218100	-1.94629900	4.04314300
C	-5.20053000	2.46280900	-0.66391300
C	-1.57106100	4.87723700	3.35571300
H	-1.52954300	0.53354600	-1.45552300
H	-1.15070200	2.07849400	-0.76196300
H	-3.54224600	0.28204200	-0.13613200
H	-3.12726000	1.62448700	0.92060900
H	0.92396600	2.07009700	1.70978600
H	0.16206900	1.01563000	2.87506400
H	-1.36871600	3.13529500	1.26035900
H	-1.98928700	2.24064600	2.63522300
H	-0.32520800	-1.61229600	1.96703700
H	-1.48089200	-1.73353400	0.64525000
H	-1.99508600	-0.04449100	3.16237200
H	-3.15727200	-0.45743800	1.91035900
H	-1.79242900	-2.40827100	3.82254900
H	-2.78773300	-2.90994800	2.46895200
H	-4.12988600	-2.86047600	4.59455200
H	-3.78145300	-1.13940700	4.77547100
H	-4.75833600	-1.70069600	3.41838600
H	-3.68594200	1.84288900	-2.07141600
H	-3.20188600	3.18167800	-1.04780500
H	-5.69874500	3.14724900	-1.35715400
H	-5.75816300	1.52022300	-0.66439400
H	-5.28182400	2.89370800	0.34050000
H	0.36815000	4.18632900	2.71539500
H	-0.26617200	3.32817600	4.10341600
H	-1.18677300	5.66294900	4.01201000
H	-1.84845700	5.34631400	2.40482500
H	-2.49207400	4.49160100	3.80620200
C	0.84617500	2.46923900	-2.51538400
N	-0.14866100	3.21500200	-2.99381000
C	-0.57093400	4.24363200	-2.24157700
C	1.04274800	3.77153900	-0.53442600
C	-0.00251300	4.55326200	-1.01043600
H	1.14774600	1.63798700	-3.15249200
H	-1.39109600	4.83472800	-2.64599800
H	1.49617700	4.02081600	0.42080500
H	-0.36488700	5.39903800	-0.43090500
B	3.24911400	-2.26560300	1.25747600
C	2.56550400	1.76955400	-0.79564400
O	2.89038600	-1.07605500	1.81335400
O	4.54947700	-2.65694400	1.25377600
C	3.32581600	2.08574900	0.38257000
C	4.46871100	1.41081000	0.72356000
C	4.95598200	0.35925800	-0.09013100
C	3.09355300	0.69925600	-1.61485900
C	4.30147400	0.03501300	-1.25516700
H	3.00269500	2.89732500	1.03009400
H	5.01387200	1.65927300	1.62943400
O	6.07916700	-0.27647700	0.38892600
H	2.76117300	0.58220000	-2.64592000
H	4.66702000	-0.75404200	-1.90438700
C	6.72041200	-1.16401100	-0.51197700
H	7.63052800	-1.50042200	-0.01441600
H	6.08923300	-2.03264400	-0.73687600
H	6.97903500	-0.65521600	-1.44896000
H	5.11364200	-1.91352400	1.50570000
Na	-0.17966500	-2.20454800	-2.1687440
O	-2.11019700	-2.87969400	-1.29134000
C	-3.27775900	-2.28993400	-1.33481200
C	-4.23716400	-2.44076100	-0.29769400
C	-3.65867500	-1.45649700	-2.41987700
C	-5.48327900	-1.82725800	-0.35666300
H	-3.97468600	-3.05824900	0.56348900
C	-4.90593200	-0.84707900	-2.47025600
H	-2.94329800	-1.30738400	-3.22968600
C	-5.83751900	-1.03016100	-1.44618500
H	-6.19014600	-1.97561000	0.45830800
H	-5.15787200	-0.21773800	-3.32237500
H	-6.81455600	-0.55823900	-1.49493500
H	2.03884200	-0.73238200	1.47696800

Ni[P(n-Bu)$_3$][Na$_2$CO$_3$OPh-B(OH)$_2$],

Ni	-0.60913300	-0.22766200	0.73784200
P	1.47469400	0.12149200	0.32159700
O	-3.56991500	1.74967000	-0.94972500
C	-4.53700700	1.72546900	0.07455200
O	-4.16180900	1.94632000	1.25259400
O	-5.67587000	1.41648100	-0.32592300
Na	-4.70473700	-0.22078800	-1.8309740
C	1.98446100	-0.60934900	-1.31417900
C	2.14773400	1.85620700	0.26564800
C	2.55457600	-0.75368100	1.55586300
C	3.94828700	-1.23506000	1.17117000
C	4.64054000	-1.97026300	2.31202200
C	3.61943200	2.13352400	0.54876000
C	3.95060300	3.61957600	0.49720800
C	3.25834000	-0.15074900	-2.01382900
C	3.46060300	-0.84560400	-3.35458300
C	4.71756100	-0.39003800	-4.07410800
C	6.02065100	-2.47982800	1.93699200
C	5.40538800	3.91416000	0.81687700
H	1.95885700	-1.61851400	1.87769600
H	2.60773600	-0.09717100	2.43572500

H	3.88019600	-1.90553800	0.30230300
H	4.57813400	-0.39492200	0.85189100
H	1.53662900	2.42370200	0.97990300
H	1.87149300	2.25924500	-0.72064600
H	3.88457800	1.74103600	1.54122800
H	4.25985100	1.59733000	-0.16362600
H	1.13315800	-0.44701500	-1.99090100
H	1.99563300	-1.69733500	-1.15922800
H	3.22513200	0.93666600	-2.17580600
H	4.13806700	-0.32941500	-1.38218900
H	2.58047300	-0.66842400	-3.98770200
H	3.49433600	-1.93186400	-3.19290900
H	4.84741900	-0.89775900	-5.03412100
H	4.69284600	0.68720400	-4.27198500
H	5.61163000	-0.58794700	-3.47288500
H	4.00750800	-2.80723300	2.63731600
H	4.71262200	-1.29960900	3.17951400
H	6.50301900	-3.00485600	2.76626000
H	5.96996800	-3.17495000	1.09187800
H	6.67980200	-1.65673000	1.64001400
H	3.29700800	4.15832200	1.19700900
H	3.69952500	4.00795100	-0.49957300
H	5.62636600	4.98440600	0.77331000
H	5.66827600	3.56408000	1.82113700
H	6.07613300	3.40992500	0.11266400
B	-2.21199500	1.59463800	-0.68408300
O	-1.43405400	1.32671800	-1.77015600
O	-1.67780100	1.69633000	0.57385400
H	-0.55211200	1.07968600	-1.45019700
H	-2.44423400	1.82631600	1.18203100
Na	-5.40525500	-0.03293700	1.7024440
O	-4.22600400	-1.10399400	0.16536600
C	-3.03614800	-1.64760000	0.09150400
C	-2.62675300	-2.40385300	-1.02371300
C	-2.08926100	-1.49420800	1.17841900
C	-1.38107100	-3.07483400	-1.05021300
H	-3.34688200	-2.57773100	-1.82587800
C	-0.80480500	-2.15802700	1.12470700
H	-2.50335700	-1.17261400	2.13977300
C	-0.49505700	-2.99013000	-0.00053500
H	-1.13667000	-3.69326900	-1.91320500
H	-0.25747900	-2.32970000	2.05612100
H	0.44474100	-3.53978800	-0.01769100

Supplementary Methods

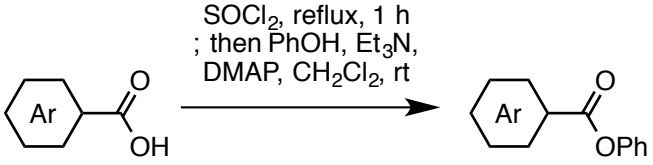
1. General

Unless otherwise noted, all materials including dry solvents were obtained from commercial suppliers and used as received. $Ni(OAc)_2 \cdot 4H_2O$ and P(*n*-Bu)$_3$ were obtained from Kanto Chemicals. Na_2CO_3 was obtained from Wako Chemicals. Toluene was purified by Glass Contour. Anisole and 1,4-dioxane were distilled with Na/ketyl before the use. Phenyl nicotinate (**1A**)[1], phenyl 2-naphthoate (**1B**)[1], phenyl thiophene-2-carboxylate (**1K**)[1], phenyl thiophene-3-carboxylate (**1L**)[1], phenyl furan-3-carboxylate (**1N**)[1], phenyl furan-2-carboxylate (**1O**)[1], phenyl 2-phenylthiazole-4-carboxylate (**1R**)[1], phenyl isonicotinate (**1T**)[1], phenyl 2-phenylquinoline-4-carboxylate (**1V**)[1], phenyl picolinatephenyl (**1AC**)[1], pyrazine-2-carboxylate (**1AD**)[1], 4-oxo-4*H*-chromene-2-carboxylic acid (**1AB**)[2], 5-(methoxycarbonyl)nicotinic acid (**1AA**)[3], and 4-methylpiperazine-1-carbothioamide (**1S**)[4] were synthesized according to procedures reported in the literature. Phenyl 3-methylbenzoate (**1J**)[5], phenyl 4-fluorobenzoate (**1G**)[6], methyl phenyl terephthalate (**1F**)[7], phenyl 4-methylbenzoate (**1H**)[7], phenyl 1-naphthoate (**1C**)[8], phenyl 2-methoxybenzoate (**1E**)[8], and phenyl quinoline-3-carboxylate (**1W**)[8] were synthesized by known procedures using the corresponding carboxylic acids, phenol, EDC·HCl, and DMAP, and the spectra matched with those of reported compounds in the literature. Unless otherwise noted, all reactions were performed with dry solvents under an atmosphere of N_2 gas in dried glassware using standard vacuum-line techniques. All coupling reactions were performed in 20-mL glass vessel tubes equipped with J. Young® O-ring tap and heated in an 8-well reaction block (heater + magnetic stirrer) unless otherwise noted. All work-up and purification procedures were carried out with reagent-grade solvents in air.

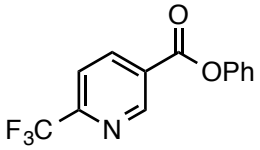
Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F_{254} precoated plates (0.25 mm). The developed chromatogram was analyzed by UV lamp (254 nm). Flash column chromatography was performed with E. Merck silica gel 60 (230–400 mesh) or Biotage Isolera® equipped with Biotage SNAP Cartridge KP-Sil columns using hexane/EtOAc as an eluent. Preparative thin-layer chromatography (PTLC) was performed using Wakogel B5-F silica coated plates (0.75 mm) prepared in our laboratory. Preparative high performance liquid chromatography (preparative HPLC) was performed with a Biotage Isolera®, one equipped with Biotage SNAP Cartridge KP-C18-HS columns using acetonitrile/water as an eluent. Preparative gel permeation chromatography (GPC) was performed with a JAI LC-9204 instrument equipped with JAIGEL-1H/JAIGEL-2H columns using chloroform as an eluent. Gas chromatography (GC) analysis was conducted on a Shimadzu GC-2010 instrument equipped with a HP-5 column (30 m × 0.25 mm, Hewlett-Packard) with dodecane as an internal standard. GCMS analysis was conducted on a Shimadzu GCMS-QP2010 instrument equipped with a HP-5 column (30 m × 0.25 mm, Hewlett-Packard). High-resolution mass spectra (HRMS) were obtained from a JEOL JMS-T100TD instrument (DART), Thermo Scientific Exactive Plus Orbitrap MS (ESI) and MSI.TOKYO Inc. MULTUM-FAB (FAB). Nuclear magnetic resonance (NMR) spectra were recorded on a JEOL JNM-ECA-400 (^{1}H 400 MHz, ^{13}C 100 MHz) and JNM-ECA-600 (^{1}H 600 MHz, ^{13}C 150 MHz) spectrometer. Chemical shifts for ^{1}H NMR are expressed in parts per million (ppm) relative to tetramethylsilane (δ 0.00 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, t = triplet, td = triplet of doublets, q = quartet, m = multiplet, br = broad signal), coupling constant (Hz), and integration.

2. Preparation of Arenecarboxylic Acid Phenyl Esters 1

2-1. Method A



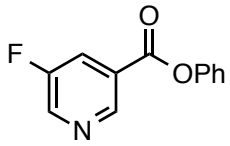
Thionyl chloride (0.5 M) was added to the carboxylic acid (1.0 equiv) and the mixture was refluxed for 1 h. The solution was concentrated *in vacuo*. To the residue were added CH_2Cl_2 (0.5 M), phenol (1.0 equiv), and then *N*,*N*-dimethyl-4-aminopyridine (DMAP: 1 mol%). After cooling the mixture to 0 °C, triethylamine (Et_3N: 1.2 equiv) was slowly added and then the reaction mixture was warmed to room temperature. After stirring the mixture for 1 h, $NaHCO_3$aq was added to the resulting mixture to quench the reaction. The mixture was extracted three times with CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, and then filtrated. The filtrate was concentrated *in vacuo* and the residue was purified by recrystallization or flash column chromatography to afford the corresponding phenyl ester **1**.



1X

Phenyl 6-(trifluoromethyl)nicotinate (1X)

Following the method A, purification by recrystallization (hexane) afforded **1X** as a white solid (741 mg, 88% yield; 3.15 mmol scale). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.48 (s, 1H), 8.64 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 8.0 Hz, 2H), 7.33 (t, J = 8.0 Hz, 1H), 7.24 (d, J = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 162.6, 151.7 (q, $J_{C–F}$ = 35 Hz), 151.4, 150.2, 139.3, 129.7, 128.1, 126.5, 121.4, 121.0 (q, $J_{C–F}$ = 279 Hz), 120.3 (q, $J_{C–F}$ = 3.0 Hz); HRMS (DART) *m*/*z* calcd for $C_{13}H_9F_3NO_2$ $[M+H]^+$: 268.0585, found: 268.0585.

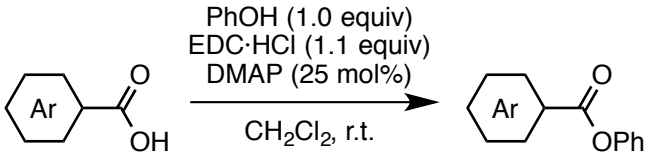


1Y

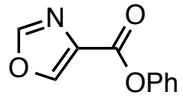
Phenyl 5-fluoronicotinate (1Y)

Following the method A, purification by flash column chromatography (hexane/EtOAc = 5:1) afforded **1Y** as a white solid (470 mg, 77% yield; 2.65 mmol scale). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.22 (s, 1H), 8.72 (d, J = 2.8 Hz, 1H), 8.16–8.11 (m, 1H), 7.45 (t, J = 8.0 Hz, 2H), 7.30 (t, J = 8.0 Hz, 1H), 7.23 (d, J = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 161.5 (d, $J_{C–F}$ = 238 Hz), 157.7, 150.3, 147.0 (d, $J_{C–F}$ = 4.0 Hz), 142.6 (d, $J_{C–F}$ = 24 Hz), 129.6, 126.9 (d, $J_{C–F}$ = 3.0 Hz), 126.4, 124.0 (d, $J_{C–F}$ = 20 Hz), 121.3; HRMS (DART) *m*/*z* calcd for $C_{12}H_9FNO_2$ $[M+H]^+$: 218.0617, found: 218.0620.

