Copper-catalyzed 1,6-conjugate addition of *para*-quinone methides with diborylmethane

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Supporting Information

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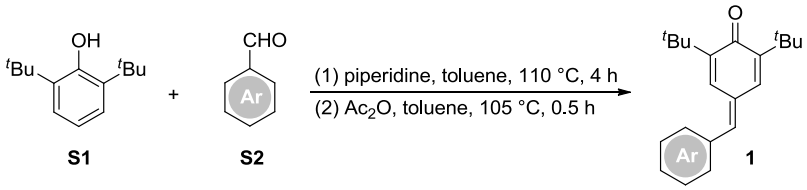
I. General Information

All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using dry solvents. Anhydrous toluene were freshly distilled from sodium. Unless otherwise stated, chemicals and reagents were used as received. Flash column chromatography was performed over silica gel (200-300 mesh) purchased from *Qindao Bangkai Co., China.* ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV 500 MHz NMR spectrometer using residue solvent peaks as an internal standard (^{1}H NMR: $CHCl_3$ at 7.26 ppm, ^{13}C NMR: $CDCl_3$ at 77.0 ppm). HRMS were recorded on an Agilent 6545 Q-TOF LC/MS instrument with electrospray ionization (ESI) technique.

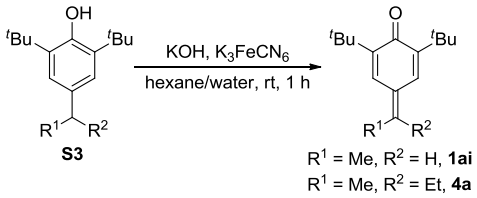
II. Preparation of Materials

2.1. Synthesis of *p*-Quinone Methide Substrates



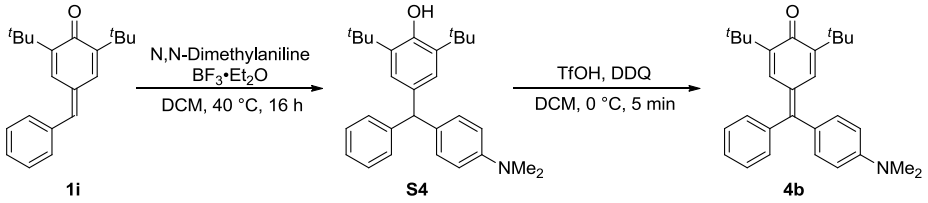
p-Quinone methide substrates **1a**-**1ah**, **1aj** were synthesized according to the literature reported procedure.[1] They are known compounds.

2.2. Synthesis of *p*-Quinone Methide 1ai and 4a



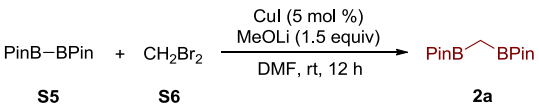
p-Quinone methide **1ai** and **4a** were synthesized according to the literature reported procedure.[2] They are known compounds.

2.3. Synthesis of *p*-Quinone Methide 4b



p-Quinone methide **4b** was synthesized according to the literature reported procedure.[3] It is a known compound.

2.4. Synthesis of Diborylmethane 2a

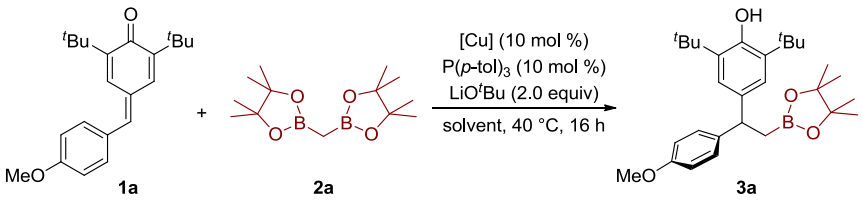


[1] D. Richter, N. Hampel, T. Singer, A. R. Ofial, H. Mayr, *Eur. J. Org. Chem*. **2009,** *19*, 3203.
[2] Z.-Q. Liu, P.-S. You, L.-D. Zhang, D.-Q. Liu, S.-S. Liu, X.-Y. Guan, *Molecules* **2020**, *25*, 539.
[3] S. Gao, X. Xu, Z. Yuan, H. Zhou, H. Yao, A. Lin, *Eur. J. Org. Chem.* **2016**, 3006.

Diborylmethane **2a** was synthesized according to the literature reported procedure.[4] It is a known compound.

III. Screening of Reaction Conditions

Table S1. Screening of Solvents and Copper Catalysts

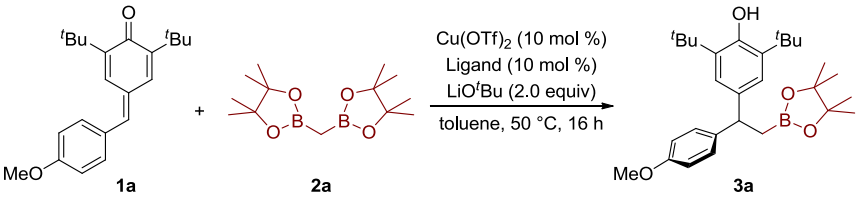


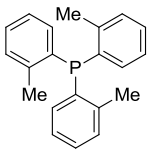
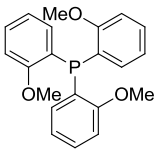
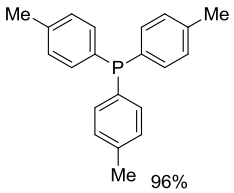
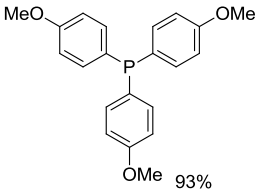
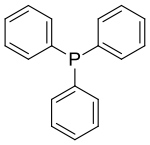
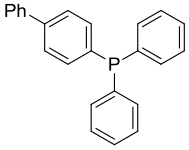
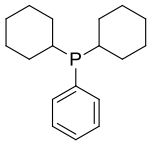
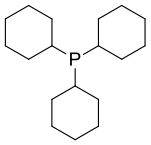
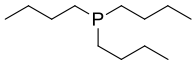
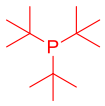
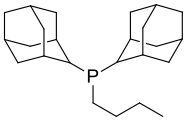
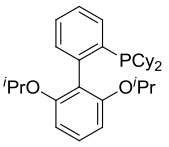
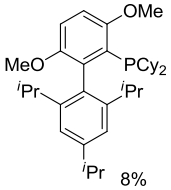
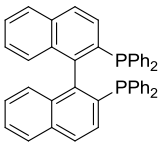
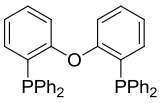
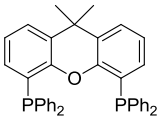
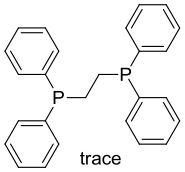
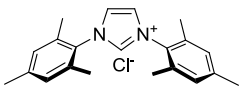
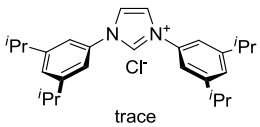
entry	solvent	[Cu]	yield (%)
1	THF	$Cu(OTf)_2$	trace
2	MeCN	$Cu(OTf)_2$	trace
3	dioxane	$Cu(OTf)_2$	20
4	hexane	$Cu(OTf)_2$	trace
5	toluene	$Cu(OTf)_2$	84
6	toluene	CuSCN	trace
7	toluene	CuCl	67
8	toluene	CuBr	< 5
9	toluene	CuI	< 5
10	toluene	CuTc	44
11	toluene	Cu_2O	trace
12	toluene	$CuCl_2$	30
13	toluene	$CuBr_2$	trace
14	toluene	CuF_2	trace
15	toluene	$Cu(NO_3)_2$	36
16	toluene	$Cu(acac)_2$	49
17	toluene	$Cu(OAc)_2$	73
18	toluene	none	0
19[a]	toluene	$Cu(OTf)_2$	95
20[b]	toluene	$Cu(OTf)_2$	93
21[c]	toluene	$Cu(OTf)_2$	16

a: the reaction was performed at 50 °C
b: the reaction was performed at 60 °C
c: the reaction was performed at rt

[4] X. Liu, T. M. Deaton, F. Haeffner, J. P. Morken, *Angew. Chem., Int. Ed.* **2017**, *56*, 11485.

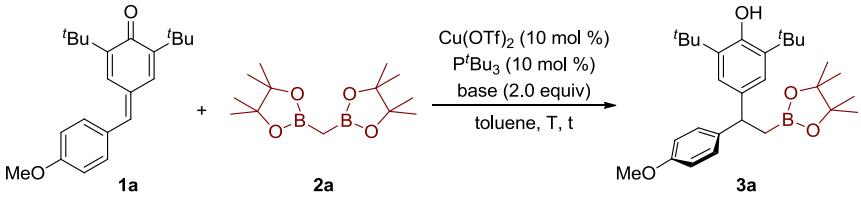
Table S2. Screening of Ligands



 87%	 97%	 96%	 93%
 66%	 96%	 89%	 73%
 28%	 99%	 92%	 49%
 8%	 trace (trace[a])	 trace	 trace
 trace	 trace	 trace	none 0%

a: 5 mol% of ligand was used

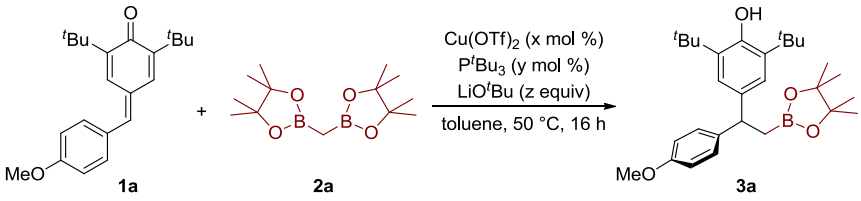
Table S3. Screening of Base and Other Reaction Conditions



entry	base	**T** (°C)	t (h)	yield (%)
1	LiO^tBu	50	16	98
2	NaO^tBu	50	16	69
3	KO^tBu	50	16	97
4	LiOMe	50	16	77
5	NaOMe	50	16	17
6	LiOH	50	16	50
7	KF	50	16	19
8	Cs_2CO_3	50	16	64
9	LiO^tBu	60	16	94
10	LiO^tBu	40	20	89
11	LiO^tBu	rt	20	15
12	LiO^tBu	50	12	93
13	LiO^tBu	50	8	82
14[a]	LiO^tBu	50	16	trace
15[b]	NaO^tBu	50	16	0
16[b]	KO^tBu	50	16	0

a: The reaction was performed under air b: Without $Cu(OTf)_2$ and P^tBu_3

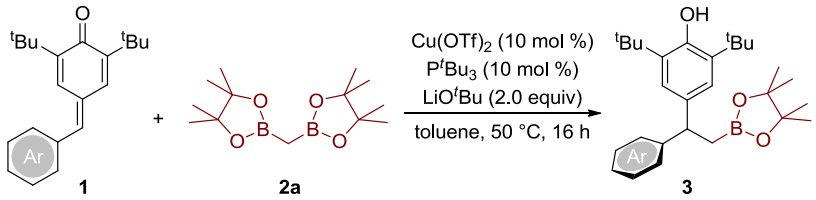
Table S4. Screening of the Equivalents of Catalyst/Ligand/Base



entry	x	y	z	yield (%)
1	5	5	2	78
2	5	10	2	75
3	10	10	2	99
4	10	20	2	97
5	10	10	1	66
6	10	10	1.5	96
7	10	10	2.5	93
8[a]	10	10	2	43
9[b]	10	10	2	92

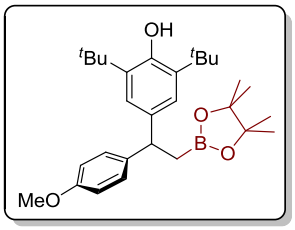
a: 1.0 equiv of **2a** was used b: 2.0 equiv of **2a** was used

IV. 1,6-Conjugate Addition of Diborylmethane



An oven-dried Schlenk tube equipped with a Teflon sealed cap was charged with $Cu(OTf)_2$ (1.8 mg, 0.005 mmol, 10 mol%), LiO^tBu (8.0 mg, 0.1 mmol, 2.0 equiv), *p*-quinone methide substrates (0.05 mmol) and a stir bar. Then a solution of diboryl methane (33.5 mg, 0.125 mmol, 2.5 equiv) and P^tBu_3 (15 μL, 10% in pentane) in anhydrous toluene (0.5 mL) was added to the tube. The tube was degased and refilled with nitrogen for 3 times, sealed, and then heated at 50 °C for 16 hours. The reaction was quenched with saturated NH_4Cl and the aqueous layer was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were dried with Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate) to afford the pure product.

2,6-di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) ethyl)phenol (3a)



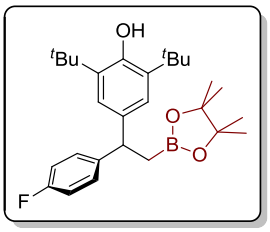
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.7 Hz, 2H), 7.12 (s, 2H), 6.84 (d, *J* = 8.7 Hz, 1H), 5.03 (s, 1H), 4.18 (t, *J* = 8.6 Hz, 1H), 3.79 (s, 3H), 1.61 (d, *J* = 8.6 Hz, 2H), 1.45 (s, 18H), 1.08 (s, 6H), 1.07 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 157.6, 151.8, 139.6, 137.3, 135.3, 128.4, 124.1, 113.5, 82.9, 55.2, 45.9, 34.3, 30.3, 24.57, 24.56.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.26.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{29}H_{43}BO_4Na$: 489.3147, found: 489.3145.

2,6-di-*tert*-butyl-4-(1-(4-fluorophenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)eth yl)phenol (3b)



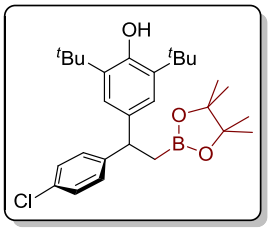
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.23 (m, 2H), 7.07 (s, 2H), 6.98 – 6.92 (m, 2H), 5.03 (s, 1H), 4.18 (t, *J* = 8.6 Hz, 1H), 1.58 (d, *J* = 8.6 Hz, 2H), 1.42 (s, 18H), 1.05 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 161.1 (d, *J* = 243.0 Hz), 151.9, 142.9 (d, *J* = 3.1 Hz), 136.9, 135.4, 128.9 (d, *J* = 7.8 Hz), 124.0, 114.8 (d, *J* = 20.9 Hz), 83.0, 45.9, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.51.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{28}H_{40}FBO_3Na$: 477.2947, found: 477.2953.

2,6-di-*tert*-butyl-4-(1-(4-chlorophenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)et hyl)phenol (3c)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 (s, 4H), 7.06 (s, 2H), 5.04 (s, 1H), 4.17 (t, *J* = 8.6 Hz, 1H), 1.57 (d, *J* = 8.6 Hz, 2H), 1.42 (s, 18H), 1.06 (s, 6H), 1.06 (s, 6H).

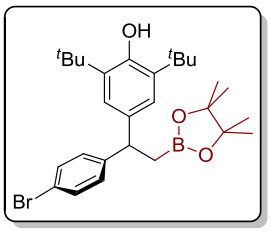
^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 145.8, 136.4, 135.5, 131.3,

128.9, 128.2, 124.1, 83.1, 46.0, 34.3, 30.3, 24.58, 24.55.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.79.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{28}H_{40}ClBO_3Na$: 493.2651, found: 493.2655.

4-(1-(4-bromophenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)-2,6-di-*tert*-butylphenol (3d)



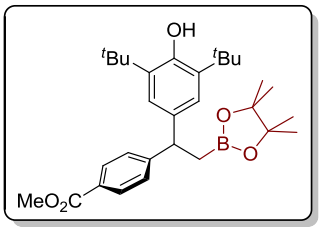
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.4 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.06 (s, 2H), 5.04 (s, 1H), 4.16 (t, *J* = 8.5 Hz, 1H), 1.57 (d, *J* = 8.5 Hz, 2H), 1.42 (s, 18H), 1.06 (s, 6H), 1.06 (s, sH).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 146.4, 136.3, 135.5, 131.1, 129.3, 124.1, 119.3, 83.1, 46.1, 34.3, 30.3, 24.57, 24.56.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.18.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{28}H_{40}BrBO_3Na$: 537.2146, found: 537.2152.

4-(1-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)benzoate (3e)



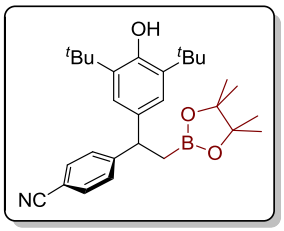
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.07 (s, 2H), 5.04 (s, 1H), 4.25 (t, *J* = 8.5 Hz, 1H), 3.90 (s, 3H), 1.61 (d, *J* = 8.5 Hz, 2H), 1.41 (s, 18H), 1.05 (s, 6H), 1.05 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 167.2, 152.7, 152.0, 136.1, 135.5, 129.6, 127.61, 127.57, 124.1, 83.1, 51.9, 46.7, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 35.11.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{43}BO_5Na$: 517.3096, found: 517.3093.

4-(1-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)benzonitrile (3f)



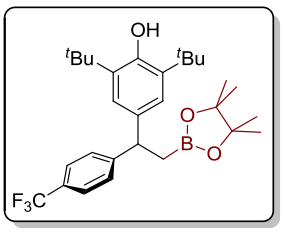
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.04 (s, 2H), 5.08 (s, 1H), 4.24 (t, *J* = 8.5 Hz, 1H), 1.59 (dd, *J* = 8.5, 3.2 Hz, 2H), 1.42 (s, 18H), 1.05 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.9, 152.2, 135.7, 135.3, 132.1, 128.3, 124.1, 119.2, 109.4, 83.2, 46.7, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.57.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{29}H_{40}BNO_3Na$: 484.2993, found: 484.2997.

2,6-di-*tert*-butyl-4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1-(4-(trifluoromethyl)phenyl)ethyl)phenol (3g)



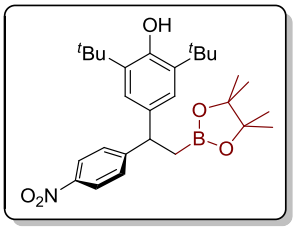
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.1 Hz, 2H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.09 (s, 2H), 5.06 (s, 1H), 4.25 (t, *J* = 8.6 Hz, 1H), 1.62 (dd, *J* = 4.3, 2.1 Hz, 2H), 1.43 (s, 18H), 1.06 (s, 6H), 1.05 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 151.5, 135.8, 135.6, 127.9 (q, *J* = 31.6 Hz), 127.8, 125.1 (q, *J* = 3.7 Hz), 124.4 (q, *J* = 273.4 Hz), 124.1, 83.1, 46.5, 34.4, 30.3, 24.54, 24.52.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.81.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{29}H_{40}BF_3O_3Na$: 527.2915, found: 527.2924.

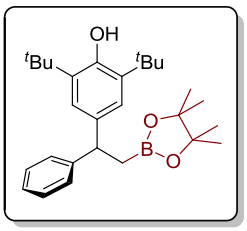
2,6-di-*tert*-butyl-4-(1-(4-nitrophenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3h)



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.8 Hz, 2H), 7.45 (d, *J* = 8.8 Hz, 2H), 7.05 (s, 2H), 5.09 (s, 1H), 4.30 (t, *J* = 8.5 Hz, 1H), 1.62 (d, *J* = 8.5 Hz, 1H), 1.42 (s, 18H), 1.06 (s, 6H), 1.06 (s, 6H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 155.2, 152.3, 146.1, 135.8, 135.2, 128.3, 124.1, 123.5, 83.2, 46.5, 34.4, 30.3, 24.57, 24.55.
^{11}B NMR (160 MHz, $CDCl_3$) δ 33.52.

HRMS: (ESI$^+$) [M+Na]$^+$ calcd for $C_{28}H_{40}BNO_5Na$: 504.2892, found: 504.2896.

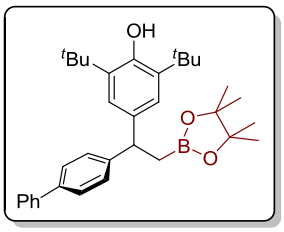
2,6-di-*tert*-butyl-4-(1-phenyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3i)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 1H), 7.18 – 7.13 (m, 1H), 7.12 (s, 2H), 5.02 (s, 1H), 4.21 (t, *J* = 8.7 Hz, 1H), 1.62 (d, *J* = 8.7 Hz, 2H), 1.43 (s, 18H), 1.06 (s, 6H), 1.05 (s, 6H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 147.2, 136.9, 135.3, 128.1, 127.5, 125.6, 124.2, 82.9, 46.7, 34.3, 30.3, 24.54, 24.53.
^{11}B NMR (160 MHz, $CDCl_3$) δ 33.72.

HRMS: (ESI$^+$) [M+Na]$^+$ calcd for $C_{28}H_{41}BO_3Na$: 459.3041, found: 459.3049.

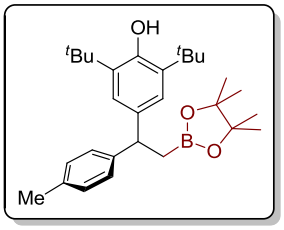
4-(1-([1,1'-biphenyl]-4-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)-2,6-di-*tert*-butylphenol (3j)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.56 (m, 2H), 7.52 (d, *J* = 8.3 Hz, 2H), 7.43 (dd, *J* = 8.3, 7.0 Hz, 2H), 7.40 (d, *J* = 8.3 Hz, 2H), 7.36 – 7.31 (m, 1H), 7.16 (s, 2H), 5.03 (s, 1H), 4.25 (t, *J* = 8.6 Hz, 1H), 1.65 (d, *J* = 8.6 Hz, 2H), 1.44 (s, 18H), 1.06 (s, 6H), 1.05 (s, 6H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 146.5, 141.2, 138.5, 136.8, 135.4, 128.6, 127.9, 126.93, 126.88, 126.86, 124.2, 83.0, 46.4, 34.4, 30.3, 24.6, 24.5.
^{11}B NMR (160 MHz, $CDCl_3$) δ 33.72.

HRMS: (ESI$^+$) [M+Na]$^+$ calcd for $C_{34}H_{45}BO_3Na$: 535.3354, found: 535.3360.

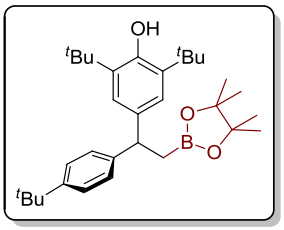
2,6-di-*tert*-butyl-4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1-(p-tolyl)ethyl)phenol (3k)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.1 Hz, 2H), 7.12 (s, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 5.00 (s, 1H), 4.17 (t, *J* = 8.7 Hz, 1H), 2.31 (s, 3H), 1.60 (dd, *J* = 8.7, 2.6 Hz, 2H), 1.43 (s, 18H), 1.06 (s, 6H), 1.04 (s, 6H).
^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 144.4, 137.0, 135.2, 134.9, 128.8, 127.3, 124.1, 82.9, 46.3, 34.3, 30.3, 24.6, 24.5, 20.9.
^{11}B NMR (160 MHz, $CDCl_3$) δ 33.27.

HRMS: (ESI$^+$) [M+H]$^+$ calcd for $C_{29}H_{44}BO_3$: 451.3378, found: 451.3388.

2,6-di-*tert*-butyl-4-(1-(4-(tert-butyl)phenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3l)



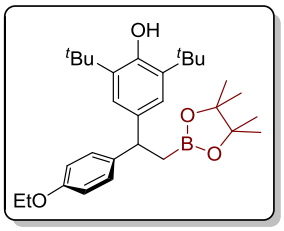
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 8.5 Hz, 2H), 7.14 (s, 2H), 5.00 (s, 1H), 4.15 (t, *J* = 8.7 Hz, 1H), 1.61 (d, *J* = 8.7 Hz, 2H), 1.43 (s, 18H), 1.30 (s, 9H), 1.03 (s, 6H), 1.00 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 148.3, 144.3, 136.9, 135.2, 127.0, 125.0, 124.2, 82.9, 46.4, 34.32, 34.26, 31.4, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.91.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{32}H_{49}BO_3Na$: 515.3667, found: 515.3662.

2,6-di-*tert*-butyl-4-(1-(4-ethoxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3m)



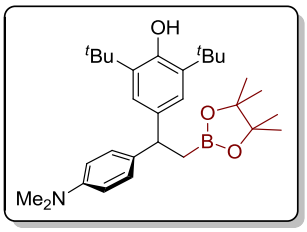
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.7 Hz, 2H), 7.09 (s, 2H), 6.81 (d, *J* = 8.7 Hz, 2H), 5.00 (s, 1H), 4.14 (t, *J* = 8.6 Hz, 1H), 4.01 (q, *J* = 7.0 Hz, 2H), 1.58 (d, *J* = 8.6 Hz, 2H), 1.42 (s, 18H), 1.40 (t, *J* = 7.0 Hz, 3H), 1.05 (s, 6H), 1.04 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9, 151.7, 139.4, 137.4, 135.3, 128.4, 124.1, 114.2, 82.9, 63.4, 45.9, 34.3, 30.33, 24.6, 24.6, 14.9.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.70.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{45}BO_3Na$: 503.3303, found: 503.3308.

2,6-di-*tert*-butyl-4-(1-(4-(dimethylamino)phenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3n)



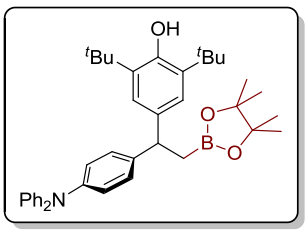
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.7 Hz, 2H), 7.11 (s, 2H), 6.69 (d, *J* = 8.7 Hz, 2H), 4.97 (s, 1H), 4.11 (t, *J* = 8.7 Hz, 1H), 2.90 (s, 6H), 1.58 (dd, *J* = 8.7, 1.2 Hz, 2H), 1.42 (s, 18H), 1.06 (s, 6H), 1.03 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 148.9, 137.5, 136.1, 135.1, 127.9, 124.1, 113.0, 82.8, 45.8, 41.0, 34.3, 30.3, 24.7, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.05.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{46}BNO_3Na$: 502.3463, found: 502.3468.

2,6-di-*tert*-butyl-4-(1-(4-(diphenylamino)phenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3o)



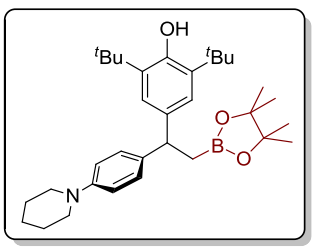
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 – 7.18 (m, 6H), 7.12 (s, 2H), 7.09 – 7.04 (m, 4H), 7.04 – 7.00 (m, 2H), 6.98 (tt, *J* = 7.3, 1.2 Hz, 2H), 5.04 (s, 1H), 4.17 (t, *J* = 8.6 Hz, 1H), 1.61 (d, *J* = 8.6 Hz, 1H), 1.44 (s, 18H), 1.09 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 148.0, 145.4, 142.0, 137.3, 135.3, 129.0, 128.5, 124.6, 124.2, 123.6, 122.2, 83.0, 46.1, 34.4, 30.3, 24.6, 24.6.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.10.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{46}BNO_3Na$: 626.3776, found: 626.3773.

2,6-di-*tert*-butyl-4-(1-(4-(piperidin-1-yl)phenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3p)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.5 Hz, 2H), 7.09 (s, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 4.98 (s, 1H), 4.11 (t, *J* = 8.7 Hz, 1H), 3.17 – 3.01 (m, 4H), 1.79 – 1.67 (m, 4H), 1.57 (d, *J* = 8.7 Hz, 2H), 1.59 – 1.52 (m, 2H), 1.41 (s, 18H), 1.05 (s, 6H), 1.03 (s, 6H).

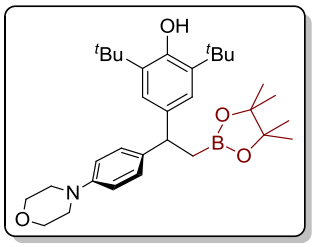
^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 150.4, 138.5, 137.5, 135.2, 128.0, 124.1, 116.7, 82.9, 51.2, 45.9, 34.3, 30.3, 25.9, 24.7, 24.6,

24.6.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.78.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{33}H_{50}BNO_3Na$: 542.3776, found: 542.3779.

2,6-di-*tert*-butyl-4-(1-(4-morpholinophenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3q)



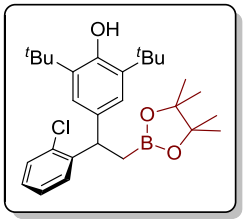
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.5 Hz, 2H), 7.09 (s, 2H), 6.84 (d, *J* = 8.5 Hz, 2H), 5.00 (s, 1H), 4.13 (t, *J* = 8.6 Hz, 1H), 3.93 – 3.81 (m, 4H), 3.11 (dd, *J* = 5.8, 3.8 Hz, 4H), 1.58 (d, *J* = 8.6 Hz, 2H), 1.42 (s, 18H), 1.05 (s, 6H), 1.04 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 149.3, 139.3, 137.2, 135.3, 128.1, 124.1, 115.8, 82.9, 67.0, 49.8, 45.9, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 35.03.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{32}H_{48}BNO_4Na$: 544.3569, found: 544.3572.

2,6-di-*tert*-butyl-4-(1-(2-chlorophenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3r)



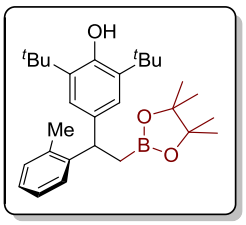
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.32 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.21 (td, *J* = 7.6, 1.4 Hz, 1H), 7.16 (s, 2H), 7.08 (td, *J* = 7.7, 1.7 Hz, 1H), 5.02 (s, 1H), 4.74 (t, *J* = 8.7 Hz, 1H), 1.64 (dd, *J* = 15.2, 8.7 Hz, 1H), 1.57 (dd, *J* = 15.2, 8.7 Hz, 1H), 1.42 (s, 18H), 1.03 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 144.5, 135.5, 135.2, 133.7, 129.4, 128.3, 126.79, 126.75, 124.5, 83.0, 42.2, 34.3, 30.3, 24.48, 24.46.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.68.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{28}H_{40}ClBO_3Na$: 493.2651, found: 493.2656.

2,6-di-*tert*-butyl-4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1-(o-tolyl)ethyl)phenol (3s)



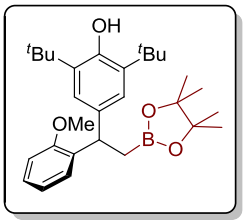
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.18 (td, *J* = 7.4, 1.8 Hz, 1H), 7.12 – 7.03 (m, 2H), 7.09 (s, 2H), 4.99 (s, 1H), 4.40 (t, *J* = 8.6 Hz, 1H), 2.40 (s, 3H), 1.60 (d, *J* = 8.6 Hz, 2H), 1.41 (s, 18H), 1.05 (s, 6H), 1.01 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.6, 145.0, 136.7, 135.8, 135.2, 130.0, 126.6, 125.9, 125.5, 124.3, 82.9, 42.0, 34.3, 30.3, 24.6, 24.5, 20.1.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.90.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{29}H_{43}BO_3Na$: 473.3197, found: 473.3203.

2,6-di-*tert*-butyl-4-(1-(2-methoxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3t)



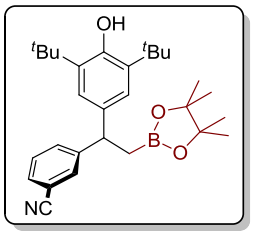
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.19 (s, 2H), 7.14 (td, *J* = 7.8, 1.7 Hz, 1H), 6.91 (td, *J* = 7.5, 1.1 Hz, 1H), 6.83 (dd, *J* = 8.1, 1.1 Hz, 1H), 4.98 (s, 1H), 4.66 (t, *J* = 8.8 Hz, 1H), 3.84 (s, 3H), 1.61 (dd, *J* = 16.9, 8.8 Hz, 2H), 1.43 (s, 18H), 1.02 (s, 6H), 1.02 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.7, 151.6, 136.6, 135.8, 134.9, 127.5, 126.5, 124.6, 120.4, 110.4, 82.8, 55.3, 38.9, 34.3, 30.4, 24.51, 24.45.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.61.

HRMS: (ESI$^+$) [M+Na]$^+$ calcd for $C_{29}H_{43}BO_4Na$: 489.3147, found: 489.3151.

3-(1-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)benzonitrile (3u)



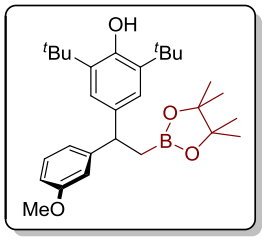
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (t, *J* = 1.8 Hz, 1H), 7.54 (dt, *J* = 7.9, 1.6 Hz, 1H), 7.45 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.05 (s, 2H), 5.09 (s, 1H), 4.23 (t, *J* = 8.5 Hz, 1H), 1.59 (dd, *J* = 8.5, 4.0 Hz, 2H), 1.43 (s, 18H), 1.07 (s, 6H), 1.06 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.2, 148.8, 135.7, 135.4, 132.1, 131.3, 129.5, 128.9, 124.1, 119.2, 112.0, 83.2, 46.2, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.12.

HRMS: (ESI$^+$) [M+Na]$^+$ calcd for $C_{29}H_{40}BNO_3Na$: 484.2993, found: 484.2999.

2,6-di-*tert*-butyl-4-(1-(3-methoxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3v)



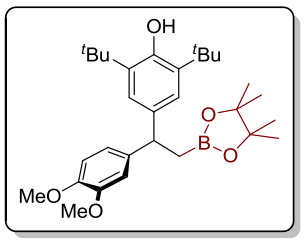
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (t, *J* = 7.9 Hz, 1H), 7.12 (s, 2H), 6.93 (dt, *J* = 7.7, 1.1 Hz, 1H), 6.87 (t, *J* = 2.1 Hz, 1H), 6.73 – 6.67 (m, 1H), 5.01 (s, 1H), 4.17 (t, *J* = 8.6 Hz, 1H), 3.79 (s, 3H), 1.60 (d, *J* = 8.6 Hz, 2H), 1.42 (s, 18H), 1.06 (s, 6H), 1.04 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 159.4, 151.9, 149.1, 136.7, 135.3, 129.0, 124.2, 120.0, 113.4, 111.0, 82.9, 55.1, 46.8, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.66.

HRMS: (ESI$^+$) [M+Na]$^+$ calcd for $C_{29}H_{43}BO_4Na$: 489.3147, found: 489.3154.

2,6-di-*tert*-butyl-4-(1-(3,4-dimethoxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3w)



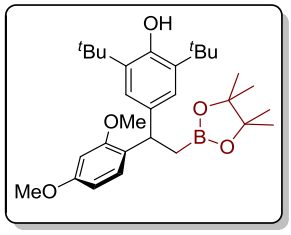
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.11 (s, 2H), 6.88 (d, *J* = 2.1 Hz, 1H), 6.86 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.79 (d, *J* = 8.2 Hz, 1H), 5.01 (s, 1H), 4.14 (t, *J* = 8.6 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 1.59 (dd, *J* = 8.6, 1.8 Hz, 2H), 1.42 (s, 18H), 1.05 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 148.5, 147.0, 140.1, 137.2, 135.3, 124.0, 119.4, 111.1, 111.0, 83.0, 55.9, 55.7, 46.3, 34.3, 30.3, 24.60, 24.57.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.03.

HRMS: (ESI$^+$) [M+Na]$^+$ calcd for $C_{30}H_{45}BO_5Na$: 519.3252, found: 519.3258.

2,6-di-*tert*-butyl-4-(1-(2,4-dimethoxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3x)



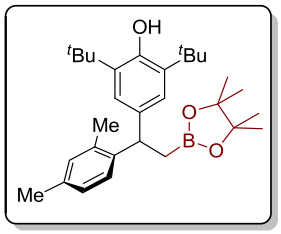
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.11 (s, 2H), 6.88 (d, *J* = 2.1 Hz, 1H), 6.86 (dd, *J* = 8.2, 2.1 Hz, 1H), 6.79 (d, *J* = 8.2 Hz, 1H), 5.01 (s, 1H), 4.14 (t, *J* = 8.6 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 1.59 (dd, *J* = 8.6, 1.7 Hz, 2H), 1.42 (s, 18H), 1.05 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 148.4, 146.9, 140.0, 137.1, 135.3, 124.0, 119.3, 111.1, 111.0, 82.9, 55.9, 55.7, 46.3, 34.3, 30.3, 24.59, 24.55.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.86.

HRMS: (ESI$^+$) [M+Na]$^+$ calcd for $C_{30}H_{45}BO_5Na$: 519.3252, found: 519.3259.

2,6-di-*tert*-butyl-4-(1-(2,4-dimethylphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3y)



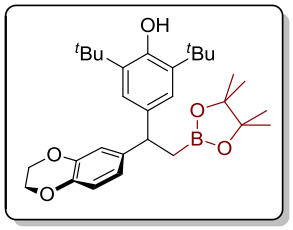
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 1H), 7.09 (s, 2H), 6.99 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.91 (d, *J* = 1.9 Hz, 1H), 4.97 (s, 1H), 4.36 (t, *J* = 8.6 Hz, 1H), 2.37 (s, 3H), 2.27 (s, 3H), 1.58 (d, *J* = 8.6 Hz, 2H), 1.41 (s, 18H), 1.04 (s, 6H), 1.02 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.6, 142.1, 136.9, 135.4, 135.1, 134.7, 130.8, 126.5, 126.4, 124.3, 82.9, 41.7, 34.3, 30.3, 24.6, 24.5, 20.8, 20.0.

^{11}B NMR (160 MHz, $CDCl_3$) δ 35.21.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{45}BO_3Na$: 487.3354, found: 487.3360.

2,6-di-*tert*-butyl-4-(1-(2,3-dihydrobenzo[b][1,4]dioxin-7-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3z)



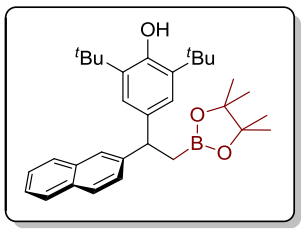
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.09 (s, 2H), 6.83 – 6.78 (m, 2H), 6.77 – 6.74 (m, 1H), 5.00 (s, 1H), 4.27 – 4.20 (m, 4H), 4.08 (t, *J* = 8.6 Hz, 1H), 1.55 (dd, *J* = 8.6, 6.2 Hz, 2H), 1.42 (s, 18H), 1.06 (s, 6H), 1.04 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 143.0, 141.4, 141.1, 136.9, 135.3, 124.1, 120.3, 116.7, 116.2, 82.9, 64.4, 64.3, 46.0, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.45.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{43}BO_5Na$: 517.3096, found: 517.3102.

2,6-di-*tert*-butyl-4-(1-(naphthalen-2-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3aa)



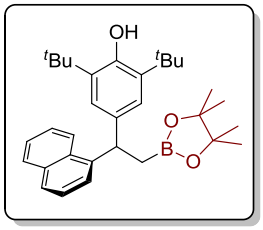
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 – 7.80 (m, 1H), 7.79 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.78 – 7.76 (m, 1H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.48 – 7.39 (m, 3H), 7.16 (s, 2H), 5.03 (s, 1H), 4.38 (t, *J* = 8.5 Hz, 1H), 1.71 (dd, *J* = 8.5, 5.3 Hz, 2H), 1.43 (s, 18H), 1.03 (s, 6H), 1.03 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 144.8, 136.8, 135.4, 133.5, 132.0, 127.7, 127.7, 127.5, 126.8, 125.6, 125.2, 125.0, 124.3, 83.0, 46.7, 34.3, 30.3, 24.57, 24.55.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.99.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{32}H_{43}BO_3Na$: 503.3197, found: 503.3202.

2,6-di-*tert*-butyl-4-(1-(naphthalen-1-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3ab)



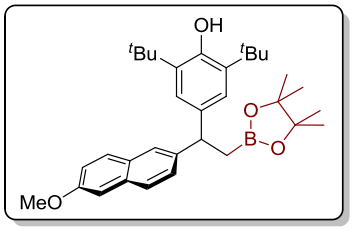
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.5 Hz, 1H), 7.84 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.48 – 7.41 (m, 2H), 7.18 (s, 2H), 5.05 (t, *J* = 8.5 Hz, 1H), 5.00 (s, 1H), 1.76 (dd, *J* = 15.3, 8.5 Hz, 1H), 1.70 (dd, *J* = 15.3, 8.5 Hz, 1H), 1.40 (s, 18H), 1.02 (s, 6H), 0.97 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 143.2, 136.6, 135.2, 133.9, 131.7, 128.6, 126.4, 125.5, 125.4, 125.1, 124.5, 124.2, 124.1, 82.9, 41.5, 34.3, 30.3, 24.50, 24.47.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{32}H_{43}BO_3Na$: 503.3197, found: 503.3206.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.86.

2,6-di-*tert*-butyl-4-(1-(6-methoxynaphthalen-2-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3ac)



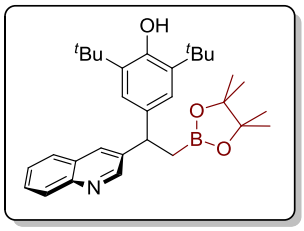
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 9.1 Hz, 1H), 7.69 (d, *J* = 2.4 Hz, 1H), 7.64 (d, *J* = 8.5 Hz, 1H), 7.40 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.15 (s, 2H), 7.12 (dd, *J* = 8.8, 2.5 Hz, 1H), 7.10 (d, *J* = 2.5 Hz, 1H), 5.02 (s, 1H), 4.34 (t, *J* = 8.6 Hz, 1H), 3.92 (s, 3H), 1.68 (dd, *J* = 8.6, 7.2 Hz, 2H), 1.42 (s, 18H), 1.03 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 151.8, 142.5, 137.0, 135.3, 132.9, 129.2, 129.0, 127.3, 126.6, 125.1, 124.3, 118.3, 105.6, 83.0, 55.2, 46.5, 34.3, 30.3, 24.58, 24.56.

^{11}B NMR (160 MHz, $CDCl_3$) δ 34.35.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{33}H_{45}BO_4Na$: 539.3303, found: 539.3300.

2,6-di-*tert*-butyl-4-(1-(quinoline-2-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3ad)



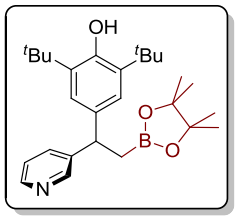
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.89 (d, *J* = 2.3 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 8.02 (d, *J* = 2.2 Hz, 1H), 7.79 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.65 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.52 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.14 (s, 2H), 5.08 (s, 1H), 4.42 (t, *J* = 8.5 Hz, 1H), 1.72 (d, *J* = 8.5 Hz, 2H), 1.42 (s, 18H), 1.04 (s, 6H), 1.04 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.2, 152.0, 146.5, 140.1, 135.8, 135.5, 132.7, 128.9, 128.5, 128.1, 127.6, 126.4, 124.2, 83.2, 44.3, 34.3, 30.3, 24.58, 24.56.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.50.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{31}H_{42}BO_4Na$: 510.3150, found: 510.3153.

2,6-di-*tert*-butyl-4-(1-(pyridin-3-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3ae)



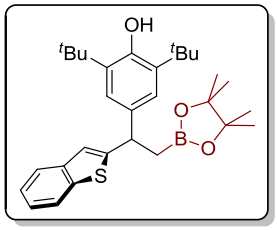
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 2.3 Hz, 1H), 8.41 (dd, *J* = 4.9, 1.6 Hz, 1H), 7.59 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.20 (ddd, *J* = 7.9, 4.8, 0.9 Hz, 1H), 7.08 (s, 2H), 5.07 (s, 1H), 4.22 (t, *J* = 8.6 Hz, 1H), 1.61 (dd, *J* = 8.6, 3.3 Hz, 2H), 1.42 (s, 18H), 1.06 (s, 6H), 1.05 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 149.4, 147.1, 142.5, 135.7, 135.6, 134.8, 124.1, 123.2, 83.2, 44.2, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.86.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{27}H_{40}BNO_3Na$: 460.2993, found: 460.2998.

4-(1-(benzo[*b*]thiophen-2-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)-2,6-di-*tert*-butylphenol (3af)



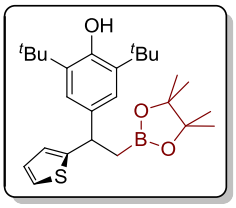
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (ddd, *J* = 7.3, 5.5, 1.6 Hz, 2H), 7.36 – 7.29 (m, 2H), 7.24 (d, *J* = 0.9 Hz, 1H), 7.16 (s, 2H), 5.01 (s, 1H), 4.55 (t, *J* = 8.5 Hz, 1H), 1.76 (dd, *J* = 15.3, 8.5 Hz, 1H), 1.66 (dd, *J* = 15.3, *J* = 8.5 Hz, 1H), 1.41 (s, 18H), 1.08 (s, 6H), 1.01 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 142.3, 140.6, 138.7, 135.7, 135.4, 124.2, 123.9, 123.5, 122.6, 122.6, 120.9, 83.0, 40.7, 34.3, 30.3, 24.6, 24.5.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.4.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{41}BO_3SNa$: 515.2762, found: 515.2768.

2,6-di-*tert*-butyl-4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1-(thiophen-2-yl)ethyl)phenol (3ag)



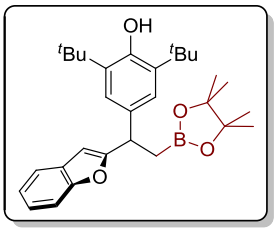
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (s, 2H), 7.10 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.89 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.82 (dt, *J* = 3.5, 1.2 Hz, 1H), 5.04 (s, 1H), 4.41 (t, *J* = 8.5 Hz, 1H), 1.69 (dd, *J* = 15.2, 8.5 Hz, 1H), 1.63 (dd, *J* = 15.2, 8.5 Hz, 1H), 1.43 (s, 18H), 1.07 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 152.1, 136.5, 135.4, 126.3, 124.0, 123.1, 122.9, 83.1, 42.3, 34.3, 30.3, 24.59, 24.56.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.71.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{26}H_{39}O_3SNa$: 465.2605, found: 465.2613.

4-(1-(benzo[b]furan-2-yl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)-2,6-di-*tert*-butylphenol (3ah)



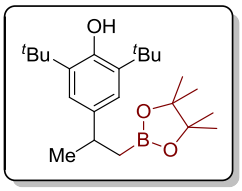
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 – 7.45 (m, 1H), 7.43 – 7.38 (m, 1H), 7.23 – 7.14 (m, 2H), 7.17 (s, 2H), 6.37 (d, *J* = 1.0 Hz, 1H), 5.08 (s, 1H), 4.31 (t, *J* = 8.3 Hz, 1H), 1.72 (dd, *J* = 15.4, 8.3 Hz, 1H), 1.56 (dd, *J* = 15.4, 8.3 Hz, 1H), 1.44 (s, 18H), 1.13 (s, 6H), 1.11 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 163.5, 154.8, 152.4, 135.5, 133.9, 128.9, 124.4, 123.0, 122.2, 120.3, 110.9, 101.5, 83.2, 41.0, 34.4, 30.3, 24.7, 24.6.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.51.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{41}BO_4Na$: 499.2990, found: 499.2997.

2,6-di-*tert*-butyl-4-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propan-2-yl)phenol (3ai)



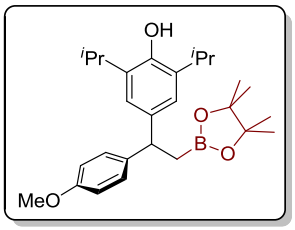
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.06 (s, 2H), 5.01 (s, 1H), 2.98 (dp, *J* = 8.7, 6.9 Hz, 1H), 1.45 (s, 18H), 1.28 (d, *J* = 6.9 Hz, 3H), 1.18 (s, 12H), 1.16 (d, *J* = 8.7 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.6, 139.7, 135.3, 123.1, 82.9, 35.7, 34.4, 30.4, 25.3, 24.8, 24.7.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.99.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{23}H_{39}BO_3Na$: 397.2884, found: 397.2887.

2,6-diisopropyl-4-(1-(4-methoxyphenyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenol (3aj)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (d, *J* = 8.7 Hz, 2H), 6.97 (s, 2H), 6.81 (d, *J* = 8.7 Hz, 2H), 4.63 (s, 1H), 4.17 (t, *J* = 8.6 Hz, 1H), 3.78 (s, 3H), 3.12 (hept, *J* = 6.9 Hz, 2H), 1.58 (d, *J* = 8.6 Hz, 2H), 1.25 (d, *J* = 6.9 Hz, 6H), 1.24 (d, *J* = 6.9 Hz, 7H), 1.07 (s, 6H), 1.05 (s, 6H).

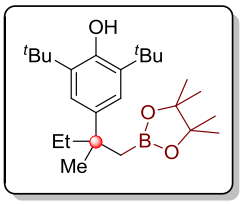
^{13}C NMR (125 MHz, $CDCl_3$) δ 157.5, 148.0, 139.6, 138.6, 133.1, 128.4, 122.6, 113.5, 83.0, 55.2, 45.6, 27.3, 24.7, 24.6, 24.5, 22.8, 22.7.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.89.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{27}H_{39}BO_4Na$: 461.2834, found: 461.2834.

