Tropylium Promoted Hydroboration Reactions: Mechanistic Insights via Experimental and Computational Studies

Supporting Information: Part 1 - Experimental

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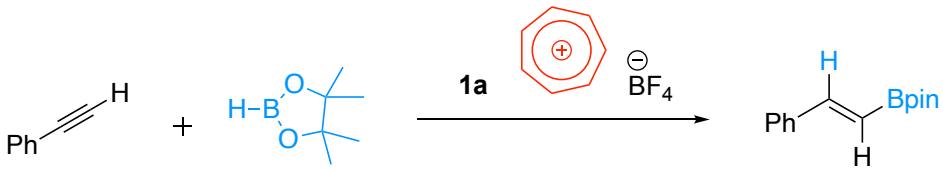
Optimization Studies

Table S1. Optimization of reaction conditions (solvent).[a]



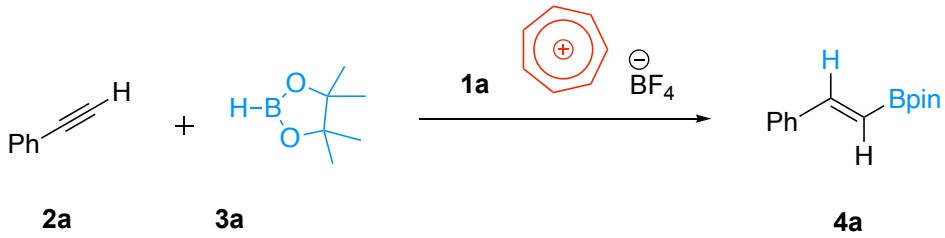
2a **3a** **4a**

Entry	Solvent	Temp. (°C)	Molar ratio	Yield of **4a**, %[b]
1	DCE	50	1:1.5	**94**
2	DCM	50	1:1.5	87
3	Chloroform	50	1:1.5	< 10, n.d
4	MeCN	50	1:1.5	traces
5	THF	50	1:1.5	traces
6	Toluene	50	1:1.5	**95**
7	Neat	50	1:1.5	**98**

[a] Phenylacetylene (0.5 mmol), tropylium tetrafluoroborate **1a** as catalyst (0.05 mmol, 10 mol%), HBpin (0.75 mmol, 1.5 equiv), solvent (2 mL), 12 h. [b] Yields of the isolated product **4a**. DCE = 1,2-dichloroethane; DCM = dichloromethane; MeCN = acetonitrile; THF = tetrahydrofuran. HBpin = 4,4,5,5-tetramethyl-1,3,2-dioxaborolane. n.d = not determined. The *trans*-isomer was formed exclusively.

General optimization procedure for Table S1: To a mixture of phenylacetylene (0.5 mmol) and 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin, ~ 96 mg, 0.75 mmol, 1.5 equiv) in a reaction vial containing solvent (2 mL) equipped with a stirrer bar was added tropylium tetrafluoroborate catalyst (~ 9 mg, 0.05 mmol, 10 mol%). The reaction mixture was heated to 50 °C for 12 h, with the reaction progress monitored by TLC. The product was purified by flash column chromatography (silica-gel, EtOAc/hexanes).

Table S2. Optimization of reaction conditions (catalyst loading).[a]



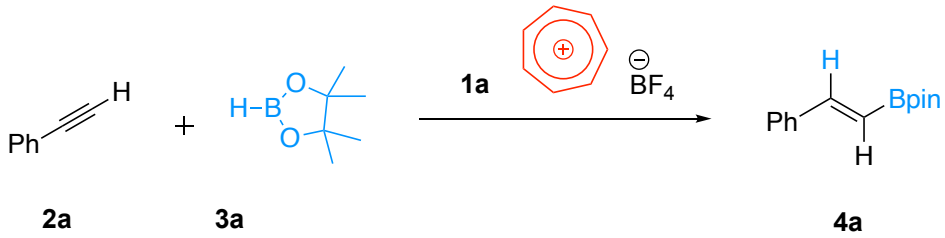
2a **3a** **4a**

Entry	Solvent	Cat. (mol%)	Temp. (°C)	Molar ratio	Yield of **4a**, %[b]
1	DCE	1	50	1:1.5	< 20, n.d
2	DCE	2	50	1:1.5	< 20, n.d
3	DCE	5	50	1:1.5	73
4	DCE	10	50	1:1.5	**94**
5	Toluene	1	50	1:1.5	< 20, n.d
6	Toluene	2	50	1:1.5	< 20, n.d
7	Toluene	5	50	1:1.5	74
8	Toluene	10	50	1:1.5	**95**
9	Neat	10	50	1:1.5	**98**

[a] Phenylacetylene (0.5 mmol), tropylium tetrafluoroborate **1a** as catalyst, HBpin (0.75 mmol, 1.5 equiv), solvent (2 mL), 12 h. [b] Yields of the isolated product **4a**. DCE = 1,2-dichloroethane; HBpin = 4,4,5,5-tetramethyl-1,3,2-dioxaborolane. n.d = not determined. The *trans*-isomer was formed exclusively.

General optimization procedure for Table S2: To a mixture of phenylacetylene (0.5 mmol) and 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin, ~ 96 mg, 0.75 mmol, 1.5 equiv) in a reaction vial containing solvent (2 mL) equipped with a stirrer bar was added tropylium tetrafluoroborate catalyst. The reaction mixture was heated to 50 °C for 12 h, with the reaction progress monitored by TLC. The product was purified by flash column chromatography (silica-gel, EtOAc/hexanes).

Table S3. Optimization of reaction conditions (temperature).[a]



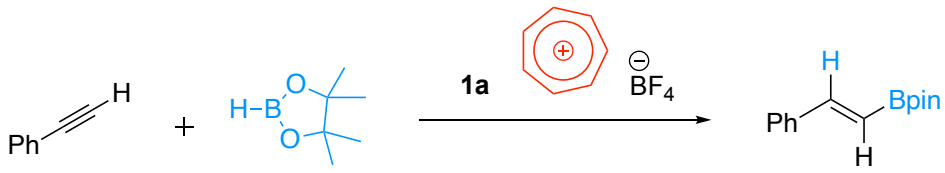
2a **3a** **4a**

Entry	Solvent	Temp. (°C)	Molar ratio	Yield of **4a**, %[b]
1	DCE	RT	1:1.5	50
2	DCE	40	1:1.5	73
3	DCE	50	1:1.5	94
4	DCE	70	1:1.5	**95**
5	DCE	90	1:1.5	81
6	Neat	50	1:1.5	98
7	Neat	70	1:1.5	**99**

[a] Phenylacetylene (0.5 mmol), tropylium tetrafluoroborate **1a** as catalyst (0.05 mmol, 10 mol%), HBpin (0.75 mmol, 1.5 equiv), solvent (2 mL), 12 h. [b] Yields of the isolated product **4a**. DCE = 1,2-dichloroethane; HBpin = 4,4,5,5-tetramethyl-1,3,2-dioxaborolane. The *trans*-isomer was formed exclusively.

General optimization procedure for Table S3: To a mixture of phenylacetylene (0.5 mmol) and 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin, ~ 96 mg, 0.75 mmol, 1.5 equiv) in a reaction vial containing solvent (2 mL) equipped with a stirrer bar was added tropylium tetrafluoroborate catalyst (~ 9 mg, 0.05 mmol, 10 mol%). The reaction mixture was heated for 12 h at different temperatures, with the reaction progress monitored by TLC. The product was purified by flash column chromatography (silica-gel, EtOAc/hexanes).

Table S4. Optimization of reaction conditions (catalyst loading and stoichiometry of HBpin in neat condition).[a]



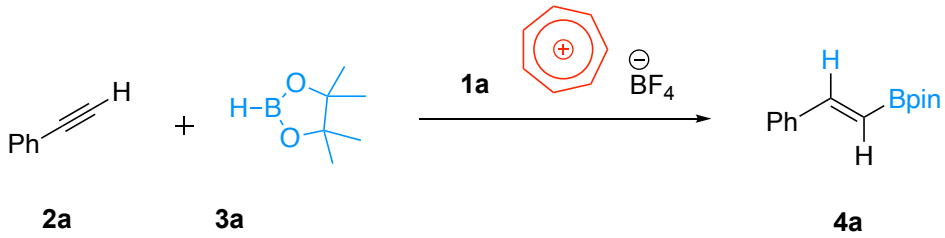
2a **3a** **4a**

Entry	Cat. (mol%)	Temp. (°C)	Molar ratio	Yield of **4a**, %[b]
1	1	50	1:1.5	89
2	2	50	1:1.5	94
3	5	50	1:1.5	98
4	10	50	1:1.5	98
5	1	70	1:1.5	92
6	2	70	1:1.5	**99**
7	5	70	1:1.5	**99**
8	10	70	1:1.5	99
9	5	70	1:1.2	**99**
10	5	70	1:1.0	91

[a] Phenylacetylene (0.5 mmol), tropylium tetrafluoroborate **1a** as catalyst, HBpin (0.75 mmol, 1.5 equiv), neat, 12 h. [b] Yields of the isolated product **4a**; HBpin = 4,4,5,5-tetramethyl-1,3,2-dioxaborolane. The *trans*-isomer was formed exclusively.

General optimization procedure for Table S4: To a mixture of phenylacetylene (0.5 mmol) and 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin, ~ 96 mg, 0.75 mmol, 1.5 equiv) in a reaction vial equipped with a stirrer bar was added tropylium tetrafluoroborate catalyst. The reaction mixture was heated to 50 °C or 70 °C for 12 h, with the reaction progress monitored by TLC. The product was purified by flash column chromatography (silica-gel, EtOAc/hexanes).

Table S5. Optimization of reaction conditions (time).[a]



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

Entry	Temp. (°C)	Time (h)	Molar ratio	Yield of **4a**, %[b]
1	70	2	1:1.2	15
2	70	4	1:1.2	63
3	70	6	1:1.2	**99**
4	70	8	1:1.2	**99**

[a] Phenylacetylene (0.5 mmol), tropylium tetrafluoroborate as catalyst (0.01 mmol, 2 mol%), HBpin (0.6 mmol, 1.2 equiv), neat, 2, 4, 6, 8 h. [b] Yields of the isolated product **4a**; HBpin = 4,4,5,5-tetramethyl-1,3,2-dioxaborolane. The *trans*-isomer was formed exclusively.

General optimization procedure for Table S5: To a mixture of phenylacetylene (0.5 mmol) and 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin, ~ 76.8 mg, 0.6 mmol, 1.2 equiv) in a reaction vial equipped with a stirrer bar was added tropylium tetrafluoroborate catalyst (~ 1.8 mg, 0.01 mmol, 2 mol%). The reaction mixture was heated to 70 °C for 2, 4, 6 or 8 h, with the reaction progress monitored by TLC. The product was purified by flash column chromatography (silica-gel, EtOAc/hexanes).