2-2. Method B



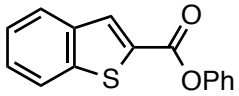
To a round-bottomed flask with the carboxylic acid (1.0 equiv) were added phenol (1.0 equiv), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC·HCl: 1.1 equiv), *N,N*-dimethyl-4-aminopyridine (DMAP: 0.25 equiv) and CH_2Cl_2 (0.5 M). After stirring the mixture for several hours with monitoring reaction progress with TLC, the reaction was quenched with saturated $NaHCO_3$aq and extracted three times with CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, filtrated, and concentrated *in vacuo*. The residue was purified by recrystallization or flash column chromatography to afford the corresponding phenyl ester **1**.



1Q

Phenyl oxazole-4-carboxylate (1Q)

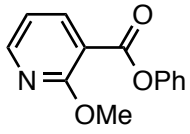
Following the method B, purification by flash column chromatography (hexane/EtOAc = 5:1) afforded **1Q** as a white solid (800 mg, 96% yield; 4.4 mmol scale). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.45 (s, 1H), 8.02 (s, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.2, 151.6, 150.1, 145.1, 132.7, 129.5, 126.2, 121.5; HRMS (DART) *m*/*z* calcd for $C_{10}H_8NO_3$ $[M+H]^+$: 190.0504, found: 190.0505.



1P

Phenyl benzo[*b*]thiophene-2-carboxylate (1P)

Following the method B, purification by recrystallization (hexane) afforded **1P** as a white solid (708 mg, 93% yield; 3.0 mmol scale). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.25 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.50 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.47–7.40 (m, 3H), 7.31–7.23 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 161.2, 150.6, 142.6, 138.6, 132.7, 131.9, 129.5, 127.3, 126.1, 125.7, 125.1, 122.8, 121.6; HRMS (DART) *m*/*z* calcd for $C_{15}H_{11}O_2S$ $[M+H]^+$: 255.0480, found: 255.0477.

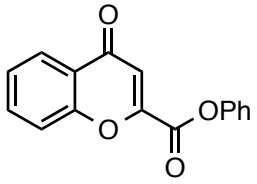


1AA

Phenyl 2-methoxynicotinate (1AA)

Following the method B, purification by flash column chromatography (hexane/EtOAc = 7:1) afforded **1AA** as colorless liquid (1.22 g, 91% yield; 6.0 mmol scale). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.38 (d, *J* = 5.2 Hz, 1H), 8.35 (d, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.01 (dd, *J* = 7.6, 5.2 Hz, 1H), 4.08 (s, 3H); ^{13}C NMR

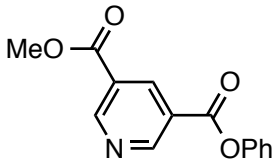
($CDCl_3$, 100 MHz) δ 163.4, 163.0, 151.6, 150.8, 141.8, 129.5, 126.0, 121.8, 116.5, 113.4, 54.3; HRMS (DART) *m*/*z* calcd for $C_{13}H_{12}NO_3$ $[M+H]^+$: 230.0817, found: 230.0819.



1AB

Phenyl 4-oxo-4*H*-chromene-2-carboxylate (1AB)

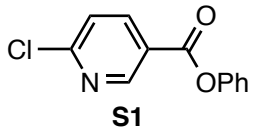
Following the method B, purification by flash column chromatography (hexane/EtOAc = 10:1) afforded **1AB** as a yellow solid (462 mg, 30% yield; 5.8 mmol scale). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.78 (t, *J* = 8.8 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.51–7.43 (m, 3H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.31 (s, 1H), 7.25 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 178.2, 159.1, 156.0, 151.6, 150.0, 134.9, 129.7, 126.7, 126.1, 125.8, 124.4, 121.1, 118.8, 115.7; HRMS (DART) *m*/*z* calcd for $C_{16}H_{11}O_4$ $[M+H]^+$: 267.0657, found: 267,0654.



1Z

3-Methyl 5-phenyl pyridine-3,5-dicarboxylate (1Z)

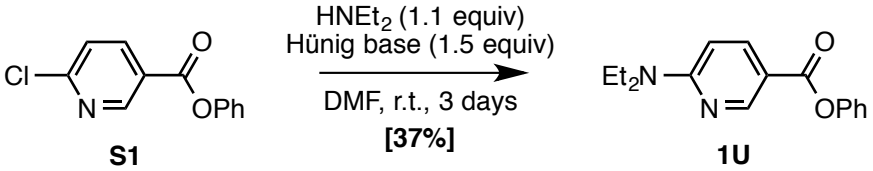
Following the method B, purification by recrystallization from hexane afforded **1Z** as a white solid (570 mg, 44% yield; 5.0 mmol scale). ^1H NMR ($CDCl_3$, 400 MHz) δ 9.53 (d, *J* = 0.8 Hz, 1H), 9.44 (d, *J* = 2.0 Hz, 1H), 9.03 (dd, *J* = 2.0, 0.8 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.32 (t, *J* = 8.0 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 4.02 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.8, 163.0, 154.7, 154.6, 150.3, 138.5, 129.6, 126.4, 126.1, 125.6, 121.4, 52.8; HRMS (DART) *m*/*z* calcd for $C_{14}H_{12}NO_4$ $[M+H]^+$: 258.0766, found: 258.0770.



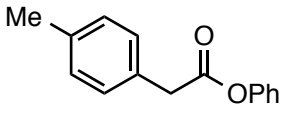
S1

Phenyl 6-chloronicotinate (S1)

Following the method B, purification by recrystallization (hexane) afforded **S1** as a white solid (1.82 g, 79% yield; 10 mmol scale). ^1H NMR ($CDCl_3$, 400 MHz) δ 9.17 (d, *J* = 2.8 Hz, 1H), 8.39 (dd, *J* = 8.4, 2.8 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.46 (dd, *J* = 8.0, 7.6 Hz, 2H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.0, 156.3, 151.6, 150.3, 140.0, 129.6, 126.4, 124.6, 124.4, 121.4; HRMS (DART) *m*/*z* calcd for $C_{12}H_9ClNO_2$ $[M+H]^+$: 234.0322, found: 234.0318.



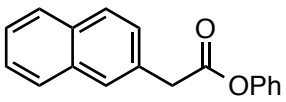
To a solution of phenyl 6-chloronicotinate (**S1**: 467 mg, 2.0 mmol) in DMF (4.0 mL) were added diethylamine (160.9 mg, 2.2 mmol, 1.1 equiv) and *N,N*-diisopropylethylamine (Hünig base: 510 mL, 3.0 mmol, 1.5 equiv). The mixture was stirred for 3 days at room temperature. The reaction was quenched with NH_4Claq and extracted four times with EtOAc. The combined organic layers were washed with brine, and then dried over Na_2SO_4. After filtration of the organic layer, the mixture was concentrated *in vacuo*. Purification by flash column chromatography (hexane/EtOAc = 15:1 to 10:1) afforded **1U** as a white solid (198 mg, 37% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.96 (d, *J* = 2.0 Hz, 1H), 8.08 (dd, *J* = 9.2, 2.0 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 6.48 (d, *J* = 9.2 Hz, 1H), 3.59 (q, *J* = 7.2 Hz, 4H), 1.22 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.8, 159.5, 152.3, 151.0, 138.4, 129.3, 125.5, 121.8, 112.2, 104.4, 42.9, 12.8; HRMS (DART) *m*/*z* calcd for $C_{16}H_{19}N_2O_2$ $[M+H]^+$: 271.1447, found: 271.1451.



1AG

Phenyl 2-(*p*-tolyl)acetate (1AG)

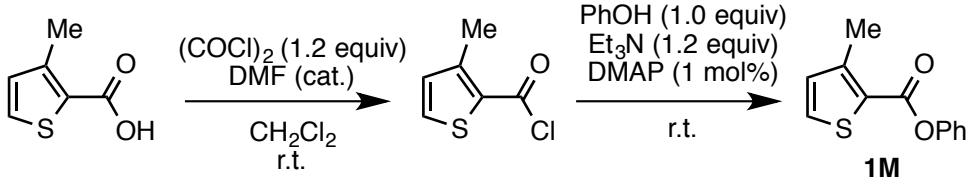
Following the method B, purification by flash column chromatography (hexane/EtOAc = 20:1) afforded **1AG** as colorless oil (1.12 g, 99% yield; 5 mmol scale). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.34 (t, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 7.6 Hz, 2H), 3.81 (s, 2H), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.2, 150.8, 137.0, 130.4, 129.4, 129.3, 129.1, 125.8, 121.4, 41.0, 21.1; HRMS (ESI) *m*/*z* calcd for $C_{15}H_{14}O_2Na$ $[M+Na]^+$: 249.0886, found: 249.0876.



1AH

Phenyl 2-(naphthalen-2-yl)acetate (1AH)

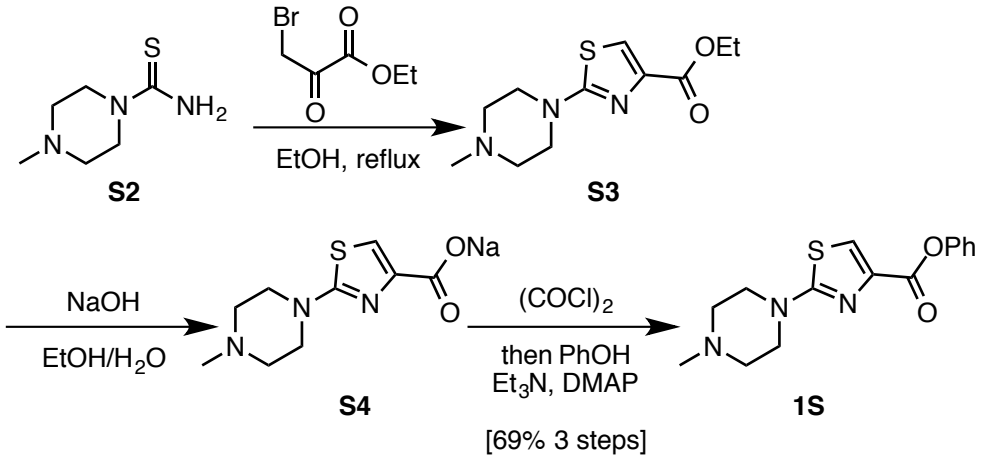
Following the method B, purification by recrystallization (hexane) afforded **1AH** as a white solid (1.10 g, 76% yield; 5 mmol scale). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.88–7.80 (m, 4H), 7.54–7.44 (m, 3H), 7.35 (dd, *J* = 8.0, 7.6 Hz, 2H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 2H), 4.02 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.0, 150.7, 133.5, 132.6, 130.9, 129.4, 128.4, 128.1, 127.71, 127.67, 127.2, 126.3, 126.0, 125.9, 121.4, 41.6; HRMS (ESI) *m*/*z* calcd for $C_{18}H_{14}O_2Na$ $[M+Na]^+$: 285.0886, found: 285.0876.



1M

Phenyl 3-methylthiophene-2-carboxylate (1M)

To a solution of 3-methylthiophene-2-carboxylic acid (713 mg, 5.0 mmol, 1.0 equiv) in CH_2Cl_2 (10 mL) were added oxalyl chloride (762 mg, 6.0 mmol, 1.2 equiv) and a portion of DMF. After stirring for 1.5 h at room temperature, phenol (470 mg, 5.0 mmol, 1.0 equiv) and *N,N*-dimethyl-4-aminopyridine (DMAP: 6.1 mg, 0.05 mmol, 1 mol%) were added to the mixture. Triethylamine (Et_3N: 470 mg, 6.0 mmol, 1.2 equiv) was slowly added to the mixture at 0 °C. After stirring the solution overnight, the reaction mixture was quenched with saturated $NaHCO_3$aq and extracted three times with CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, filtrated, and concentrated *in vacuo*. Purification by flash column chromatography (hexane/EtOAc = 20:1) afforded **1M** as brown oil (990 mg, 91% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.49 (d, *J* = 5.2 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 2H), 7.26 (t, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.99 (d, *J* = 5.2 Hz, 1H), 2.61 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 161.1, 150.5, 148.0, 131.9, 131.1, 129.4, 125.9, 125.6, 121.8, 16.1; HRMS (DART) *m*/*z* calcd for $C_{12}H_{11}O_2S$ $[M+H]^+$: 219.0480, found: 219.0483.



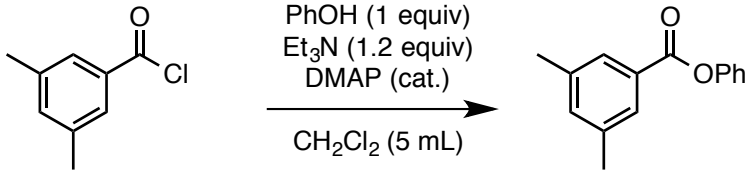
Phenyl 2-(4-methylpiperazin-1-yl)thiazole-4-carboxylate (1S)

A mixture of 4-methylpiperazine-1-carbothioamide (1.1 g, 6.7 mmol, 1.0 equiv) and ethyl 3-bromo-2-oxopropanoate (935 mL, 7.4 mmol, 1.1 equiv) in EtOH (10 mL) was refluxed overnight. After cooling to room temperature, the mixture was concentrated *in vacuo*. $NaHCO_3$aq was added to the resulted solid and the mixture was extracted with Et_2O. The combined organic layer was dried over $MgSO_4$, filtrated, and concentrated *in vacuo* to afford ethyl 2-(4-methylpiperazin-1-yl)thiazole-4-carboxylate (**S3**: 1.57 g, 91% yield) as orange oil. **S3** was used without further purification.

The obtained oil **S3** (1.57 g, 6.1 mmol) was treated with NaOH (270 mg, 6.7 mmol, 1.1 equiv) in EtOH/H_2O (10 mL/5 mL) at room temperature. After stirring overnight, the mixture was concentrated *in vacuo* to afford sodium 2-(4-methylpiperazin-1-yl)thiazole-4-carboxylate **S4** (1.53 g, quant.) as a yellow solid.

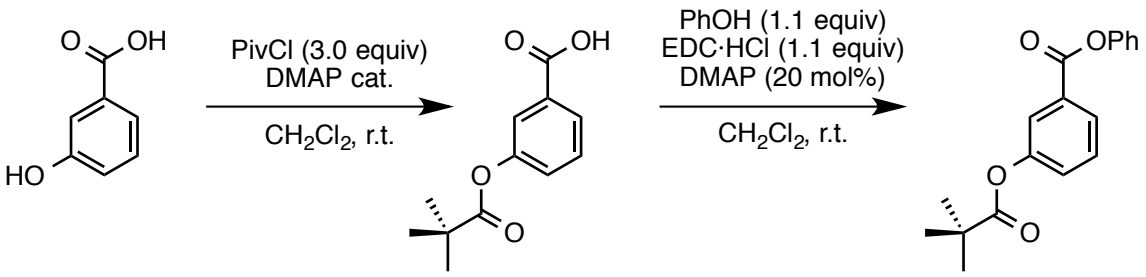
To a solution of the sodium carboxylate **S4** (1.53 g, 6.14 mmol) in CH_2Cl_2 (20 mL) were added oxalyl chloride (791 mL, 9.2 mmol, 1.5 equiv) and a portion of DMF. After stirring for 1.5

h, phenol (866 mg, 9.2 mmol, 1.5 equiv) and *N,N*-dimethyl-4-aminopyridine (DMAP: 10.0 mg, 0.05 mmol, 1 mol%) were added to the mixture. Then, triethylamine (Et_3N: 1.72 mL, 12 mmol, 2.0 equiv) was slowly added to the mixture at 0 °C. After stirring the solution overnight, the reaction mixture was quenched with saturated $NaHCO_3$aq and extracted three times with CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, filtrated, and concentrated *in vacuo*. Purification by flash column chromatography ($CHCl_3$/MeOH = 20:1) and then preparative HPLC (H_2O/MeCN) afforded phenyl 2-(4-methylpiperazin-1-yl)thiazole-4-carboxylate **1S** as a brown solid (1.38 g, 74% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.67 (s, 1H), 7.40 (dd, *J* = 8.0, 7.6 Hz, 2H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 2H), 3.59 (t, *J* = 4.8 Hz, 4H), 2.53 (t, *J* = 4.8 Hz, 4H), 2.34 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.9, 159.9, 150.7, 143.0, 129.4, 125.8, 121.7, 118.2, 54.1, 48.3, 46.1; HRMS (DART) *m*/*z* calcd for $C_{15}H_{18}N_3O_2S$ $[M+H]^+$: 304.1120, found: 304.1125.