2,6-di-*tert*-butyl-4-(2-methyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butan-2-yl)phenol (5a)

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (s, 2H), 4.98 (s, 1H), 1.68 (dh, *J* = 20.9, 7.4 Hz, 3H), 1.45



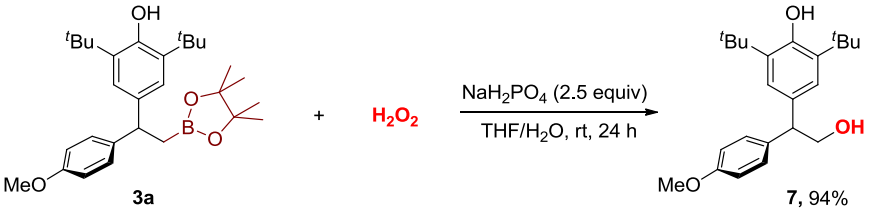
(s, 18H), 1.40 (s, 3H), 1.30 (d, J = 14.9 Hz, 2H), 1.15 (d, J = 14.9 Hz, 1H), 1.10 (s, 6H), 1.06 (s, 6H), 0.72 (t, J = 7.4 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 139.9, 134.4, 122.8, 82.5, 39.3, 38.0, 34.5, 30.5, 26.5, 24.8, 24.5, 9.2.

^{11}B NMR (160 MHz, $CDCl_3$) δ 33.57.

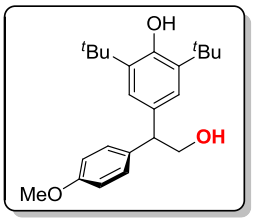
HRMS: (ESI$^+$) $[M+Na]^+$ calcd for $C_{25}H_{43}BO_3Na$: 425.3197, found: 425.3192.

V. Synthesis of compound 7



To a solution **3a** (23.3 mg, 0.05 mmol) in anhydrous THF (0.5 mL) was added a solution of NaH_2PO_4 (15.0 mg, 0.125 mmol, 2.5 equiv) in water (0.5 mL). The reaction mixture was then cooled to 0 °C and H_2O_2 (30% wt% in H_2O, 0.5 mL) was added. After stirring at room temperature for additional 24 hours, the reaction was quenched with saturated NH_4Cl and extracted with ethyl acetate (3 × 10 mL). The combined organic layers were dried with Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 3/1) to afford the pure product.

2,6-di-*tert*-butyl-4-(2-hydroxy-1-(4-methoxyphenyl)ethyl)phenol (7)

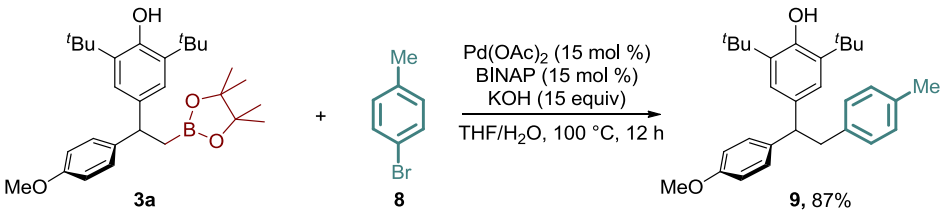


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (d, J = 8.7 Hz, 2H), 7.07 (s, 2H), 6.90 (d, J = 8.7 Hz, 2H), 5.14 (s, 1H), 4.10 (d, J = 1.6 Hz, 3H), 3.82 (s, 3H), 1.51 (b, 1H), 1.44 (s, 18H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 158.3, 152.5, 136.0, 133.9, 131.8, 129.2, 124.7, 114.0, 66.7, 55.2, 52.9, 34.4, 30.3.

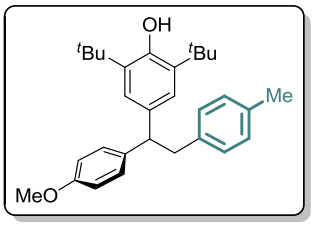
HRMS: (ESI$^+$) $[M+Na]^+$ calcd for $C_{23}H_{32}O_3Na$: 379.2244, found: 379.2249.

VI. Synthesis of compound 9



An oven-dried Schlenk tube was charged with compound **3a** (23.3 mg, 0.05 mmol), $Pd(OAc)_2$ (1.7 mg, 15 mol %), BINAP (4.7 mg, 15 mol %), and KOH (42.0 mg, 0.75 mol, 15 equiv). The tube was sealed, degased and refilled with N_2 for 3 times. Then a solution of 1-bromo-4-methylbenzene (25.7 mg, 0.15 mmol, 3 equiv) in THF (1.0 mL) and water (0.1 mL) were injected into the tube via syringes. The tube was heated at 100 °C for 12 hours. After completion, the reaction mixture was filtered through a pad of Celite and Na_2SO_4. The filtride was washed with ethyl acetate for 3 times (3 × 10 mL). The combined organic solvents were concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 20/1) to afford the pure product.

2,6-di-*tert*-butyl-4-(1-(4-methoxyphenyl)-2-(p-tolyl)ethyl)phenol (9)



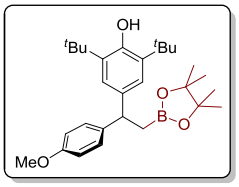
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.15 (d, *J* = 8.7 Hz, 2H), 7.00 (d, *J* = 7.8 Hz, 2H), 6.97 (s, 2H), 6.89 (d, *J* = 7.8 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 5.04 (s, 1H), 4.08 (t, *J* = 7.8 Hz, 1H), 3.80 (s, 3H), 3.25 (qd, *J* = 13.5, 7.8 Hz, 2H), 2.30 (s, 3H), 1.41 (s, 18H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 157.7, 151.8, 137.7, 137.1, 135.6, 135.3, 135.0, 129.0, 129.0, 128.6, 124.4, 113.5, 55.2, 52.4, 42.7, 34.3, 30.3, 21.0.

HRMS: (ESI^+) $[M+Na]^+$ calcd for $C_{30}H_{38}O_2Na$: 453.2764, found: 453.2766.

VII. NMR Spectra

Please refer to next pages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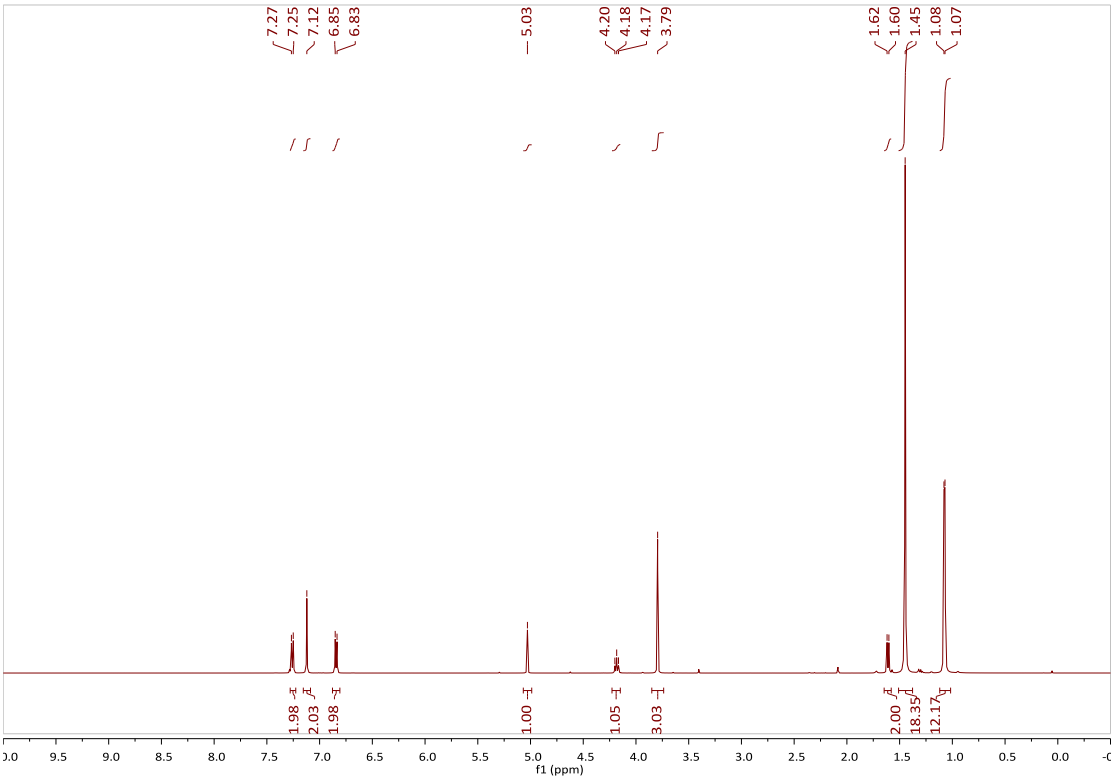
O
B
O
MeO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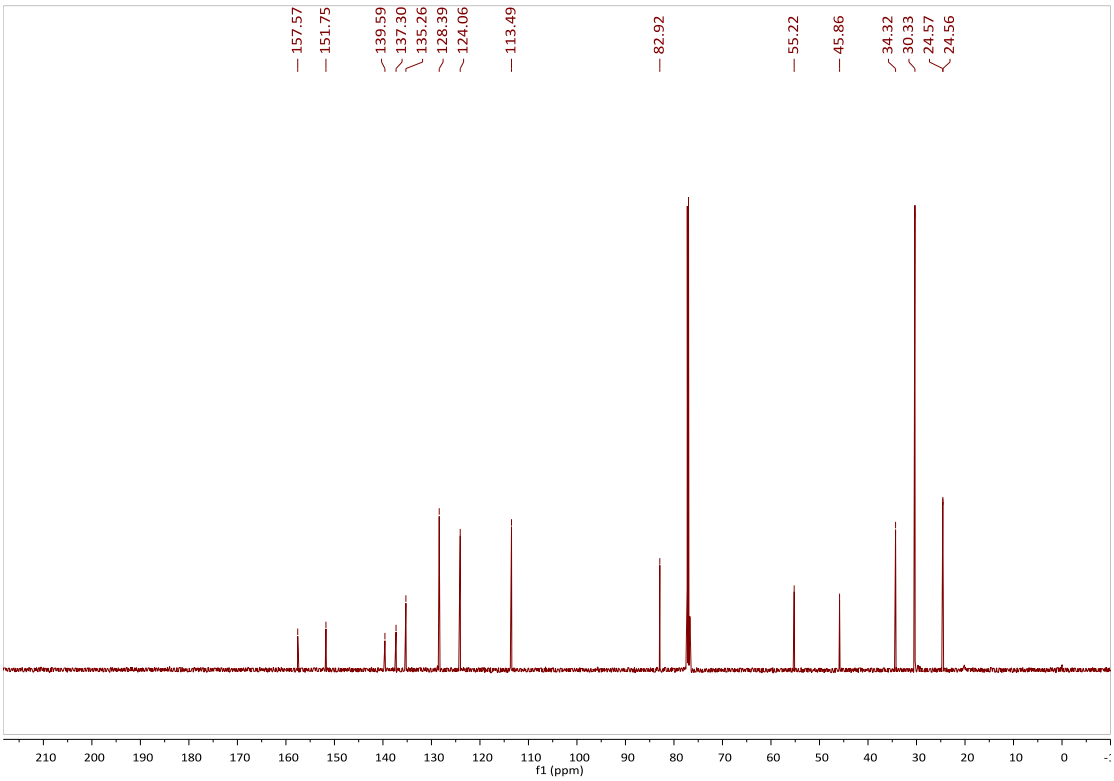
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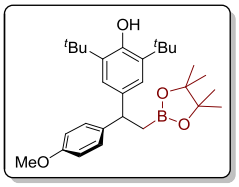
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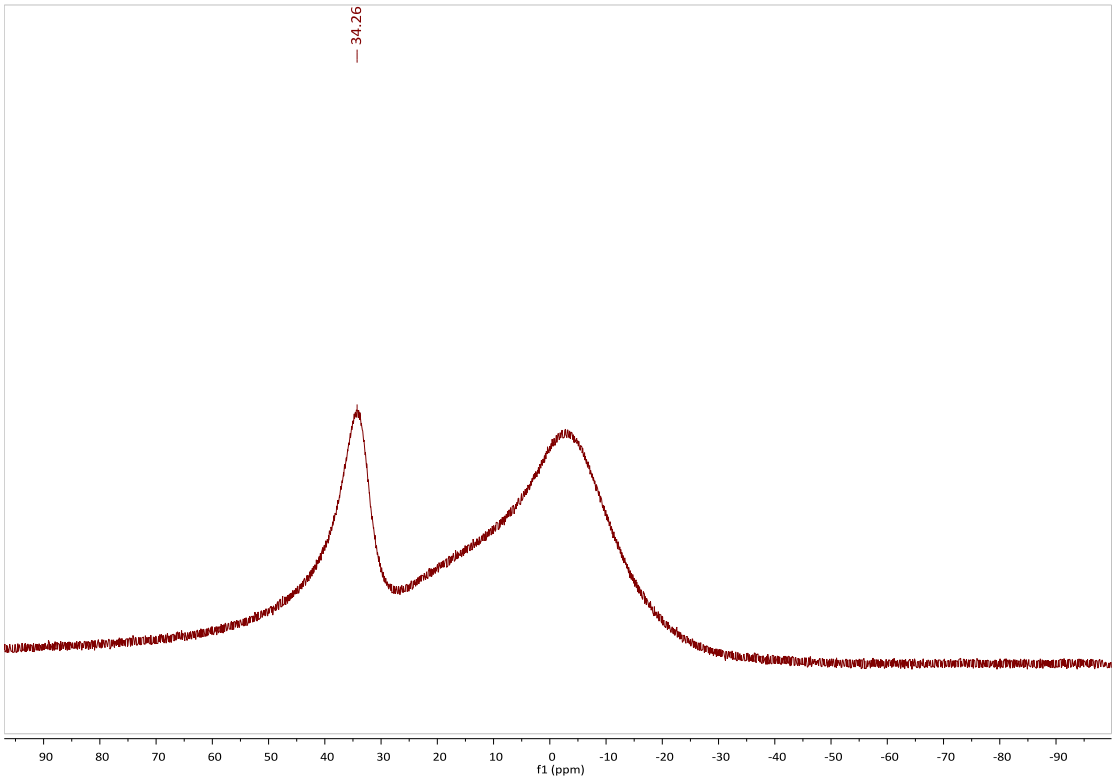
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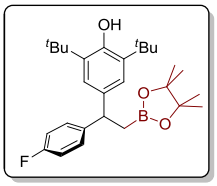
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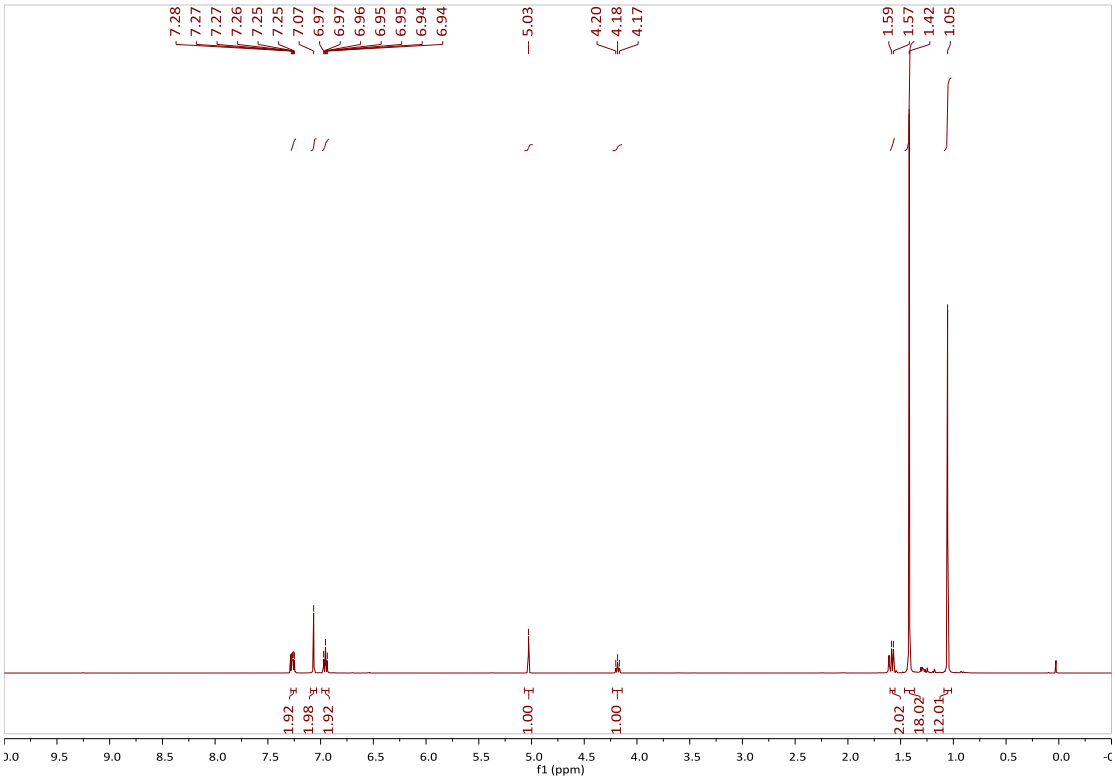
O
F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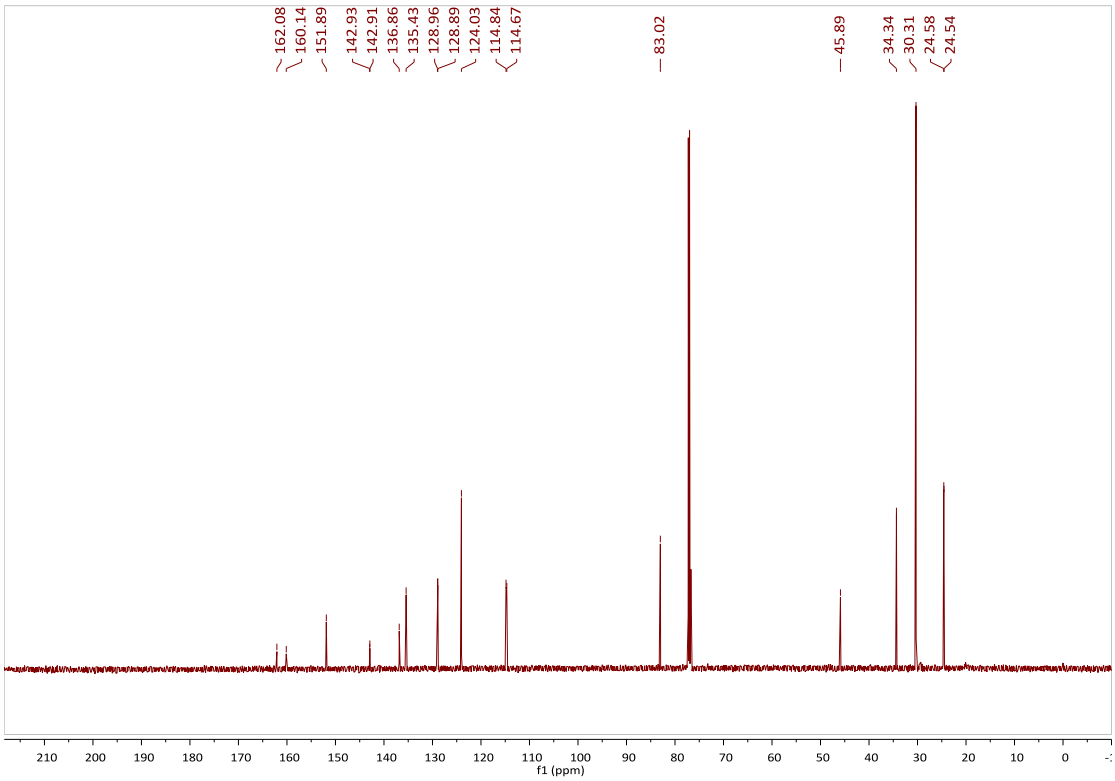
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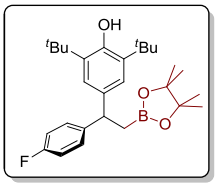
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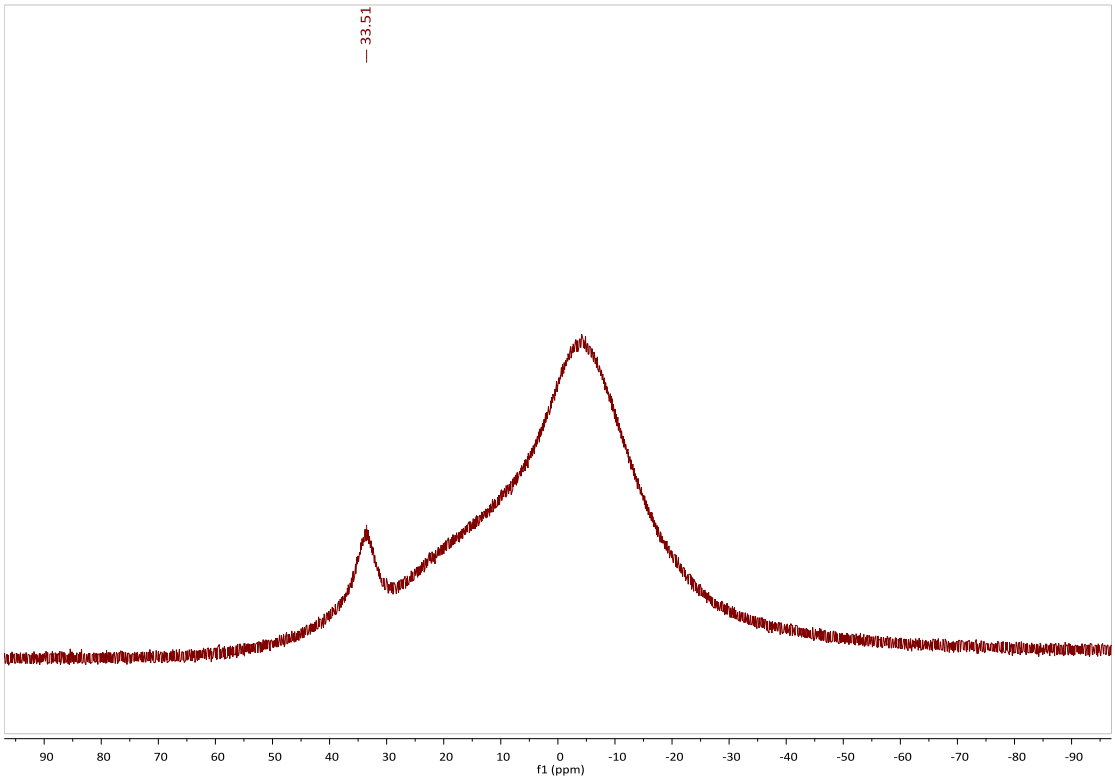
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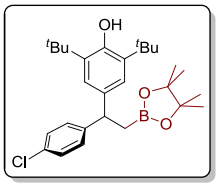
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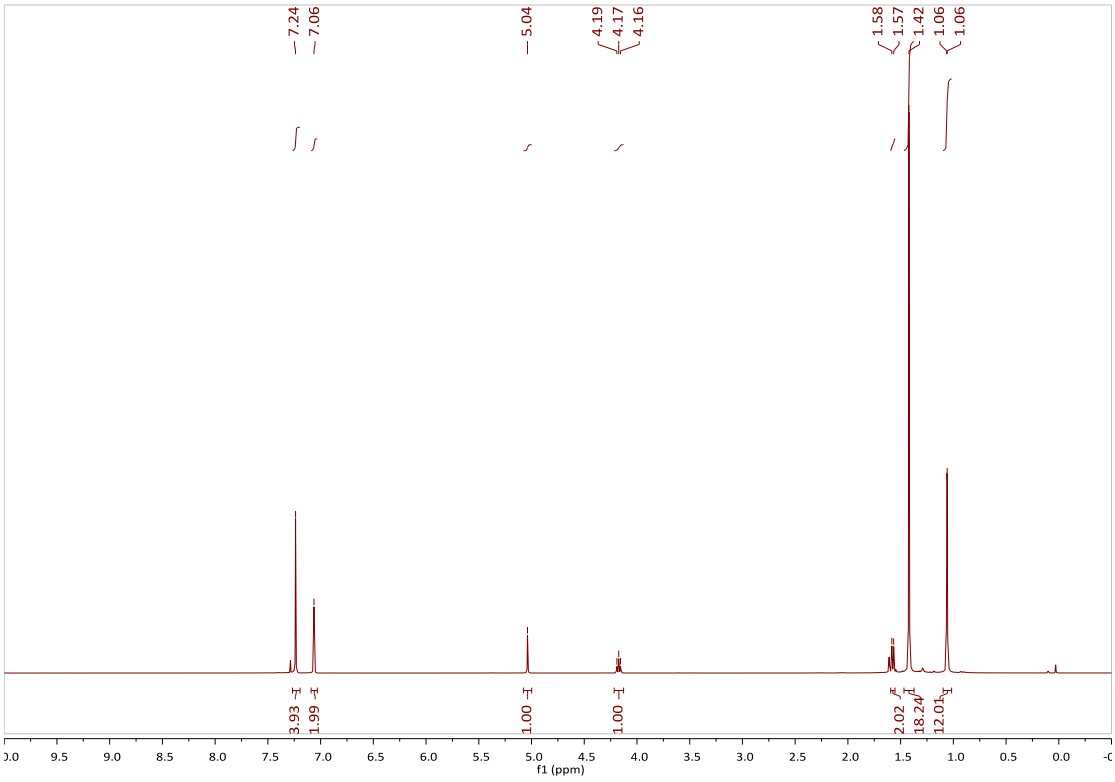
B
O
Cl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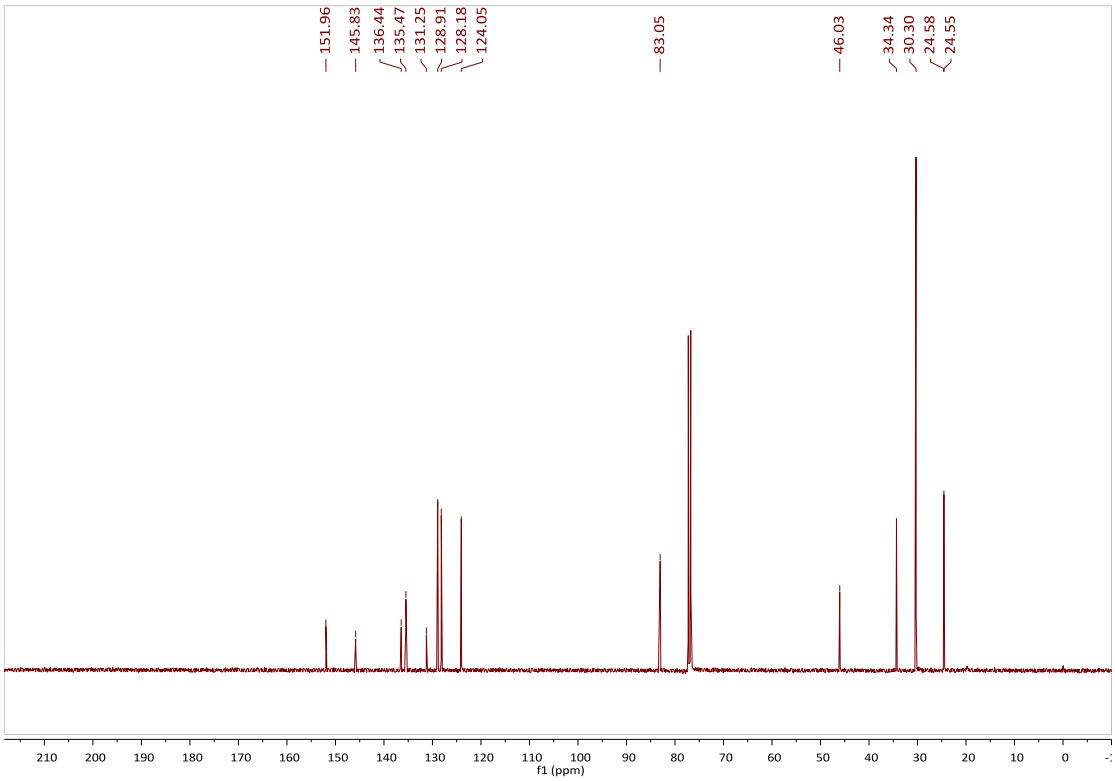
f1 (ppm)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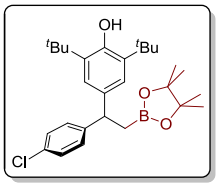
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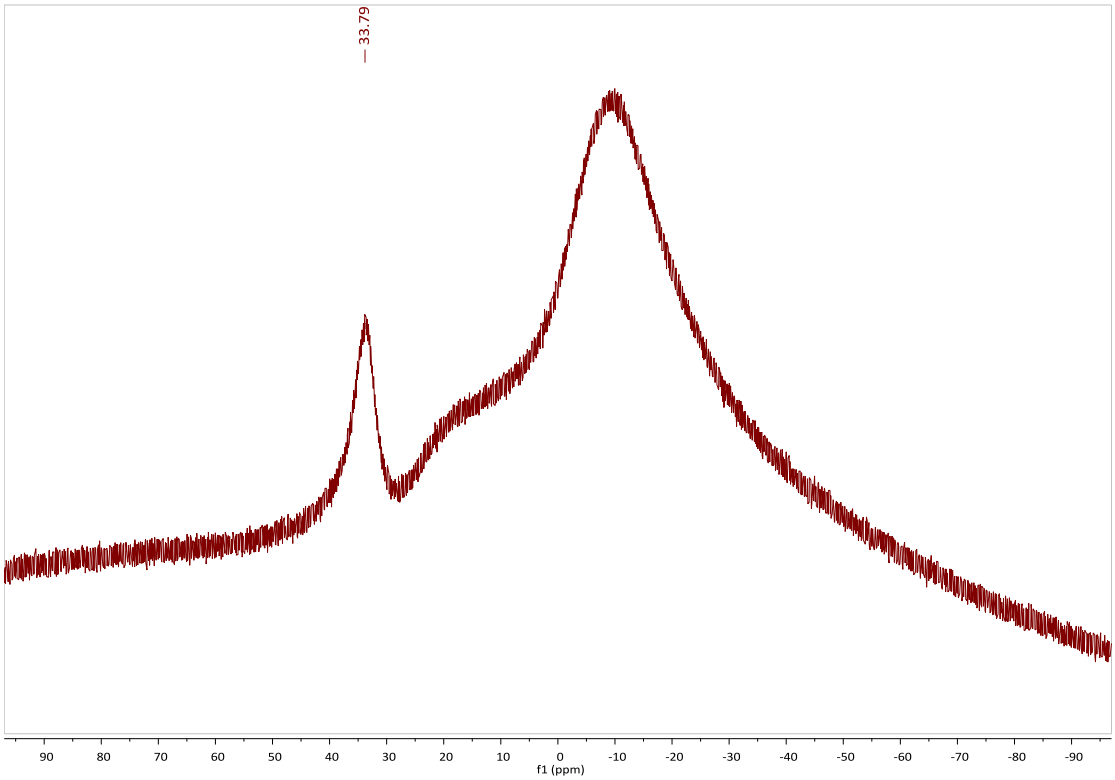
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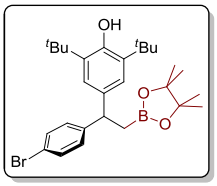
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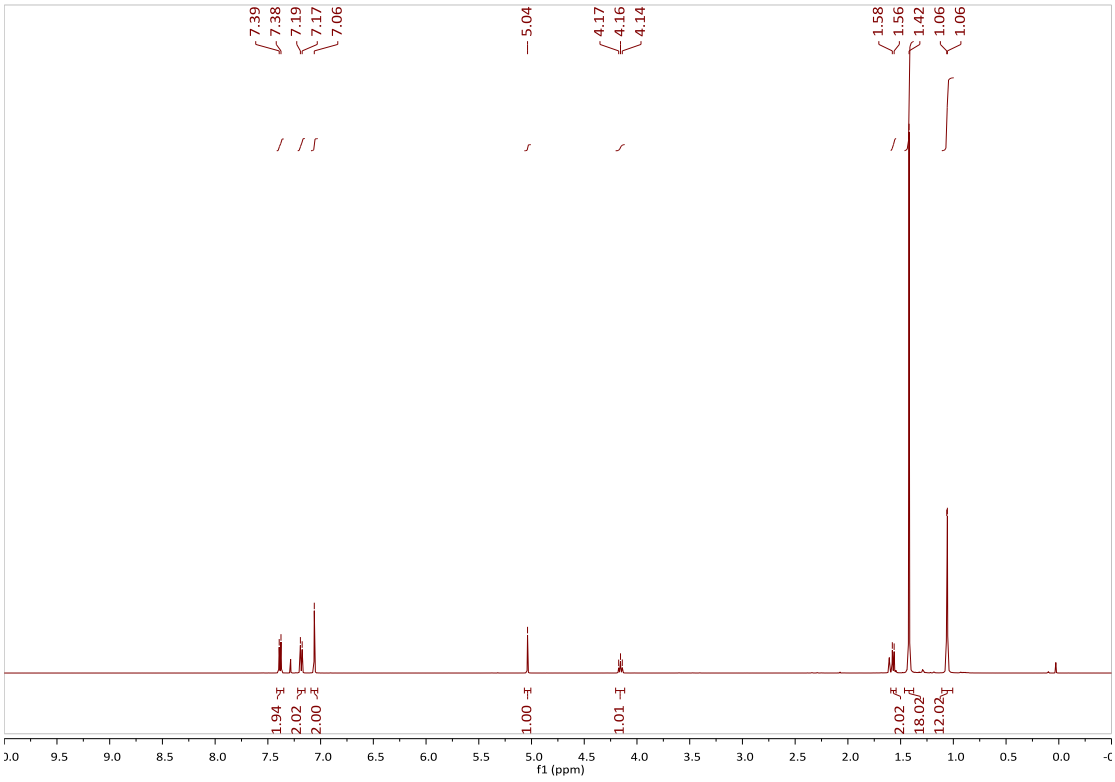
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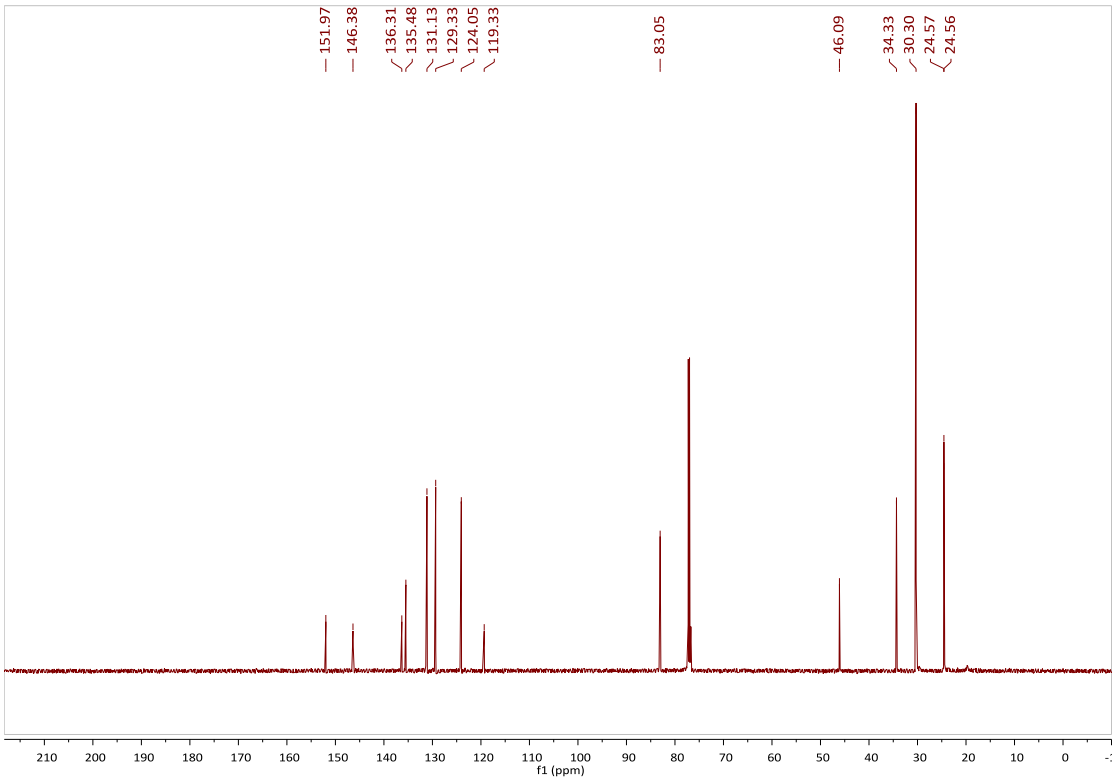
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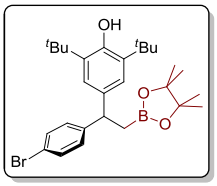
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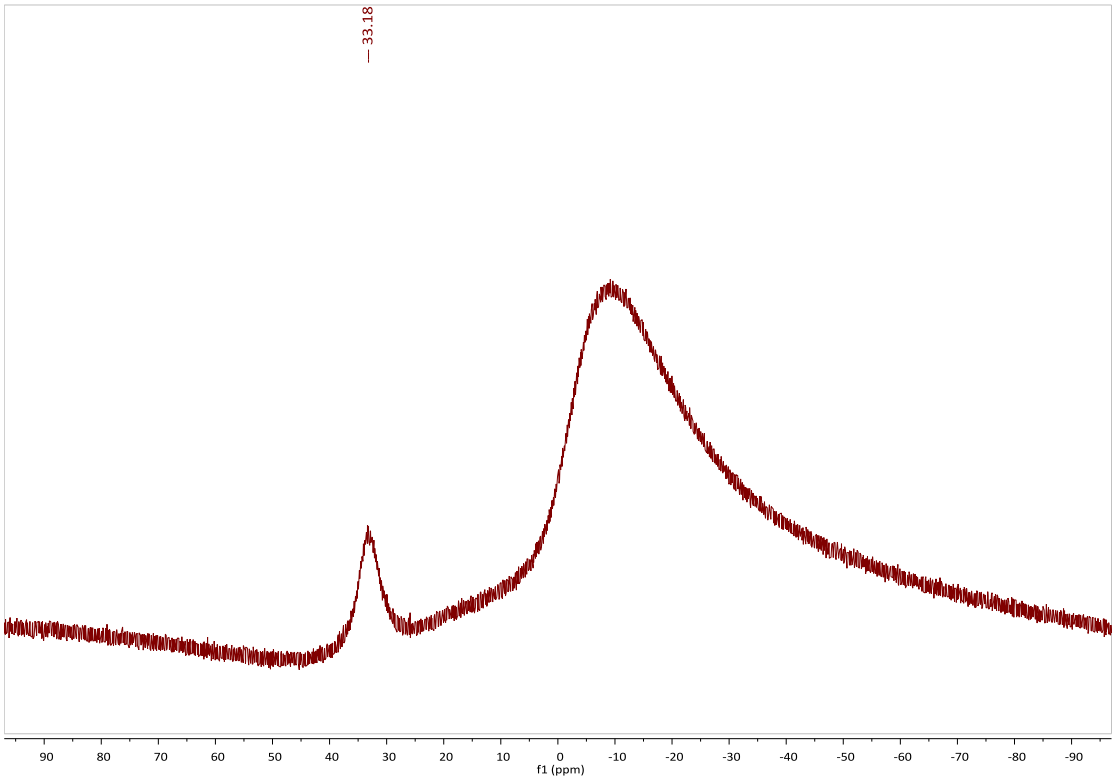
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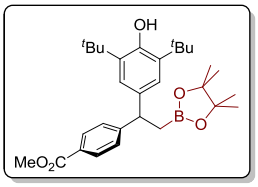
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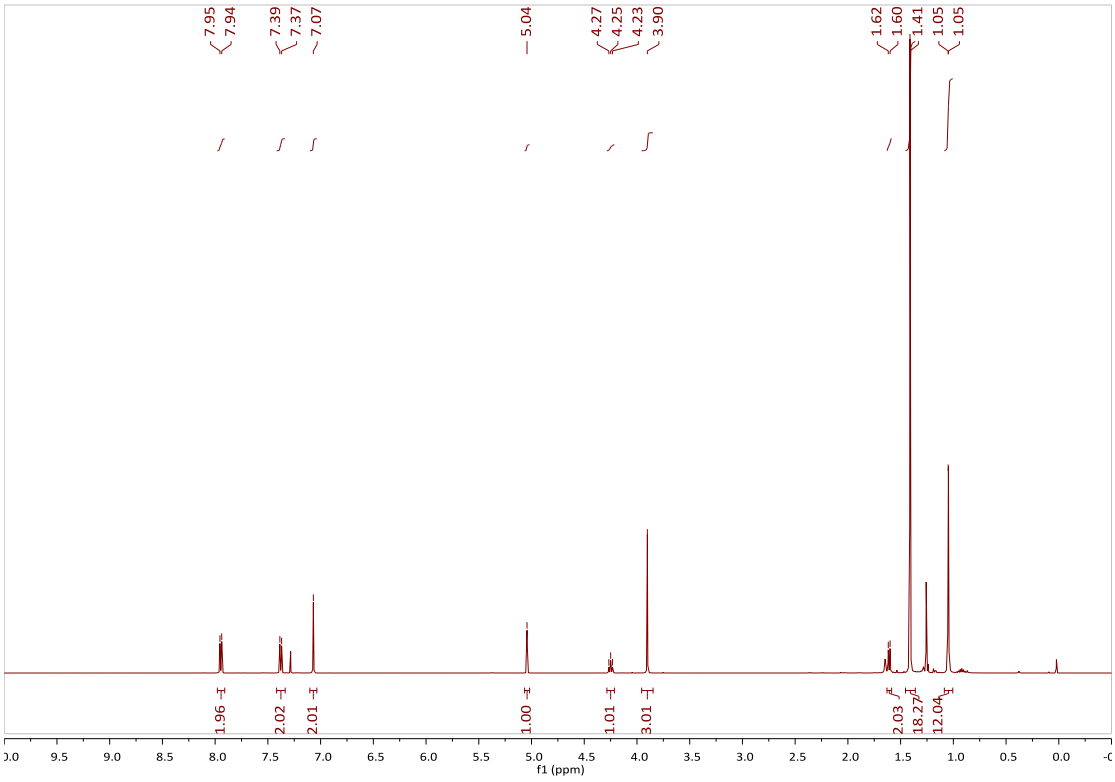
MeO2C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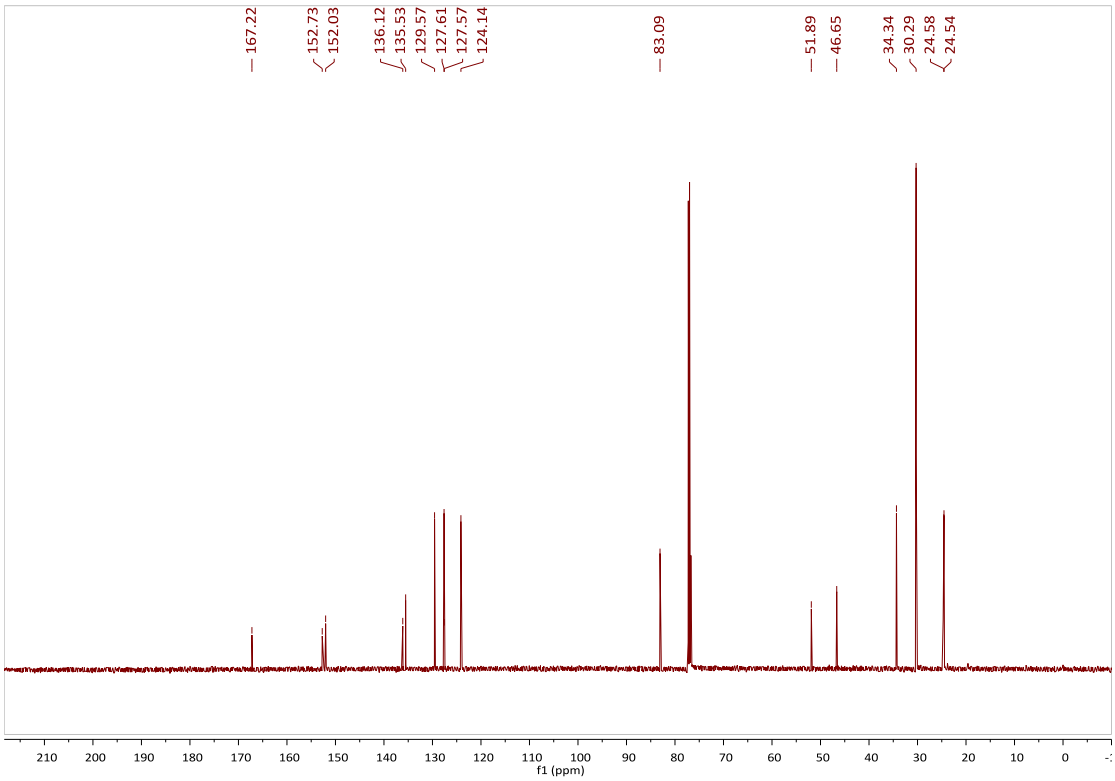
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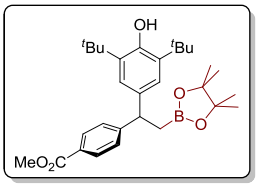
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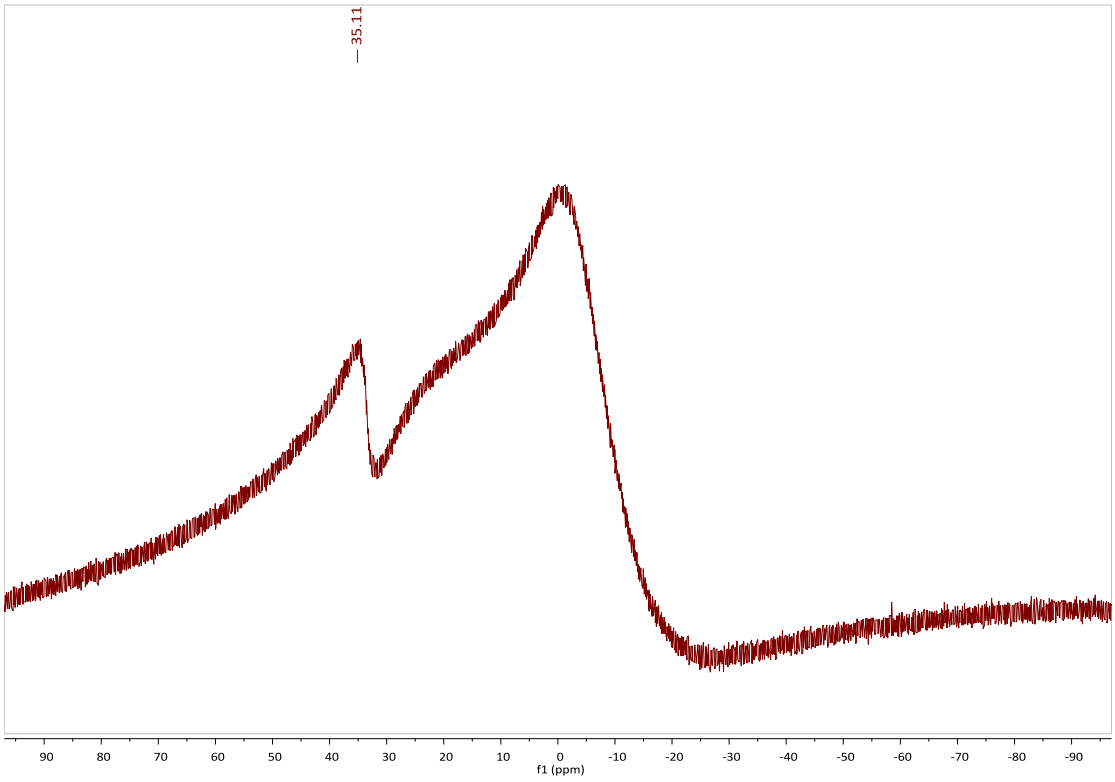
B
O
MeO2C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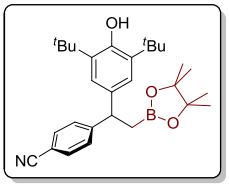
f1 (ppm)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B
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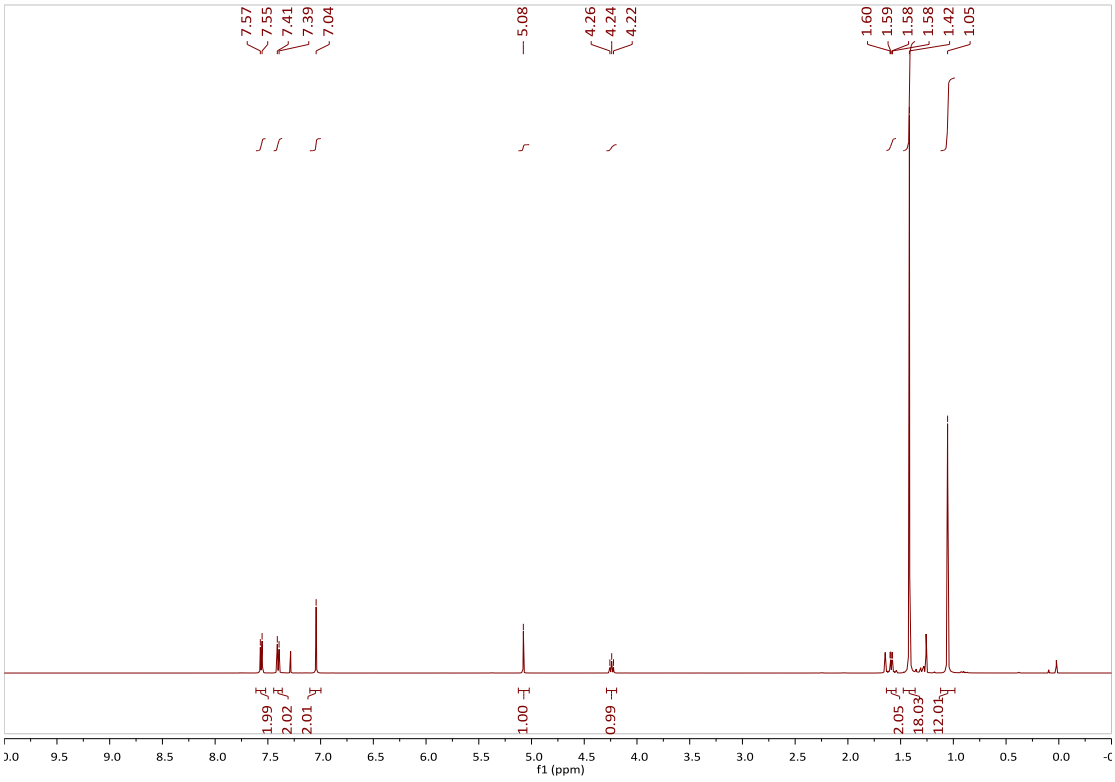
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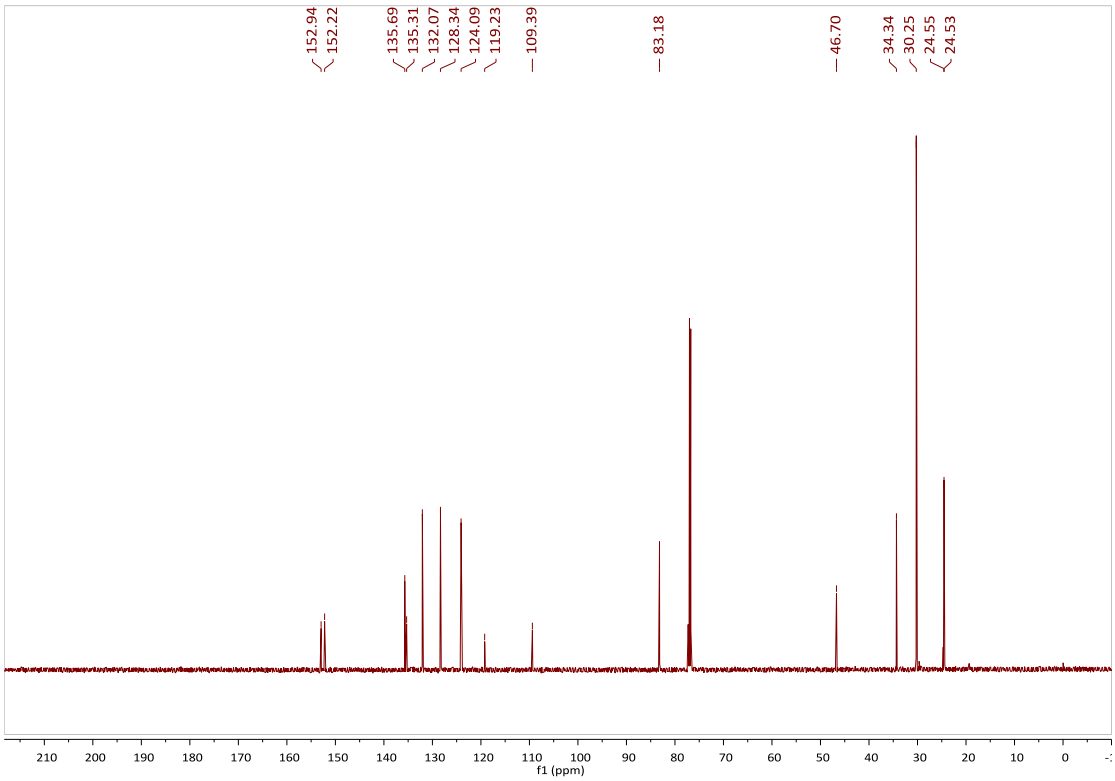
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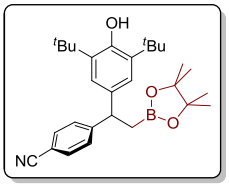
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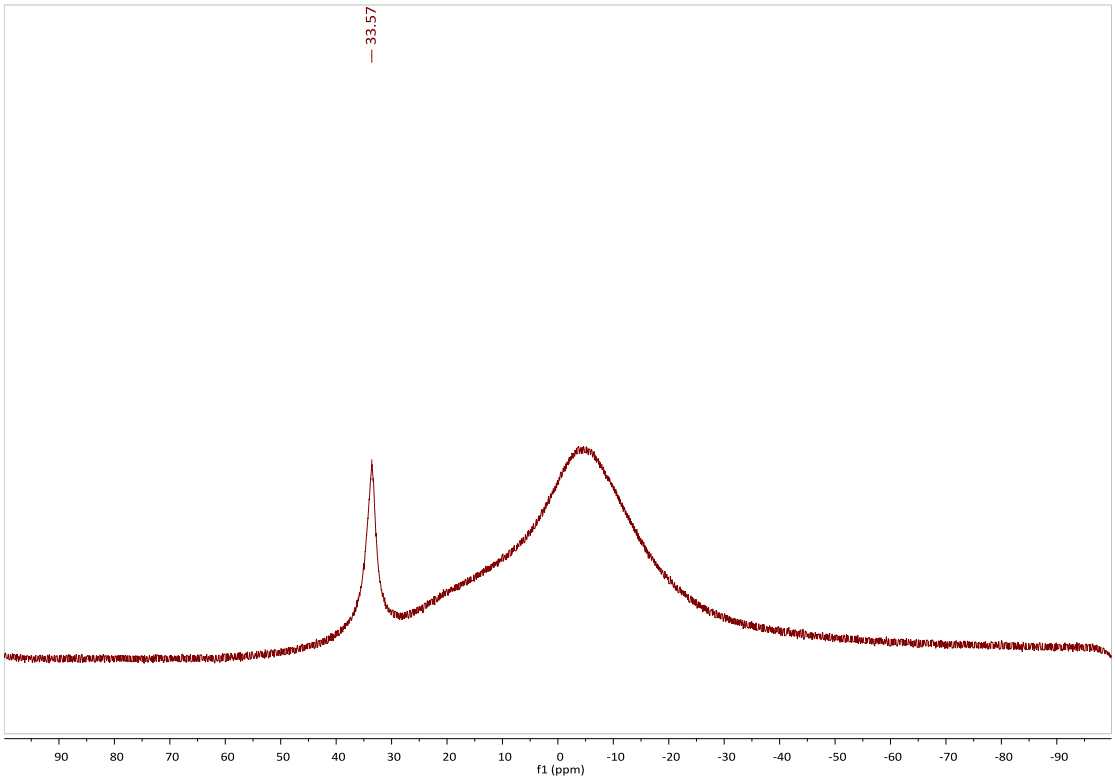
NC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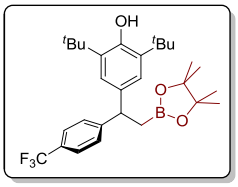
f1 (ppm)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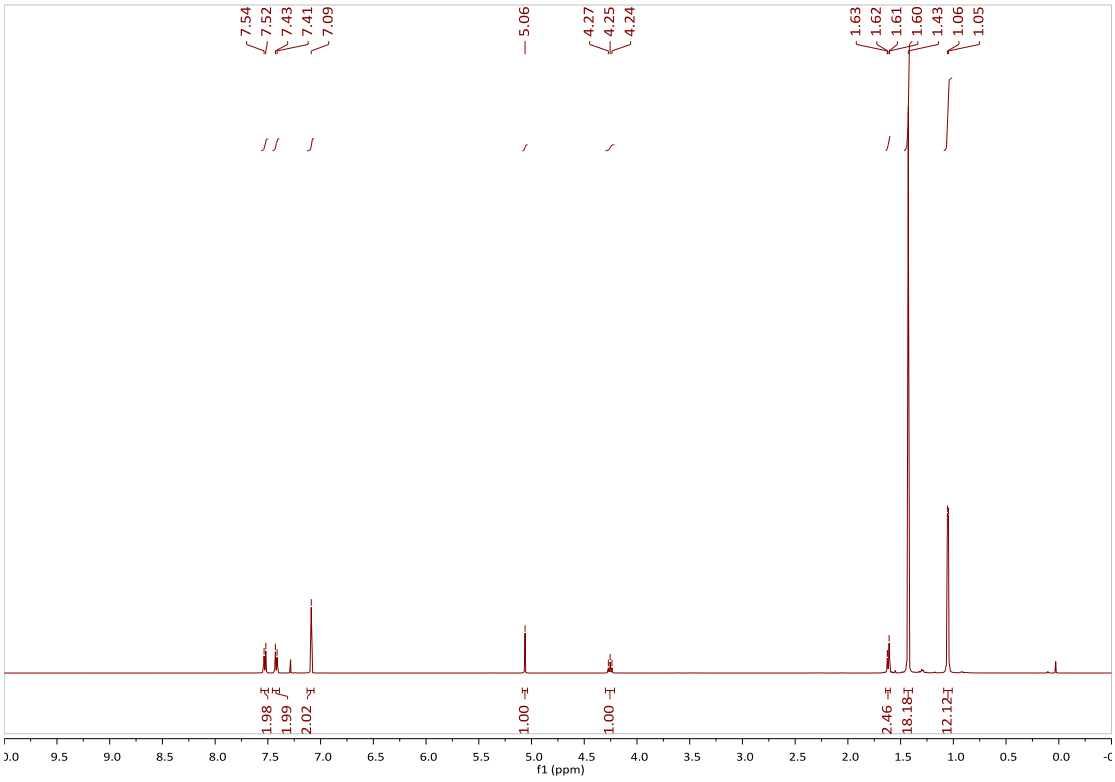
O
F3C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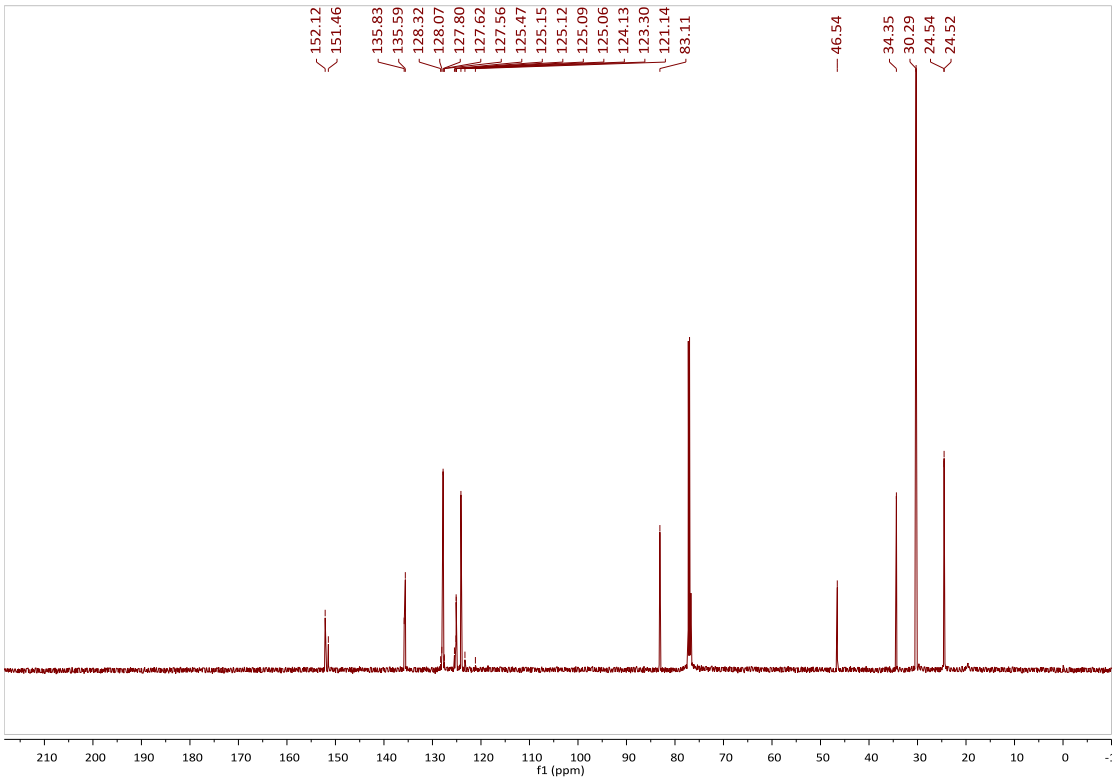
7.52
7.43
7.41
7.09
5.06
4.27
4.25
4.24
1.63
1.62
1.61
1.60
1.43
1.06
1.05
1.98
1.99
2.02
1.00
1.00
2.46
18.18
12.12
f1 (ppm)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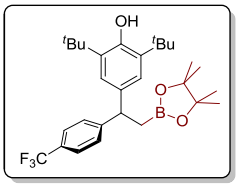
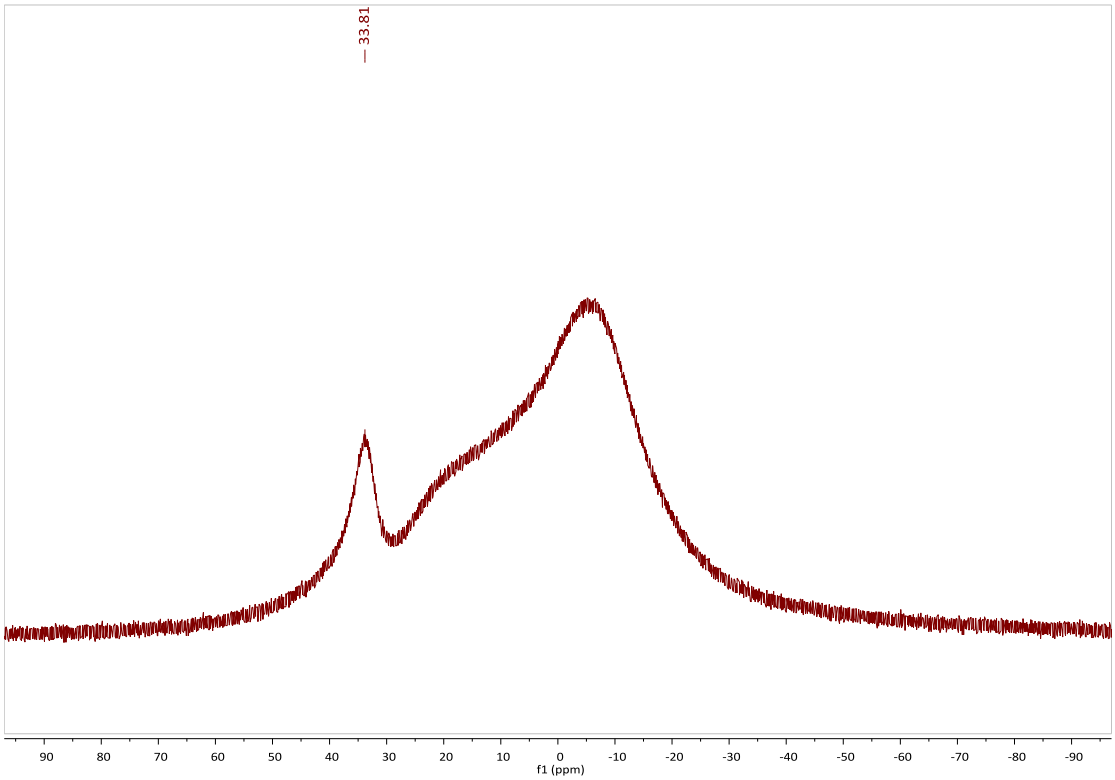
151.46
135.83
135.59
128.32
128.07
127.80
127.62
127.56
125.47
125.15
125.12
125.09
125.06
124.13
123.30
121.14
83.11
46.54
34.35
30.29
24.54
24.52
f1 (ppm)


