Supplementary Materials

The Improved *para*-selective C(sp^2)-H Borylation of Anisole Derivatives Enabled by Bulky Lewis Acid

Dai-Yu Li [1,2], Rui-Mu Yu [1,2], Jin-Ping Li [1,2], Deng-Feng Yang [2], Qi Pang [1,*] and Hong-Liang Li [2,*]

[1] School of Chemistry and Chemical Engineering, Guangxi University, Daxue Road, Nanning 53004, China; 2114391039@st.gxu.edu.cn (D.-Y.L.); 2114391125@st.gxu.edu.cn (R.-M.Y.); 2214301040@st.gxu.edu.cn (J.-P.L.)

[2] Guangxi Key Laboratory of Marine Natural Products and Combinatorial Biosynthesis Chemistry, Guangxi Academic of Marine Sciences, Guangxi Academy of Sciences, Nanning 53007, China; dengfengyang@163.com

* Correspondence: qipang@gxu.edu.cn (Q.P.); hongliang-li@gxas.cn (H.-L.L.)

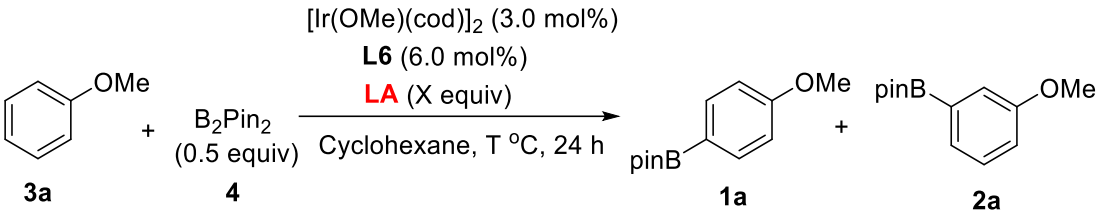
Table of Contents

1. General information

All reactions were carried out in a dry and degassed solvent under N_2 atmosphere. Compounds $B(Mes)_3$, B_2Pin_2, $[Ir(OMe)(cod)]_2$, were purchased from Aldrich and Bide Pharmatech, and used without further purification unless otherwise noted. Anhydrous solvents such as cyclohexane and tetrahydrofuran were distilled and degassed refluxing over CaH_2 or the combination of sodium/benzophenone ketyl. Reactions were monitored by thin-layer chromatography (TLC) visualizing with UV-light (254 nm). Organic solutions were concentrated under reduced pressure using a rotary evaporator (30 °C, <50 torr). NMR spectra were recorded on 400 MHz (400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR), and 800 MHz (800 MHz for ^{1}H NMR, 201 MHz for ^{13}C NMR) spectrometers. Proton and carbon chemical shifts are reported relative to the solvent used as an internal reference. The boron-bearing carbon atom was not observed due to quadrupolar relaxation. ESI-MS spectra were measured on a spectrometer for HRMS.

2. Optimization of reaction condition

Tabel S1. Screening of the loading amount of Lewis acid and reaction temperature

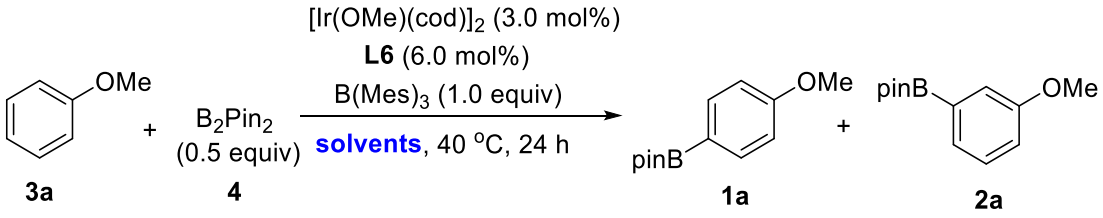


3a **4** **1a** **2a**

Entry	$B(Mes)_3$ (X eq.)	T °C	Yield(%) **1a**	Yield(%) **2a**	Ratio (para : meta)
1	--	40 °C	15%	33%	32 : 68
2	0.5	40 °C	30%	11%	72 : 28
3	**1.0**	**40 °C**	**46%**	**8%**	**84 : 16**
4	1.5	40 °C	39%	11%	79 : 21
5	1.0	60 °C	44%	17%	73 : 27
6	1.0	80 °C	28%	32%	47 : 53
7	1.0	100 °C	22%	33%	41 : 59

[a] Yields and selectivities were calculated by ^{1}H-NMR with 1,2-dichoromethane as internal standard

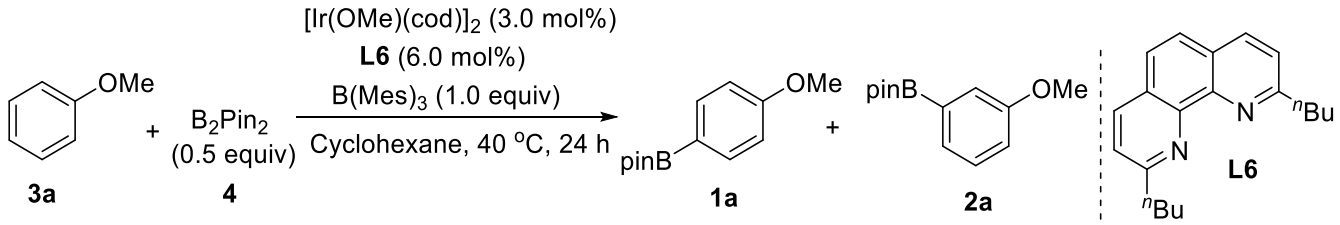
Tabel S2. Screening of different solvents



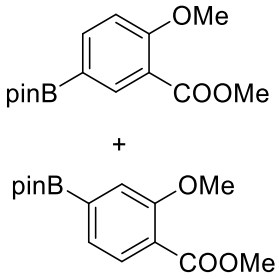
Entry	solvent	Yield(%) 1a	Yield(%) 2a	Ratio (para : meta)
1	hexane	30%	8%	80 : 20
2	p-xylene	37%	10%	78 : 22
3	THF	34%	23%	60 : 40
4	diethylether	29%	14%	67 : 33
5	EtOAc	trace	--	--
6	CH_2Cl_2	--	--	--
7	1,2-dichloroethane	--	--	--

[a] Yields and selectivities were calculated by ^{1}H-NMR with 1,2-dichoromethane as internal standard

3. General procedure for *para*-selective C-H borylation of anisole derivatives (1a-1x)

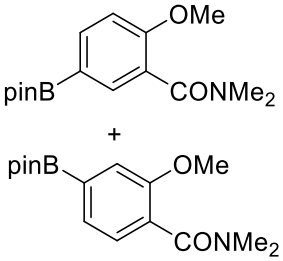


methyl 2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (1l + 2l)



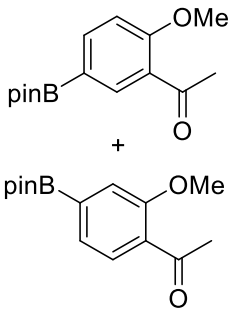
The mixture of product (90 mg, 63% yield, *para*/*meta* = 60 : 40); *para*-borylated product **1l** was obtained by further purification of the crude mixture by GPC (54 mg); the data of **1l**: ^{1}H NMR (800 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.90 (d, *J* = 8.3 Hz, 1H), 6.96 (d, *J* = 8.4 Hz, 1H), 3.92 (s, 3H), 3.88 (s, 3H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 166.5, 161.4, 140.2, 138.3, 119.6, 111.1, 83.8, 55.9, 51.9, 24.8; the data of **2l**: ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.37 (s, 1H), 3.93 (s, 3H), 3.88 (d, *J* = 1.4 Hz, 3H), 1.34 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 166.7, 158.2, 130.7, 126.4, 122.3, 117.5, 84.2, 56.0, 52.0, 24.8; IR (KBr, ν / cm^{-1}) 1728, 1358, 1232, 1145, 1085, 972, 853, 683; HRMS (ESI^+) Calcd for $C_{15}H_{22}BO_5^+$ ($[M+H]^+$) 293.1555, Found 293.1561.

2-methoxy-N,N-dimethyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzamide (1m + 2m)



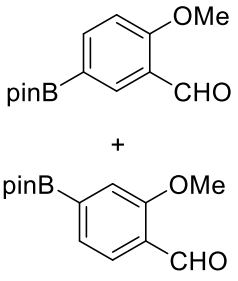
The mixture of product (64 mg, 42% yield, *para*/*meta* = 68 : 32); *para*-borylated product **1m** was obtained by further purification of the crude mixture by GPC (46 mg); the data of **1m**: ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.3 Hz, 1H), 7.68 (s, 1H), 6.89 (d, *J* = 8.3 Hz, 1H), 3.84 (s, 3H), 3.09 (s, 3H), 2.83 (s, 3H), 1.31 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 169.4, 157.7, 137.2, 134.5, 125.8, 110.1, 83.7, 55.5, 38.3, 34.7, 24.8; the data of **2m**: ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.4 Hz, 1H), 7.31 (s, 1H), 7.22 (d, *J* = 7.2 Hz, 1H), 3.87 (s, 3H), 3.10 (s, 3H), 2.81 (s, 3H), 1.34 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 169.3, 154.7, 129.1, 127.4, 127.2, 116.4, 84.0, 55.6, 38.1, 34.6, 24.8; IR (KBr, ν / cm^{-1}) 1633, 1507, 1387, 1236, 1141, 1028, 964, 852, 773, 689; HRMS (ESI^+) Calcd for $C_{16}H_{25}BNO_4^+$ ($[M+H]^+$) 306.1871, Found 306.1868.

1-(2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)ethan-1-one (1n + 2n)



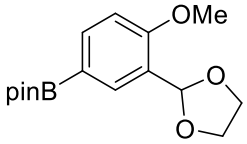
The mixture of product (78 mg, 57% yield, *para*/*meta* = 73 : 27); *para*-borylated product **1n** was obtained by further purification of the crude mixture by GPC (49 mg); the data of **1n**: ^{1}H NMR (800 MHz, $CDCl_3$) δ 8.14 (d, *J* = 1.7 Hz, 1H), 7.89 (dd, *J* = 8.3, 1.7 Hz, 1H), 6.95 (d, *J* = 8.3 Hz, 1H), 3.93 (s, 3H), 2.59 (s, 3H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 200.1, 160.9, 140.2, 137.2, 128.1, 110.8, 83.8, 55.5, 31.6, 24.8; the data of **2n**: ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.37 (s, 1H), 3.94 (s, 3H), 2.60 (s, 3H), 1.34 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 200.3, 158.0, 130.5, 129.3, 126.8, 117.2, 84.2, 55.5, 31.8, 24.8; IR (KBr, ν / cm^{-1}) 1670, 1395, 1351, 1229, 1142, 1023, 966, 852, 687; HRMS (ESI^+) Calcd for $C_{15}H_{22}BO_4^+$ ($[M+H]^+$) 277.1606, Found 277.1657.

2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde (1o + 2o)



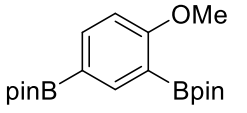
The mixture of product (68 mg, 52% yield, *para*/*meta* = 70 : 30); *para*-borylated product **1o** was obtained by further purification of the crude mixture by GPC (47 mg); the data of **1o**: ^{1}H NMR (800 MHz, $CDCl_3$) δ 10.44 (s, 1H), 8.28 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 3.95 (s, 3H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 189.8, 163.8, 142.4, 136.4, 124.3, 110.9, 83.9, 55.7, 24.8; the data of **2o**: ^{1}H NMR (800 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.80 (d, *J* = 7.5 Hz, 1H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.40 (s, 1H), 3.97 (s, 3H), 1.36 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 190.2, 161.0, 127.5, 126.8, 117.4, 84.3, 55.7, 24.9; IR (KBr, ν / cm^{-1}) 1675, 1403, 1358, 1231, 1027, 906, 805, 685; HRMS (ESI^+) Calcd for $C_{14}H_{20}BO_4^+$ ($[M+H]^+$) 263.1449, Found 263.1451.

2-(3-(1,3-dioxolan-2-yl)-4-methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1p)



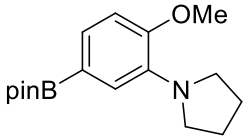
The mixture of product (61 mg, 40% yield, *para*/*meta* = 80 : 20); *para*-borylated product **1p** was obtained by further purification of the crude mixture by GPC (49 mg); ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.79 (d, *J* = 8.3 Hz, 1H), 6.89 (d, *J* = 8.3 Hz, 1H), 6.15 (s, 1H), 4.17 – 4.14 (m, 2H), 4.04 – 4.01 (m, 2H), 3.88 (s, 3H), 1.32 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 160.2, 137.5, 133.7, 125.1, 109.9, 99.3, 83.5, 65.3, 55.5, 24.8; IR (KBr, ν / cm^{-1}) 1417, 1376, 1232, 1141, 1029, 967, 851, 692; HRMS (ESI^+) Calcd for $C_{16}H_{24}BO_5^+$ ($[M+H]^+$) 307.1711, Found 307.1705.

2,2'-(4-methoxy-1,3-phenylene)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (1q)



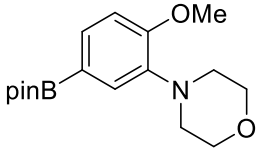
The mixture of product (99 mg, 55% yield, *para*/*meta* = 82 : 18); *para*-borylated product **1q** was obtained by further purification of the crude mixture by GPC (81 mg); ^{1}H NMR (800 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.85 (d, *J* = 8.3 Hz, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 3.84 (s, 3H), 1.35 (s, 13H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 166.6, 143.5, 139.6, 109.5, 83.5, 83.4, 55.6, 24.8, 24.7; IR (KBr, ν / cm^{-1}) 1596, 1357, 1318, 1249, 1139, 1025, 965, 849, 647; HRMS (ESI^+) Calcd for $C_{19}H_{31}BO_2O_5^+$ ($[M+H]^+$) 361.2352, Found 361.2348.

1-(2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)pyrrolidine (1r)



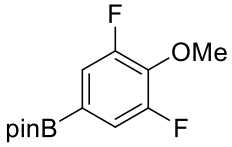
The mixture of product (71 mg, 47% yield, *para*/*meta* = 80 : 20); *para*-borylated product **1r** was obtained by further purification of the crude mixture by GPC (57 mg); ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.9 Hz, 1H), 7.24 (s, 1H), 6.85 (d, *J* = 8.0 Hz, 1H), 3.86 (s, 3H), 3.32 – 3.28 (m, 4H), 1.95 – 1.89 (m, 4H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 153.4, 139.3, 127.8, 121.6, 110.5, 83.4, 55.3, 50.6, 24.8, 24.6; IR (KBr, ν / cm^{-1}) 2927, 1414, 1354, 1234, 1138, 1022, 989, 849, 807, 684; HRMS (ESI^+) Calcd for $C_{17}H_{27}BNO_3^+$ ($[M+H]^+$) 304.2079, Found 304.2082.

4-(2-methoxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)morpholine (1s)



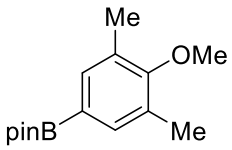
The mixture of product (80 mg, 50% yield, *para*/*meta* = 79 : 21); *para*-borylated product **1s** was obtained by further purification of the crude mixture by GPC (63 mg); ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 1H), 7.35 (s, 1H), 6.87 (d, *J* = 8.1 Hz, 1H), 3.91 – 3.87 (m, 7H), 3.09 (t, *J* = 4.6 Hz, 4H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 154.9, 140.4, 130.8, 124.0, 110.5, 83.6, 67.2, 55.4, 51.2, 24.8; IR (KBr, ν / cm^{-1}) 2918, 1645, 1457, 1353, 1236, 1097, 964, 852, 689; HRMS (ESI^+) Calcd for $C_{17}H_{27}BNO_4^+$ ($[M+H]^+$) 320.2028, Found 320.2035.

2-(3,5-difluoro-4-methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1t)



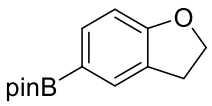
The para-borylated product (88 mg, 65% yield, *para*/*meta* = 100/0); ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.31 (s, 1H), 7.30 (s, 1H), 4.03 (s, 4H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 155.7 (d, *J* = 6.0 Hz), 154.5 (d, *J* = 6.0 Hz), 118.1 (d, *J* = 4.0 Hz), 117.9 (d, *J* = 4.0 Hz), 84.3, 61.6, 24.8; IR (KBr, ν / cm^{-1}) 1417, 1376, 1232, 1141, 1029, 967, 851, 692; HRMS (ESI^+) Calcd for $C_{13}H_{18}BF_2O_3^+$ ($[M+H]^+$) 271.1312, Found 271.1299.

2-(4-methoxy-3,5-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1u)



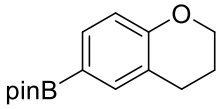
The para-borylated product (81 mg, 62% yield, *para*/*meta* = 100/0); ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.49 (s, 2H), 3.73 (s, 3H), 2.29 (s, 6H), 1.34 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 159.8, 135.6, 130.3, 83.6, 59.6, 24.8, 15.9; IR (KBr, ν / cm^{-1}) 1603, 1339, 1212, 1012, 962, 850, 692; HRMS (ESI^+) Calcd for $C_{15}H_{24}BO_3^+$ ($[M+H]^+$) 263.1813, Found 263.1798.

2-(2,3-dihydrobenzofuran-5-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1v)



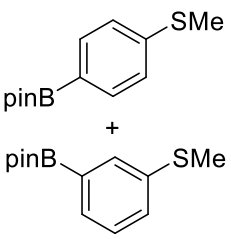
The mixture of product (69 mg, 56% yield, *para*/*meta* = 75 : 25); *para*-borylated product **1v** was obtained by further purification of the crude mixture by GPC (52 mg); ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.66 (s, 1H), 7.61 (d, *J* = 9.5 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 4.57 (t, *J* = 8.7 Hz, 2H), 3.19 (t, *J* = 8.7 Hz, 2H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 162.8, 135.5, 131.5, 126.5, 109.0, 83.5, 71.3, 29.2, 24.8; IR (KBr, ν / cm^{-1}) 1417, 1376, 1232, 1141, 1029, 967, 851, 692; HRMS (ESI^+) Calcd for $C_{14}H_{20}BO_3^+$ ($[M+H]^+$) 247.1500, Found 247.1508.

2-(chroman-6-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1w)



The mixture of product (70 mg, 54% yield, *para*/*meta* = 71 : 29); *para*-borylated product **1w** was obtained by further purification of the crude mixture by GPC (50 mg); ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.52 (s, 1H), 6.78 (d, *J* = 8.1 Hz, 1H), 4.22 – 4.18 (m, 2H), 2.79 (t, *J* = 6.5 Hz, 2H), 2.02 – 1.98 (m, 2H), 1.33 (s, 12H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 157.7, 136.9, 134.0, 121.6, 116.2, 83.5, 66.6, 24.8, 24.7, 22.3; IR (KBr, ν / cm^{-1}) 1458, 1363, 1120, 954, 863, 787, 756, 659; HRMS (ESI^+) Calcd for $C_{15}H_{22}BO_3^+$ ($[M+H]^+$) 261.1657, Found 261.1650.

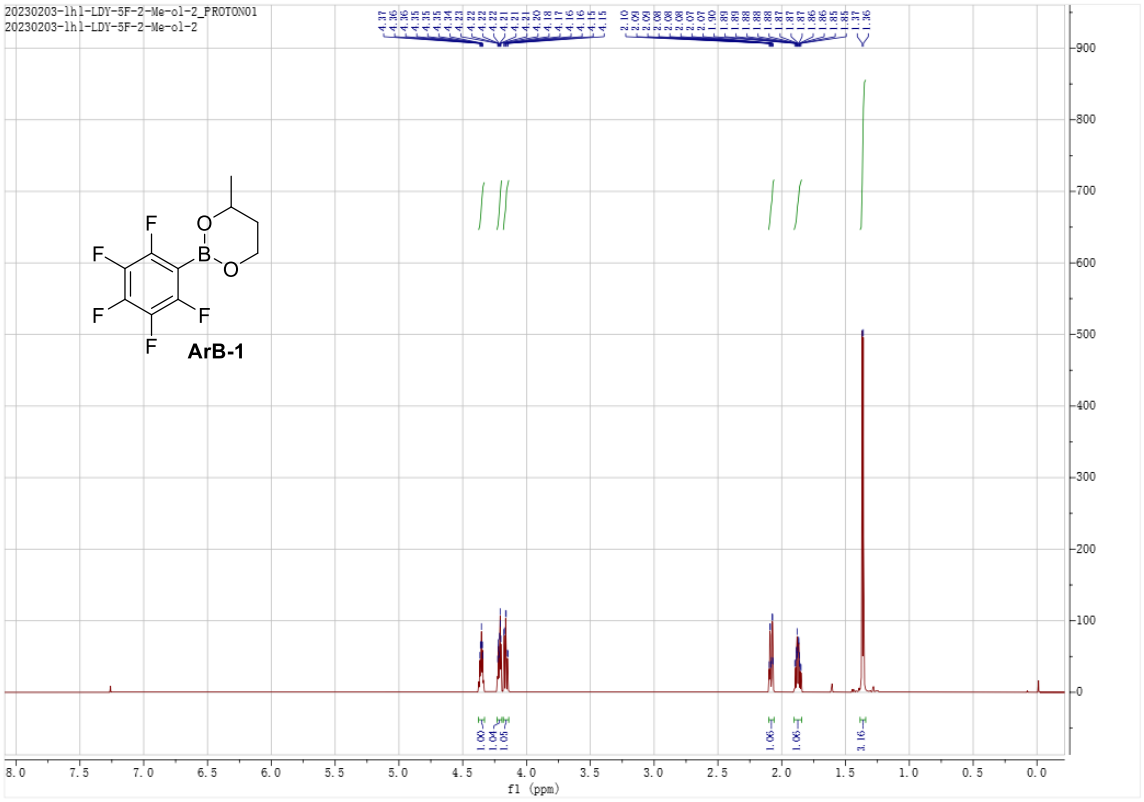
4,4,5,5-tetramethyl-2-(4-(methylthio)phenyl)-1,3,2-dioxaborolane (1x + 2x)

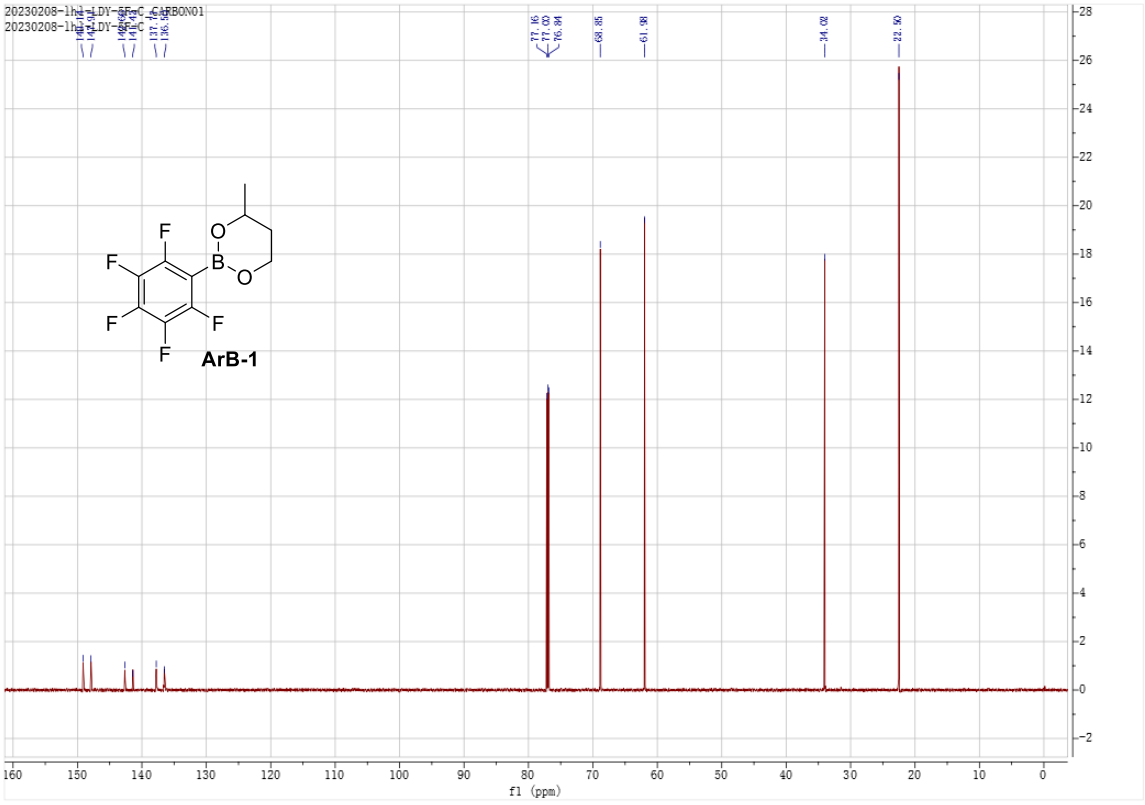


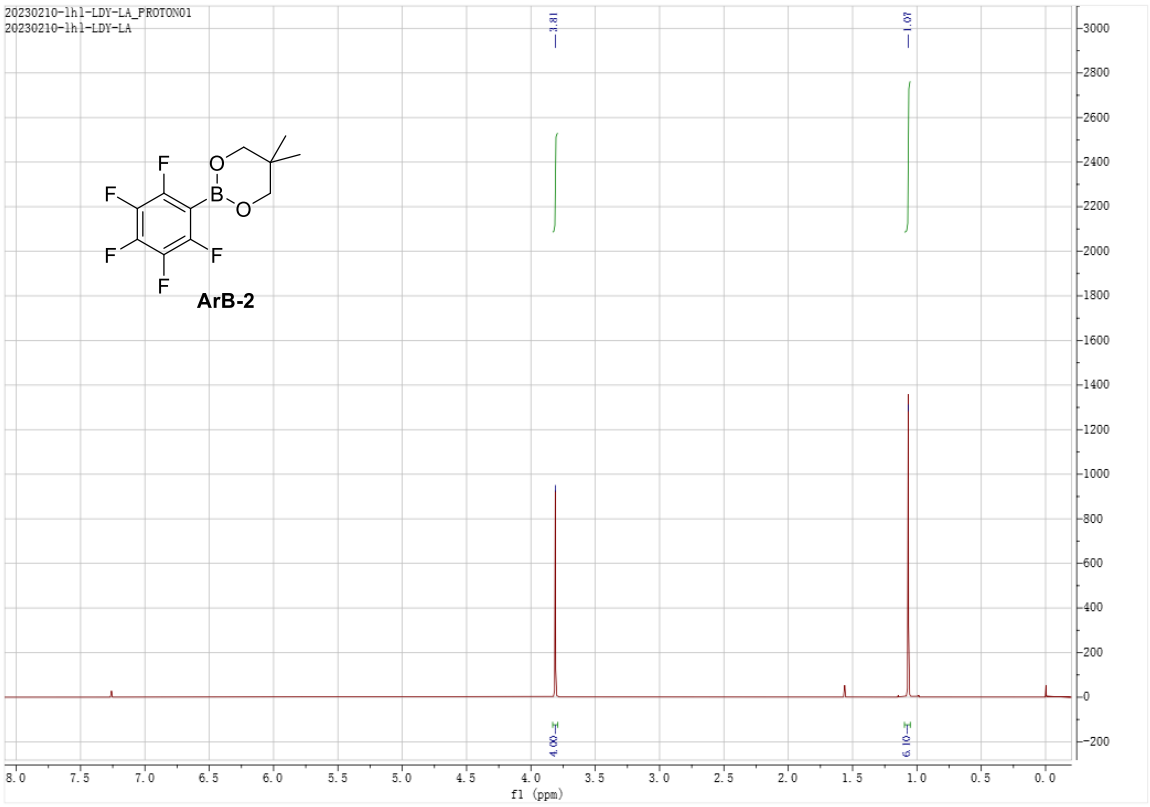
The mixture of product (75 mg, 60% yield, *para*/*meta* = 40 : 60); *para*-borylated product **1x** was obtained by further purification of the crude mixture by GPC (30 mg); the data of **1x**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 2H), 7.28 (d,

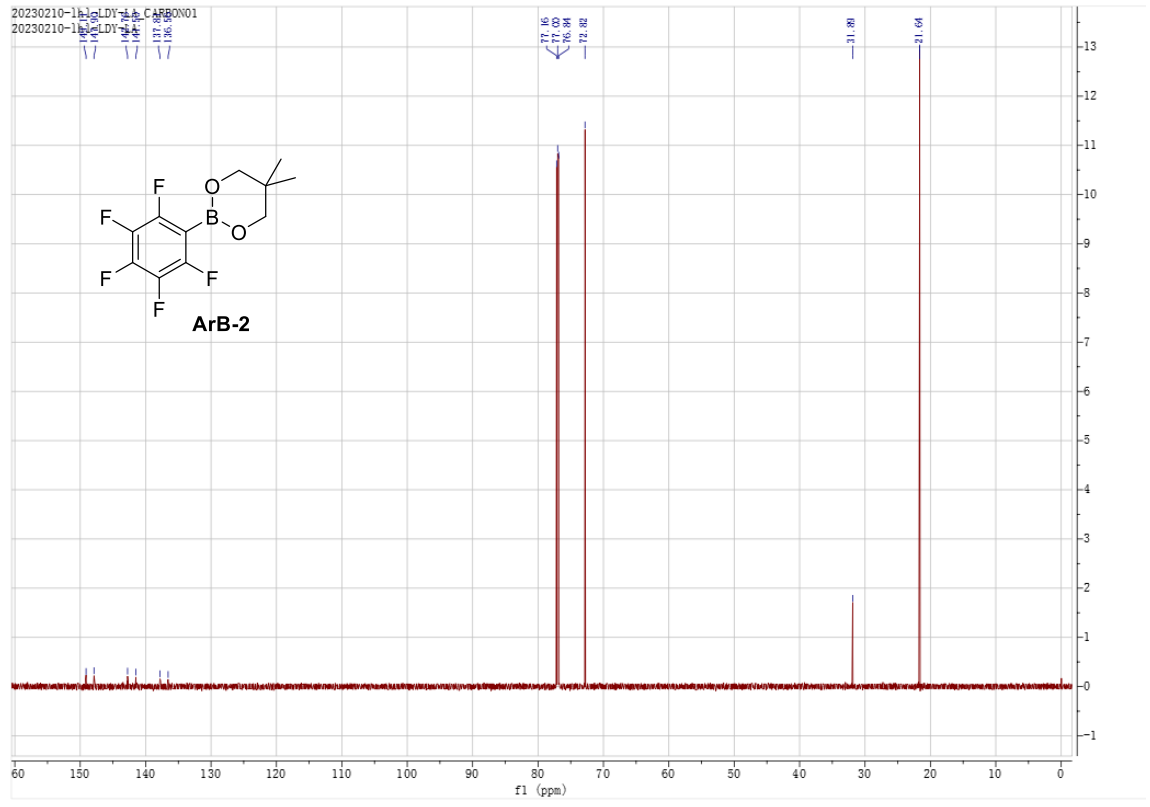
J = 8.2 Hz, 2H), 2.53 (s, 3H), 1.38 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 135.3, 125.2, 83.9, 25.1, 15.2; the data of **2x**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.54 (d, *J* = 7.3 Hz, 1H), 7.31 (d, *J* = 6.9 Hz, 1H), 7.24-7.28 (m, 1H), 2.46 (s, 3H), 1.31 (s, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.0, 132.9, 131.6, 129.7, 128.4, 84.1, 25.0, 16.0; IR (KBr, ν / cm^{-1}) 2974, 1583, 1348, 1048, 863, 791; HRMS (ESI^+) Calcd for $C_{13}H_{19}BO_2SNa$ ($[M+Na]^+$ 273.1091, Found 273.1104.