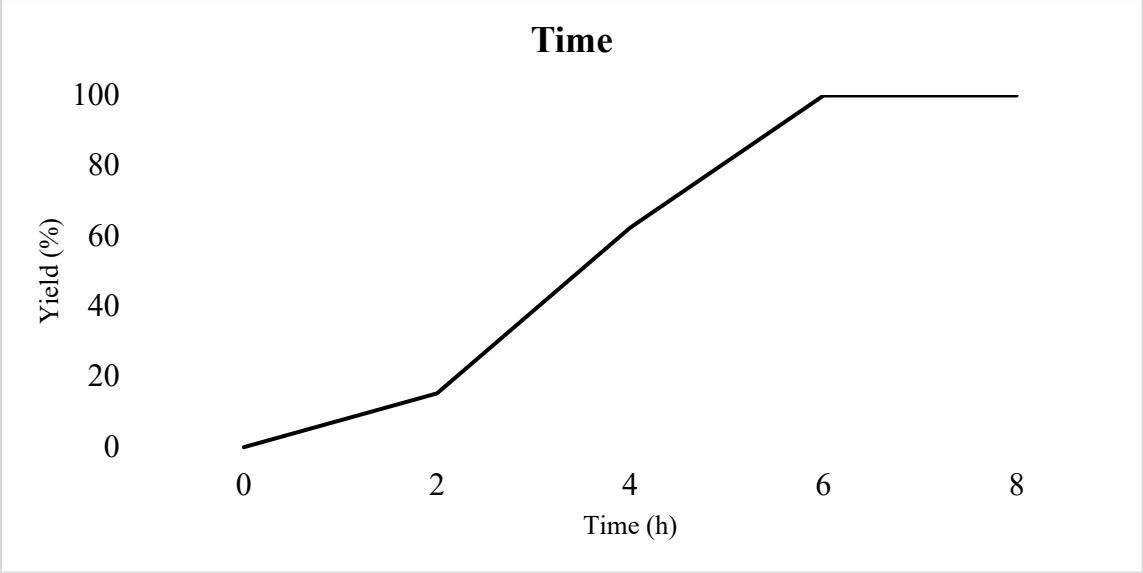
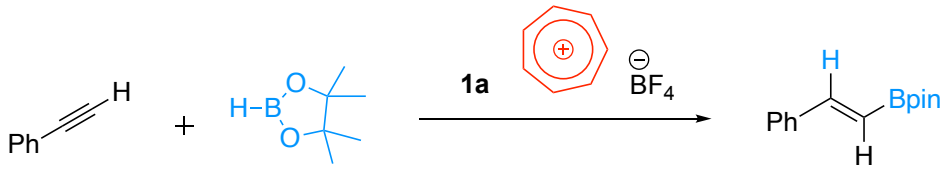

Time
100
80
60
40
20
0
Yield (%)
0
2
4
6
8
Time (h)

Table S6. Optimization of reaction conditions.[a] (no catalyst)

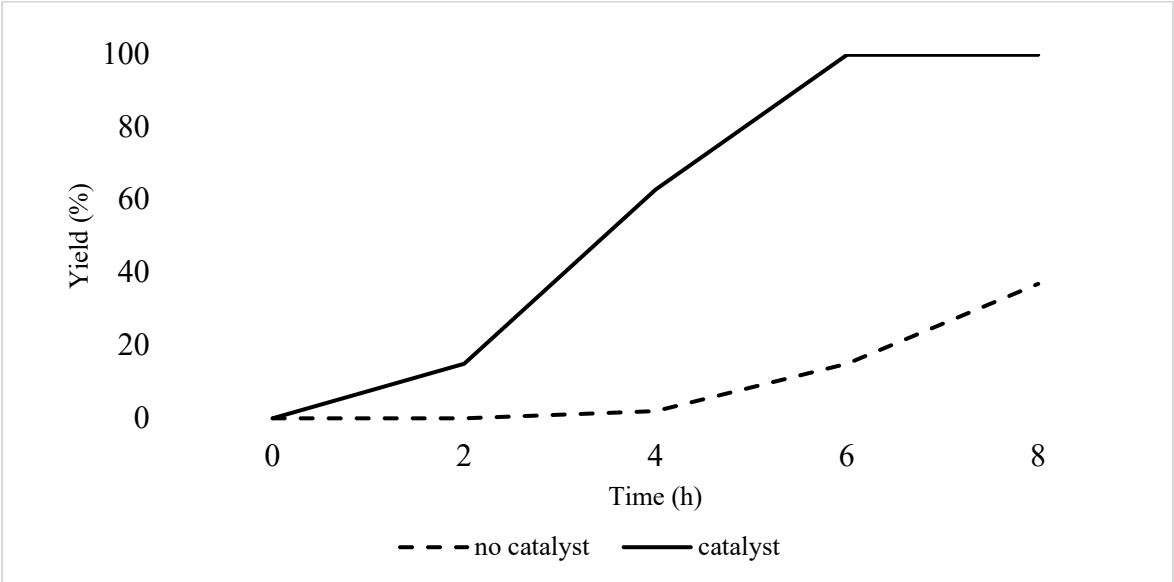


2a **3a** **4a**

Entry	Temp. (°C)	Time (h)	Molar ratio	Yield of **4a**, %[b]
1	70	2	1:1.2	0
2	70	4	1:1.2	2
3	70	6	1:1.2	15
4	70	8	1:1.2	37

[a] Phenylacetylene (0.5 mmol), HBpin (0.6 mmol, 1.2 equiv), neat, 2, 4, 6 or 8 h. [b] Yields of the isolated product **4a**; HBpin = 4,4,5,5-tetramethyl-1,3,2-dioxaborolane. The *trans*-isomer was formed exclusively.

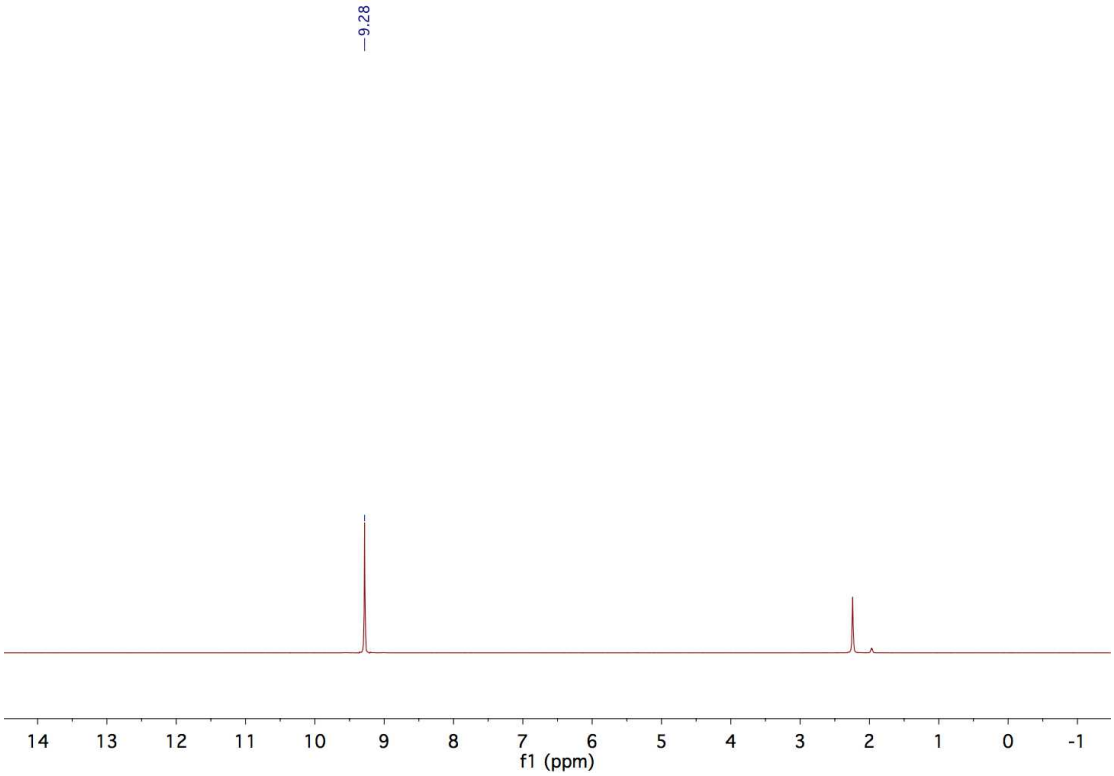
General optimization procedure for Table S6: To a mixture of phenylacetylene (0.5 mmol) and 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin, ~ 76.8 mg, 0.6 mmol, 1.2 equiv) in a reaction vial equipped with a stirrer bar was heated to 70 °C for 2, 4, 6 and 8 h, with the reaction progress monitored by TLC. The product was purified by flash column chromatography (silica-gel, EtOAc/hexanes).



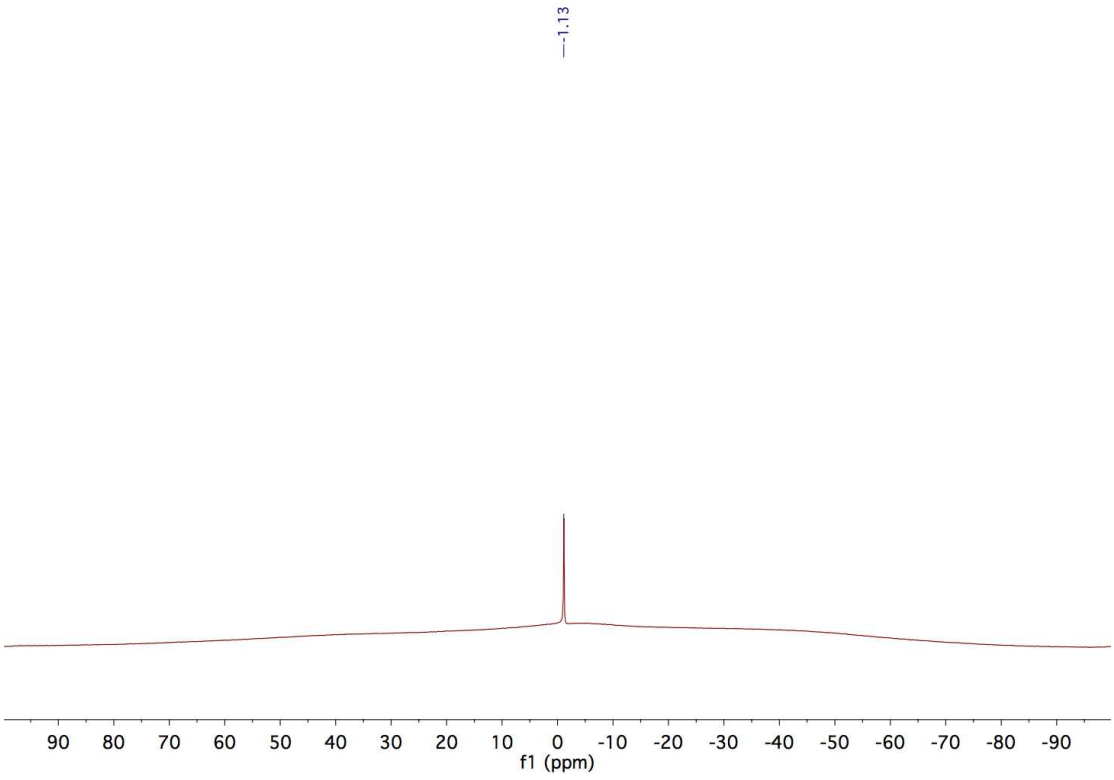
NMR Spectra for Mechanistic Studies

Tropylium tetrafluoroborate 1a

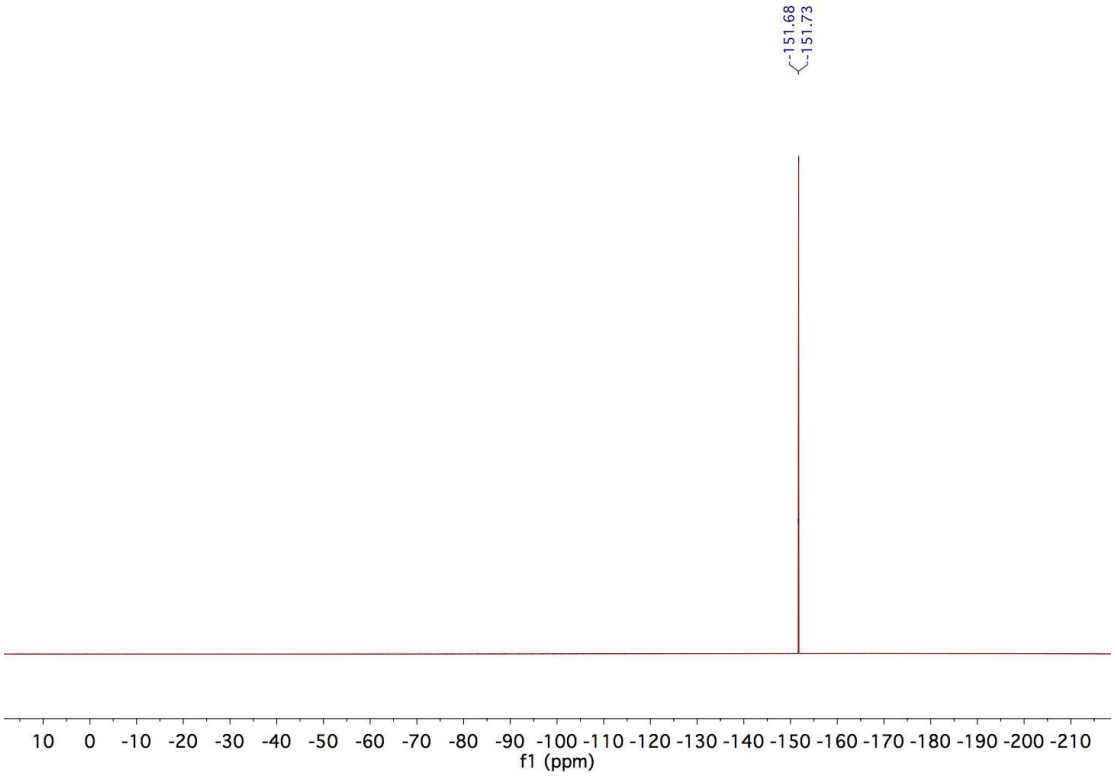
^{1}H NMR (400 MHz, CD_3CN, 298K)