OH
tBu
tBu
O
B
O
F3C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60
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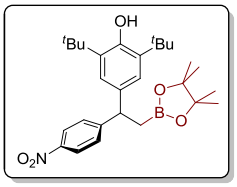
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)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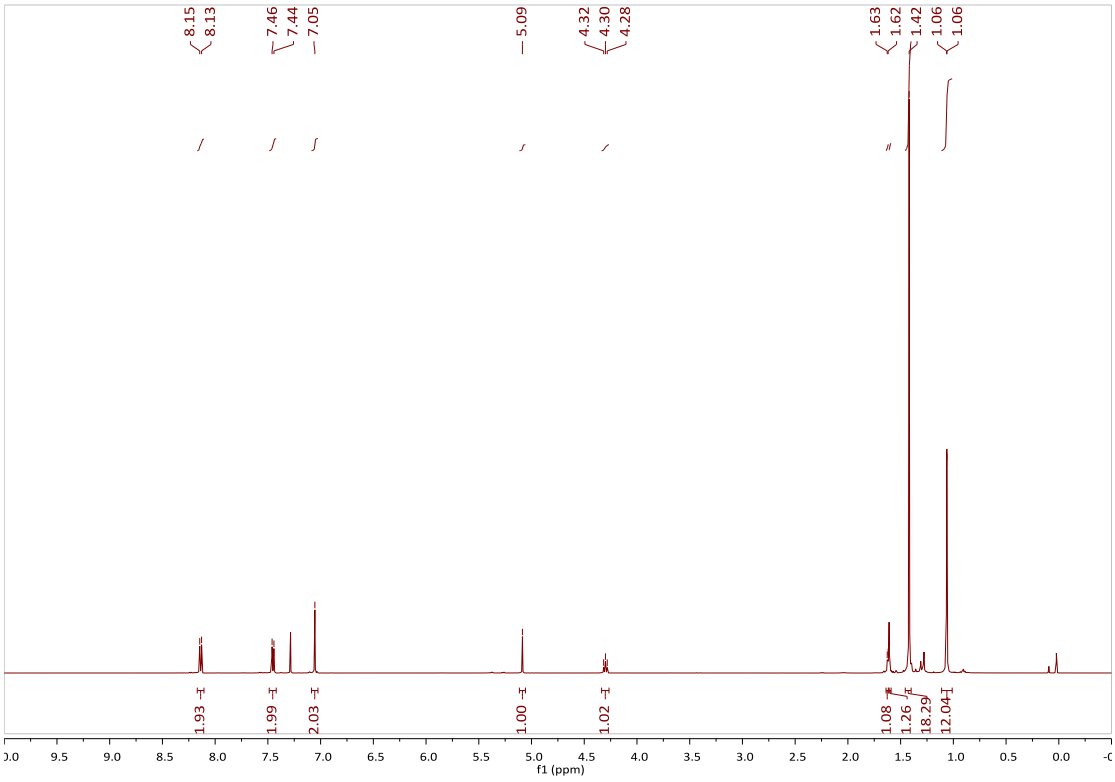
tBu
tBu
O
B
O
O2N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8.13
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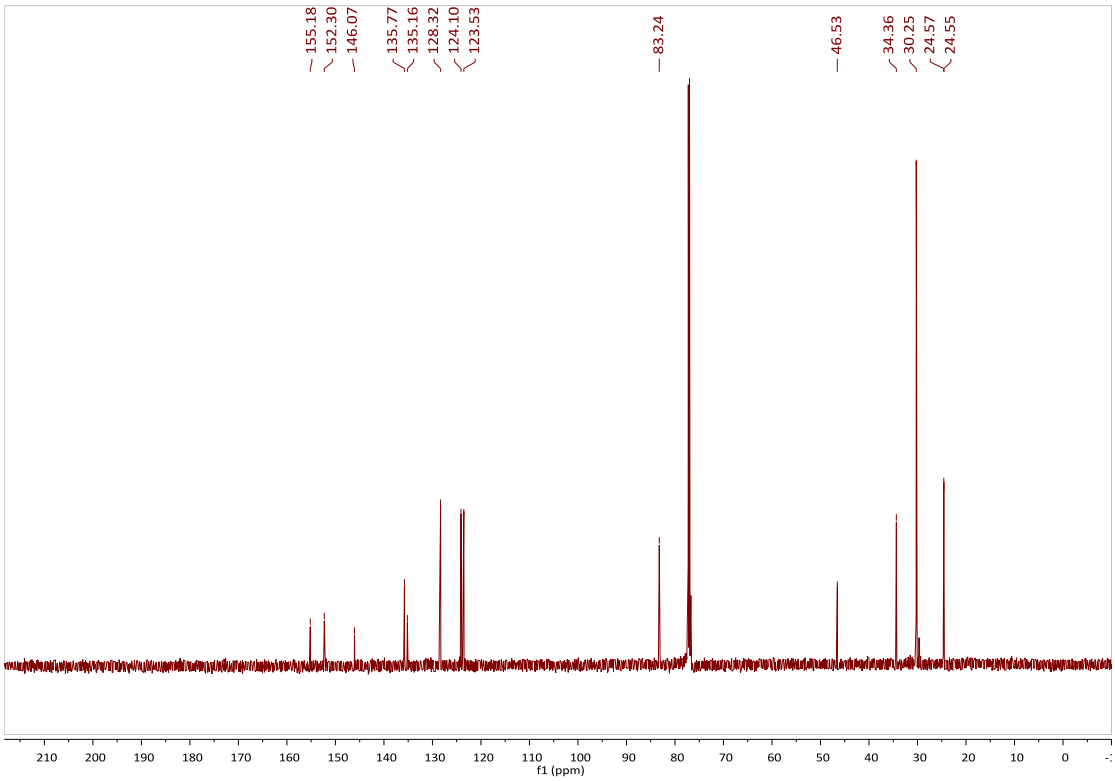
7.05
5.09
4.32
4.30
4.28
1.63
1.62
1.42
1.06
1.06
1.93
1.99
2.03
1.00
1.02
1.08
1.26
18.29
12.04
f1 (ppm)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152.30
146.07
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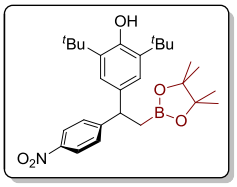
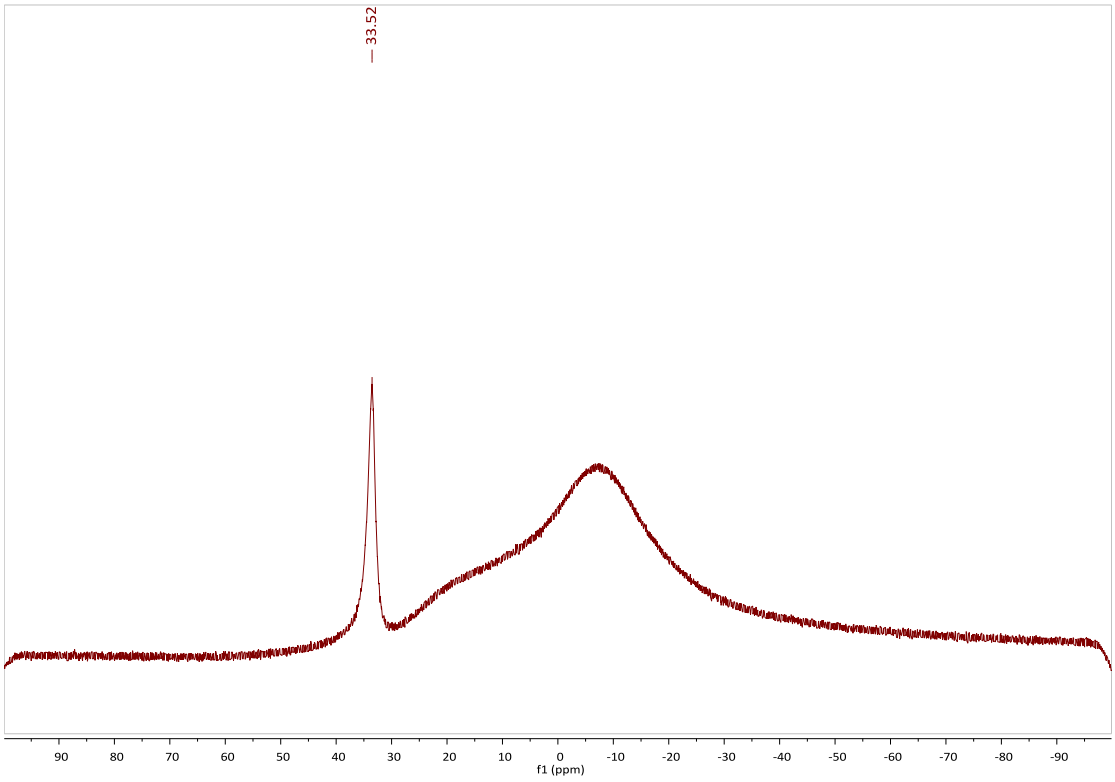
135.16
128.32
124.10
123.53
83.24
46.53
34.36
30.25
24.57
24.55
f1 (ppm)


OH
tBu
tBu
O
B
O
O2N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90
80
70
60
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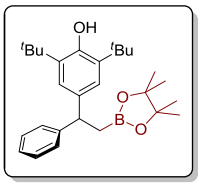
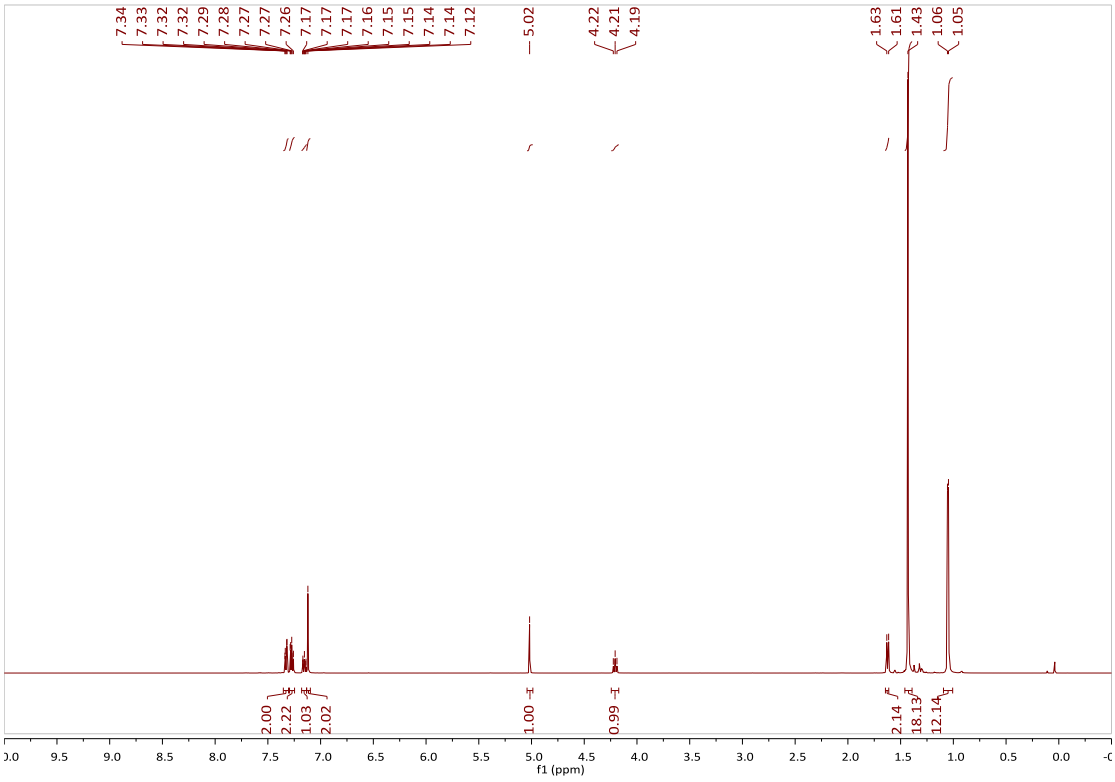
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O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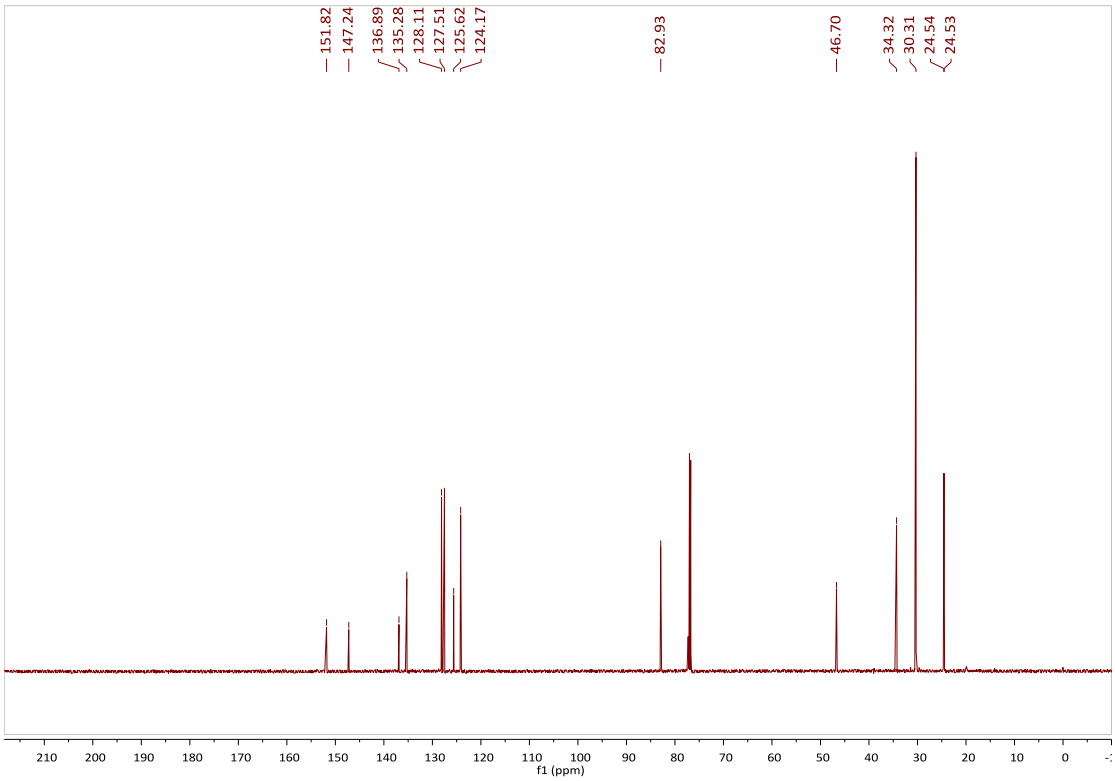
7.33
7.32
7.32
7.29
7.28
7.27
7.27
7.26
7.17
7.17
7.17
7.16
7.15
7.15
7.14
7.14
7.12
5.02
4.22
4.21
4.19
1.63
1.61
1.43
1.06
1.05
2.00
2.22
1.03
2.02
1.00
0.99
2.14
18.13
12.14
f1 (ppm)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147.24
136.89
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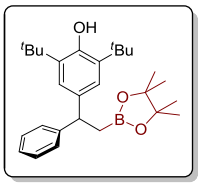
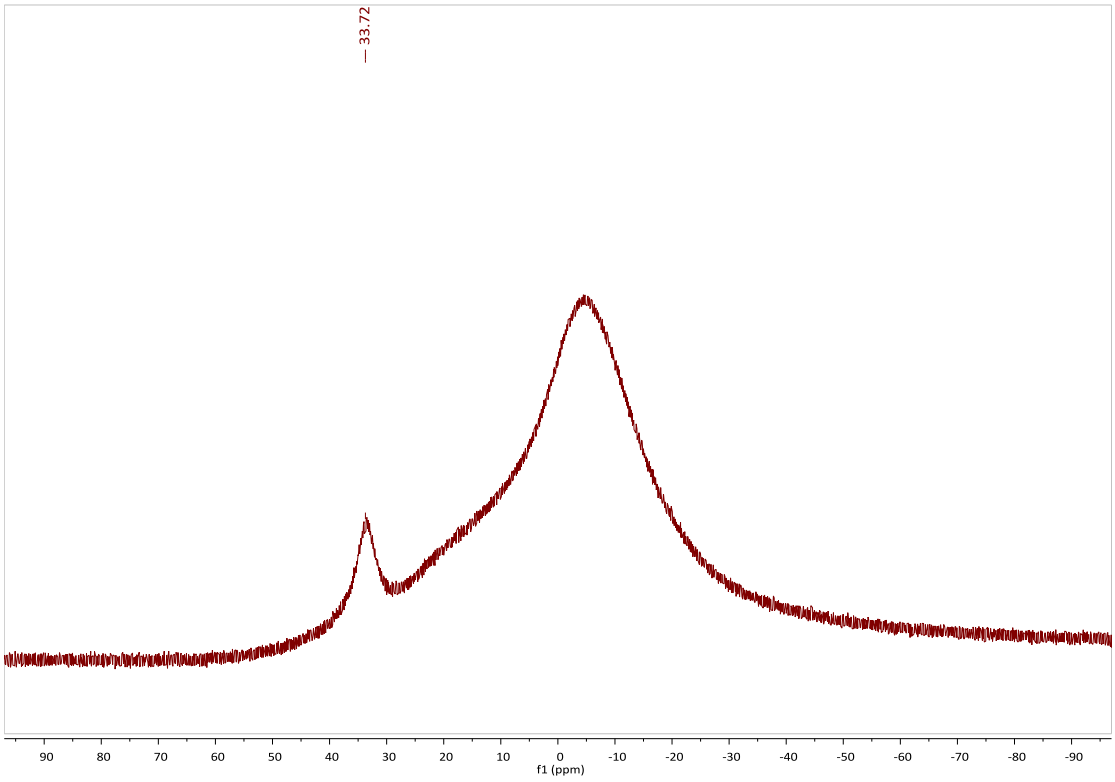
125.62
124.17
82.93
46.70
34.32
30.31
24.54
24.53
f1 (ppm)


OH
tBu
tBu
O
B
O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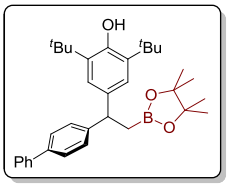
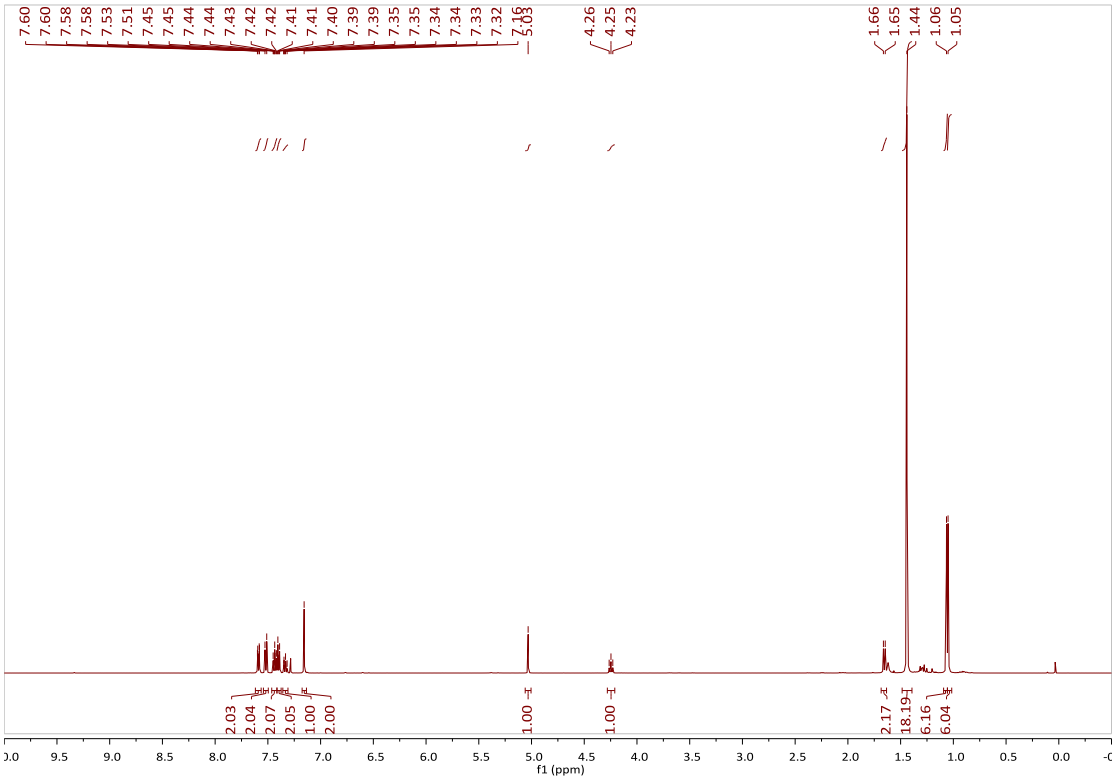
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
Ph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7.60
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7.58
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7.51
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7.45
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7.44
7.43
7.42
7.42
7.41
7.41
7.40
7.39
7.39
7.35
7.35
7.34
7.34
7.33
7.32
7.16
5.03
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4.25
4.23
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1.06
1.05
2.03
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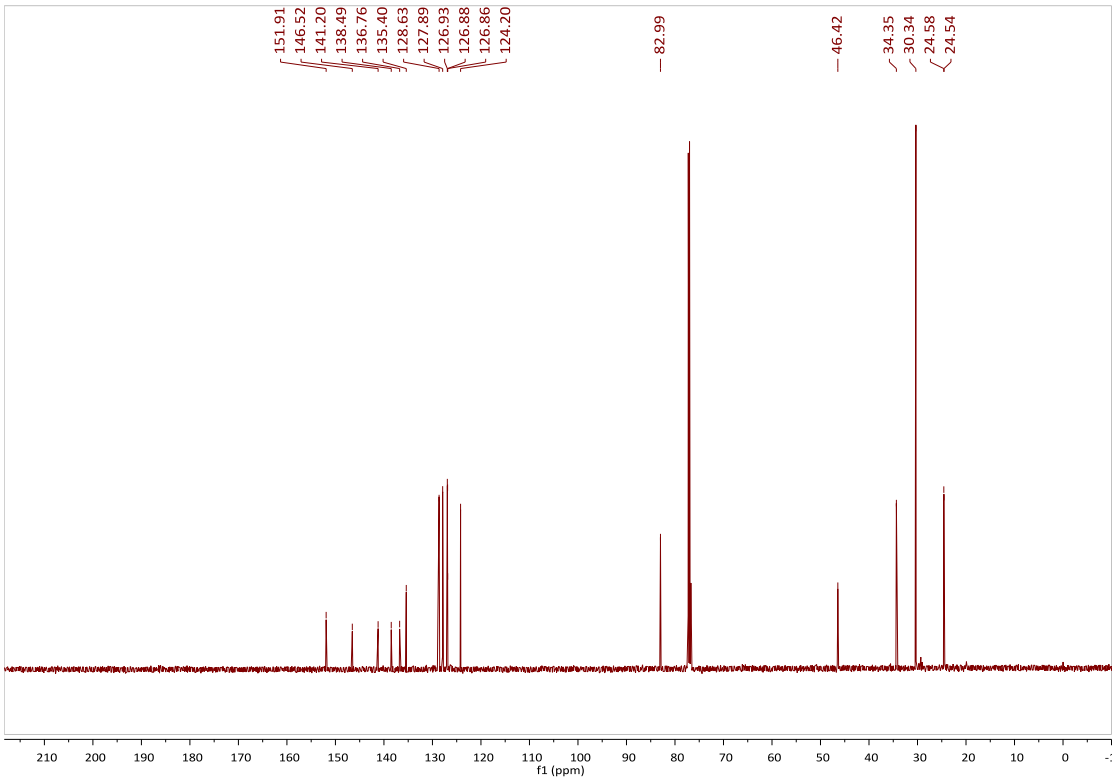
2.17
18.19
6.16
6.04
f1 (ppm)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135.40
128.63
127.89
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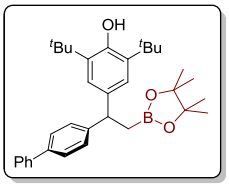
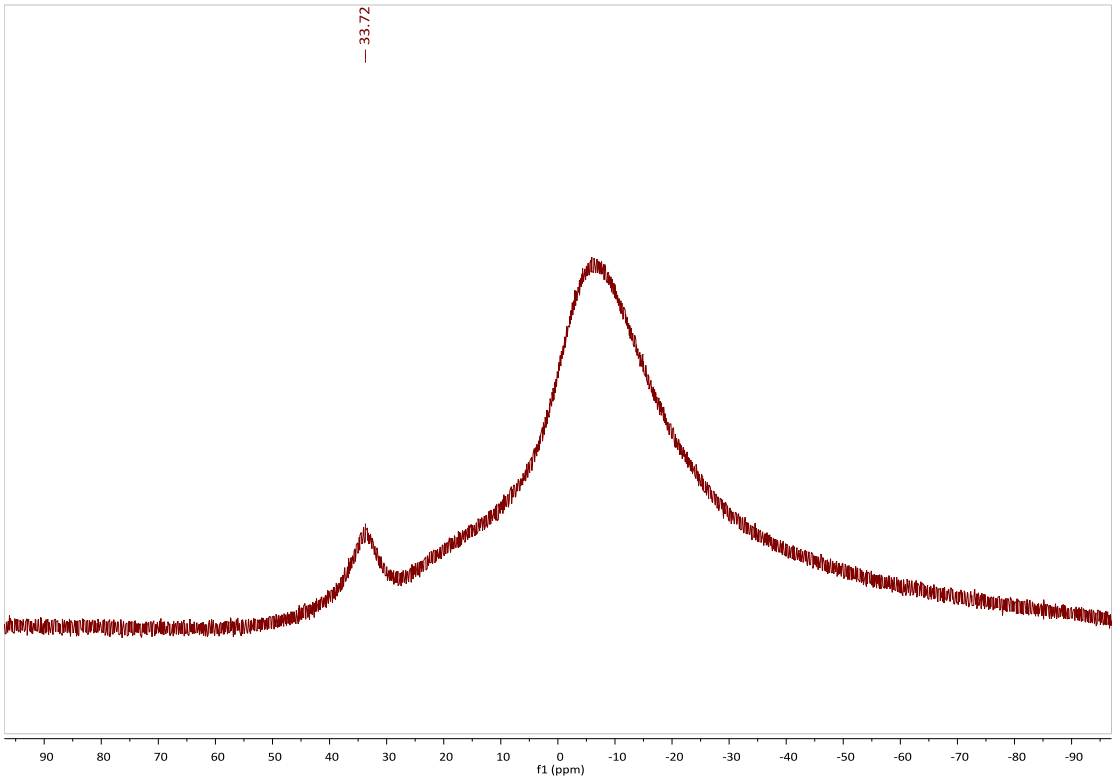
126.86
124.20
82.99
46.42
34.35
30.34
24.58
24.54
f1 (ppm)


OH
tBu
tBu
O
B
O
Ph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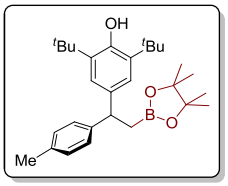
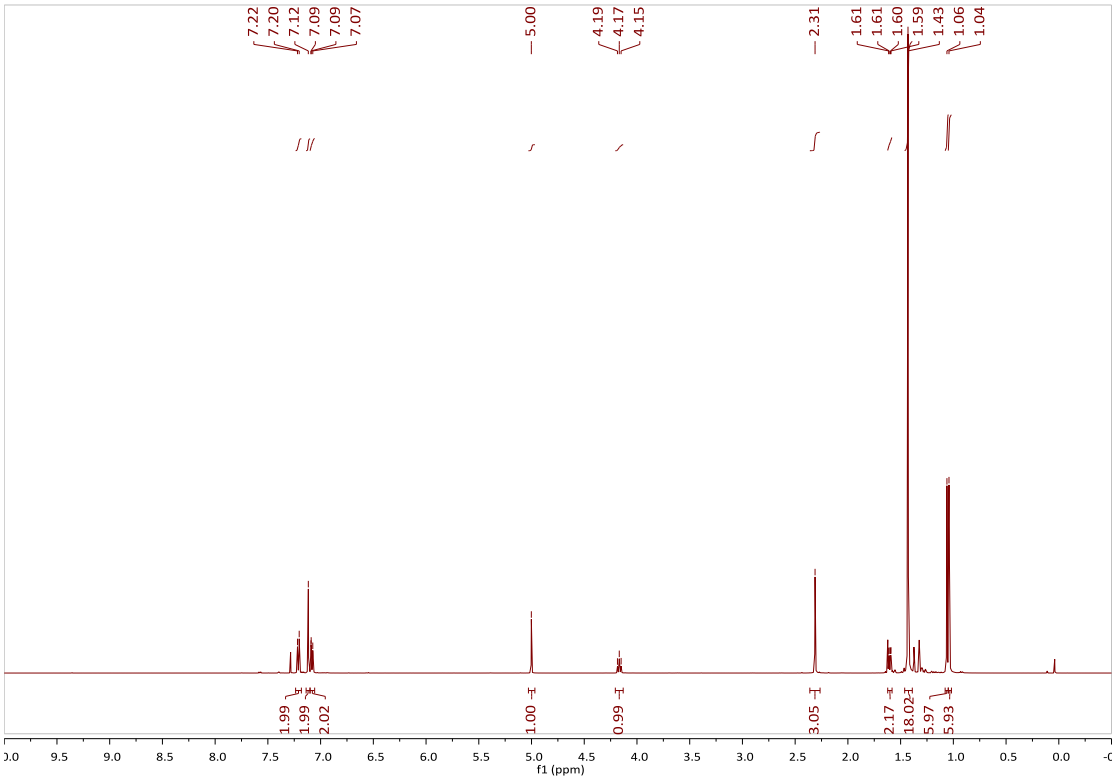
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
Me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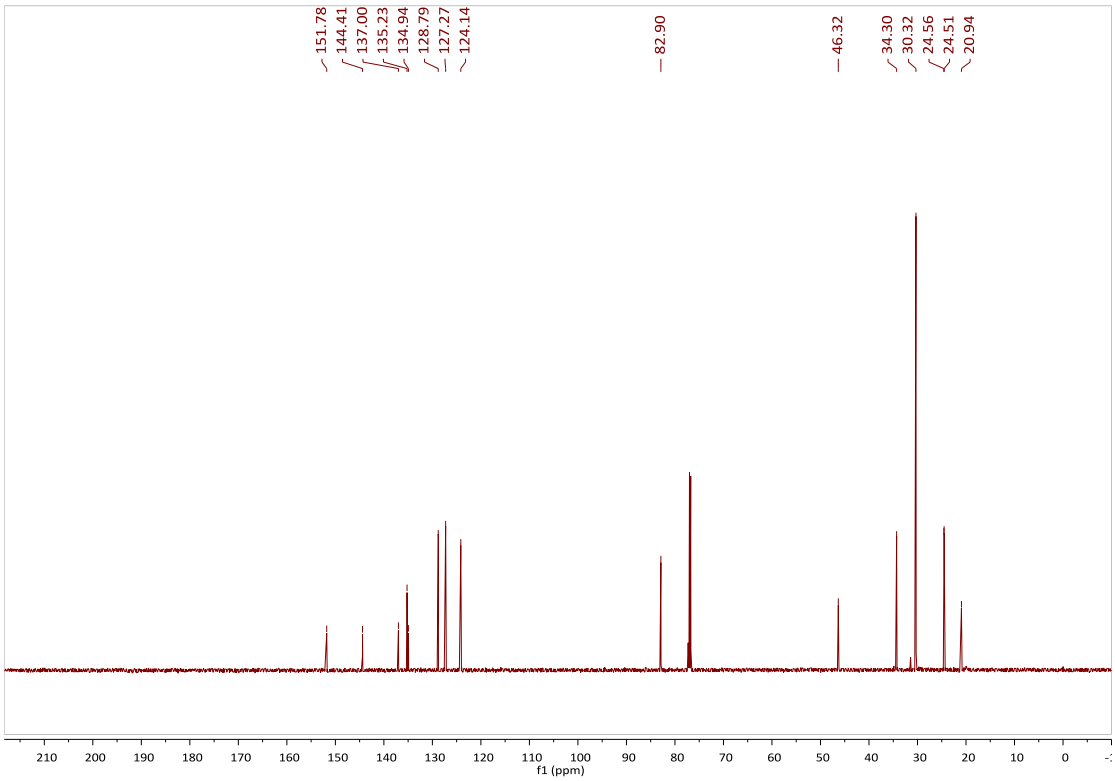
7.20
7.12
7.09
7.09
7.07
5.00
4.19
4.17
4.15
2.31
1.61
1.61
1.60
1.59
1.43
1.06
1.04
1.99
1.99
2.02
1.00
0.99
3.05
2.17
18.02
5.97
5.93
f1 (ppm)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128.79
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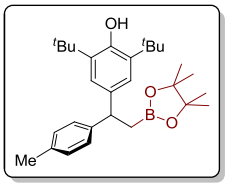
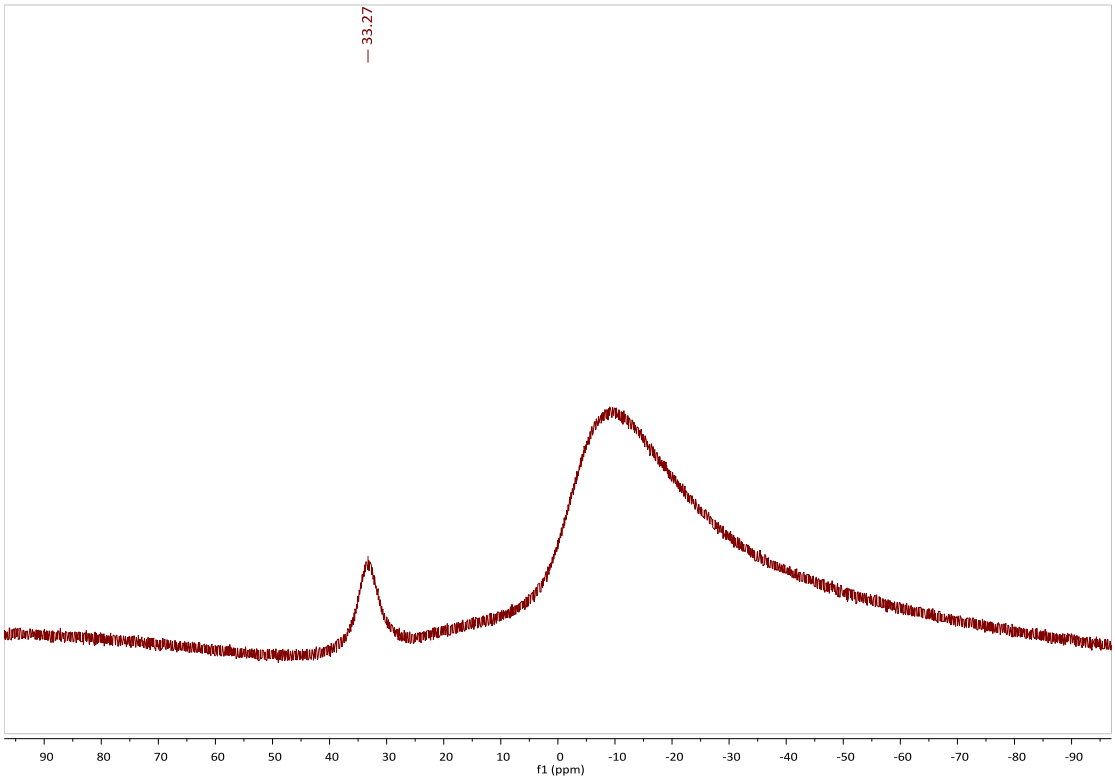
124.14
82.90
46.32
34.30
30.32
24.56
24.51
20.94
f1 (ppm)