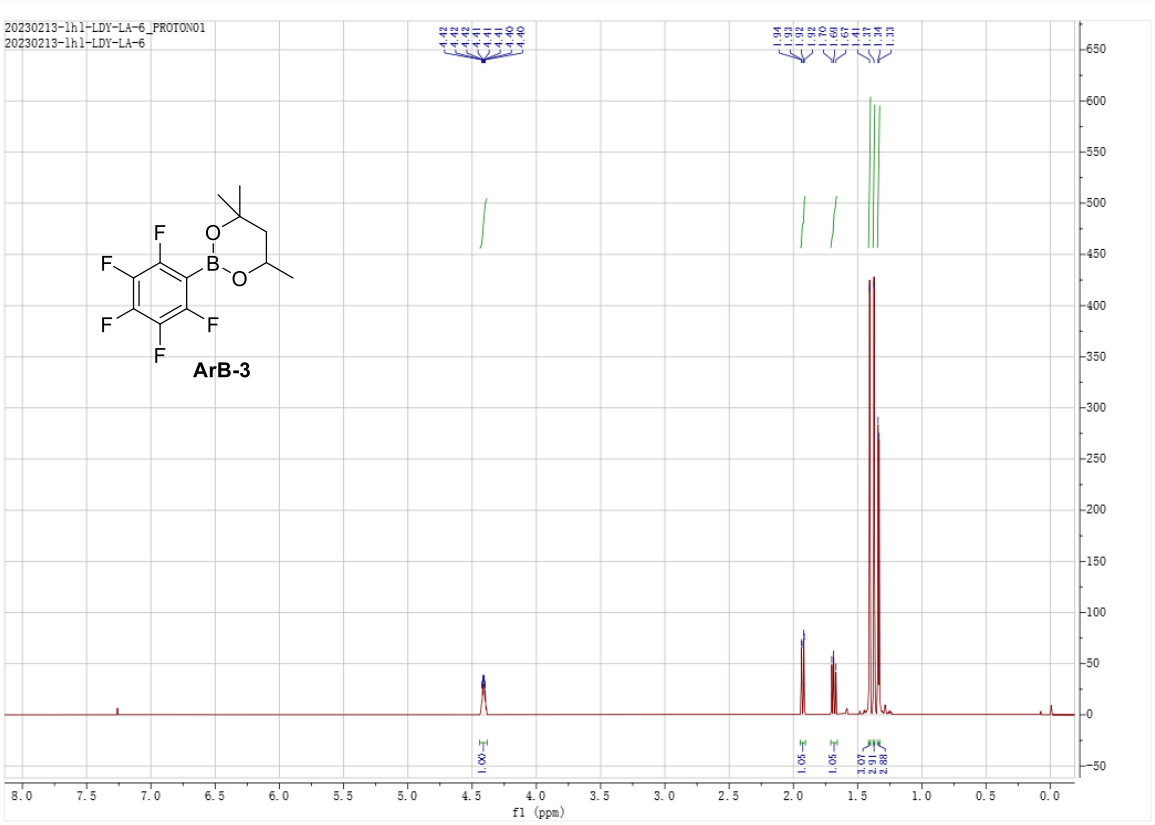
4. ^{1}H-NMR and ^{13}C-NMR Chart

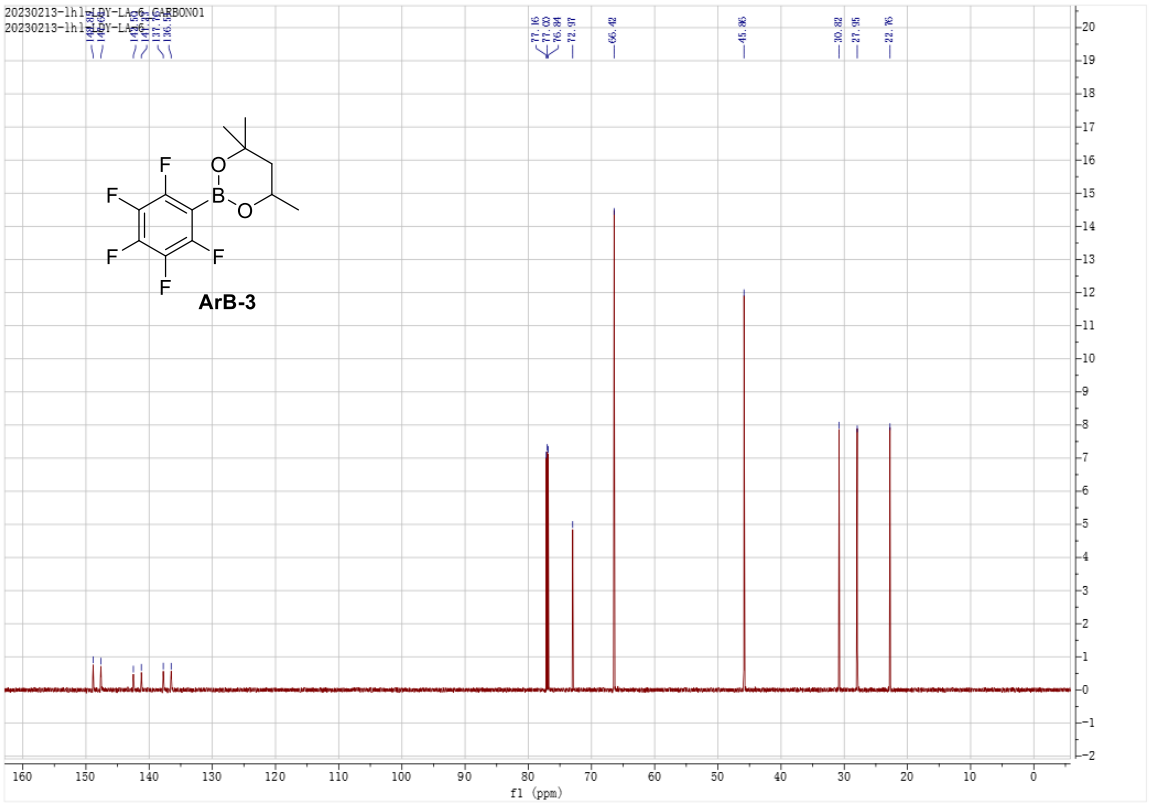


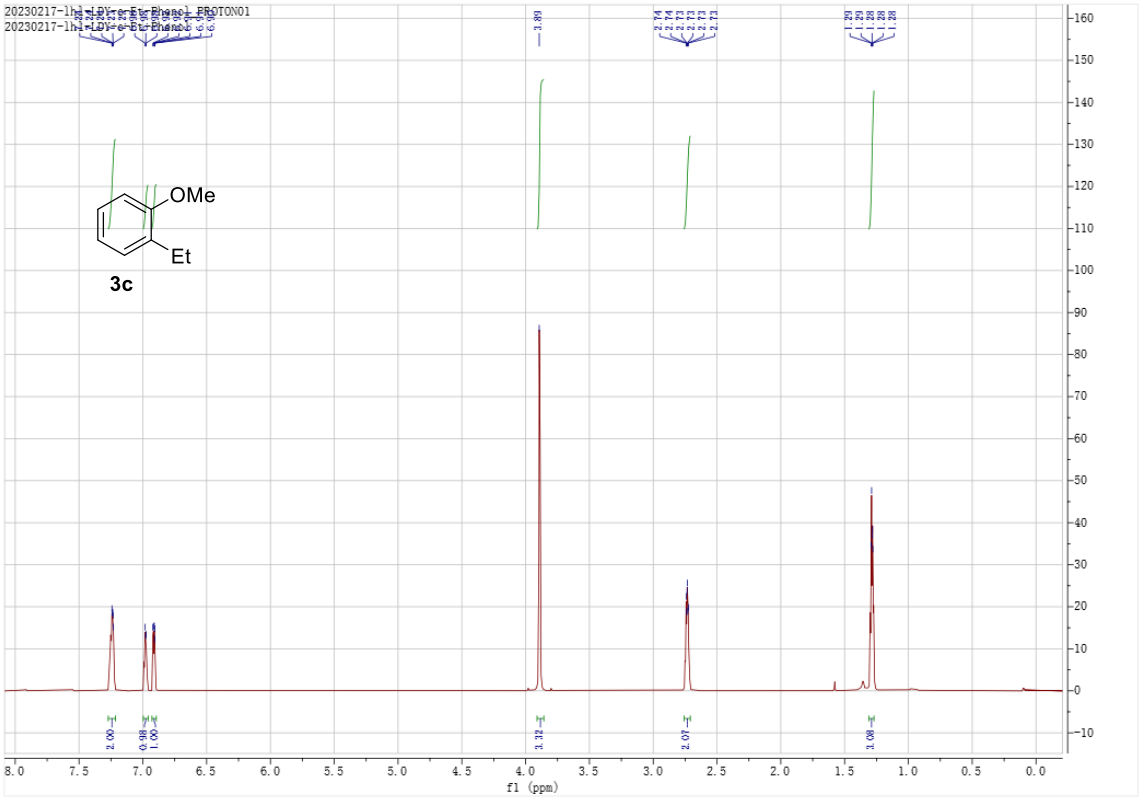


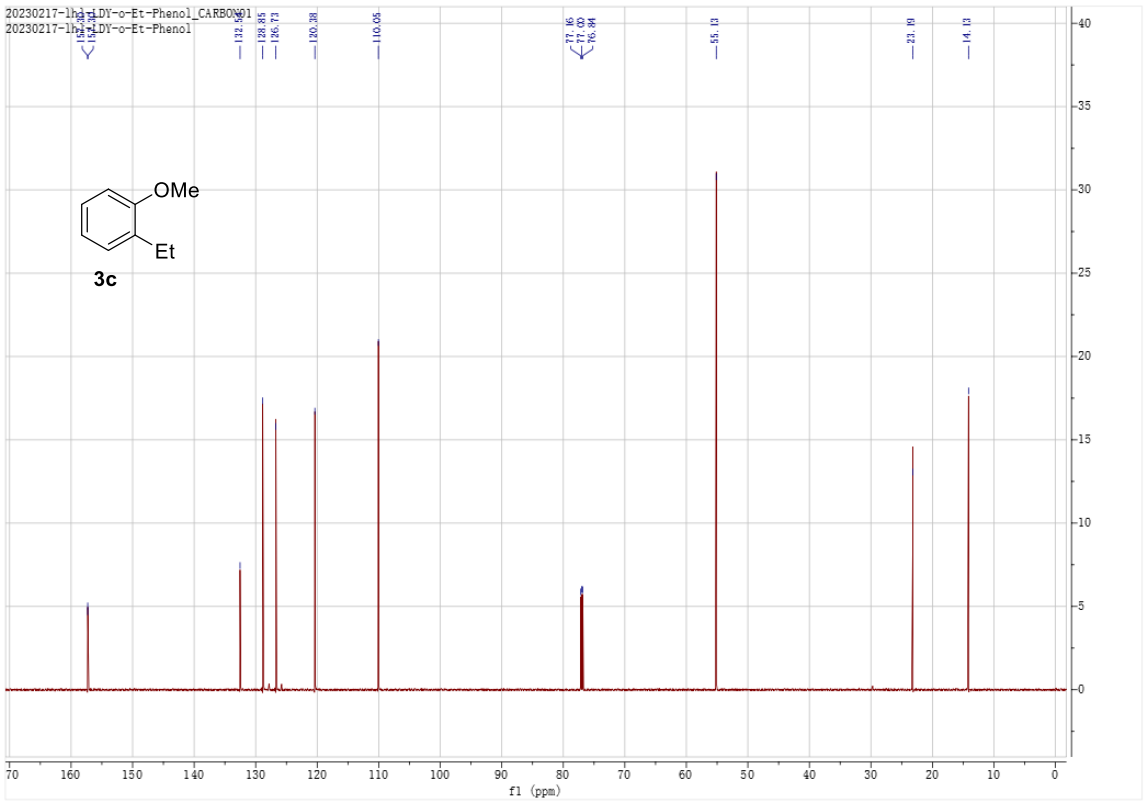

20230210-lh1-LDY-LA_PROTON01
20230210-lh1-LDY-LA
3.81
1.07
4.00
6.10
F
O
B
O
F
F
F
F
ArB-2
f1 (ppm)

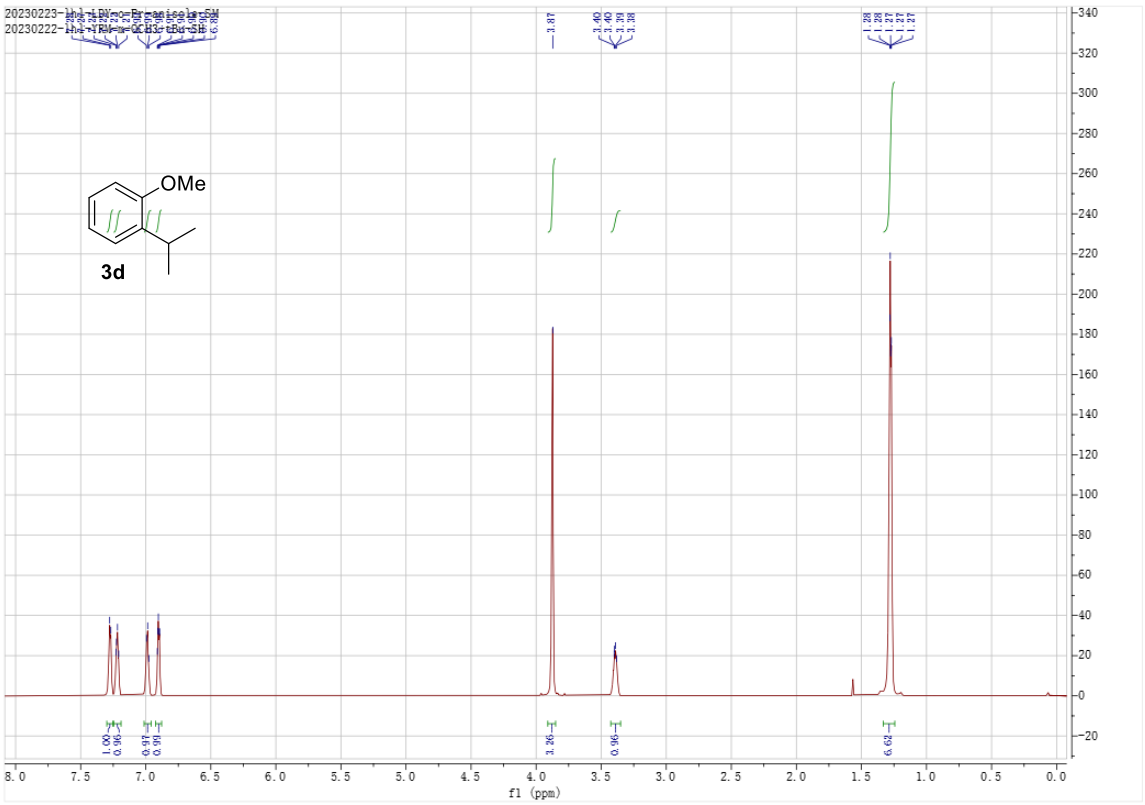

77.16
77.00
76.84
72.82
31.89
21.64
F
O
B
O
F
F
F
F
ArB-2
f1 (ppm)

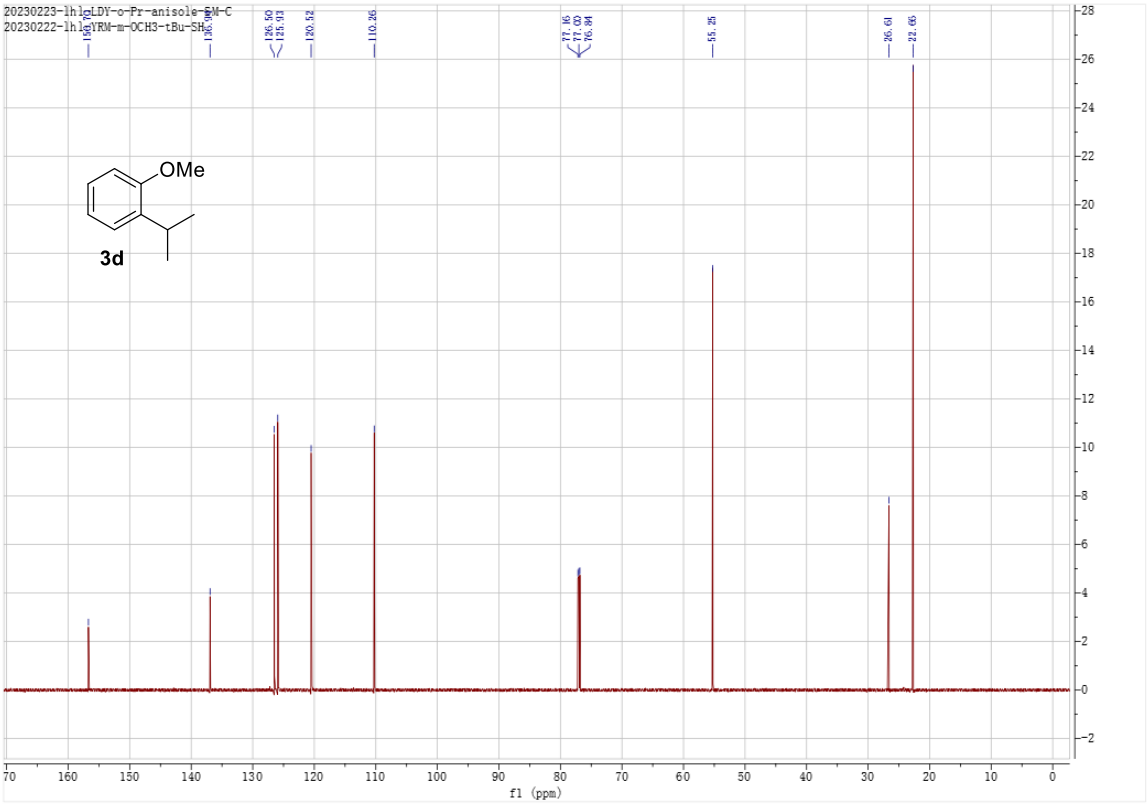

20230213-1h1-LDY-LA-6_PROTON01
20230213-1h1-LDY-LA-6
ArB-3
f1 (ppm)

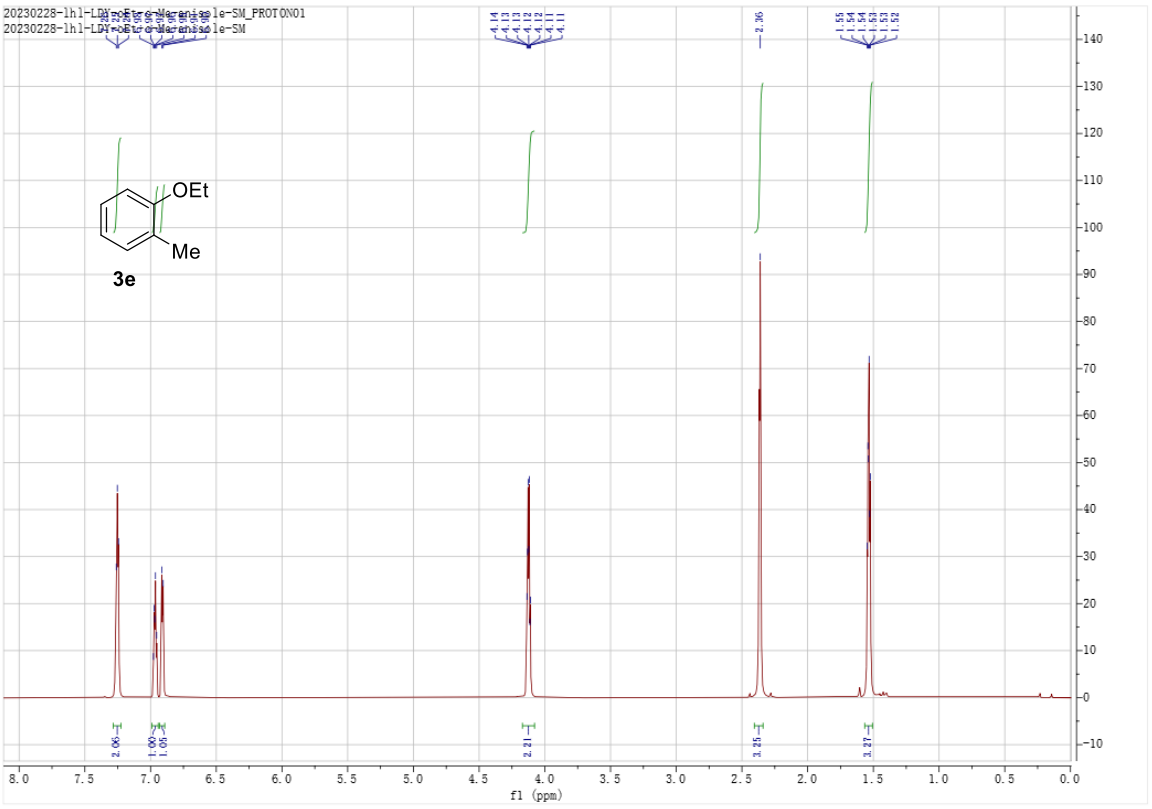

20230213-1h1-LDY-LA-6_CARBON01
ArB-3
f1 (ppm)

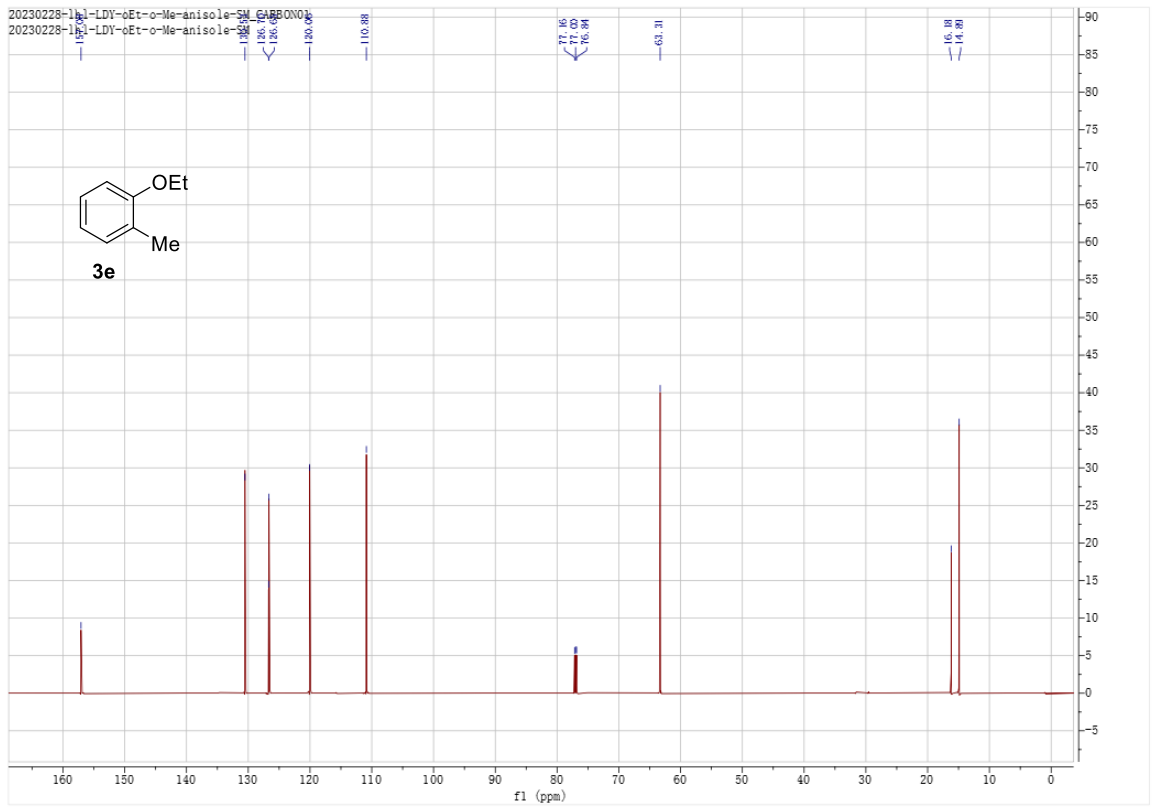

OMe
Et
3c
fl (ppm)

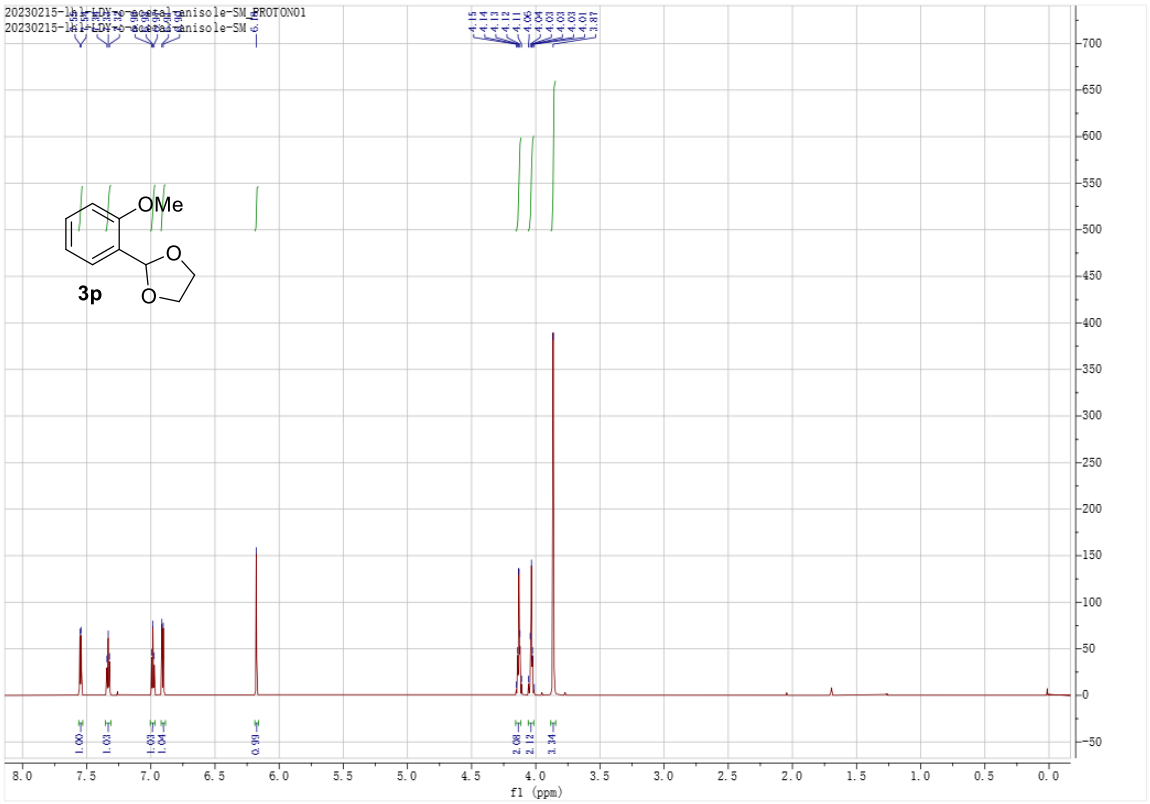

OMe
Et
3c
fl (ppm)

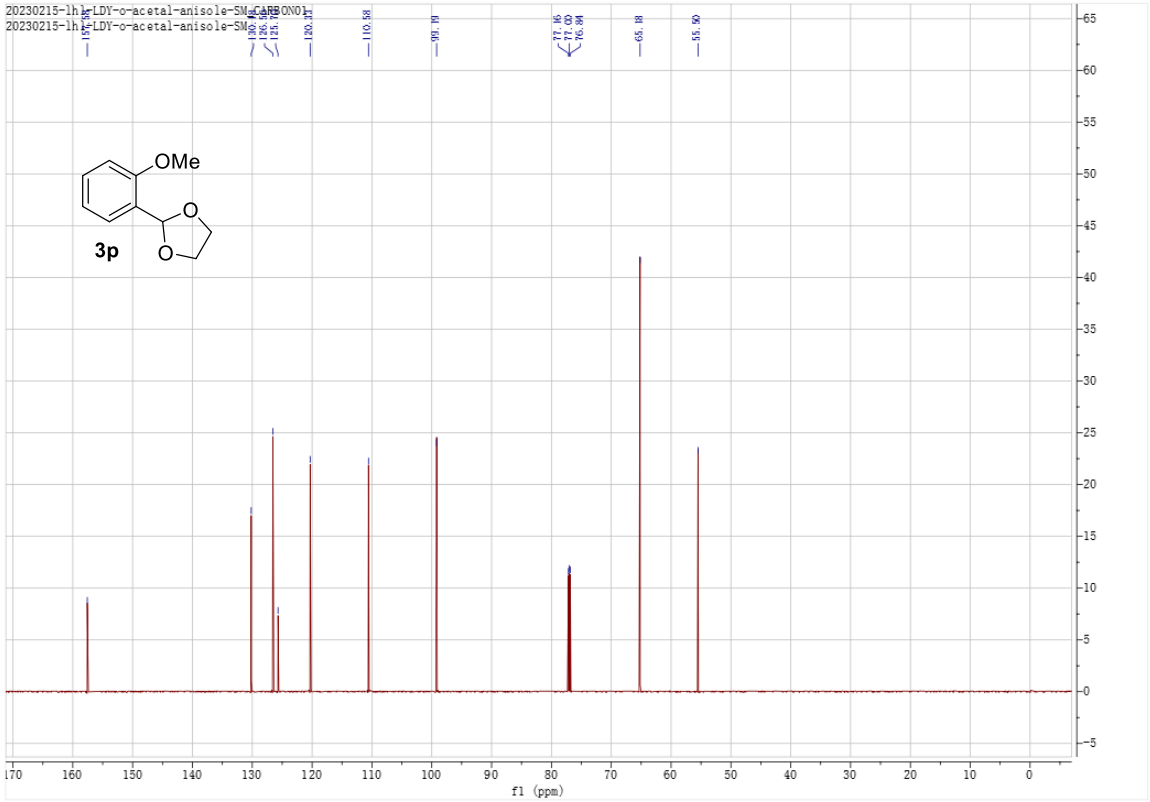

OMe
3d
f1 (ppm)

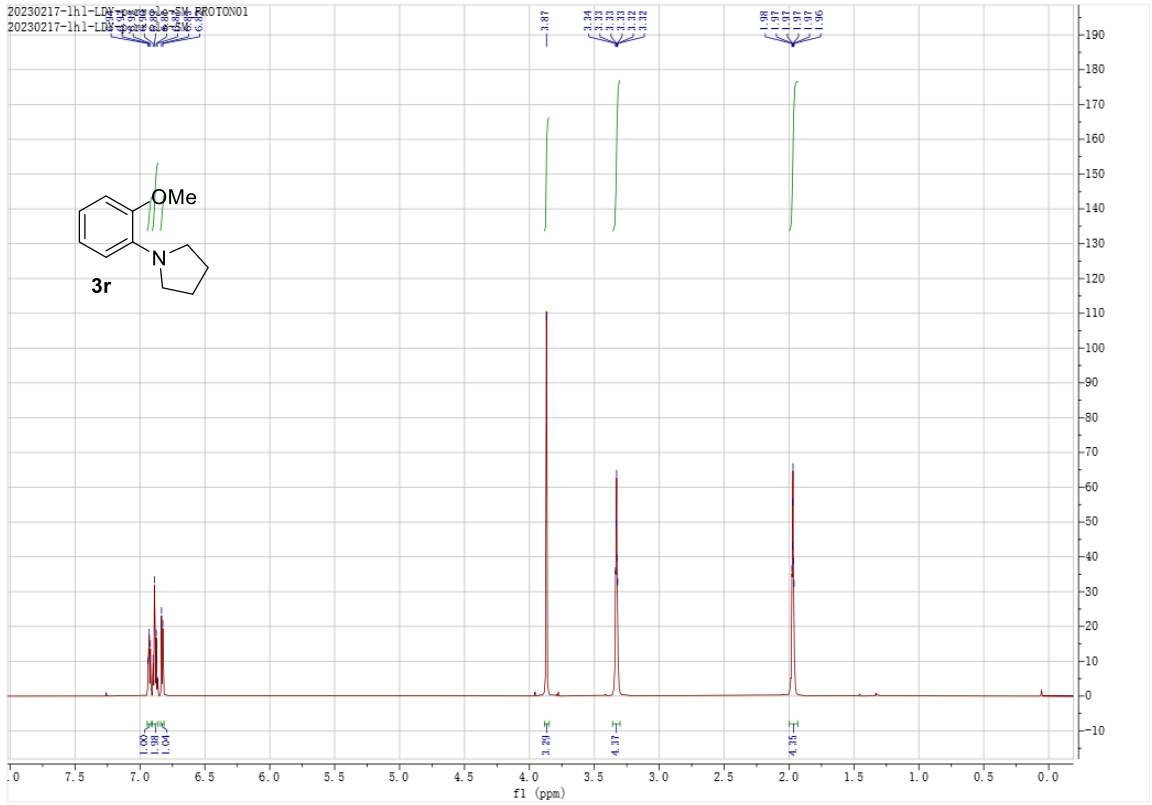

OMe
3d
f1 (ppm)