1D

To a solution of phenol (470 mg, 5.0 mmol, 1.0 equiv), DMAP (6.0 mg, 0.05 mmol, 1 mol%) and Et_3N (607 mg, 6.0 mmol, 1.2 equiv) in CH_2Cl_2 (5 mL) was slowly added 3,5-dimethylbenzoyl chloride (0.74 mL, 5.0 mmol, 1.0 equiv) at 0 °C. After stirring for 3 h, the reaction mixture was quenched with saturated $NaHCO_3$aq and extracted three times with CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, filtrated, and concentrated *in vacuo*. Purification by flash column chromatography (hexane/EtOAc = 50:1) afforded **1D** as colorless liquid (1.13 g, quant). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.83 (s, 2H), 7.43 (t, *J* = 8.4 Hz, 2H), 7.30–7.24 (m, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 2.41 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.5, 151.0, 138.3, 135.2, 129.5, 129.4, 127.9, 125.8, 121.7, 21.2; HRMS (DART) *m*/*z* calcd for $C_{15}H_{15}O_2$ $[M+H]^+$: 227.1072, found: 227.1075.

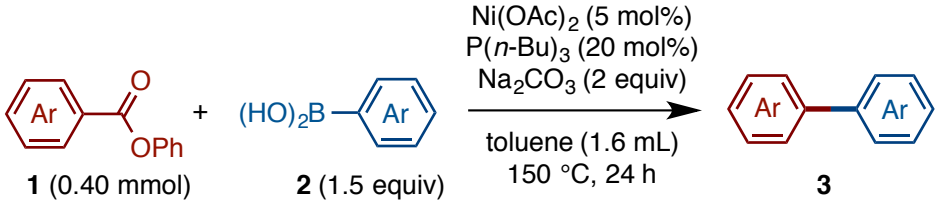


S5 **4**

To a solution of 3-hydroxybenzoic acid (1.38 g, 10 mmol) and DMAP (12.0 mg, 0.1 mmol, 1 mol%) in pyridine (12 mL) was added pivaloyl chloride (3.62 g, 30 mmol, 3.0 equiv) at 0 °C. This solution was allowed to warm to room temperature and stirred for 1 h. To the mixture was carefully added water (30 mL) and stirred overnight at room temperature. This solution was extracted three times with CH_2Cl_2. The combined organic layer was washed with 2.0M H_2SO_4 (20 mL) three times. The organic layer was dried over Na_2SO_4 and filtrated. The filtrate was concentrated *in vacuo* to afford 3-(pivaloyloxy)benzoic acid (**S5**: 2.15 g, 97% yield) as a white solid.

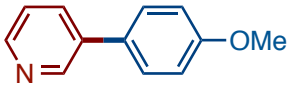
A mixture of **S5** (2.15 g, 9.7 mmol, 1.0 equiv), phenol (1.0 g, 10.7 mmol, 1.1 equiv), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC·HCl: 2.0 g, 10.7 mmol, 1.1 equiv), and *N,N*-dimethylaminopyridine (DMAP: 237 mg, 1.9 mmol, 0.2 equiv) in CH_2Cl_2 (20 mL) was stirred for 3 h at room temperature. After quenching the reaction with $NaHCO_3$aq, the mixture was extracted three times with CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, filtrated, and then concentrated *in vacuo*. The residue was purified by flash column chromatography (hexane/EtOAc = 20:1) to afford phenyl 3-(pivaloyloxy)benzoate **4** as a white solid (2.56 g, 88% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.07 (d, J = 8.0 Hz, 1H), 7.88 (s, 1H), 7.52 (t, J = 8.0 Hz, 1H), 7.43 (t, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 1H), 7.27 (t, J = 8.0 Hz, 1H), 7.20 (d, J = 8.0 Hz, 2H), 1.36 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 176.9, 164.3, 151.2, 150.8, 131.0, 129.54, 129.50, 127.4, 127.0, 126.0, 123.3, 121.6, 39.1, 27.1; HRMS (DART) *m/z* calcd for $C_{18}H_{19}O_4$ $[M+H]^+$: 299.1283, found: 299.1285.

3. Procedure for the Ni-Catalyzed Decarbonylative Cross-Coupling of 1 and 2



1 (0.40 mmol) **2** (1.5 equiv) **3**

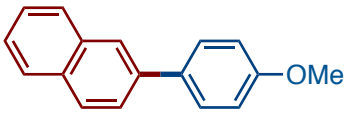
General Procedure: A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar and $Ni(OAc)_2·4H_2O$ (5.0 mg, 0.020 mmol, 5 mol%) was dried with a heatgun under reduced pressure and filled with N_2 gas after cooling to room temperature. To this vessel was added phenyl arenecarboxylic acid phenyl ester **1** (0.40 mmol, 1.0 equiv), arylboronic acid **2** (0.60 mmol, 1.5 equiv), and Na_2CO_3 (84.8 mg, 0.8 mmol, 2.0 equiv). The vessel was vacuumed and refilled N_2 gas three times. To this was added P(*n*-Bu)$_3$ (19.0 mL, 0.08 mmol, 20 mol%) and toluene (1.6 mL). The vessel was sealed with O-ring tap and then heated at 150 °C for 24 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a short silica gel pad with EtOAc. The filtrate was concentrated and the residue was purified by flash column chromatography or PTLC to afford the corresponding cross-coupling product **3**.



3Aa

3-(4-Methoxyphenyl)pyridine (3Aa)[9]

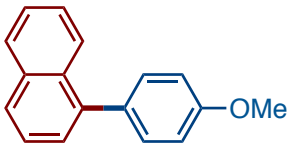
Purification by flash column chromatography (hexane/Et_2O = 2:1) afforded **3Aa** as a white solid (using 5 mol% catalyst, for 24 h; 69.7 mg, 95% yield: using 3 mol% catalyst, for 48 h; 73.4 mg, >99% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.82 (d, J = 2.4 Hz, 1H), 8.55 (d, J = 4.8 Hz, 1H), 7.83 (dd, J = 8.0, 2.4 Hz, 1H), 7.53 (d, J = 9.2 Hz, 2H), 7.34 (dd, J = 8.0, 4.8 Hz, 1H), 7.02 (d, J = 9.2 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.7, 147.9, 147.8, 136.2, 133.8, 130.2, 128.1, 123.4, 114.5, 55.3; HRMS (ESI) *m/z* calcd for $C_{12}H_{12}NO$ $[M+H]^+$: 186.0913, found: 186.0912.



3Ba

2-(4-Methoxyphenyl)naphthalene (3Ba)[10]

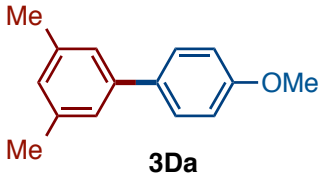
Purification by flash column chromatography (hexane/$CHCl_3$ = 5:1) afforded **3Ba** as a white solid (84.9 mg, 91% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.98 (s, 1H), 7.91–7.82 (m, 3H), 7.71 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 2H), 7.52–7.42 (m, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.2, 138.1, 133.7, 133.6, 132.3, 128.4, 128.3, 128.0, 127.6, 126.2, 125.6, 125.4, 125.0, 114.3, 55.4; HRMS (DART) *m*/*z* calcd for $C_{17}H_{15}O$ $[M+H]^+$: 235.1123, found: 235.1120.



3Ca

1-(4-Methoxyphenyl)naphthalene (3Ca)[11]

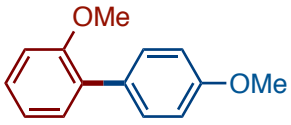
Purification by flash column chromatography (hexane/EtOAc = 100:1) afforded **3Ca** as a white solid (90.2 mg, 96% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.92 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.85–7.35 (m, 6H), 6.99 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.9, 139.9, 133.8, 133.1, 131.8, 131.1, 128.2, 127.3, 126.9, 126.0, 125.9, 125.7, 125.4, 113.7, 55.3; HRMS (DART) *m*/*z* calcd for $C_{17}H_{15}O$ $[M+H]^+$: 235.1123, found: 235.1122.



3Da

4'-Methoxy-3,5-dimethyl-1,1'-biphenyl (3Da) [12]

Purification by flash column chromatography (hexane/EtOAc = 100:1) afforded **3Da** as colorless liquid (63.8 mg, 75% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.49 (d, *J* = 9.2 Hz, 2H), 7.16 (s, 2H), 6.97–6.91 (m, 3H), 3.81 (s, 3H), 2.35 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.0, 140.8, 138.1, 133.9, 128.3, 128.1, 124.6, 114.0, 55.2, 21.4; HRMS (DART) *m*/*z* calcd for $C_{15}H_{17}O$ $[M+H]^+$: 213.1279, found: 213.1277.

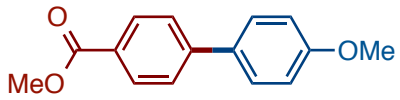


3Ea

2,4'-Dimethoxy-1,1'-biphenyl (3Ea)[13]

Purification by PTLC (hexane/EtOAc= 20:1) afforded **3Ea** as colorless oil (66.1 mg, 77% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.46 (d, *J* = 8.8 Hz, 2H), 7.32–7.25 (m, 2H), 7.00 (dd, *J* =

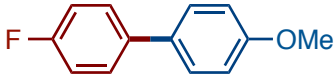
8.0, 7.2 Hz, 1H), 6.97–6.91 (m, 3H), 3.82 (s, 3H), 3.79 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.6, 156.4, 130.8, 130.63, 130.55, 130.2, 128.1, 120.8, 113.4, 111.1, 55.5, 55.2; HRMS (DART) *m/z* calcd for $C_{14}H_{15}O_2$ $[M+H]^+$: 215.1072, found: 215.1076.



3Fa

Methyl 4'-methoxy-[1,1'-biphenyl]-4-carboxylate (3Fa)[14]

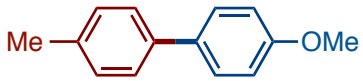
Purification by flash column chromatography (hexane/$CHCl_3$ = 4:1 to 1:1) afforded **3Fa** as a white solid (85.0 mg, 88% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.07 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 3.92 (s, 3H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 167.0, 159.8, 145.1, 132.3, 130.0, 128.3, 128.2, 126.4, 114.3, 55.3, 52.0; HRMS (DART) *m/z* calcd for $C_{15}H_{15}O_3$ $[M+H]^+$: 243.1021, found: 243.1019.



3Ga

4-Fluoro-4'-methoxy-1,1'-biphenyl (3Ga)[9]

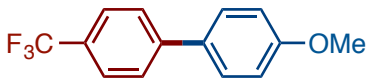
Purification by flash column chromatography (hexane/$CHCl_3$ = 10:1 to 4:1) afforded **3Ga** as a white solid (68.9 mg, 85% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.51–7.43 (m, 4H), 7.12–7.06 (m, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 162.1 (d, J_{C-F} = 249 Hz), 159.1, 136.9 (d, J_{C-F} = 4.0 Hz), 132.8, 128.2 (d, J_{C-F} = 8.0 Hz), 128.0, 115.5 (d, J_{C-F} = 21 Hz), 114.2, 55.3; HRMS (DART) *m/z* calcd for $C_{13}H_{12}FO$ $[M+H]^+$: 203.0872, found: 203.0870.



3Ha

4-Methoxy-4'-methyl-1,1'-biphenyl (3Ha)[15]

Purification by flash column chromatography (hexane/$CHCl_3$ = 10:1 to 4:1) afforded **3Ha** as a white solid (70.3 mg, 89% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.50 (d, *J* = 8.8 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.84 (s, 3H), 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.9, 137.9, 136.3, 133.7, 129.4, 127.9, 126.6, 114.1, 55.3, 21.0; HRMS (DART) *m/z* calcd for $C_{14}H_{15}O$ $[M+H]^+$: 199.1123, found: 199.1121.

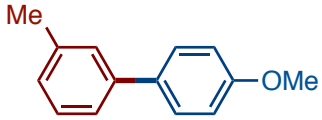


3Ia

4-Methoxy-4'-(trifluoromethyl)-1,1'-biphenyl (3Ia)[9]

The reaction was conducted at 160 °C. Purification by flash column chromatography (hexane/$CHCl_3$ = 4:1) afforded **3Ia** as a white solid (99.5 mg, 99% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.67–7.62 (m, 4H), 7.53 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H); ^{13}C

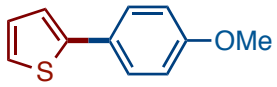
NMR ($CDCl_3$, 100 MHz) δ 159.8, 144.3, 132.1, 128.7 (q, J_{C-F} = 33 Hz), 128.3, 126.8, 125.7 (q, J_{C-F} = 4 Hz), 124.4 (q, J_{C-F} = 276 Hz), 114.4, 55.3; HRMS (DART) *m/z* calcd for $C_{14}H_{12}F_3O$ $[M+H]^+$: 253.0840, found: 253.0838.



3Ja

4'-Methoxy-3-methyl-1,1'-biphenyl (3Ja)[16]

Purification by PTLC (hexane/EtOAc = 20:1) afforded **3Ja** as a white solid (57.8 mg, 73% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.51 (d, *J* = 9.2 Hz, 2H), 7.38–7.25 (m, 3H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.94 (d, *J* = 9.2 Hz, 2H), 3.80 (s, 3H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.0, 140.7, 138.2, 133.8, 128.6, 128.1, 127.5, 127.4, 123.8, 114.1, 55.2, 21.5; HRMS (DART) *m/z* calcd for $C_{14}H_{15}O$ $[M+H]^+$: 199.1123, found: 199.1120.



3Ka

2-(4-Methoxyphenyl)thiophene (3Ka)[12]

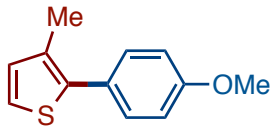
Purification by PTLC (hexane/EtOAc = 30:1) afforded **3Ka** as a white solid (59.3 mg, 78% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.53 (d, *J* = 8.4 Hz, 2H), 7.21–7.16 (m, 2H), 7.03 (d, *J* = 4.4 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.1, 144.3, 127.9, 127.23, 127.16, 123.8, 122.0, 114.2, 55.3; HRMS (ESI) *m/z* calcd for $C_{11}H_{11}OS$ $[M+H]^+$: 191.0525, found: 191.0522.