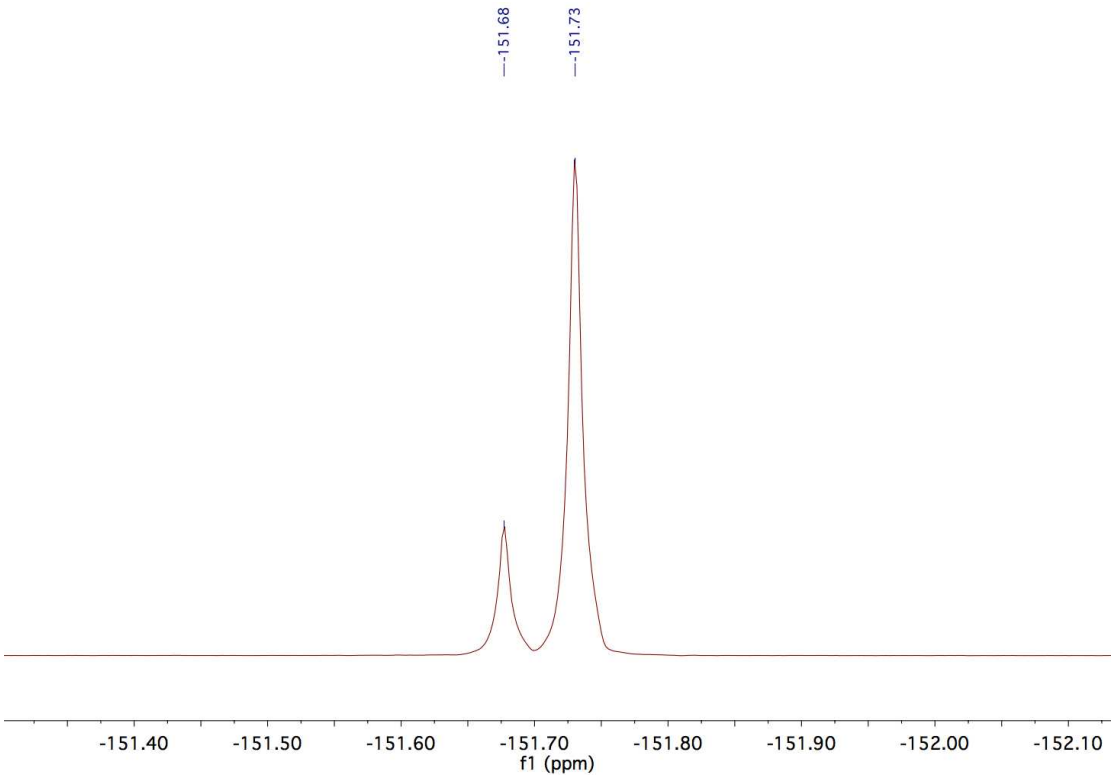


^{11}B NMR (128 MHz, CD_3CN, 298K)



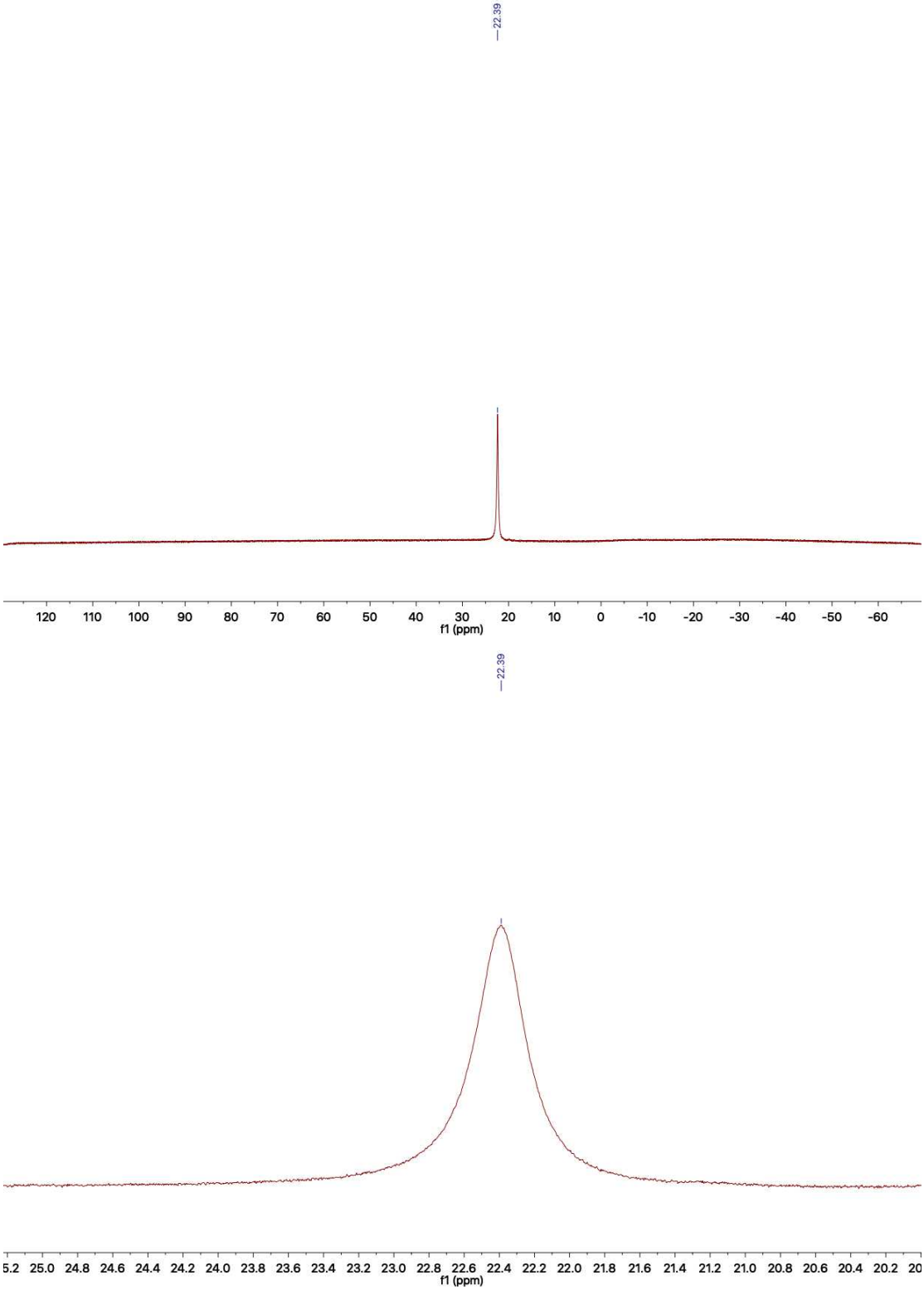
^{19}F NMR (376.5 MHz, CD_3CN, 298K)



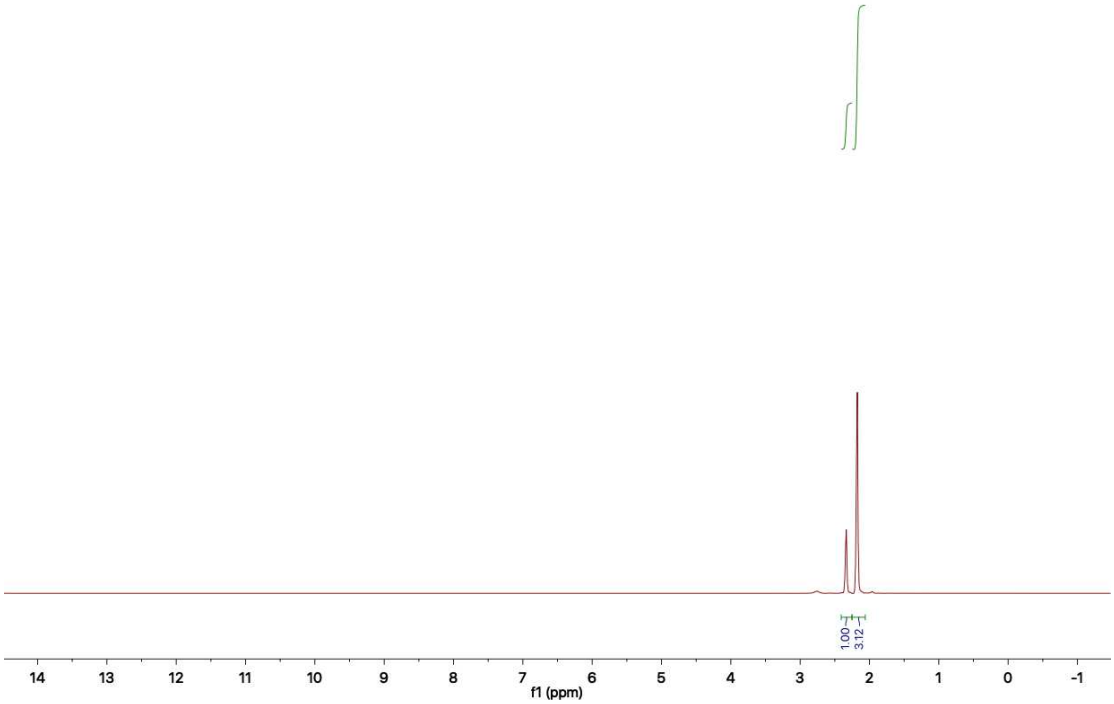


HBpin 3

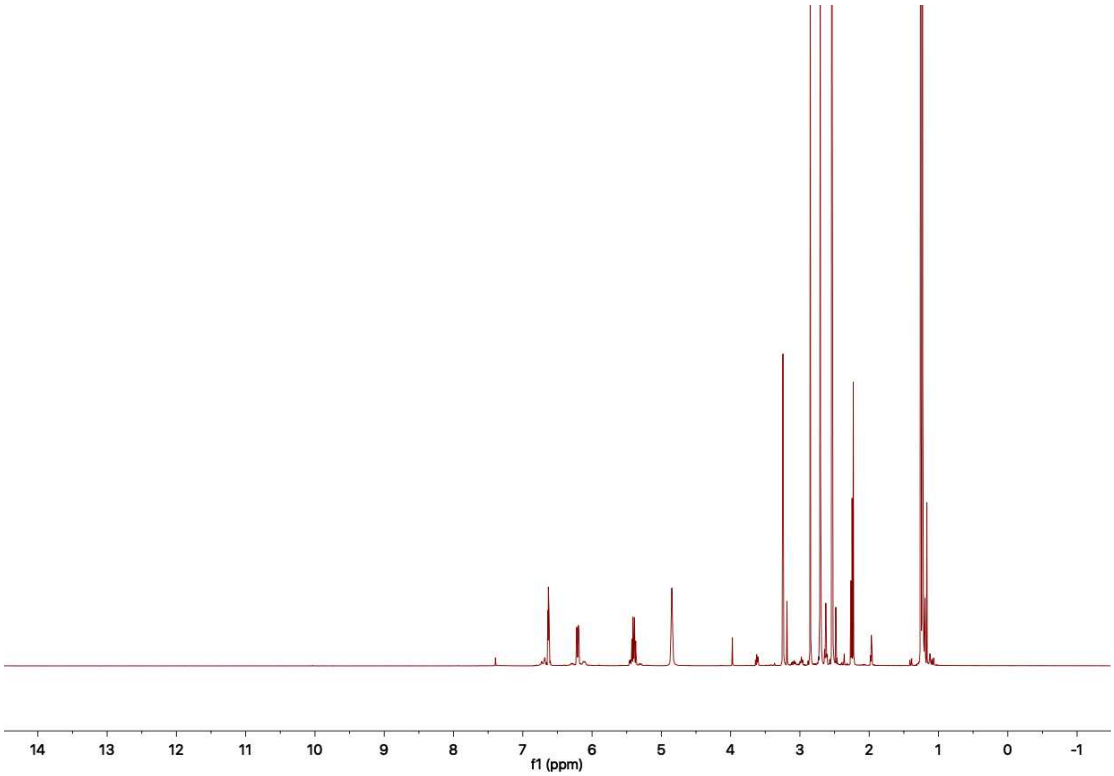
^{11}B NMR (128 MHz, CD_3CN, 298K)