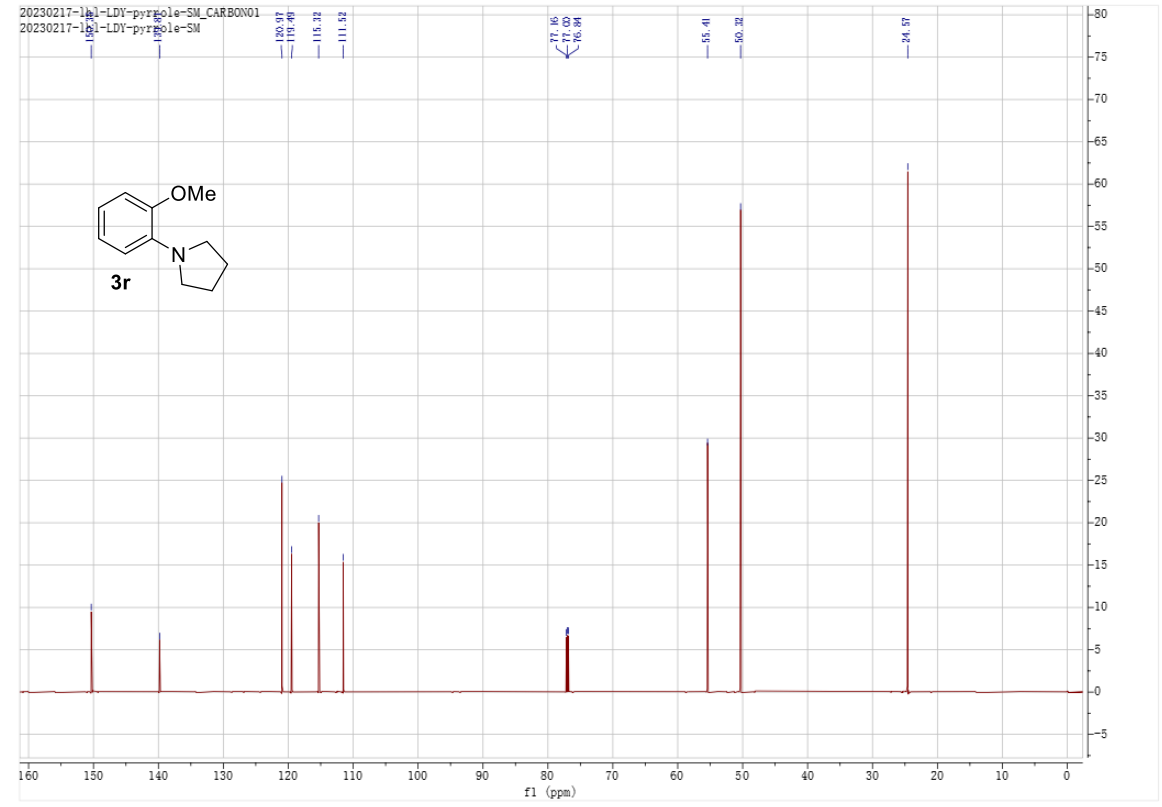

OEt
Me
3e
f1 (ppm)

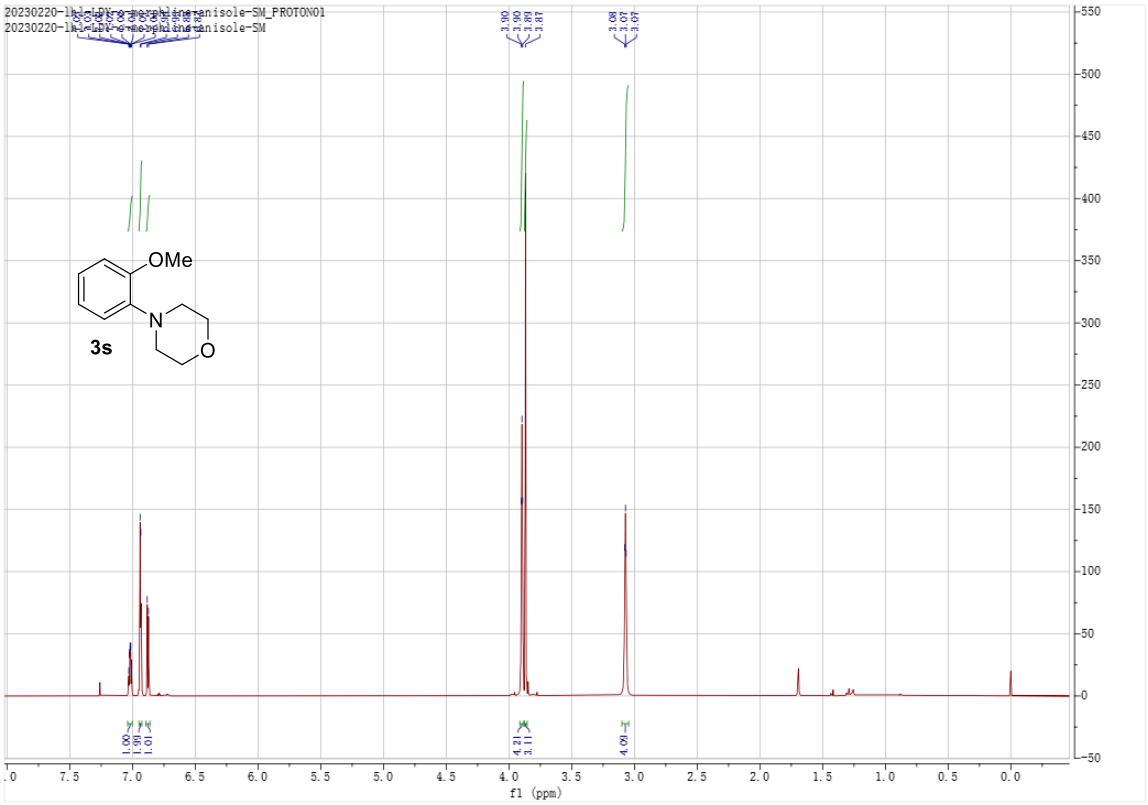

OEt
Me
3e
f1 (ppm)

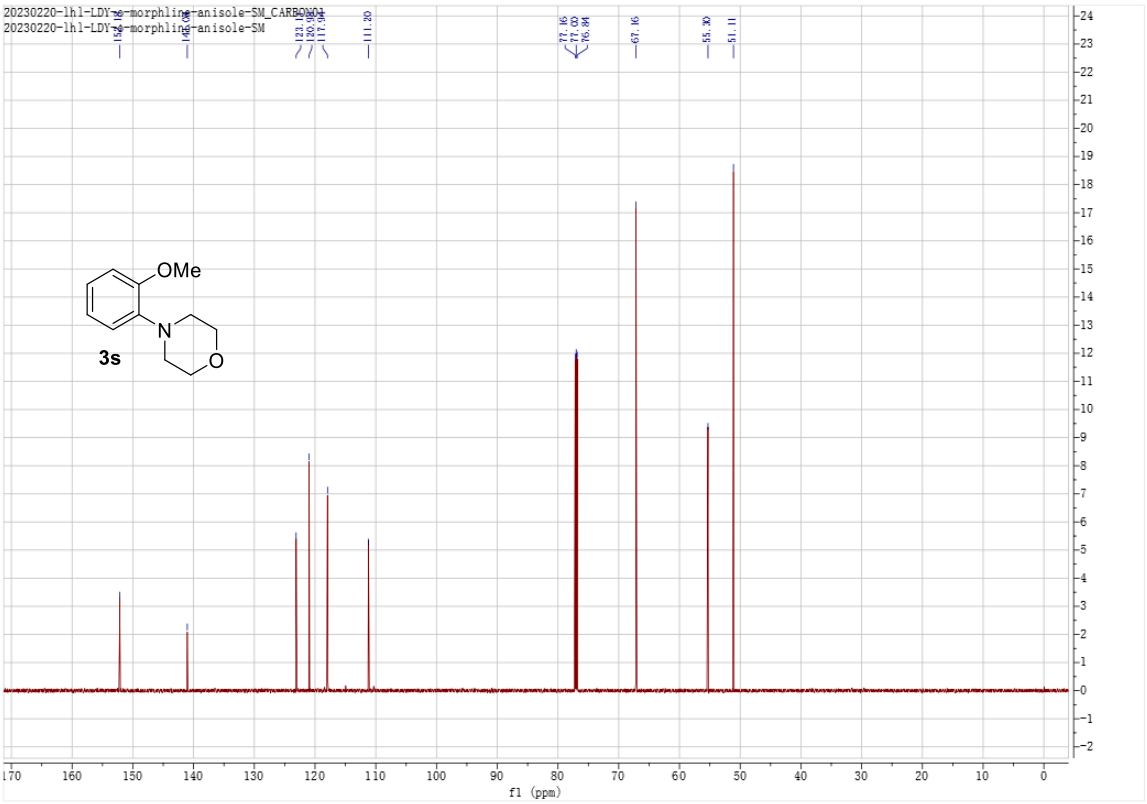

OMe
O
O
3p
f1 (ppm)

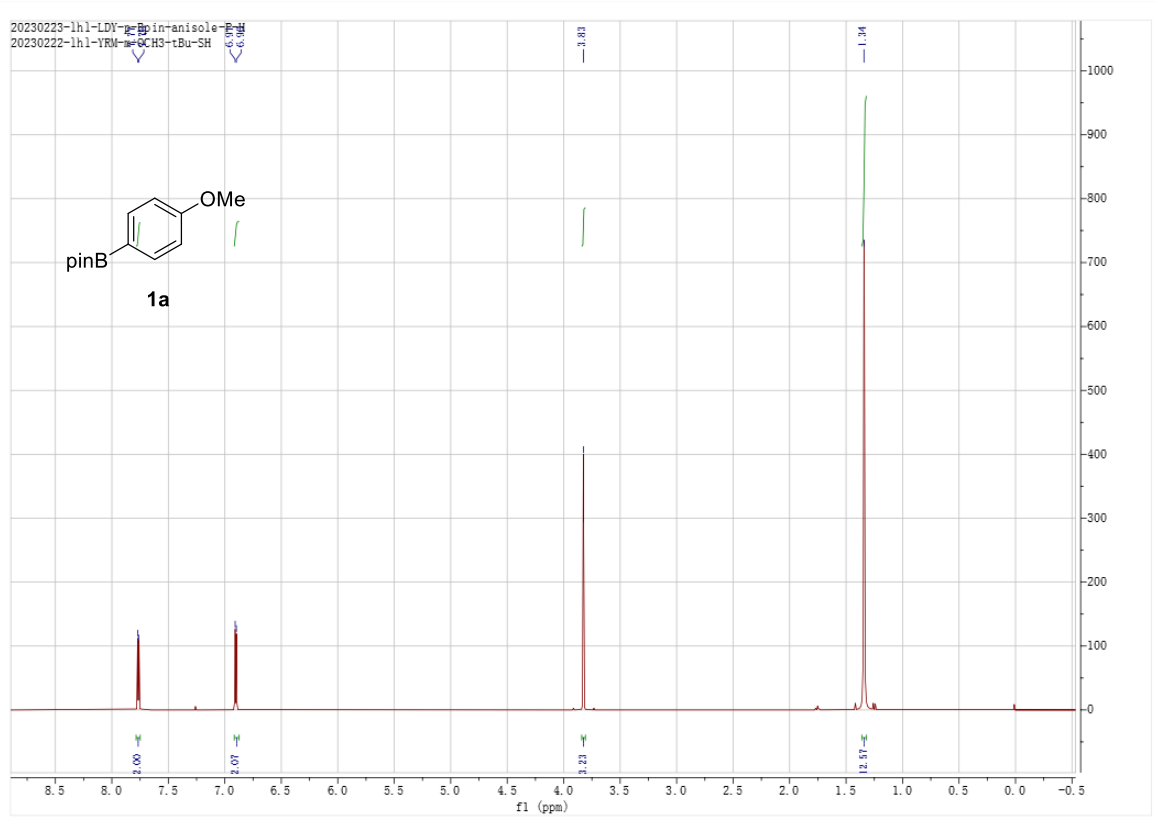

OMe
O
O
3p
f1 (ppm)

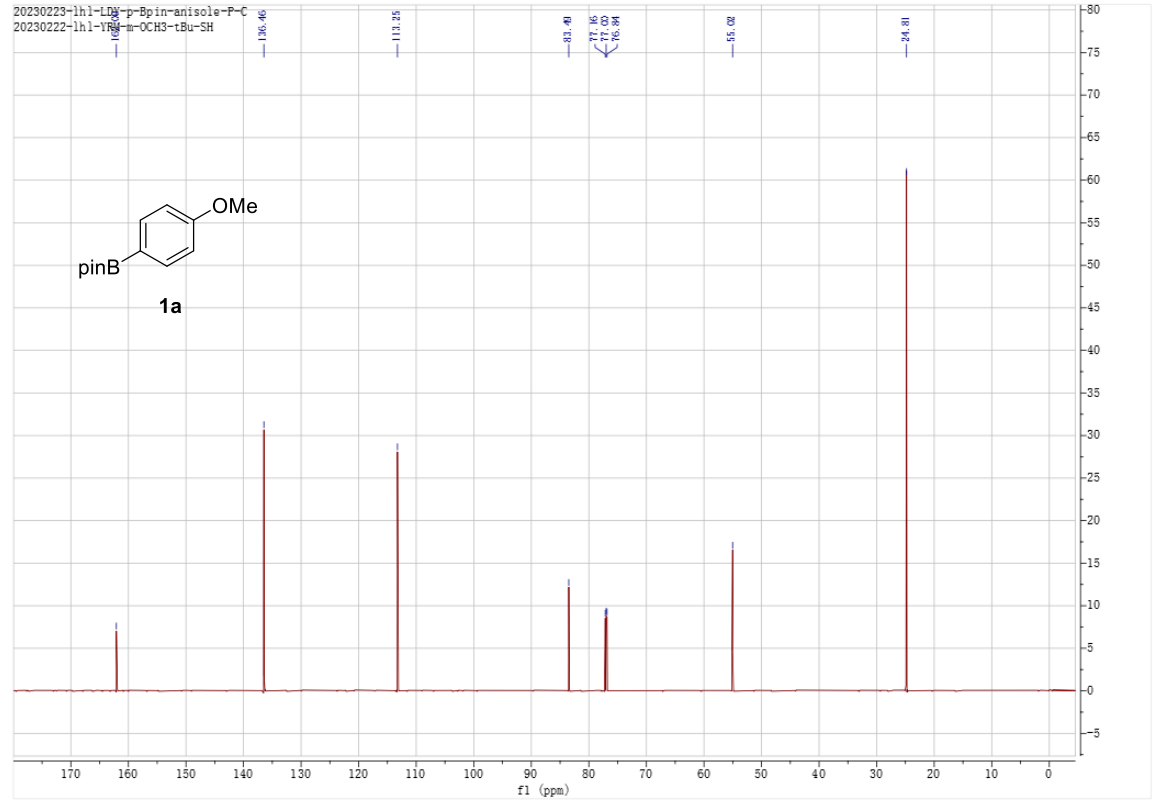

OMe
N
3r
f1 (ppm)

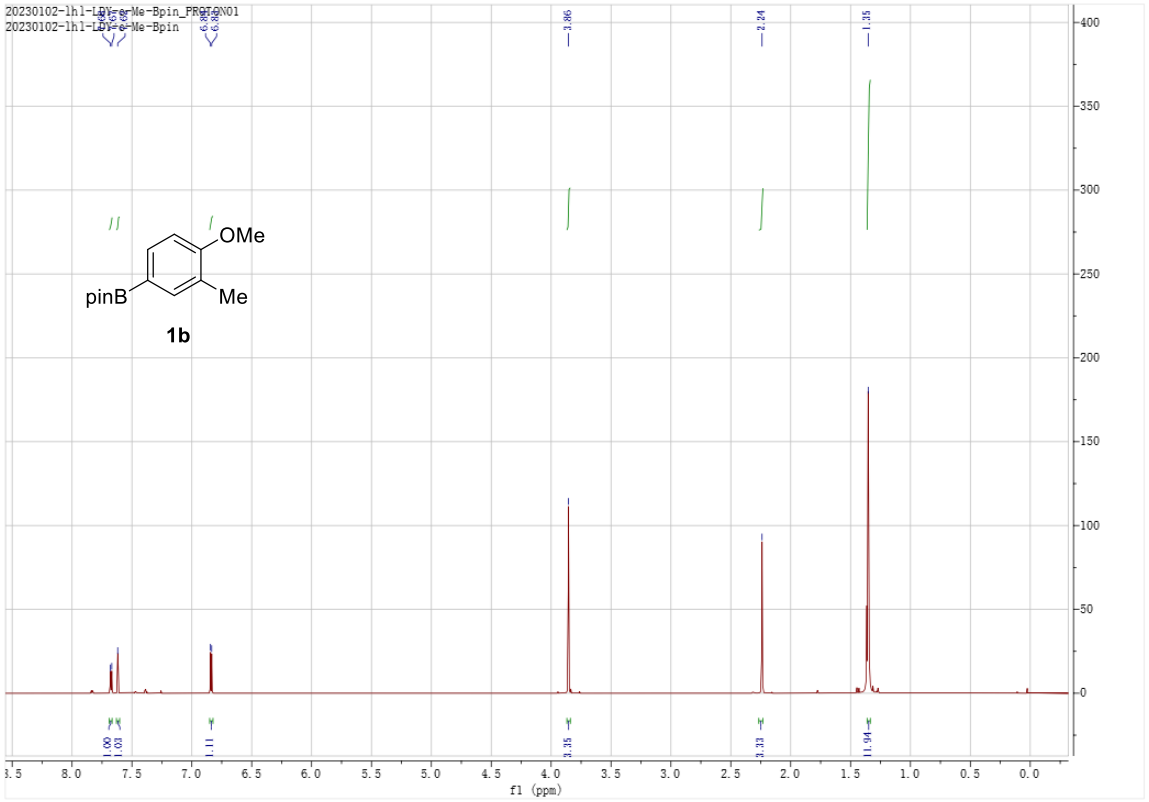

OMe
N
3r
f1 (ppm)

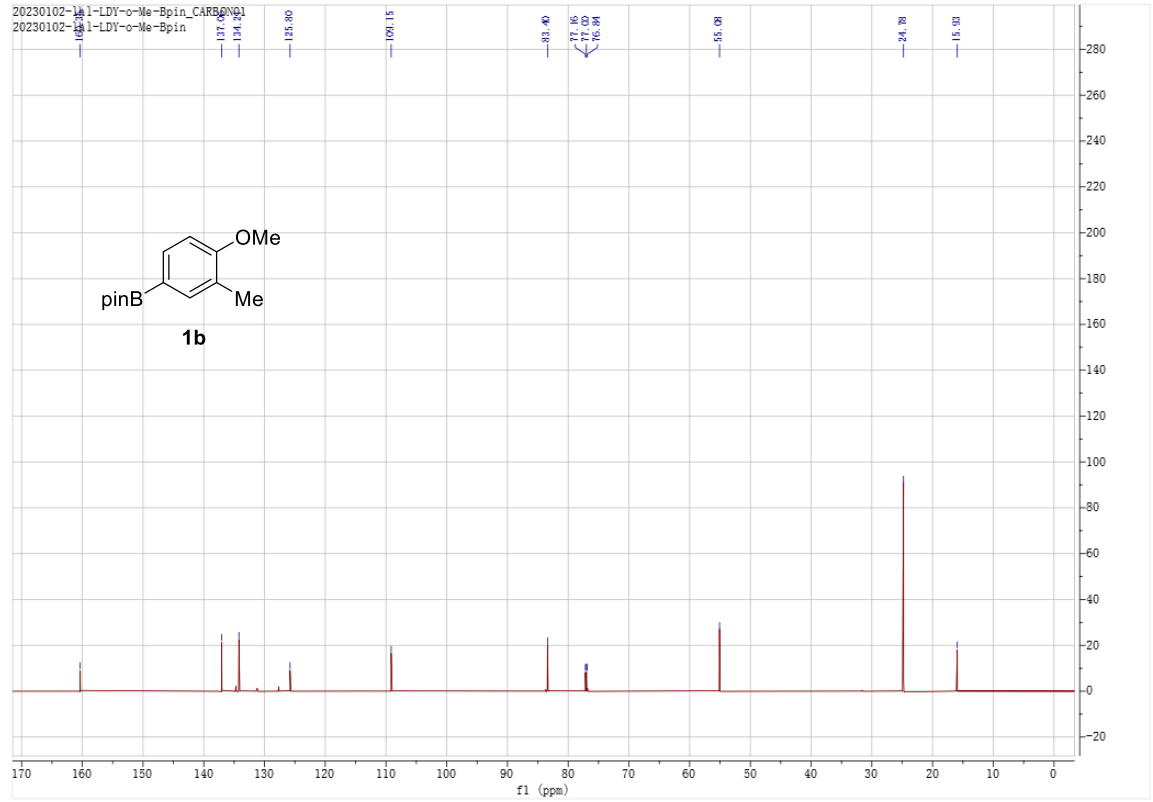

OMe
N
O
3s
f1 (ppm)

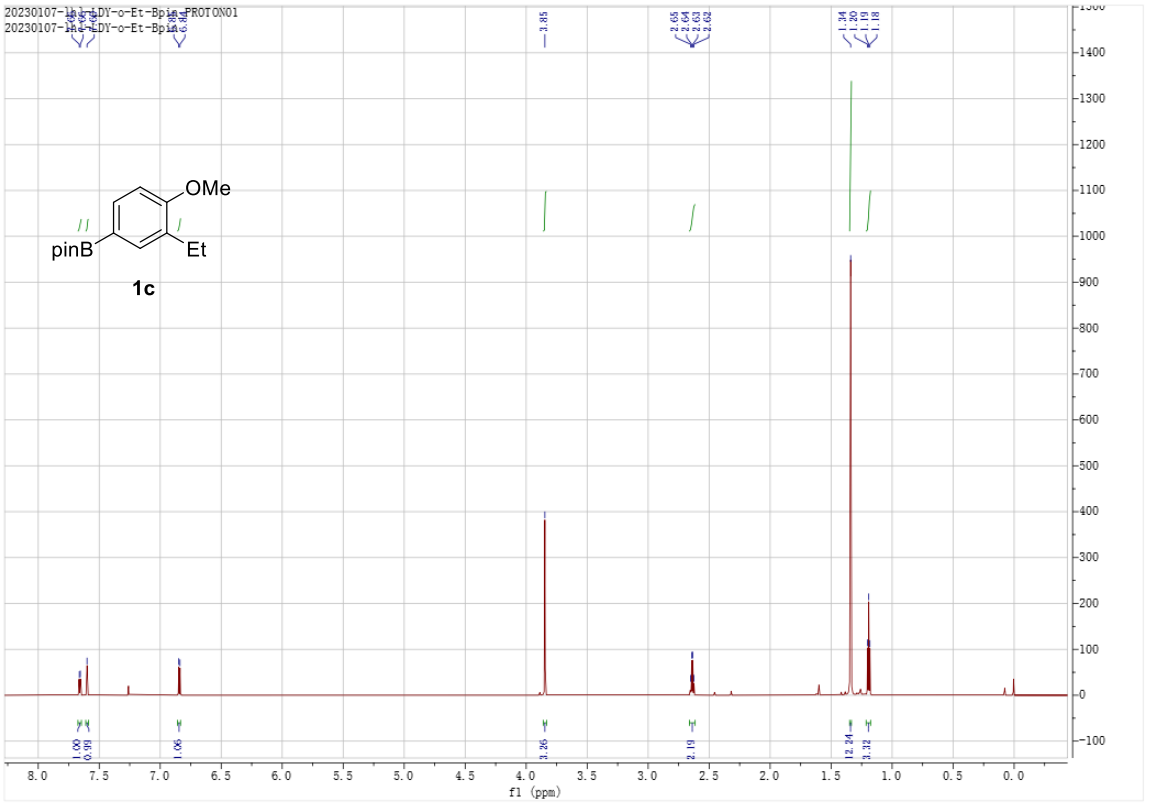

OMe
N
O
3s
f1 (ppm)

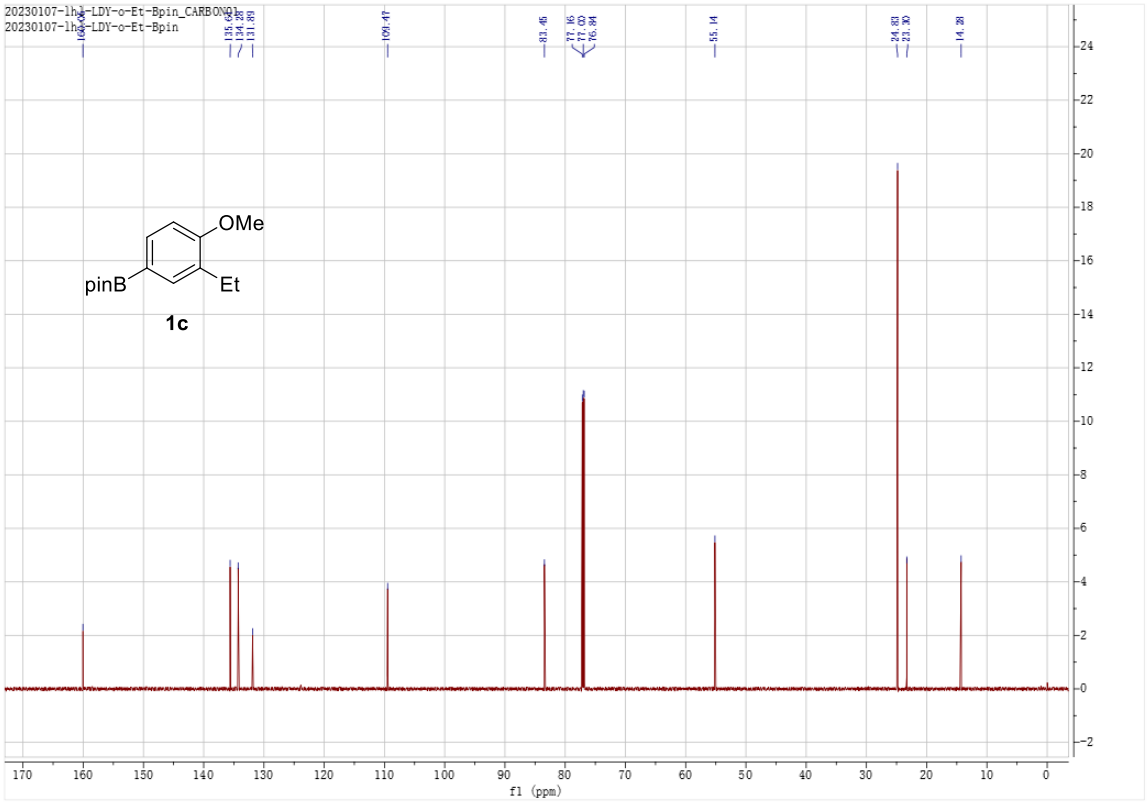

OMe
pinB
1a
f1 (ppm)

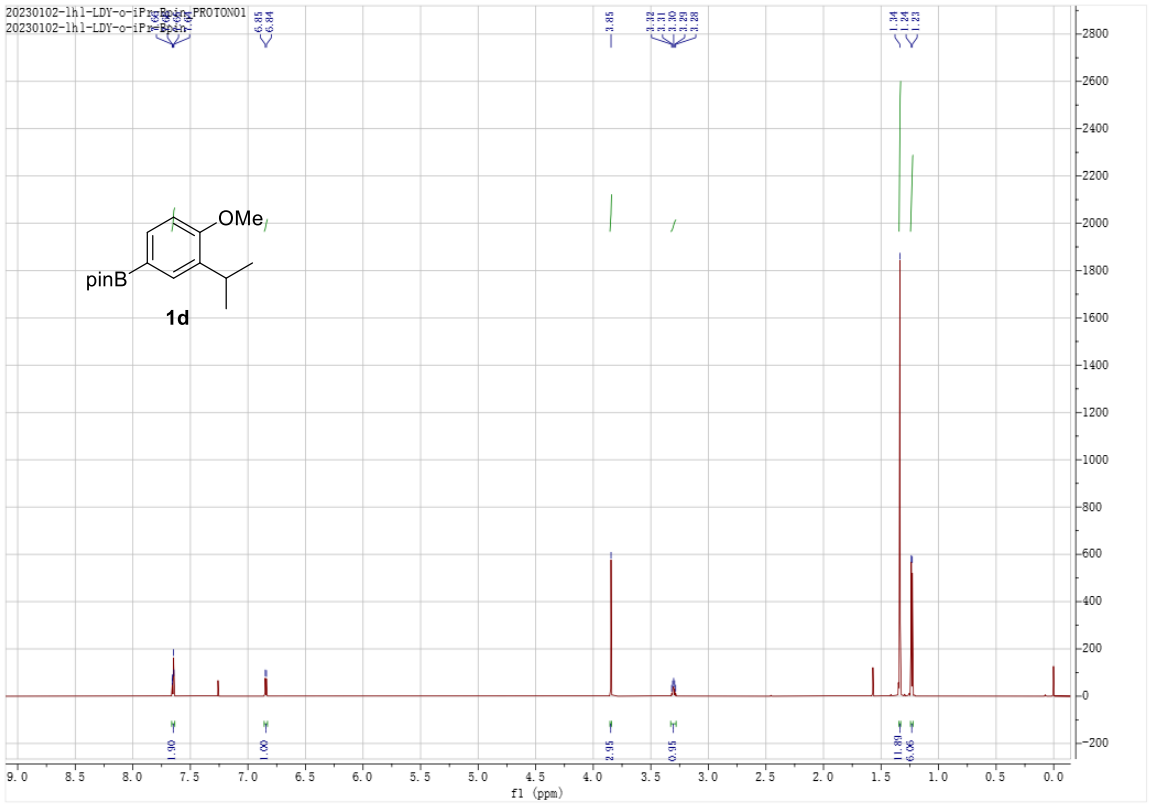

OMe
pinB
1a
f1 (ppm)

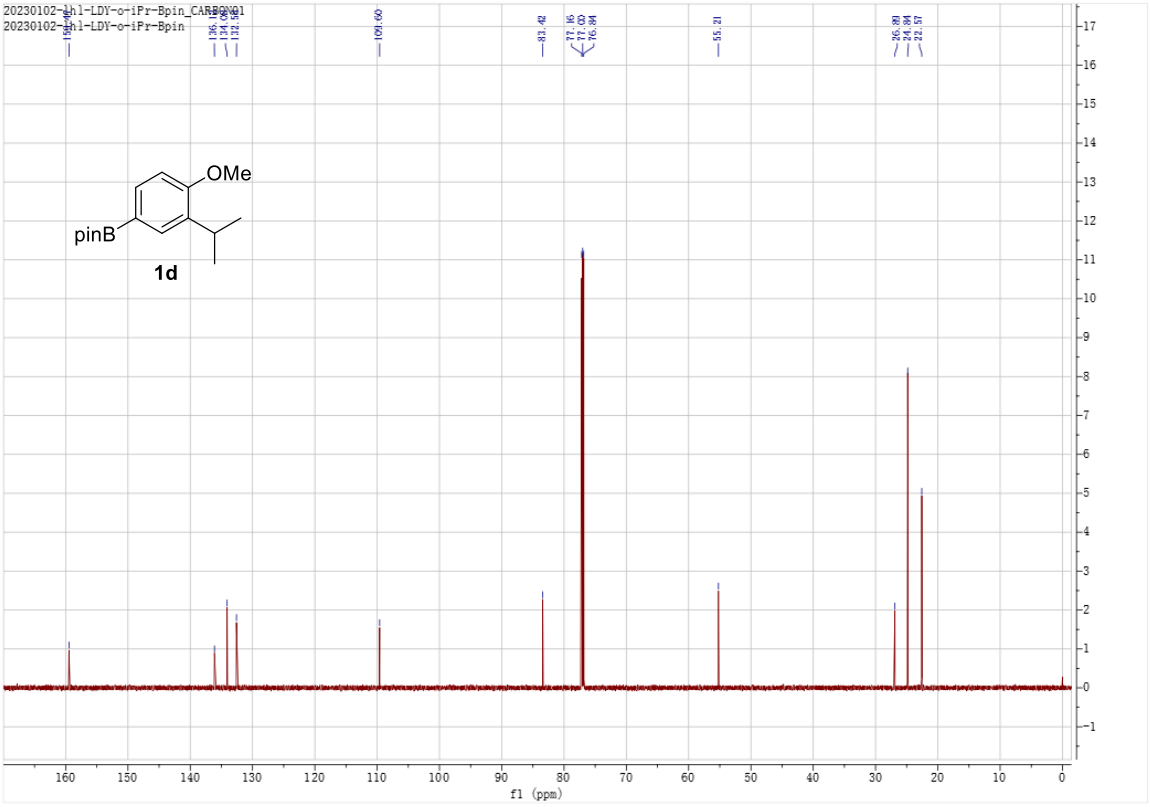

OMe
pinB
Me
1b
f1 (ppm)