OH
tBu
tBu
O
B
O
Me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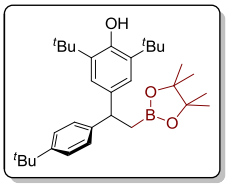
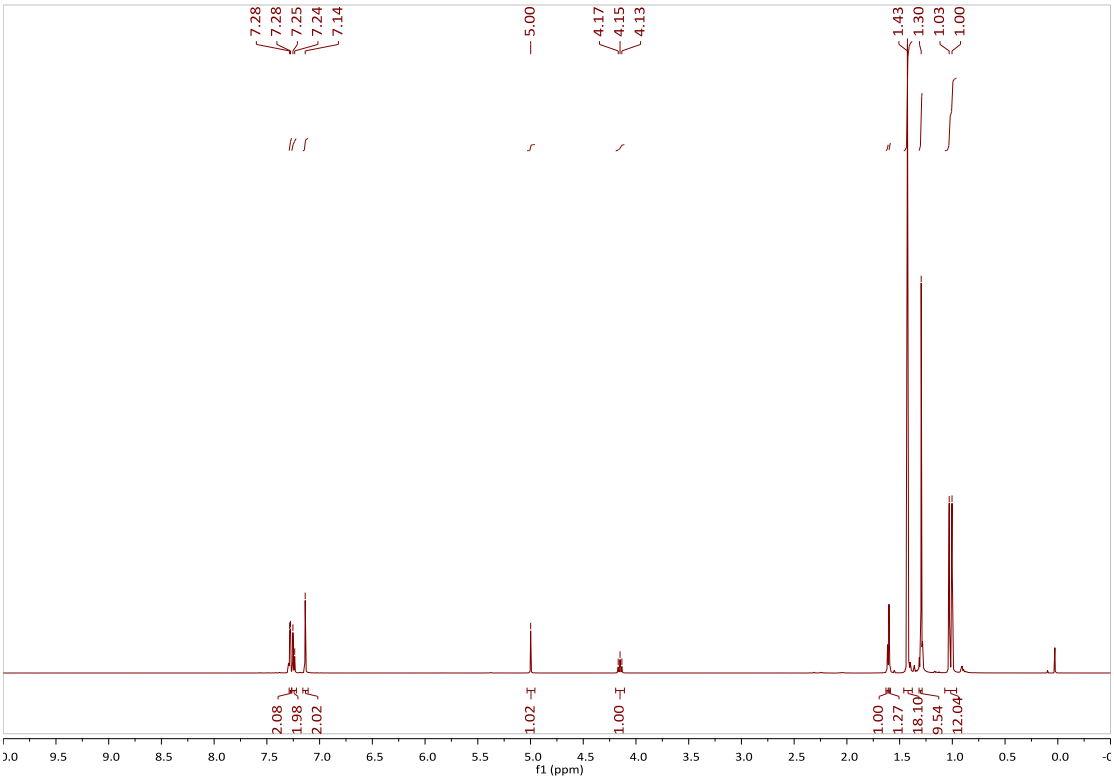
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
tBu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7.28
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7.24
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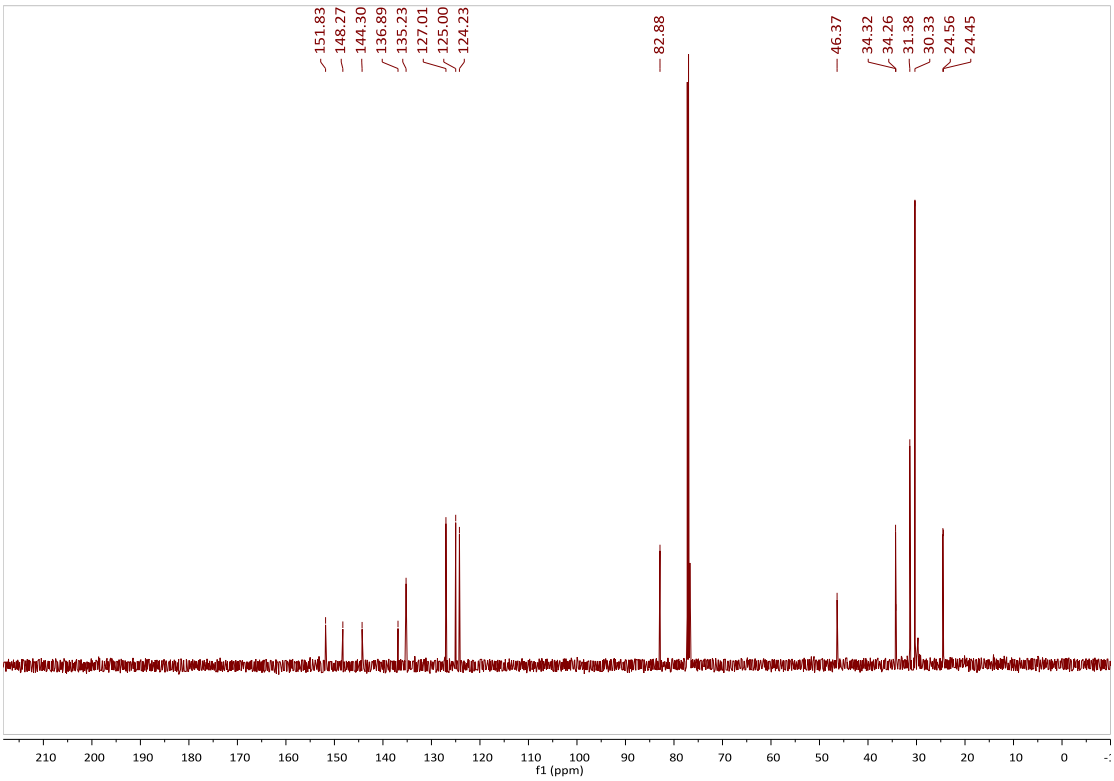
4.17
4.15
4.13
1.43
1.30
1.03
1.00
2.08
1.98
2.02
1.02
1.00
1.00
1.27
18.10
9.54
12.04
f1 (ppm)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136.89
135.23
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125.00
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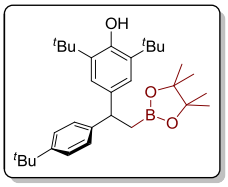
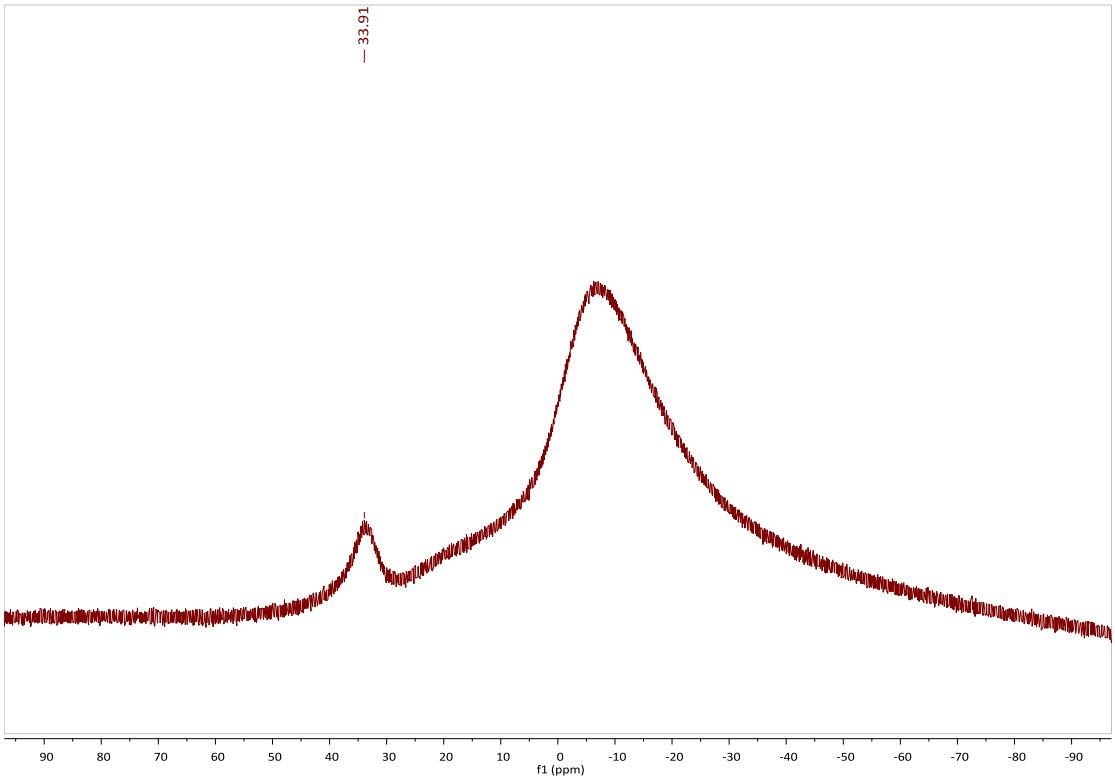
82.88
46.37
34.32
34.26
31.38
30.33
24.56
24.45
f1 (ppm)


OH
tBu
tBu
O
B
O
tBu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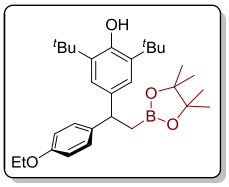
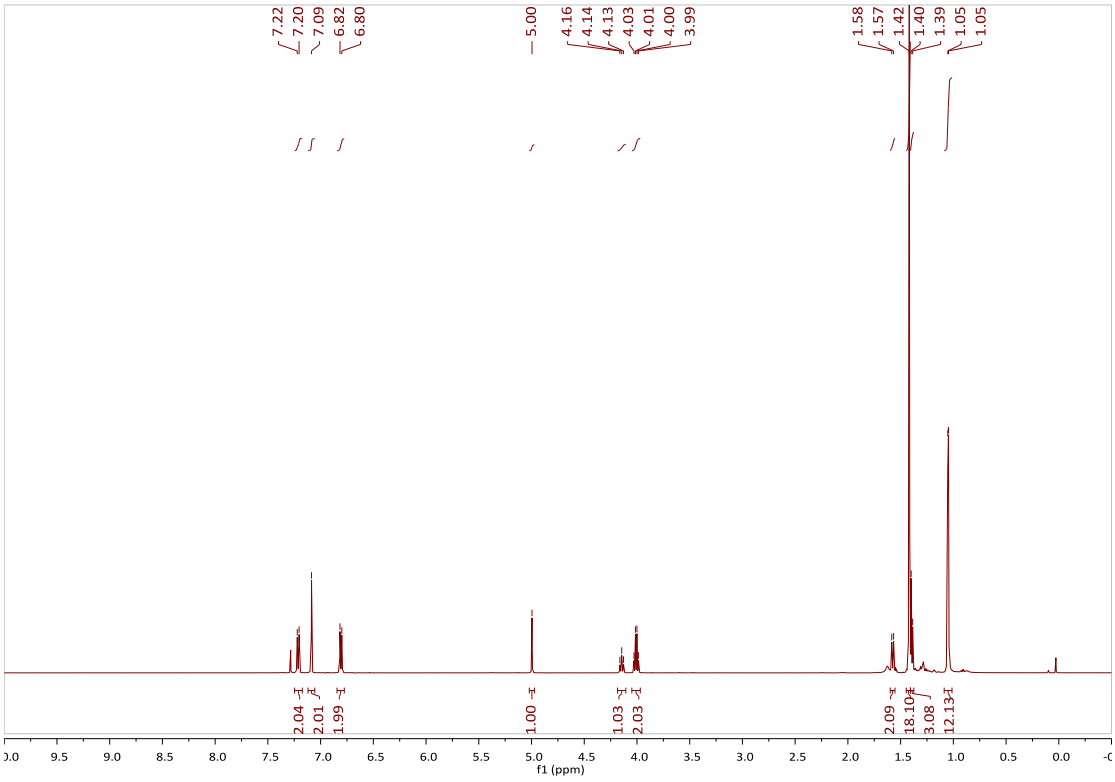
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
EtO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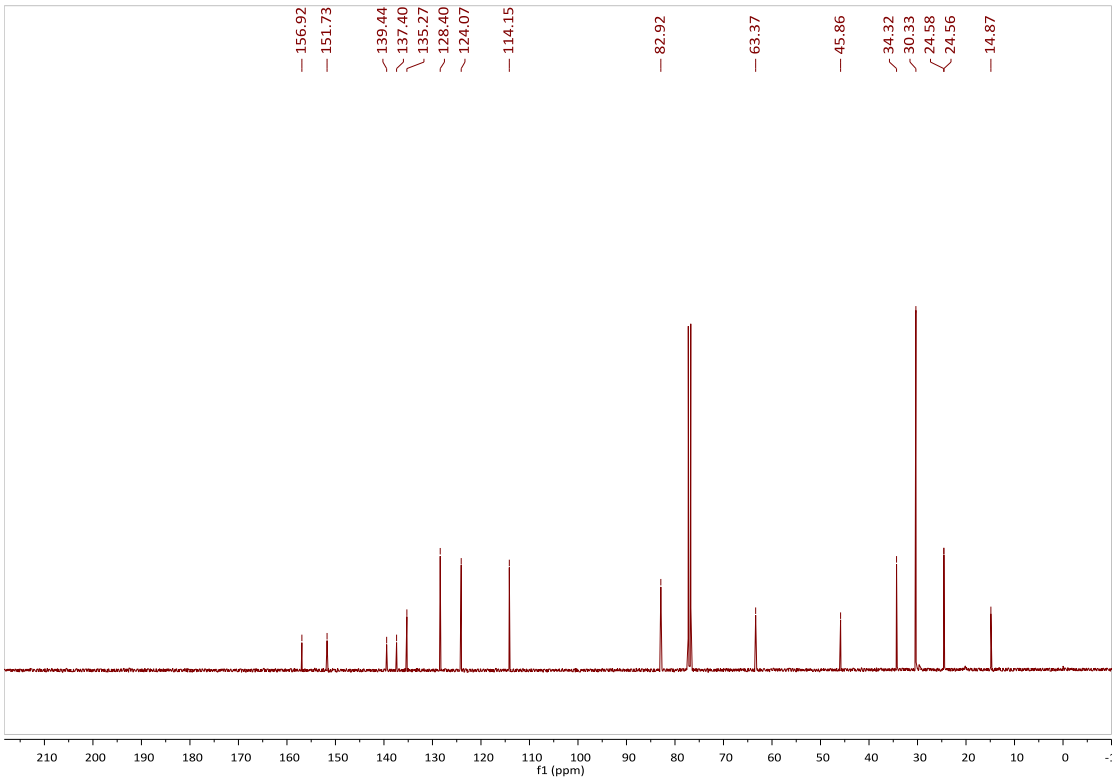
6.82
6.80
5.00
4.16
4.14
4.13
4.03
4.01
4.00
3.99
1.58
1.57
1.42
1.40
1.39
1.05
1.05
2.04
2.01
1.99
1.00
1.03
2.03
2.09
18.10
3.08
12.13
f1 (ppm)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128.40
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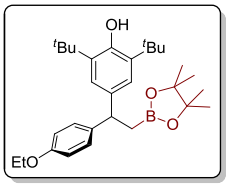
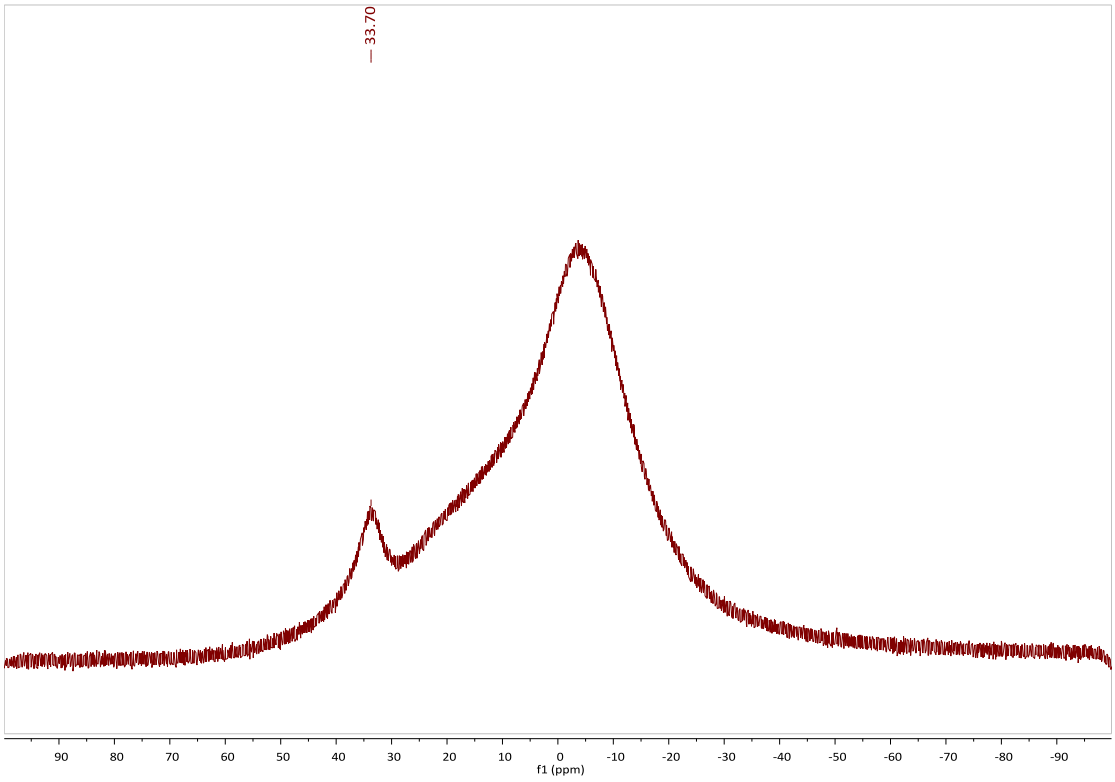
82.92
63.37
45.86
34.32
30.33
24.58
24.56
14.87
f1 (ppm)


OH
tBu
tBu
O
B
O
EtO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60
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30
20
10
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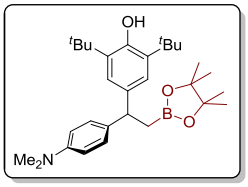
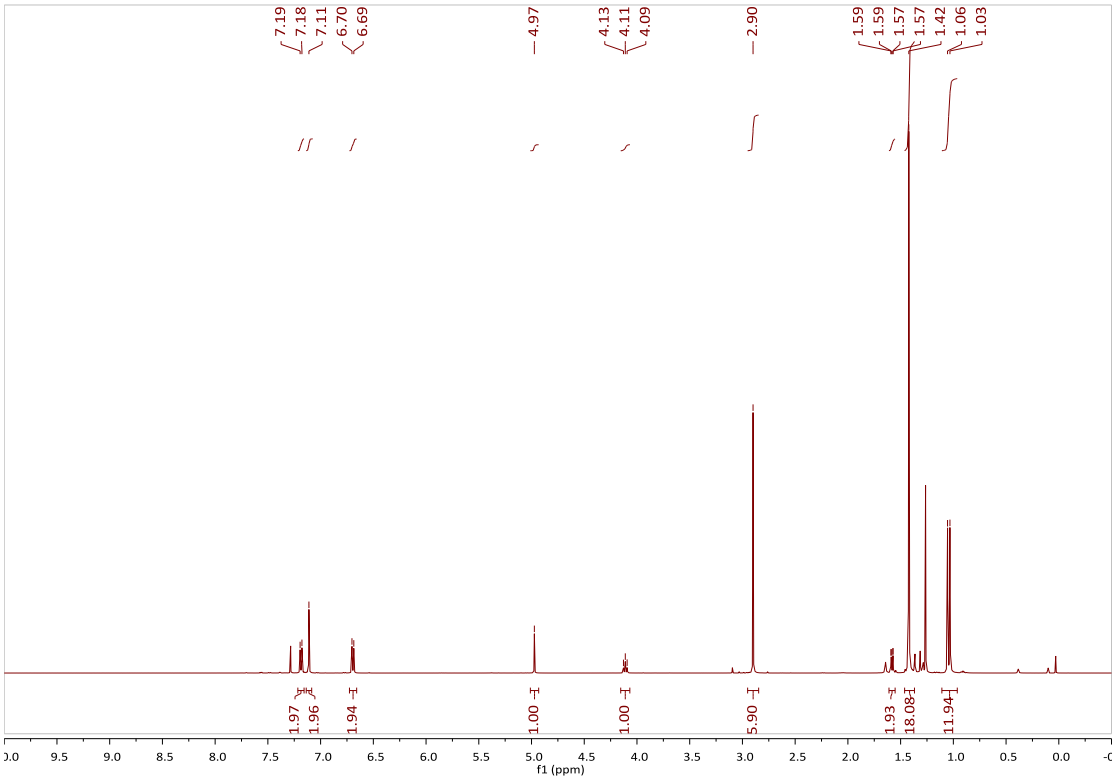
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
Me2N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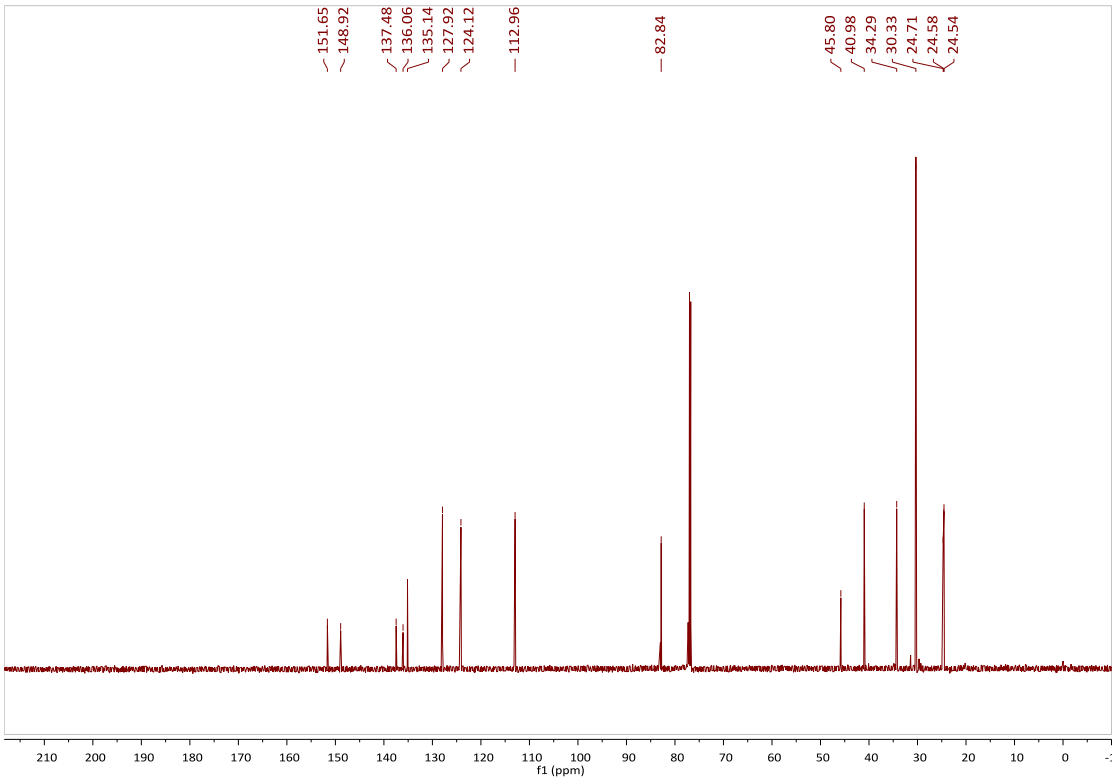
7.18
7.11
6.70
6.69
4.97
4.13
4.11
4.09
2.90
1.59
1.59
1.57
1.57
1.42
1.06
1.03
1.97
1.96
1.94
1.00
1.00
5.90
1.93
18.08
11.94
f1 (ppm)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136.06
135.14
127.92
124.12
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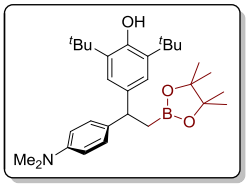
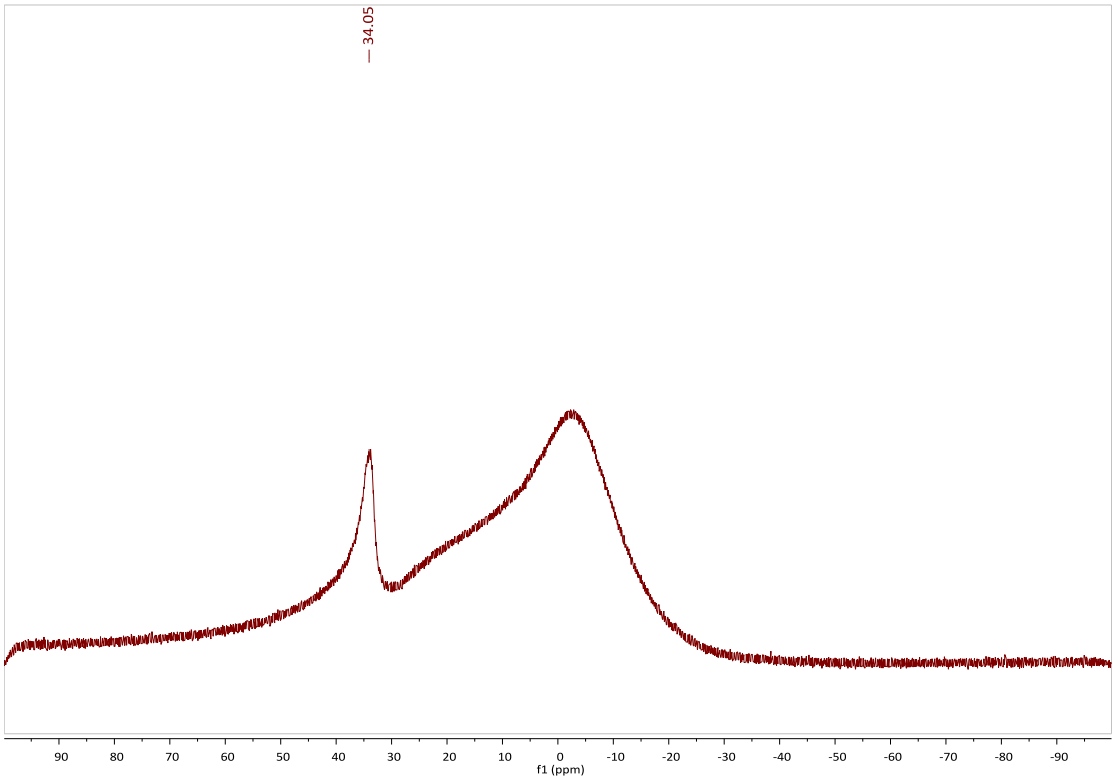
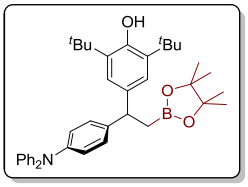
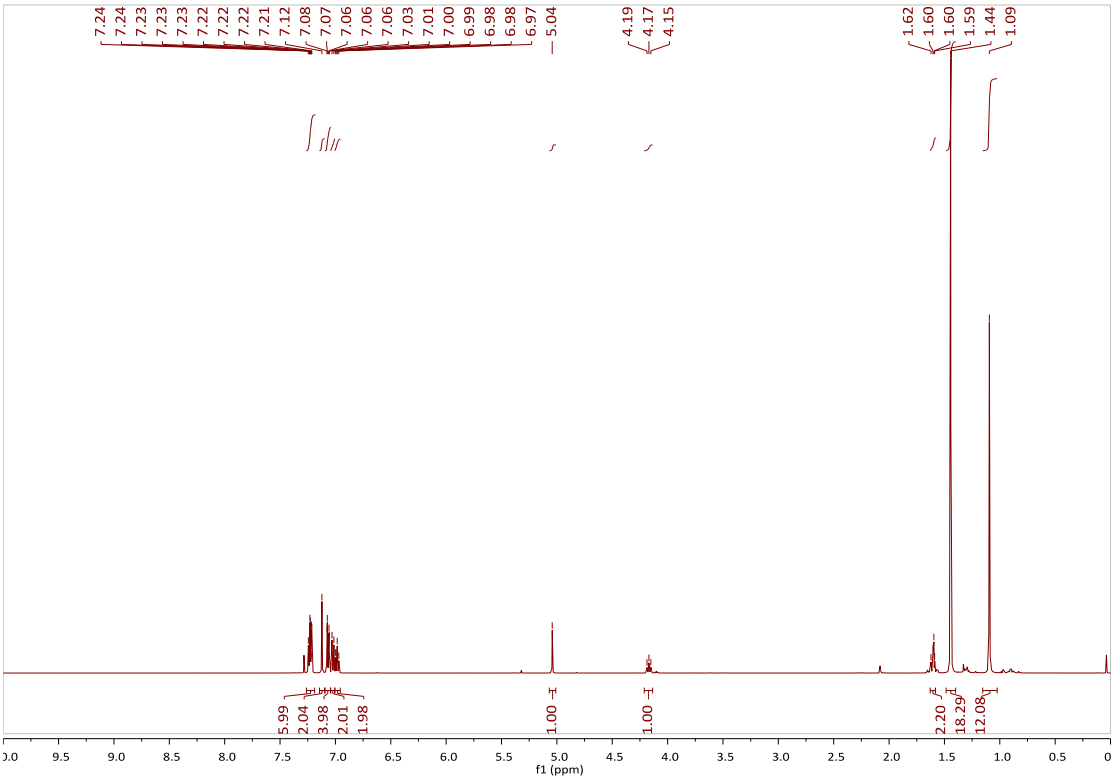
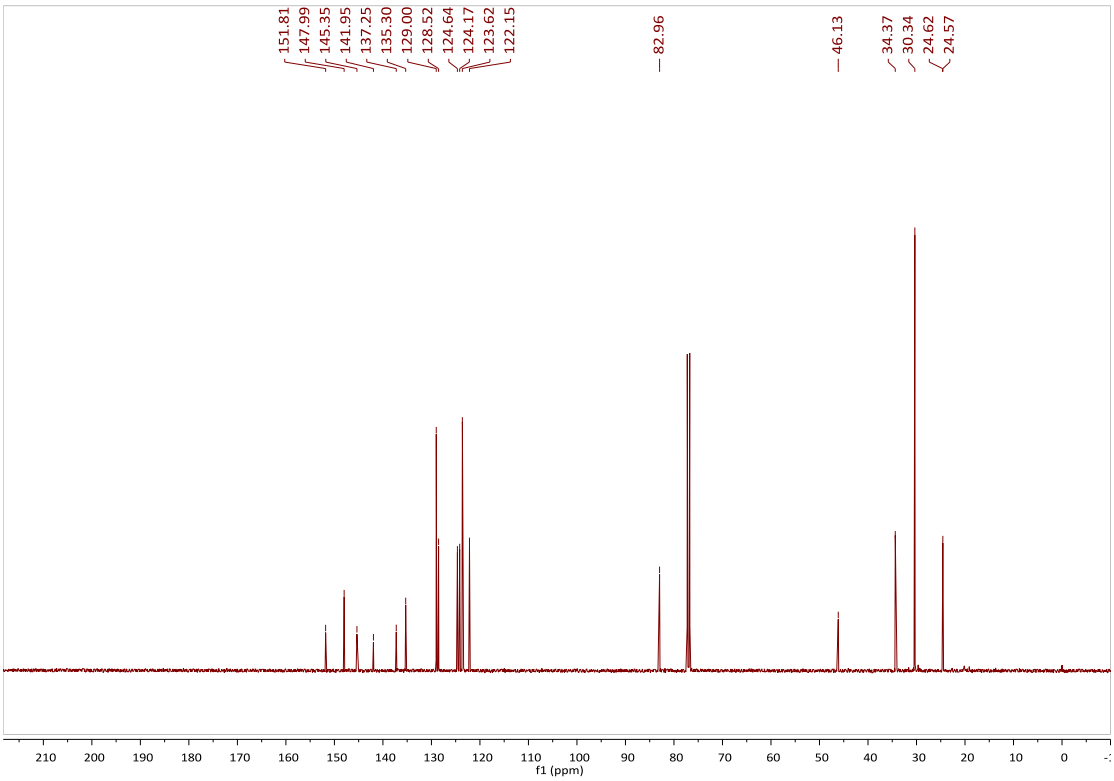
82.84
45.80
40.98
34.29
30.33
24.71
24.58
24.54
f1 (ppm)

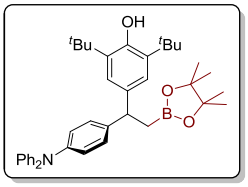

OH
tBu
tBu
O
B
O
Me2N

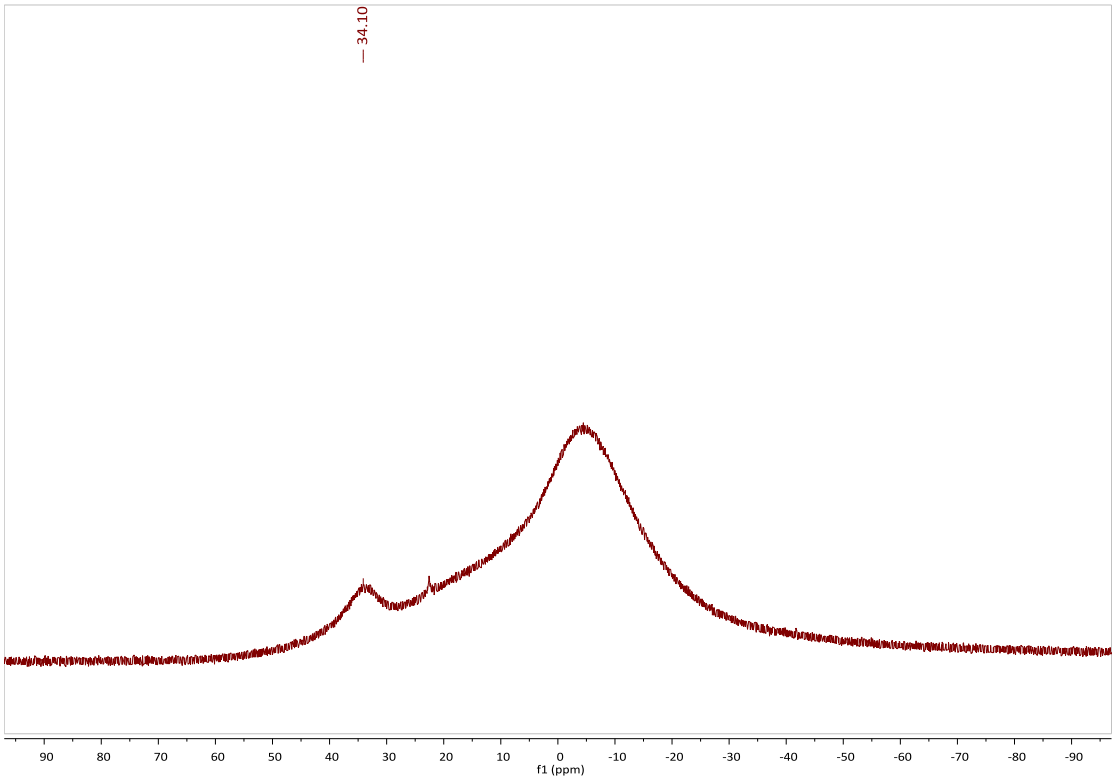

34.05
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
Ph2N


7.24 7.24 7.23 7.23 7.23 7.22 7.22 7.22 7.21 7.12 7.08 7.07 7.06 7.06 7.06 7.03 7.01 7.00 6.99 6.98 6.98 6.97 5.04
4.19 4.17 4.15
1.62 1.60 1.60 1.59 1.44 1.09
5.99 2.04 3.98 2.01 1.98 1.00 1.00 2.20 18.29 12.08
f1 (ppm)


151.81 147.99 145.35 141.95 137.25 135.30 129.00 128.52 124.64 124.17 123.62 122.15
82.96
46.13
34.37 30.34 24.62 24.57
f1 (ppm)


OH
tBu
tBu
O
B
O
Ph2N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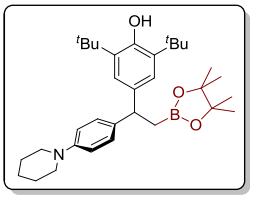
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)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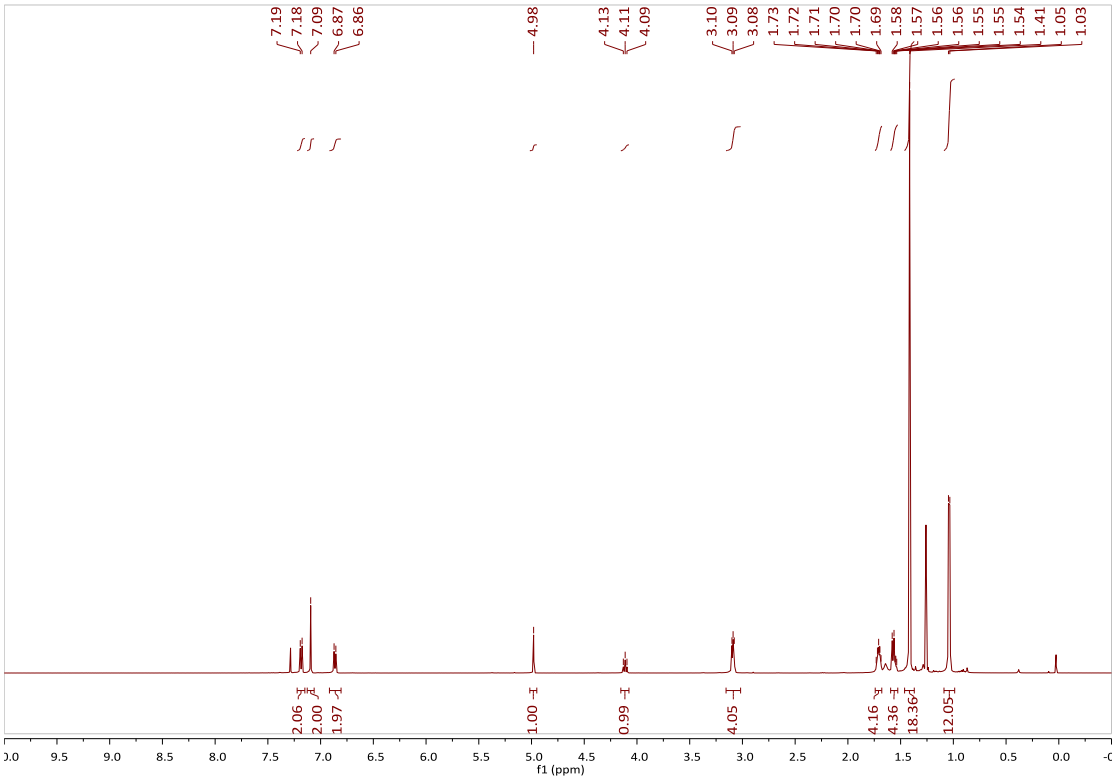
tBu
tBu
O
B
O
N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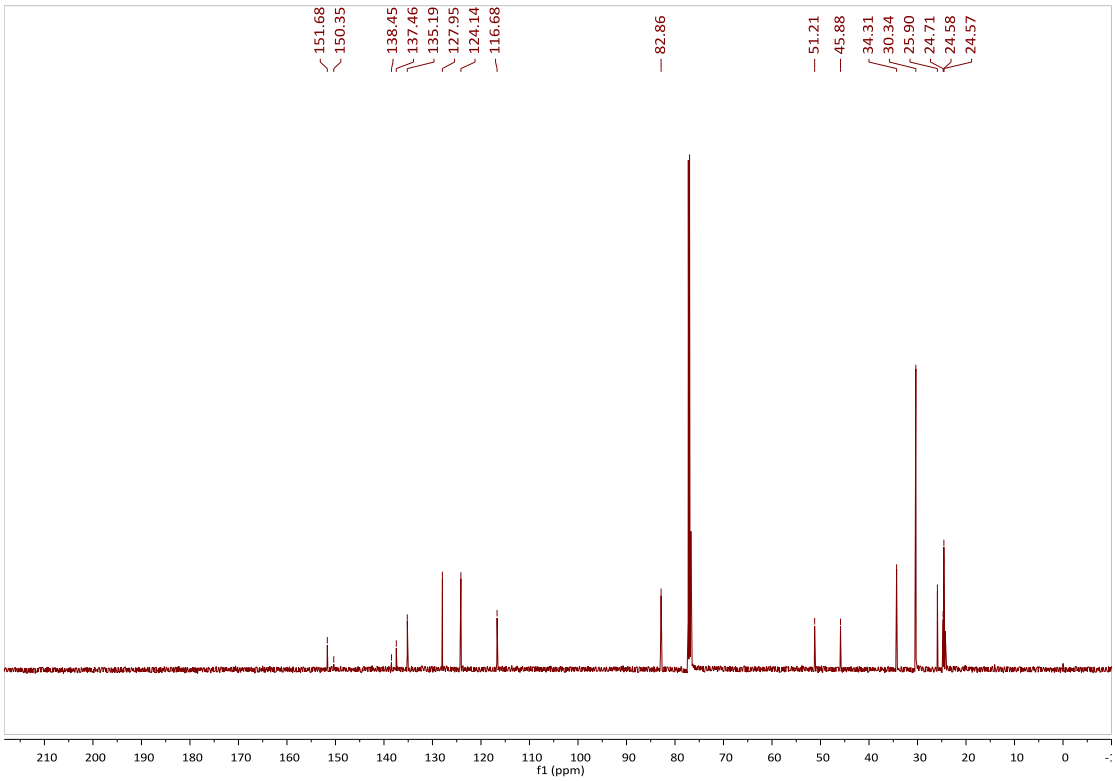
7.18
7.09
6.87
6.86
4.98
4.13
4.11
4.09
3.10
3.09
3.08
1.73
1.72
1.71
1.70
1.70
1.69
1.58
1.57
1.56
1.56
1.55
1.55
1.54
1.41
1.05
1.03
2.06
2.00
1.97
1.00
0.99
4.05
4.16
4.36
18.36
12.05
f1 (ppm)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135.19
127.95
124.14
116.68
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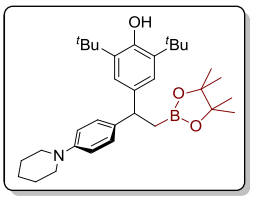
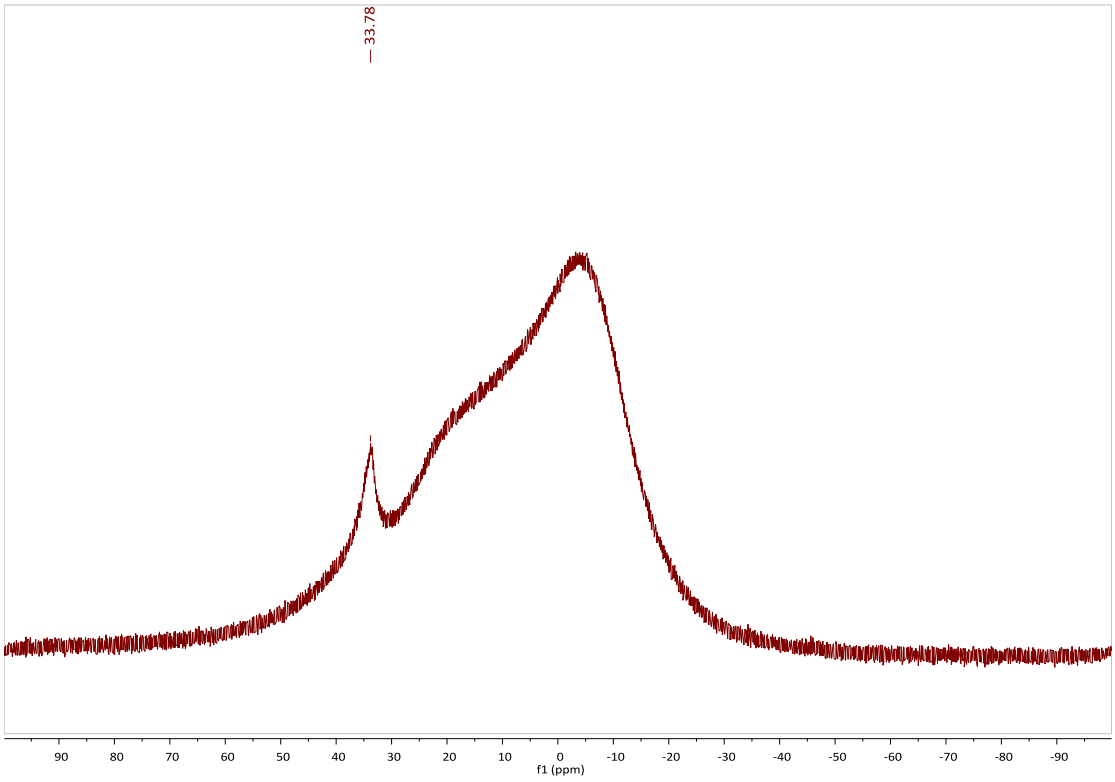
51.21
45.88
34.31
30.34
25.90
24.71
24.58
24.57
f1 (ppm)


OH
tBu
tBu
O
B
O
N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60
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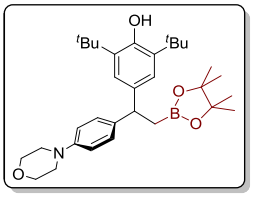
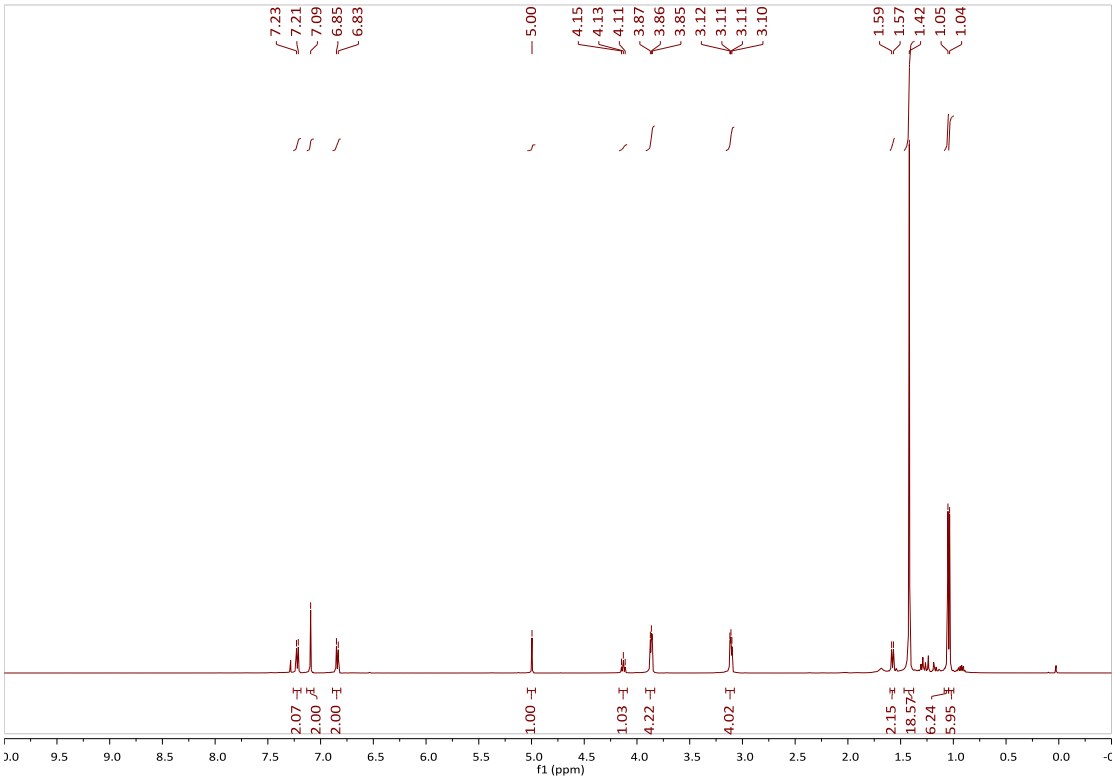
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
N
O