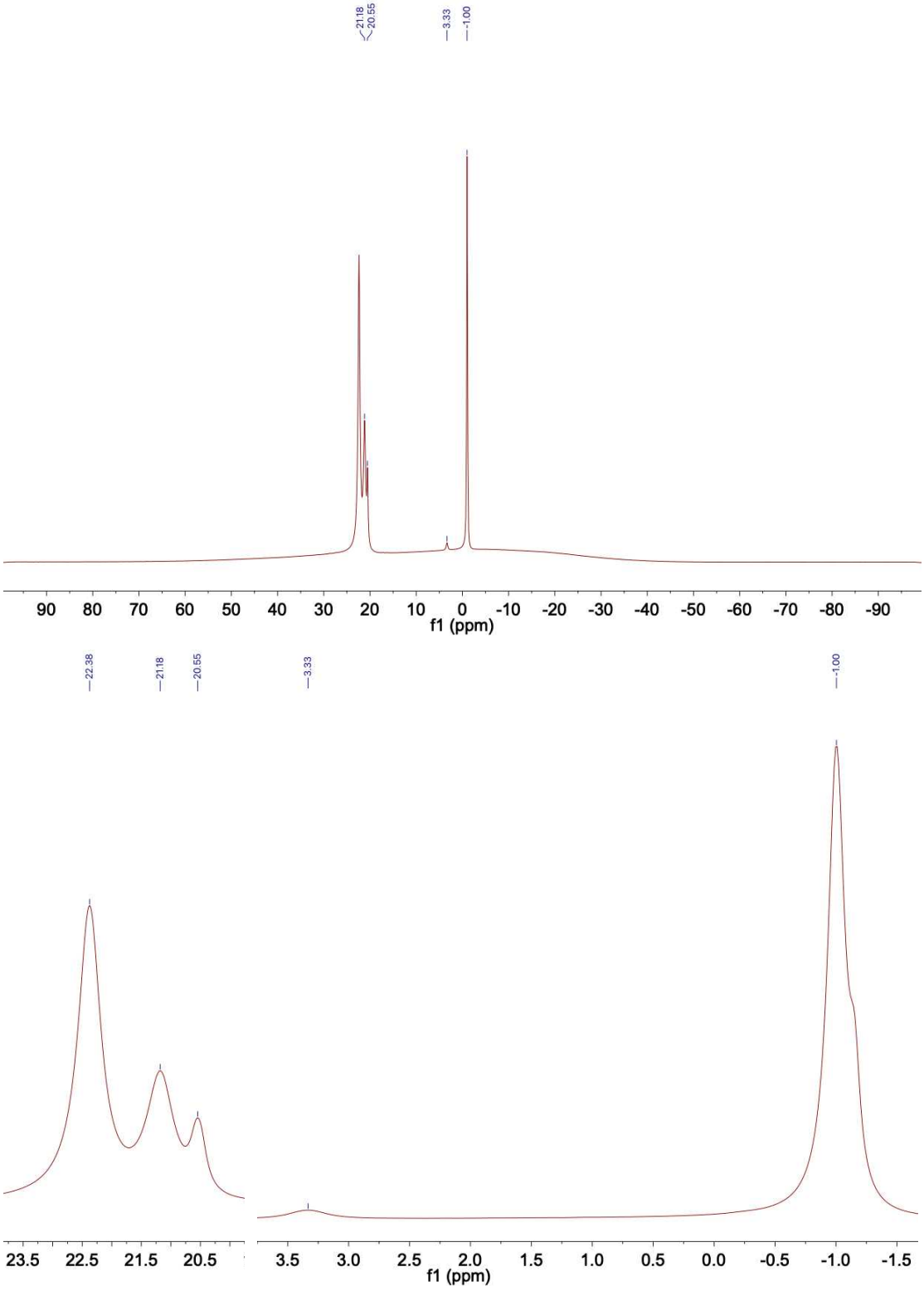
TMEDA ^{1}H NMR (400 MHz, CD_3CN, 298K)



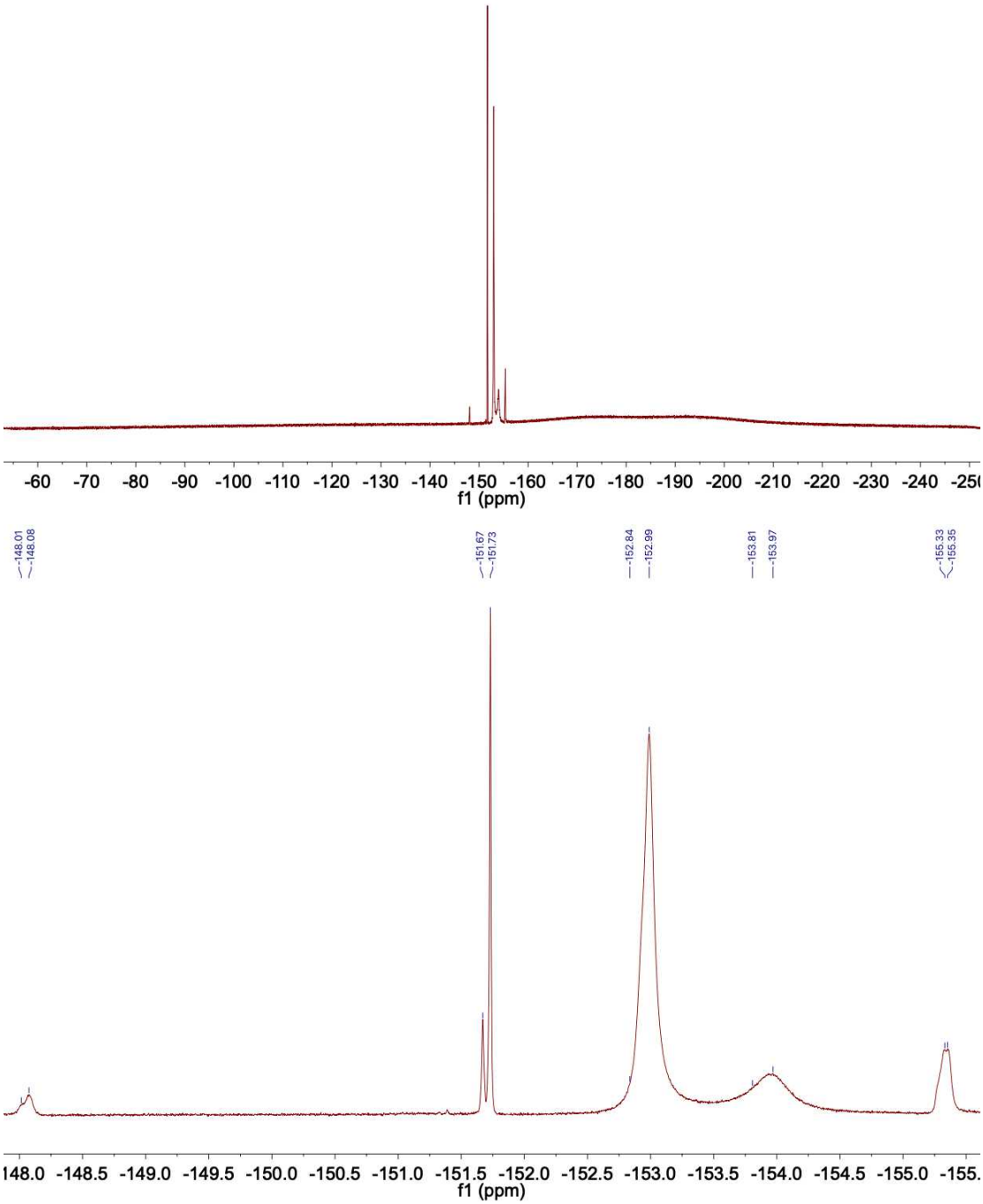
TMEDA + Trop.BF_4 + HBpin ^{1}H NMR (400 MHz, CD_3CN, 298K)



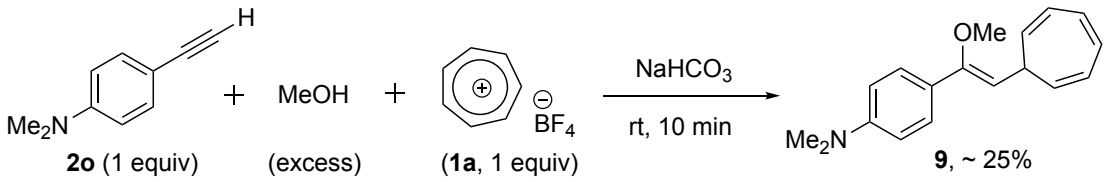
Trop.BF_4 + HBpin (rt, 30 min) ^{11}B NMR (128 MHz, CD_3CN, 298K)



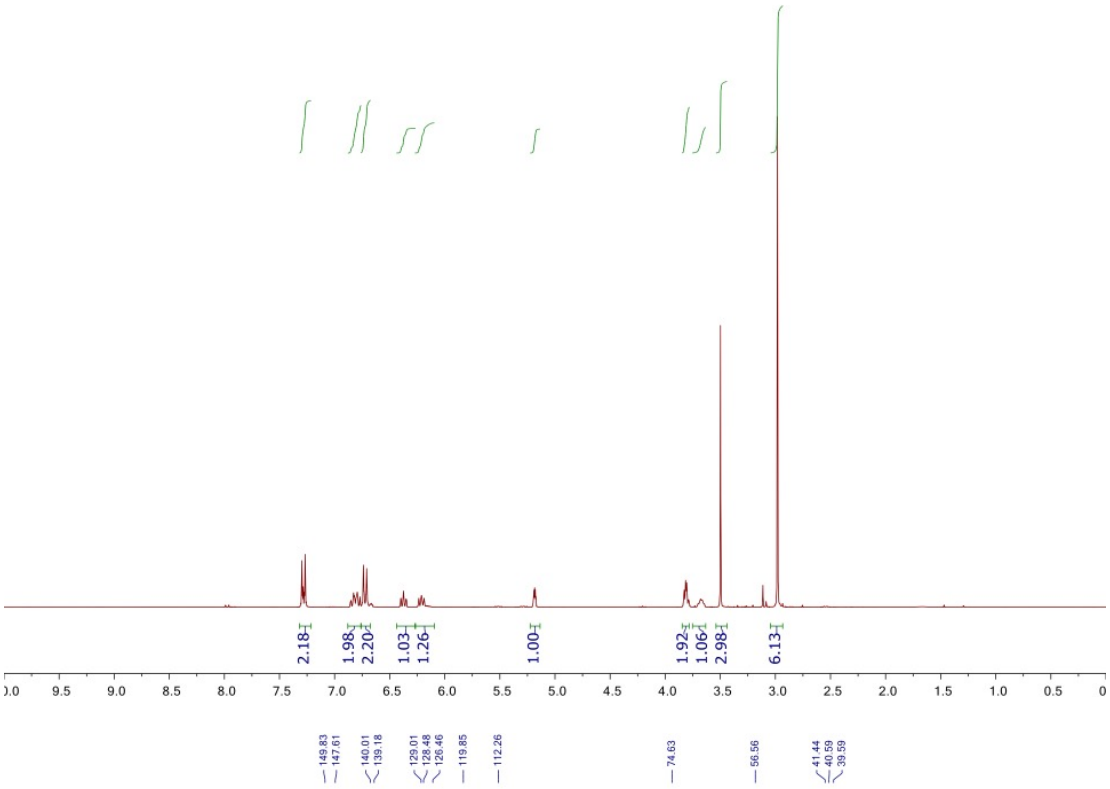
Trop.BF_4 + HBpin (rt, 30 min) ^{19}F NMR (376.5 MHz, CD_3CN, 298K)