3La

3-(4-Methoxyphenyl)thiophene (3La)[17]

Purification by flash column chromatography (hexane/EtOAc = 100:1) afforded **3La** as a white solid (50.6 mg, 66% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.52 (d, *J* = 7.6 Hz, 2H), 7.38–7.30 (m, 3H), 6.92 (d, *J* = 7.6 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.8, 142.0, 128.7, 127.5, 126.2, 126.0, 118.9, 114.1, 55.3; HRMS (DART) *m/z* calcd for $C_{11}H_{10}OS$ $[M+H]^+$: 191.0531, found: 191.0533.



3Ma

2-(4-Methoxyphenyl)-3-methylthiophene (3Ma)

Purification by flash column chromatography (hexane/EtOAc = 100:1) afforded **3Ma** as colorless liquid (49.4 mg, 60% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 7.37 (d, *J* = 7.6 Hz, 2H),

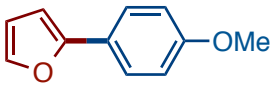
7.13 (d, J = 5.6 Hz, 1H), 6.93 (d, J = 7.6 Hz, 2H), 6.88 (d, J = 5.6 Hz, 1H), 3.81 (s, 3H), 2.28 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.8, 137.6, 132.5, 130.9, 130.2, 127.1, 122.6, 113.9, 55.2, 14.8; HRMS (ESI) m/z calcd for $C_{12}H_{13}OS$ $[M+H]^+$: 205.0682, found: 205.0680



3Na

3-(4-Methoxyphenyl)furan (3Na)[12]

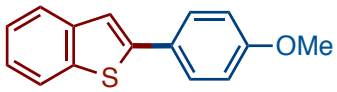
Purification by flash column chromatography (hexane/EtOAc = 100:1) afforded **3Na** as a white solid (46.9 mg, 67% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.65 (d, J = 1.6 Hz, 1H), 7.44 (t, J = 1.6 Hz, 1H), 7.40 (d, J = 8.8 Hz, 2H), 6.91 (d, J = 8.8 Hz, 2H), 6.64 (d, J = 1.6 Hz, 1H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.7, 143.5, 137.6, 127.0, 126.0, 125.0, 114.2, 108.8, 55.3; HRMS (ESI) m/z calcd for $C_{11}H_{11}O_2$ $[M+H]^+$: 175.0754, found: 175.0752.



3Oa

2-(4-Methoxyphenyl)furan (3Oa)[18]

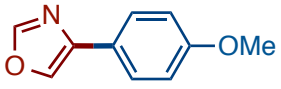
The reaction was conducted using 1.2 equiv of Na_2CO_3. Purification by flash column chromatography (hexane/EtOAc = 100:1) afforded **3Oa** as a white solid (51.0 mg, 73% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.60 (d, J = 8.8 Hz, 2H), 7.41 (d, J = 1.6 Hz, 1H), 6.91 (d, J = 8.8 Hz, 2H), 6.50 (d, J = 3.2 Hz, 1H), 6.43 (dd, J = 3.2, 1.6 Hz, 1H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.0, 154.0, 141.3, 125.2, 124.0, 114.0, 111.5, 103.3, 55.3; HRMS (ESI) m/z calcd for $C_{11}H_{11}O_2$ $[M+H]^+$: 175.0754, found: 175.0752.



3Pa

2-(4-Methoxyphenyl)benzo[*b*]thiophene (3Pa)[19]

Purification by precipitation of the crude mixture in Et_2O and filtration of the suspension afforded **3Pa** as a white solid (91.7 mg, 95% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.80 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 7.2 Hz, 1H), 7.64 (d, J = 8.8 Hz, 2H), 7.42 (s, 1H), 7.36–7.25 (m, 2H), 6.96 (d, J = 8.8 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.8, 144.1, 140.9, 139.1, 127.7, 127.0, 124.4, 123.9, 123.2, 122.2, 118.2, 114.3, 55.4; HRMS (ESI) m/z calcd for $C_{15}H_{13}OS$ $[M+H]^+$: 241.0682, found: 241.0678.

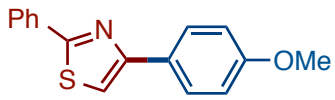


3Qa

4-(4-Methoxyphenyl)oxazole (3Qa)[20]

Purification by PTLC (hexane/EtOAc = 5:1) afforded **3Qa** as a white solid (35.5 mg, 50% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.91 (s, 1H), 7.86 (s, 1H), 7.68 (d, J = 8.4 Hz, 2H), 6.95 (d,

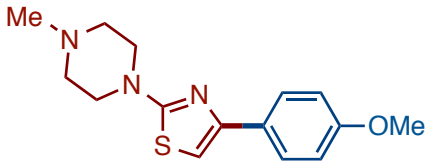
J = 8.4 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.6, 151.2, 140.2, 132.6, 126.9, 123.4, 114.2, 55.3; HRMS (ESI) m/z calcd for $C_{10}H_{10}NO_2$ $[M+H]^+$: 176.0706, found: 176.0704.



3Ra

4-(4-Methoxyphenyl)-2-phenylthiazole (3Ra)[21]

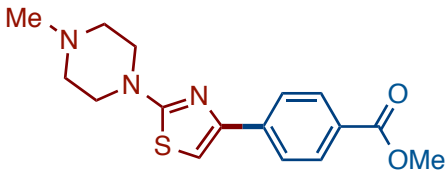
The reaction was conducted at 160 °C. Purification by PTLC (hexane/$CHCl_3$ = 1:1) afforded **3Ra** as a white solid (86.8 mg, 81% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.03 (dd, J = 8.4, 2.0 Hz, 2H), 7.92 (d, J = 8.4 Hz, 2H), 7.47–7.38 (m, 3H), 7.31 (s, 1H), 6.96 (d, J = 7.2 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 167.6, 159.6, 156.0, 133.8, 129.9, 128.9, 127.7, 127.5, 126.5, 114.0, 110.9, 55.3; HRMS (DART) m/z calcd for $C_{16}H_{14}NOS$ $[M+H]^+$: 268.0796, found: 268.0795.



3Sa

4-(4-Methoxyphenyl)-2-(4-methylpiperazin-1-yl)thiazole (3Sa)

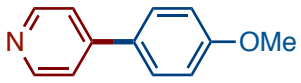
Purification by PTLC ($CHCl_3$/MeOH = 50:1) afforded **3Sa** as a yellow solid (54.5 mg, 47% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.76 (d, J = 8.4 Hz, 2H), 6.90 (d, J = 8.4 Hz, 2H), 6.62 (s, 1H), 3.82 (s, 3H), 3.56 (t, J = 5.2 Hz, 4H), 2.54 (t, J = 5.2 Hz, 4H), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.9, 159.2, 151.6, 128.1, 127.3, 113.8, 99.6, 55.2, 54.5, 48.2, 46.2; HRMS (DART) m/z calcd for $C_{15}H_{20}N_3OS$ $[M+H]^+$: 290.1327, found: 290.1329.



3Si

Methyl 4-(2-(4-methylpiperazin-1-yl)thiazol-4-yl)benzoate (3Si)

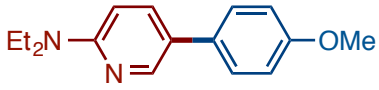
The reaction was conducted at 160 °C. Purification by PTLC ($CHCl_3$/MeOH = 50:1) afforded **3Si** as a brown solid (63.2 mg, 51% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.03 (d, J = 8.4 Hz, 2H), 7.90 (d, J = 8.4 Hz, 2H), 6.91 (s, 1H), 3.92 (s, 3H), 3.59 (t, J = 5.2 Hz, 4H), 2.55 (t, J = 5.2 Hz, 4H), 2.36 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.0, 167.0, 150.8, 139.1, 129.9, 128.8, 125.8, 103.7, 54.2, 52.0, 48.3, 46.2; HRMS (DART) m/z calcd for $C_{16}H_{20}N_3O_2S$ $[M+H]^+$: 318.1276, found: 318.1275.



3Ta

4-(4-Methoxyphenyl)pyridine (3Ta)[22]

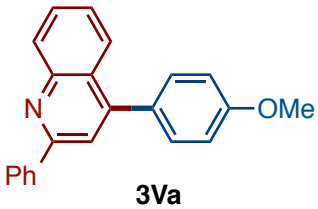
The reaction was conducted using 1.5 equiv of Et_3N instead of Na_2CO_3. Purification by flash column chromatography (hexane/Et_2O = 1:1) afforded **3Ta** as a white solid (69.7 mg, 94% yield). ^{1}H NMR ($CDCl_3$, 600 MHz) δ 8.62 (d, *J* = 6.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 6.4 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 160.5, 150.1, 147.7, 130.3, 128.1, 121.0, 114.5, 55.3; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{12}NO$ $[M+H]^+$: 186.0913, found: 186.0910.



3Ua

***N*,*N*-Diethyl-5-(4-methoxyphenyl)pyridin-2-amine (3Ua)**

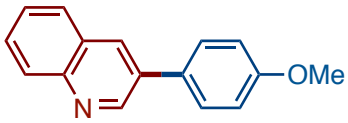
Purification by PTLC (hexane/EtOAc = 10:1) and then GPC afforded **3Ua** as a white solid (64.3 mg, 63% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.37 (d, *J* = 2.4 Hz, 1H), 7.60 (dd, *J* = 9.2, 2.4 Hz, 1H), 7.41 (d, *J* = 9.2 Hz, 2H), 6.95 (d, *J* = 9.2 Hz, 2H), 6.51 (d, *J* = 9.2 Hz, 1H), 3.82 (s, 3H), 3.52 (q, *J* = 7.2 Hz, 4H), 1.20 (t, *J* =7.2 Hz, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.4, 156.4, 145.9, 135.5, 131.4, 126.9, 123.6, 114.2, 105.3, 55.3, 42.5, 13.0; HRMS (DART) *m*/*z* calcd for $C_{16}H_{21}N_2O$ $[M+H]^+$: 257.1654, found: 257.1658.



3Va

4-(4-Methoxyphenyl)-2-phenylquinoline (3Va)[23]

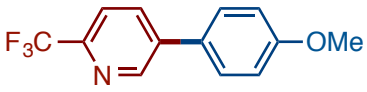
The reaction was conducted using 1.5 equiv of Et_3N instead of Na_2CO_3. Purification by flash column chromatography (hexane/EtOAc = 30:1) afforded **3Va** as a white solid (125.6 mg, >99% yield). ^{1}H NMR ($CDCl_3$, 600 MHz) δ 8.23 (d, *J* = 8.4 Hz, 1H), 8.18 (d, *J* = 7.2 Hz, 2H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.79 (s, 1H), 7.71 (td, *J* = 8.4, 1.2 Hz, 1H), 7.54–7.42 (m, 6H), 7.07, (d, *J* = 8.4 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 159.8, 156.9, 148.9, 148.8, 139.7, 130.8, 130.6, 130.1, 129.4, 129.2, 128.8, 127.5, 126.2, 125.9, 125.6, 119.3, 114.0, 55.4; HRMS (DART) *m*/*z* calcd for $C_{22}H_{18}NO$ $[M+H]^+$: 312.1388, found: 312.1389.



3Wa

3-(4-Methoxyphenyl)quinoline (3Wa)[13]

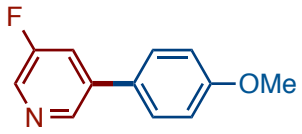
Purification by PTLC (hexane/EtOAc = 5:1) afforded **3Wa** as a white solid (98.7 mg, >99% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.16 (d, *J* = 2.4 Hz, 1H), 8.21 (d, *J* = 2.4 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.68 (dd, *J* = 8.4, 7.8 Hz, 1H), 7.63 (d, *J* = 9.2 Hz, 2H), 7.54 (dd, *J* = 8.4, 7.8 Hz, 1H), 7.03 (d, *J* = 9.2 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.7, 149.8, 146.9, 133.3, 132.3, 130.2, 129.1, 129.0, 128.4, 128.0, 127.8, 126.8, 114.6, 55.3; HRMS (ESI) *m*/*z* calcd for $C_{16}H_{14}NO$ $[M+H]^+$: 236.1070, found: 236.1073.



3Xa

5-(4-Methoxyphenyl)-2-(trifluoromethyl)pyridine (3Xa)

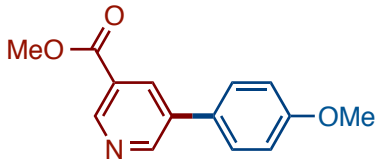
The reaction was conducted using 1.5 equiv of Et_3N instead of Na_2CO_3. Purification by flash column chromatography (hexane/EtOAc = 10:1) afforded **3Xa** as a white solid (89 mg, 88% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.90 (s, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.54 (d, J = 9.0 Hz, 2H), 7.03 (d, J = 9.0 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.4, 148.0, 146.0 (q, J_{C-F} = 35 Hz), 139.0, 134.7, 128.6, 128.4, 121.7 (q, J_{C-F} = 275 Hz), 120.3, 114.8, 55.3; HRMS (DART) *m*/*z* calcd for $C_{13}H_{11}F_3NO$ $[M+H]^+$: 254.0793, found: 254.0790.



3Ya

3-Fluoro-5-(4-methoxyphenyl)pyridine (3Ya)

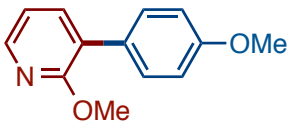
Purification by PTLC (hexane/EtOAc = 4:1) afforded **3Ya** as a white solid (75.2 mg, 92% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.62 (s, 1H), 8.39 (s, 1H), 7.54–7.47 (m, 3H), 6.99 (d, J = 8.8 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.0, 159.6 (d, J_{C-F} = 260 Hz), 143.6 (d, J_{C-F} = 4 Hz), 137.7 (d, J_{C-F} = 4 Hz), 135.7 (d, J_{C-F} = 24 Hz), 128.5, 128.2, 120.2 (d, J_{C-F} = 19 Hz), 114.5, 55.2; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{11}FNO$ $[M+H]^+$: 204.0819, found: 204.0820.



3Za

Methyl 5-(4-methoxyphenyl)nicotinate (3Za)

The reaction was conducted using 1.2 equiv of Na_2CO_3. Purification by flash column chromatography (hexane/EtOAc = 4:1) afforded **3Za** as a white solid (85.8 mg, 88% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 9.14 (s, 1H), 8.96 (d, J = 2.0 Hz, 1H), 8.43 (d, J = 2.0 Hz, 1H), 7.56 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.0 Hz, 2H), 3.98 (s, 3H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.8, 160.0, 151.3, 148.6, 135.9, 134.5, 128.8, 128.2, 125.8, 114.6, 55.3, 52.4; HRMS (DART) *m*/*z* calcd for $C_{14}H_{14}NO_3$ $[M+H]^+$: 244.0974, found: 244.0971.

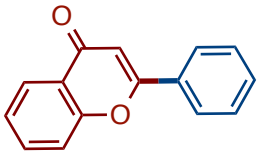


3AAa

2-Methoxy-3-(4-methoxyphenyl)pyridine (3AAa)[24]

Purification by PTLC (hexane/EtOAc = 10:1) afforded **3AAa** as a white solid (72.4 mg, 84% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.12 (dd, J = 4.8, 1.2 Hz, 1H), 7.57 (dd, J = 8.0, 1.2

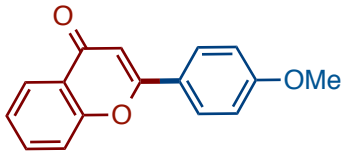
Hz, 1H), 7.50 (d, J = 8.0 Hz, 2H), 6.99–6.92 (m, 3H), 3.97 (s, 3H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.8, 159.0, 145.1, 138.1, 130.2, 129.0, 124.3, 117.1, 113.6, 55.2, 53.5; HRMS (ESI) m/z calcd for $C_{13}H_{14}NO_2$ $[M+H]^+$: 216.1019, found: 216.1020.