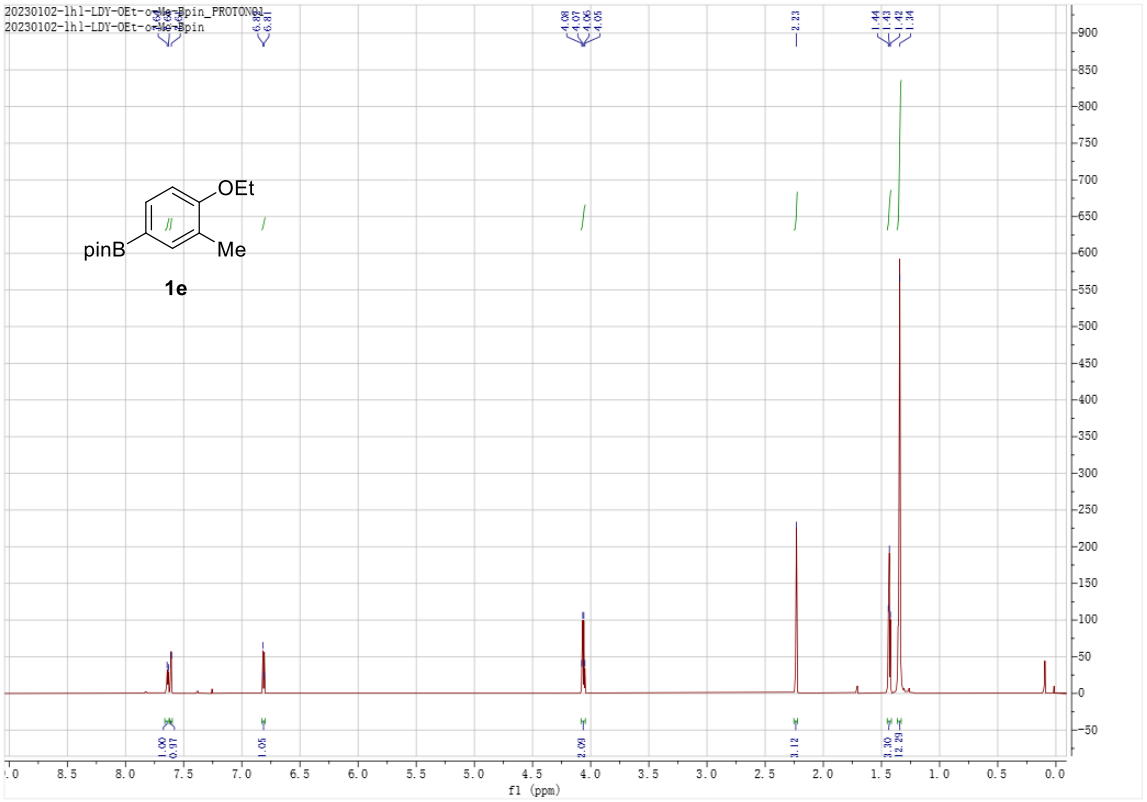

OMe
pinB
Me
1b
f1 (ppm)

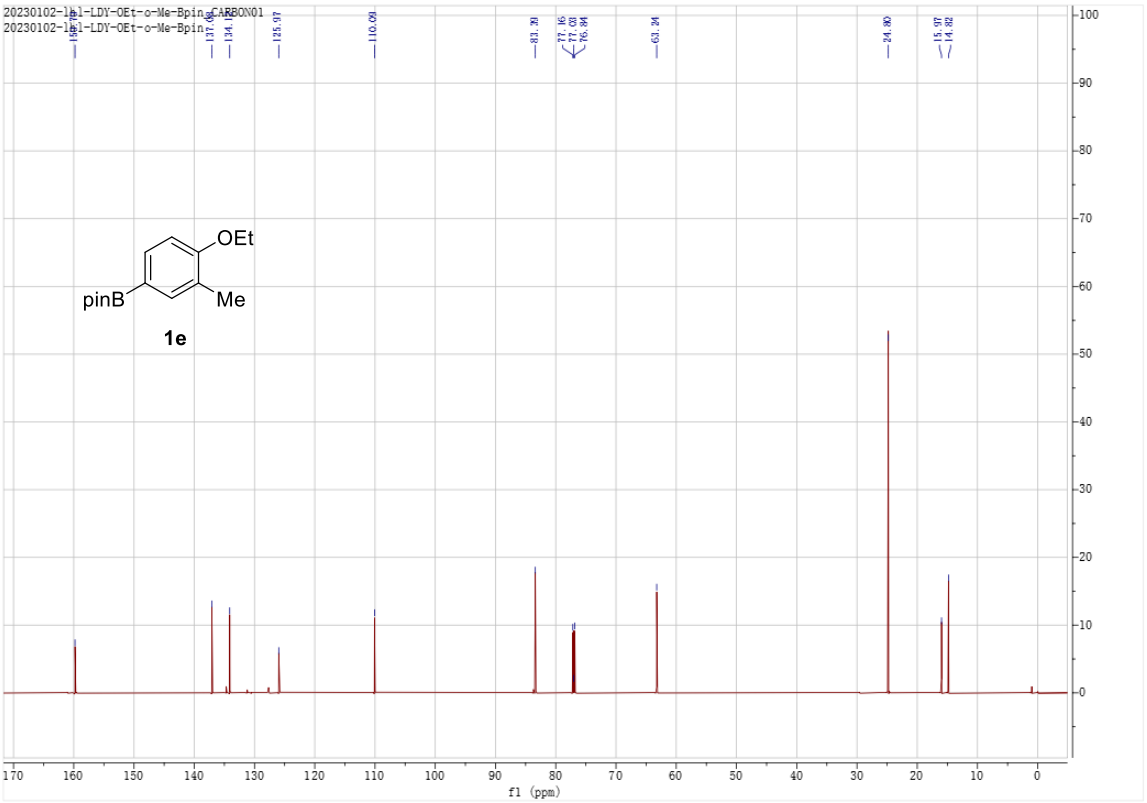

OMe
pinB
Et
1c
f1 (ppm)

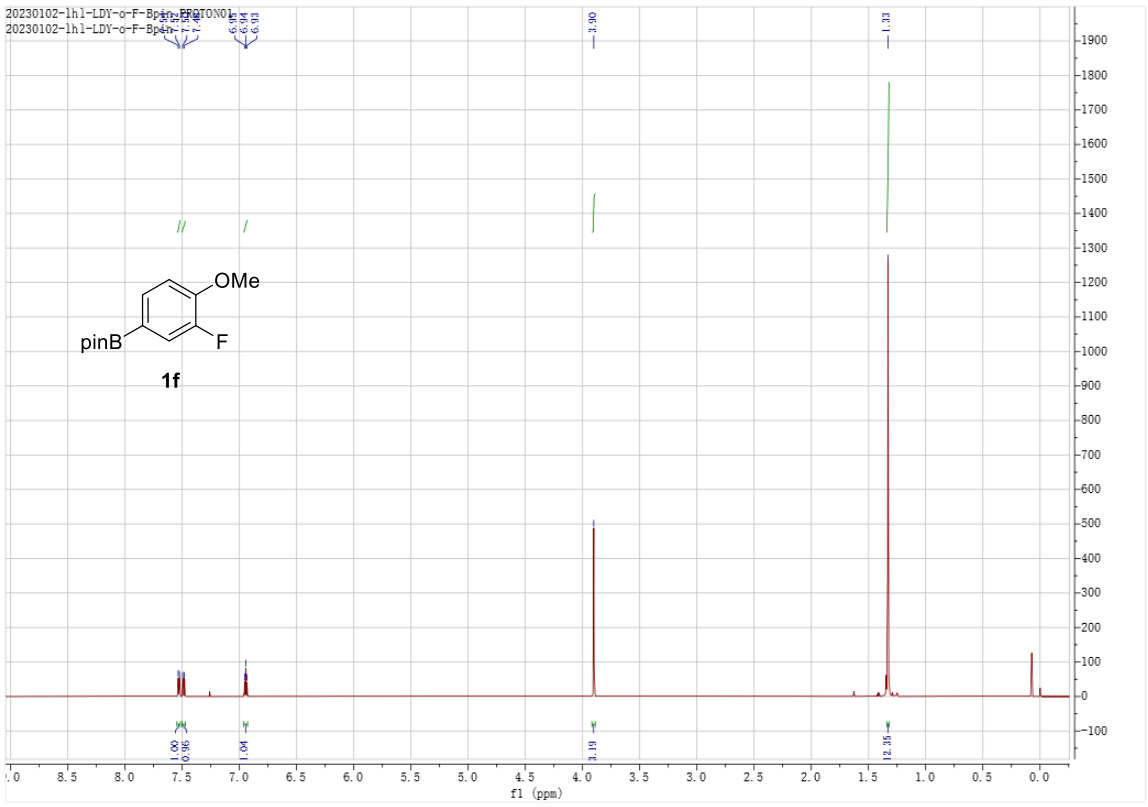

OMe
pinB
Et
1c
f1 (ppm)

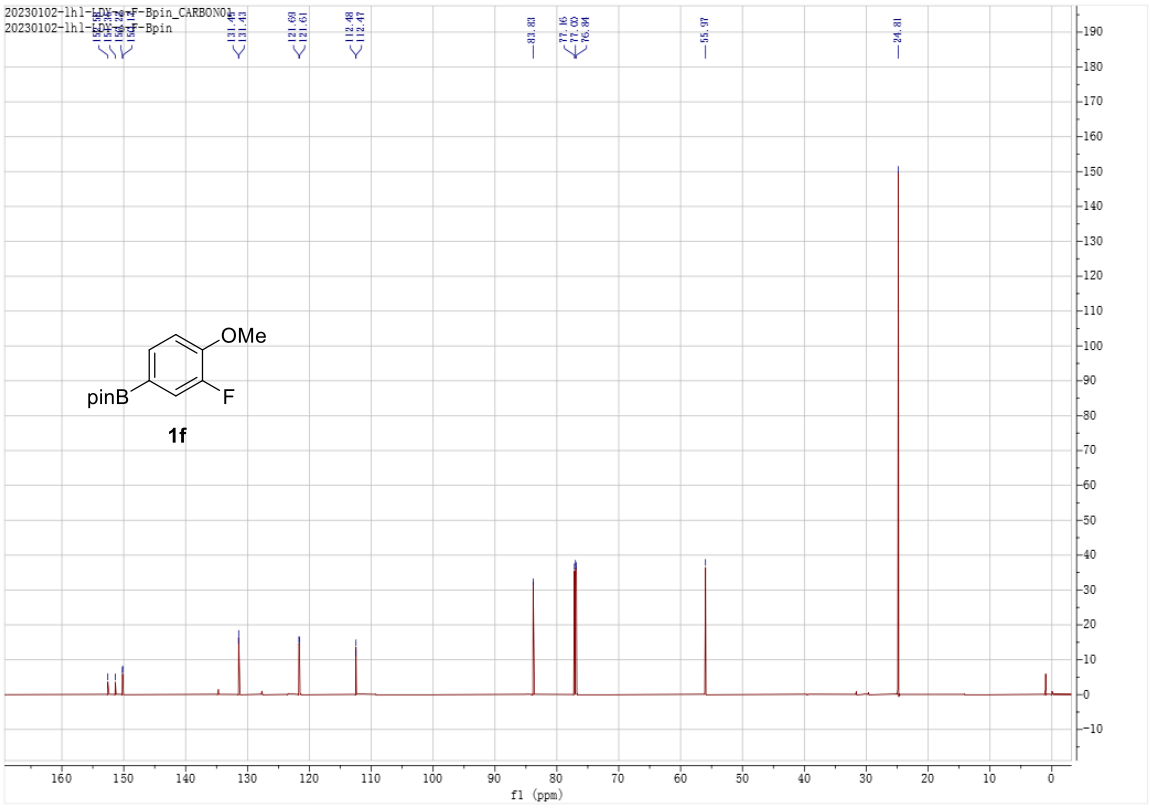

OMe
pinB
1d
f1 (ppm)

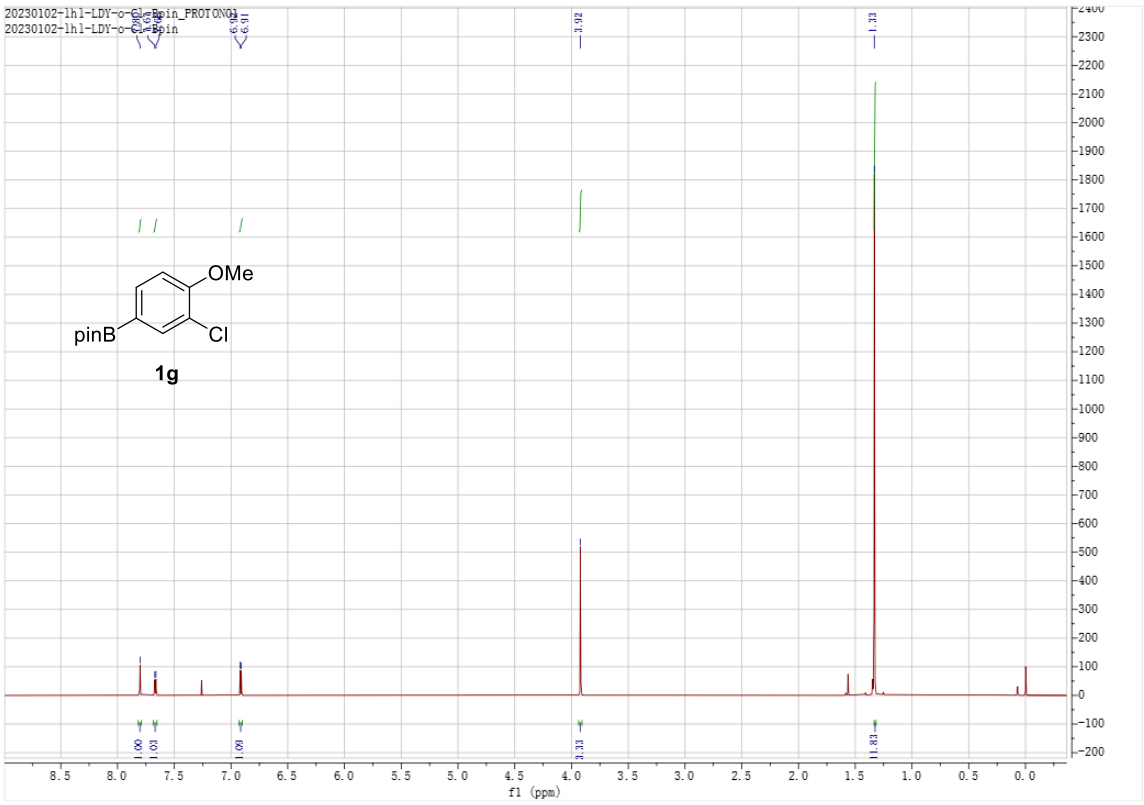

OMe
pinB
1d
f1 (ppm)

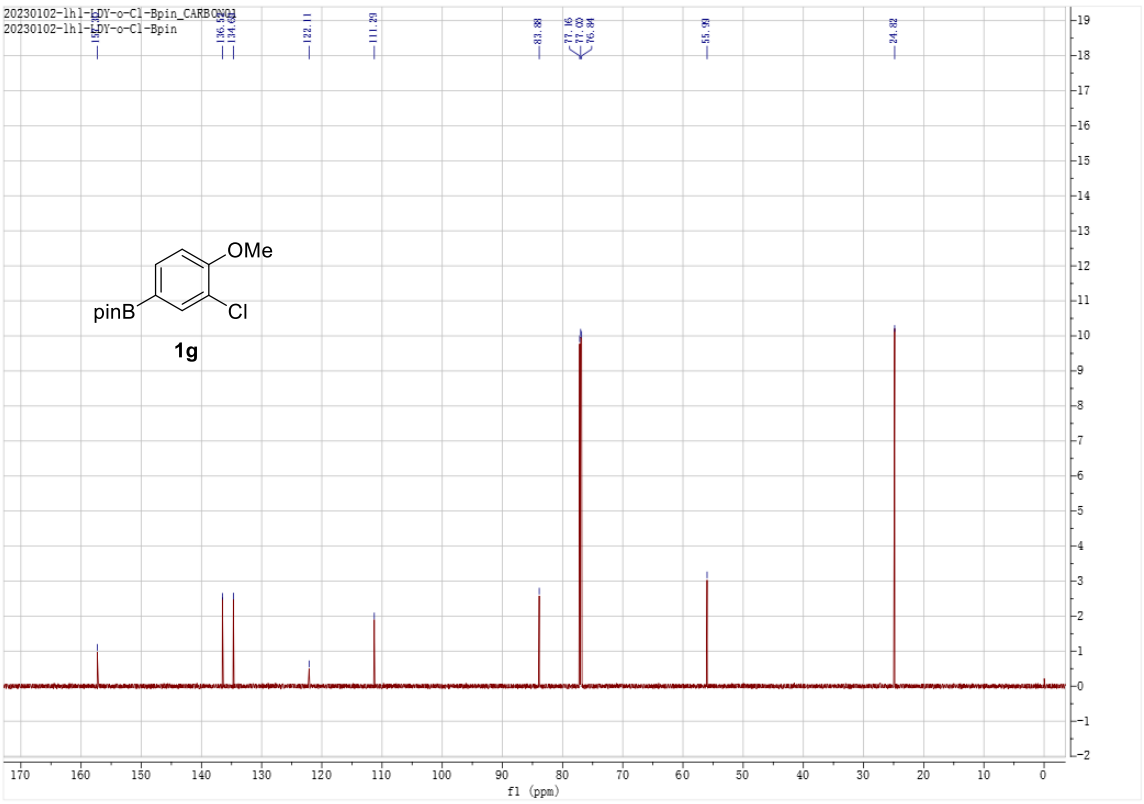

OEt
pinB
Me
1e
f1 (ppm)

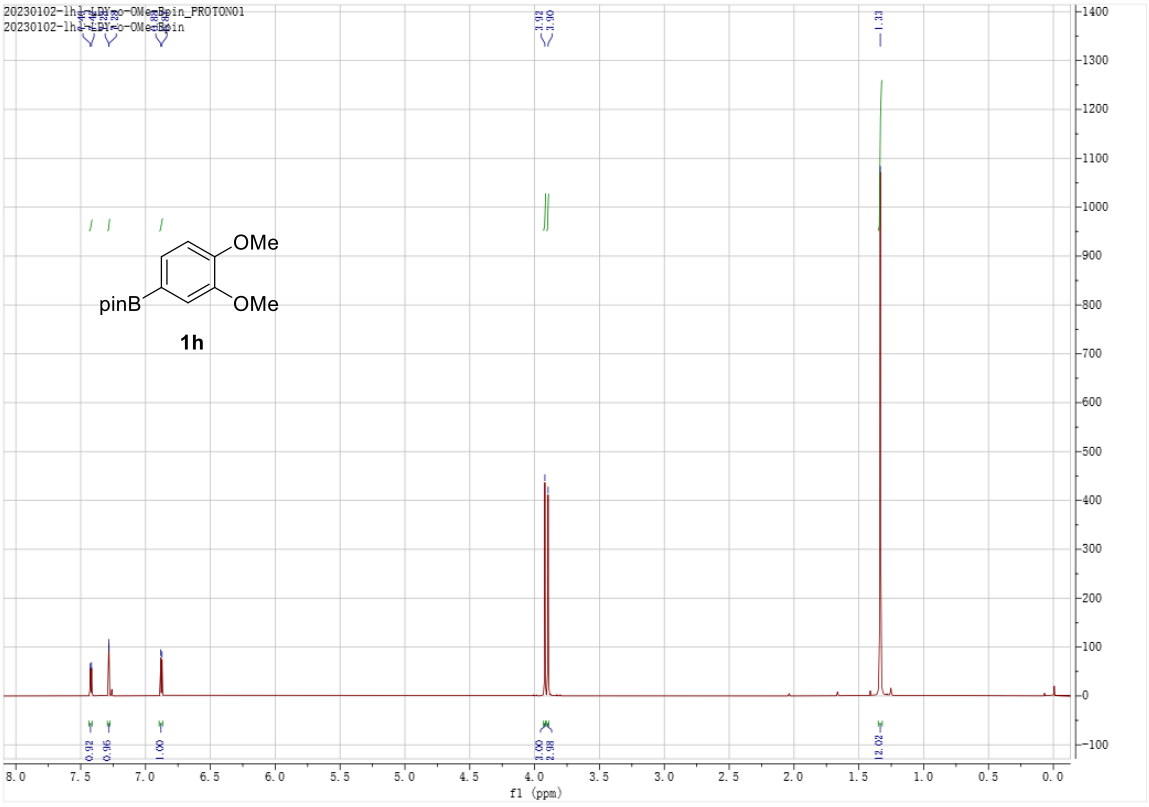

OEt
pinB
Me
1e
f1 (ppm)

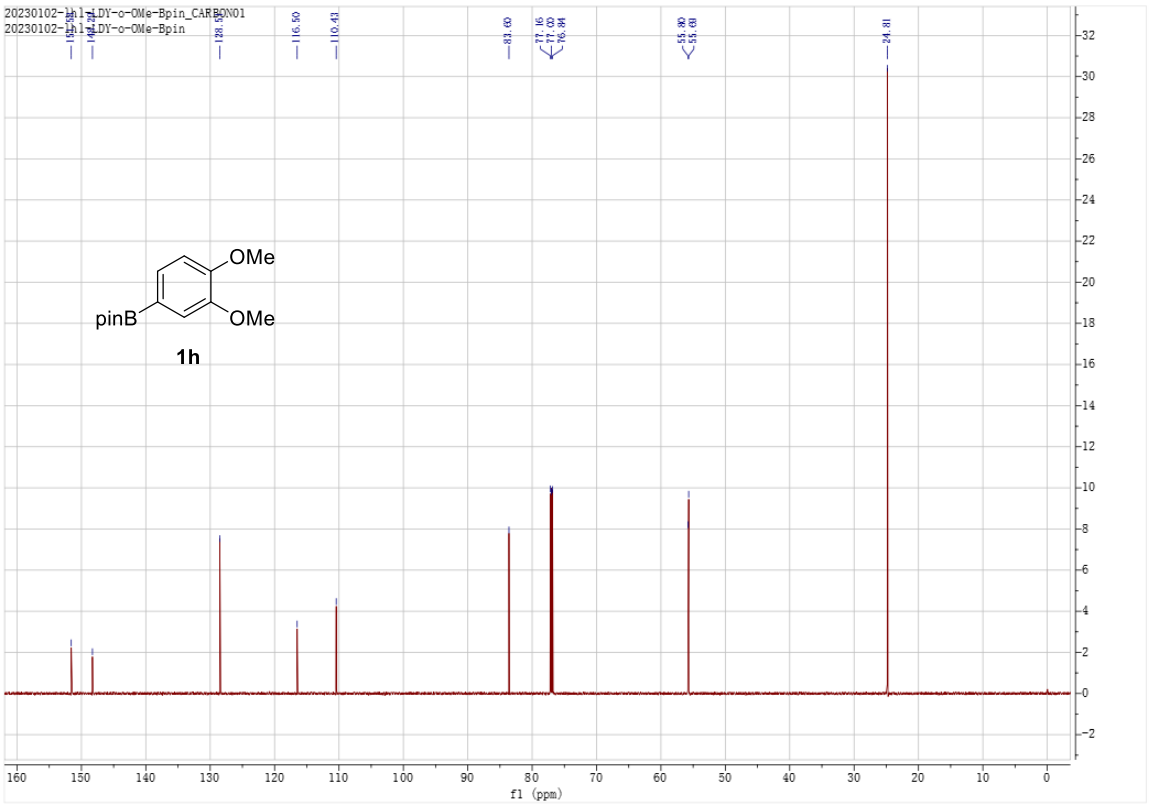

OMe
pinB
F
1f
f1 (ppm)

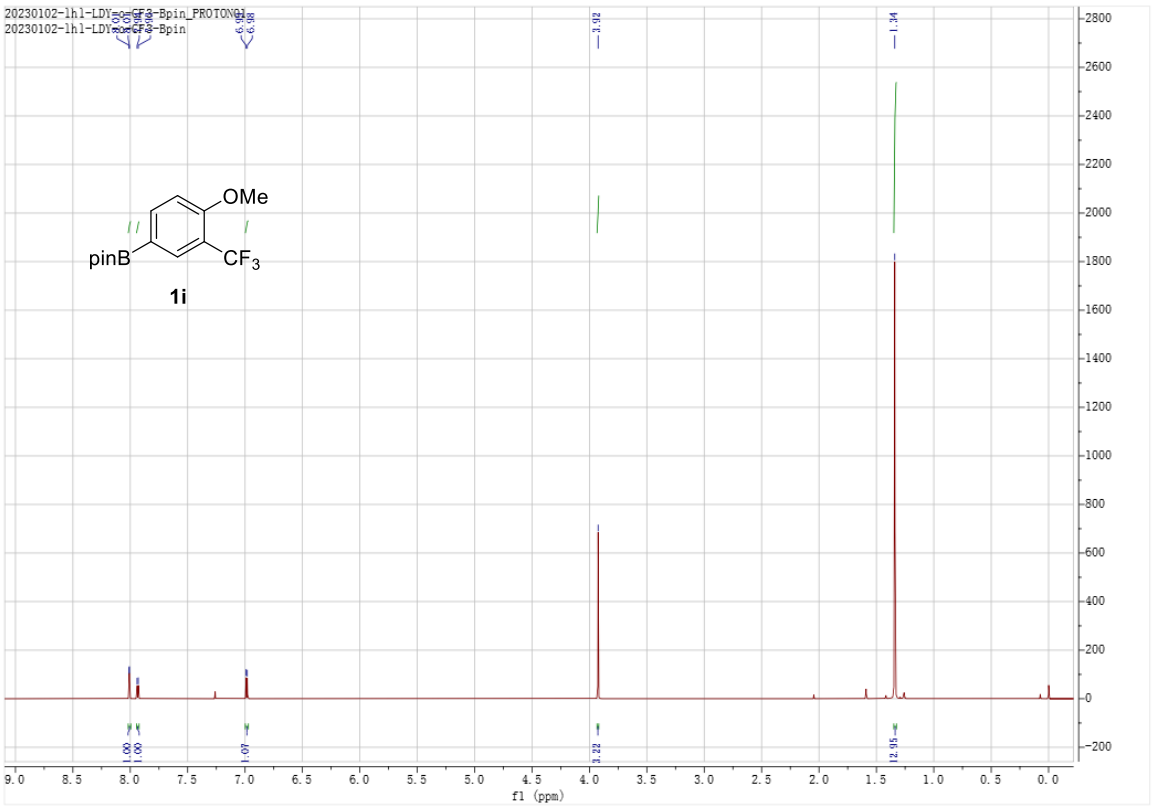

OMe
pinB
F
1f
f1 (ppm)

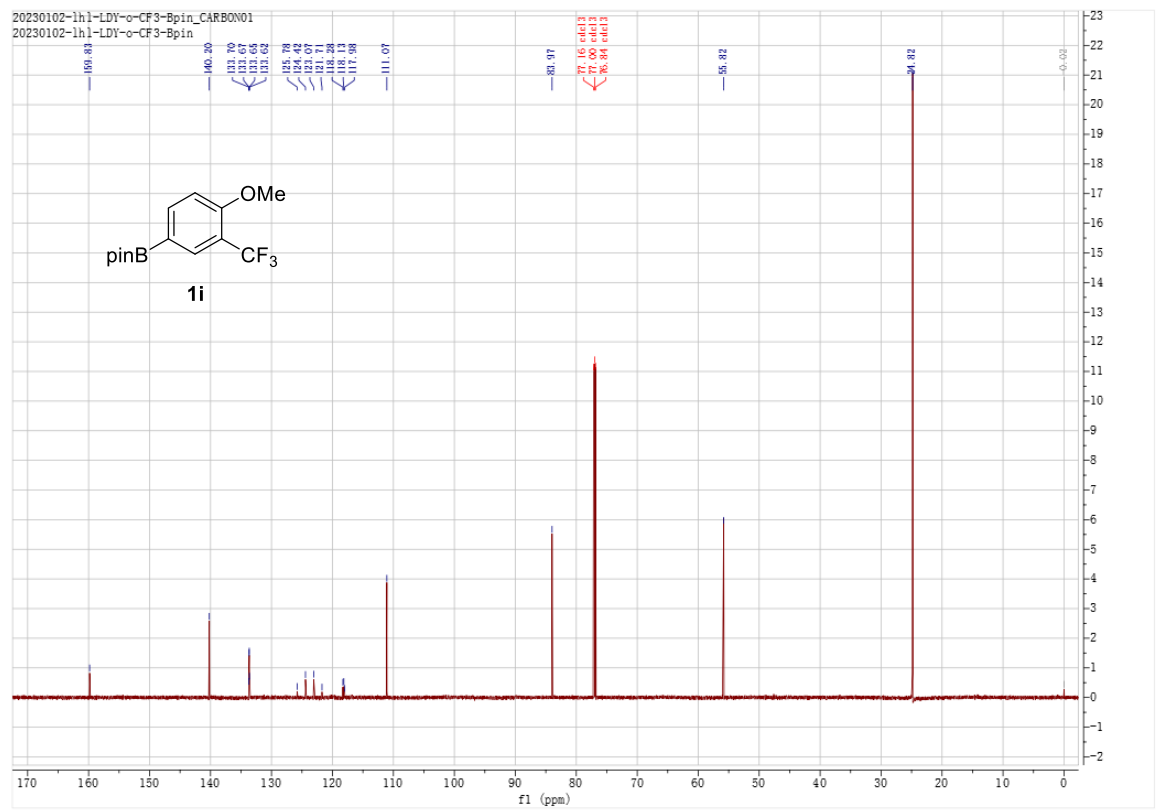

20230102-lh1-LDY-o-Cl-Bpin_PROTON01
20230102-lh1-LDY-o-Cl-Bpin
OMe
pinB
Cl
1g
f1 (ppm)

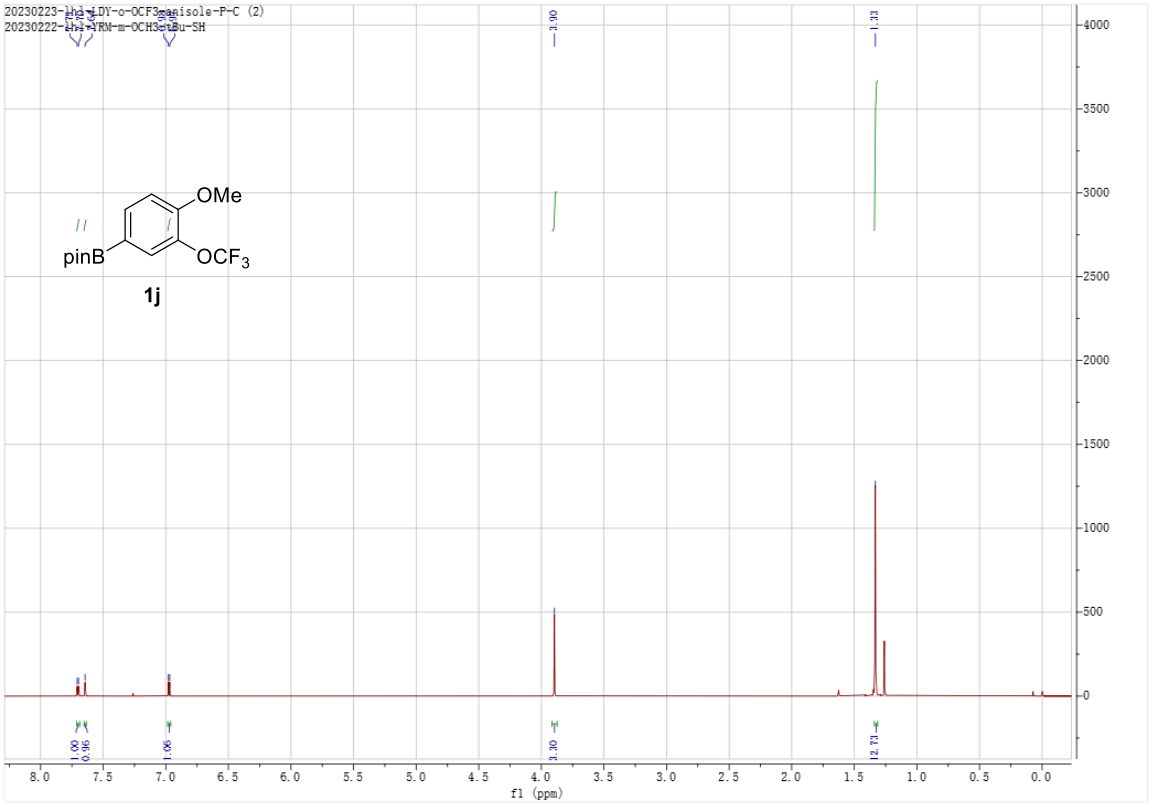

20230102-lh1-LDY-o-Cl-Bpin_CARBON01
20230102-lh1-LDY-o-Cl-Bpin
OMe
pinB
Cl
1g
f1 (ppm)