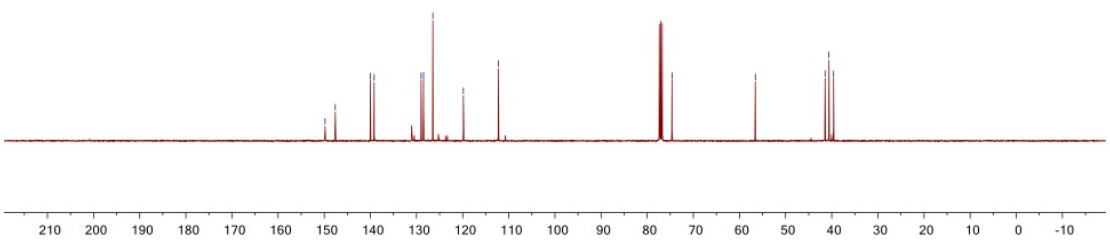


NMR Spectra of Compound 9 (Scheme 4)



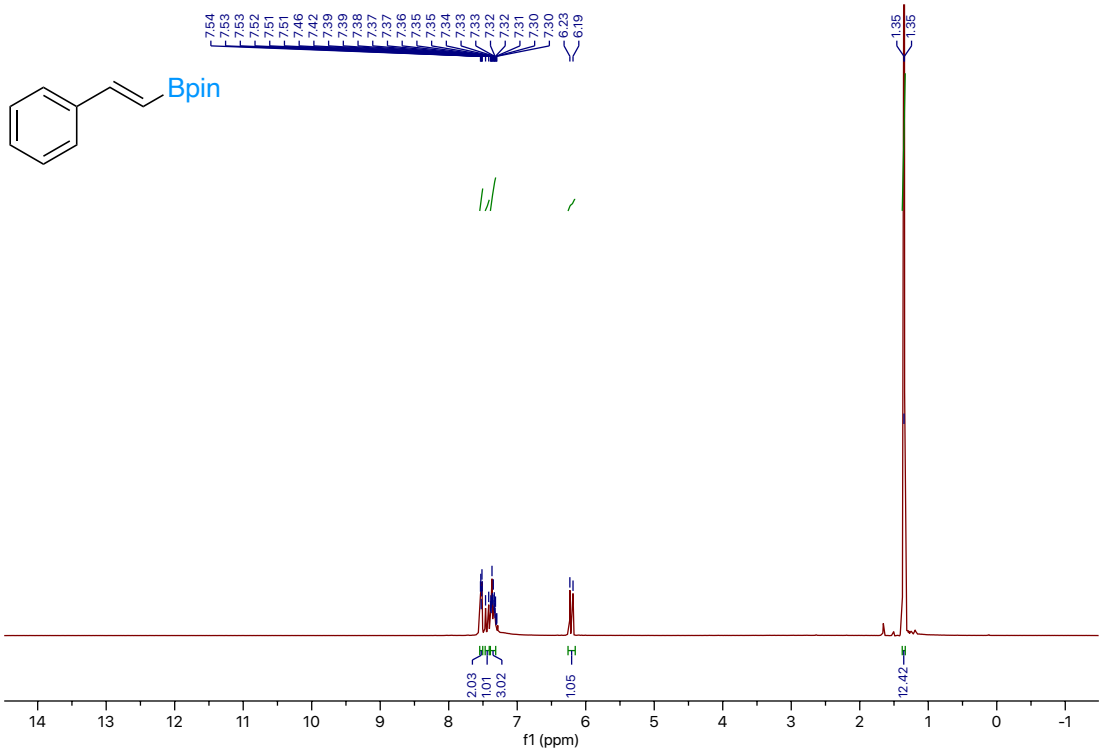
2o (1 equiv) (excess) (**1a**, 1 equiv) **9**, ~ 25%

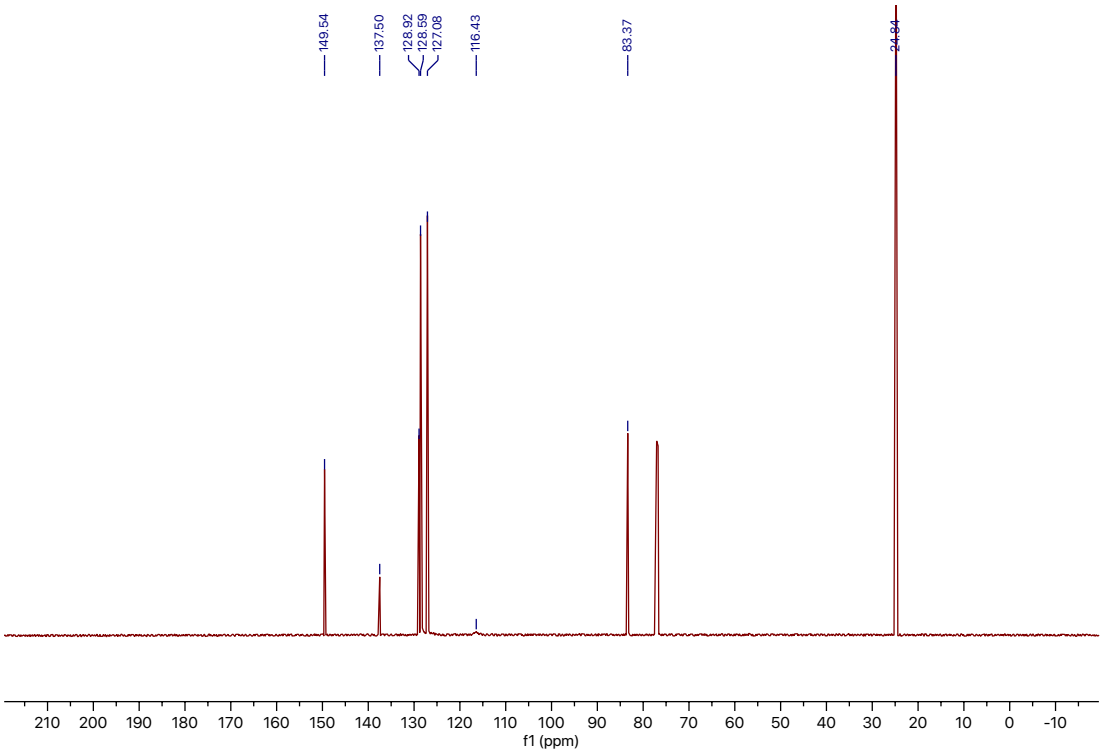


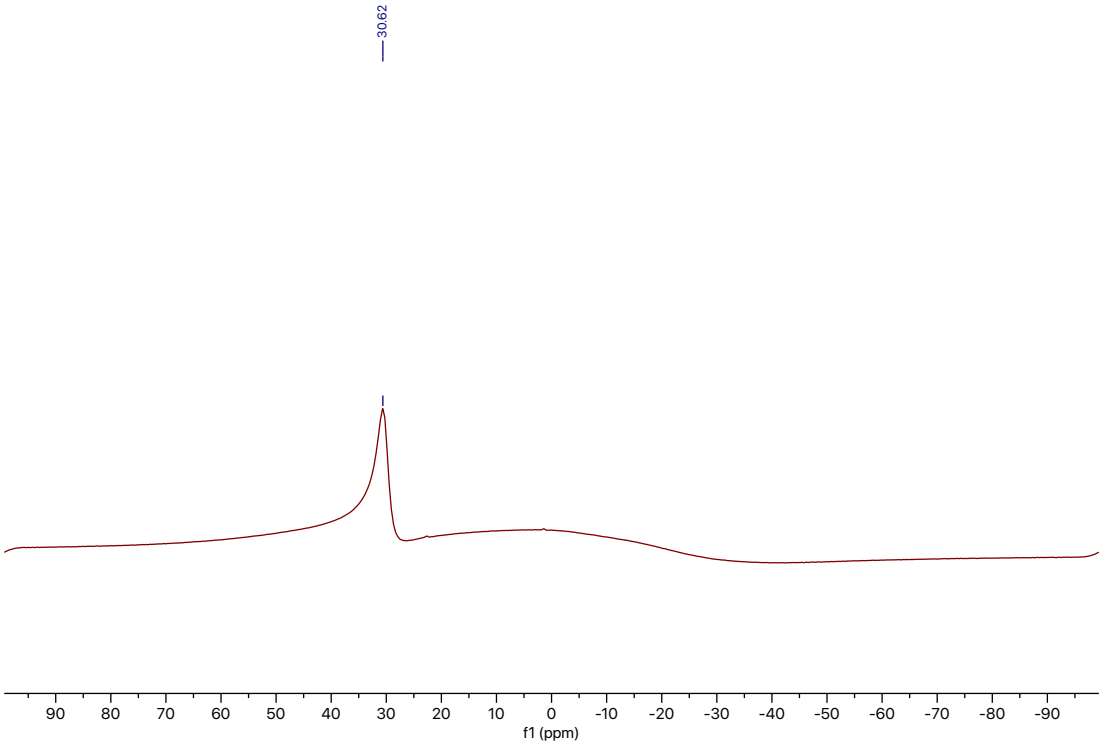


NMR Spectra of Hydroboration Products

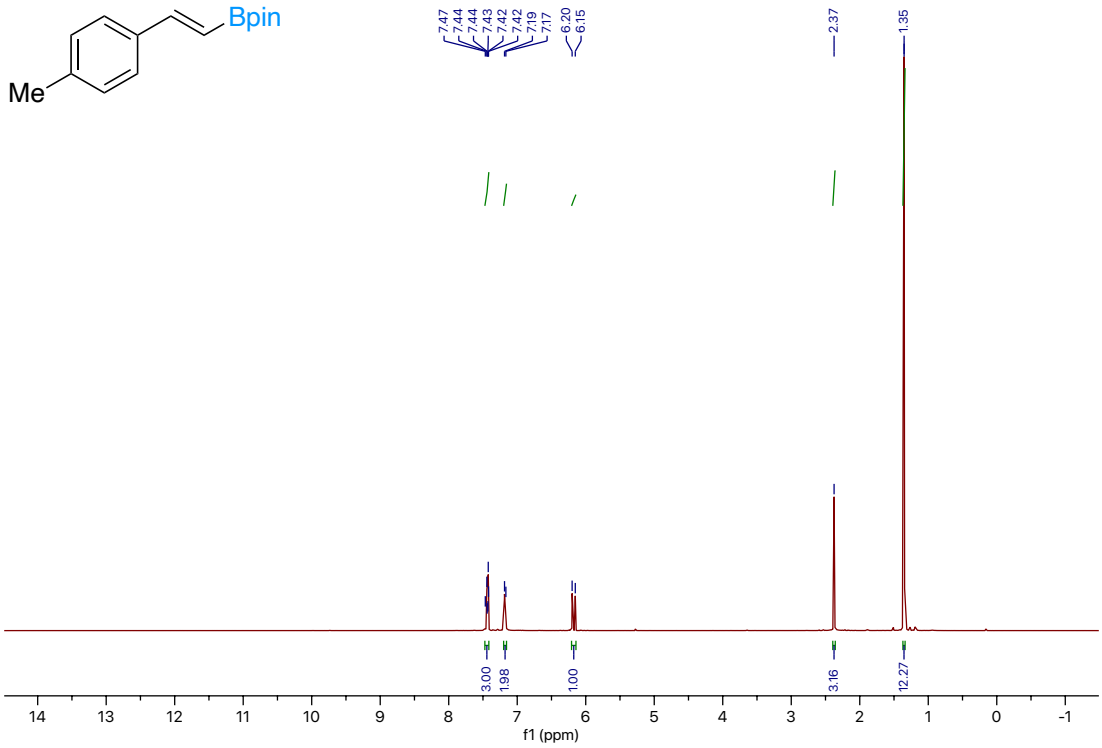
(*E*)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane (4a): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