3ABh

2-Phenyl-4*H*-chromen-4-one (3ABh)[25]

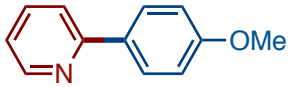
Purification by flash column chromatography (hexane/EtOAc = 6:1) afforded **3ABh** as a white solid (80.0 mg, 90% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.22 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 7.6 Hz, 2H), 7.68 (dd, J = 8.0, 7.6 Hz, 1H), 7.60–7.46 (m, 4H), 7.40 (dd, J = 8.0, 7.6 Hz, 1H), 6.81 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 178.3, 163.2, 156.1, 133.7, 131.6, 131.5, 128.9, 126.2, 125.6, 125.1, 123.8, 118.0, 107.5; HRMS (ESI) m/z calcd for $C_{15}H_{11}O$ $[M+H]^+$: 223.0754, found: 223.0756.



3ABa

2-(4-Methoxyphenyl)-4*H*-chromen-4-one (3ABa)[25]

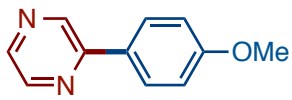
Purification by PTLC (hexane/Et_2O = 1:1, hexane/EtOAc= 3:1, and then $CHCl_3$) afforded **3ABa** as a white solid (100.8 mg, >99% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.21 (d, J = 7.6 Hz, 1H), 7.86 (d, J = 8.0 Hz, 2H), 7.66 (dd, J = 7.6, 7.2 Hz, 1H), 7.52 (d, J = 7.6 Hz, 1H), 7.39 (dd, J = 7.6, 7.2 Hz, 1H), 6.99 (d, J = 8.0 Hz, 2H), 6.72 (s, 1H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 178.2, 163.3, 162.3, 156.1, 133.5, 127.9, 125.5, 125.0, 123.9, 117.9, 114.4, 106.1, 55.4; HRMS (DART) m/z calcd for $C_{16}H_{13}O_3$ $[M+H]^+$: 253.0865, found: 253.0861.



3ACa

2-(4-Methoxyphenyl)pyridine (3ACa)[26]

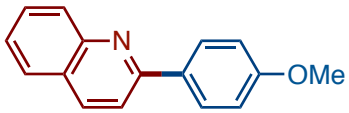
Purification by flash column chromatography (hexane/Et_2O = 5:1 to 7:3) afforded **3ACa** as a white solid (9.0 mg, 12% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.66 (d, J = 4.4 Hz, 1H), 7.95 (d, J = 8.4 Hz, 2H), 7.75–7.64 (m, 2H), 7.17 (dd, J = 7.2, 4.4 Hz, 1H), 7.00 (d, J = 8.4 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.5, 157.1, 149.5, 136.6, 132.0, 128.1, 121.4, 119.8, 114.1, 55.3; HRMS (ESI) m/z calcd for $C_{12}H_{12}NO$ $[M+H]^+$: 186.0913, found: 186.0909.



3ADa

2-(4-Methoxyphenyl)pyrazine (3ADa)[27]

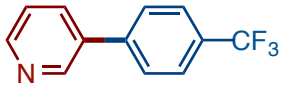
Purification by flash column chromatography (hexane/Et_2O = 1:1) afforded **3ADa** as a white solid (17.0 mg, 23% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.98 (s, 1H), 8.58 (d, J = 2.4 Hz, 1H), 8.44 (d, J = 2.4 Hz, 1H), 7.98 (d, J = 7.2 Hz, 2H), 7.03 (d, J = 7.2 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 161.1, 152.5, 144.0, 142.1, 141.6, 128.8, 128.3, 114.4, 55.4; HRMS (ESI) m/z calcd for $C_{11}H_{11}N_2O$ $[M+H]^+$: 187.0866, found: 187.0864.



3AEa

2-(4-Methoxyphenyl)quinoline (3AEa)[28]

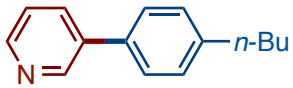
Purification by flash column chromatography (hexane/EtOAc = 20:1) afforded **3AEa** as a white solid (34.3 mg, 36% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.20–8.11 (m, 4H), 7.83 (d, J = 8.8 Hz, 1H), 7.80 (d, J = 8.8 Hz, 1H), 7.71 (td, J = 7.2, 1.2 Hz, 1H), 7.50 (td, J = 7.2, 1.2 Hz, 1H), 7.05 (d, J = 9.2 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.8, 156.9, 148.3, 136.6, 132.2, 129.6, 129.5, 128.9, 127.4, 126.9, 125.9, 118.5, 114.2, 55.4; HRMS (ESI) m/z calcd for $C_{16}H_{14}NO$ $[M+H]^+$: 236.1070, found: 236.1078.



3Ab

3-(4-(Trifluoromethyl)phenyl)pyridine (3Ab)[29]

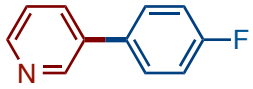
Purification by flash column chromatography (hexane/Et_2O = 2:1) afforded **3Ab** as a white solid (64.5 mg, 72% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.87 (s, 1H), 8.66 (d, J = 4.0 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.74 (d, J = 8.8 Hz, 2H), 7.68 (d, J = 8.8 Hz, 2H), 7.41 (dd, J = 8.0, 4.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 149.3, 148.3, 141.3, 135.2, 134.4, 130.2 (q, J_{C-F} = 32 Hz), 127.4, 126.0 (q, J_{C-F} = 4.0 Hz), 124.0 (q, J_{C-F} = 277 Hz), 123.6; HRMS (ESI) m/z calcd for $C_{12}H_9F_3N$ $[M+H]^+$: 224.0682, found: 224.0684.



3Ac

3-(4-Butylphenyl)pyridine (3Ac)[30]

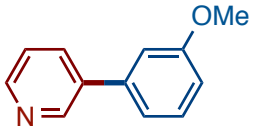
Purification by PTLC (hexane/EtOAc = 4:1) afforded **3Ac** as colorless liquid (63.0 mg, 75% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.84 (d, J = 2.4 Hz, 1H), 8.56 (dd, J = 4.8, 2.4 Hz, 1H), 7.87 (dd, J = 8.0, 4.8 Hz, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.35 (dd, J = 8.0, 4.8 Hz, 1H), 7.29 (d, J = 8.0 Hz, 2H), 2.67 (t, J = 8.0 Hz, 2H), 1.70–1.59 (m, 2H), 1.46–1.32 (m, 2H), 0.95 (t, J = 7.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.24, 148.19, 143.0, 136.6, 135.1, 134.1, 129.2, 127.0, 123.5, 35.3, 33.6, 22.4, 13.9; HRMS (ESI) m/z calcd for $C_{15}H_{18}N$ $[M+H]^+$: 212.1434, found: 212.1433.



3Ad

3-(4-Fluorophenyl)pyridine (3Ad)[29]

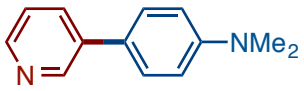
Purification by flash column chromatography (hexane/EtOAc = 6:1) afforded **3Ad** as a white solid (62.1 mg, 90% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.81 (s, 1H), 8.59 (d, J = 4.8 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.59–7.50 (m, 2H), 7.36 (dd, J = 8.0, 4.8 Hz, 1H), 7.20–7.11 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 162.8 (d, J_{C-F} = 249 Hz), 148.4, 148.1, 135.6, 134.1, 133.8, 128.7 (d, J_{C-F} = 8.0 Hz), 123.9, 116.0 (d, J_{C-F} = 21 Hz); HRMS (ESI) m/z calcd for $C_{11}H_9FN$ $[M+H]^+$: 174.0714, found: 174.0711.



3Ae

3-(3-Methoxyphenyl)pyridine (3Ae)[31]

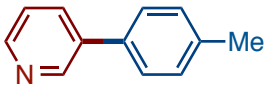
Purification by PTLC (hexane/Et_2O = 1:1) afforded **3Ae** as colorless liquid (65.2 mg, 88% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.85 (s, 1H), 8.59 (d, J = 4.8 Hz, 1H), 7.86 (dd, J = 8.0, 2.4 Hz, 1H), 7.42–7.32 (m, 2H), 7.16 (dd, J = 8.0, 4.8 Hz, 1H), 7.10 (s, 1H), 6.94 (dd, J = 8.0, 2.4 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.0, 148.6, 148.3, 139.2, 136.4, 134.3, 130.1, 123.4, 119.5, 113.3, 112.9, 55.3; HRMS (ESI) m/z calcd for $C_{12}H_{12}ON$ $[M+H]^+$: 186.0913, found: 186.0910.



3Af

***N*,*N*-Dimethyl-4-(pyridin-3-yl)aniline (3Af)**[32]

The reaction was conducted using 1.5 equiv of Et_3N instead of Na_2CO_3. Purification by flash column chromatography (hexane/EtOAc = 4:1) afforded **3Af** as a white solid (39.3 mg, 50% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.82 (s, 1H), 8.48 (d, J = 4.8 Hz, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.49 (d. J = 8.8 Hz, 2H), 7.30 (dd, J = 8.0, 4.8 Hz, 1H), 6.82 (d, J = 8.8 Hz, 2H), 3.01 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 150.4, 147.7, 147.1, 136.6, 133.2, 127.7, 125.4, 123.4, 112.8, 40.4; HRMS (ESI) m/z calcd for $C_{13}H_{15}N_2$ $[M+H]^+$: 199.1230, found: 199.1228.

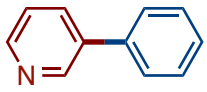


3Ag

3-(4-Methyl)pyridine (3Ag)[29]

Purification by flash column chromatography (hexane/EtOAc = 6:1) afforded **3Ag** as a white solid (64.7 mg, 96% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.84 (d, J = 2.0 Hz, 1H), 8.56 (dd, J = 4.8, 2.0 Hz, 1H), 7.85 (dd, J = 8.0, 2.0 Hz, 1H), 7.47 (d, J = 8.4 Hz, 2H), 7.34 (dd, J = 8.0, 4.8 Hz, 1H), 7.28 (d, J = 8.4 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.1

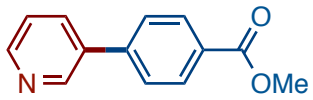
(one carbon overlap), 138.0, 136.5, 134.9, 134.1, 129.7, 126.9, 123.5, 21.1; HRMS (ESI) *m*/*z* calcd for $C_{12}H_{12}N$ $[M+H]^+$: 170.0964, found: 170.0961.



3Ah

3-Phenylpyridine (3Ah)[29]

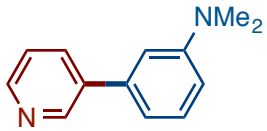
Purification by flash column chromatography (hexane/EtOAc = 4:1) afforded **3Ah** as colorless oil (50.1 mg, 81% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.86 (d, *J* = 2.4 Hz, 1H), 8.59 (d, *J* = 5.2 Hz, 1H), 7.87 (dd, *J* = 8.0, 2.4 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.48 (dd, *J* = 8.0, 2.4 Hz, 2H), 7.41 (dd, *J* = 8.0, 5.2 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.4, 148.3, 137.8, 136.6, 134.3, 129.0, 128.1, 127.1, 123.5; HRMS (ESI) *m*/*z* calcd for $C_{11}H_{10}N$ $[M+H]^+$: 156.0808, found: 156.0805.



3Ai

Methyl 4-(pyridin-3-yl)benzoate (3Ai)[33]

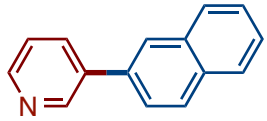
Purification by flash column chromatography (hexane/EtOAc = 5:1) afforded **3Ai** as a white solid (61.1 mg, 72% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.89 (d, *J* = 2.4 Hz, 1H), 8.65 (dd, *J* = 4.8, 2.4 Hz, 1H), 8.15 (d, *J* = 8.8 Hz, 2H), 7.92 (dd, *J* = 8.0, 2.4 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.40 (dd, *J* = 8.0, 4.8 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.6, 149.2, 148.3, 142.1, 135.4, 134.4, 130.3, 129.6, 127.0, 123.6, 52.2; HRMS (ESI) *m*/*z* calcd for $C_{13}H_{11}NO_2$ $[M+H]^+$: 214.0863, found: 214.0863.



3Aj

***N*,*N*-Dimethyl-3-(pyridin-3-yl)aniline (3Aj)**

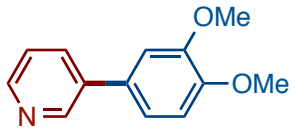
Purification by PTLC (hexane/EtOAc = 3:1) afforded **3Aj** as yellow oil (62.6 mg, 79% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.85 (d, *J* = 1.6 Hz, 1H), 8.57 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.87 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.36–7.31 (m, 2H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 2.8 Hz, 1H), 6.77 (dd, *J* = 8.4, 2.8 Hz, 1H), 3.00 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 150.9, 148.4, 148.2, 138.7, 137.5, 134.4, 129.7, 123.3, 115.4, 112.1, 111.1, 40.5; HRMS (ESI) *m*/*z* calcd for $C_{13}H_{15}N_2$ $[M+H]^+$: 199.1230, found: 199.1227.



3Ak

3-(Naphthalen-2-yl)pyridine (3Ak)[34]

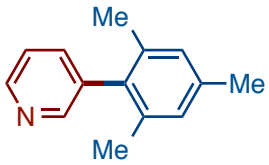
Purification by flash column chromatography (hexane/EtOAc = 5:1 to 4:1) afforded **3Ak** as a white solid (74.9 mg, 91% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.99 (d, J = 2.4 Hz, 1H), 8.63 (d, J = 4.8 Hz, 1H), 8.05 (d, J = 2.0 Hz, 1H), 8.00 (dd, J = 8.0, 2.4 Hz, 1H), 7.96 (d, J = 8.8 Hz, 1H), 7.94–7.87 (m, 2H), 7.72 (dd, J = 8.8, 2.0 Hz, 1H), 7.58–7.49 (m, 2H), 7.40 (dd, J = 8.0, 4.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.6, 148.5, 136.6, 135.2, 134.6, 133.6, 132.9, 128.9, 128.2, 127.7, 126.6, 126.4, 126.2, 125.0, 123.6; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}N$ $[M+H]^+$: 206.0964, found: 206.0964.



3Al

3-(3,4-Dimethoxyphenyl)pyridine (3Al)[35]

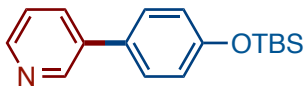
Purification by flash column chromatography (hexane/EtOAc = 1:1) afforded **3Al** as a white solid (62.6 mg, 73% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.82 (d, J = 2.0 Hz, 1H), 8.56 (dd, J = 4.8, 2.0 Hz, 1H), 7.84 (dd, J = 8.0, 2.0 Hz, 1H), 7.34 (dd, J = 8.0, 4.8 Hz, 1H), 7.14 (dd, J = 8.4, 2.0 Hz, 1H), 7.08 (d, J = 2.0 Hz, 1H), 6.97 (d, J = 8.4 Hz, 1H), 3.97 (s, 3H), 3.93 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 149.3, 149.1, 148.0, 147.9, 136.4, 133.9, 130.6, 123.4, 119.5, 111.6, 110.1, 55.9 (one peak overlap); HRMS (ESI) *m/z* calcd for $C_{13}H_{14}NO_2$ $[M+H]^+$: 216.1019, found: 216.1020.