7.23
7.21
7.09
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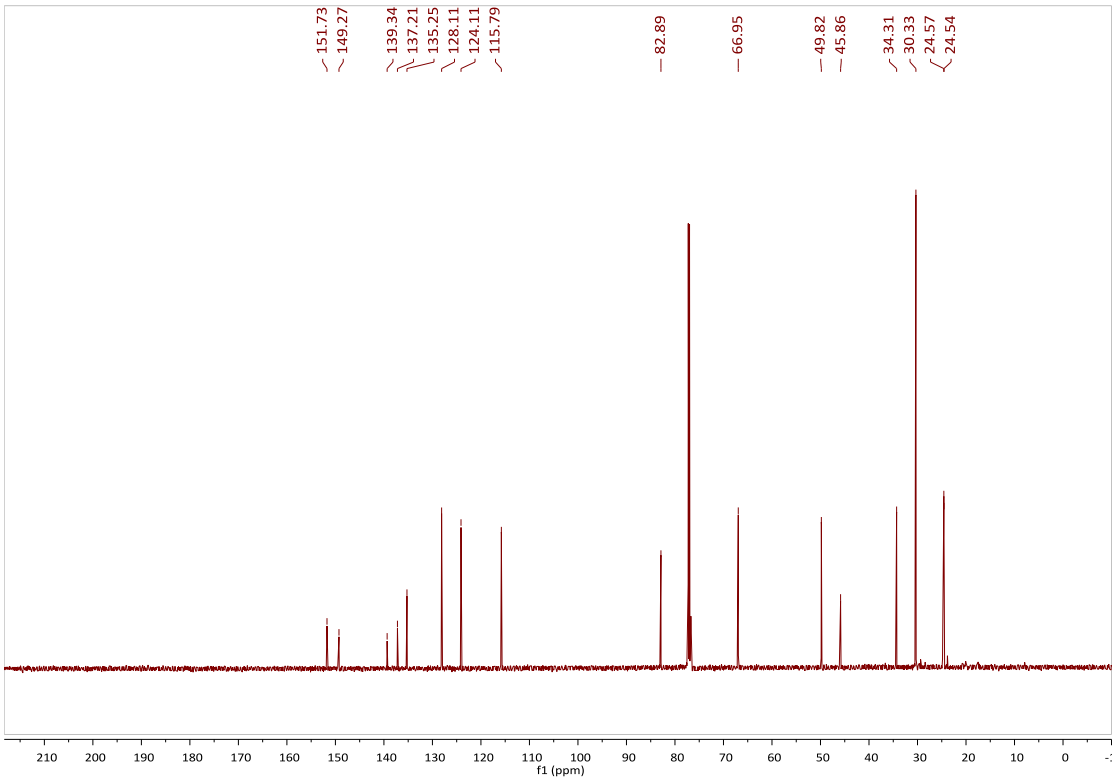
6.83
5.00
4.15
4.13
4.11
3.87
3.86
3.85
3.12
3.11
3.11
3.10
1.59
1.57
1.42
1.05
1.04
2.07
2.00
2.00
1.00
1.03
4.22
4.02
2.15
18.57
6.24
5.95
f1 (ppm)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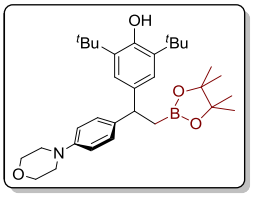
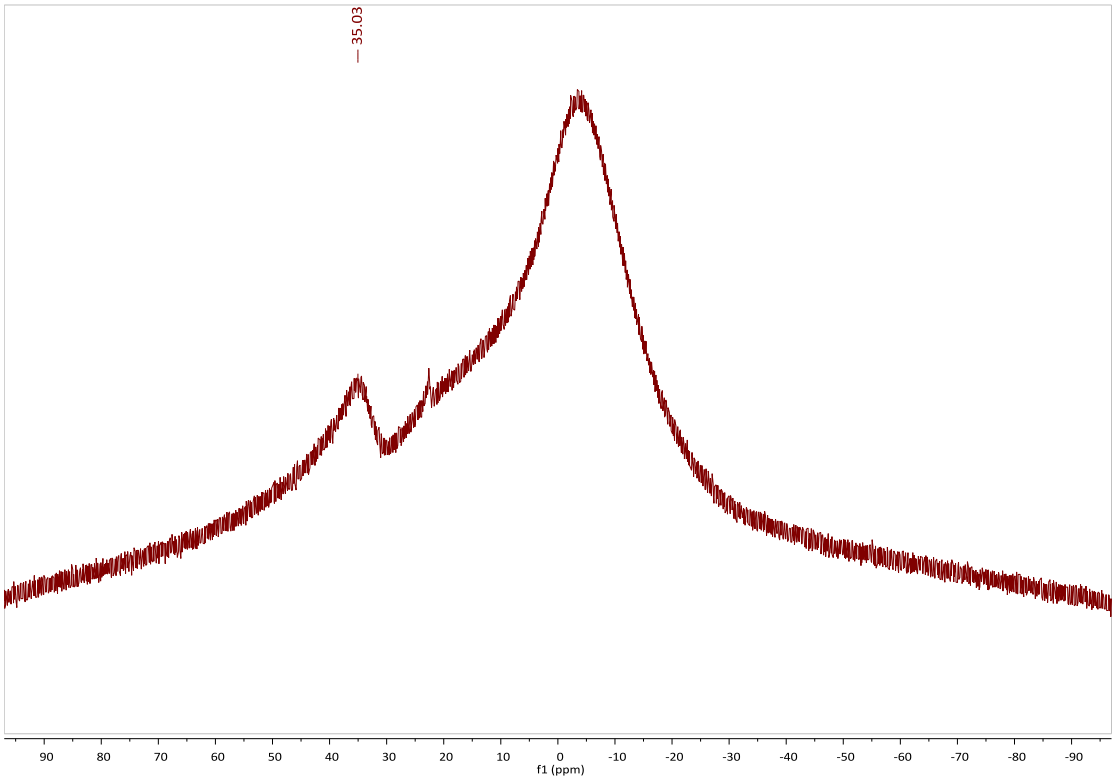
149.27
139.34
137.21
135.25
128.11
124.11
115.79
82.89
66.95
49.82
45.86
34.31
30.33
24.57
24.54
f1 (ppm)


OH
tBu
tBu
O
B
O
N
O


35.03
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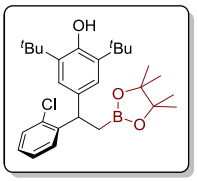
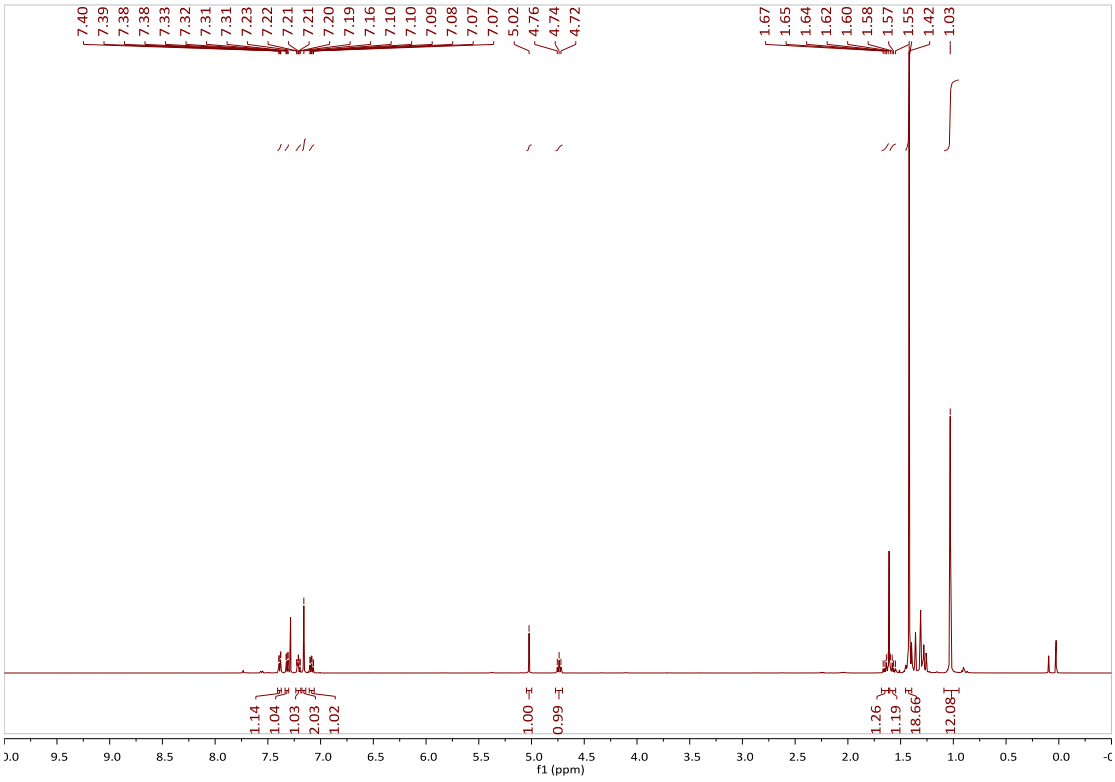
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
Cl
O
B
O


7.40
7.39
7.38
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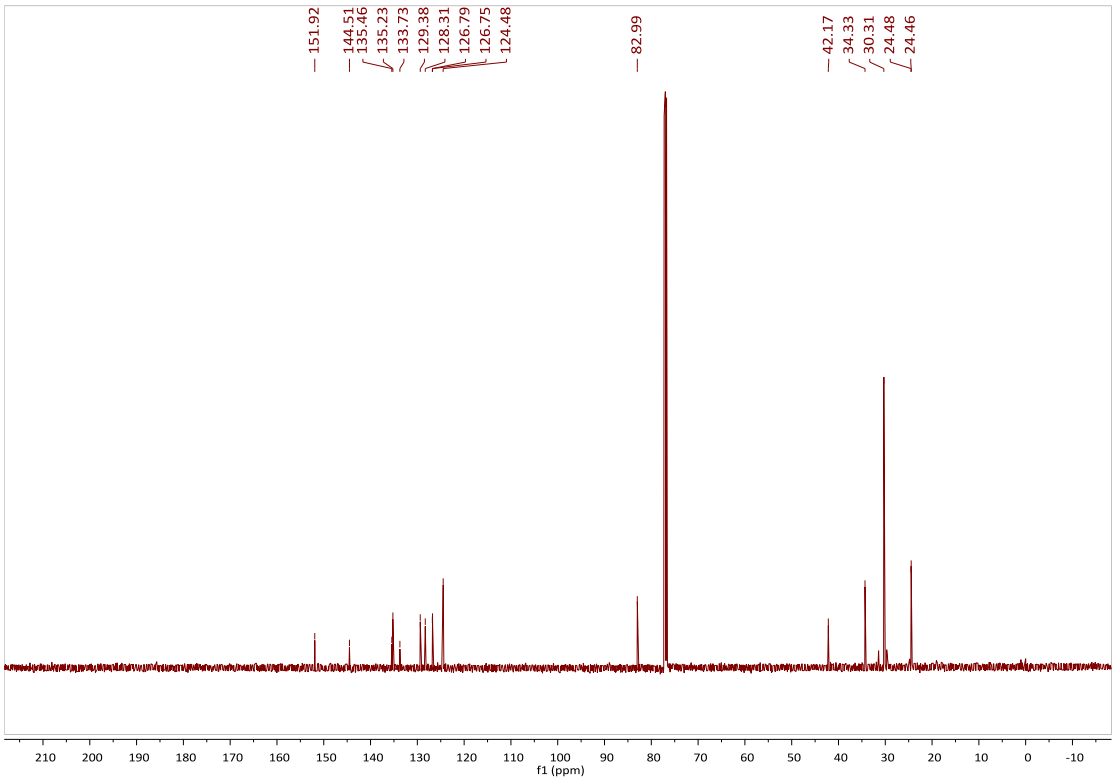
7.32
7.31
7.31
7.23
7.22
7.21
7.21
7.20
7.19
7.16
7.10
7.10
7.09
7.08
7.07
7.07
5.02
4.76
4.74
4.72
1.67
1.65
1.64
1.62
1.60
1.58
1.57
1.55
1.42
1.03
1.14
1.04
1.03
2.03
1.02
1.00
0.99
1.26
1.19
18.66
12.08
f1 (ppm)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135.23
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129.38
128.31
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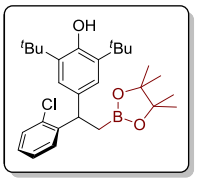
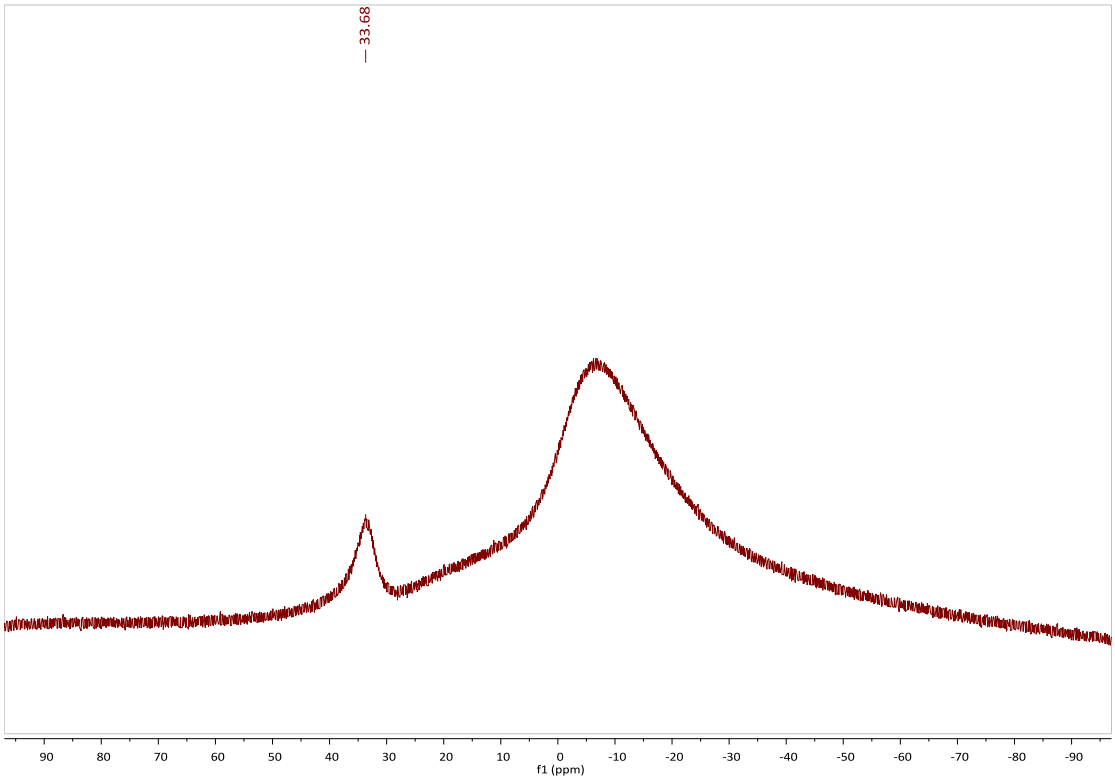
126.75
124.48
82.99
42.17
34.33
30.31
24.48
24.46
f1 (ppm)


OH
tBu
tBu
Cl
O
B
O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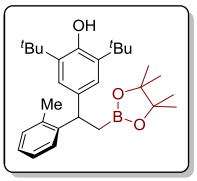
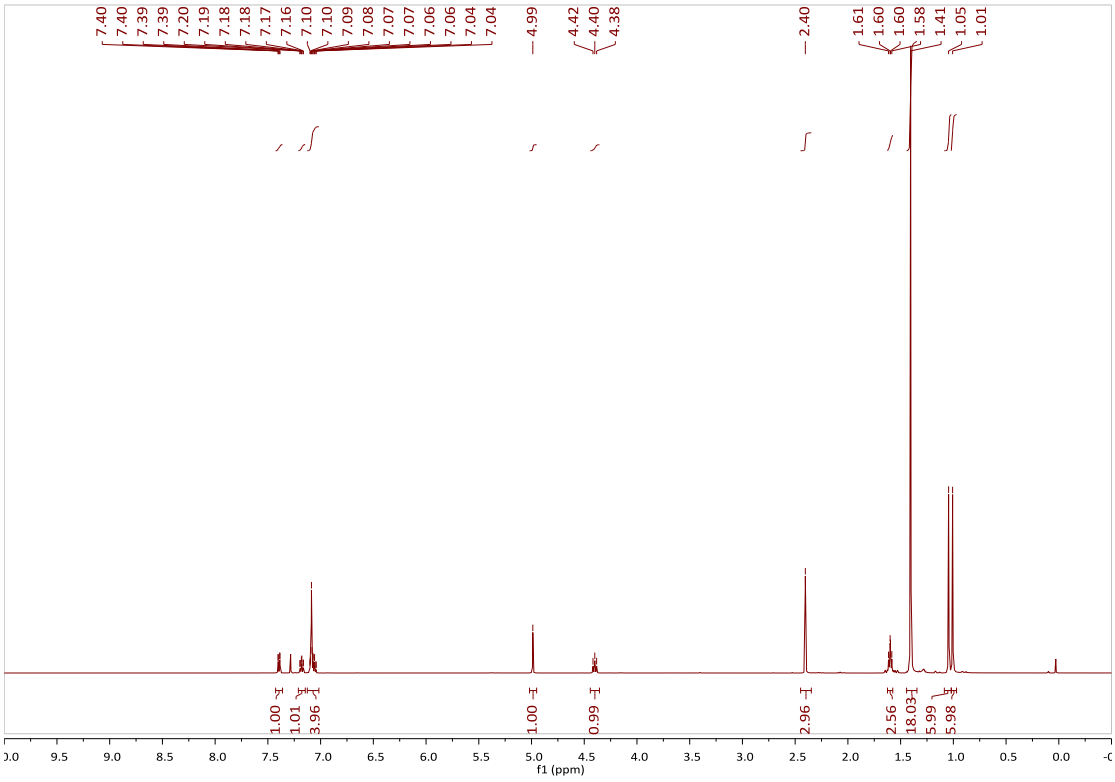
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
Me
O
B
O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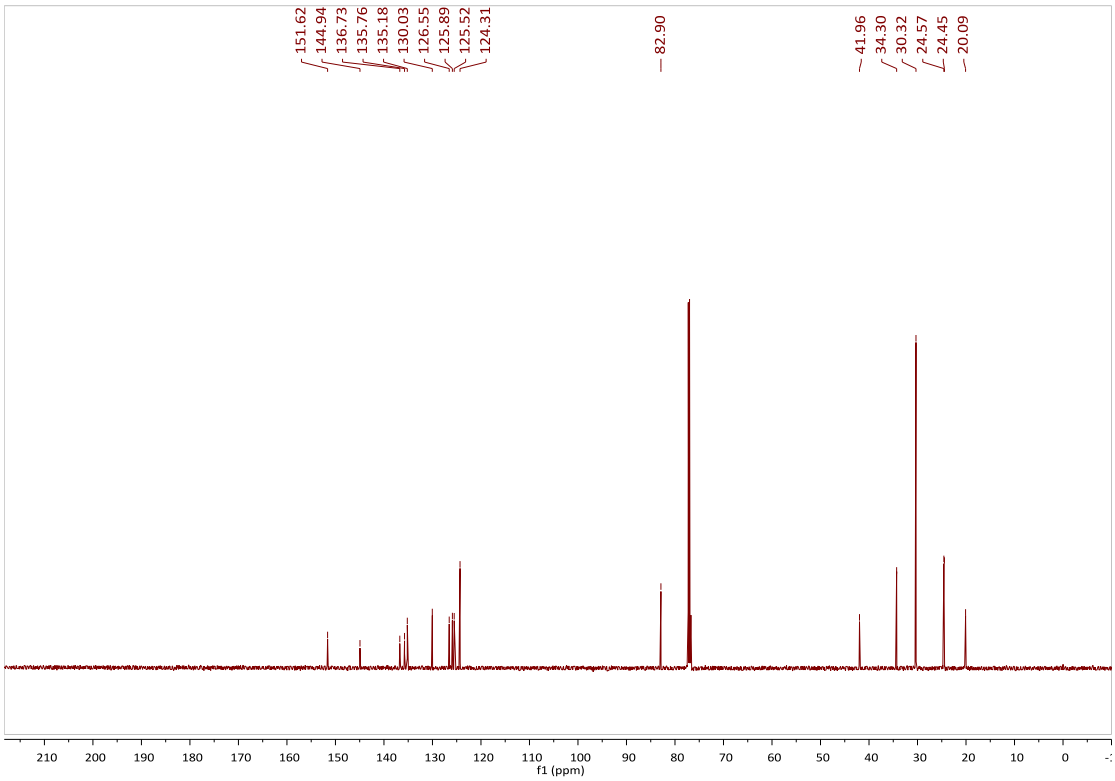
7.39
7.39
7.20
7.19
7.18
7.18
7.17
7.16
7.10
7.10
7.09
7.08
7.07
7.07
7.06
7.06
7.04
7.04
4.99
4.42
4.40
4.38
2.40
1.61
1.60
1.60
1.58
1.41
1.05
1.01
1.00
1.01
3.96
1.00
0.99
2.96
2.56
18.03
5.99
5.98
f1 (ppm)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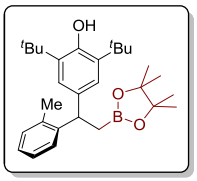
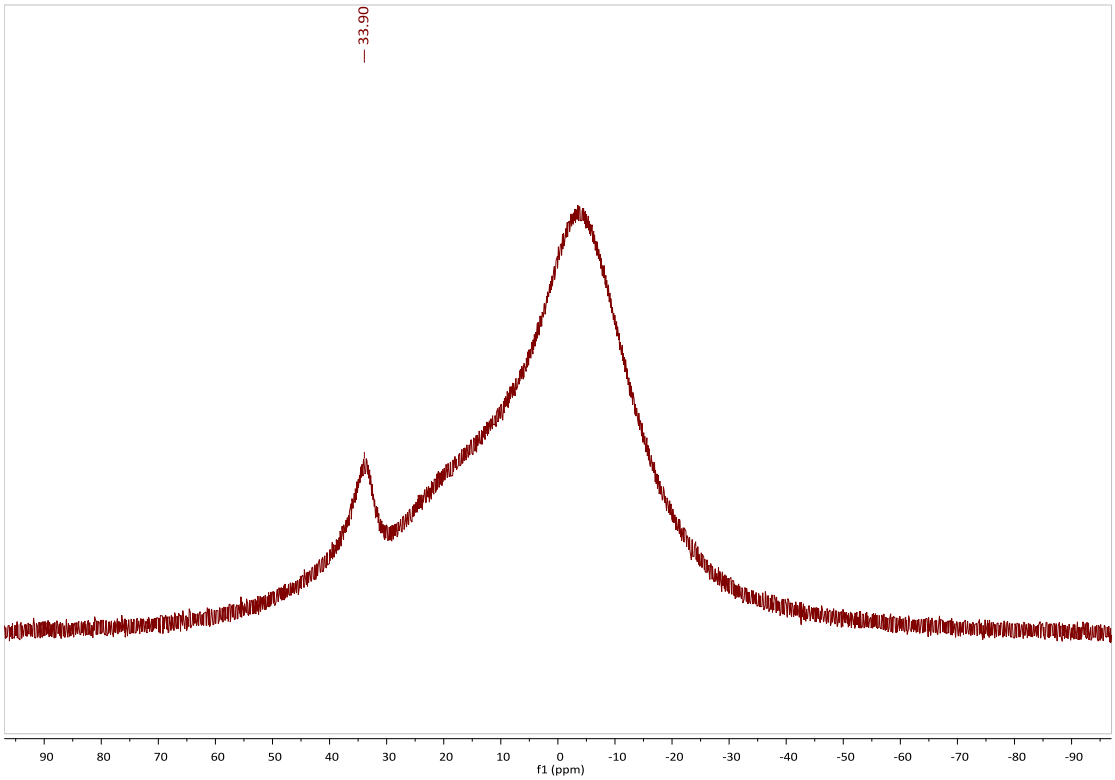
144.94
136.73
135.76
135.18
130.03
126.55
125.89
125.52
124.31
82.90
41.96
34.30
30.32
24.57
24.45
20.09
f1 (ppm)


OH
tBu
tBu
Me
O
B
O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80
70
60
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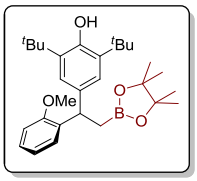
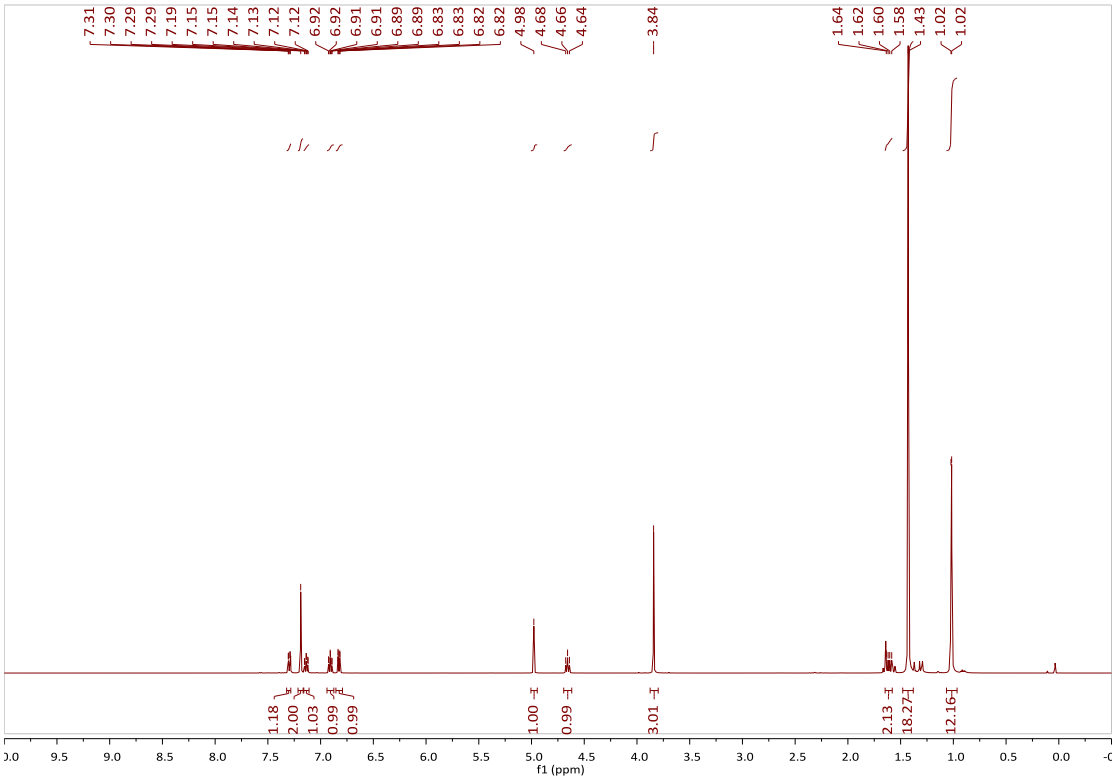
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
OMe
O
B
O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7.29
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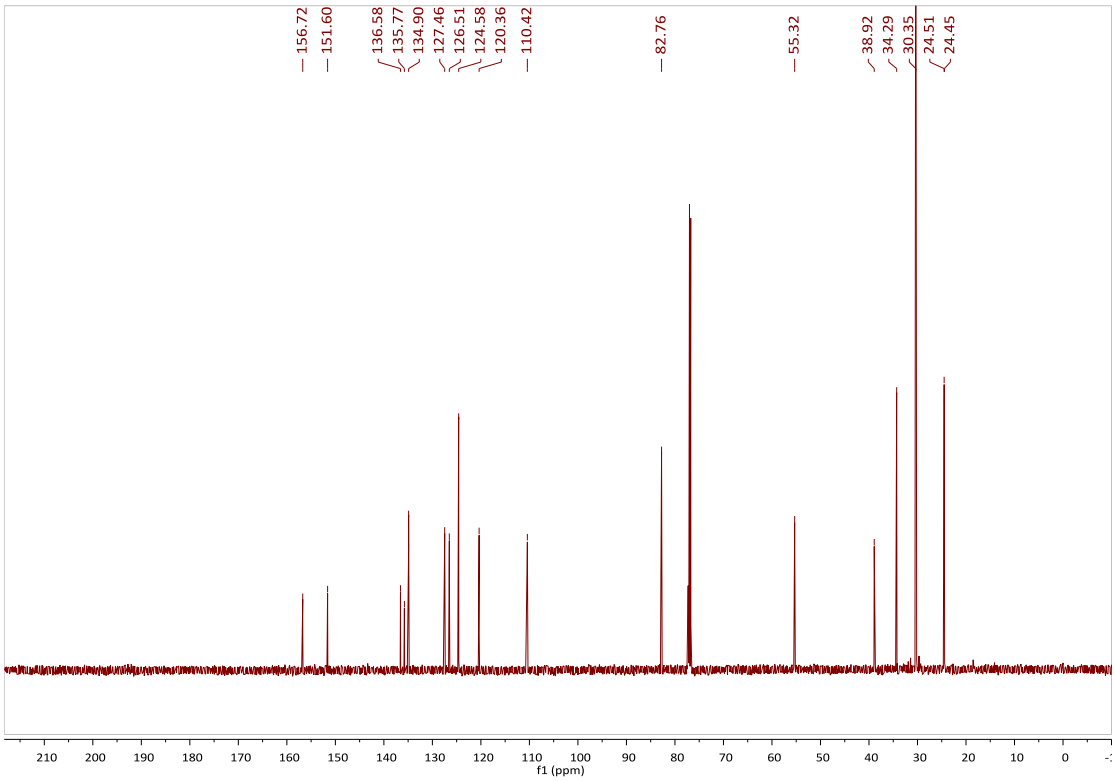
7.15
7.15
7.14
7.13
7.12
7.12
6.92
6.92
6.91
6.91
6.89
6.89
6.83
6.83
6.82
4.98
4.68
4.66
4.64
3.84
1.64
1.62
1.60
1.58
1.43
1.02
1.02
1.18
2.00
1.03
0.99
0.99
1.00
0.99
3.01
2.13
18.27
12.16
f1 (ppm)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127.46
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110.42
82.76
55.32
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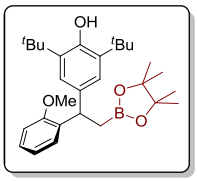
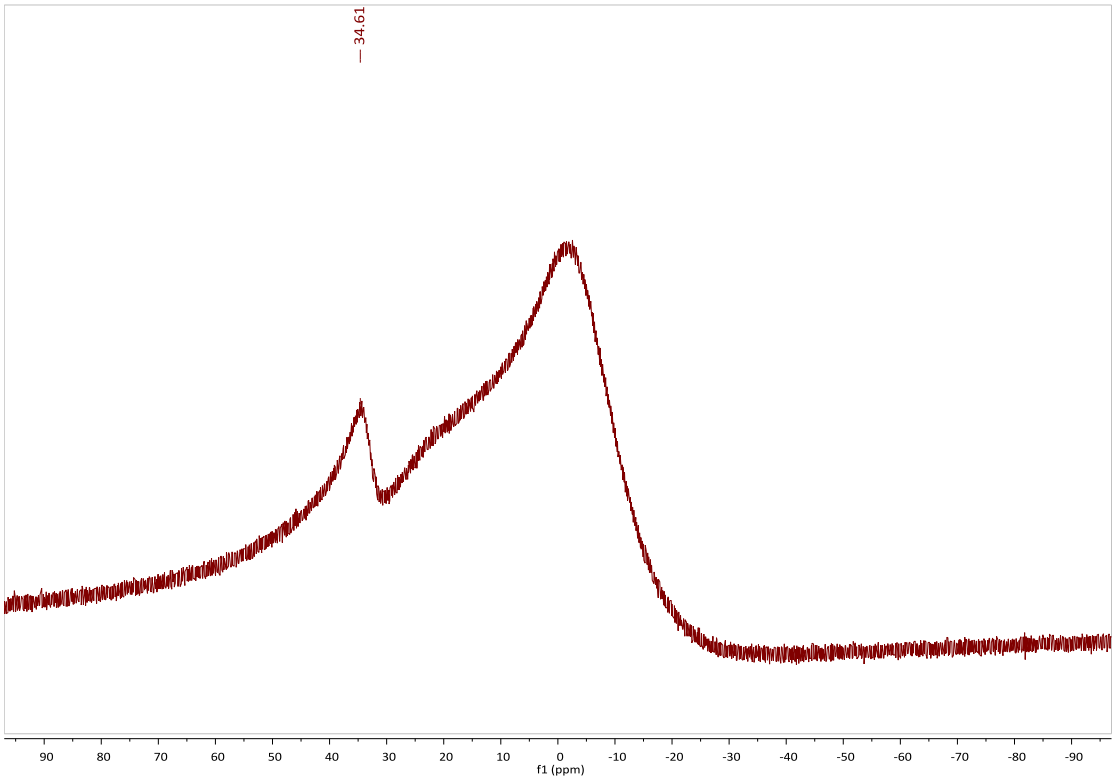
34.29
30.35
24.51
24.45
f1 (ppm)


OH
tBu
tBu
OMe
O
B
O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60
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30
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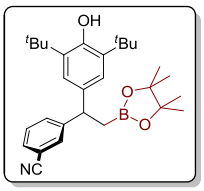
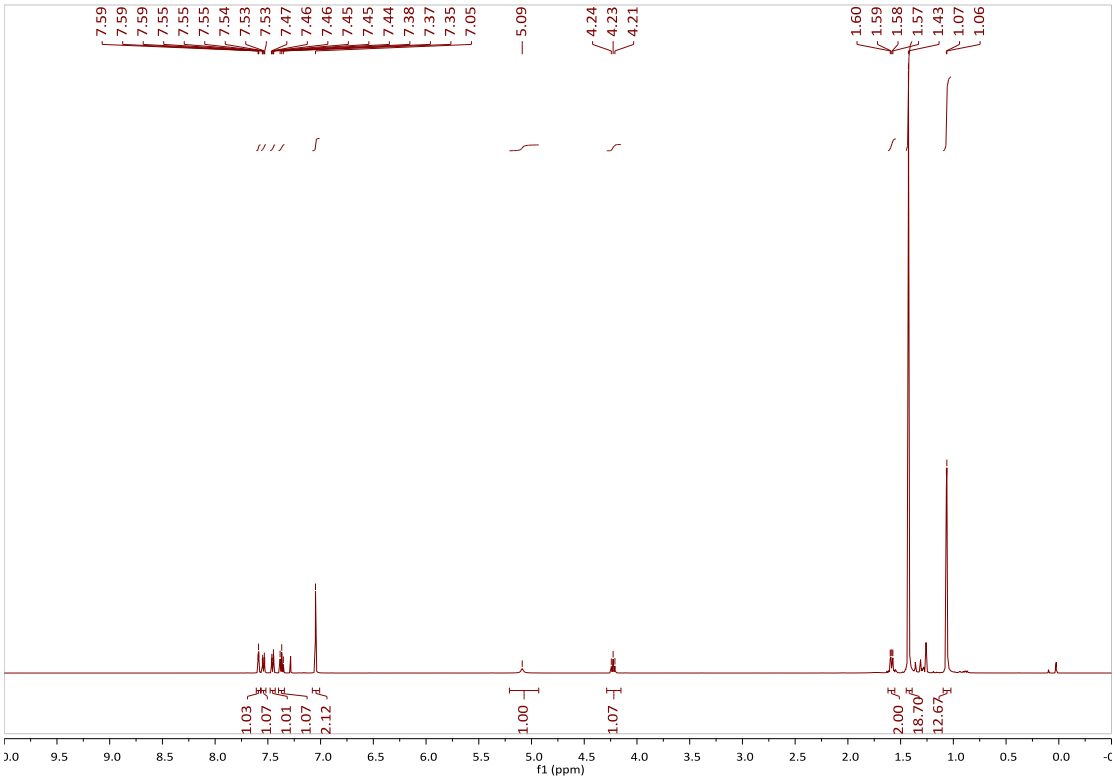
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
NC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7.55
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7.53
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7.47
7.46
7.46
7.45
7.45
7.44
7.38
7.37
7.35
7.05
5.09
4.24
4.23
4.21
1.60
1.59
1.58
1.57
1.43
1.07
1.06
1.03
1.07
1.01
1.07
2.12
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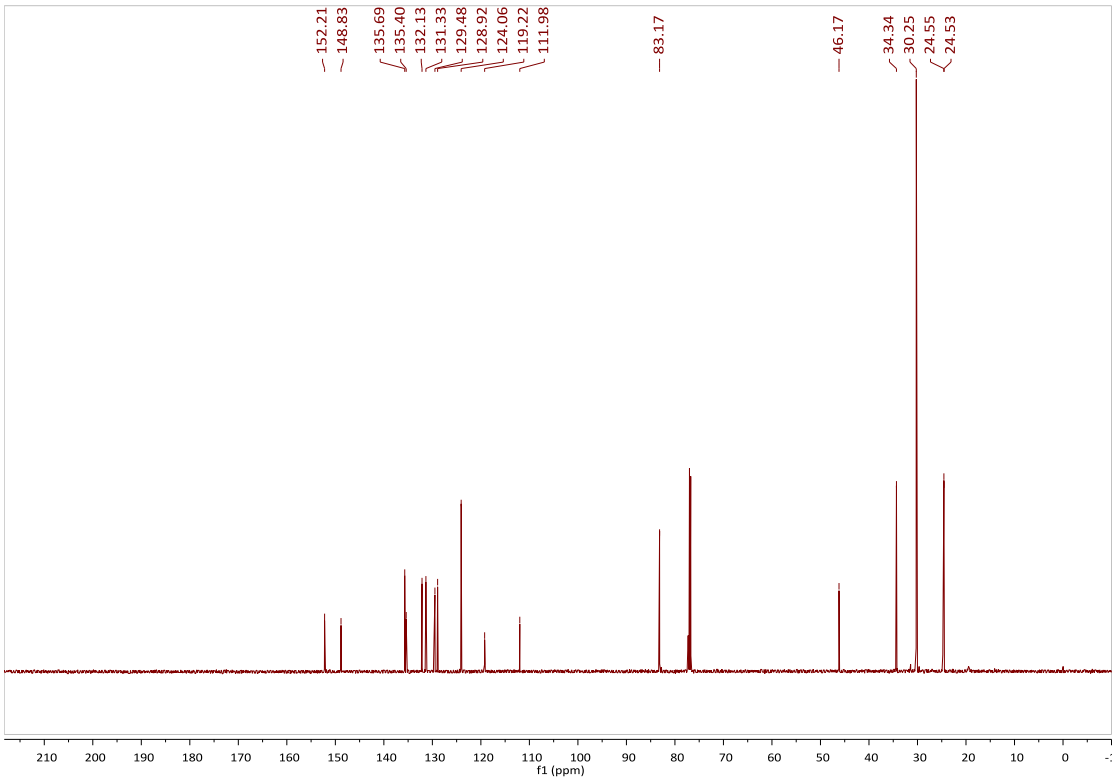
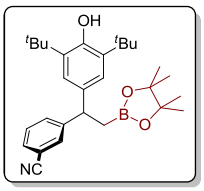
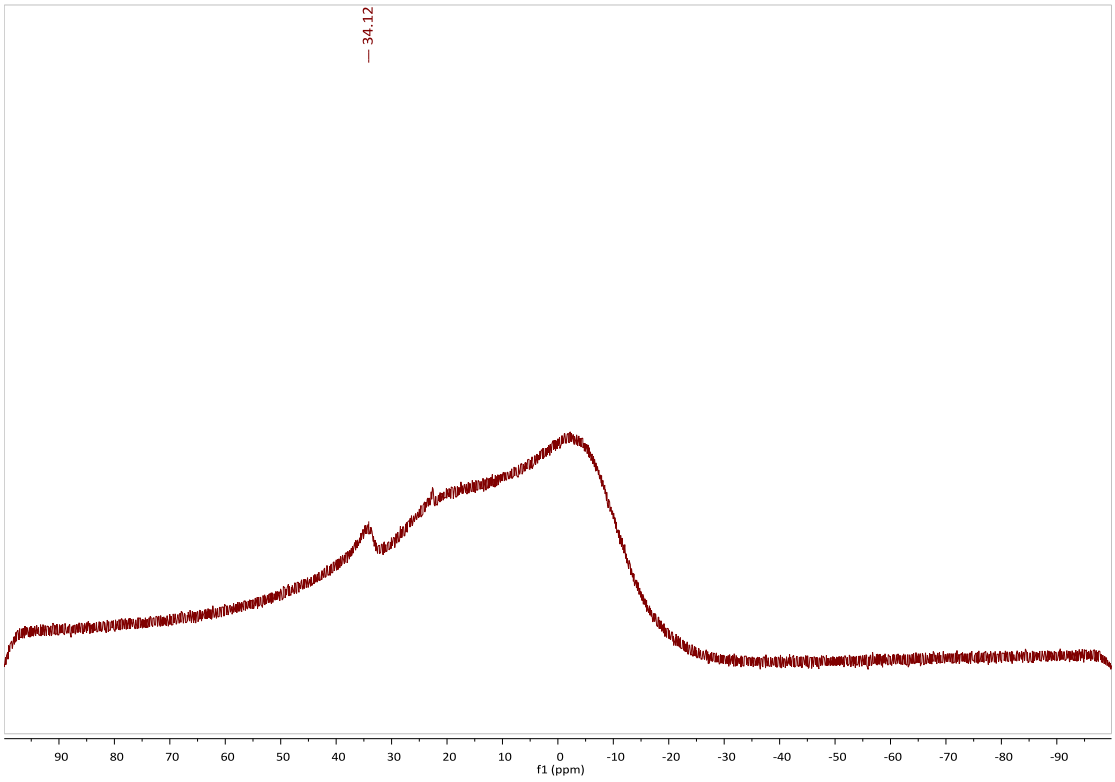
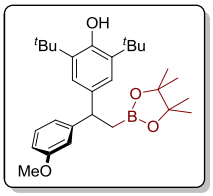
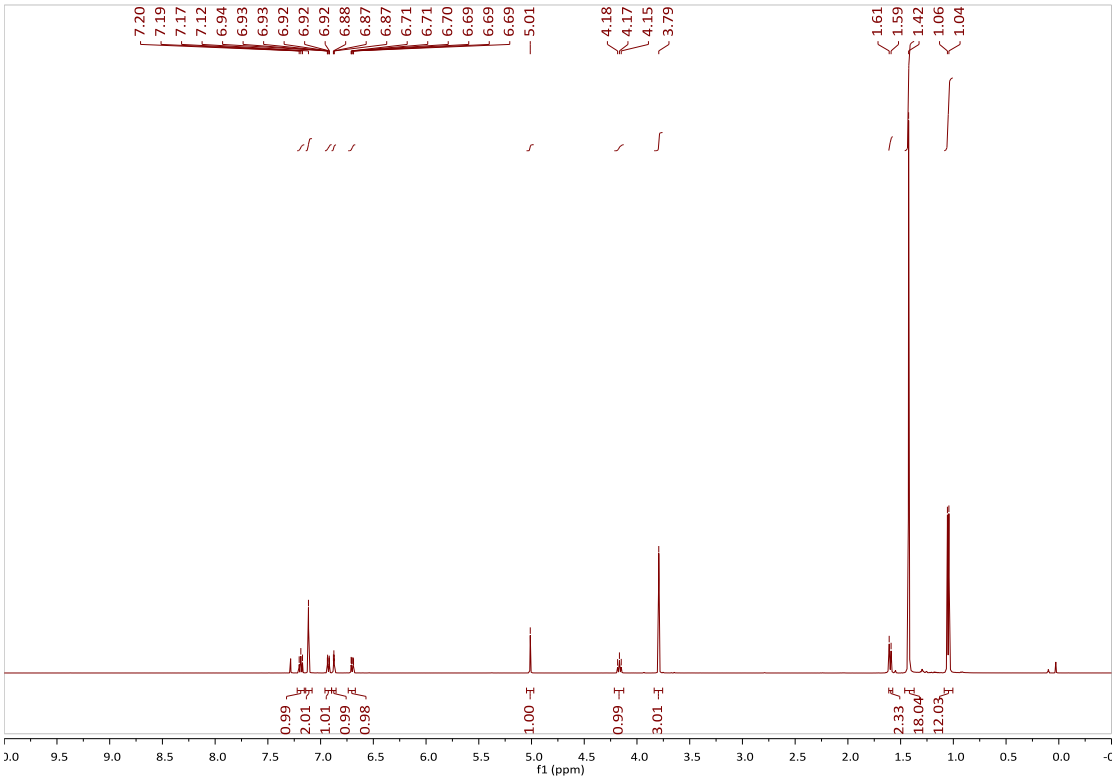
1.07
2.00
18.70
12.67
f1 (ppm)


152.21
148.83
135.69
135.40
132.13
131.33
129.48
128.92
124.06
119.22
111.98
83.17
46.17
34.34
30.25
24.55
24.53
f1 (ppm)


OH
tBu
tBu
O
B
O
NC


34.12
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
MeO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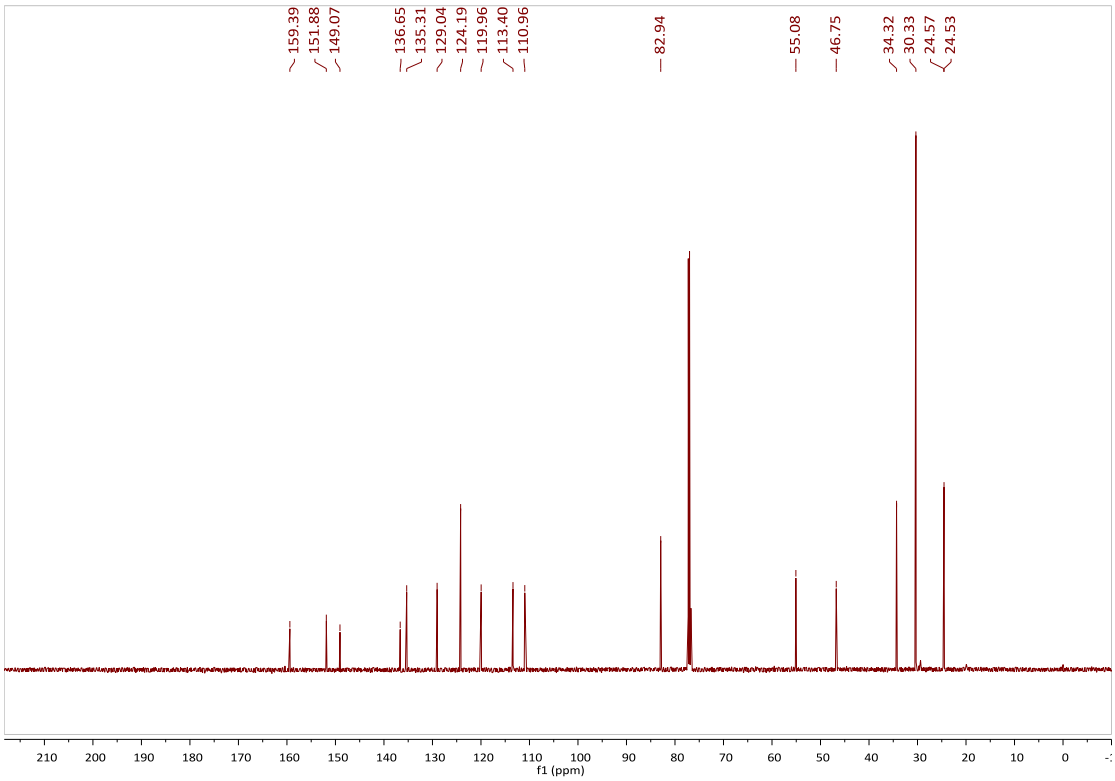
6.93
6.93
6.92
6.92
6.92
6.88
6.87
6.87
6.71
6.71
6.70
6.69
6.69
6.69
5.01
4.18
4.17
4.15
3.79
1.61
1.59
1.42
1.06
1.04
0.99
2.01
1.01
0.99
0.98
1.00
0.99
3.01
2.33
18.04
12.03
f1 (ppm)