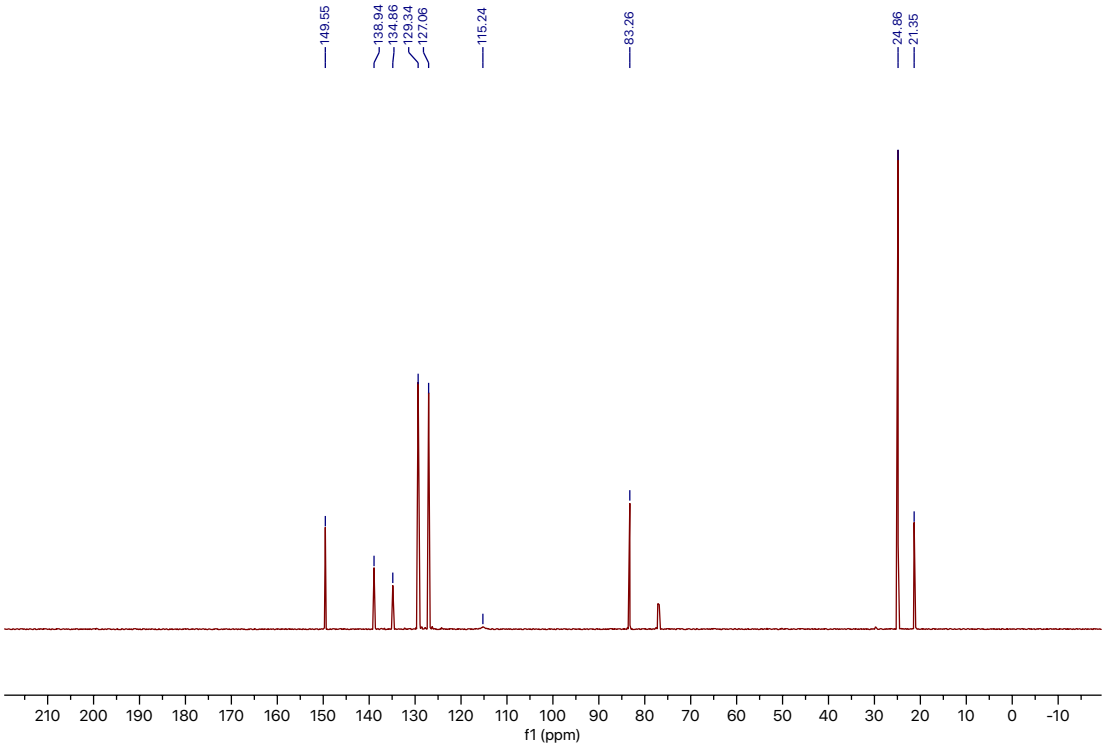


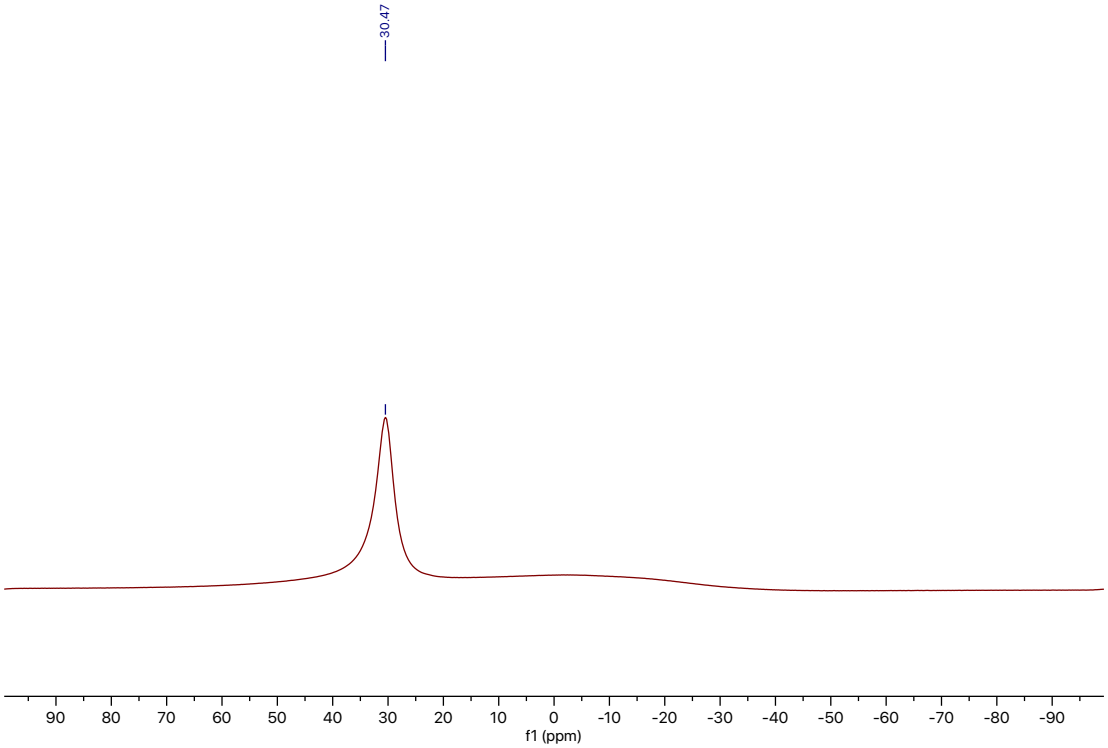




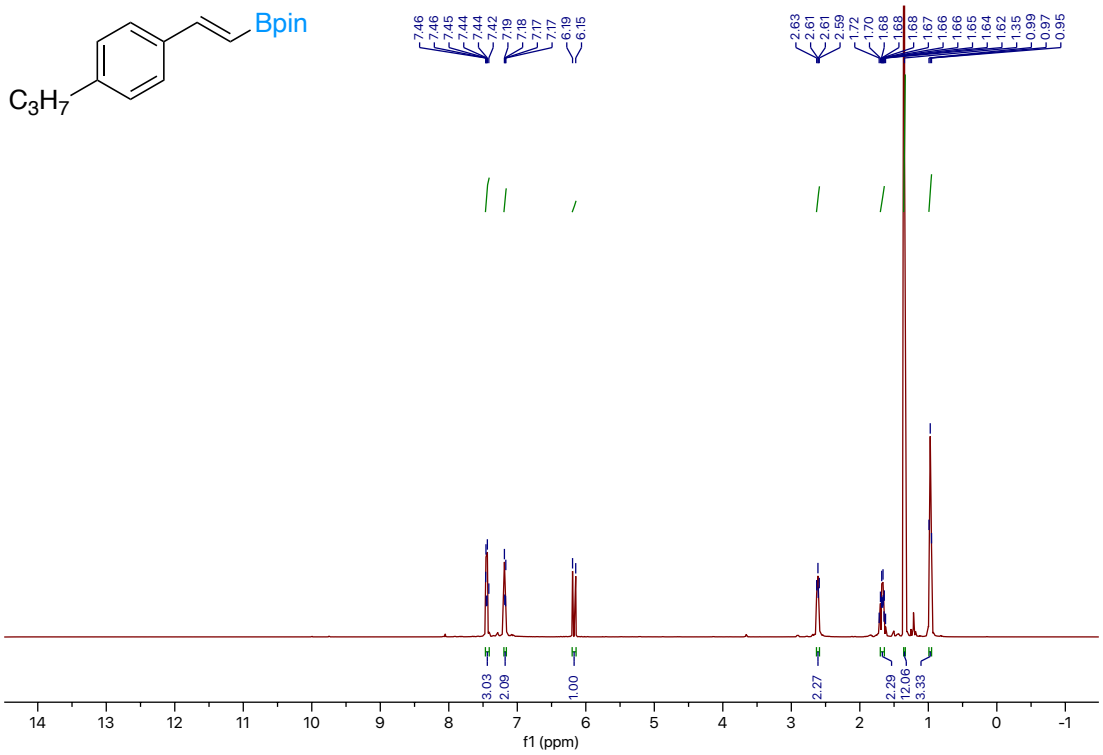
(*E*)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane (4b): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