3Am

3-Mesitylpyridine (3Am)[30]

Purification by PTLC (hexane/EtOAc = 4:1) afforded **3Am** as a white solid (52.0 mg, 66% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.59 (dd, J = 4.8, 1.6 Hz, 1H), 8.43 (d, J = 1.6 Hz, 1H), 7.50 (dd, J = 8.0, 1.6 Hz, 1H), 7.36 (dd, J = 8.0, 4.8 Hz, 1H), 6.97 (s, 2H), 2.34 (s, 3H), 2.00 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 150.3, 148.0, 137.5, 136.9, 136.6, 136.2, 135.0, 128.3, 123.3, 21.0, 20.8; HRMS (ESI) *m/z* calcd for $C_{14}H_{16}N$ $[M+H]^+$: 198.1277, found: 198.1273.

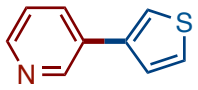


3An

3-(4-((*tert*-Butyldimethylsilyl)oxy)phenyl)pyridine (3An)

Purification by flash column chromatography (hexane/EtOAc = 5:1) afforded **3An** as colorless oil (82.4 mg, 72% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.81 (d, J = 2.4 Hz, 1H), 8.54 (d, J = 4.8 Hz, 1H), 7.82 (dd, J = 8.0, 2.4 Hz, 1H), 7.46 (d, J = 6.8 Hz, 2H), 7.32 (dd, J = 8.0, 4.8 Hz, 1H), 6.94 (d, J = 6.8 Hz, 2H), 1.01 (s, 9H), 0.24 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ

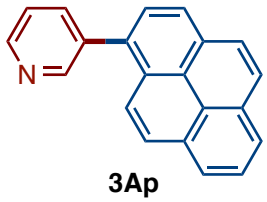
156.0, 148.0, 147.8, 136.3, 133.8, 130.8, 128.1, 123.4, 120.7, 25.6, 18.2, –4.4; HRMS (DART) *m/z* calcd for $C_{17}H_{24}NOSi$ $[M+H]^+$: 286.1627, found: 286.1621.



3Ao

3-(Thiophen-3-yl)pyridine (3Ao)[36]

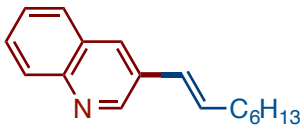
The reaction was conducted using 1.2 equiv of Na_2CO_3. Purification by PTLC (hexane/Et_2O = 1:1) and then GPC afforded **3Ao** as a white solid (41.3 mg, 64% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.88 (s, 1H), 8.53 (d, *J* = 4.4 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.52 (dd, *J* = 2.8, 1.2 Hz, 1H), 7.44 (dd, *J* = 5.2, 2.8 Hz, 1H), 7.39 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.31 (dd, *J* = 8.0, 4.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.2, 147.6, 138.7, 133.4, 131.4, 126.9, 125.8, 123.6, 121.3; HRMS (ESI) *m/z* calcd for C_9H_8NS $[M+H]^+$: 162.0372, found: 162.0369.



3Ap

3-(Pyren-1-yl)pyridine (3Ap)

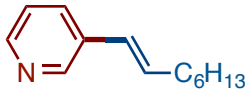
Purification by PTLC (hexane/Et_2O = 1:1) afforded **3Aq** as a yellow solid (61.7 mg, 55% yield). ^1H NMR ($CDCl_3$, 400 MHz) δ 8.88 (s, 1H), 8.72 (d, *J* = 4.8 Hz, 1H), 8.24–8.10 (m, 3H), 8.10–7.95 (m, 5H), 7.94–7.79 (m, 2H), 7.46 (dd, *J* = 8.8, 4.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 151.0, 148.4, 137.6, 136.7, 133.4, 131.3, 131.0, 130.7, 128.5, 128.0, 127.8, 127.4, 127.2, 126.1, 125.4, 125.0, 124.8, 124.64, 124.61, 124.2, 123.2; HRMS (DART) *m/z* calcd for $C_{21}H_{14}N$ $[M+H]^+$: 280.1126, found: 280.1122.



3Wq

(*E*)-3-(Oct-1-en-1-yl)quinoline (3Wq)

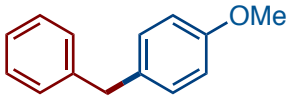
The reaction was conducted using NaCl (1.0 equiv) as additive. Purification by PTLC (hexane/EtOAc = 8:1) and then GPC afforded **3Wq** as colorless oil (57.8 mg, 57% yield). ^1H NMR ($CDCl_3$, 600 MHz) δ 8.97 (s, 1H), 8.06 (d, *J* = 8.8 Hz, 1H), 7.98 (s, 1H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.64 (t, *J* = 8.8 Hz, 1H), 7.51 (t, *J* = 8.8 Hz, 1H), 6.54–6.43 (m, 2H), 2.28 (q, *J* = 8.0 Hz, 2H), 1.56–1.46 (m, 2H), 1.42–1.27 (m, 6H), 0.91 (q, *J* = 6.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 149.4, 147.1, 134.1, 131.5, 130.8, 129.2, 128.7, 128.2, 127.6, 126.8, 126.5, 33.3, 31.7, 29.2, 28.9, 22.6, 14.1; HRMS (ESI) *m/z* calcd for $C_{17}H_{22}N$ $[M+H]^+$: 240.1747, found: 240.1752.



3Aq

(*E*)-3-(Oct-1-en-1-yl)pyridine (3Aq)[37]

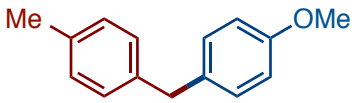
The reaction was conducted by using 1.0 equiv of NaCl as additive. Purification by PTLC (hexane/EtOAc = 5:1) afforded **3Aq** as colorless oil (35.0 mg, 46% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.56 (s, 1H), 8.42 (d, J = 4.4 Hz, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.21 (dd, J = 8.0, 4.4 Hz, 1H), 6.40–6.25 (m, 2H), 2.23 (q, J = 8.0 Hz, 2H), 1.52–1.43 (m, 2H), 1.40–1.32 (m, 6H), 0.88 (t, J = 6.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 147.94, 147.86, 133.7, 133.5, 132.3, 126.2, 123.3, 33.1, 31.7, 29.1, 28.9, 22.6, 14.1; HRMS (ESI) *m*/*z* calcd for $C_{13}H_{20}N$ $[M+H]^+$: 190.1590, found: 190.1586.



3AFa

1-Benzyl-4-methoxybenzene (3AFa)[38]

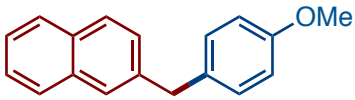
The reaction was conducted using *N,N*-dimethyl-4-aminopyridine (DMAP: 14.7 mg, 0.12 mmol, 30 mol%) as additive. Purification by PTLC (hexane/EtOAc = 20:1) afforded **3AFa** as colorless oil (36.5 mg, 46% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.27 (dd, J = 7.6, 7.2 Hz, 2H), 7.21–7.15 (m, 3H), 7.10 (d, J = 8.4 Hz, 2H), 6.82 (d, J = 8.4 Hz, 2H), 3.92 (s, 2H), 3.78 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 157.9, 141.6, 133.2, 129.8, 128.8, 128.4, 126.0, 113.9, 55.2, 41.0; HRMS (DART) *m*/*z* calcd for $C_{14}H_{15}O$ $[M+H]^+$: 199.1123, found: 199.1122.



3AGa

1-Methoxy-4-(4-methylbenzyl)benzene (3AGa)[38]

The reaction was conducted using *N,N*-dimethyl-4-aminopyridine (DMAP: 14.7 mg, 0.12 mmol, 30 mol%) as additive. Purification by PTLC (hexane/EtOAc = 20:1) afforded **3AGa** as colorless oil (30.0 mg, 35% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.12–7.03 (m, 6H), 6.81 (d, J = 8.4 Hz, 2H), 3.88 (s, 2H), 3.77 (s, 3H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 157.9, 138.5, 135.4, 133.5, 129.8, 129.1, 128.7, 113.8, 55.2, 40.6, 21.0; HRMS (FAB) *m*/*z* calcd for $C_{15}H_{16}O$ [M]: 212.1201, found: 212.1203



3AHa

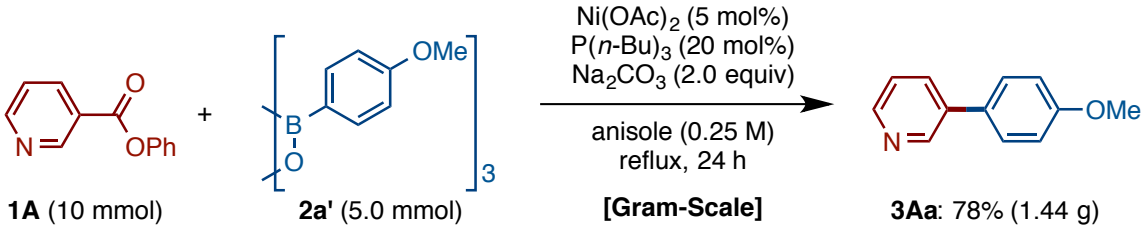
2-(4-Methoxybenzyl)naphthalene (3AHa)[38]

The reaction was conducted using *N,N*-dimethyl-4-aminopyridine (DMAP: 14.7 mg, 0.12 mmol, 30 mol%) as additive. Purification by PTLC (hexane/EtOAc = 20:1) afforded **3AHa** as a

white solid (45.8 mg, 46% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.81–7.77 (m, 3H), 7.60 (s, 1H), 7.47–7.35 (m, 2H), 7.29 (dd, J = 8.4, 1.6 Hz, 1H), 7.12 (dd, J = 8.8, 1.6 Hz, 2H), 6.82 (dd, J = 8.8, 1.6 Hz, 2H), 4.07 (s, 2H), 3.77 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.0, 139.0, 133.6, 133.0, 132.0, 129.9, 128.0, 127.6, 127.54, 127.50, 126.9, 125.9, 125.3, 113.9, 55.2, 41.2; HRMS (FAB) *m/z* calcd for $C_{18}H_{16}O$ $[M]^+$: 248.1201, found: 248.1207.

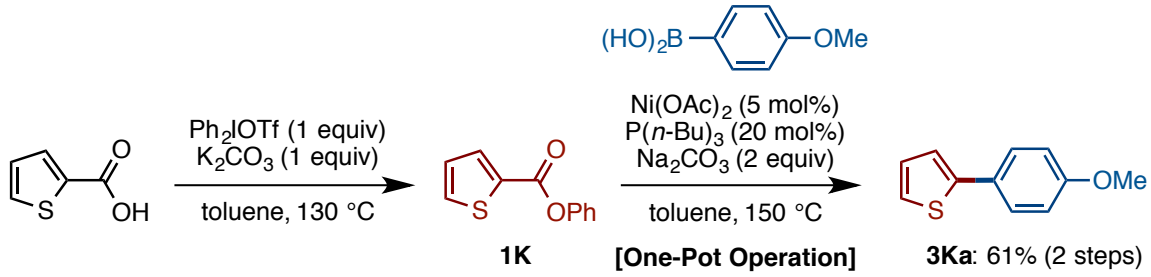
3. Gram-scale Reaction

[Gram-Scale]



A 100-mL Schlenk tube equipped with a condenser and balloon containing a magnetic stirring bar and $Ni(OAc)_2 \cdot 4H_2O$ (124 mg, 0.5 mmol, 5 mol%) was dried with a heatgun *in vacuo* and filled with N_2 gas after cooling to room temperature. To this was added phenyl nicotinate (**1A**: 1.99 g, 10 mmol, 1.0 equiv), tri(*p*-methoxyphenyl)boroxine (**2a'**: 2.00 g, 5.0 mmol, 0.5 equiv), and Na_2CO_3 (2.12 g, 20 mmol, 2.0 equiv). The tube was vacuumed and refilled N_2 gas three times. To this was added P(*n*-Bu)$_3$ (0.49 mL, 2.0 mmol, 20 mol%) and anisole (40 mL). The Schlenk cock was closed and then this mixture was refluxed for 24 h in an oil bath (oil bath temperature was 160 °C) with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a short silica gel pad with EtOAc. The filtrate was concentrated *in vacuo* and the residue was purified by flash column chromatography (hexane/Et_2O = 3:2 to 2:3) to afford 3-(4-methoxyphenyl)pyridine (**3Aa**: 1.44 g, 78% yield) as a white solid.

4. One-pot Transformation of Thiophene-2-carboxylic Acid to Biaryl 3Ka

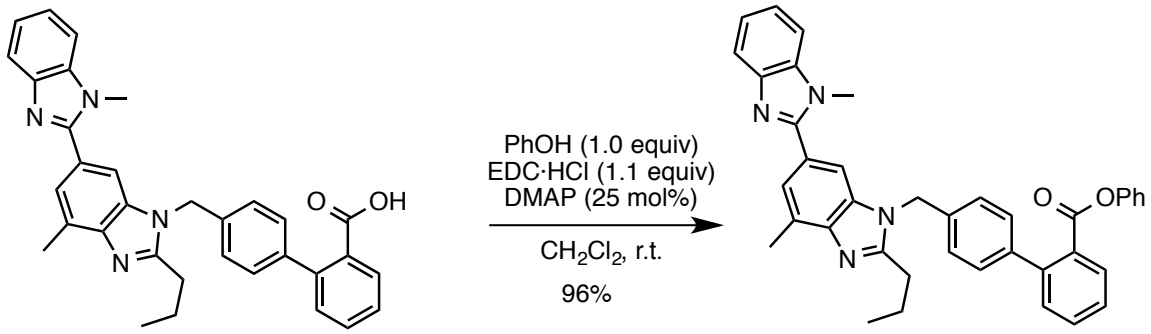


A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar was dried with heatgun under reduced pressure and filled with N_2 gas after cooling to room temperature. To this was added thiophene-2-carboxylic acid (51.3 mg, 0.40 mmol), diphenyliodonium triflate (172.0 mg, 0.40 mmol, 1.0 equiv), K_2CO_3 (55.2 mg, 0.40 mmol, 1.0 equiv), and then toluene (2.0 mL). The vessel was sealed with O-ring tap and then heated at 130 °C for 2 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, this mixture was concentrated *in vacuo* to remove toluene and iodobenzene.