159.39
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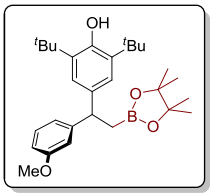
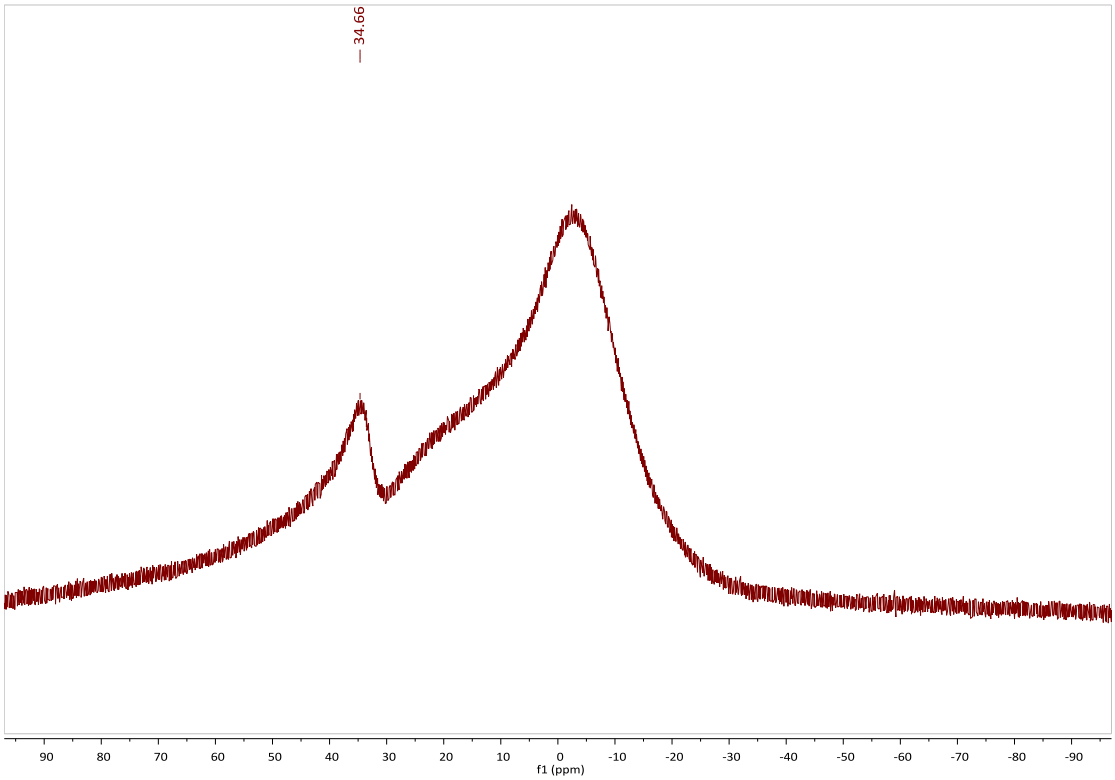
136.65
135.31
129.04
124.19
119.96
113.40
110.96
82.94
55.08
46.75
34.32
30.33
24.57
24.53
f1 (ppm)


OH
tBu
tBu
O
B
O
MeO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90
80
70
60
50
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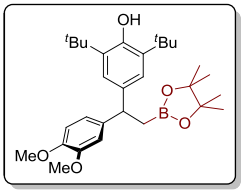
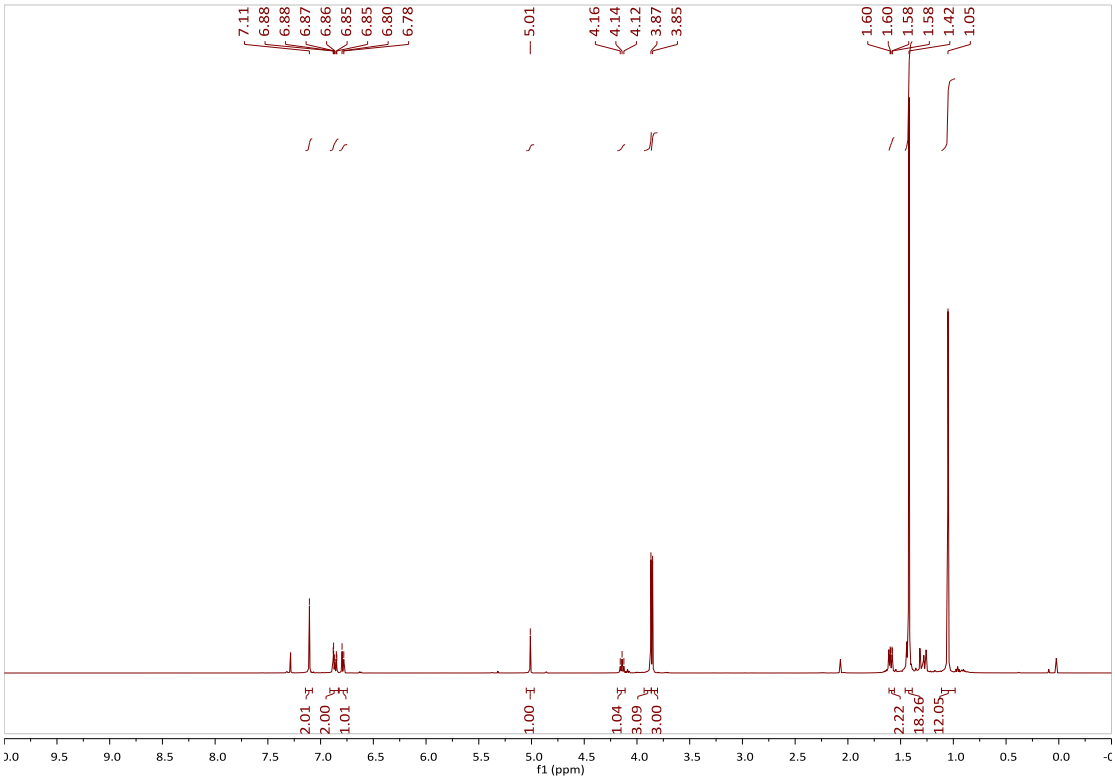
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
MeO
MeO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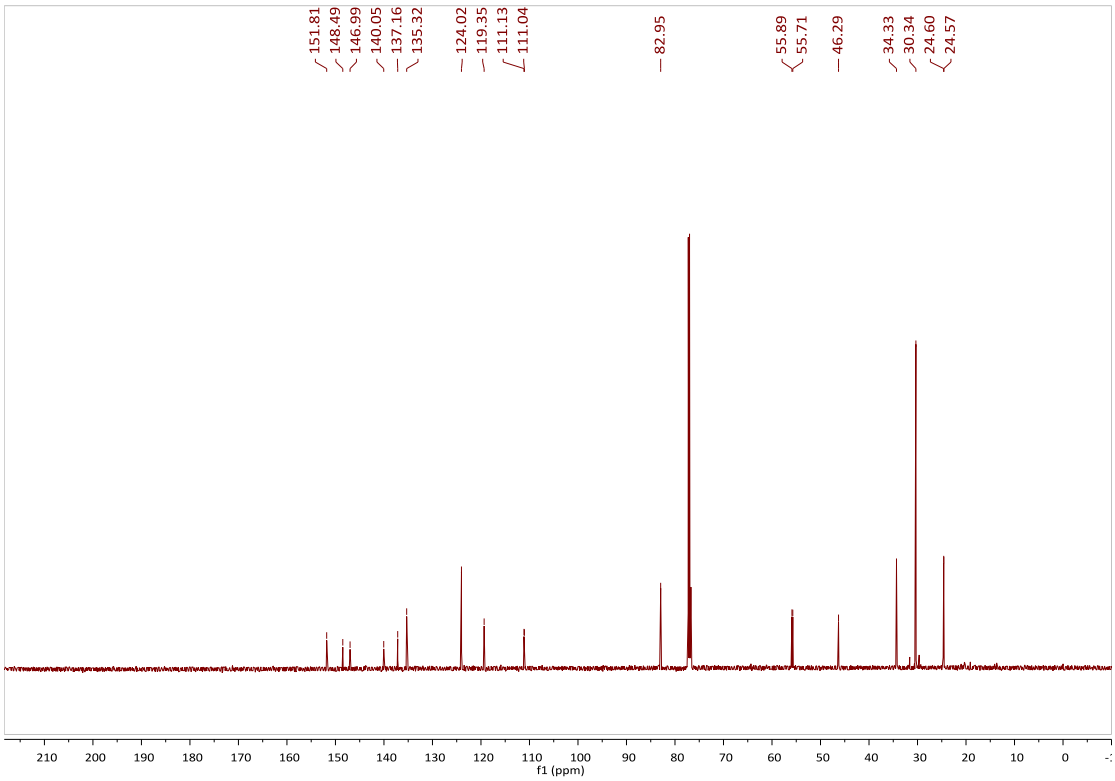
6.88
6.88
6.87
6.86
6.85
6.85
6.80
6.78
5.01
4.16
4.14
4.12
3.87
3.85
1.60
1.60
1.58
1.58
1.42
1.05
2.01
2.00
1.01
1.00
1.04
3.09
3.00
2.22
18.26
12.05
f1 (ppm)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146.99
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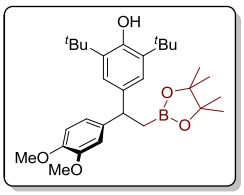
137.16
135.32
124.02
119.35
111.13
111.04
82.95
55.89
55.71
46.29
34.33
30.34
24.60
24.57
f1 (ppm)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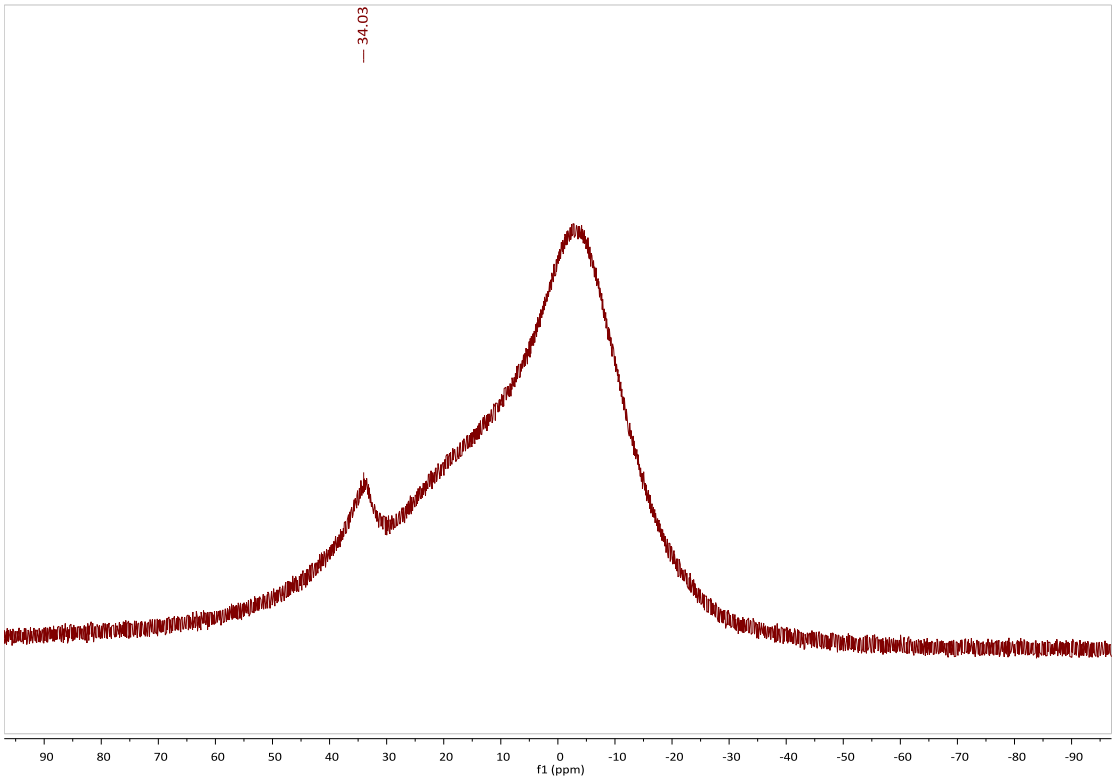
tBu
tBu
O
B
O
MeO
MeO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70
60
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30
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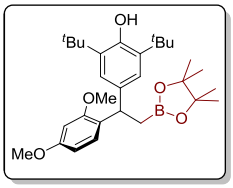
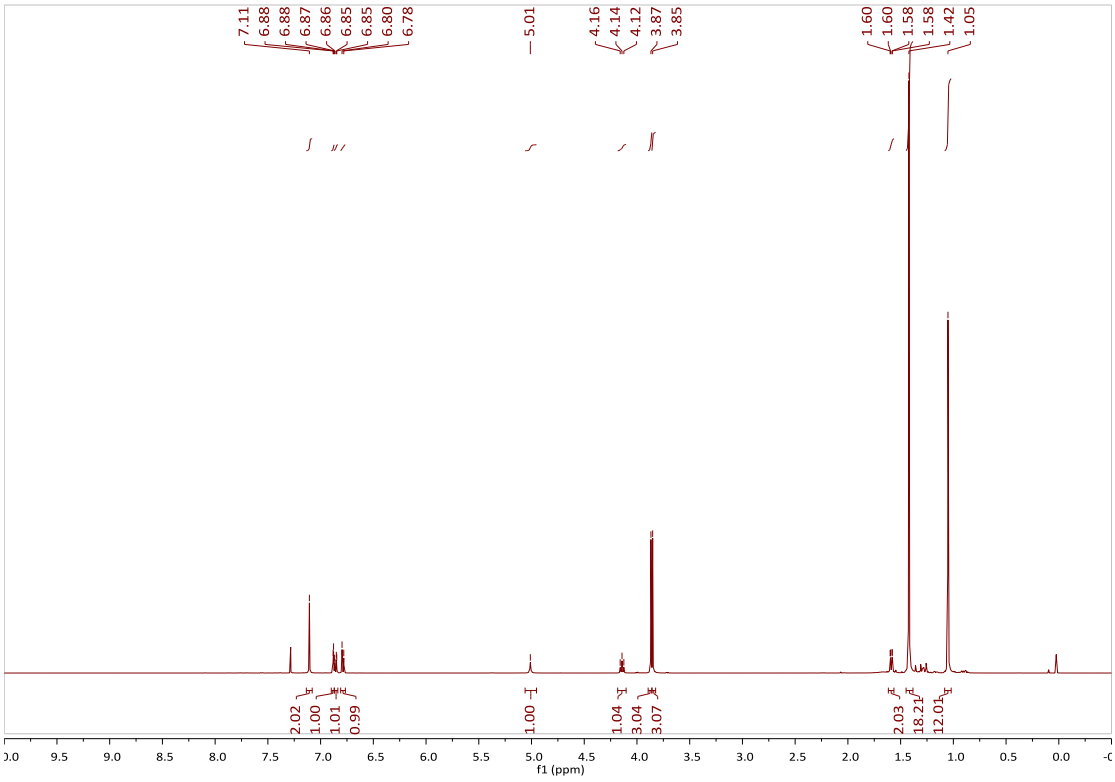
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
OMe
O
B
O
MeO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6.88
6.88
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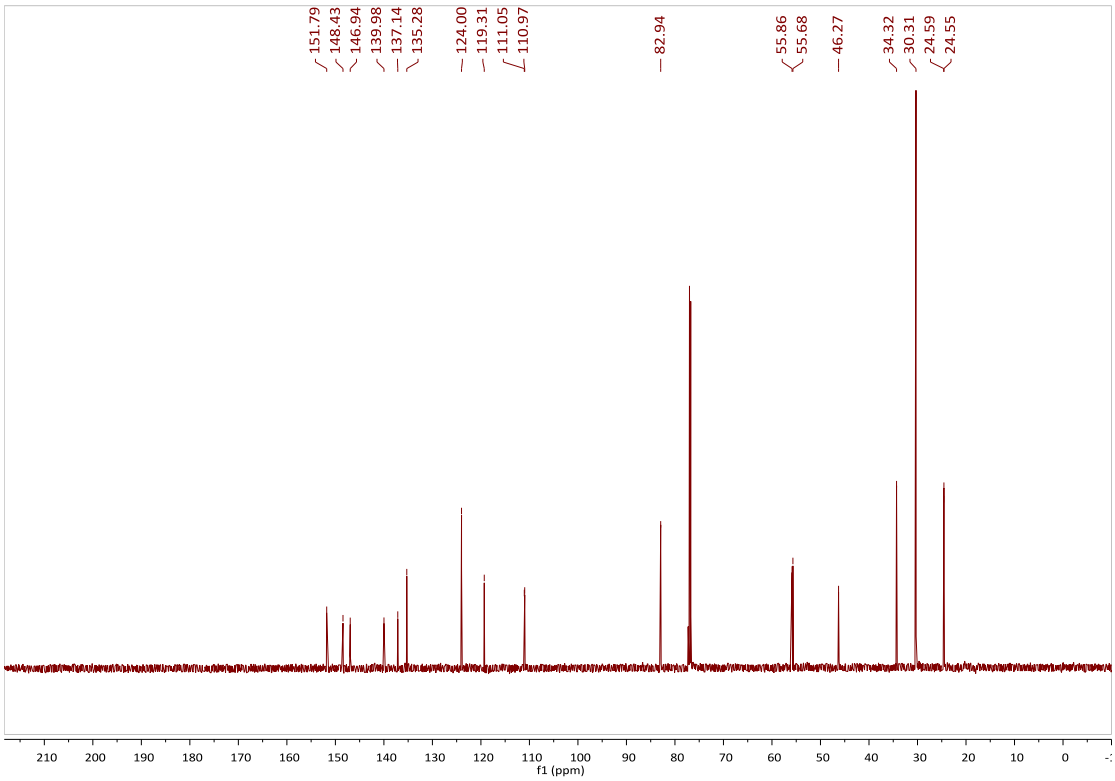
6.86
6.85
6.85
6.80
6.78
5.01
4.16
4.14
4.12
3.87
3.85
1.60
1.60
1.58
1.58
1.42
1.05
2.02
1.00
1.01
0.99
1.00
1.04
3.04
3.07
2.03
18.21
12.01
f1 (ppm)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135.28
124.00
119.31
111.05
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82.94
55.86
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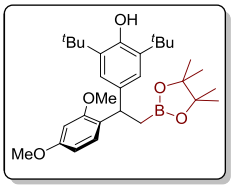
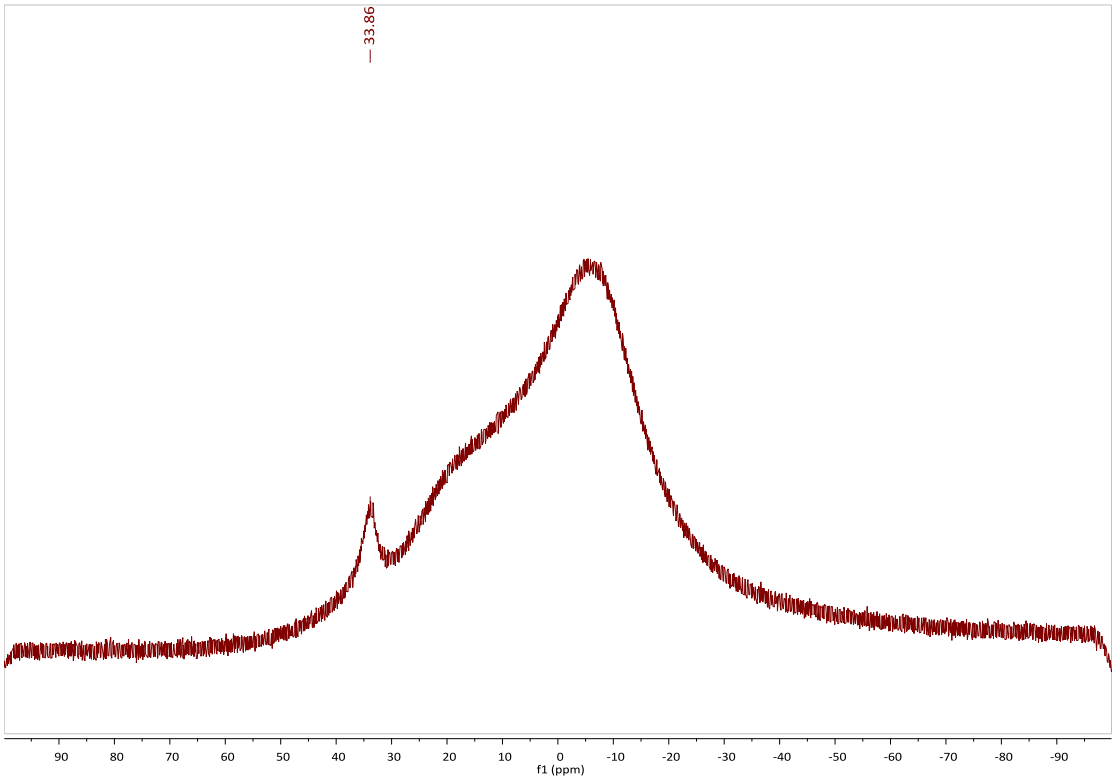
34.32
30.31
24.59
24.55
f1 (ppm)


OH
tBu
tBu
OMe
O
B
O
MeO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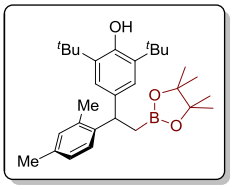
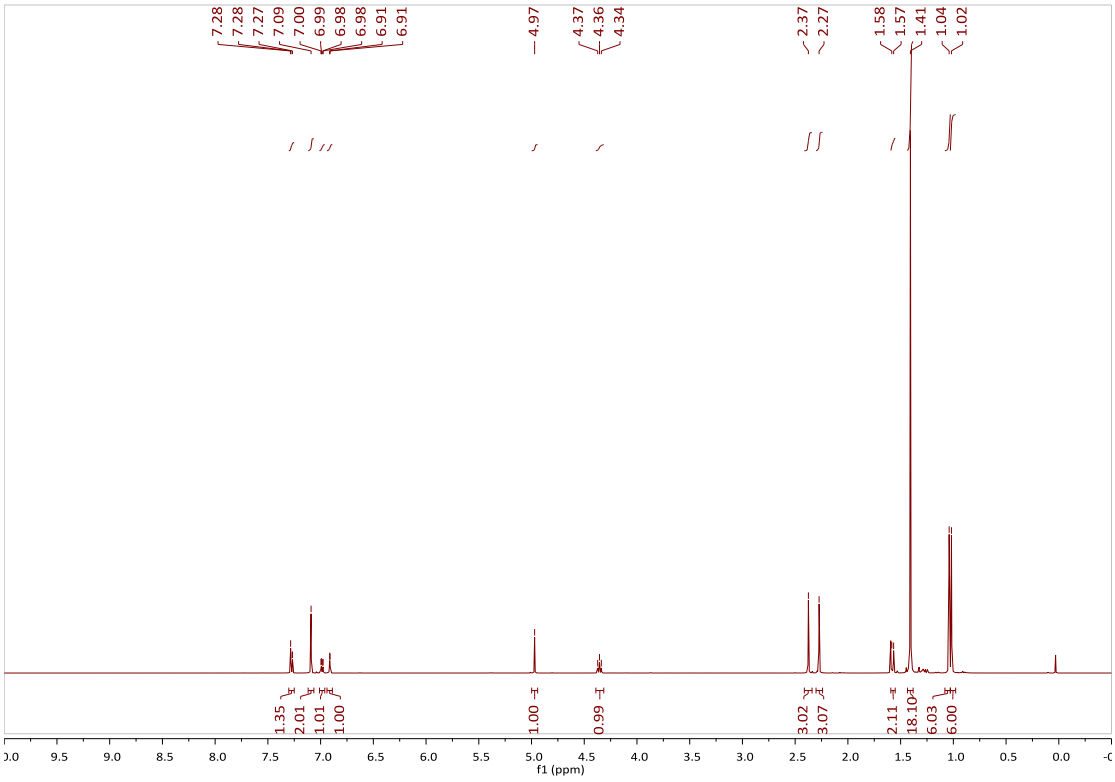
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
Me
Me
O
B
O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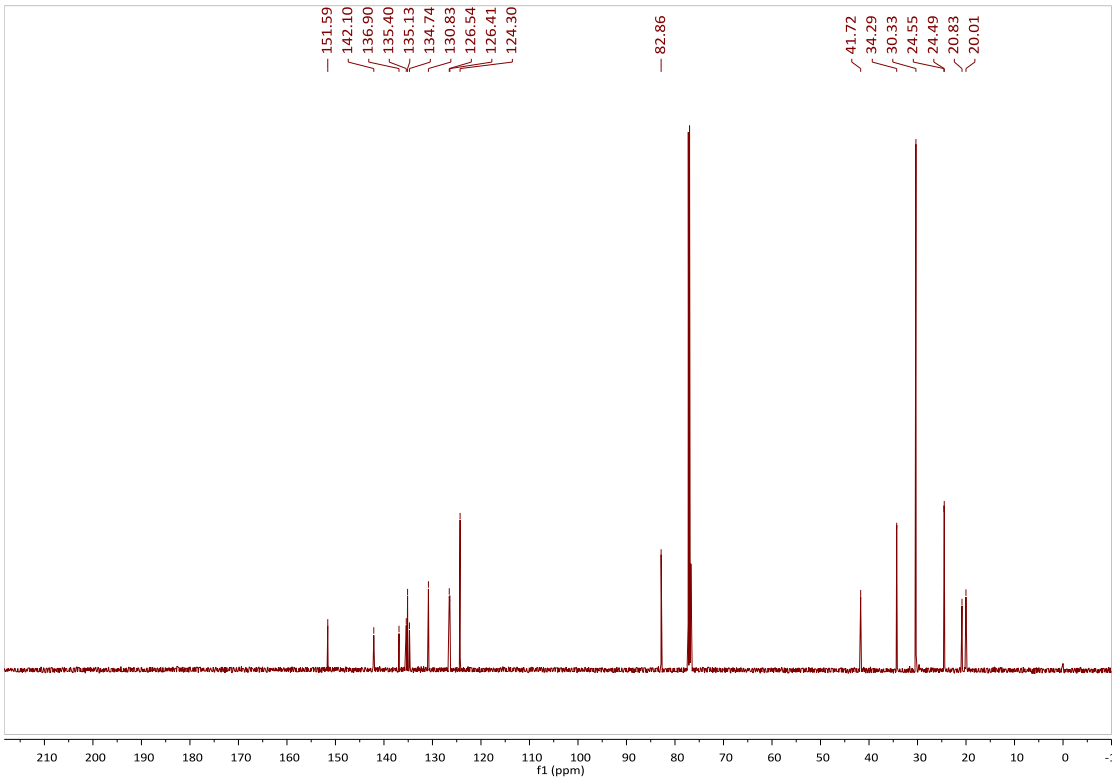
7.28
7.27
7.09
7.00
6.99
6.98
6.98
6.91
6.91
4.97
4.37
4.36
4.34
2.37
2.27
1.58
1.57
1.41
1.04
1.02
1.35
2.01
1.01
1.00
1.00
0.99
3.02
3.07
2.11
18.10
6.03
6.00
f1 (ppm)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142.10
136.90
135.40
135.13
134.74
130.83
126.54
126.41
124.30
82.86
41.72
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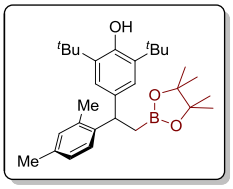
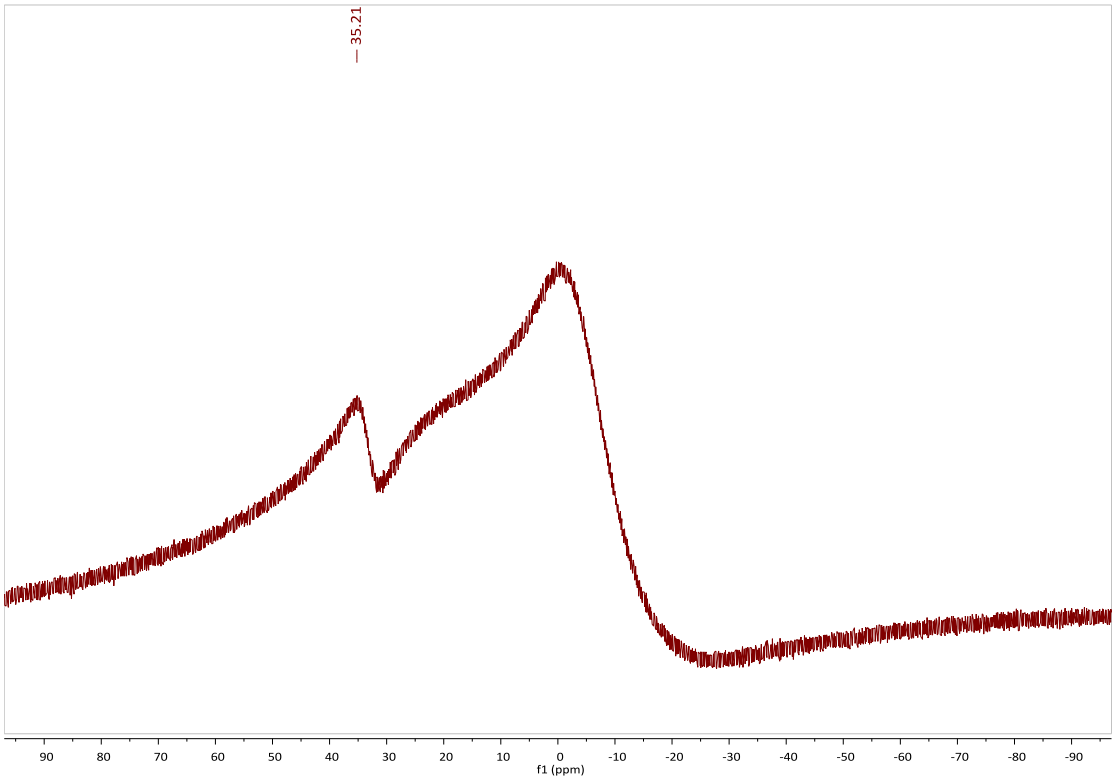
24.55
24.49
20.83
20.01
f1 (ppm)


OH
tBu
tBu
Me
Me
O
B
O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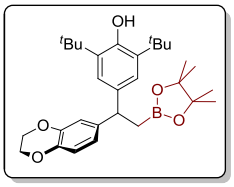
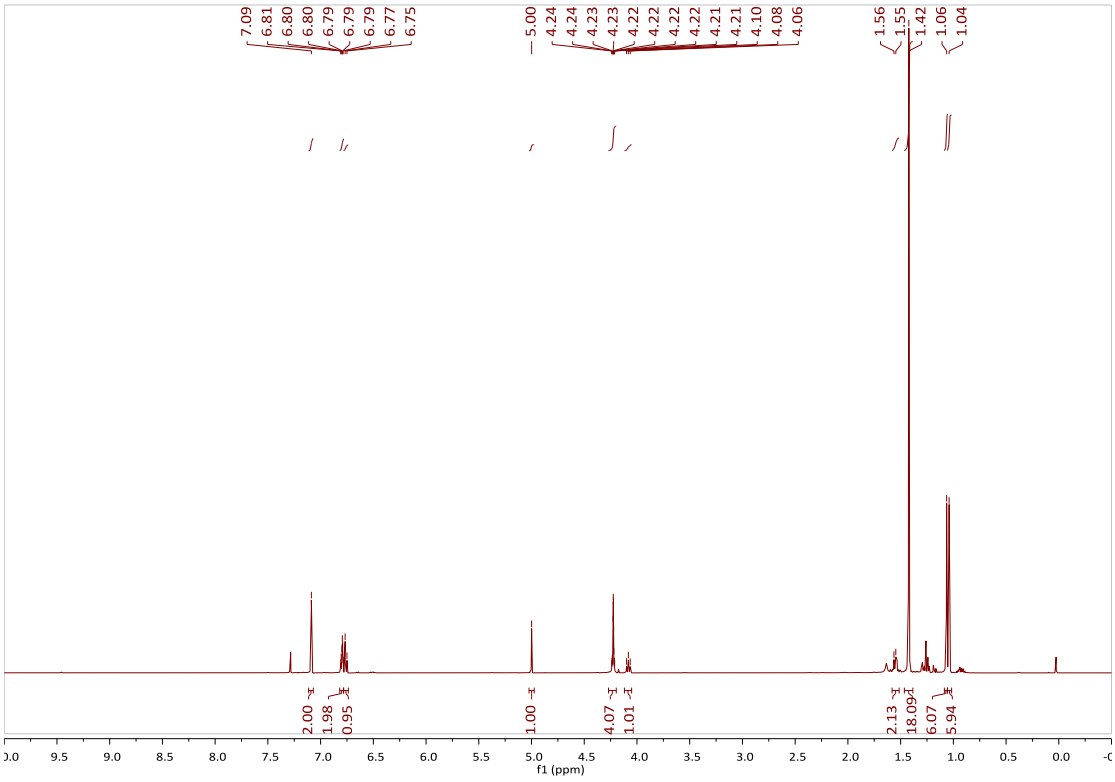
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
O
O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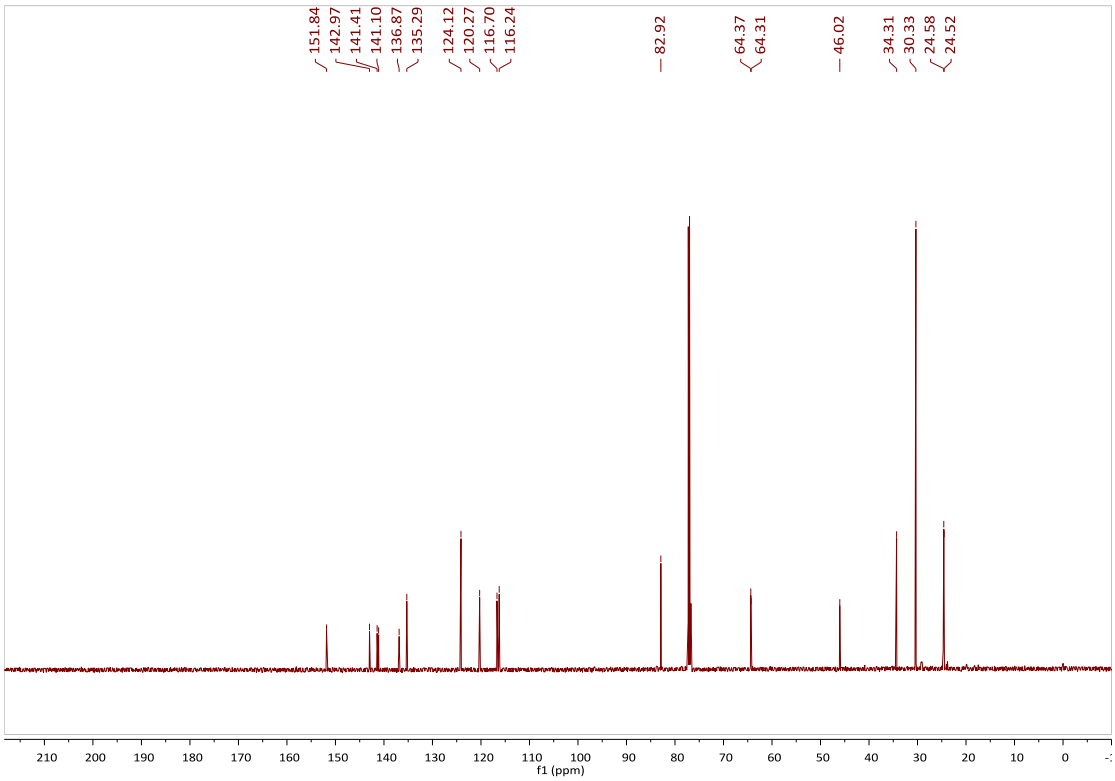
6.80
6.80
6.79
6.79
6.79
6.77
6.75
5.00
4.24
4.24
4.23
4.23
4.22
4.22
4.22
4.22
4.21
4.21
4.10
4.08
4.06
1.56
1.55
1.42
1.06
1.04
2.00
1.98
0.95
1.00
4.07
1.01
2.13
18.09
6.07
5.94
f1 (ppm)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141.10
136.87
135.29
124.12
120.27
116.70
116.24
82.92
64.37
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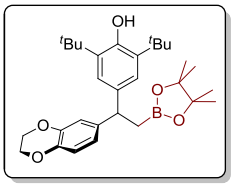
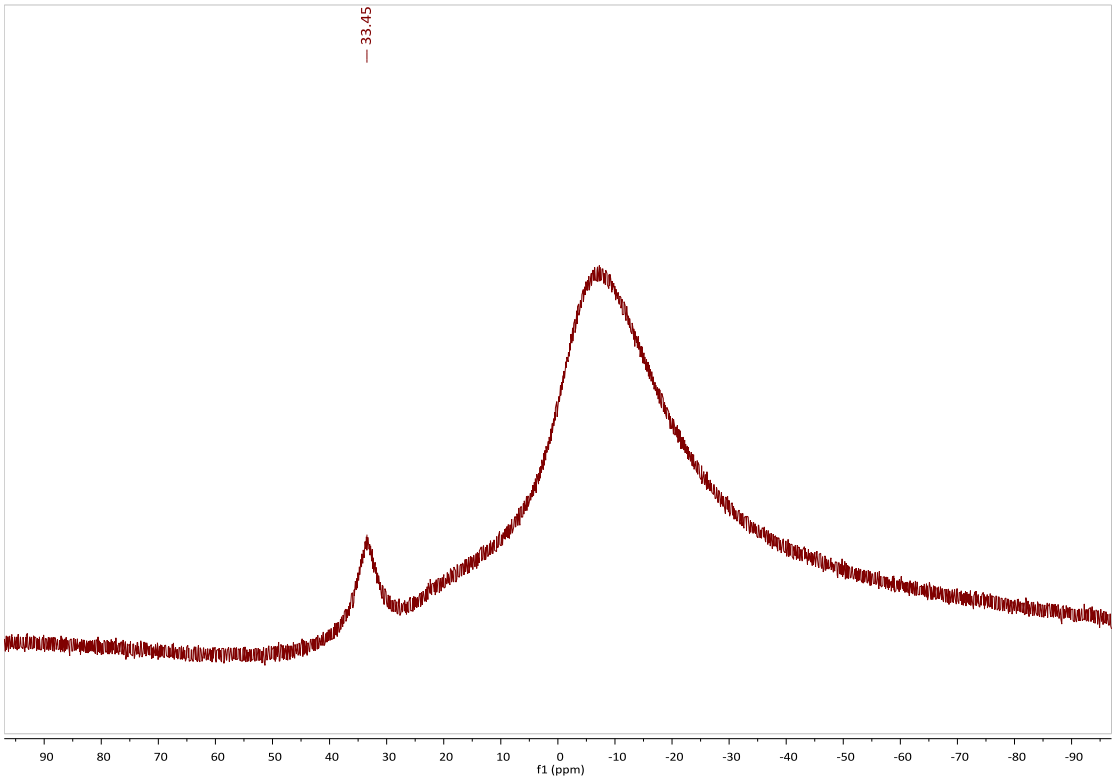
34.31
30.33
24.58
24.52
f1 (ppm)