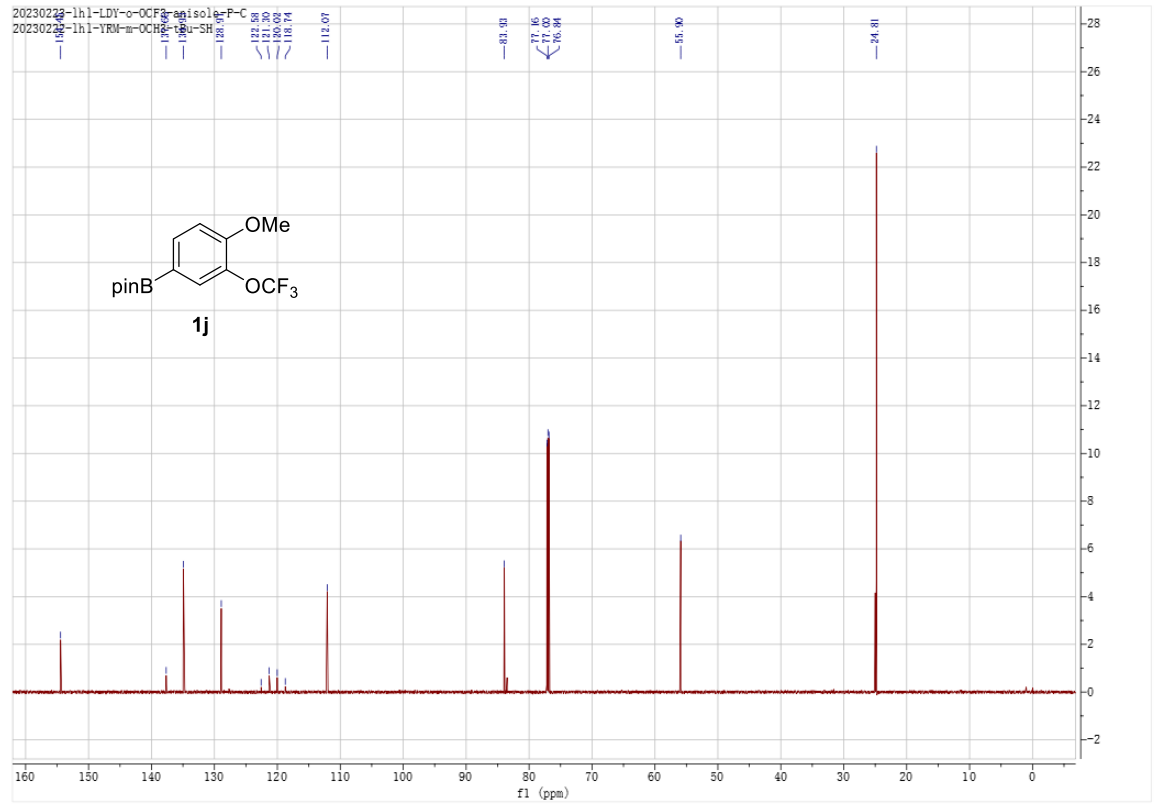

OMe
pinB
OMe
1h
f1 (ppm)

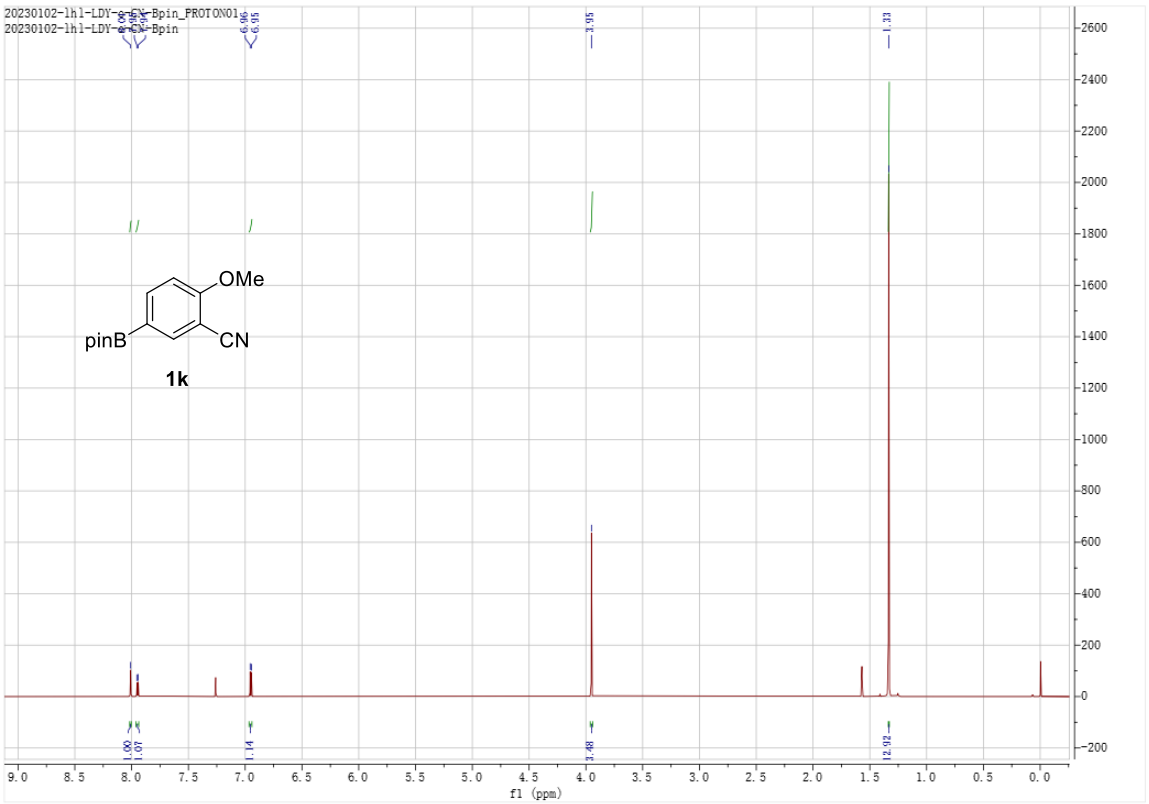

OMe
pinB
OMe
1h
f1 (ppm)

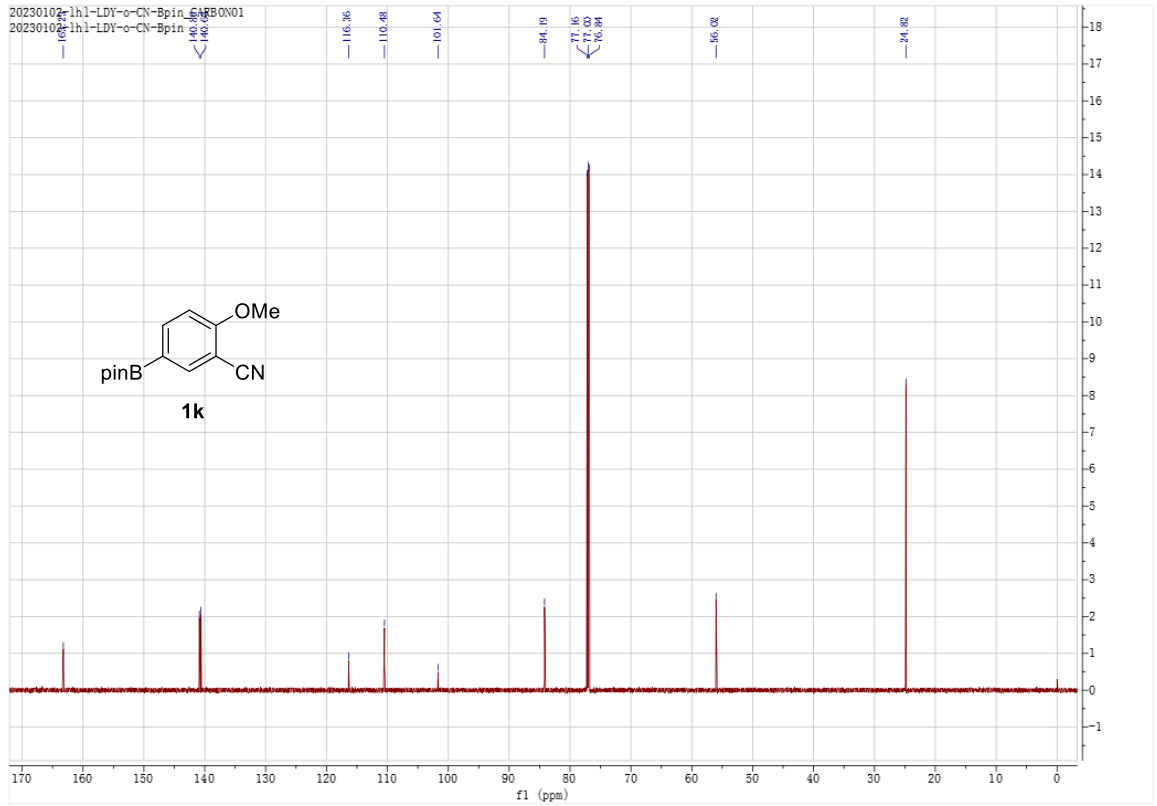

OMe
pinB
CF3
1i
f1 (ppm)

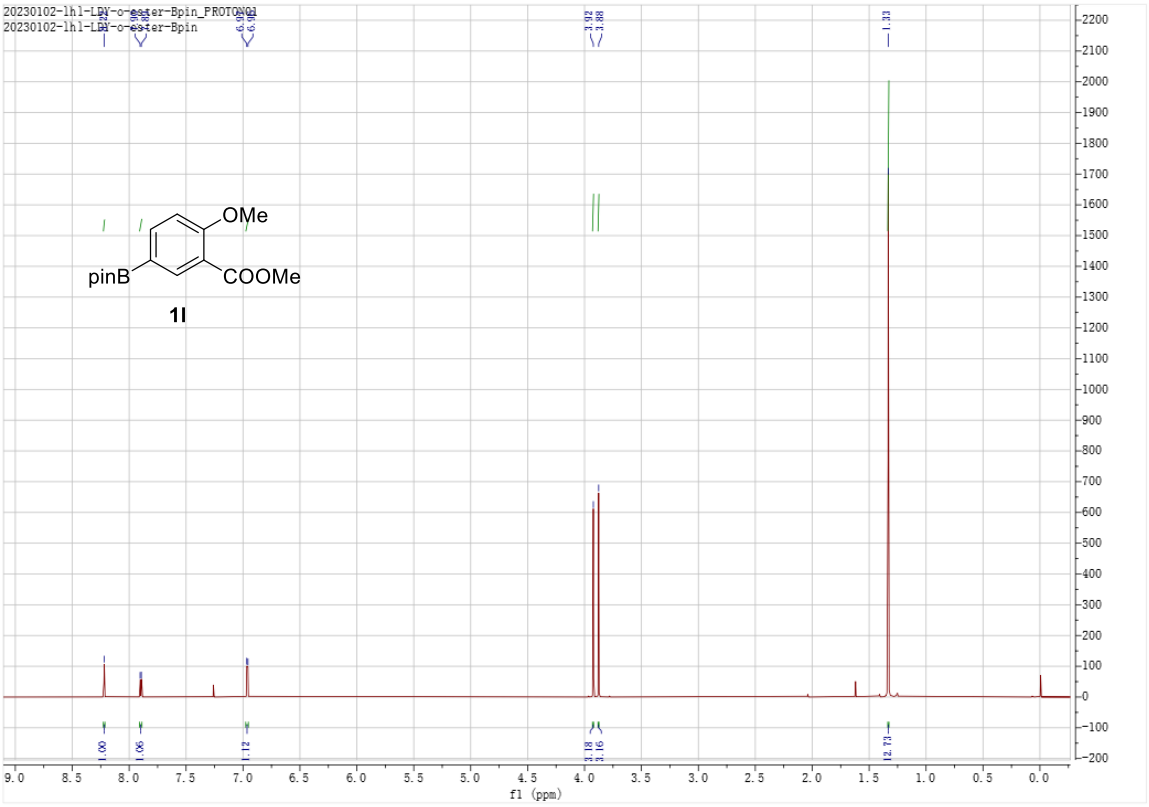

OMe
pinB
CF3
1i
f1 (ppm)

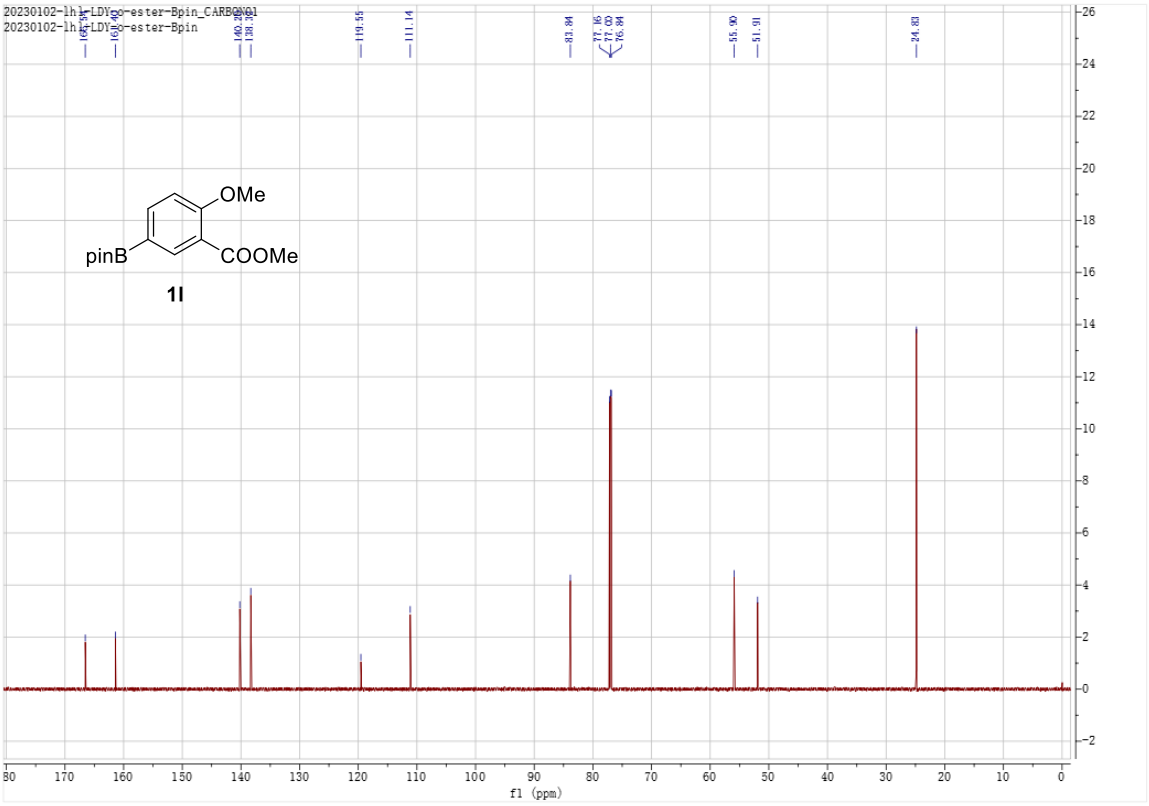

OMe
pinB
OCF3
1j
f1 (ppm)

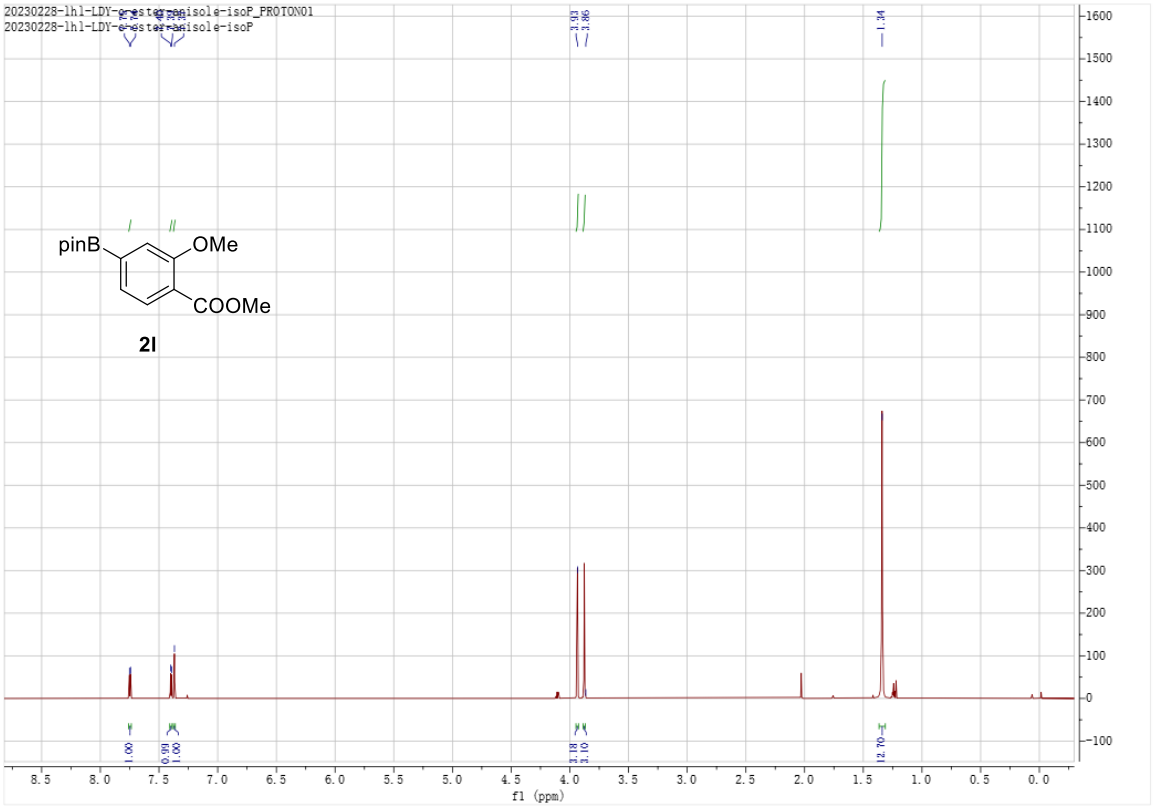

OMe
pinB
OCF3
1j
f1 (ppm)

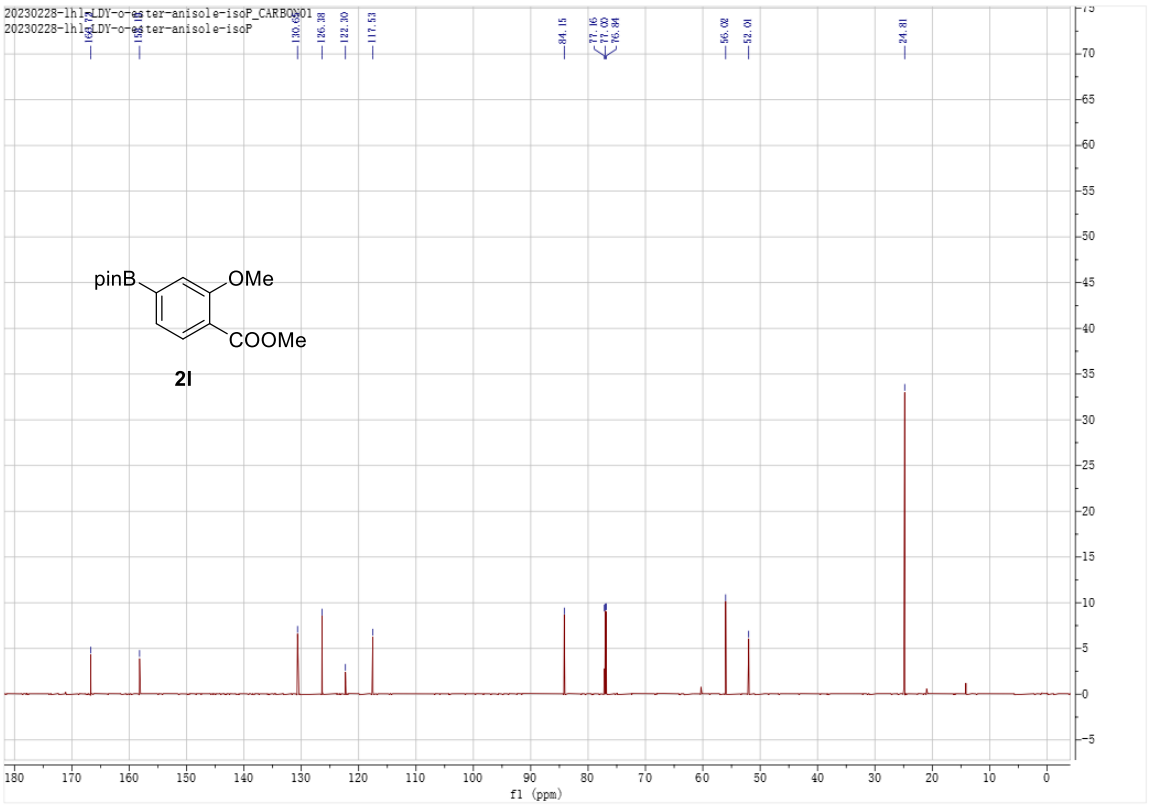

OMe
pinB
CN
1k
f1 (ppm)

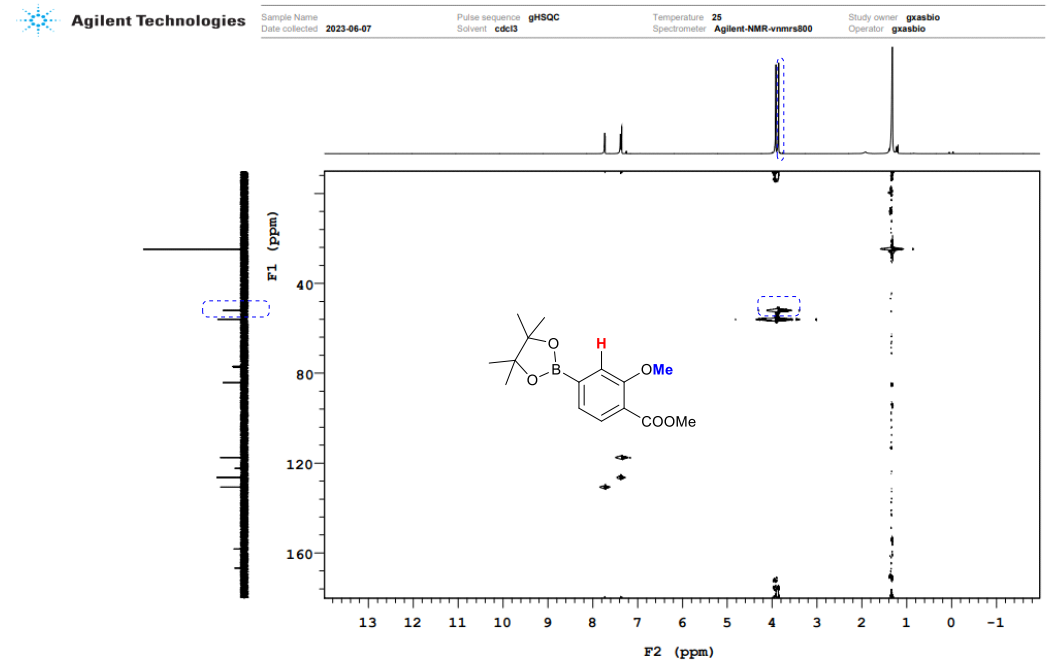

OMe
pinB
CN
1k
f1 (ppm)

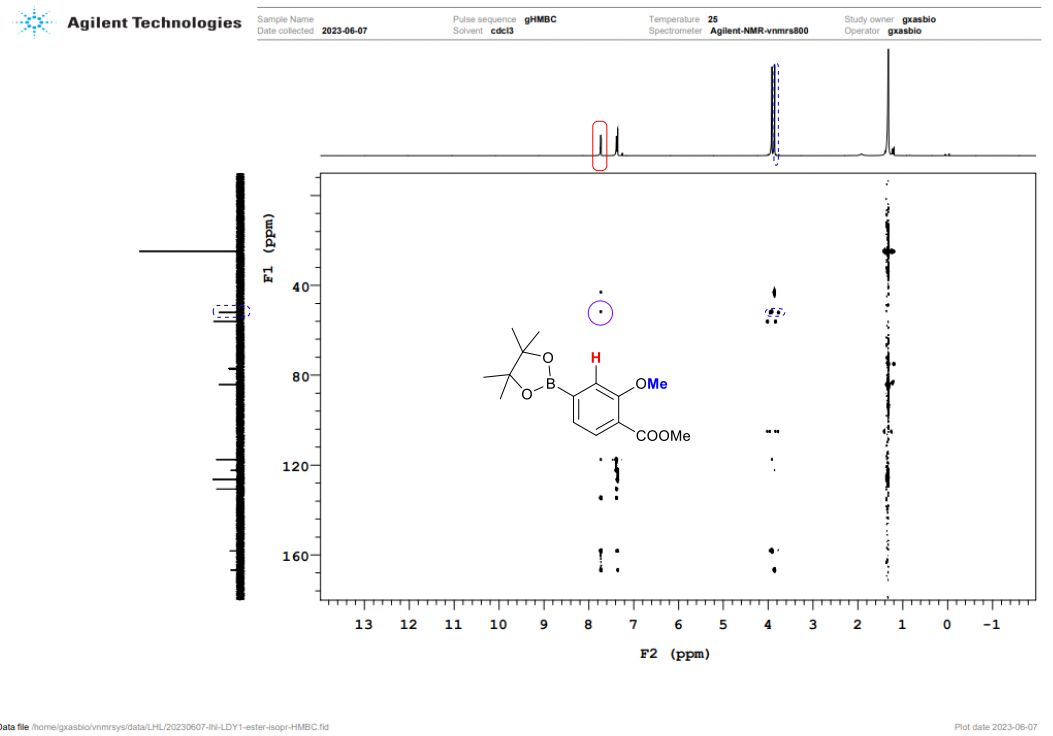

OMe
pinB
COOMe
1l
f1 (ppm)

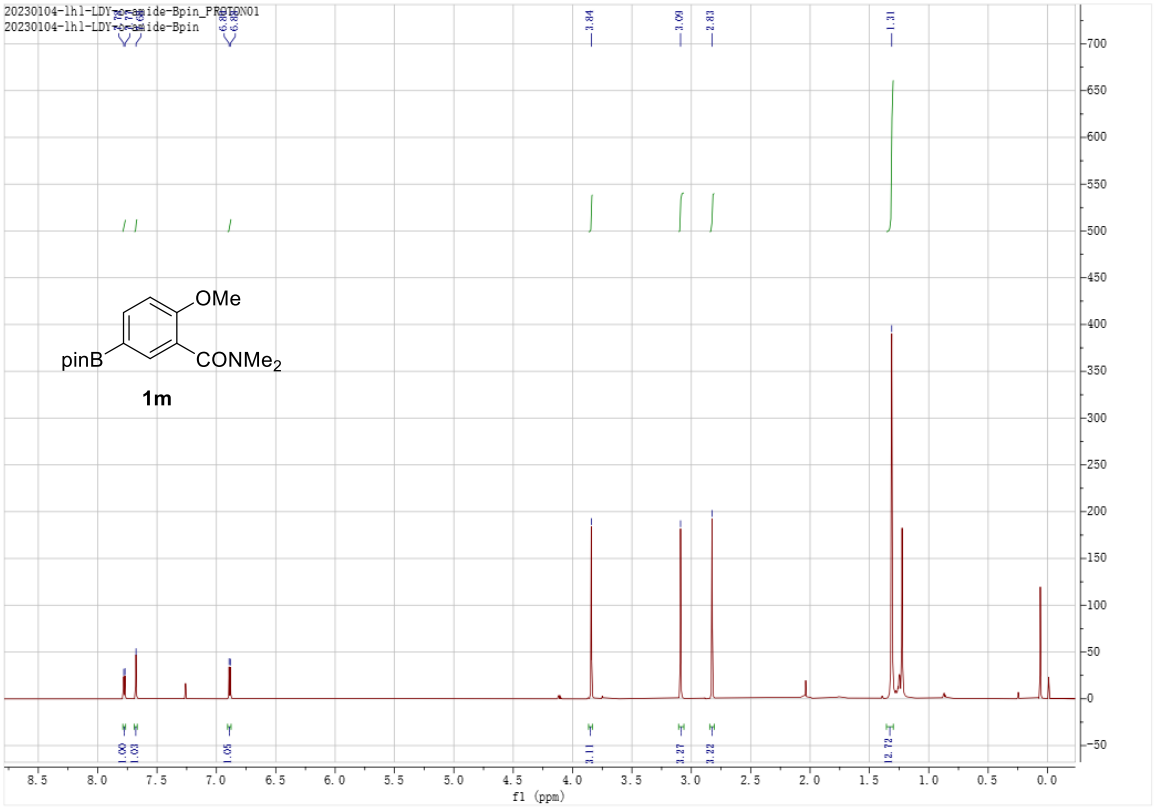

OMe
pinB
COOMe
1l
f1 (ppm)

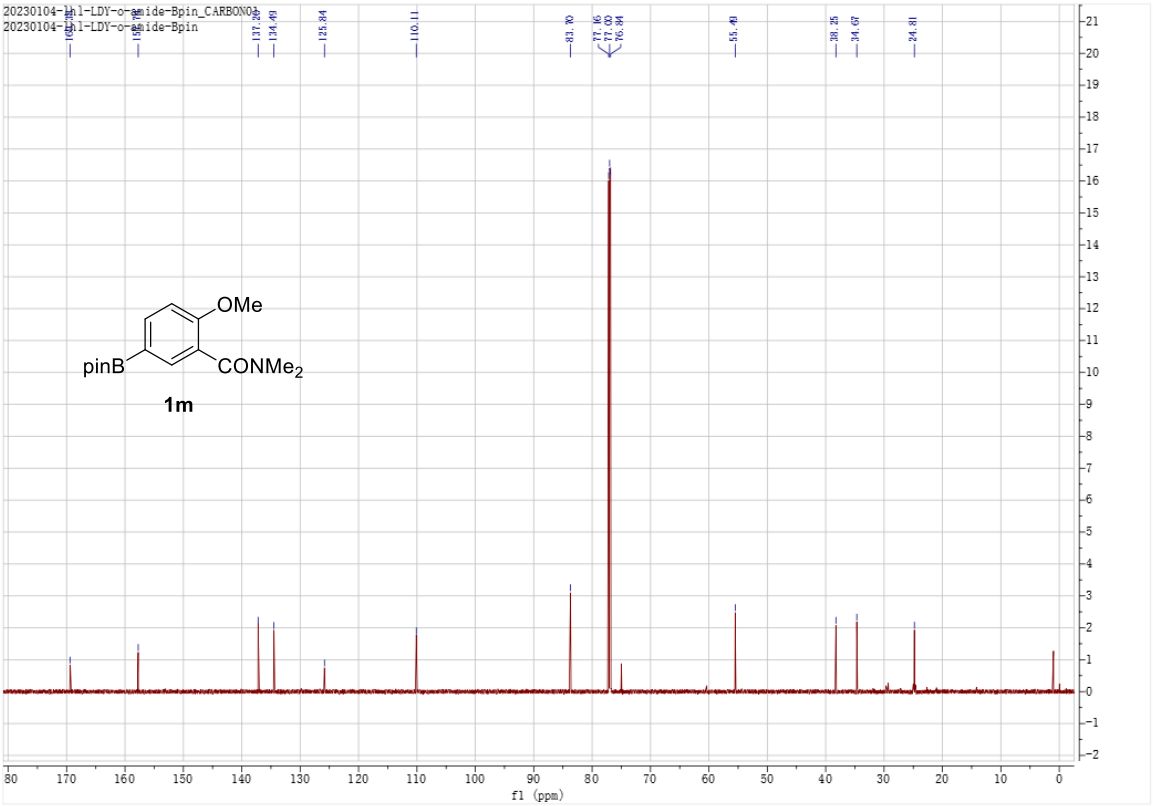

pinB
OMe
COOMe
2l
f1 (ppm)