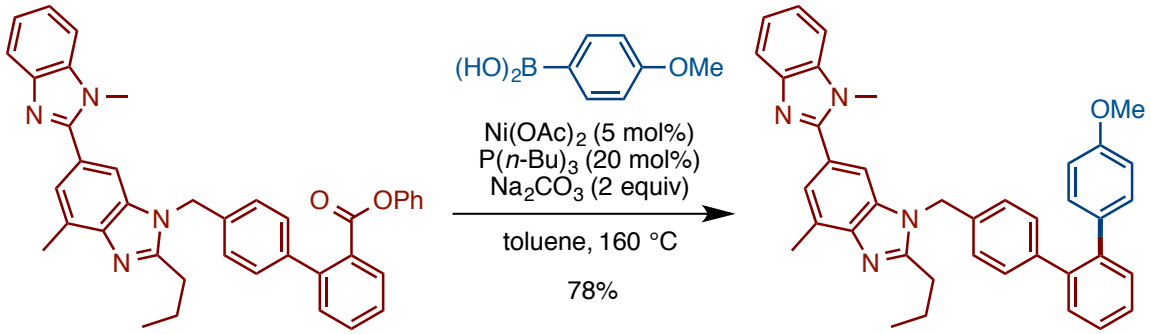
To the same tube containing obtained crude product **1K** were added $Ni(OAc)_2$ (3.5 mg, 0.02 mmol, 5 mol%), *p*-methoxyphenylboronic acid **3** (0.60 mmol, 91.9 mg, 1.5 equiv), and Na_2CO_3

(84.8 mg, 0.8 mmol, 2.0 equiv). The vessel was vacuumed and refilled N_2 gas three times. To this was added P(*n*-Bu)$_3$ (19.0 mL, 0.08 mmol, 20 mol%) and toluene (1.6 mL). The vessel was sealed with O-ring tap and then heated at 150 °C for 24 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a short silica gel pad with EtOAc. The filtrate was concentrated and the residue was purified by flash column chromatography (hexane/EtOAc = 100:1) to afford 2-(4-methoxyphenyl)thiophene (**3Ka**: 46.2 mg, 61% yield over 2 steps) as a white solid.

5. Application to the Synthesis of Telmisartan Derivtives



To a test tube equipped with screw cap containing a magnetic stirring bar were added telmisartan (772 mg, 1.5 mmol, 1.0 equiv), phenol (155 mg, 1.65 mmol, 1.1 equiv), 1-(3-dimethylaminopropyl)-3- ethylcarbodiimide hydrochloride (EDC·HCl: 316 mg, 1.65 mmol, 1.1 equiv), *N,N*-dimethyl-4-aminopyridine (DMAP: 18.3 mg, 0.15 mmol, 0.1 equiv) and CH_2Cl_2 (3.0 mL). After stirring for 6 h, the reaction mixture was quenched with saturated $NaHCO_3$aq and extracted three times with CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, filtrated, and concentrated *in vacuo*. The residue was purified by flash column chromatography (hexane/EtOAc = 2:1 to EtOAc) to afford telmisartan Ph-ester (**4**: 850 mg, 96% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.03 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.83–7.80 (m, 1H), 7.60 (td, *J* = 8.0, 1.6 Hz, 1H), 7.52–7.44 (m, 3H), 7.40–7.35 (m, 3H), 7.32–7.28 (m, 3H), 7.21 (t, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.04 (t, *J* = 8.0 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 2H), 5.45 (s, 2H), 3.71 (s, 3H), 2.91 (t, *J* = 8.0 Hz, 2H), 2.79 (s, 3H), 1.91–1.81 (m, 2H), 1.03 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.6, 156.4, 154.7, 150.6, 143.2, 142.9, 142.3, 141.1, 136.7, 135.0, 131.9, 130.9, 130.4, 129.9, 129.5, 129.25, 129.20, 127.6, 125.9, 125.7, 124.0, 123.9, 122.4, 122.3, 121.1, 119.6, 109.5, 108.8, 46.9, 31.7, 29.8, 21.8, 16.9, 14.1; HRMS (DART) *m*/*z* calcd for $C_{39}H_{35}N_4O_2$ $[M+H]^+$: 591.2760, found: 591.2770.

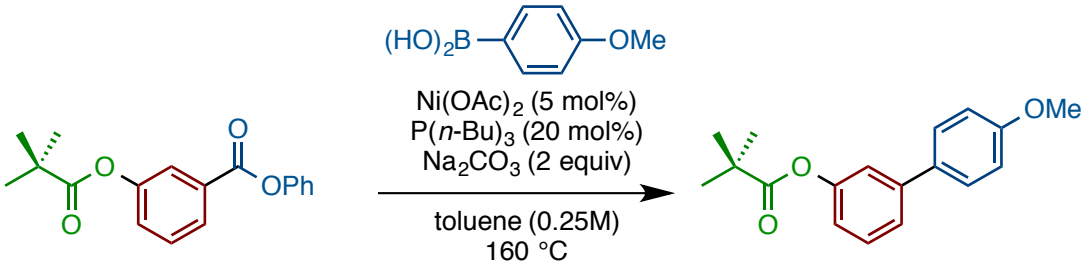


4 (telmisartan Ph-ester) **5**

A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar and $Ni(OAc)_2 \cdot 4H_2O$ (3.5 mg, 0.0125 mmol, 5 mol%) was dried with a heatgun under reduced pressure and filled with N_2 gas after cooling to room temperature. To this vessel was added telmisartan Ph-ester **4** (145 mg, 0.25 mmol, 1.0 equiv), *p*-methoxyphenylboronic acid (**2a**: 58.0 mg, 0.375 mmol, 1.5 equiv), and Na_2CO_3 (53 mg, 0.50 mmol, 2.0 equiv). The vessel was vacuumed and refilled N_2 gas three times. To this were added P(*n*-Bu)$_3$ (12.5 mL, 0.05 mmol, 20 mol%) and toluene (1.0 mL). The vessel was sealed with O-ring tap and then heated at 160 °C for 24 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through Celite® with EtOAc. The filtrate was concentrated and the residue was purified by flash column chromatography (hexane/EtOAc = 1:2 to EtOAc), followed by reverse-phase HPLC (Isolera®; H_2O/MeCN) to afford a coupling product **5** as a white solid (111 mg, 78% yield). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.84–7.81 (m, 1H), 7.51 (s, 1H), 7.44 (s, 1H), 7.40–7.28 (m, 7H), 7.10 (d, J = 8.0 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 6.94 (d, J = 8.0 Hz, 2H), 6.71 (d, J = 8.8 Hz, 2H), 5.36 (s, 2H), 3.80 (s, 3H), 3.72 (s, 3H), 2.87 (t, J = 7.6 Hz, 2H), 2.78 (s, 3H), 1.85–1.76 (m, 2H), 1.03 (t, J = 7.6 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 158.3, 156.4, 154.7, 143.1, 142.9, 141.5, 140.1, 139.5, 136.7, 135.2, 133.9, 133.6, 130.8, 130.6, 130.4, 127.6, 125.8, 123.9, 123.7, 122.4, 122.3, 119.5, 113.3, 109.5, 108.7, 55.1, 47.0, 31.8, 29.8, 21.7, 16.8, 14.0; HRMS (DART) *m/z* calcd for $C_{39}H_{37}N_4O$ $[M+H]^+$: 577.2967, found: 577.2969.

6. Orthogonal Coupling of 6, 1Q, and 10

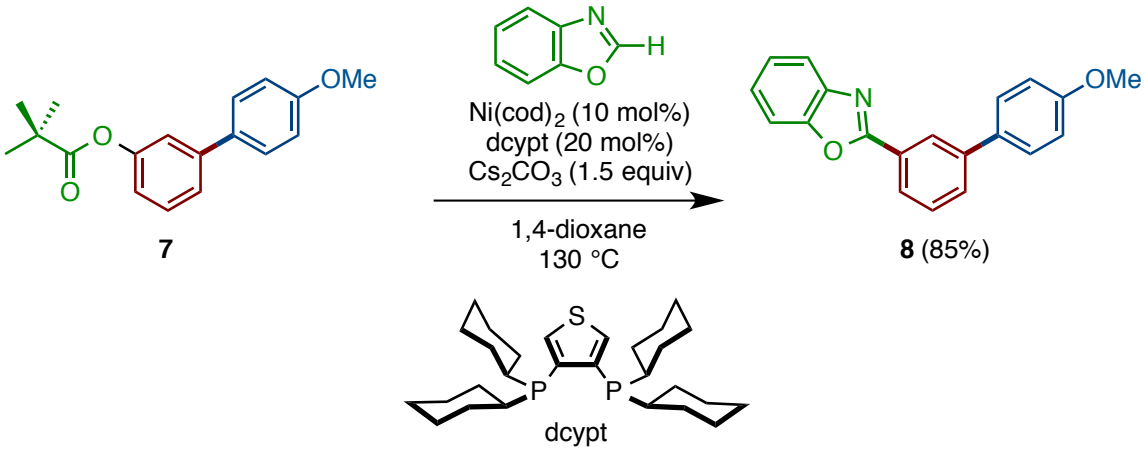
6-1. Orthogonal Coupling of 6



6 (0.40 mmol) **7** (74%)

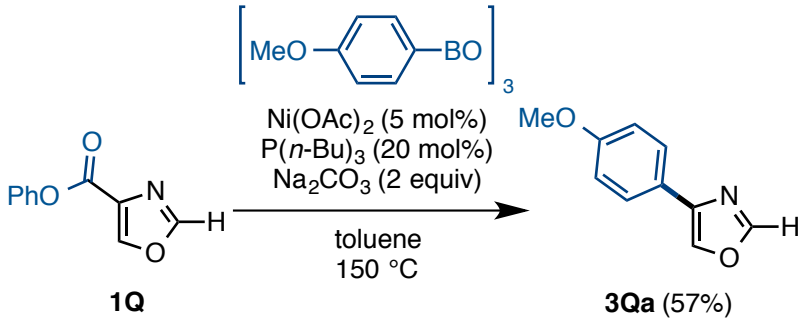
A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar and $Ni(OAc)_2 \cdot 4H_2O$ (5.0 mg, 0.020 mmol, 5 mol%) was dried with a heatgun under reduced pressure and filled with N_2 gas after cooling to room temperature. To this vessel was added phenyl 3-(pivaloyloxy)benzoate (**6**: 119.2 mg, 0.40 mmol, 1.0 equiv), *p*-methoxyphenylboronic

acid (**2a**: 91.8 mg, 0.60 mmol, 1.5 equiv), and Na_2CO_3 (85.0 mg, 0.8 mmol, 2.0 equiv). The vessel was vacuumed and refilled N_2 gas three times. To this were added P(*n*-Bu)$_3$ (20 mL, 0.08 mmol, 20 mol%) and toluene (1.6 mL). The vessel was sealed with O-ring tap and then heated at 150 °C for 24 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a short silica gel pad with EtOAc. The filtrate was concentrated *in vacuo* and the residue was purified by flash column chromatography (hexane/EtOAc = 100:1), and then GPC to afford 4'-methoxy-[1,1'-biphenyl]-3-yl pivalate **7** (84.2 mg, 74% yield) as colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.51 (d, *J* = 8.8 Hz, 2H), 7.41–7.37 (m, 2H), 7.22 (s, 1H), 7.01–6.98 (m, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 3H), 1.39 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 177.1, 159.3, 151.4, 142.4, 132.7, 129.5, 128.2, 123.9, 119.7, 119.6, 114.1, 55.3, 39.1, 27.1; HRMS (DART) *m*/*z* calcd for $C_{18}H_{21}O_3$ $[M+H]^+$: 285.1491, found: 285.1494.



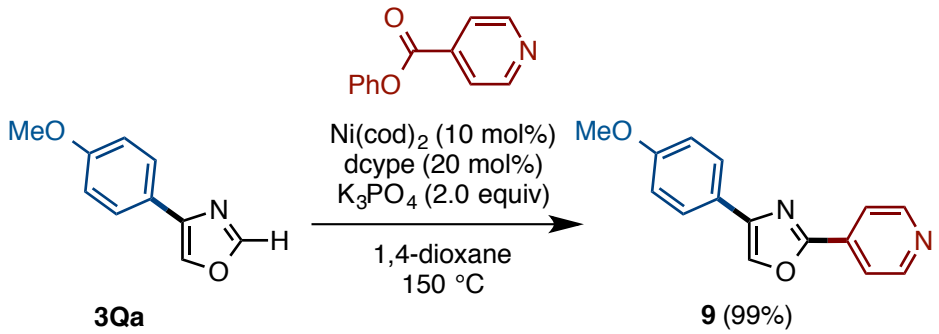
A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar and Cs_2CO_3 (146.6 mg, 0.45 mmol, 1.5 equiv) was dried with a heatgun under reduced pressure and filled with N_2 gas after cooling to room temperature. To this vessel was added 4'-methoxy-[1,1'-biphenyl]-3-yl pivalate (**7**: 85.3 mg, 0.30 mmol, 1.0 equiv) and 2,3-bis(dicyclohexylphosphine)thiophene (dcypt: 28.3 mg, 0.06 mmol, 20 mol%), and then introduced into an argon-atmosphere glovebox. To the reaction vessel was added Ni(cod)$_2$ (8.3 mg, 0.03 mmol, 10 mol%), and then taken out of the glovebox. To this tube were added benzoxazole (47.6 mg, 0.40 mmol, 1.3 equiv) and 1,4-dioxane (1.5 mL) under a stream of N_2. The vessel was sealed with O-ring tap and then heated at 130 °C for 12 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a short silica gel pad with EtOAc. The filtrate was concentrated *in vacuo* and the residue was purified by flash column chromatography (hexane/EtOAc = 100:1) to afford 2-(4'-methoxy-[1,1'-biphenyl]-3-yl)benzo[*d*]oxazole (**8**: 76.8 mg, 85% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.46 (s, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.83–7.77 (m, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.65–7.53 (m, 4H), 7.40–7.33 (m, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.0, 159.5, 150.7, 142.1, 141.5, 132.5, 129.7, 129.3, 128.2, 127.5, 125.7, 125.1, 124.6, 120.0, 114.3, 110.6, 55.3 (one peak overlap); HRMS (DART) *m*/*z* calcd for $C_{20}H_{16}NO_2$ $[M+H]^+$: 302.1181, found: 302.1178.

6-2. Orthogonal Coupling of 1Q



1Q **3Qa** (57%)

A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar and $Ni(OAc)_2 \cdot 4H_2O$ (5.0 mg, 0.020 mmol, 5 mol%) was dried with a heatgun for 1 min under reduced pressure and filled with N_2 gas after cooling to room temperature. To this vessel was added phenyl oxazole-4-carboxylate (**1Q**: 75.7 mg, 0.40 mmol, 1.0 equiv), *p*-methoxyphenylboroxine (**2a'**: 80.3 mg, 0.20 mmol, 0.50 equiv), and Na_2CO_3 (85.0 mg, 0.8 mmol, 2.0 equiv). The vessel was vacuumed and refilled with N_2 gas three times. To this were added P(*n*-Bu)$_3$ (20 mL, 0.08 mmol, 20 mol%) and toluene (1.6 mL). The vessel was sealed with O-ring tap and then heated at 150 °C for 24 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a short silica gel pad with EtOAc. The filtrate was concentrated *in vacuo* and the residue was purified by flash column chromatography by using Isolera® (hexane/EtOAc = 95:5 to 4:1), and then GPC to afford 4-(4-methoxyphenyl)oxazole (**3Qa**: 40.7 mg, 57% yield) as a white solid.