OH
tBu
tBu
O
B
O
O
O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60
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30
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10
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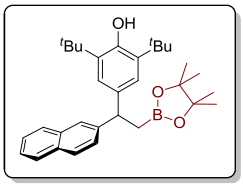
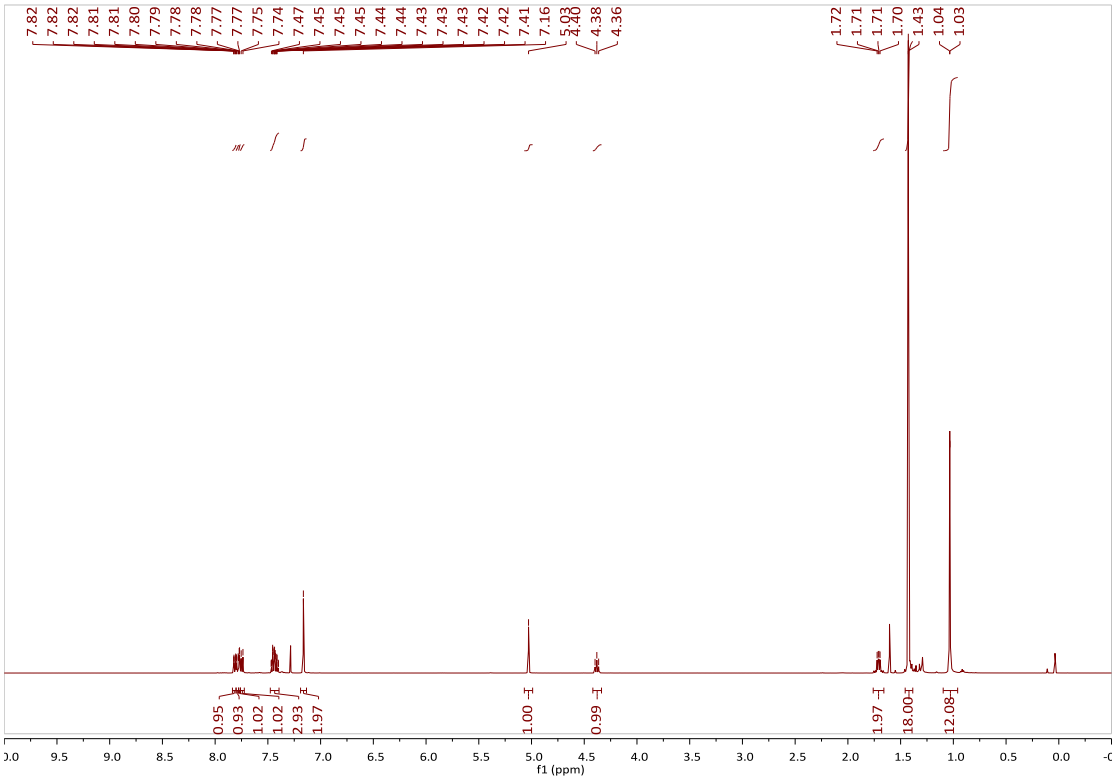
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O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7.82
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7.81
7.80
7.79
7.78
7.78
7.77
7.77
7.75
7.74
7.47
7.45
7.45
7.45
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.41
7.16
5.03
4.40
4.38
4.36
1.72
1.71
1.71
1.70
1.43
1.04
1.03
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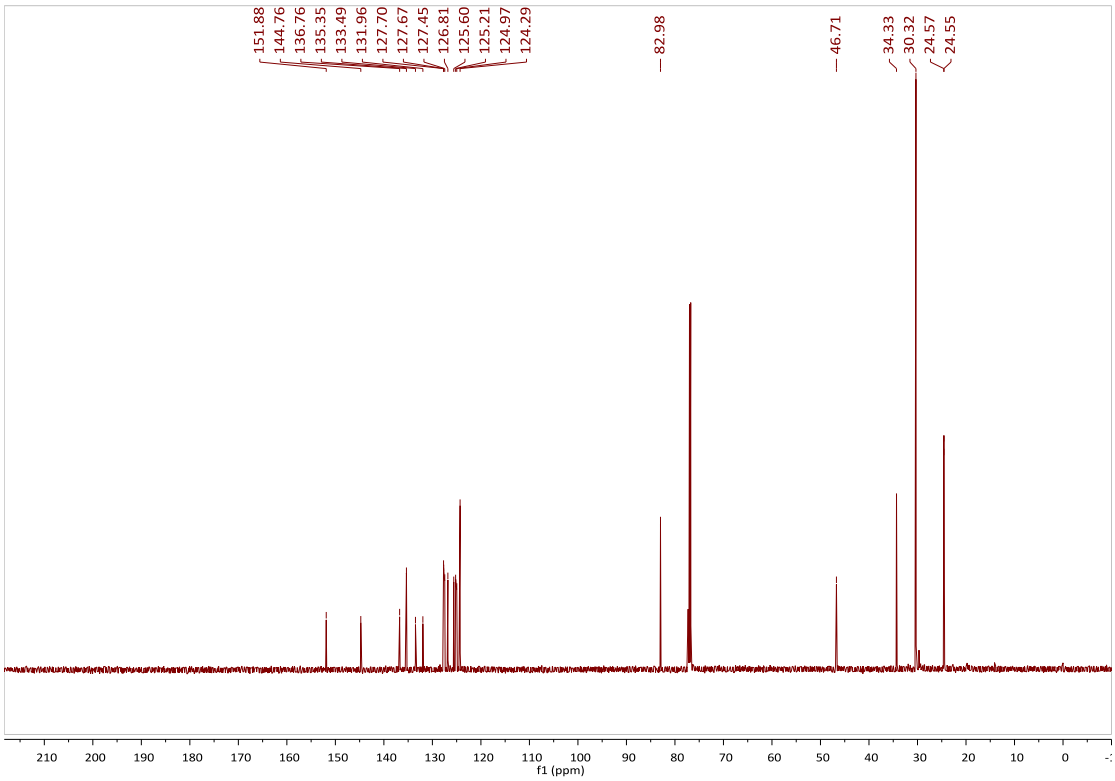
1.02
2.93
1.97
1.00
0.99
1.97
18.00
12.08
f1 (ppm)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127.70
127.67
127.45
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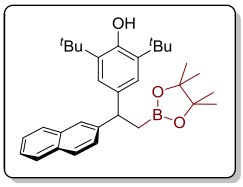
124.97
124.29
82.98
46.71
34.33
30.32
24.57
24.55
f1 (ppm)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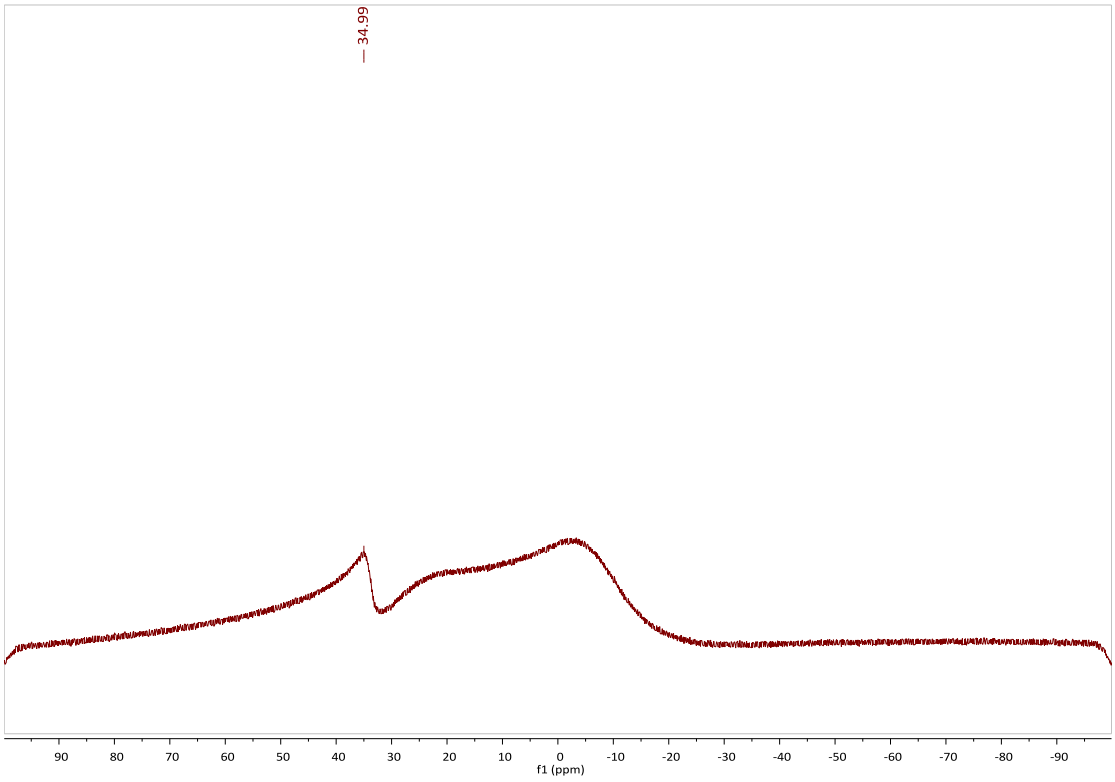
tBu
O
B
O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60
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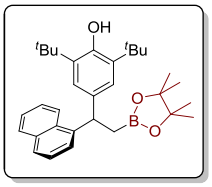
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)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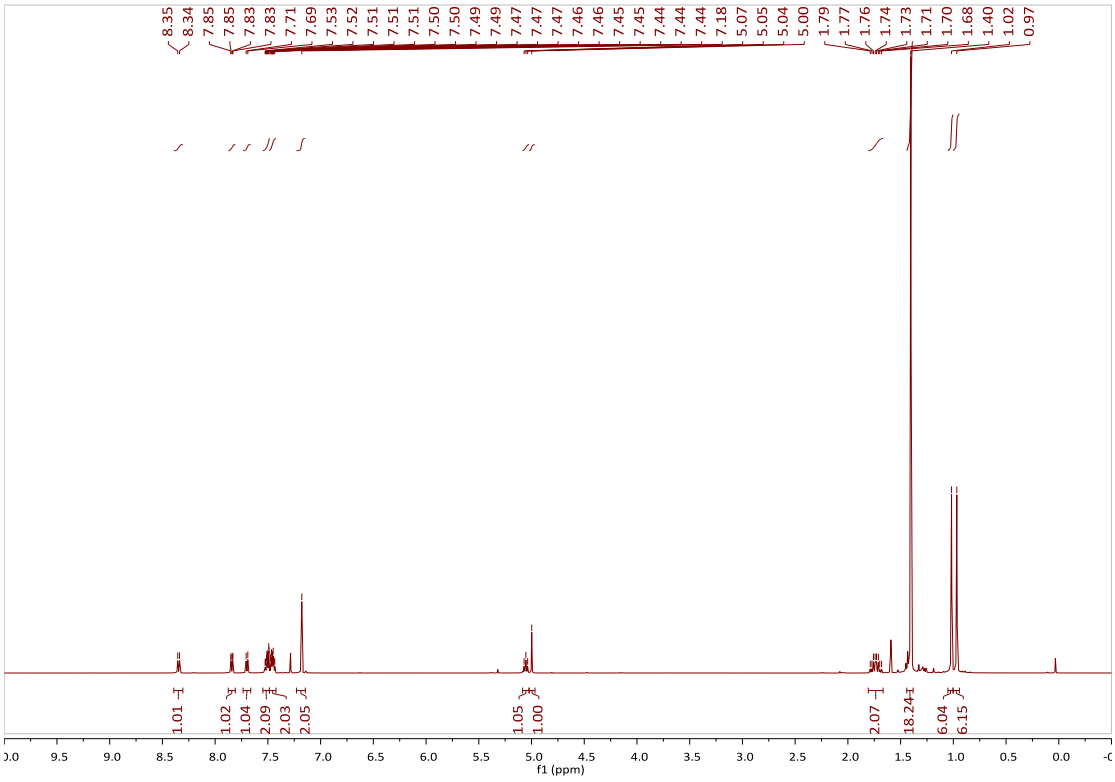
tBu
tBu
O
B
O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7.49
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7.45
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5.04
5.00
1.79
1.77
1.76
1.74
1.73
1.71
1.70
1.68
1.40
1.02
0.97
1.01
1.02
1.04
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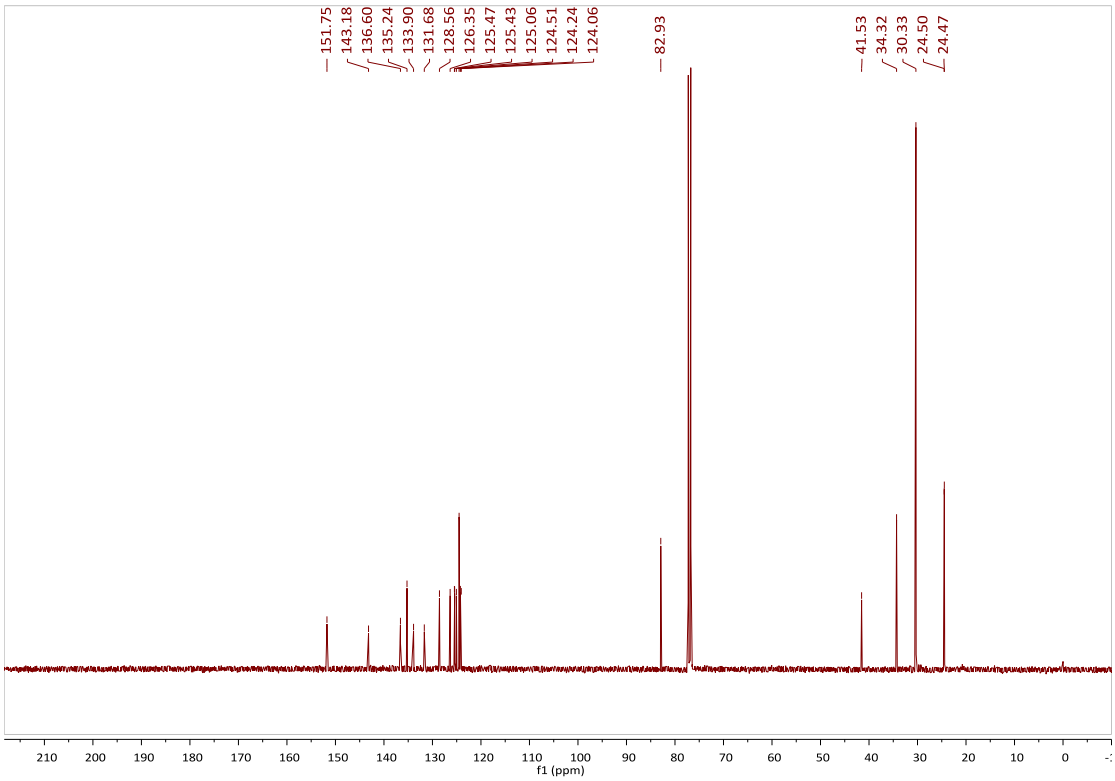
2.03
2.05
1.05
1.00
2.07
18.24
6.04
6.15
f1 (ppm)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125.47
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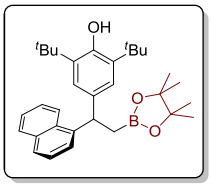
34.32
30.33
24.50
24.47
f1 (ppm)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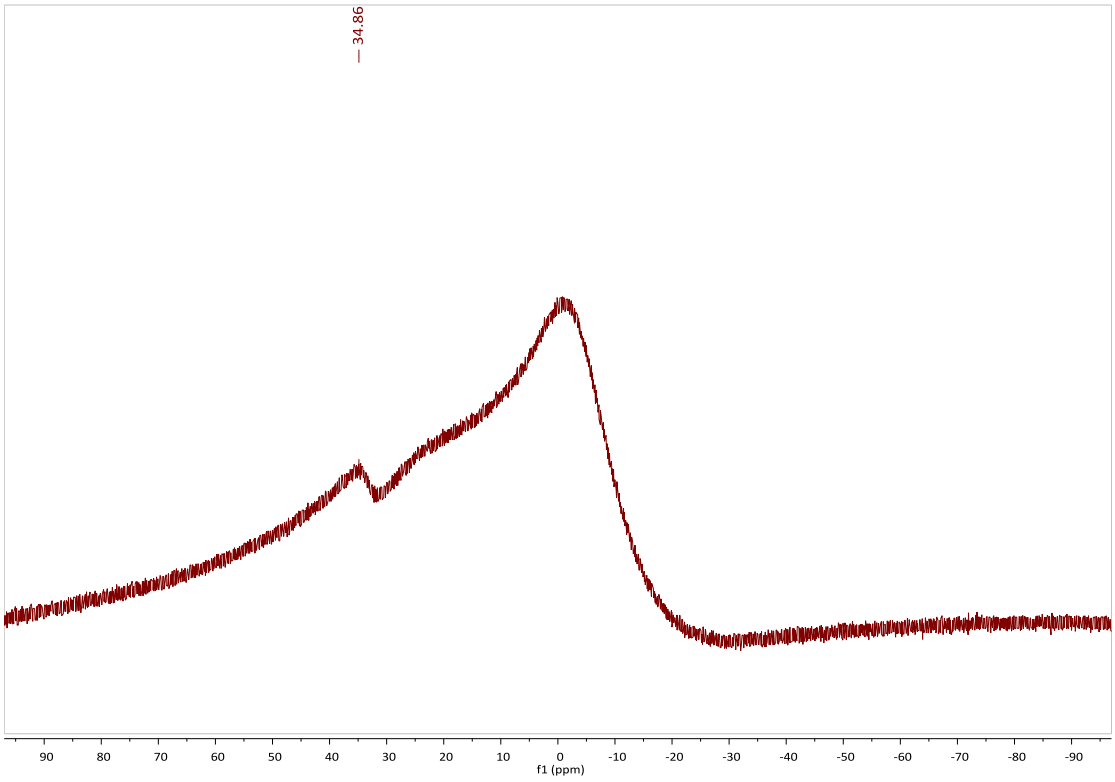
tBu
O
B
O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60
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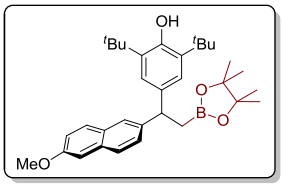
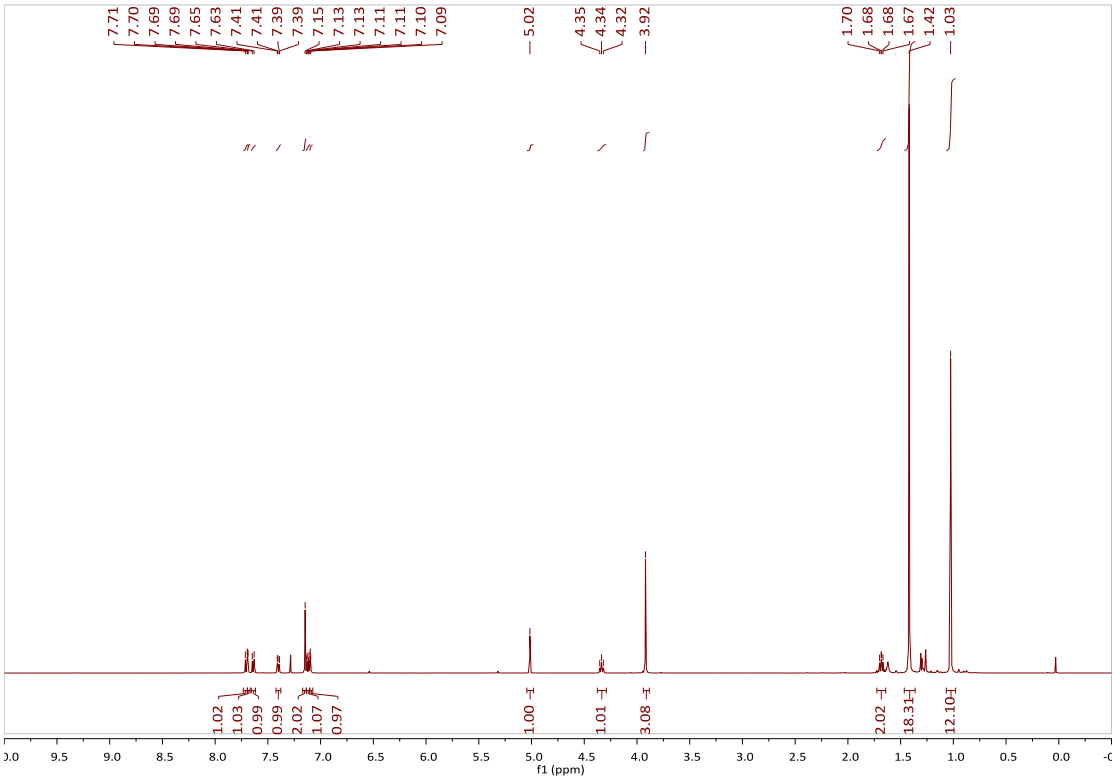
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
MeO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7.69
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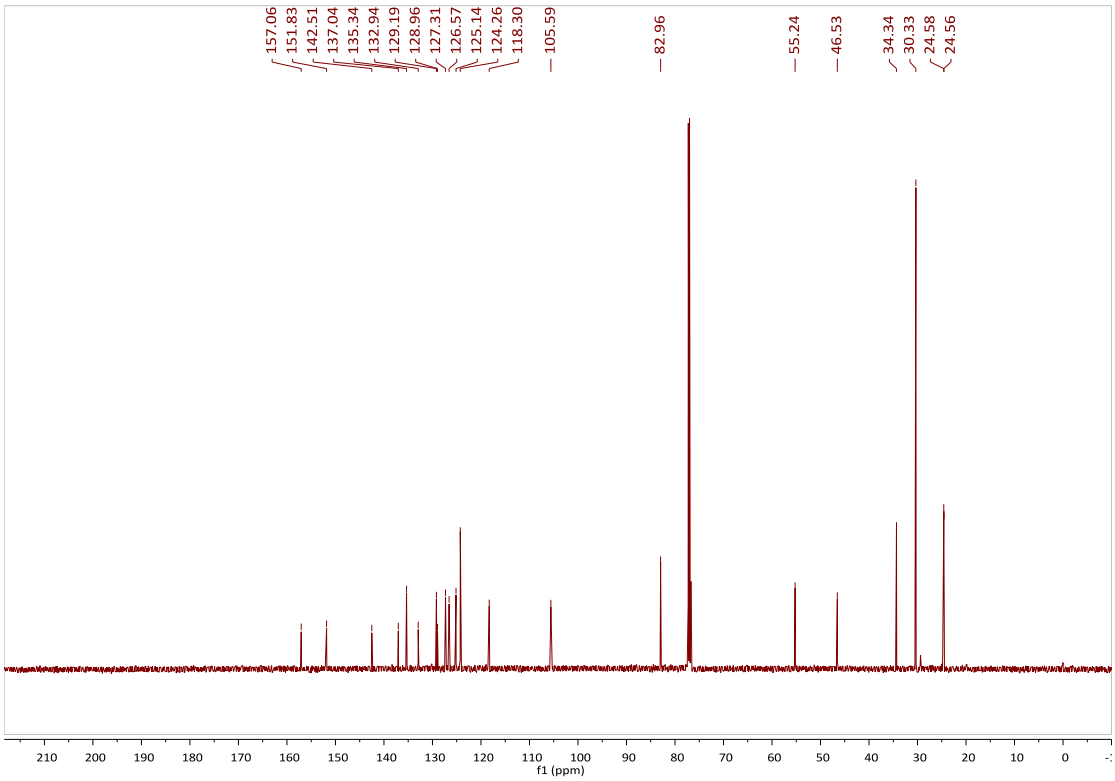
7.39
7.15
7.13
7.13
7.11
7.11
7.10
7.09
5.02
4.35
4.34
4.32
3.92
1.70
1.68
1.68
1.67
1.42
1.03
1.02
1.03
0.99
0.99
2.02
1.07
0.97
1.00
1.01
3.08
2.02
18.31
12.10
f1 (ppm)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127.31
126.57
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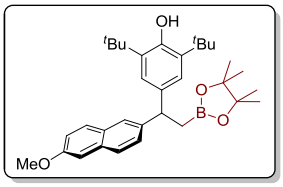
34.34
30.33
24.58
24.56
f1 (ppm)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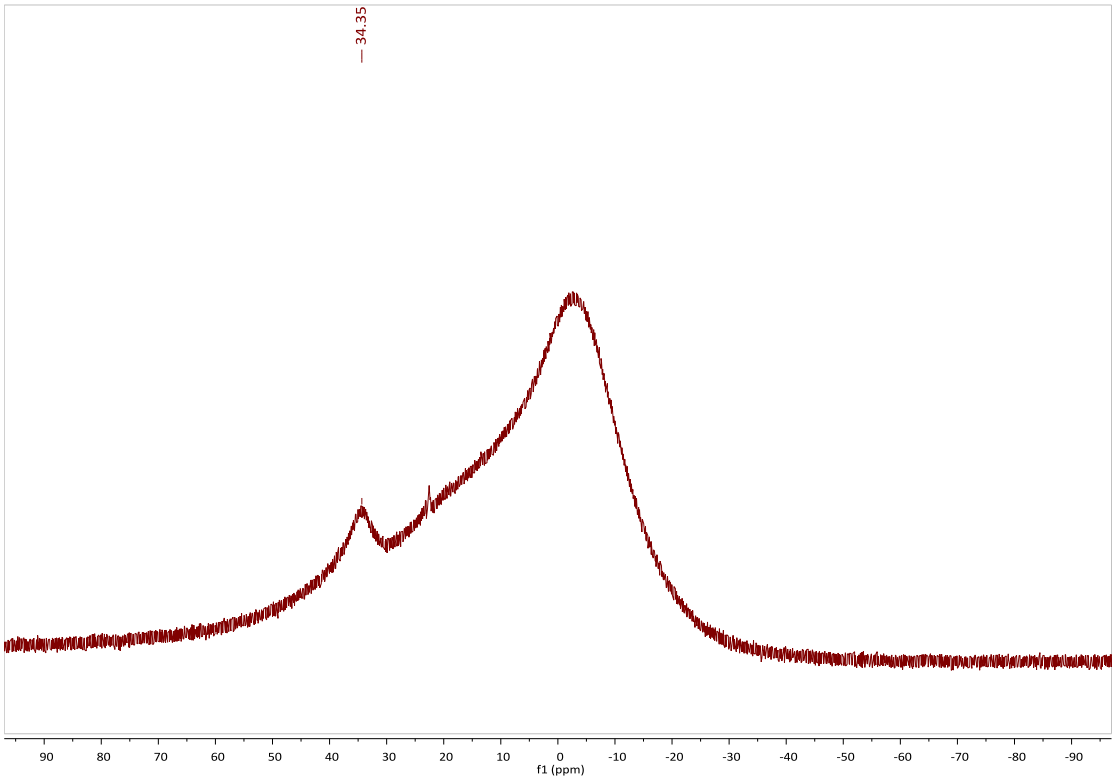
tBu
tBu
O
B
O
MeO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60
50
40
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10
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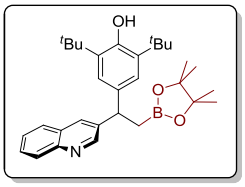
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
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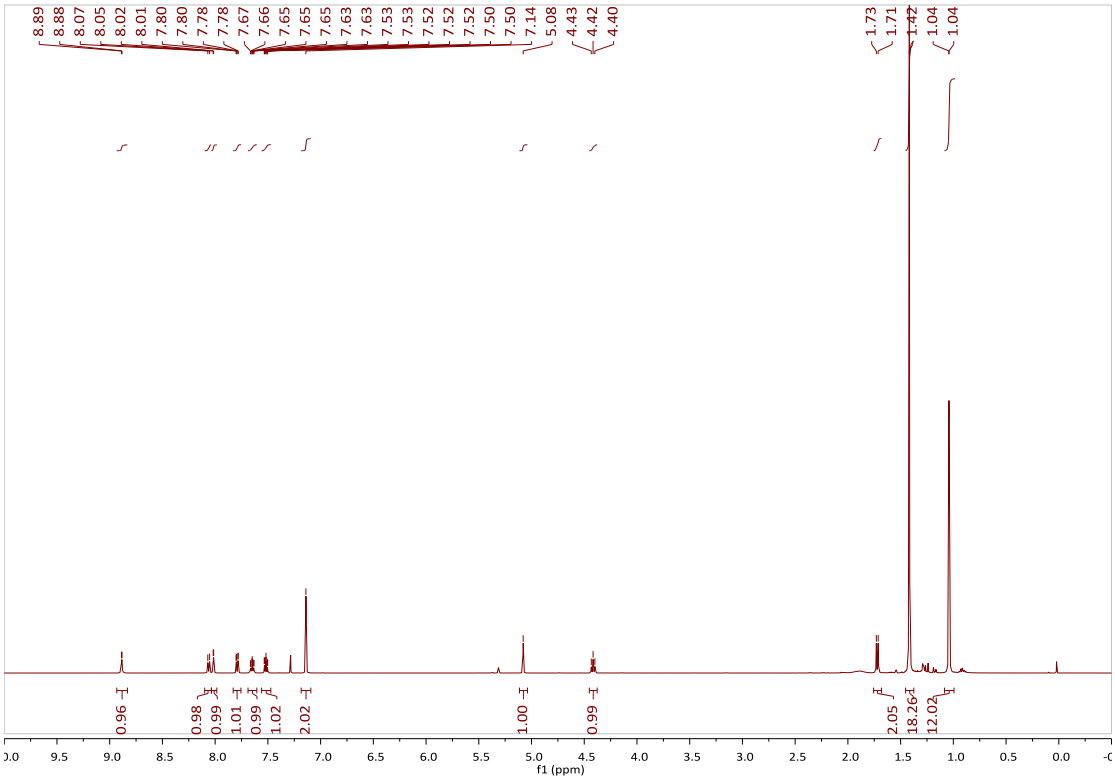
tBu
O
B
O
N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7.63
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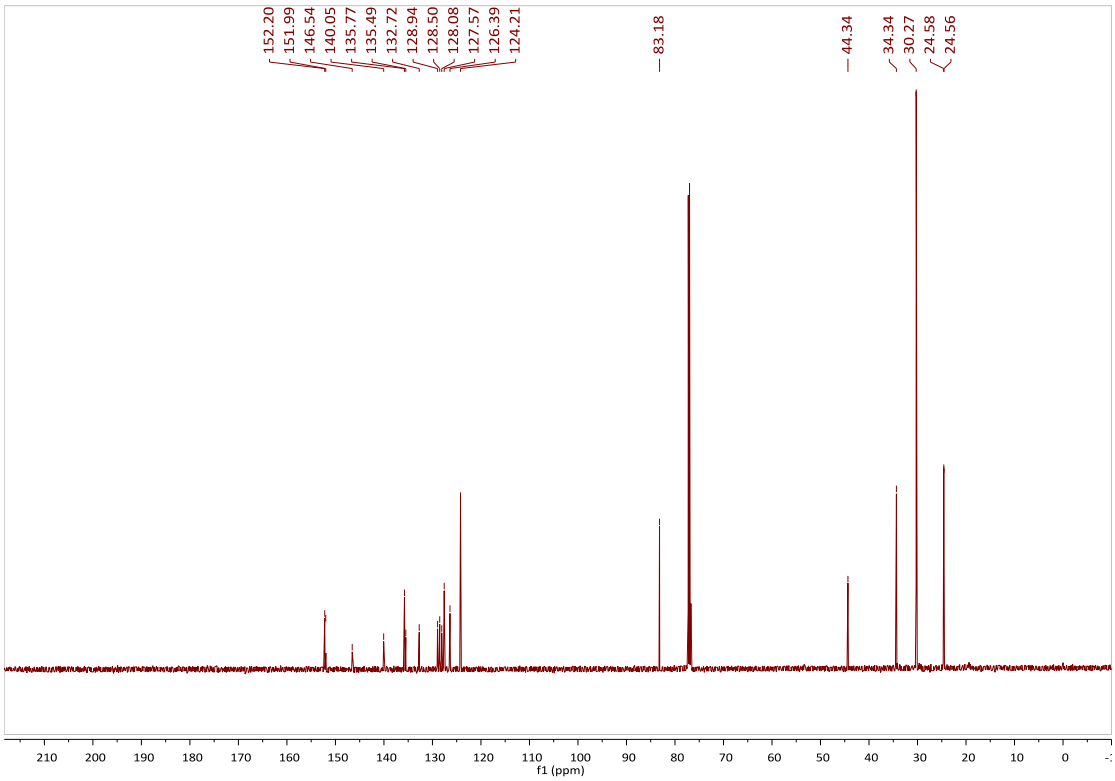
7.52
7.52
7.52
7.50
7.50
7.14
5.08
4.43
4.42
4.40
1.73
1.71
1.42
1.04
1.04
0.96
0.98
0.99
1.01
0.99
1.02
2.02
1.00
0.99
2.05
18.26
12.02
f1 (ppm)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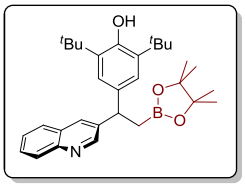
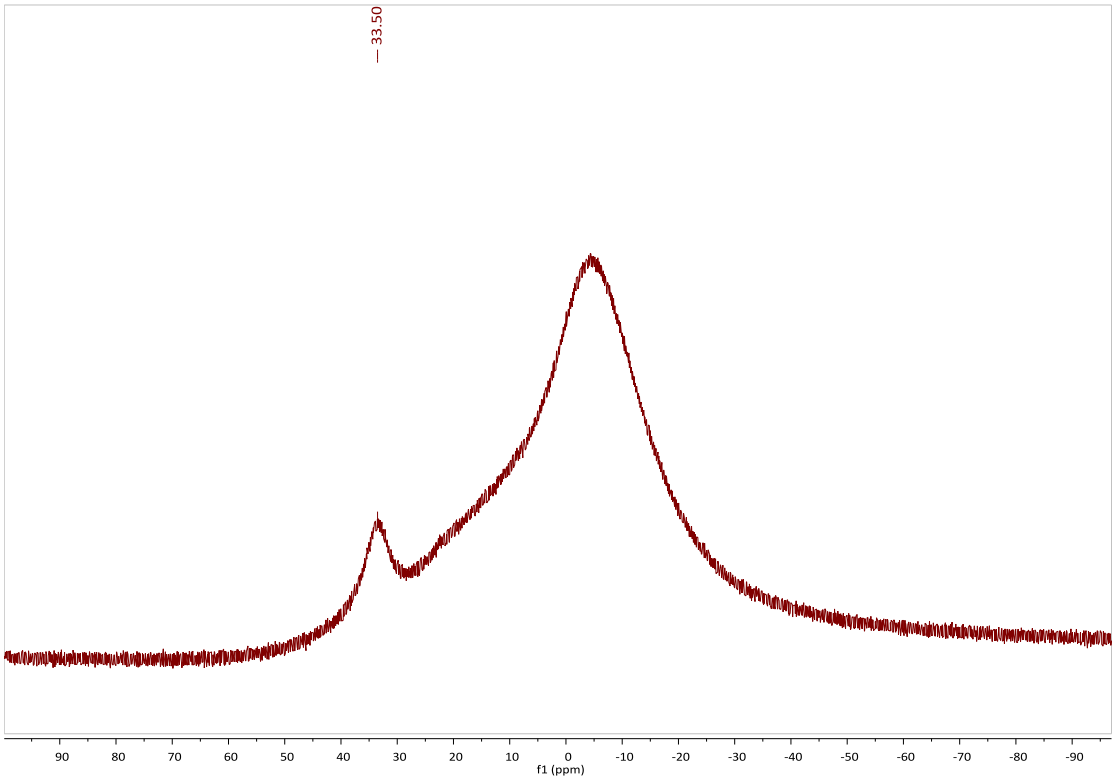
135.77
135.49
132.72
128.94
128.50
128.08
127.57
126.39
124.21
83.18
44.34
34.34
30.27
24.58
24.56
f1 (ppm)


OH
tBu
tBu
O
B
O
N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90
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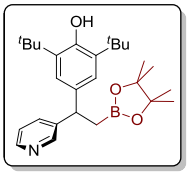
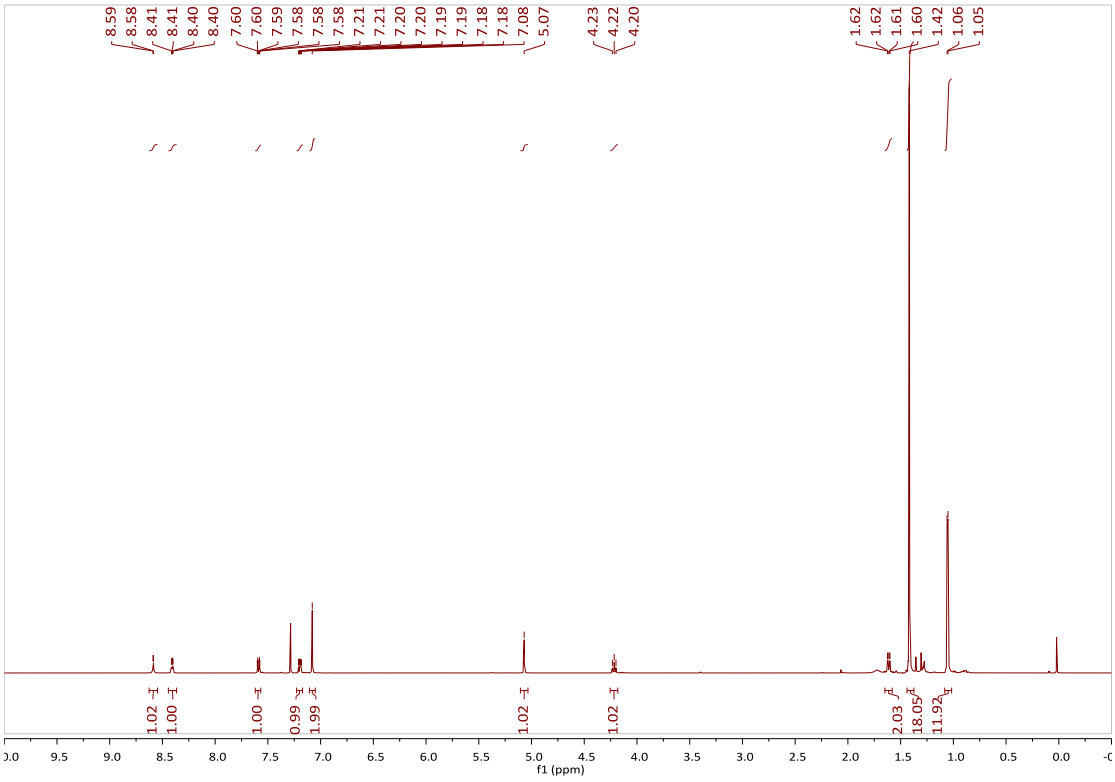
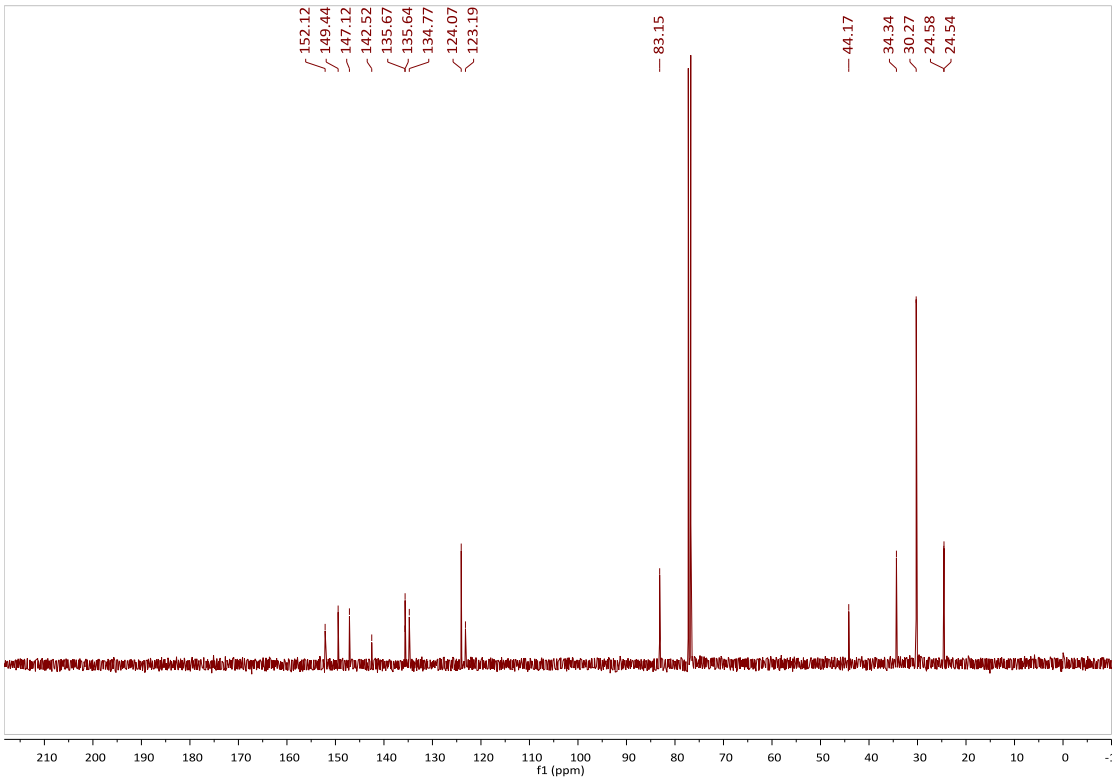
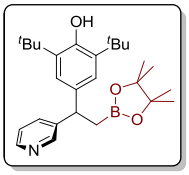
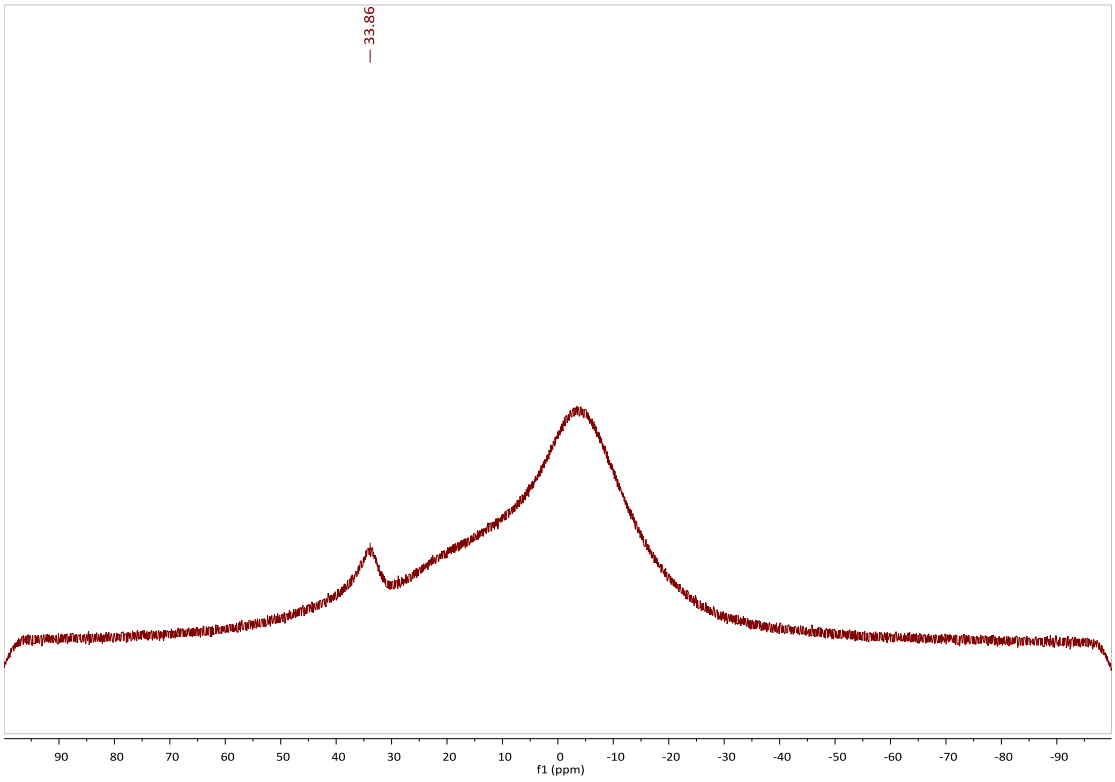
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
N


8.59
8.58
8.41
8.41
8.40
8.40
7.60
7.60
7.59
7.58
7.58
7.58
7.21
7.21
7.20
7.20
7.19
7.19
7.18
7.18
7.08
5.07
4.23
4.22
4.20
1.62
1.62
1.61
1.60
1.42
1.06
1.05
1.02
1.00
1.00
0.99
1.99
1.02
1.02
2.03
18.05
11.92
f1 (ppm)


152.12
149.44
147.12
142.52
135.67
135.64
134.77
124.07
123.19
83.15
44.17
34.34
30.27
24.58
24.54
f1 (ppm)


OH
tBu
tBu
O
B
O
N


33.86
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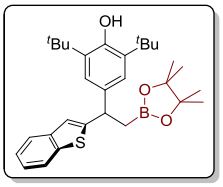
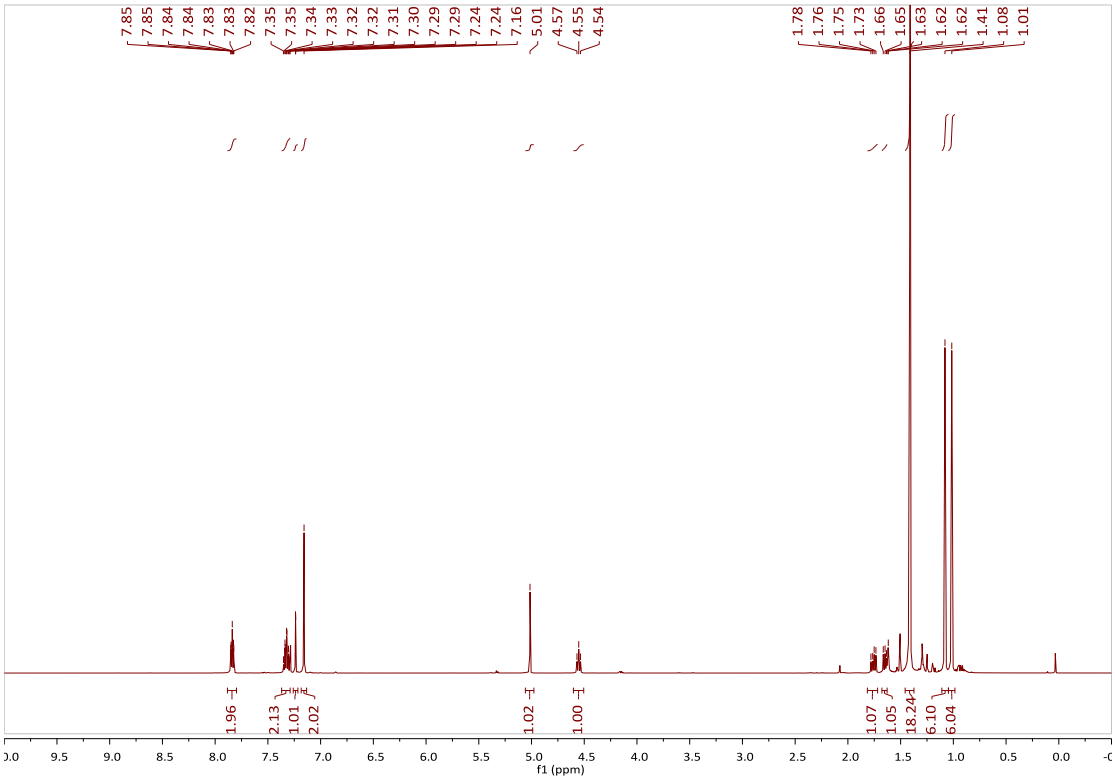
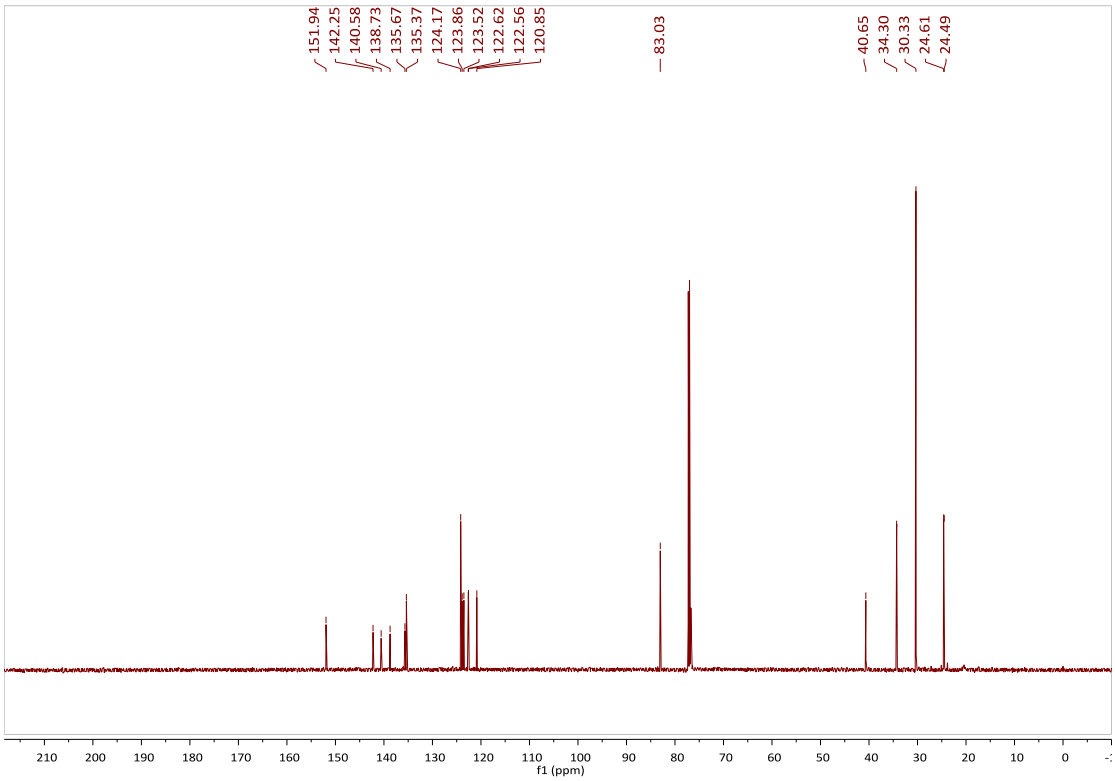
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
S


7.85
7.85
7.84
7.84
7.83
7.83
7.82
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.29
7.24
7.24
7.16
5.01
4.57
4.55
4.54
1.78
1.76
1.75
1.73
1.66
1.65
1.63
1.62
1.62
1.41
1.08
1.01
1.96
2.13
1.01
2.02
1.02
1.00
1.07
1.05
18.24
6.10
6.04
f1 (ppm)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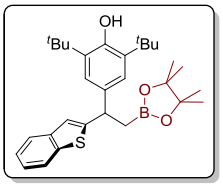
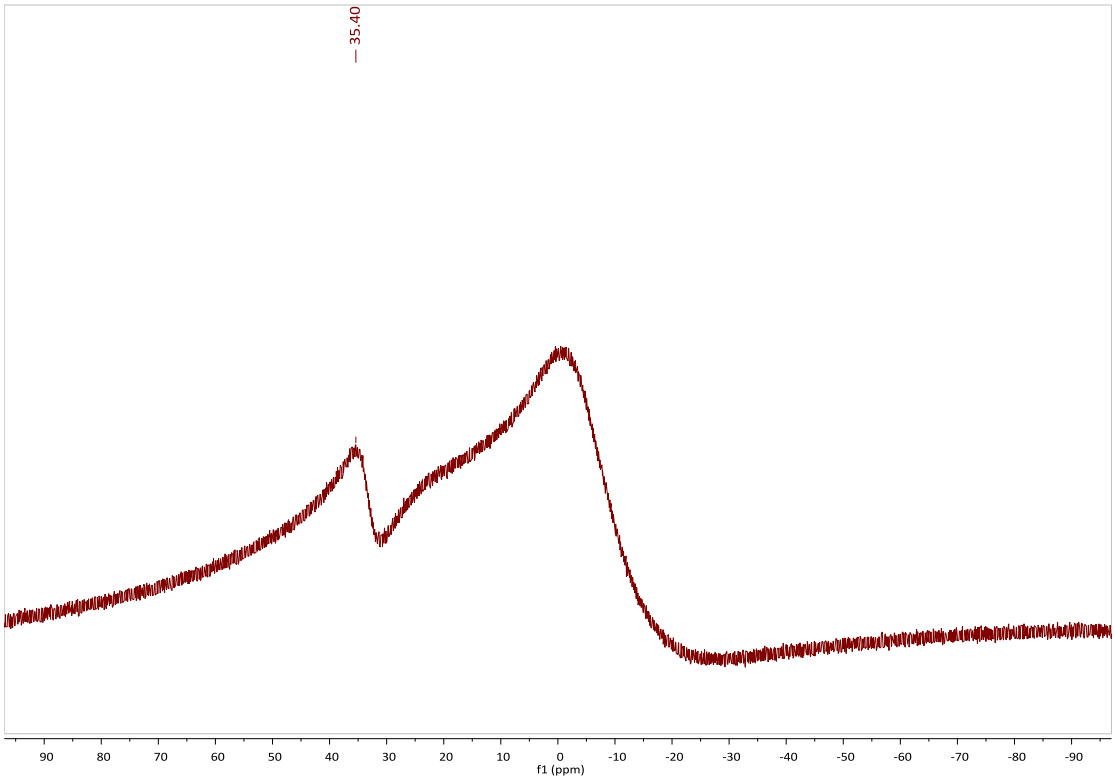
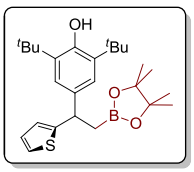
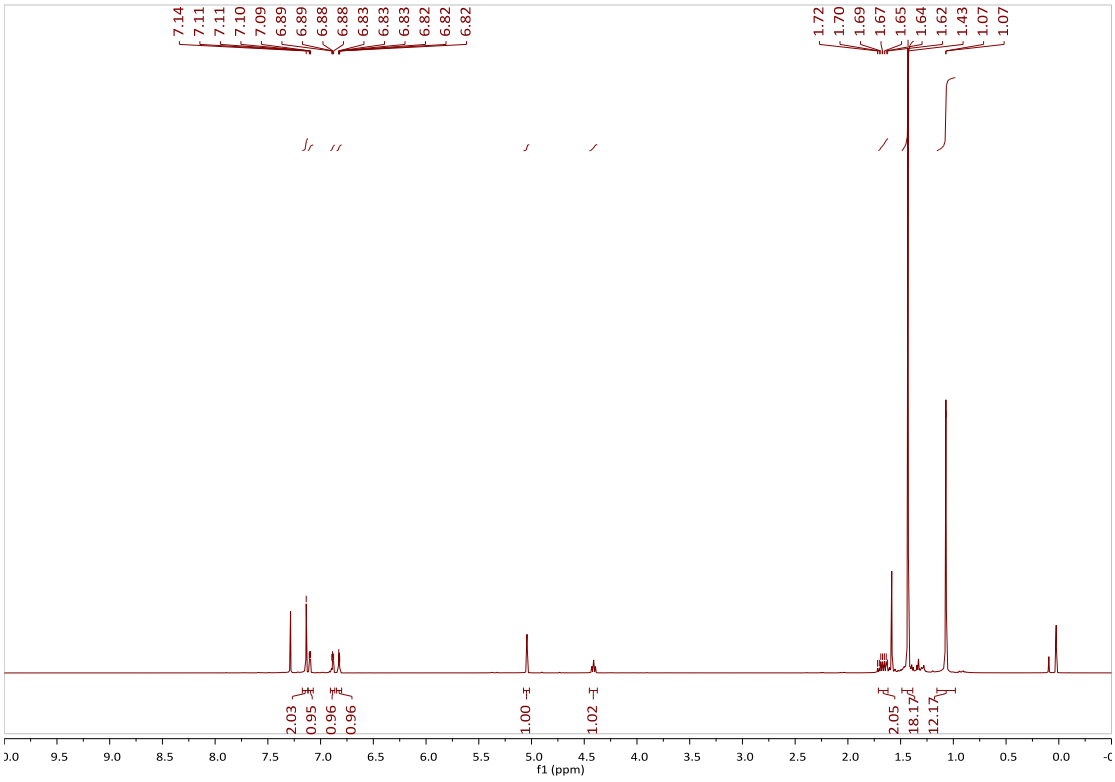
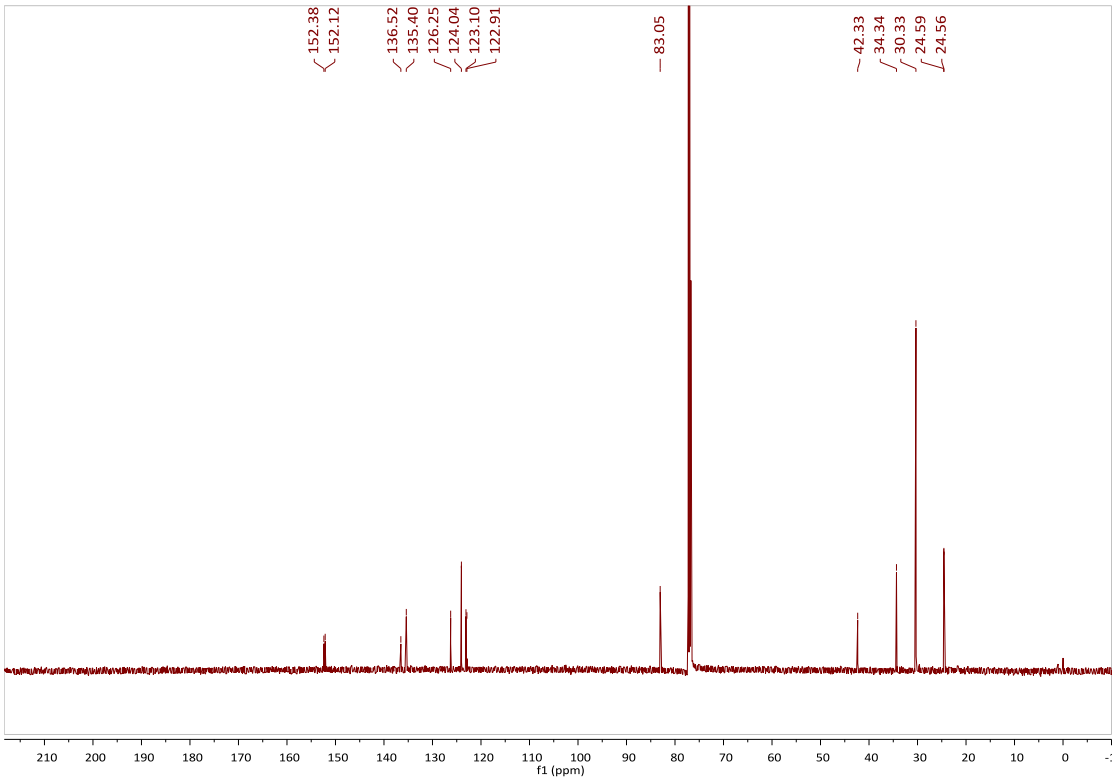
142.25
140.58
138.73
135.67
135.37
124.17
123.86
123.52
122.62
122.56
120.85
83.03
40.65
34.30
30.33
24.61
24.49
f1 (ppm)