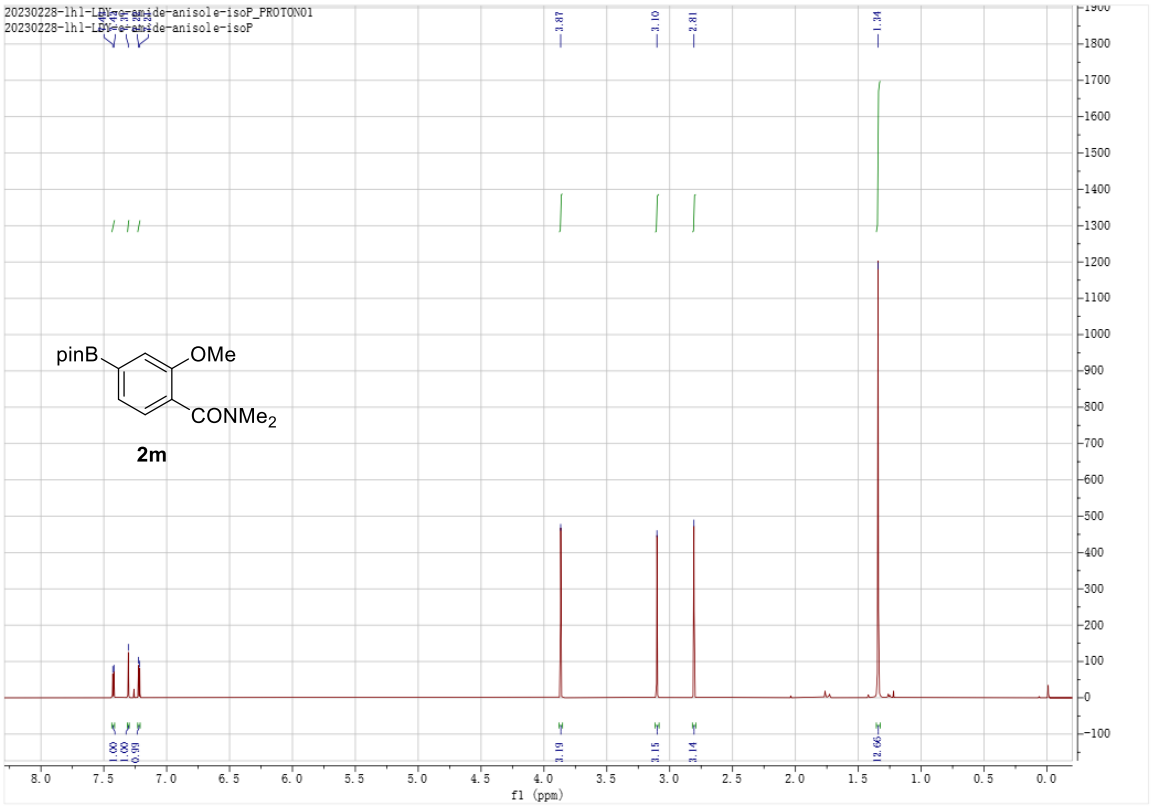

pinB
OMe
COOMe
2l
f1 (ppm)

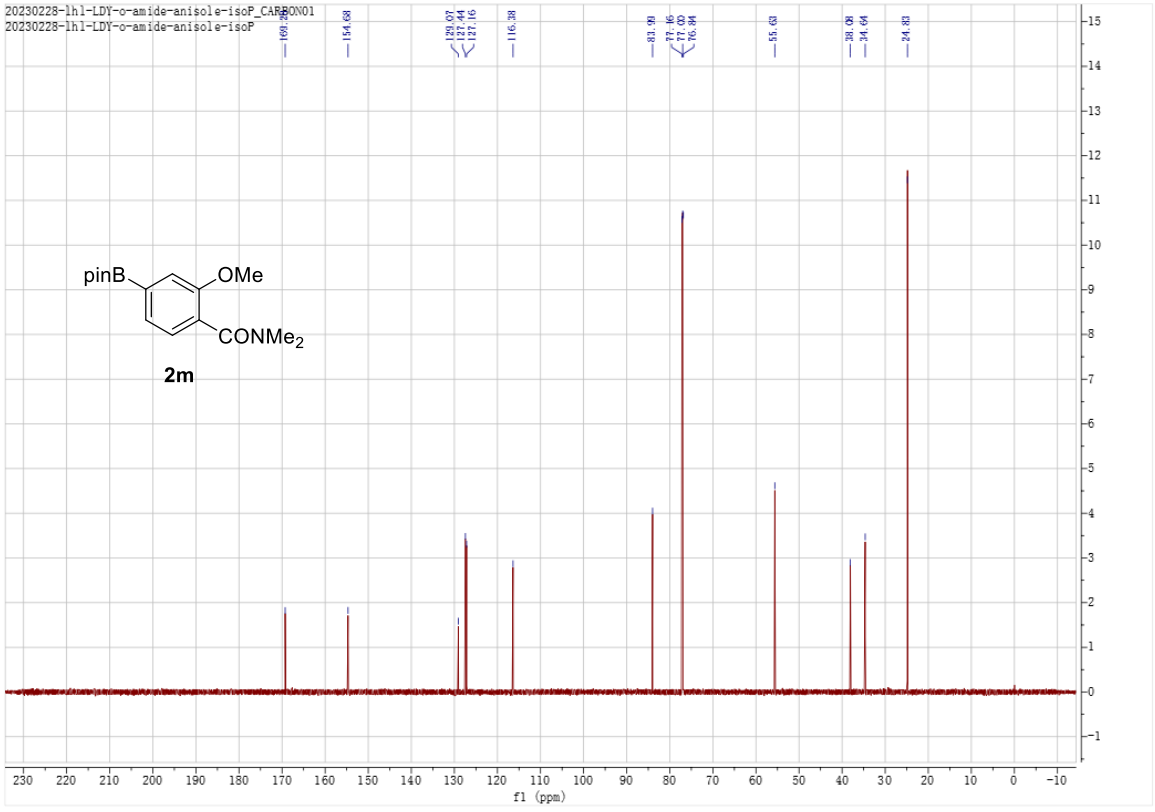

Agilent Technologies
Sample Name
Date collected 2023-06-07
Pulse sequence gHSQC
Solvent cdcl3
Temperature 25
Spectrometer Agilent-NMR-vnmrs800
Study owner gxasbio
Operator gxasbio
F1 (ppm)
F2 (ppm)
H
OMe
COOMe
Data file /home/gxasbio/vnmrsys/data/LHL/20230607-lhl-LDY1-ester-isopr-HSQC.fid
Plot date 2023-06-07

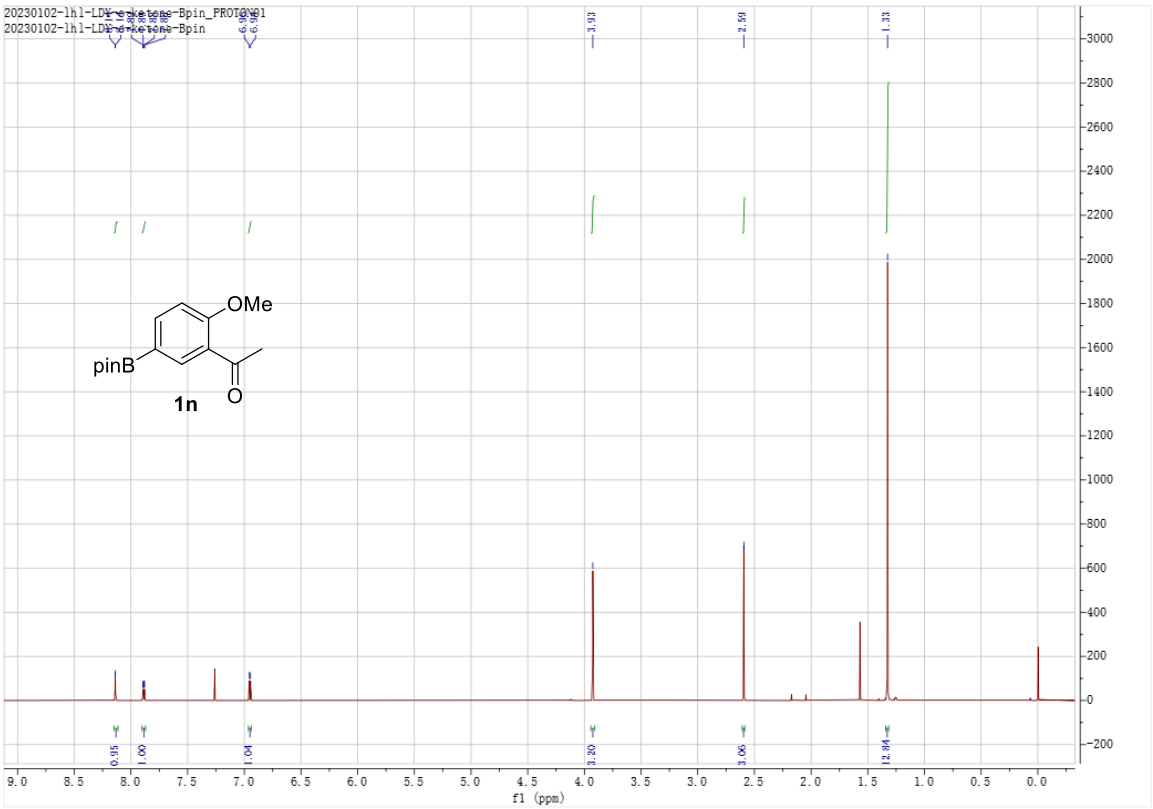

Agilent Technologies
Sample Name
Date collected 2023-06-07
Pulse sequence gHMBC
Solvent cdcl3
Temperature 25
Spectrometer Agilent-NMR-vnmrs800
Study owner gxasbio
Operator gxasbio
F1 (ppm)
F2 (ppm)
H
OMe
COOMe
Data file /home/gxasbio/vnmrsys/data/LHL/20230607-lhl-LDY1-ester-isopr-HMBC.fid
Plot date 2023-06-07

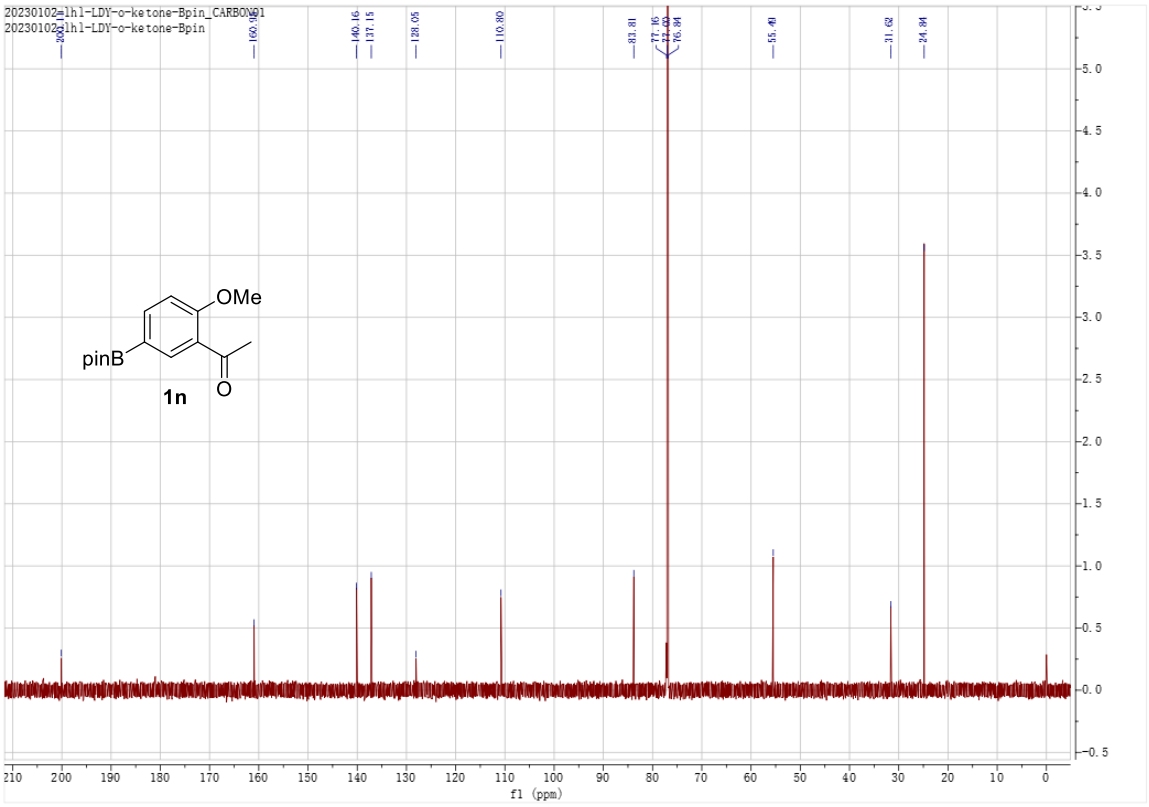

OMe
pinB
CONMe2
1m
f1 (ppm)

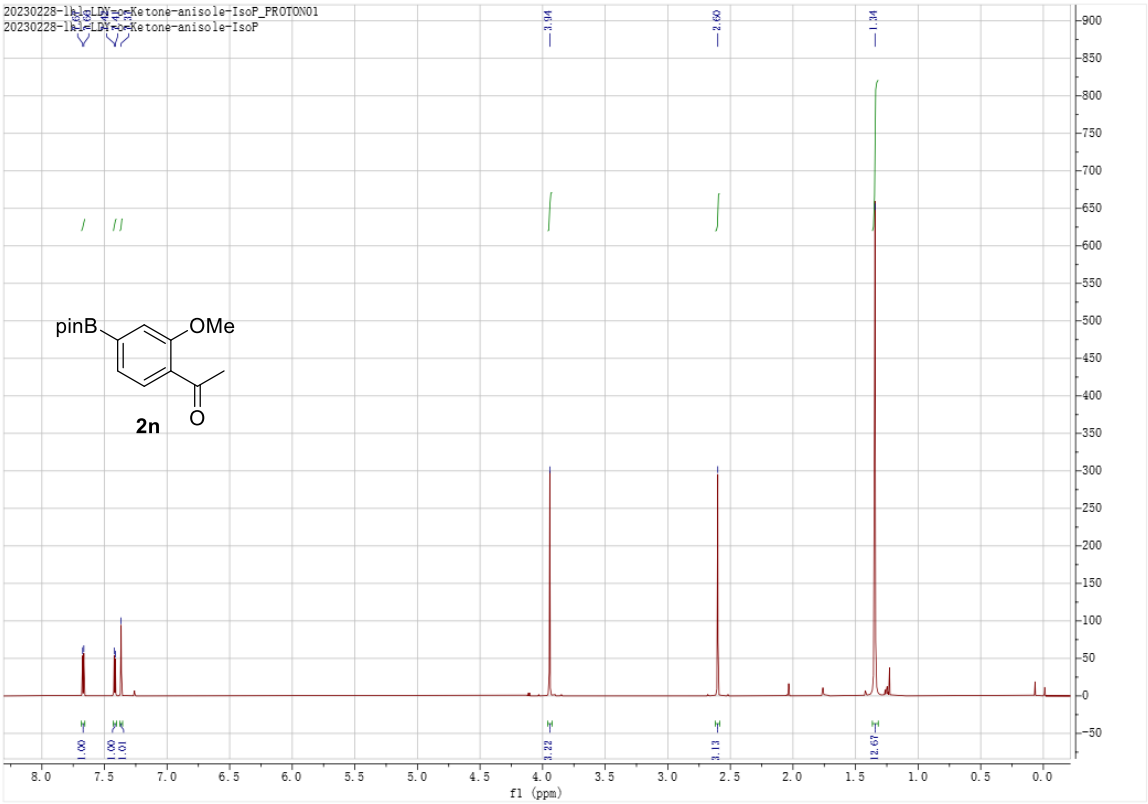

OMe
pinB
CONMe2
1m
f1 (ppm)

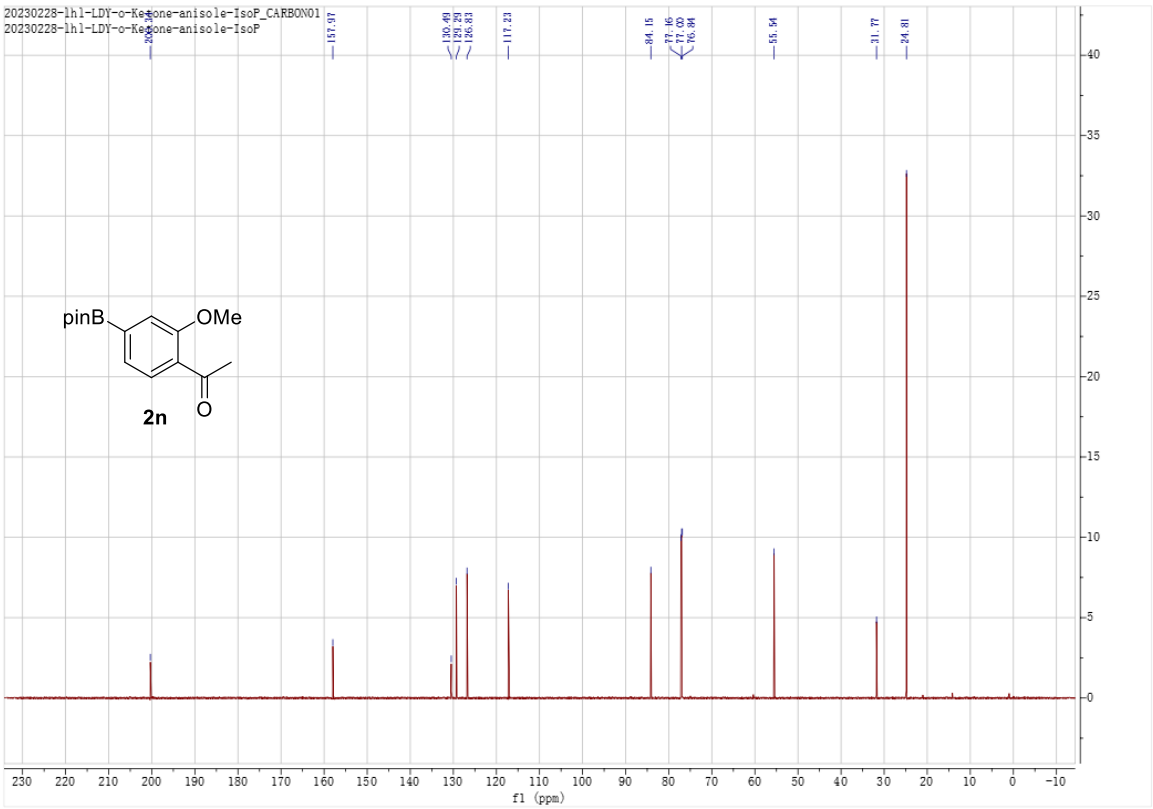

20230228-lh1-LDY-o-amide-anisole-isoP_PROTON01
20230228-lh1-LDY-o-amide-anisole-isoP
3.87
3.10
2.81
1.34
pinB
OMe
CONMe2
2m
f1 (ppm)

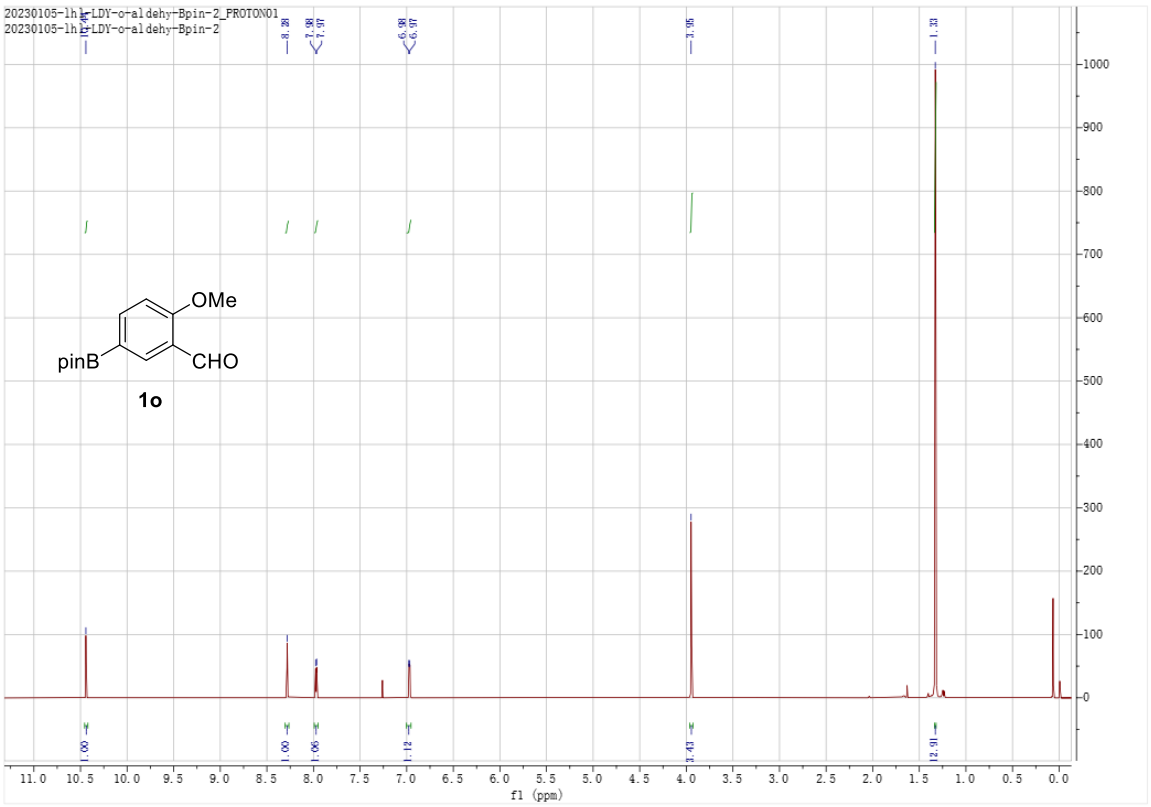

20230228-lh1-LDY-o-amide-anisole-isoP_CARBON01
20230228-lh1-LDY-o-amide-anisole-isoP
169.26
154.68
129.07
127.44
127.16
116.38
83.99
77.46
77.03
76.84
55.63
38.06
34.64
24.83
pinB
OMe
CONMe2
2m
f1 (ppm)

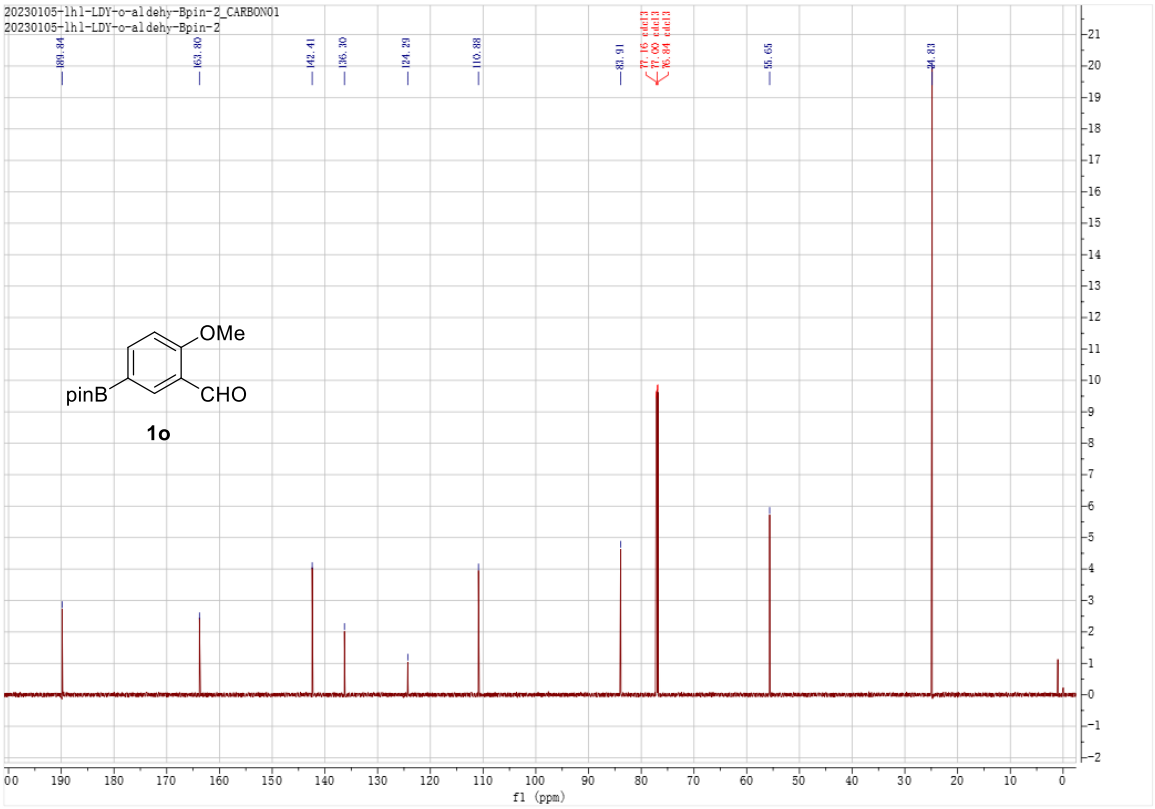

20230102-lh1-LDY-o-ketone-Bpin_PROTON01
20230102-lh1-LDY-o-ketone-Bpin
3.93
2.99
1.33
OMe
pinB
O
1n
0.95
1.00
1.04
3.20
3.06
12.84
f1 (ppm)

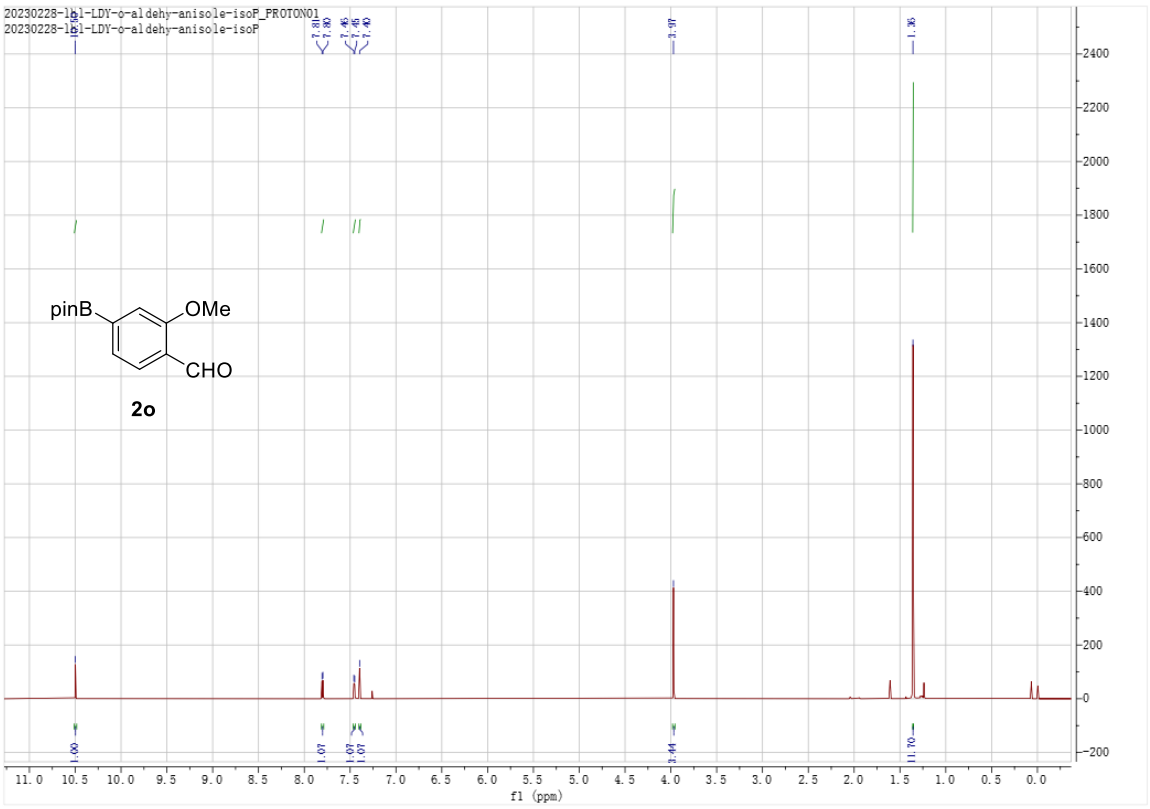

20230102-lh1-LDY-o-ketone-Bpin_CARBON01
20230102-lh1-LDY-o-ketone-Bpin
160.96
140.16
137.15
128.05
110.80
83.81
77.16
76.84
55.49
31.62
24.84
OMe
pinB
O
1n
f1 (ppm)

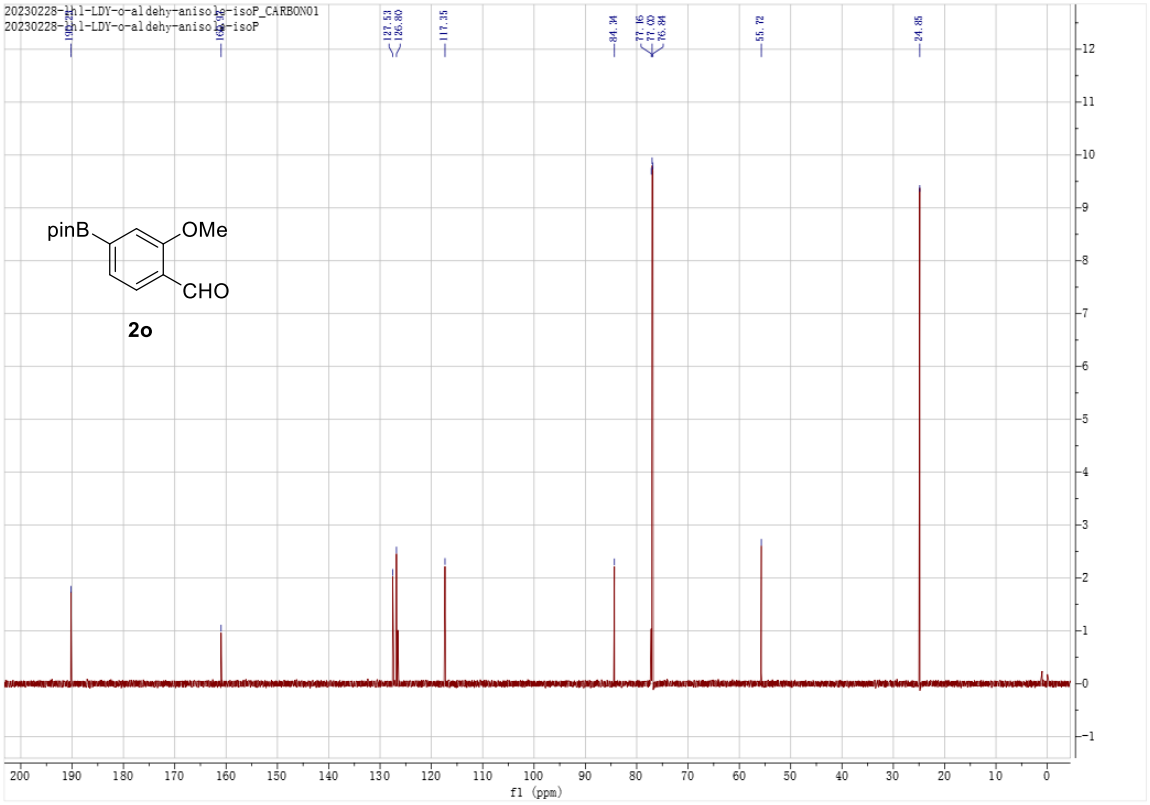

20230228-lhl-LDY-o-Ketone-anisole-IsoP_PROTON01
20230228-lhl-LDY-o-Ketone-anisole-IsoP
pinB
OMe
O
2n
f1 (ppm)