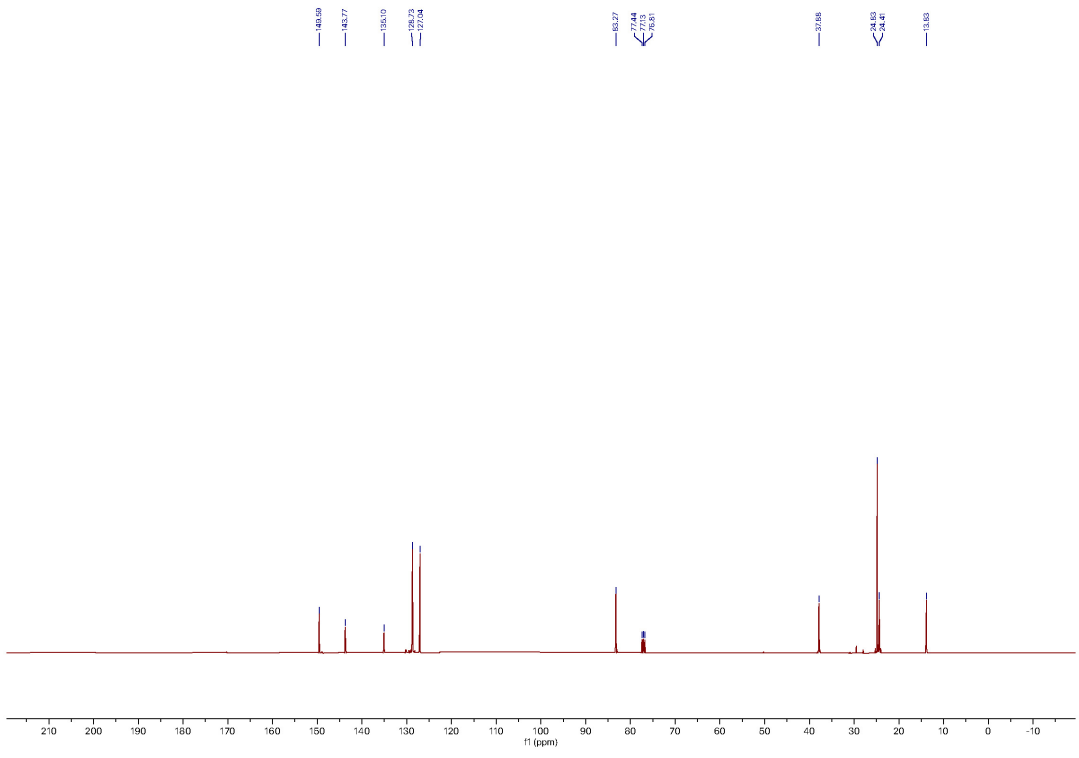


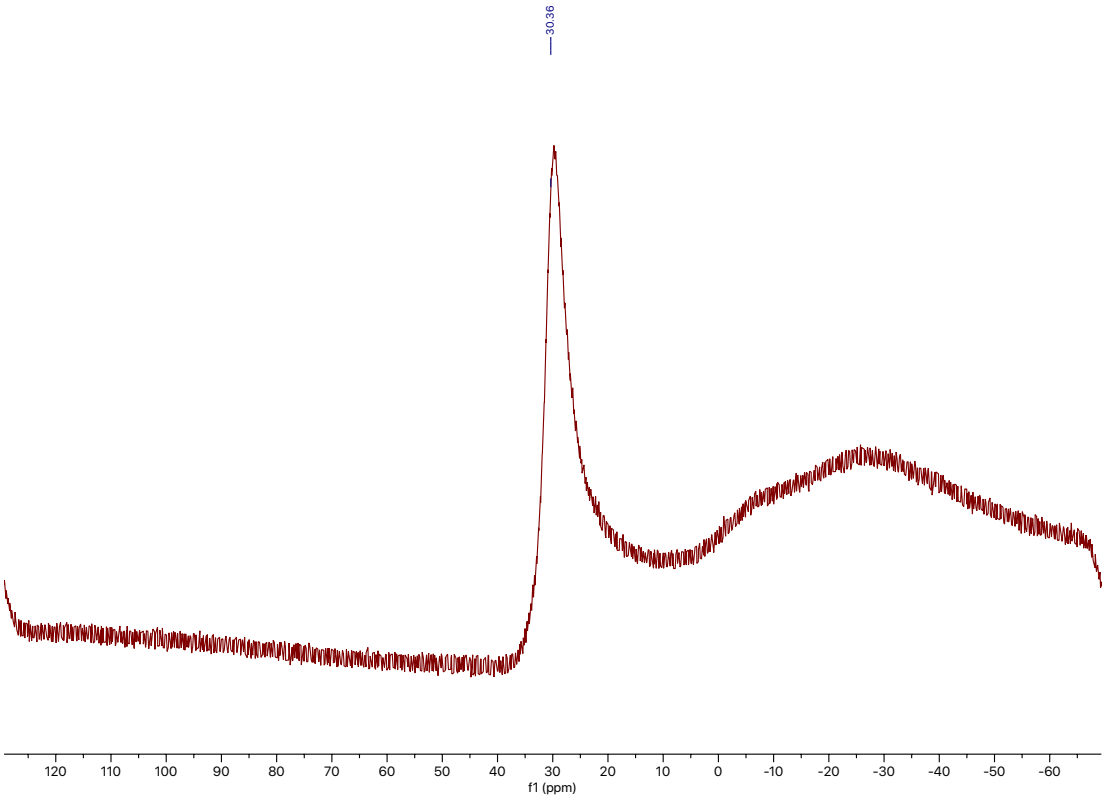

149.55
138.94
134.86
129.34
127.06
115.24
83.26
24.86
21.35
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


30.47
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

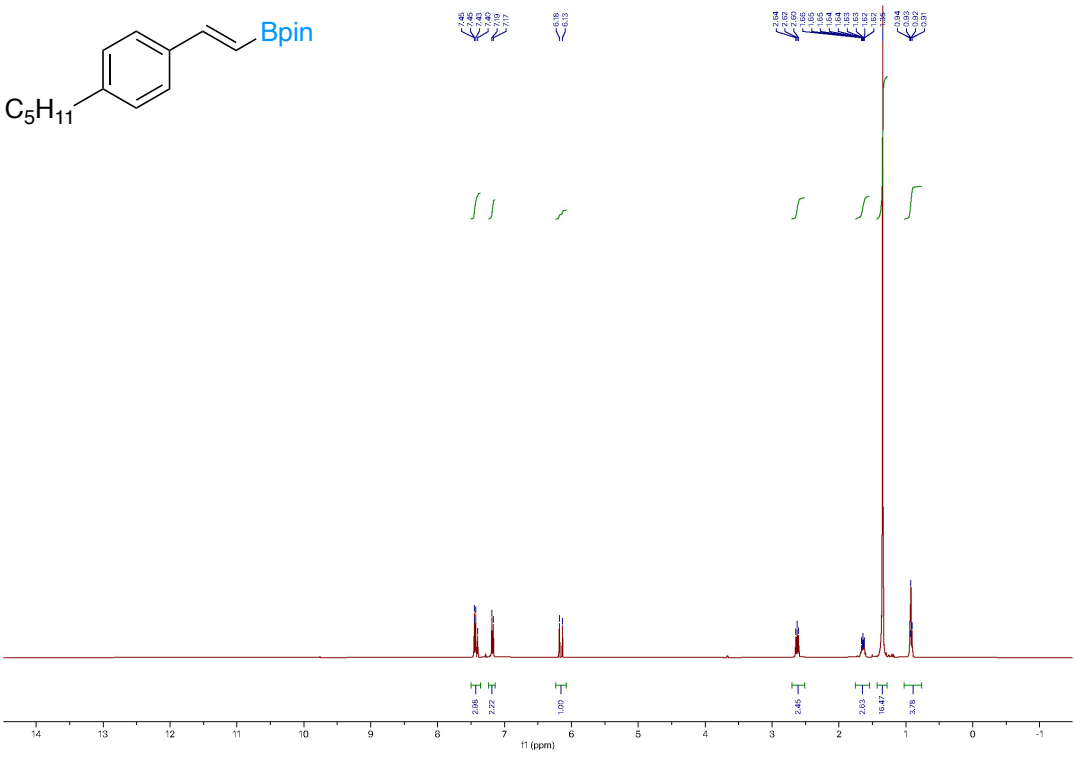
(*E*)-2-(4-propylstyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4c): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

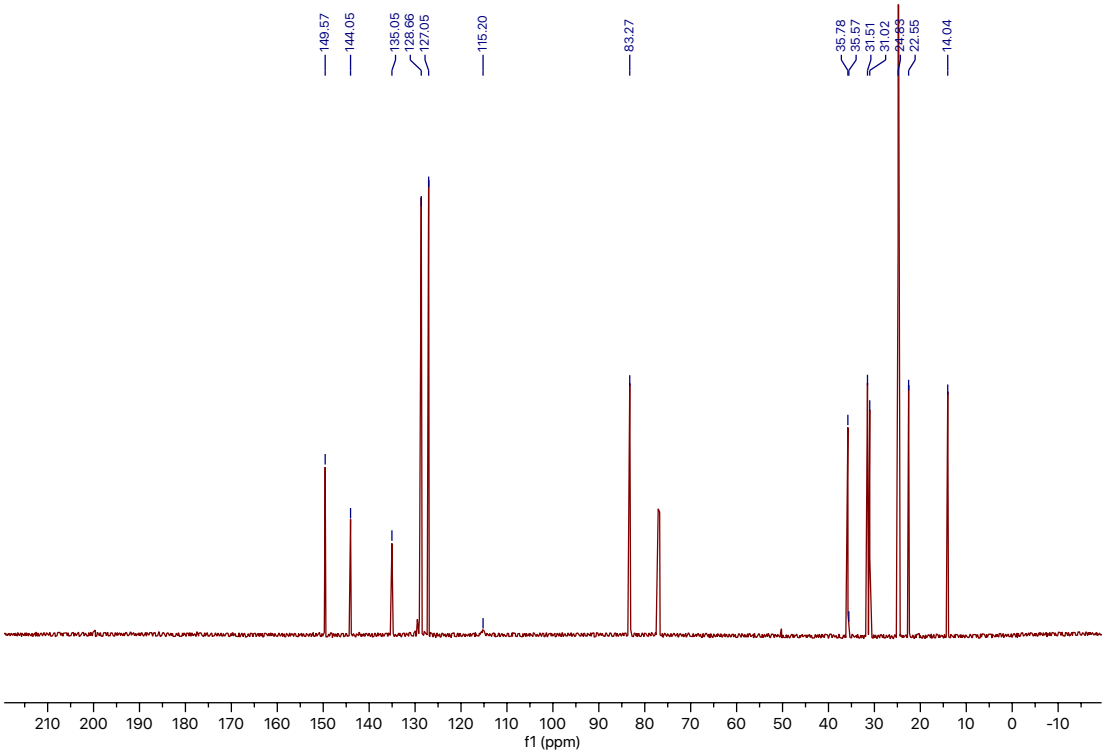


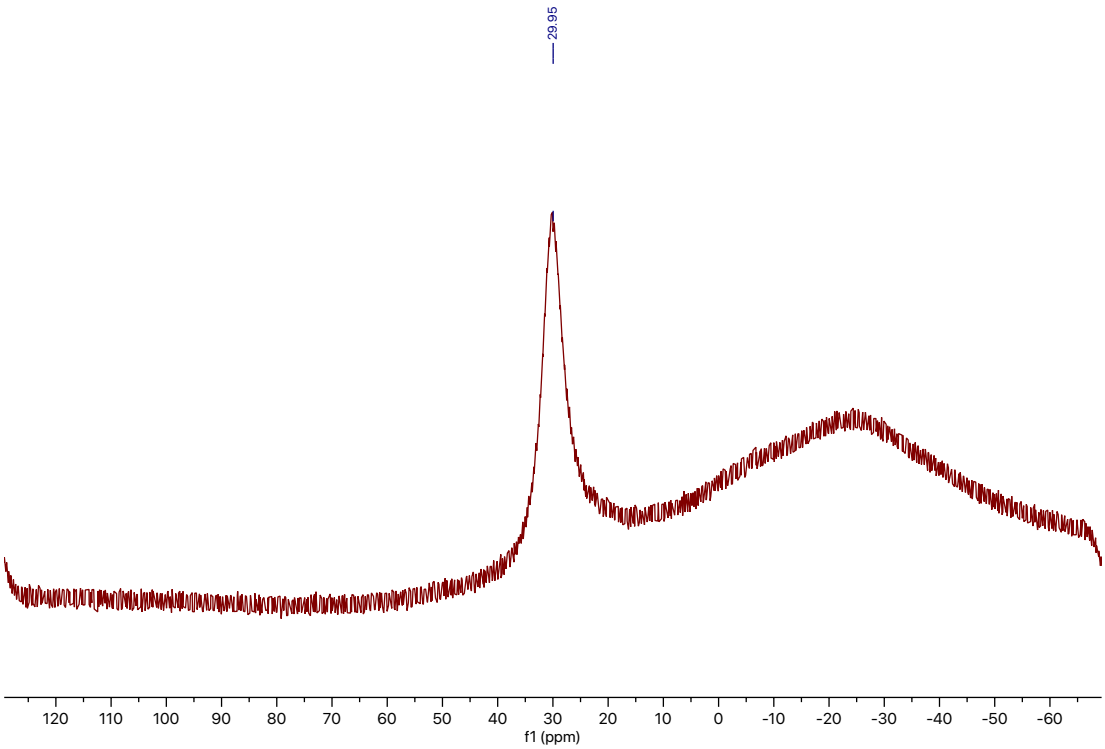




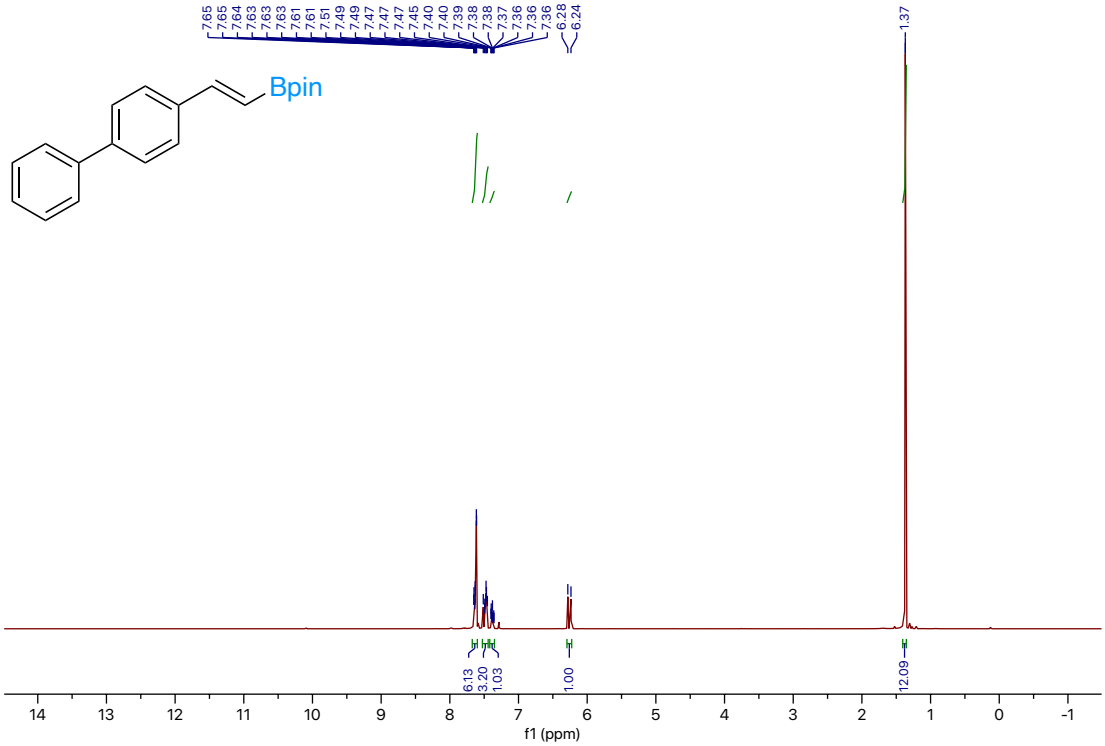
(*E*)-4,4,5,5-tetramethyl-2-(4-pentylstyryl)-1,3,2-dioxaborolane (4d): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