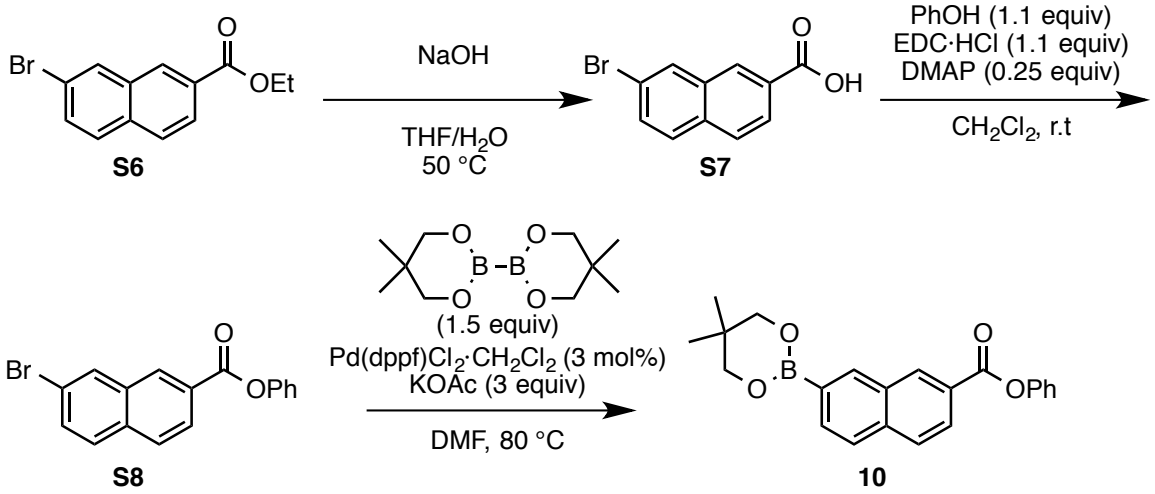


3Qa **9** (99%)

A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar and K_3PO_4 (169.8 mg, 0.80 mmol, 2.0 equiv) was dried with a heatgun for 3 minutes *in vacuo* and filled with N_2 gas after cooling to room temperature. To this vessel was added 4-(4-methoxyphenyl)oxazole (**3Qa**: 70.7 mg, 0.40 mmol, 1.0 equiv) and phenyl 4-nicotinate (119.5 mg, 0.60 mmol, 1.5 equiv), and then introduced into an argon-atmosphere glovebox. To the reaction vessel was added $Ni(cod)_2$ (11.0 mg, 0.04 mmol, 10 mol%) and 1,2-bis(dicyclohexylphosphino)ethane (dcype: 33.8 mg, 0.08 mmol, 20 mol%), and then taken out of the glovebox. To this tube was added 1,4-dioxane (1.6 mL) under a stream of N_2. The vessel was sealed with O-ring tap and then heated at 150 °C for 24 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a Celite® pad with EtOAc as an eluent. The filtrate was concentrated *in vacuo* and the residue was purified by PTLC (hexane/EtOAc = 1:1) to afford 4-(4-methoxyphenyl)-2-(pyridin-4-yl)oxazole (**9**: 100.5 mg, 99% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.76 (dd, J = 4.4, 1.2 Hz, 2H), 7.96–7.92 (m, 3H), 7.75 (dd, J = 7.2, 2.4 Hz, 2H), 6.98 (dd, J = 7.2, 2.4 Hz, 2H), 3.86 (s, 3H) ;

^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.8, 159.4, 150.5, 142.5, 134.3, 133.5, 127.0, 123.1, 120.0, 114.2, 55.3; HRMS (DART) *m/z* calcd for $C_{15}H_{13}N_2O_2$ $[M+H]^+$: 253.0977, found: 253.0972.

6-3. Orthogonal Coupling of 10

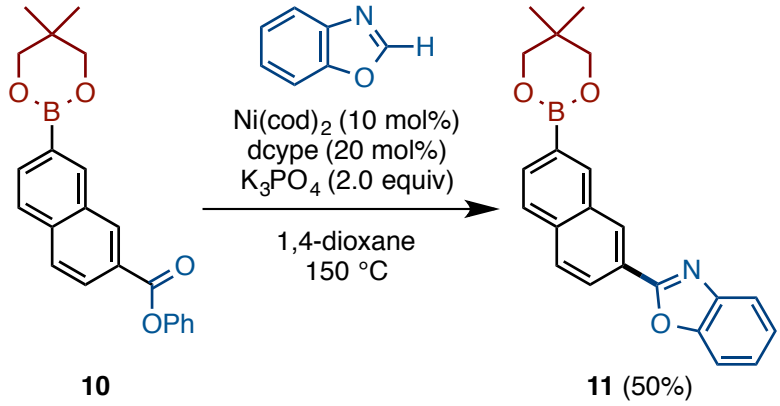


The solution of **S6** (1.95 g, 7.0 mmol, 1.0 equiv) in THF (28 mL) was treated with 1M NaOHaq (14 mL, 2.0 equiv) at 50 °C. After stirring overnight, the mixture was diluted with Et_2O and washed two times with Et_2O. 1 M HClaq was added to the combined water phase to adjust the pH to 2, and then resulted solution was extracted three times with Et_2O. The combined organic phase was concentrated *in vacuo* to afford 7-bromo-2-naphthoic acid (**S7:** 1.76 g) as a white solid. This was used without further purification.

To a round-bottomed flask with the carboxylic acid **S7** (1.76 g, 7.0 mmol, 1.0 equiv) were added phenol (725 mg, 7.7 mmol, 1.1 equiv), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC·HCl: 1.48 g, 7.7 mmol, 1.1 equiv), *N,N*-dimethyl-4-aminopyridine (DMAP: 213.8 mg, 1.75 mmol, 0.25 equiv) and CH_2Cl_2 (28 mL). After stirring the mixture for several hours with monitoring reaction progress on TLC, the reaction was quenched with saturated $NaHCO_3$aq and extracted three times with CH_2Cl_2. The combined organic layer was dried over Na_2SO_4, passed a short silica gel pad, and concentrated *in vacuo*. The residue was purified by recrystallization (hexane/CH_2Cl_2) to afford phenyl 7-bromo-2-naphthoate (**S8**: 2.15 g, 94% yield) as a white solid.

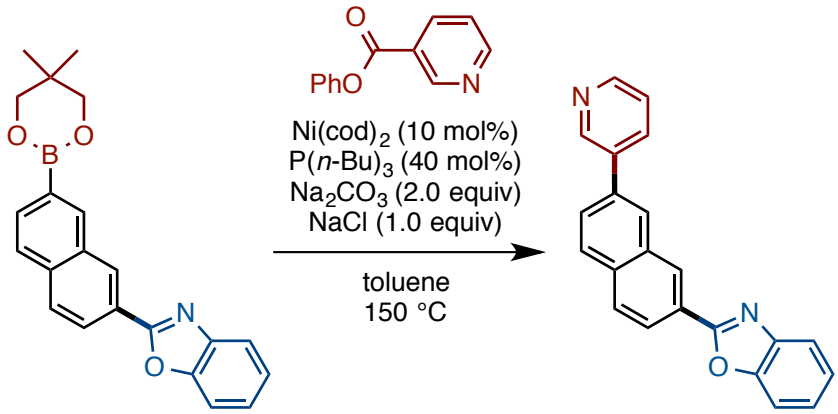
To a dried 50-mL Schlenk tube were added dehydrated KOAc (883 mg, 9.0 mmol, 3.0 equiv), phenyl 7-bromo-2-naphthoate (**S8**: 982 mg, 3.0 mmol, 1.0 equiv), Pd(dppf)Cl_2·CH_2Cl_2 (73.5 mg, 0.090 mmol, 3 mol%), and bis(neopentyl glycolato)diboron (1.01 g, 4.5 mmol, 1.5 equiv). The tube was vacuumed and filled with N_2 gas three times. DMF (12 mL) was added under a stream of N_2 gas and the mixture was heated at 80 °C for 12 h in an oil bath. After cooling the mixture to room temperature, the mixture was diluted with EtOAc and passed a silica-gel pad with EtOAc as an eluent. The mixture was washed with brine, dried over Na_2SO_4, filtered, and then concentrated *in vacuo*. The resulted crude product was purified by silica-gel column chromatography by using Isolera® (hexane/EtOAc = 10:1 to 1:1) to afford phenyl 7-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)-2-naphthoate (**10**: 940 mg, 87% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.77 (s, 1H), 8.41 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 8.01–7.91 (m, 3H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.32–7.22 (m, 3H), 3.84 (s, 4H), 1.07 (s, 6H); ^{13}C NMR ($CDCl_3$,

100 MHz) δ 165.4, 151.1, 135.2, 134.7, 133.8, 131.7, 130.9, 129.5, 129.1, 128.3, 127.3, 125.9, 125.2, 121.8, 72.5, 32.0, 21.9; HRMS (DART) *m*/*z* calcd for $C_{22}H_{22}BO_4$ $[M+H]^+$: 361.1611, found: 361.1611.



10 **11** (50%)

A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar and K_3PO_4 (169.8 mg, 0.80 mmol, 2.0 equiv) was dried with a heatgun for 3 min *in vacuo* and filled with N_2 gas after cooling to room temperature. To this vessel was added phenyl 7-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)-2-naphthoate (**10**: 144.1 mg, 0.40 mmol, 1.0 equiv), and then introduced into an argon-atmosphere glovebox. To the reaction vessel was added $Ni(cod)_2$ (11.0 mg, 0.04 mmol, 10 mol%) and 1,2-bis(dicyclohexylphosphino)ethane (dcype: 33.8 mg, 0.08 mmol, 20 mol%), and then taken out of the glovebox. To this tube were added benzoxazole (60 μL, 71.4 mg, 0.60 mmol, 1.5 equiv) and 1,4-dioxane (1.6 mL) under a stream of N_2. The vessel was sealed with O-ring tap and then heated at 150 °C for 12 h in an 8-well reaction block with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a silica-gel pad with EtOAc as an eluent. The filtrate was concentrated *in vacuo* and the residue was purified by silica-gel column chromatography by using Isolera® (hexane/EtOAc = 100:1 to EtOAc) to afford a pale yellow solid (82 mg). This solid was further purified by silica-gel column chromatography by using Isolera® (hexane/$CHCl_3$ = 4:1 to $CHCl_3$) to afford 2-(7-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)naphthalen-2-yl)benzo[*d*]oxazole (**11**: 71.3 mg, 50% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.77 (s, 1H), 8.40 (s, 1H), 8.31 (dd, *J* = 9.0, 1.2 Hz, 1H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.98–7.92 (m, 2H), 7.83–7.80 (m, 1H), 7.65–7.62 (m, 1H), 7.40–7.35 (m, 2H), 3.85 (s, 4H), 1.08 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.2, 150.8, 142.2, 134.8, 134.3, 134.1, 131.0, 129.5, 127.9, 127.7, 125.1, 124.9, 124.6, 123.7, 120.0, 110.6, 72.4, 31.9, 21.9; HRMS (DART) *m*/*z* calcd for $C_{22}H_{21}BNO_3$ $[M+H]^+$: 358.1615, found: 358.1618.



11 **12** (52%)

A 20-mL glass vessel equipped with J. Young® O-ring tap containing a magnetic stirring bar was dried with a heatgun *in vacuo* and filled with N_2 gas after cooling to room temperature. To this vessel was added a phenyl 3-nicotinate (**1A**: 59.8 mg, 0.30 mmol, 1.5 equiv), 2-(7-(5,5-dimethyl-1,3,2-dioxaborinan-2-yl)naphthalen-2-yl)benzo[*d*]oxazole (**11**: 71.4 mg, 0.20 mmol, 1.0 equiv), Na_2CO_3 (42.4 mg, 0.4 mmol, 2.0 equiv), and NaCl (11.9 mg, 0.20 mmol, 1.0 equiv). The vessel was introduced into an argon-atmosphere glovebox. To the reaction vessel was added $Ni(cod)_2$ (5.5 mg, 0.020 mmol, 10 mol%), and then taken out of the glovebox. To this were added P(*n*-Bu)$_3$ (10 mL, 0.08 mmol, 40 mol%) and toluene (0.8 mL) under a stream of N_2. The vessel was sealed with O-ring tap and then heated at 150 °C for 48 h in an oil bath with stirring. After cooling the reaction mixture to room temperature, the mixture was passed through a short silica gel pad with EtOAc. The filtrate was concentrated *in vacuo* and the residue was purified by silica-gel column chromatography by using Isolera® (hexane/EtOAc = 4:1 to EtOAc) to afford 2-(7-(pyridin-3-yl)naphthalen-2-yl)benzo[*d*]oxazole (**12**: 33.8 mg, 52% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 600 MHz) δ 9.00 (s, 1H), 8.79 (s, 1H), 8.66 (d, J = 4.2 Hz, 1H), 8.36 (d, J = 9.0 Hz, 1H), 8.10–8.07 (m, 2H), 8.05–7.98 (m, 2H), 7.84–7.75 (m, 2H), 7.64–7.60 (m, 1H), 7.45–7.41 (m, 1H), 7.40–7.34 (m, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ 162.9, 150.8, 148.9, 148.5, 142.2, 137.0, 136.1, 134.9, 134.6, 132.4, 129.9, 129.1, 127.8, 126.1, 125.3, 124.9, 124.7, 123.7, 120.1, 110.6; HRMS (DART) *m/z* calcd for $C_{22}H_{15}N_2O$ $[M+H]^+$: 323.1184, found: 323.1181.

7. Computational Details

Calculations were performed by Gaussian 09 quantum chemical package.[39] The geometries of all reported structures were optimized without symmetry constraints in toluene at the M06L level of density functional theory[40] in conjunction with the Lanl2dz basis set and corresponding Hay–Wadt ECP for Ni[41,42]. Standard 6-31G(d) basis sets were used for all other atoms. Below, this approach will be called as M06L/{Lanl2dz + [6-31G(d)]} or M06L/BS1. Solvent effects were estimated by using the PCM solvation method[43–45]. Previously, we have shown that this approach reasonable describes geometries and energetics of the Ni-complexes and Ni-catalyzed coupling reactions[46]. In order to incorporate disperse interactions into calculations we also performed geometry optimization and energy calculations of selected important intermediates and transition states at the M06/BS1 level of theory[47].

The nature of each stationary point was characterized by performing normal mode analysis at the appropriate (i.e. same as a geometry optimization) levels of theory. Relative free

energies and enthalpies of all reported structures were calculated under standard conditions (1 atm and 298.15 K). In the presented figures and tables, we give both relative Gibbs free energies and enthalpies (in kcal/mol) as ΔG/ΔH. Cartesian coordinates and total energies of all reported structures are also presented below. In this paper, we mainly discussed the M06/BS1 calculated free energies (*i.e*. ΔG values) at 298.15 K unless otherwise specified.

8. NBO Analysis of the Intermediate Complex B

NBO and molecular orbital analysis on the pre-reaction complex **B** shows the existence of a bonding between the Ni-center and C=O fragment of the substrate (called as Ni-(C=O) bond, see Supplementary Figure 159). Close examination shows that this orbital interacts with the bonding π-orbitals of the pyridine fragment and C(acyl)-O bond of substrate. The strength of these interactions are 9.1 and 1.1 kcal/mol, respectively. In addition, there exist a donor-acceptor interaction between the π-orbital of pyridine and empty orbital of Ni (Ni_{LP}*), *i.e*. E[Pyr → Ni_{LP}*], as well as between bonding C(acyl)–O orbital and empty orbital of Ni (Ni_{LP}*), *i.e*. E[(C-O)→ Ni_{LP}*]. Again, the Pyr → Ni_{LP}* interaction is calculated to be significantly larger than the (C–O)→ Ni_{LP}*. It is clear that these π-interactions collectively play a stabilization role in the C(acyl)–O activation transition state.

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