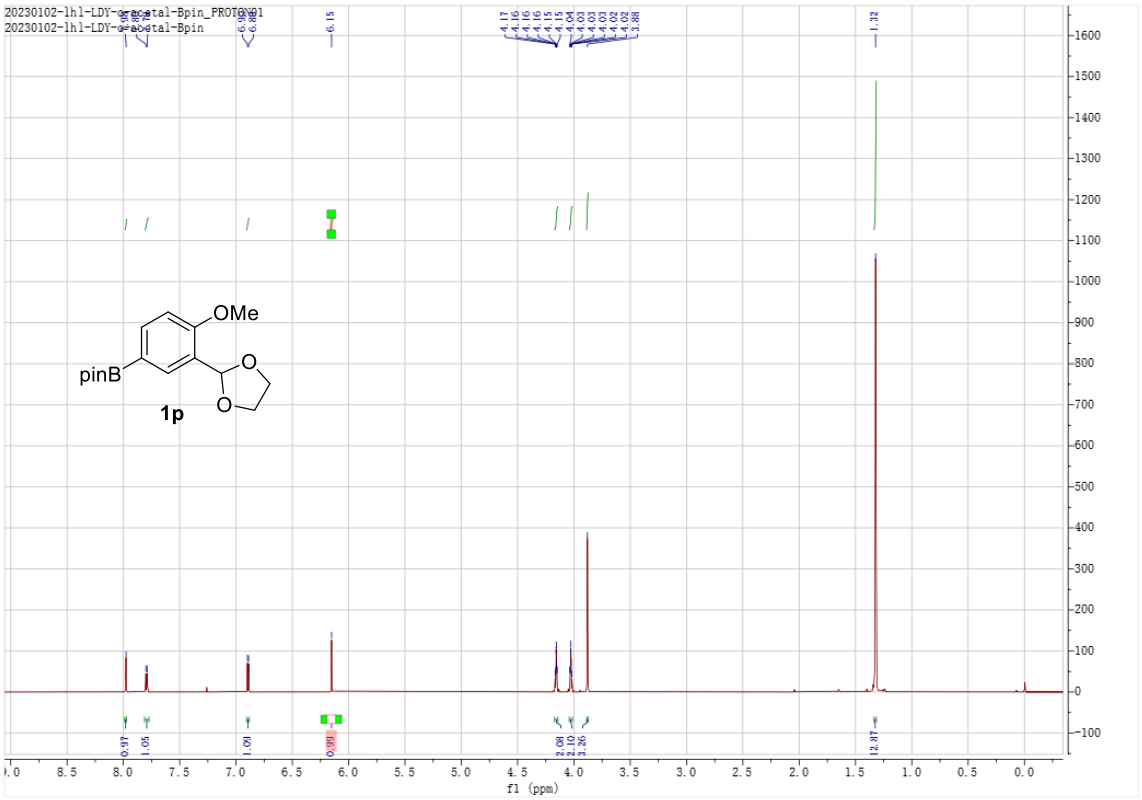

20230228-lhl-LDY-o-Ketone-anisole-IsoP_CARBON01
20230228-lhl-LDY-o-Ketone-anisole-IsoP
pinB
OMe
O
2n
f1 (ppm)

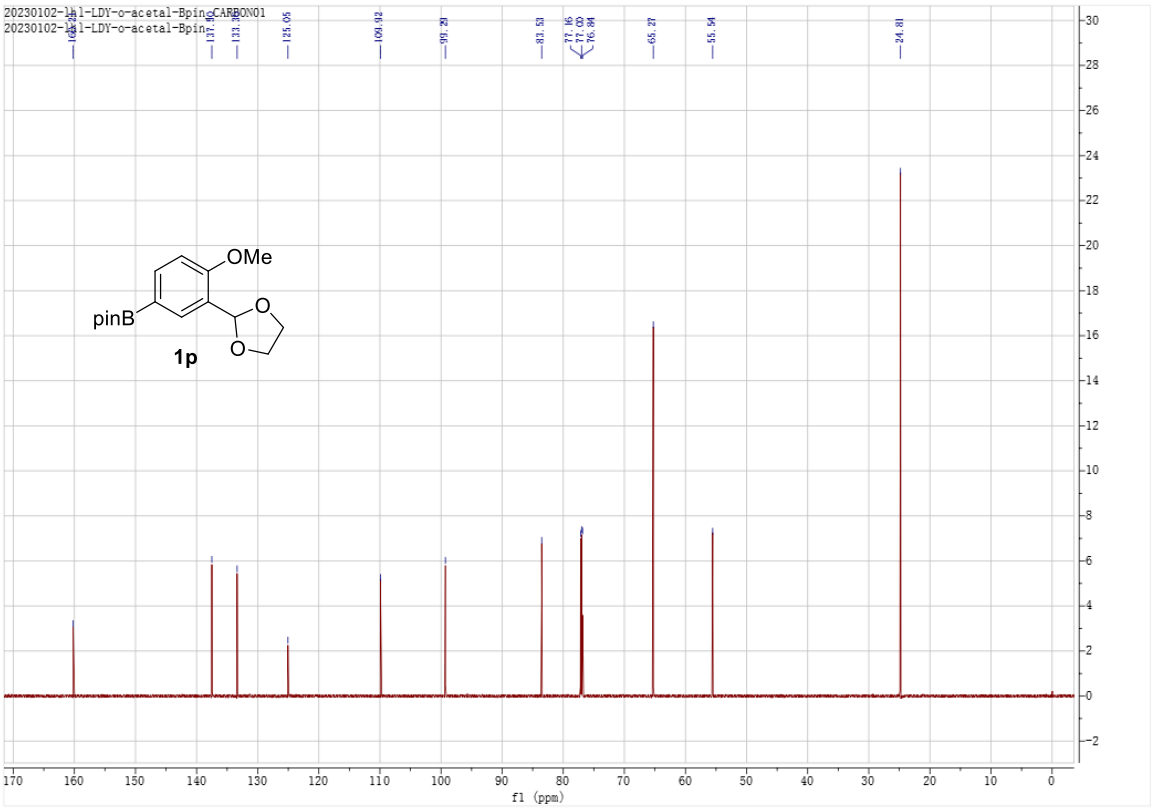

20230105-1h1-LDY-o-aldehy-Bpin-2_PROTON01
20230105-1h1-LDY-o-aldehy-Bpin-2
OMe
pinB
CHO
1o
f1 (ppm)

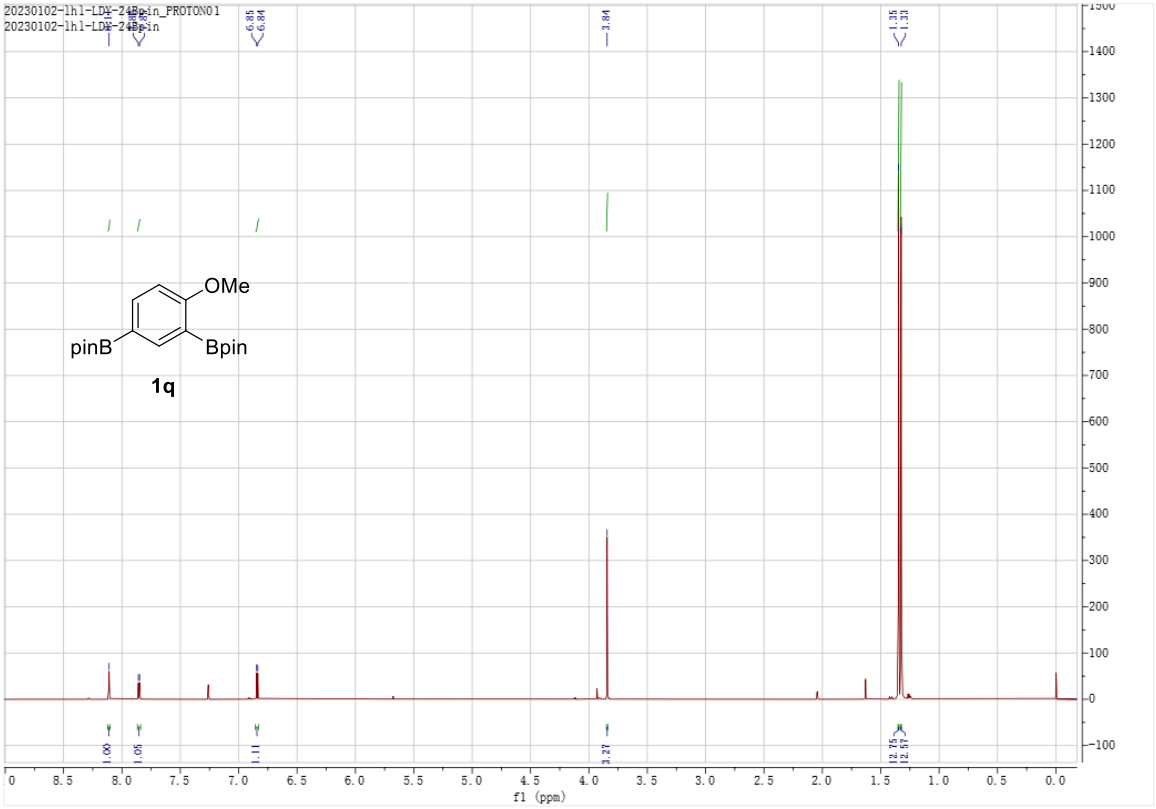

20230105-1h1-LDY-o-aldehy-Bpin-2_CARBON01
20230105-1h1-LDY-o-aldehy-Bpin-2
OMe
pinB
CHO
1o
f1 (ppm)

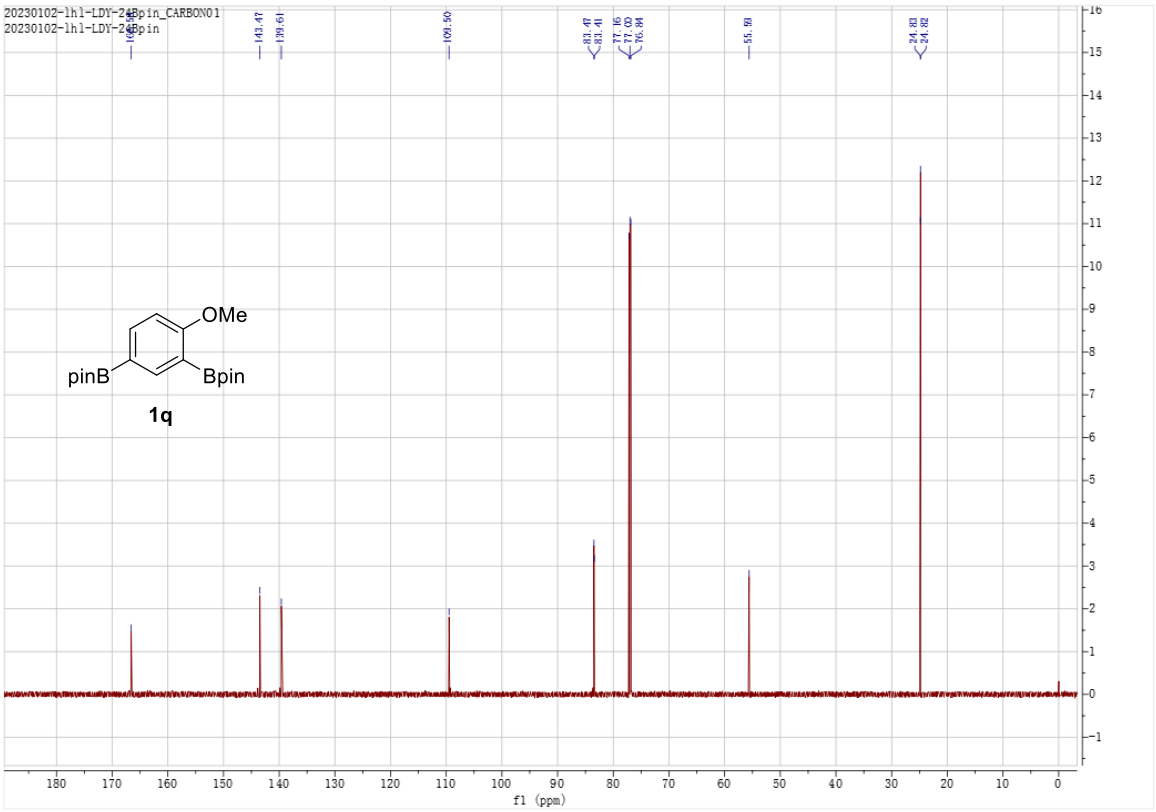

pinB
OMe
CHO
2o
f1 (ppm)

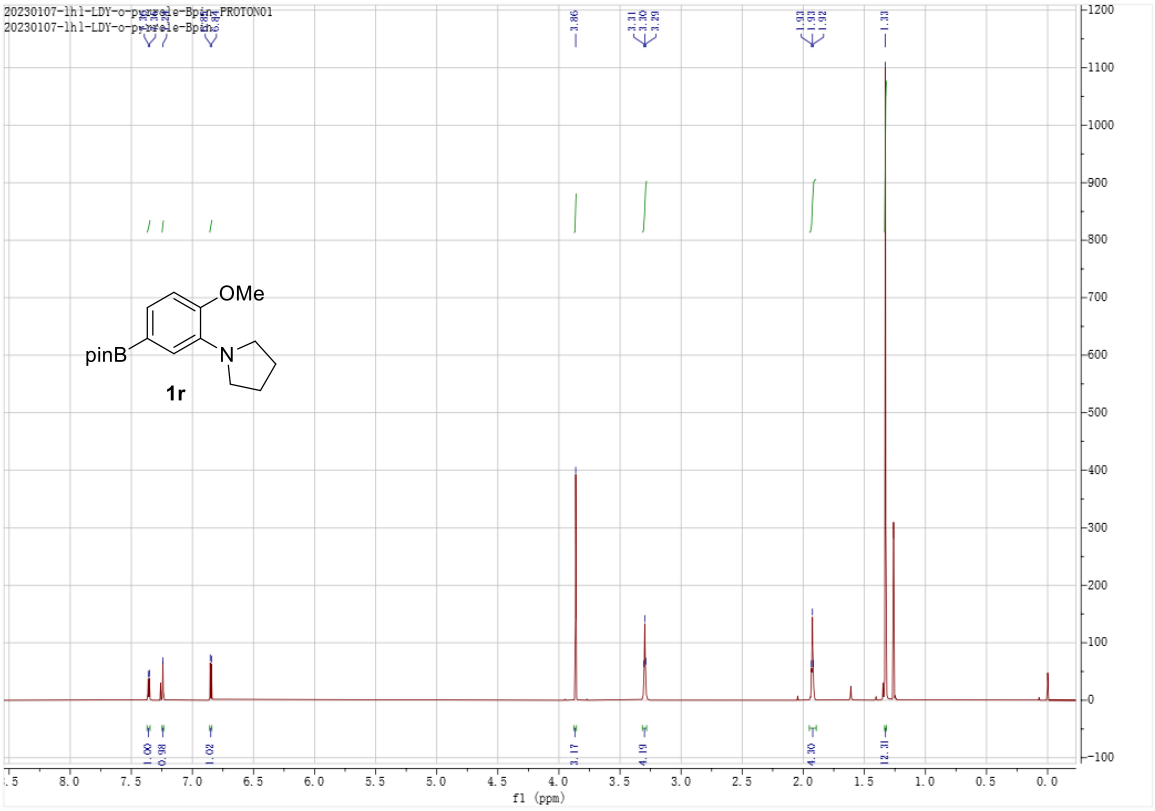

pinB
OMe
CHO
2o
f1 (ppm)

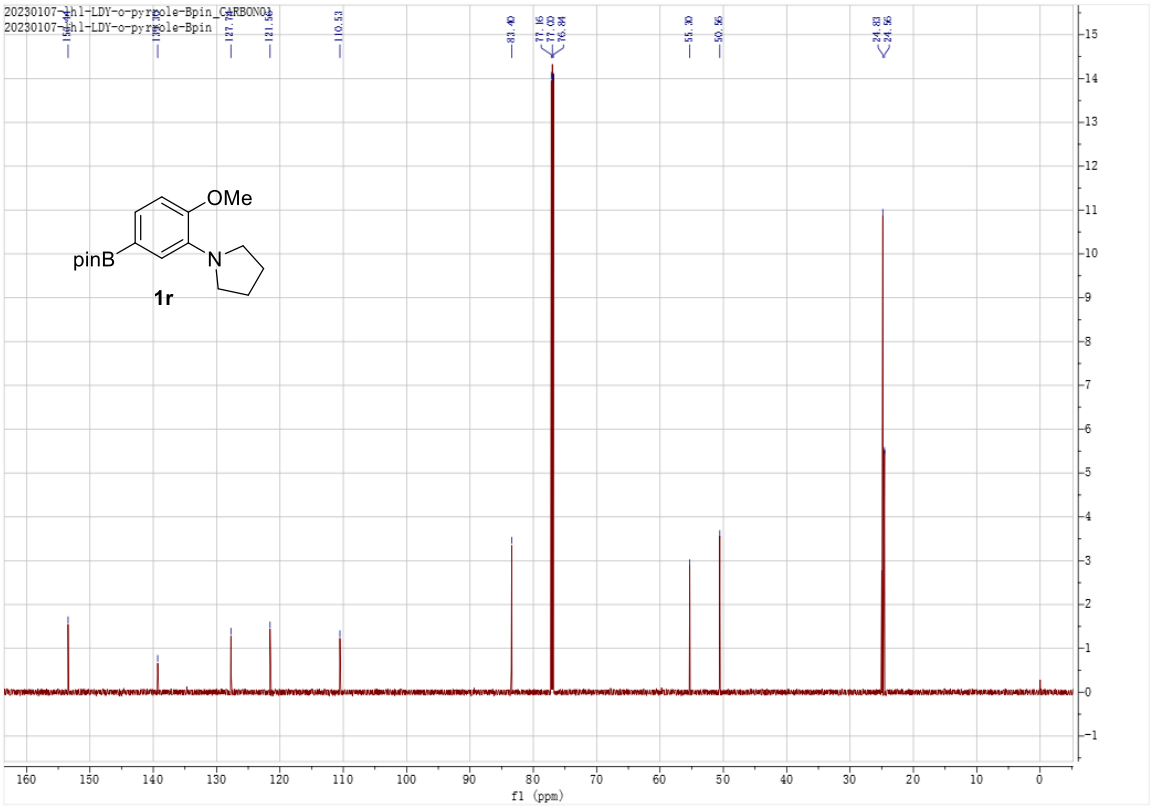

OMe
pinB
O
O
1p
f1 (ppm)

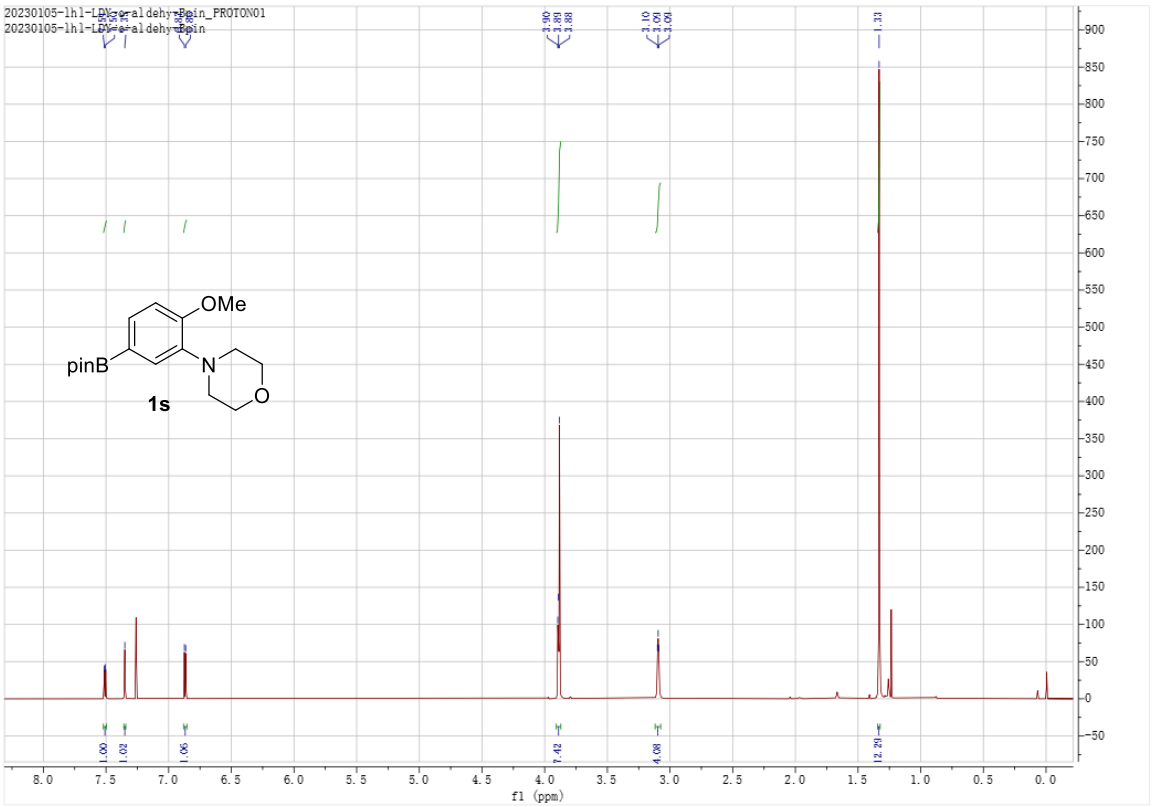

OMe
pinB
O
O
1p
f1 (ppm)

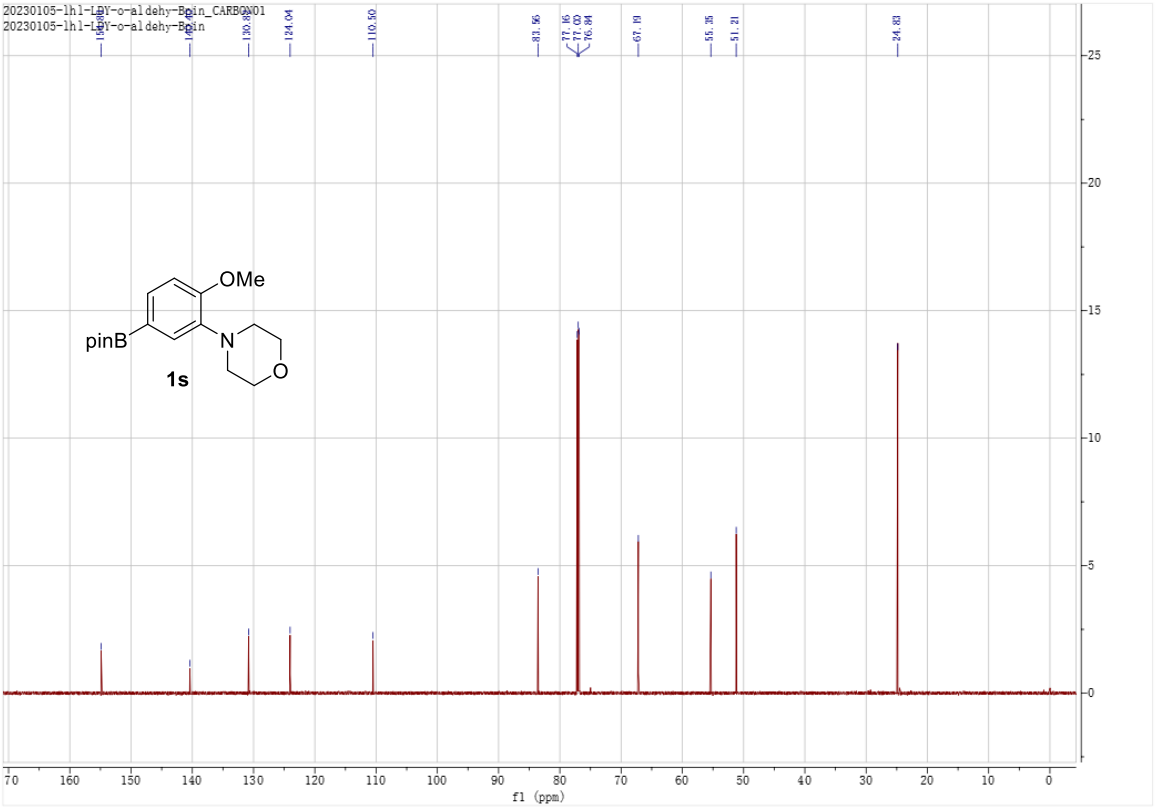

OMe
pinB
Bpin
1q
f1 (ppm)

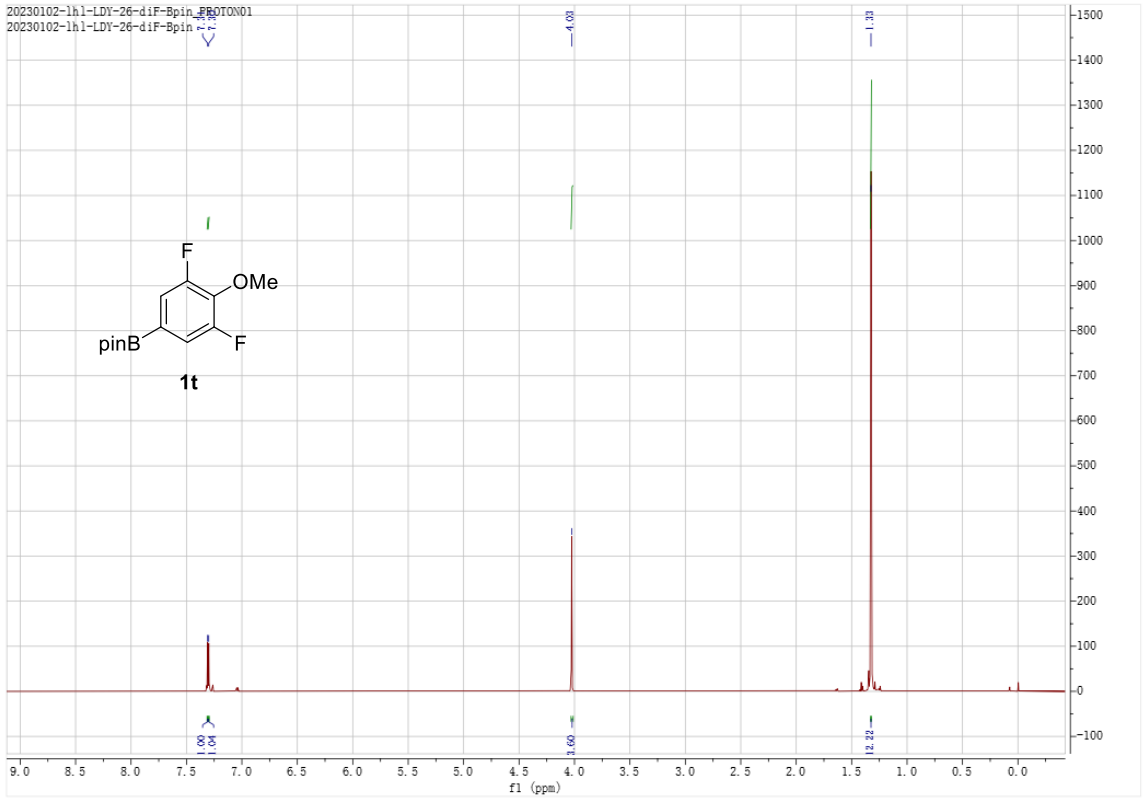

OMe
pinB
Bpin
1q
f1 (ppm)

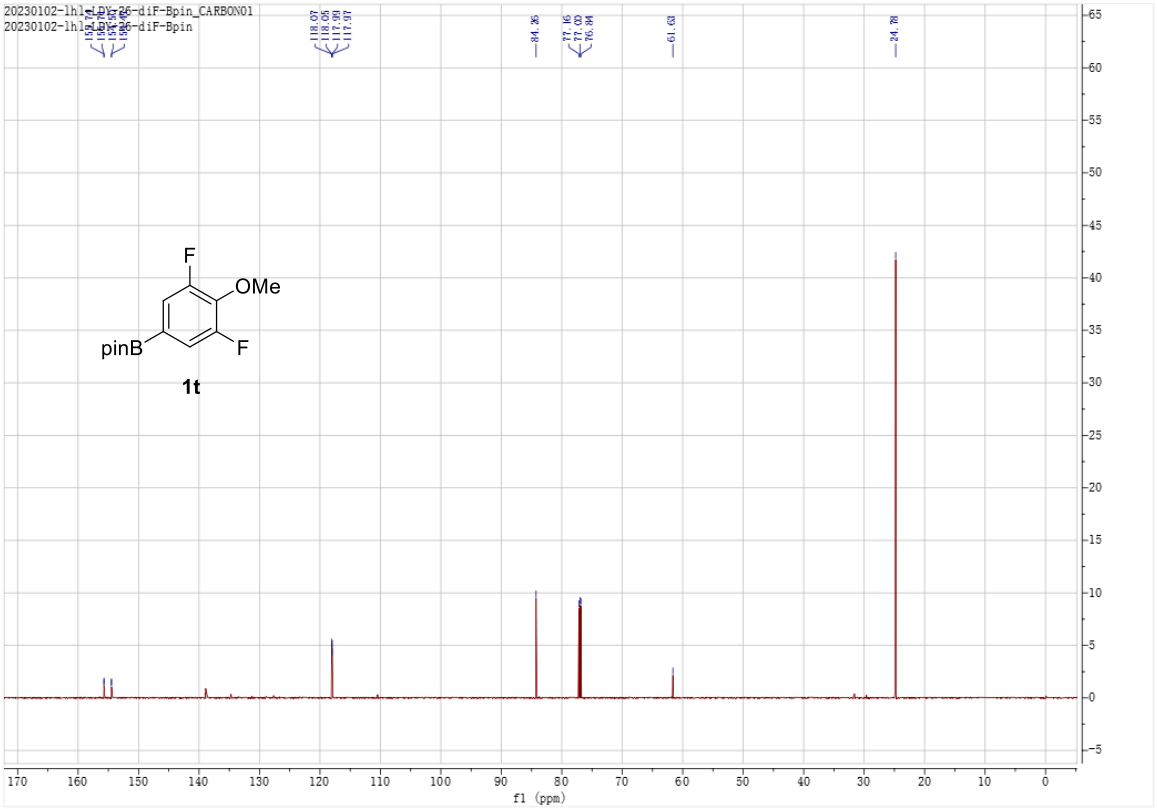

OMe
pinB
N
1r
f1 (ppm)

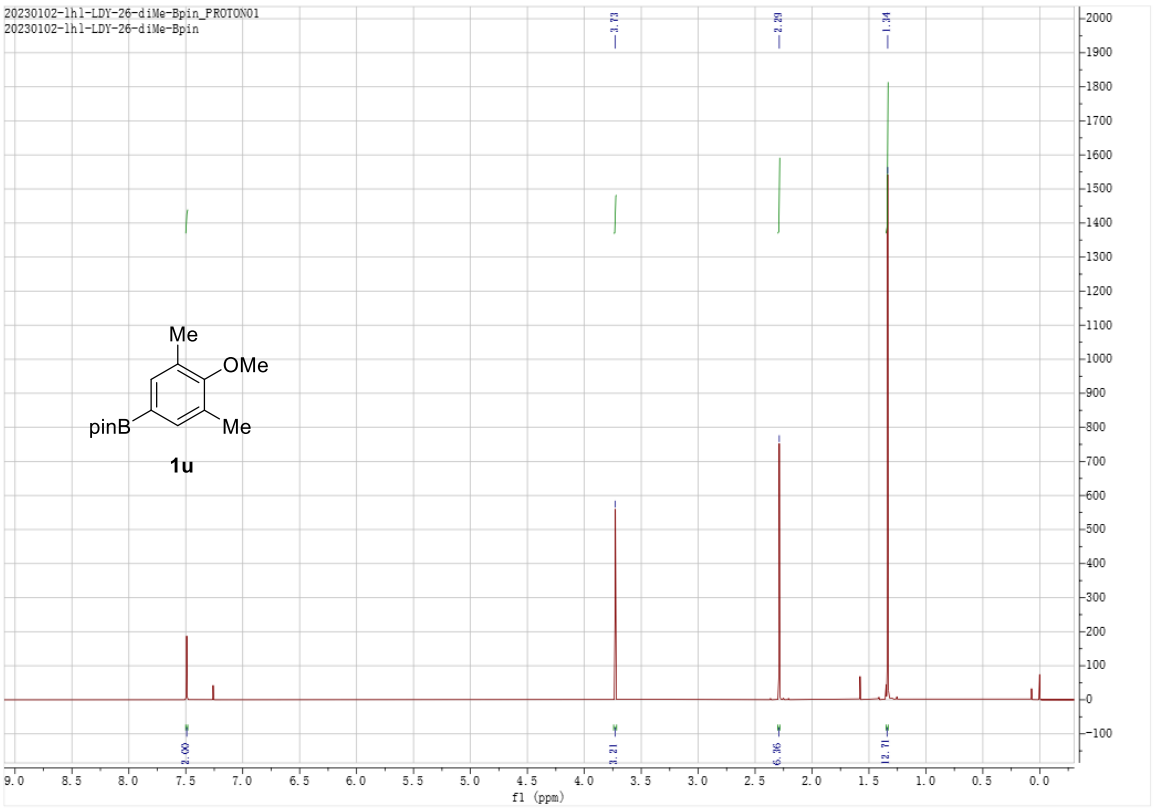

OMe
pinB
N
1r
f1 (ppm)