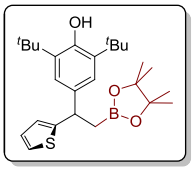

OH
tBu
tBu
O
B
O
S

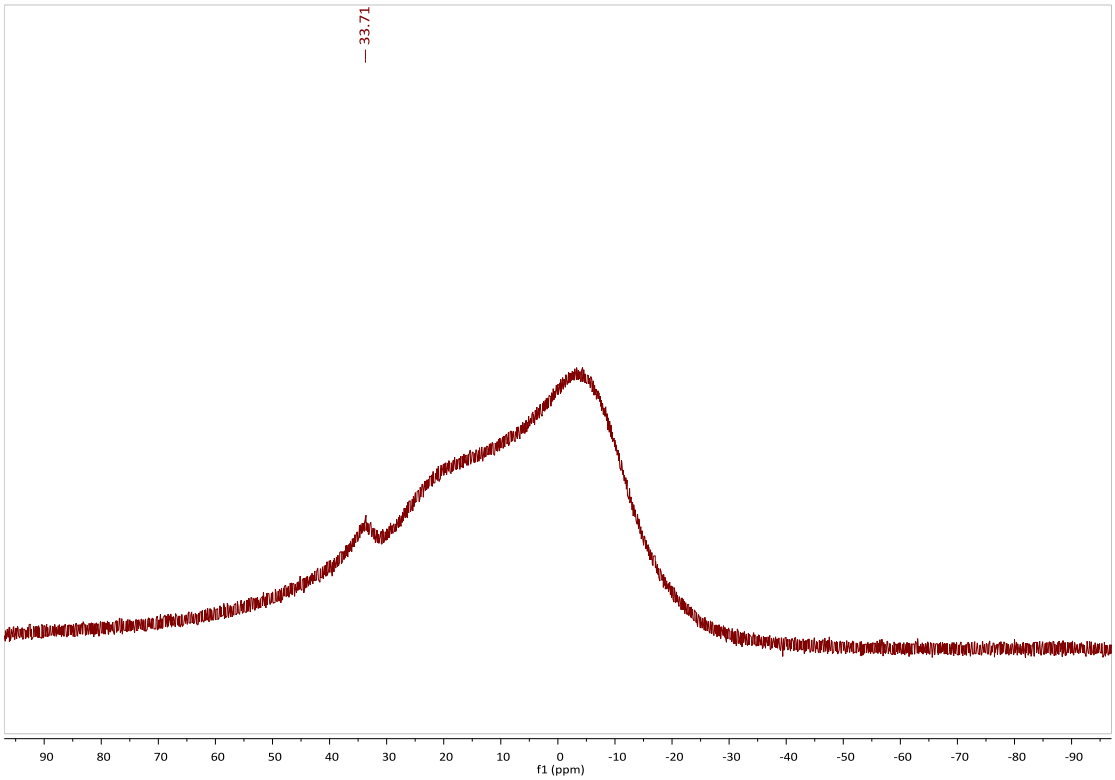

35.40
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

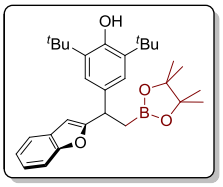

OH
tBu
tBu
O
B
O
S

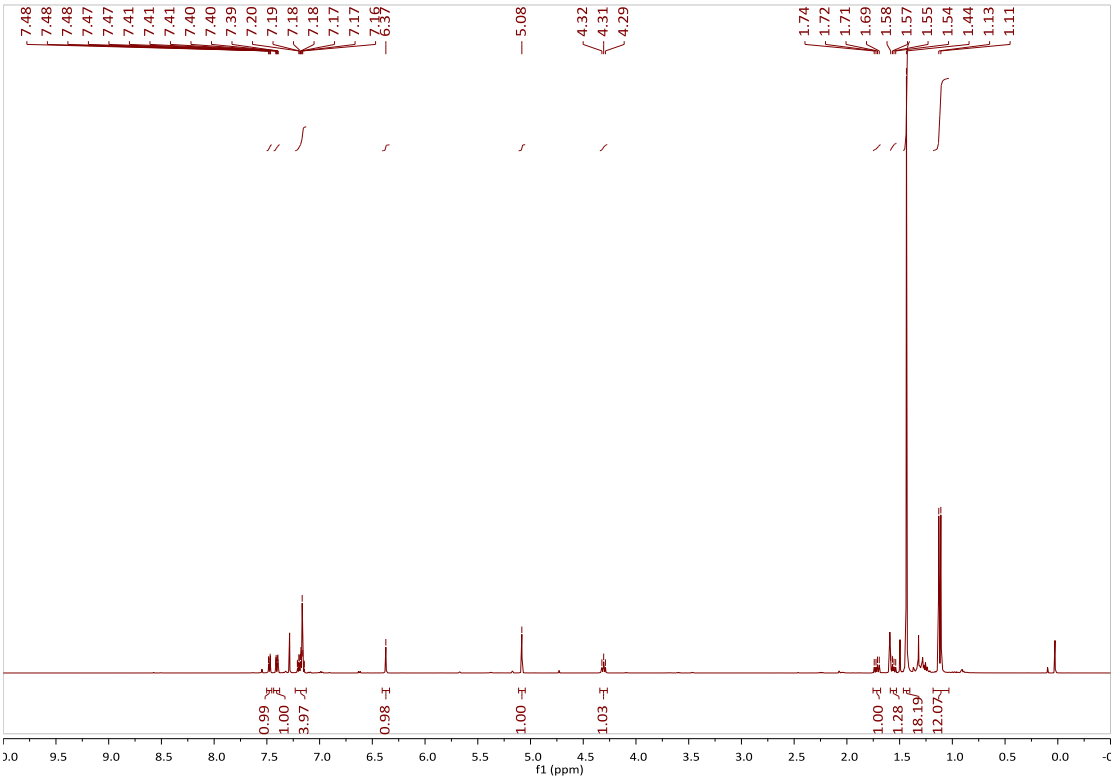

7.14
7.11
7.11
7.10
7.09
6.89
6.89
6.88
6.88
6.83
6.83
6.83
6.82
6.82
6.82
1.72
1.70
1.69
1.67
1.65
1.64
1.62
1.43
1.07
1.07
2.03
0.95
0.96
0.96
1.00
1.02
2.05
18.17
12.17
f1 (ppm)

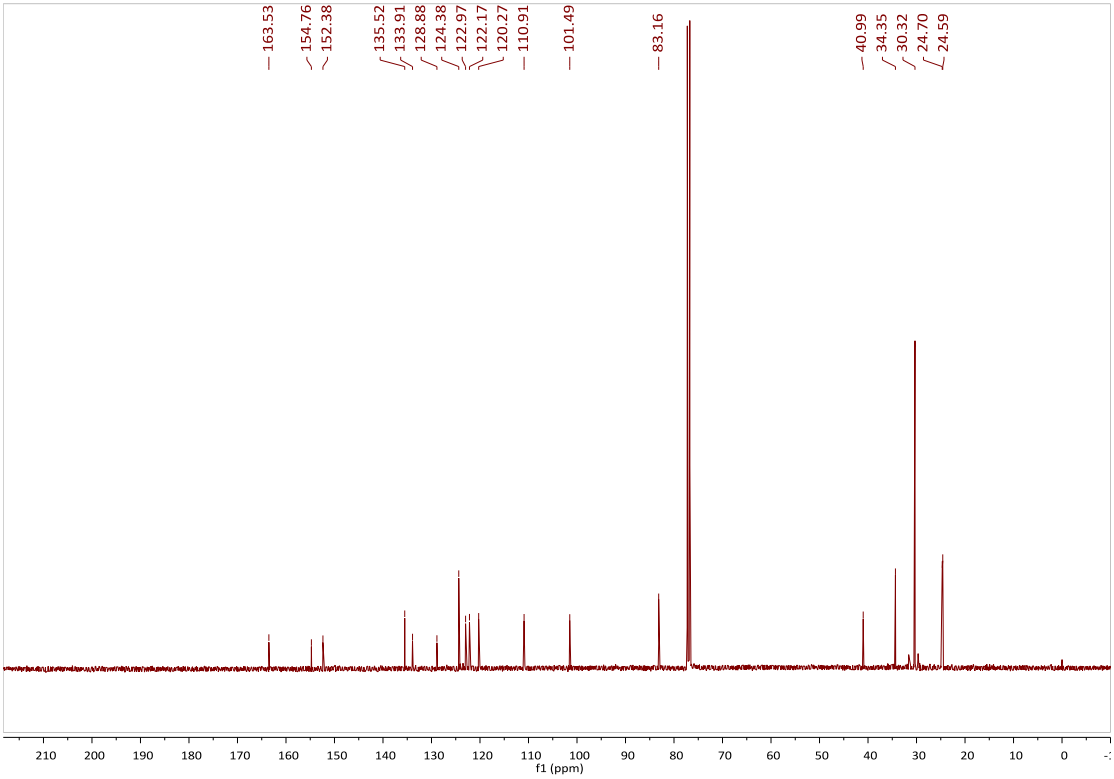

152.38
152.12
136.52
135.40
126.25
124.04
123.10
122.91
83.05
42.33
34.34
30.33
24.59
24.56
f1 (ppm)


OH
tBu
tBu
O
B
O
S


33.71
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
O


7.48
7.48
7.48
7.47
7.47
7.41
7.41
7.41
7.40
7.40
7.39
7.20
7.19
7.18
7.18
7.17
7.17
7.16
6.37
5.08
4.32
4.31
4.29
1.74
1.72
1.71
1.69
1.58
1.57
1.55
1.54
1.44
1.13
1.11
0.99
1.00
3.97
0.98
1.00
1.03
1.00
1.28
18.19
12.07
f1 (ppm)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154.76
152.38
135.52
133.91
128.88
124.38
122.97
122.17
120.27
110.91
101.49
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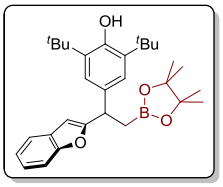
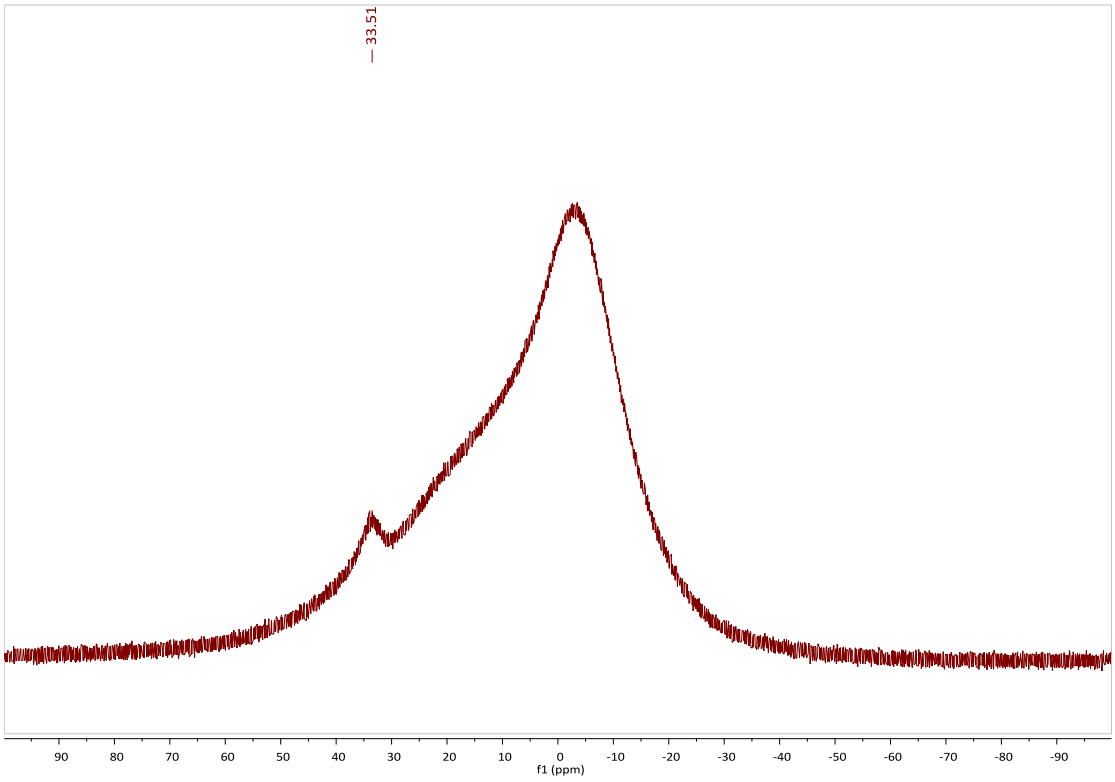
40.99
34.35
30.32
24.70
24.59
f1 (ppm)


OH
tBu
tBu
O
B
O
O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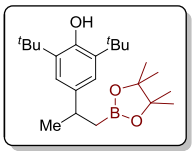
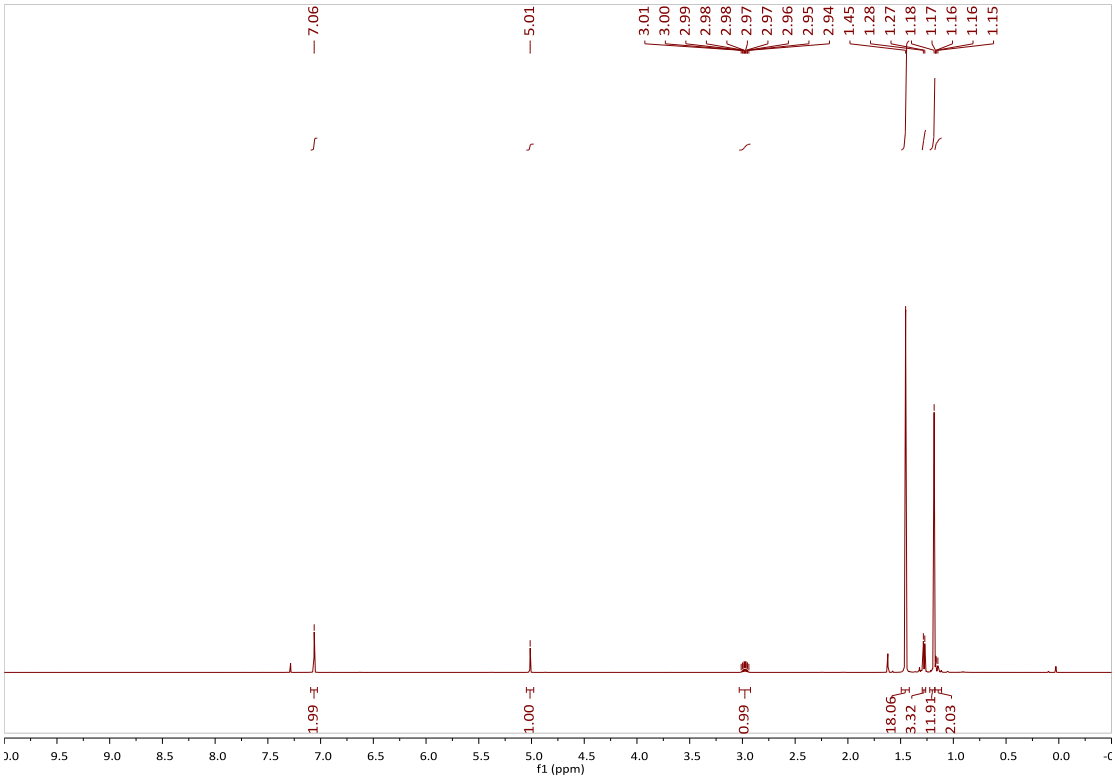
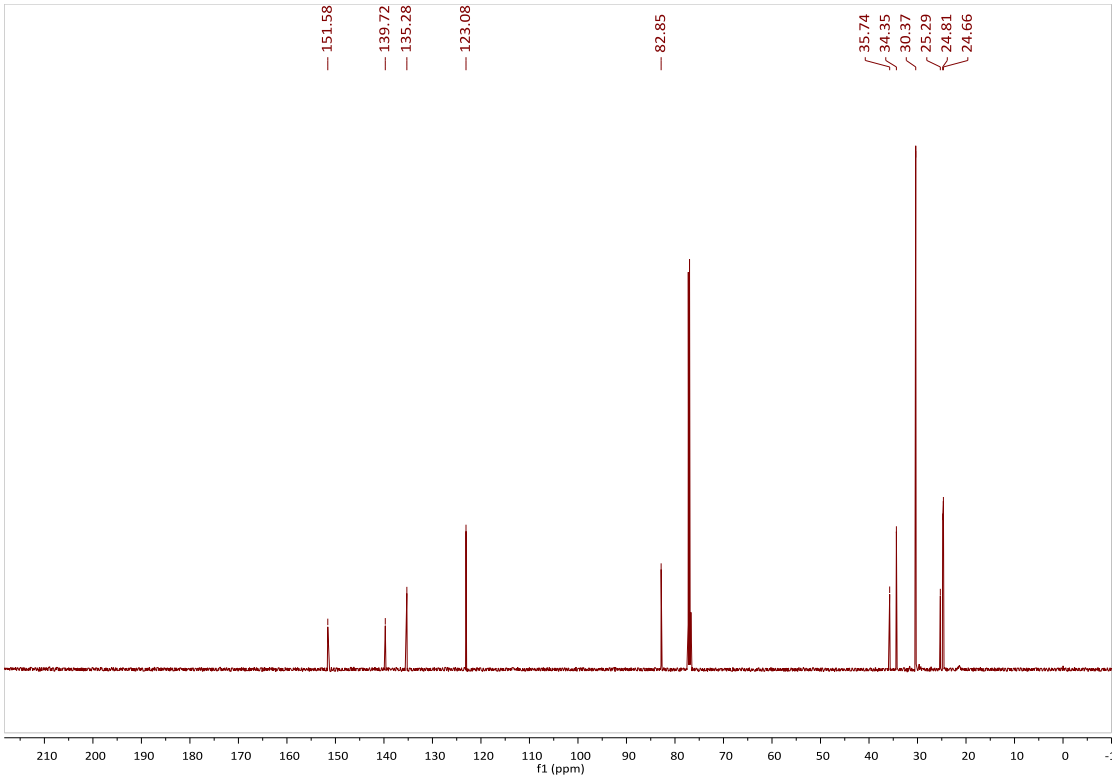
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
B
O
Me


7.06
5.01
3.01
3.00
2.99
2.98
2.98
2.97
2.97
2.96
2.95
2.94
1.45
1.28
1.27
1.18
1.17
1.16
1.16
1.15
1.99
1.00
0.99
18.06
3.32
11.91
2.03
f1 (ppm)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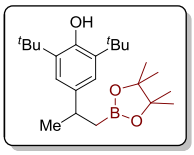
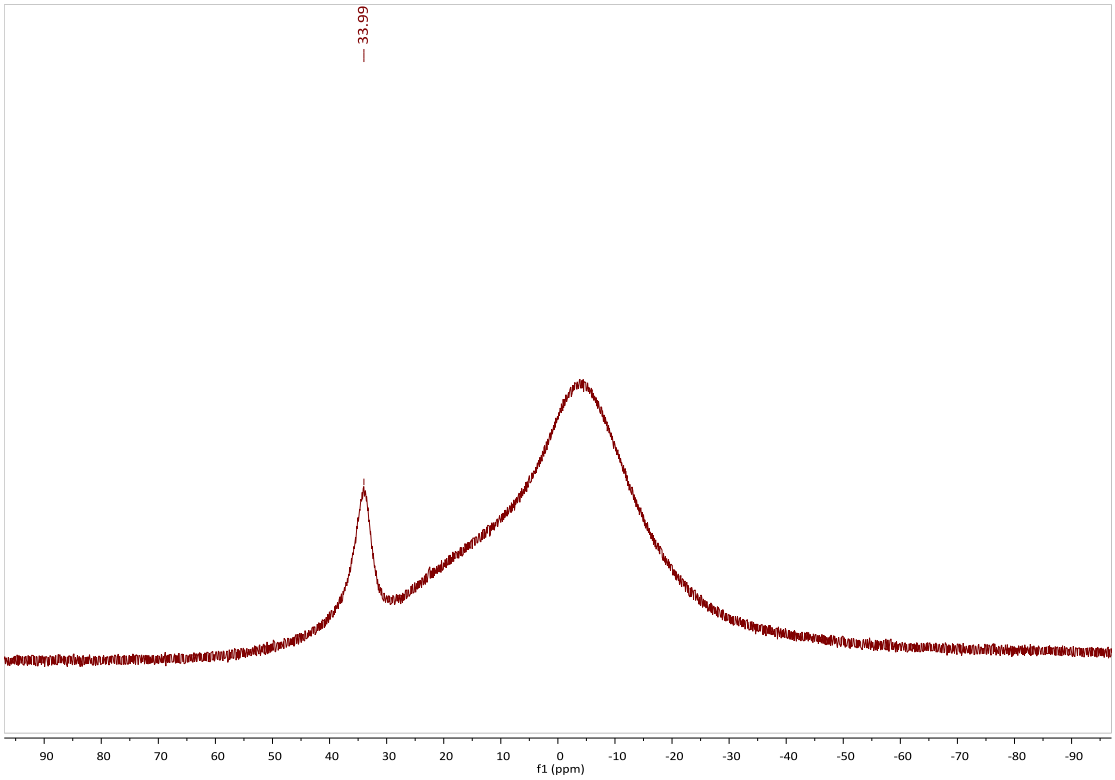
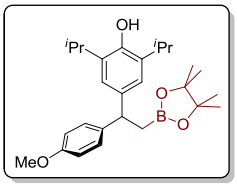
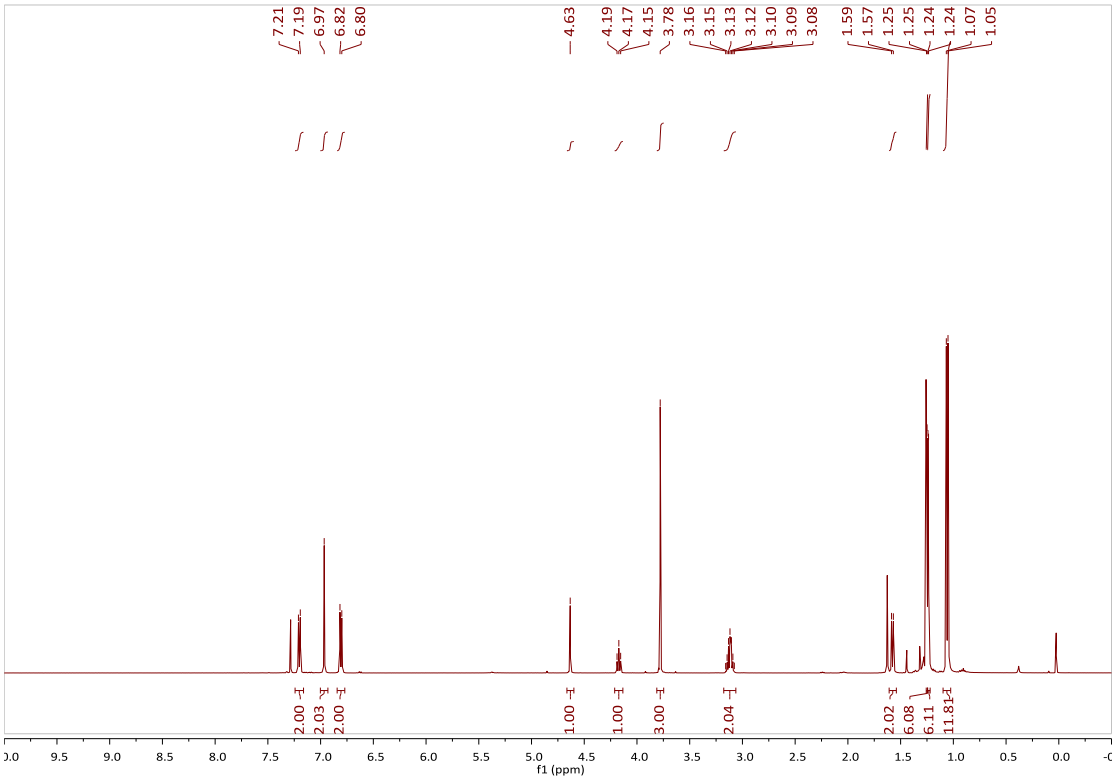
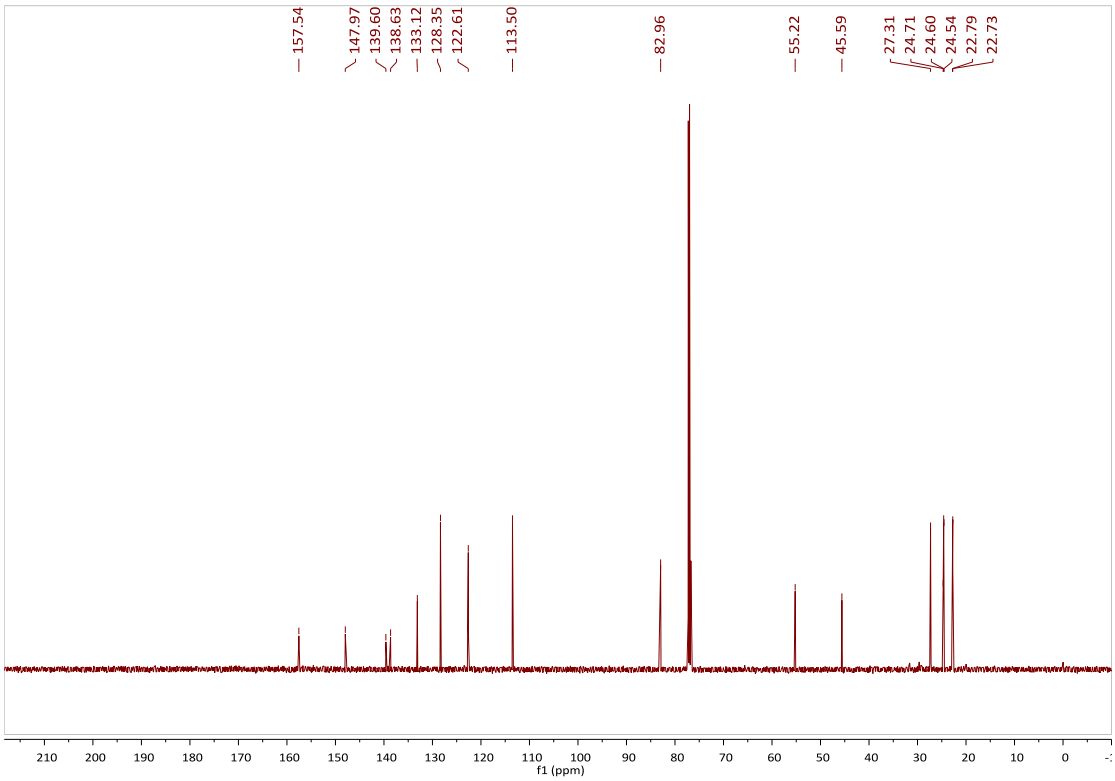
123.08
82.85
35.74
34.35
30.37
25.29
24.81
24.66
f1 (ppm)


OH
tBu
tBu
O
B
O
Me


33.99
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
iPr
iPr
O
B
O
MeO


7.21
7.19
6.97
6.82
6.80
4.63
4.19
4.17
4.15
3.78
3.16
3.15
3.13
3.12
3.10
3.09
3.08
1.59
1.57
1.25
1.25
1.24
1.24
1.07
1.05
2.00
2.03
2.00
1.00
1.00
3.00
2.04
2.02
6.08
6.11
11.81
f1 (ppm)


157.54
147.97
139.60
138.63
133.12
128.35
122.61
113.50
82.96
55.22
45.59
27.31
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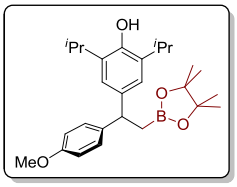
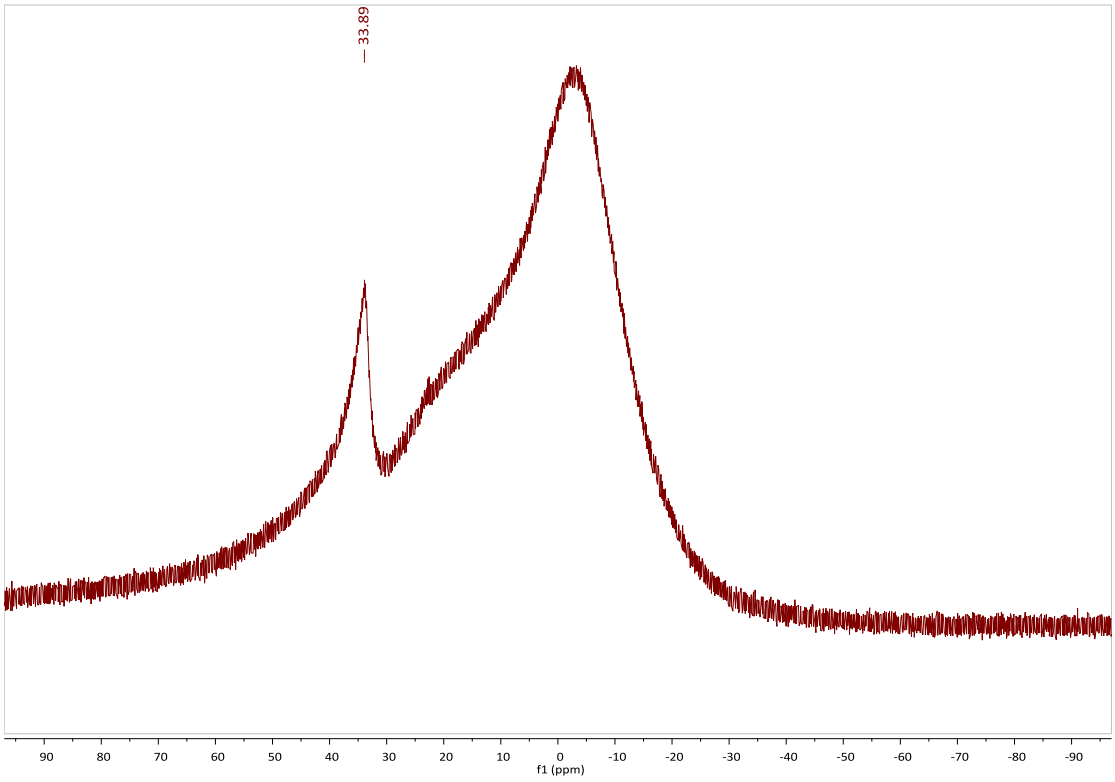
24.60
24.54
22.79
22.73
f1 (ppm)


OH
iPr
iPr
O
B
O
MeO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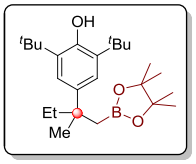
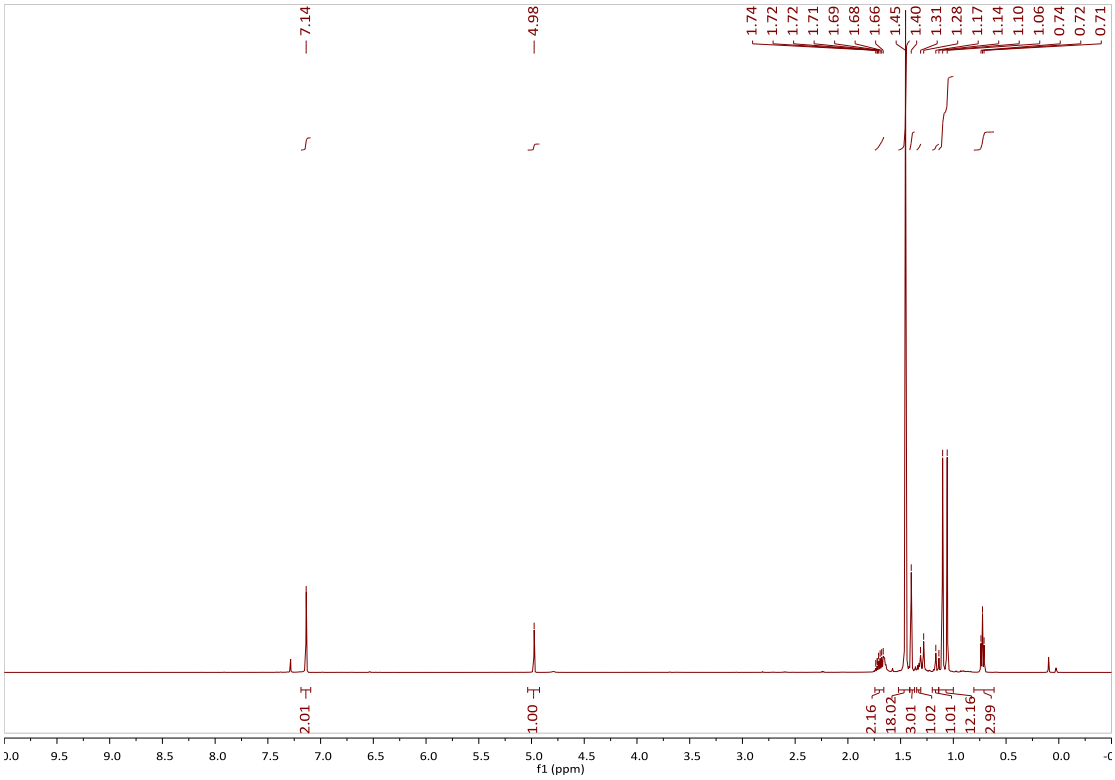
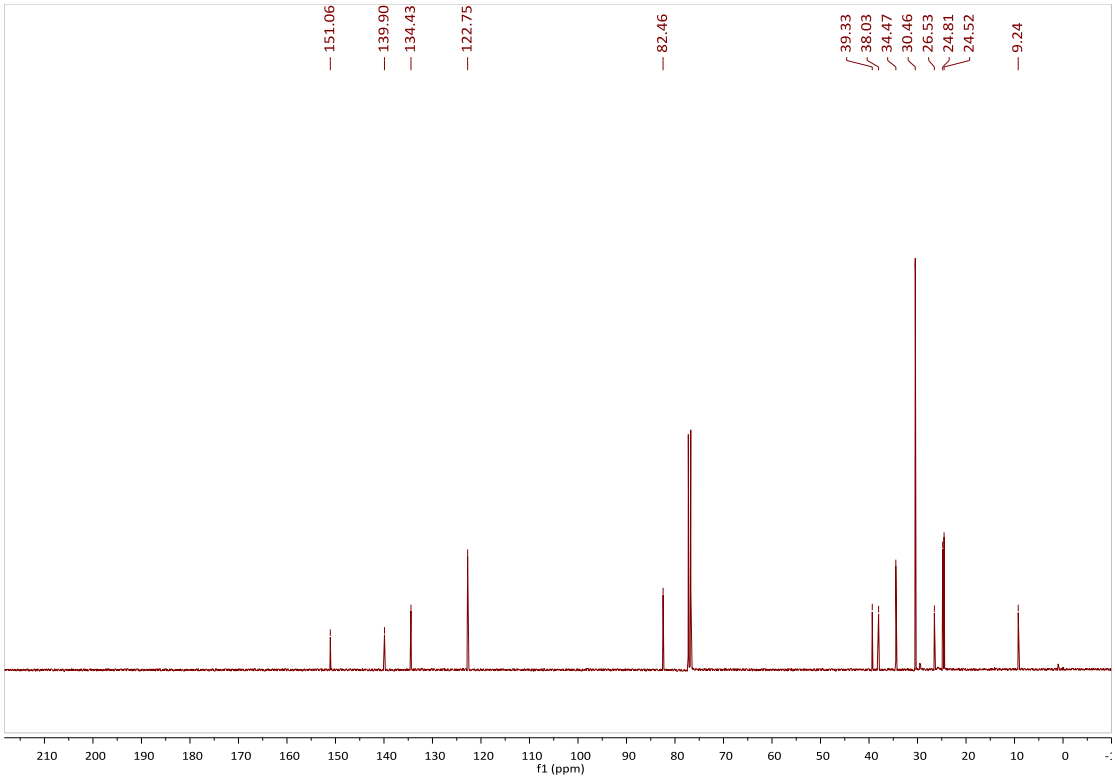
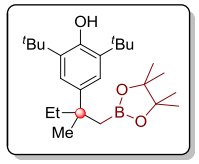
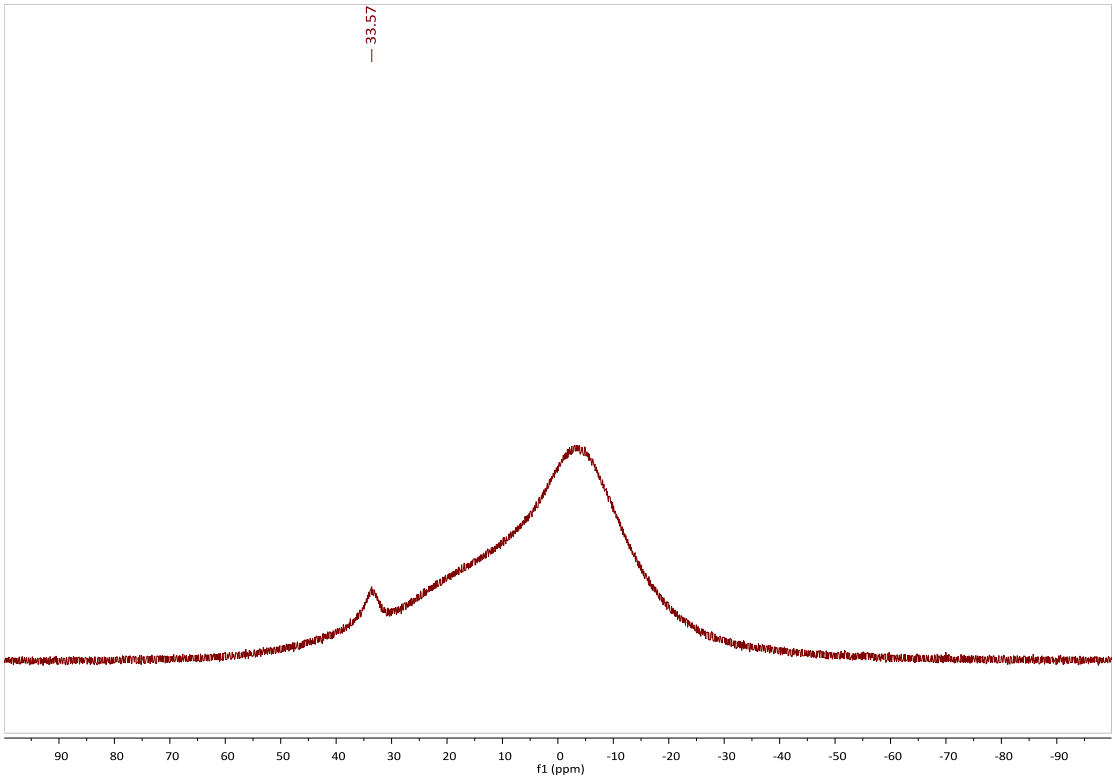
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


OH
tBu
tBu
O
Et
B
O
Me


7.14
4.98
1.74
1.72
1.72
1.71
1.69
1.68
1.66
1.45
1.40
1.31
1.28
1.17
1.14
1.10
1.06
0.74
0.72
0.71
2.01
1.00
2.16
18.02
3.01
1.02
1.01
12.16
2.99
f1 (ppm)


151.06
139.90
134.43
122.75
82.46
39.33
38.03
34.47
30.46
26.53
24.81
24.52
9.24
f1 (ppm)


OH
tBu
tBu
Et
Me
O
B
O


33.57
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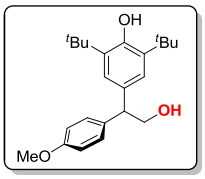
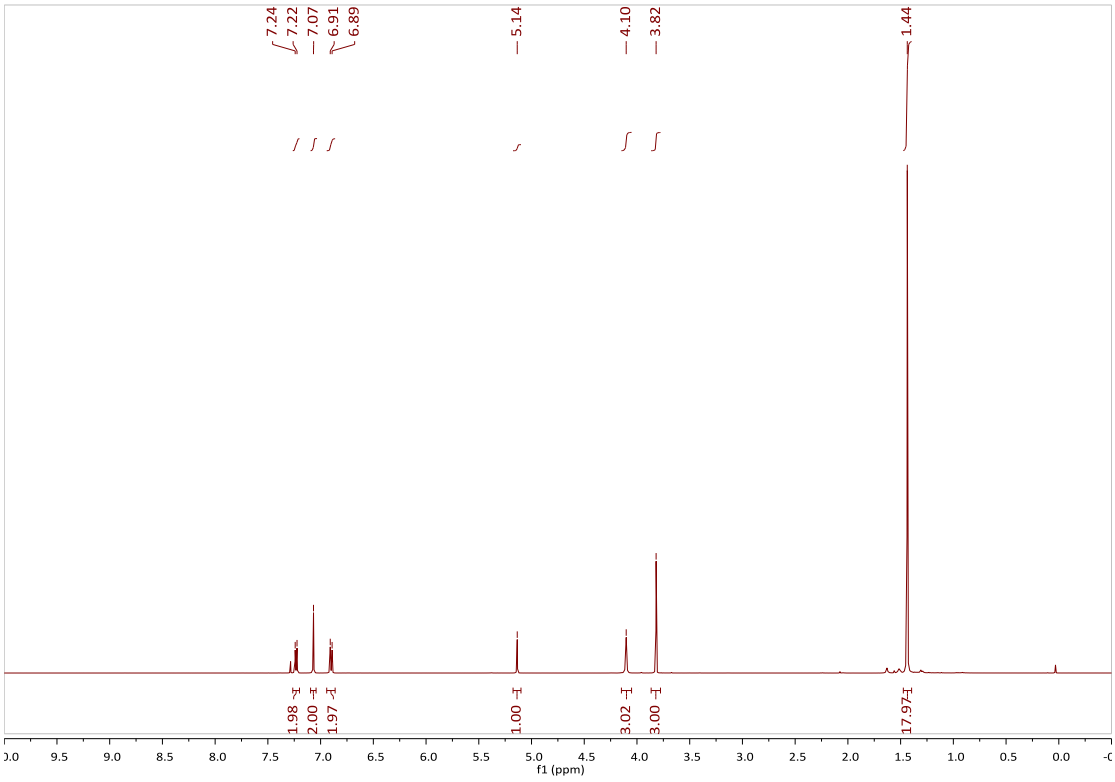
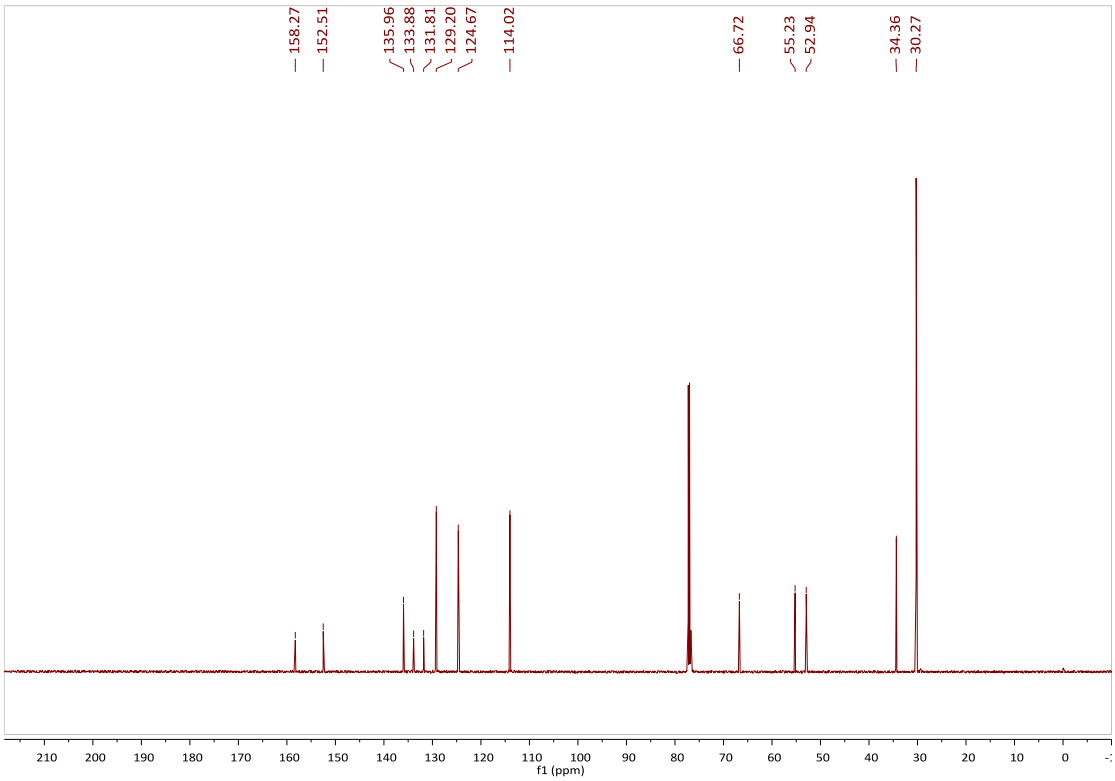
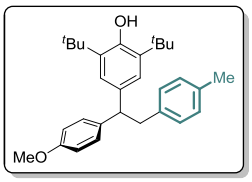
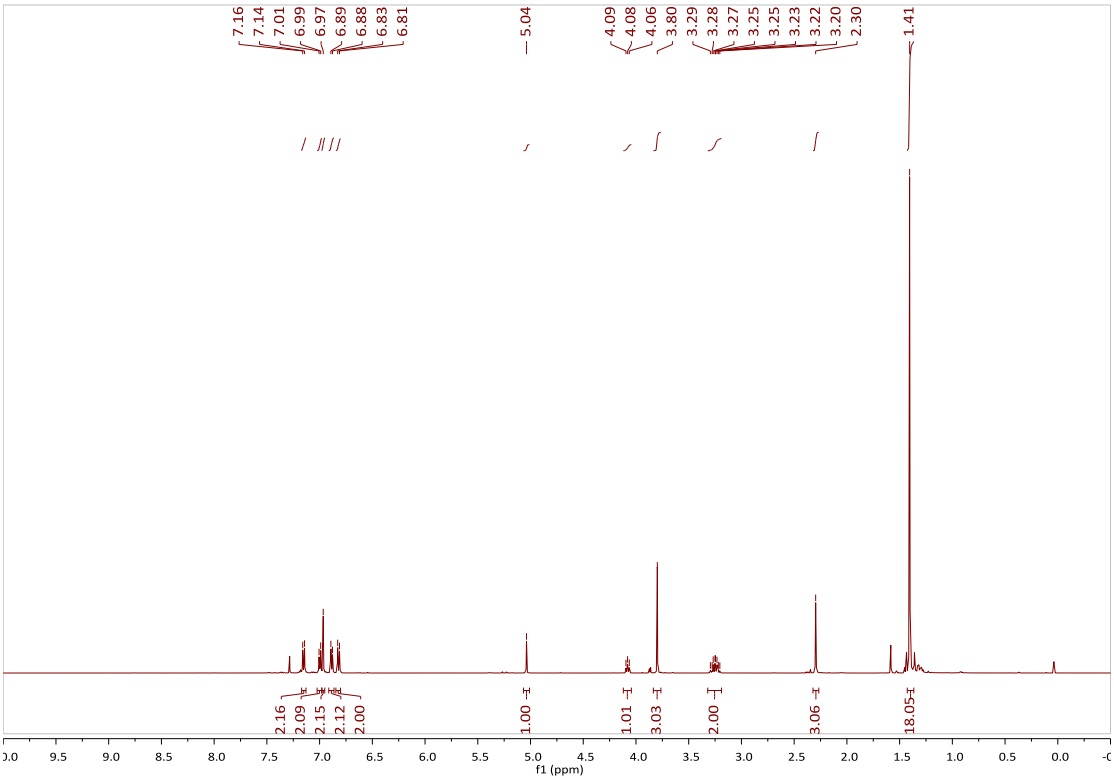
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

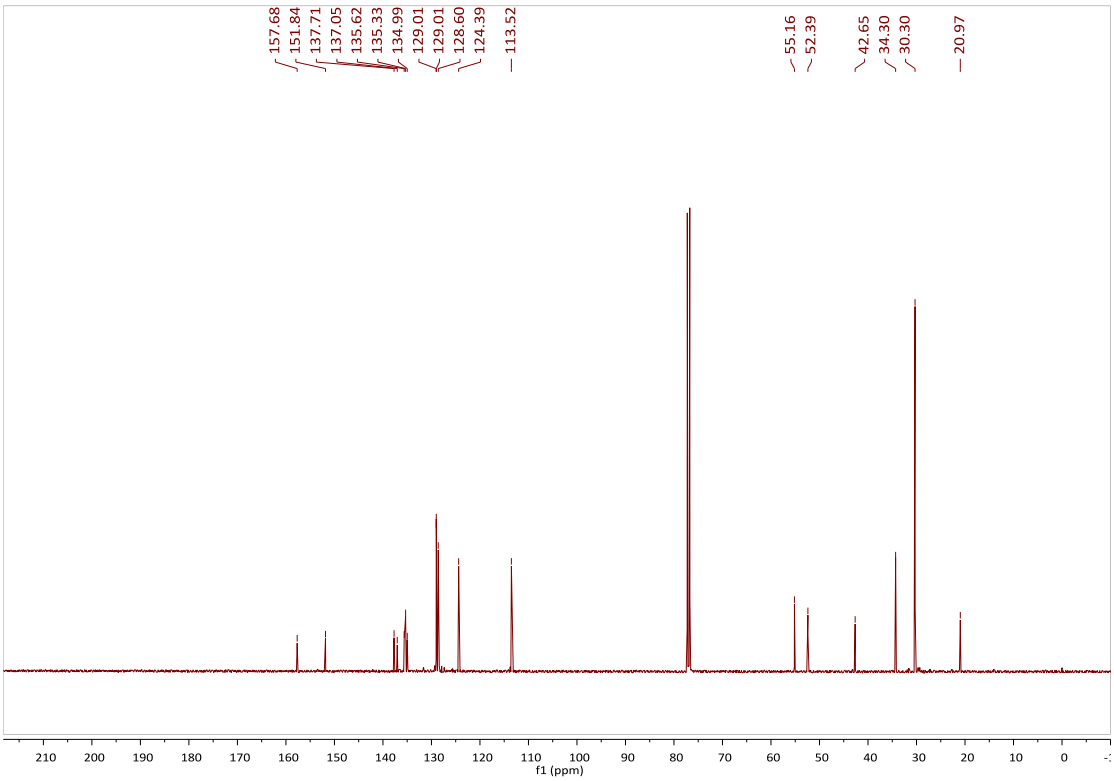

OH
tBu
tBu
OH
MeO


7.24
7.22
7.07
6.91
6.89
5.14
4.10
3.82
1.44
1.98
2.00
1.97
1.00
3.02
3.00
17.97
f1 (ppm)


158.27
152.51
135.96
133.88
131.81
129.20
124.67
114.02
66.72
55.23
52.94
34.36
30.27
f1 (ppm)


OH
tBu
tBu
Me
MeO


7.16
7.14
7.01
6.99
6.97
6.89
6.88
6.83
6.81
5.04
4.09
4.08
4.06
3.80
3.29
3.28
3.27
3.25
3.25
3.23
3.22
3.20
2.30
1.41
2.16
2.09
2.15
2.12
2.00
1.00
1.01
3.03
2.00
3.06
18.05
f1 (ppm)


157.68
151.84
137.71
137.05
135.62
135.33
134.99
129.01
129.01
128.60
124.39
113.52
55.16
52.39
42.65
34.30
30.30
20.97
f1 (ppm)