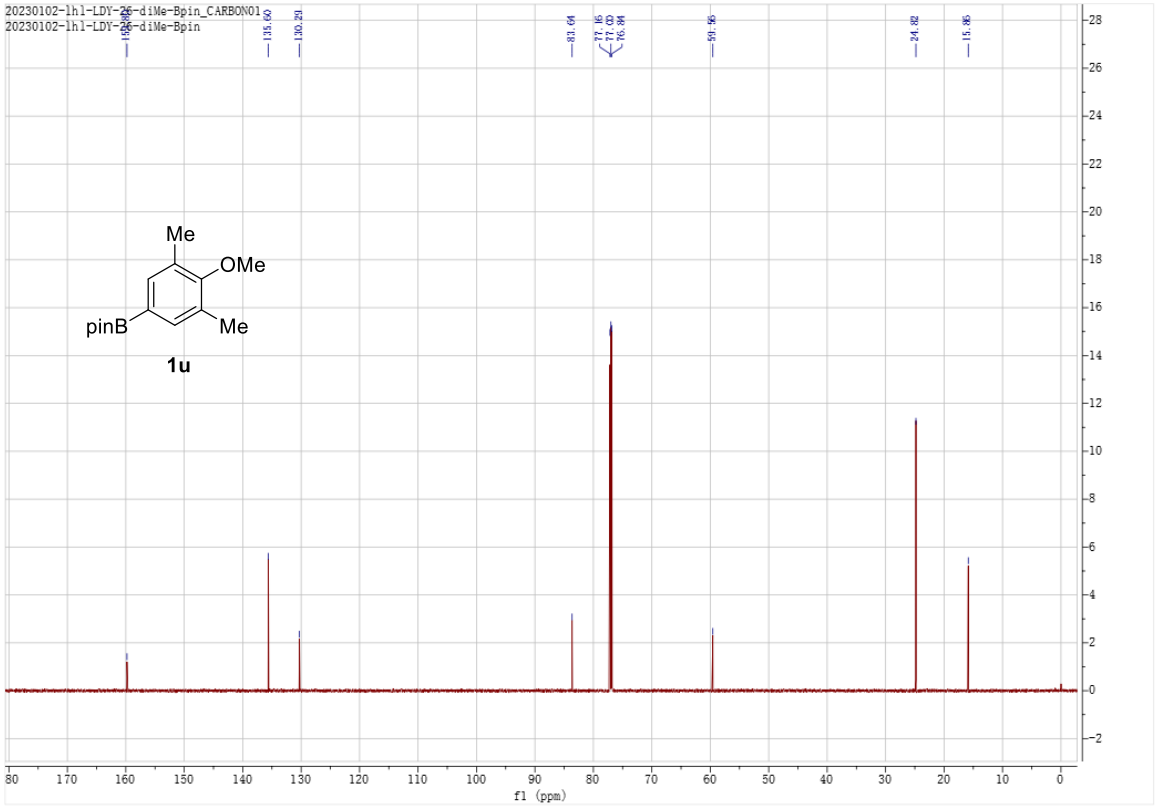

20230105-lh1-LDY-o-aldehy-Bpin_PROTON01
20230105-lh1-LDY-o-aldehy-Bpin
OMe
pinB
N
O
1s
f1 (ppm)

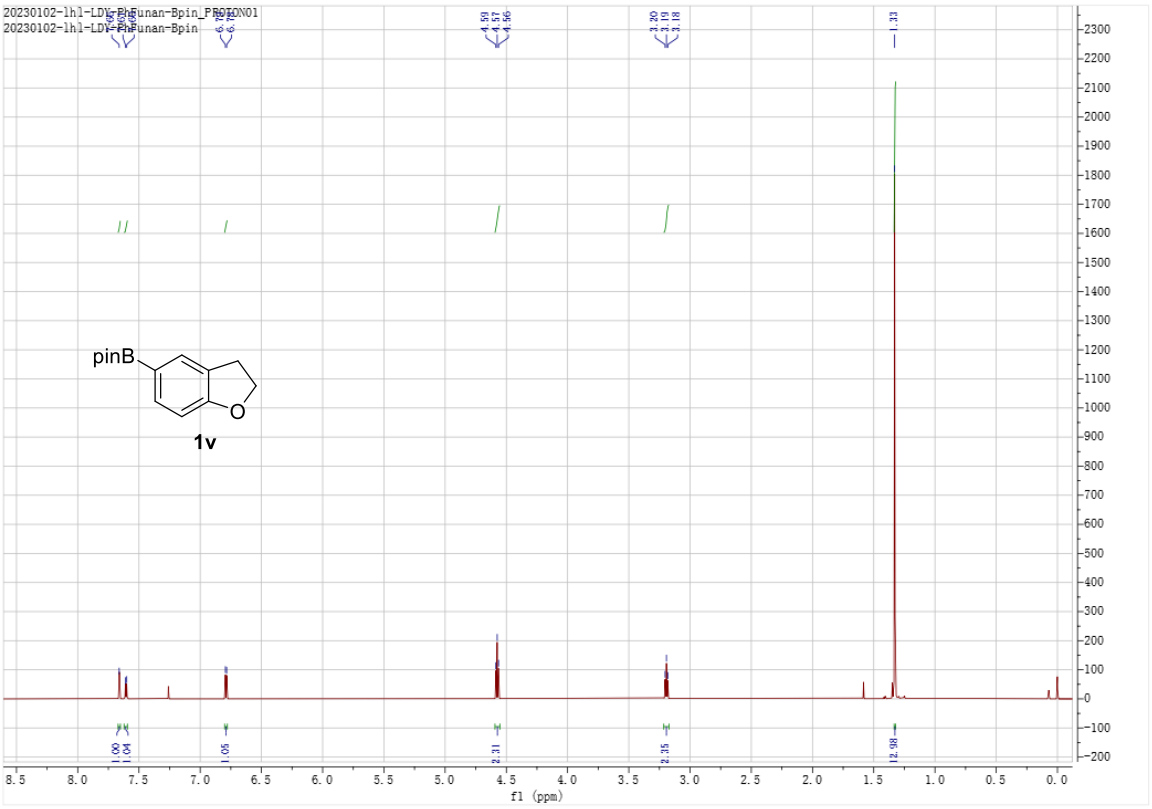

20230105-lh1-LDY-o-aldehy-Bpin_CARBON01
20230105-lh1-LDY-o-aldehy-Bpin
OMe
pinB
N
O
1s
f1 (ppm)

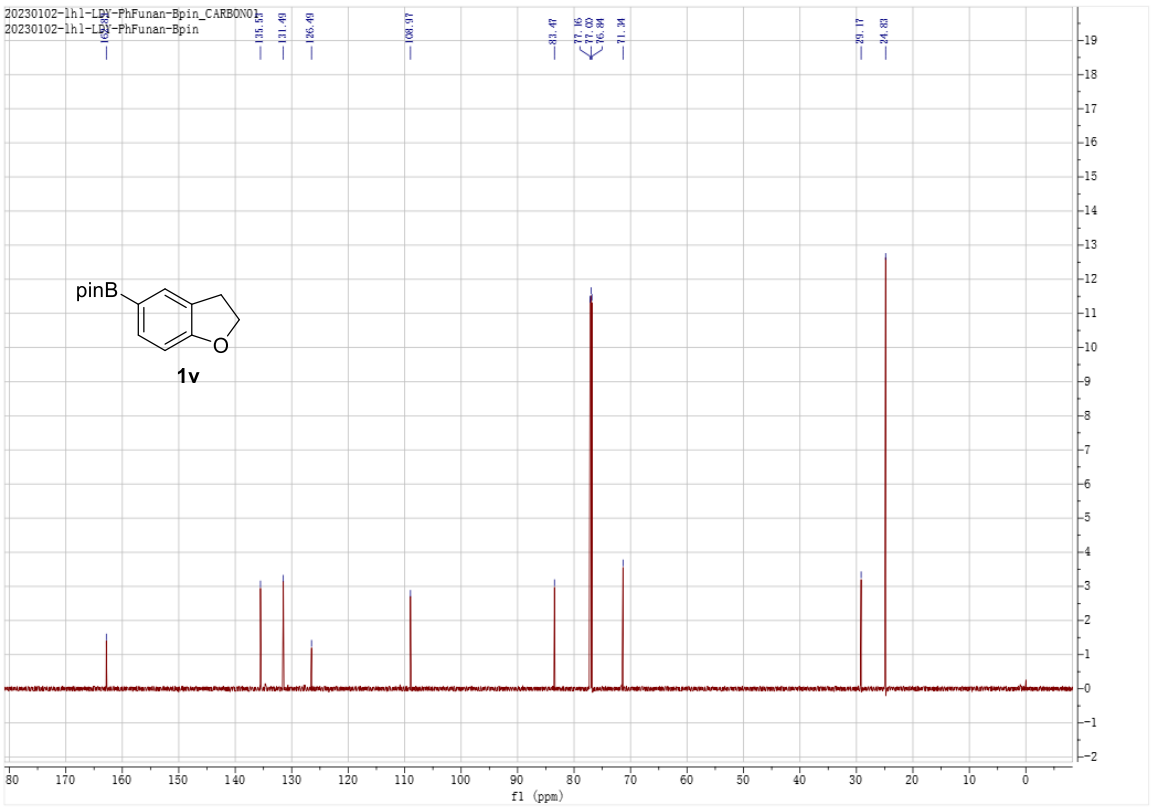

20230102-lhl-LDY-26-diF-Bpin_PROTON01
20230102-lhl-LDY-26-diF-Bpin
F
OMe
pinB
F
1t
f1 (ppm)


20230102-lhl-LDY-26-diF-Bpin_CARBON01
20230102-lhl-LDY-26-diF-Bpin
F
OMe
pinB
F
1t
f1 (ppm)

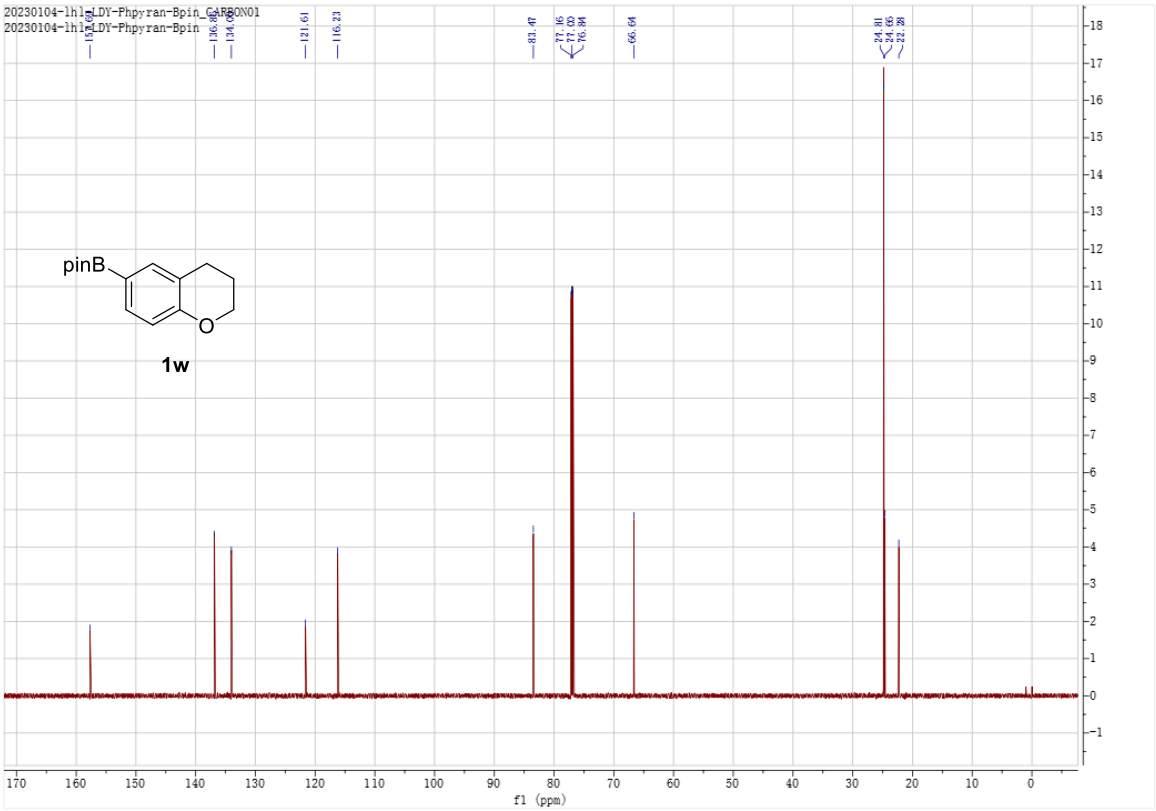

20230102-lh1-LDY-26-diMe-Bpin_PROTON01
20230102-lh1-LDY-26-diMe-Bpin
Me
OMe
pinB
Me
1u
f1 (ppm)

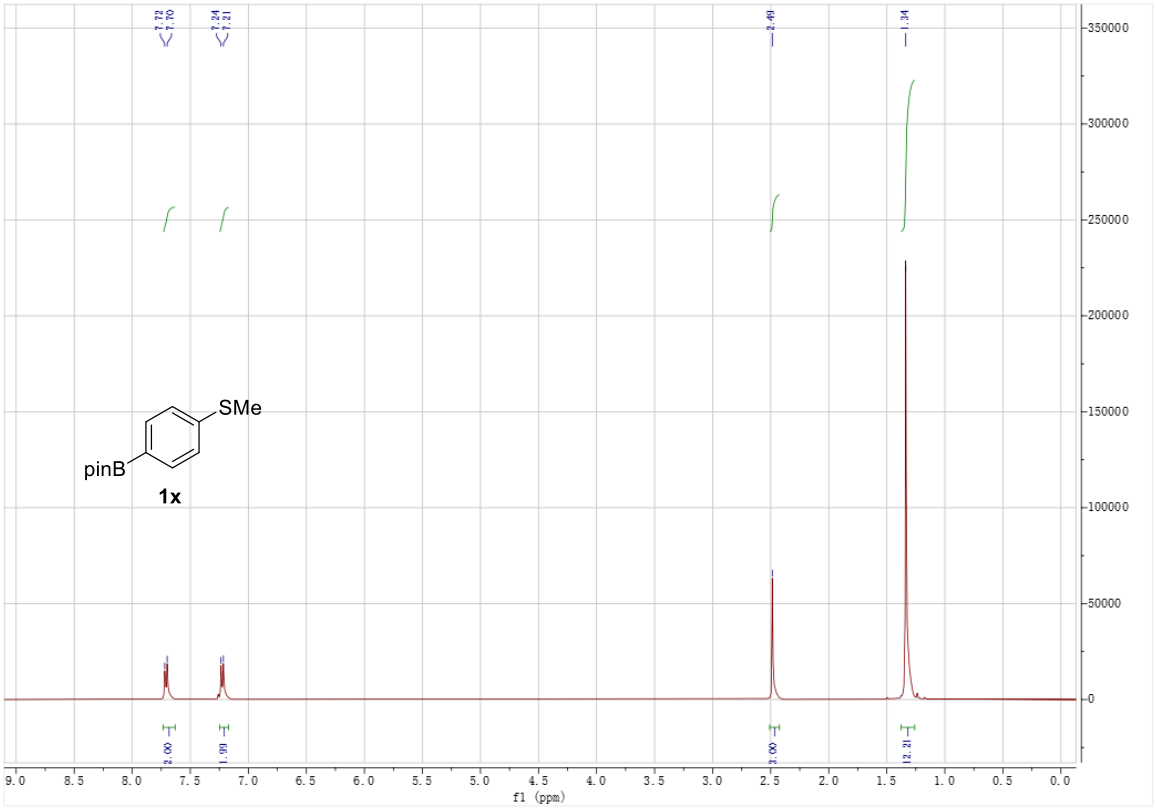

20230102-lh1-LDY-26-diMe-Bpin_CARBON01
20230102-lh1-LDY-26-diMe-Bpin
Me
OMe
pinB
Me
1u
f1 (ppm)

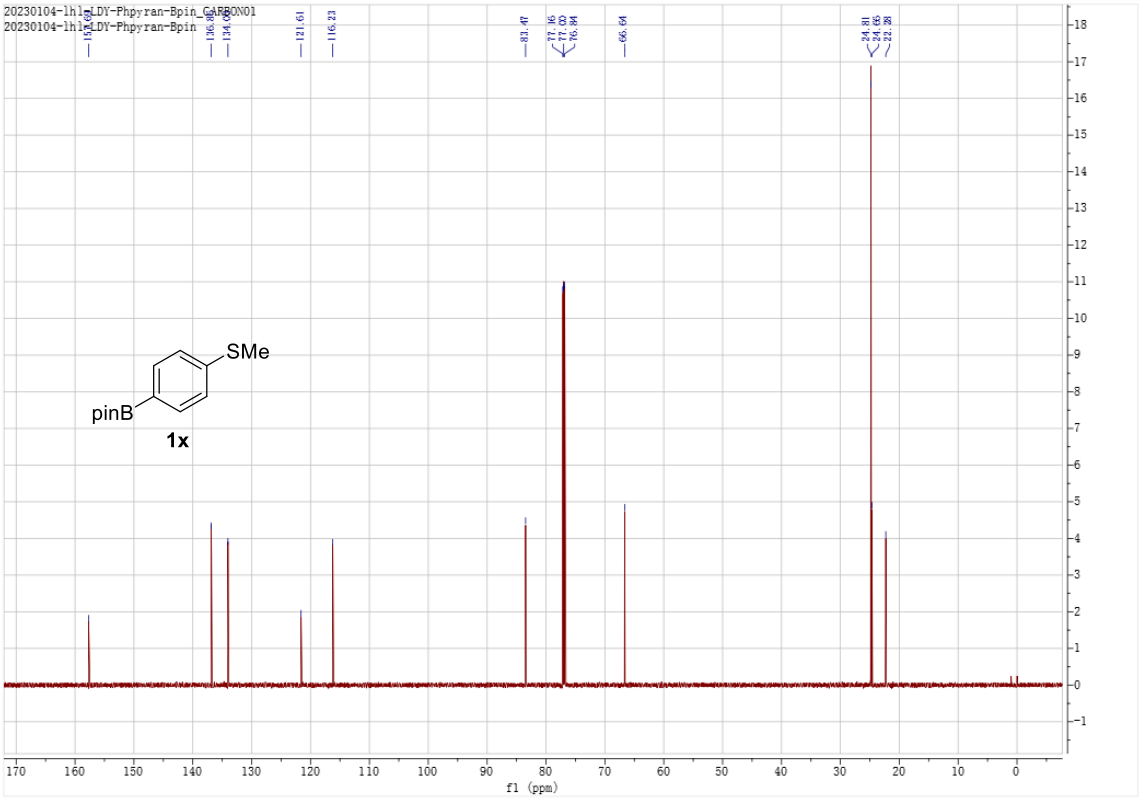

pinB
O
1v
fl (ppm)

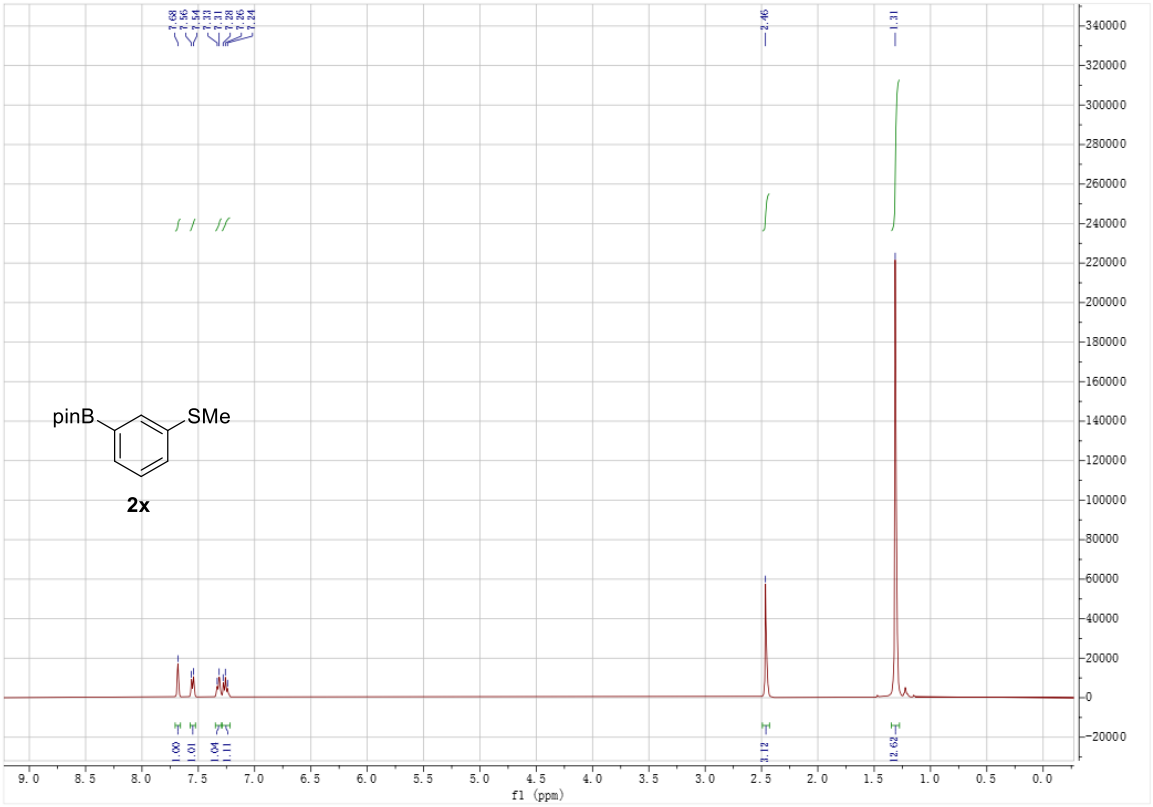

pinB
O
1v
fl (ppm)

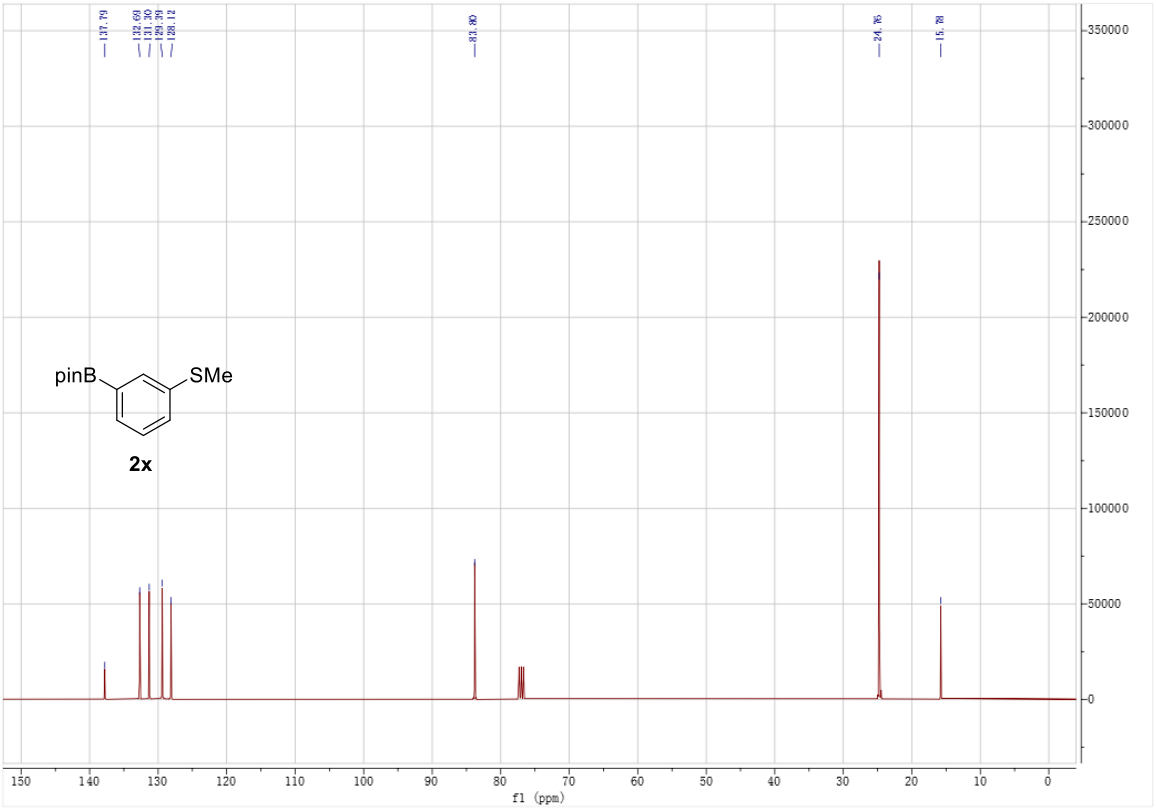

pinB
O
1w
f1 (ppm)

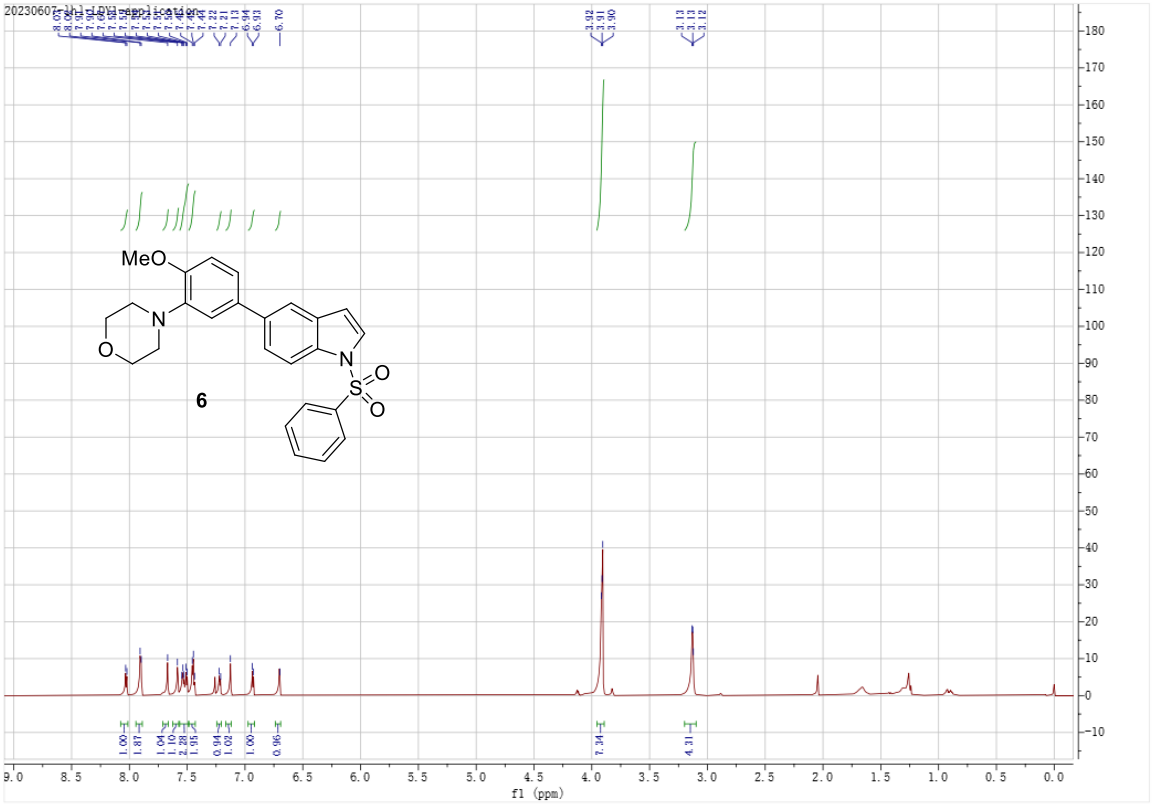

pinB
O
1w
f1 (ppm)

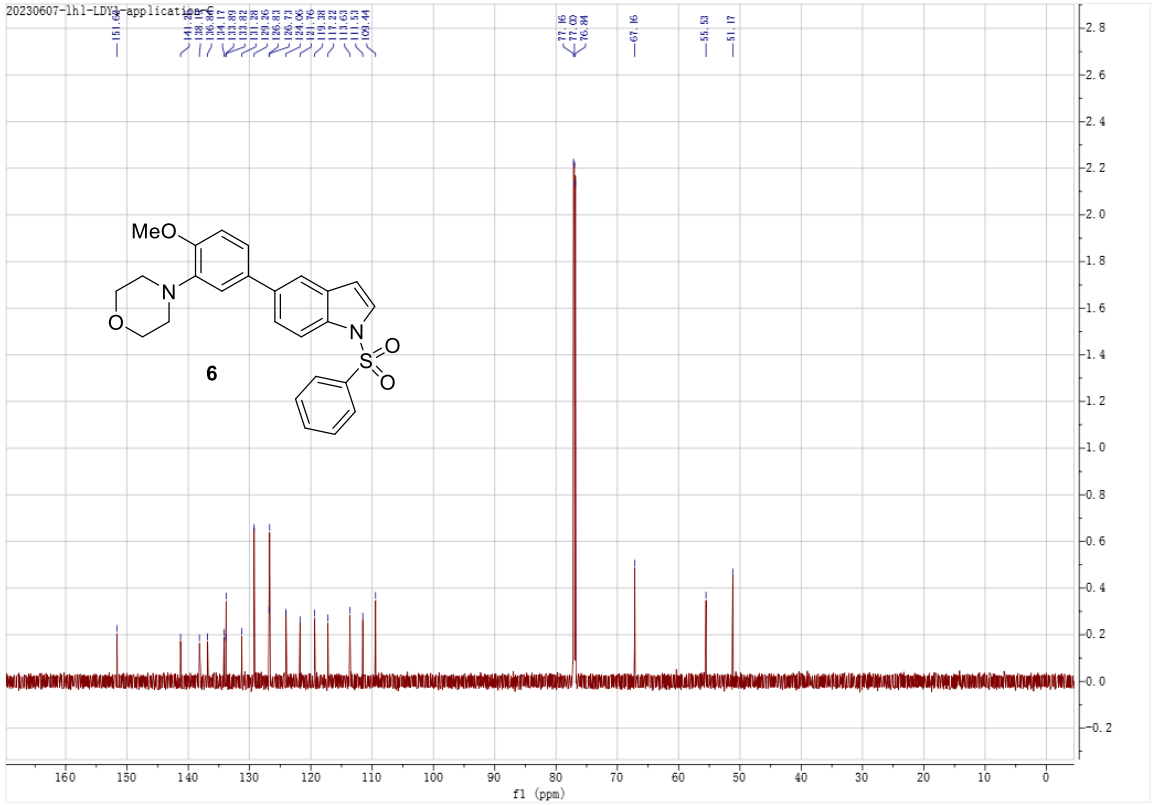

7.72
7.70
7.24
7.21
2.49
1.34
SMe
pinB
1x
2.00
1.99
3.00
12.21
f1 (ppm)


20230104-1h1c-LDY-Phpyran-Bpin_CARBON01
20230104-1h1c-LDY-Phpyran-Bpin
158.47
136.88
134.08
121.61
116.23
83.47
77.16
77.00
76.84
66.64
24.81
24.65
22.28
SMe
pinB
1x
f1 (ppm)


pinB
SMe
2x
f1 (ppm)


pinB
SMe
2x
f1 (ppm)


MeO
N
O
N
S
O
O
6
f1 (ppm)


MeO
N
O
N
S
O
O
6
f1 (ppm)