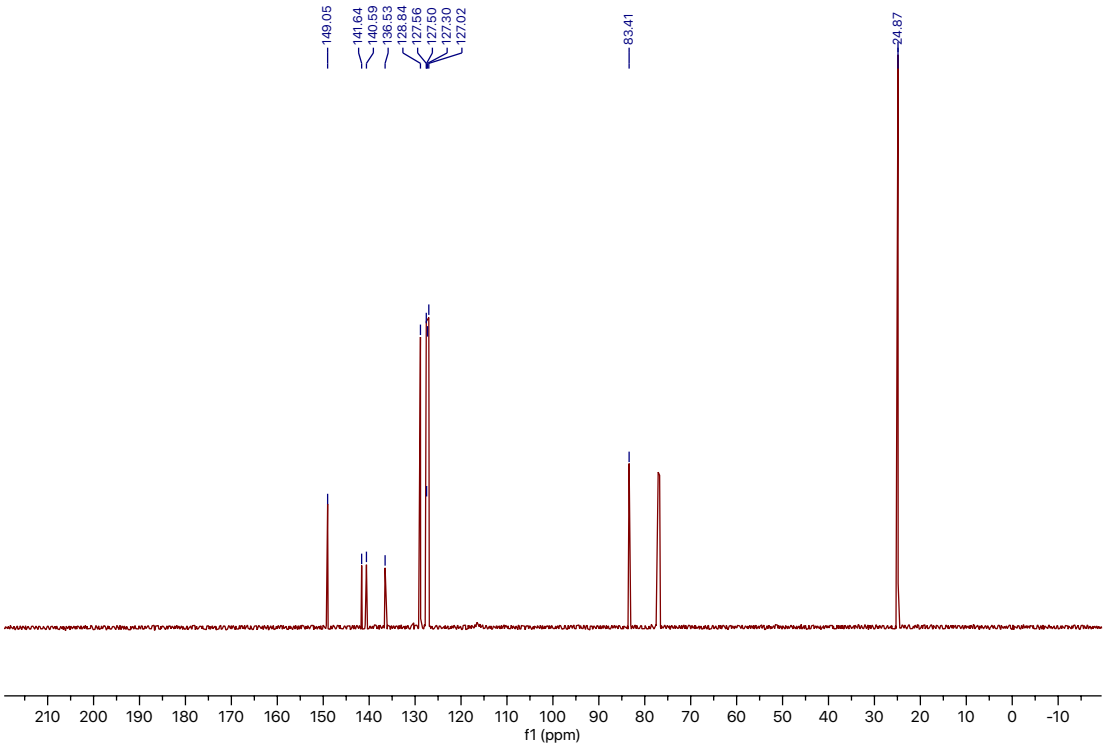


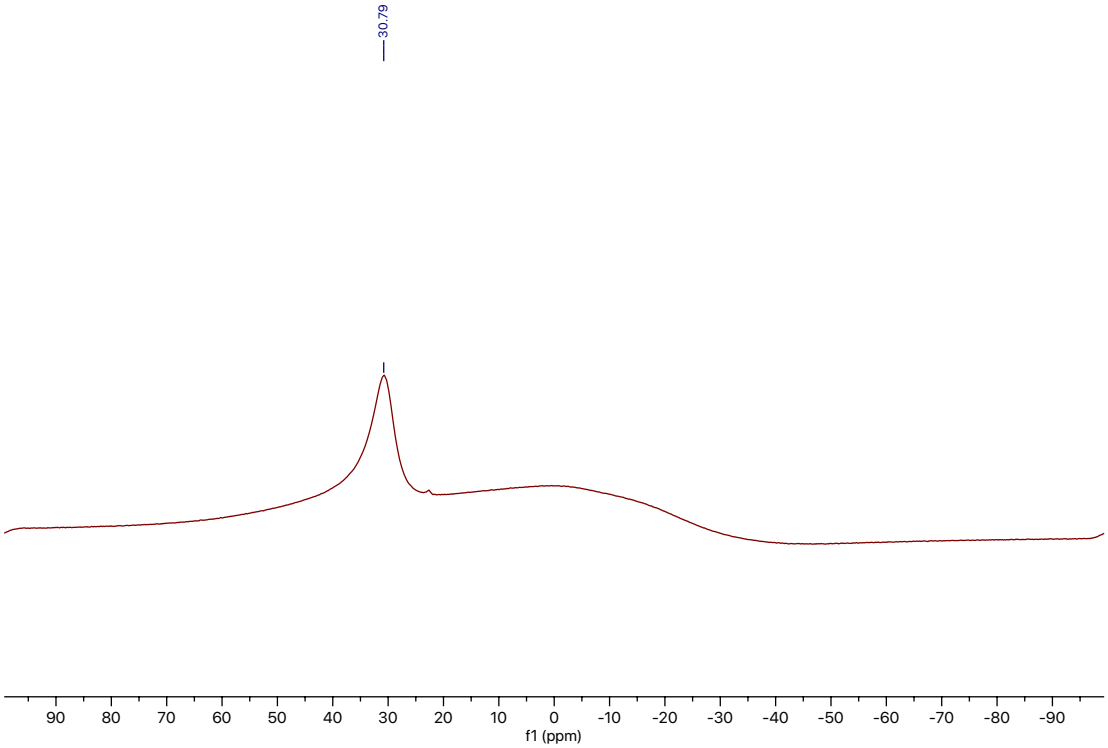

149.57
144.05
135.05
128.66
127.05
115.20
83.27
35.78
35.57
31.51
31.02
24.83
22.55
14.04
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


29.95
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60
f1 (ppm)

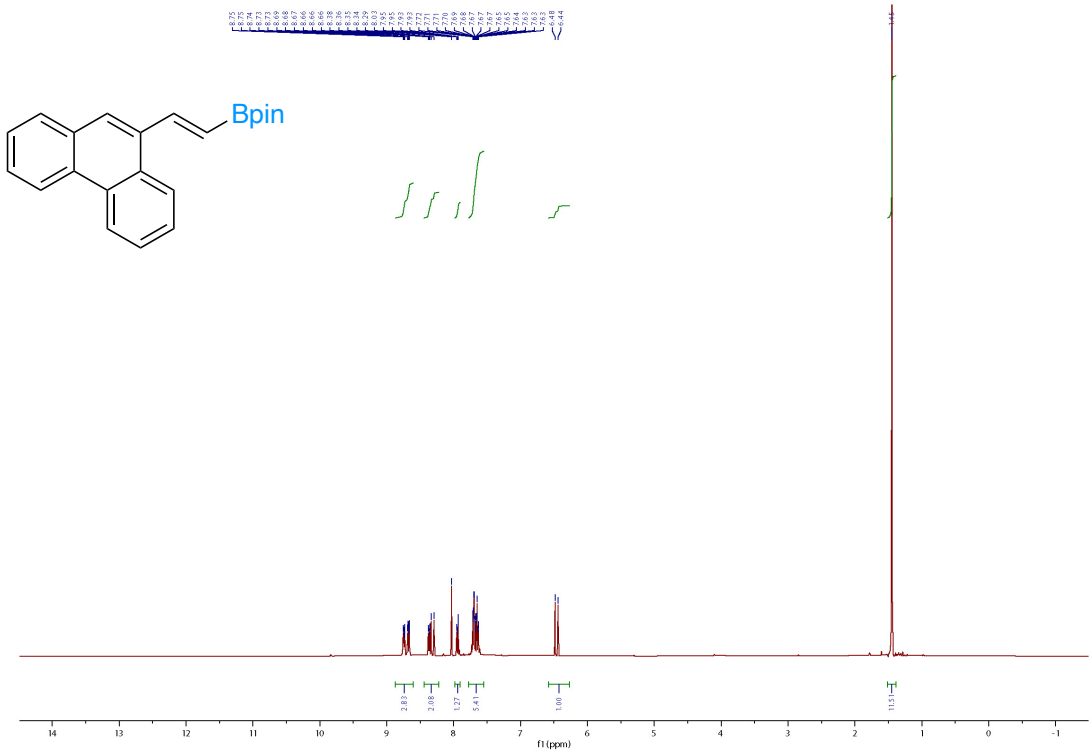
(*E*)-2-(2-([1,1'-biphenyl]-4-yl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4e): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

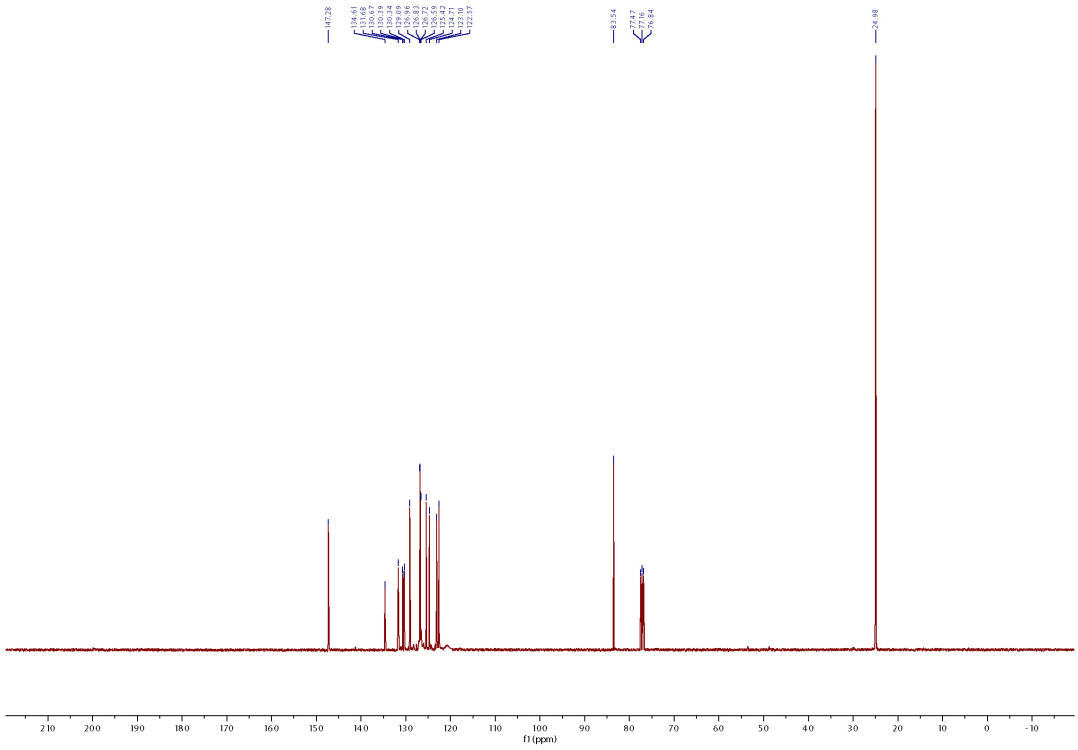


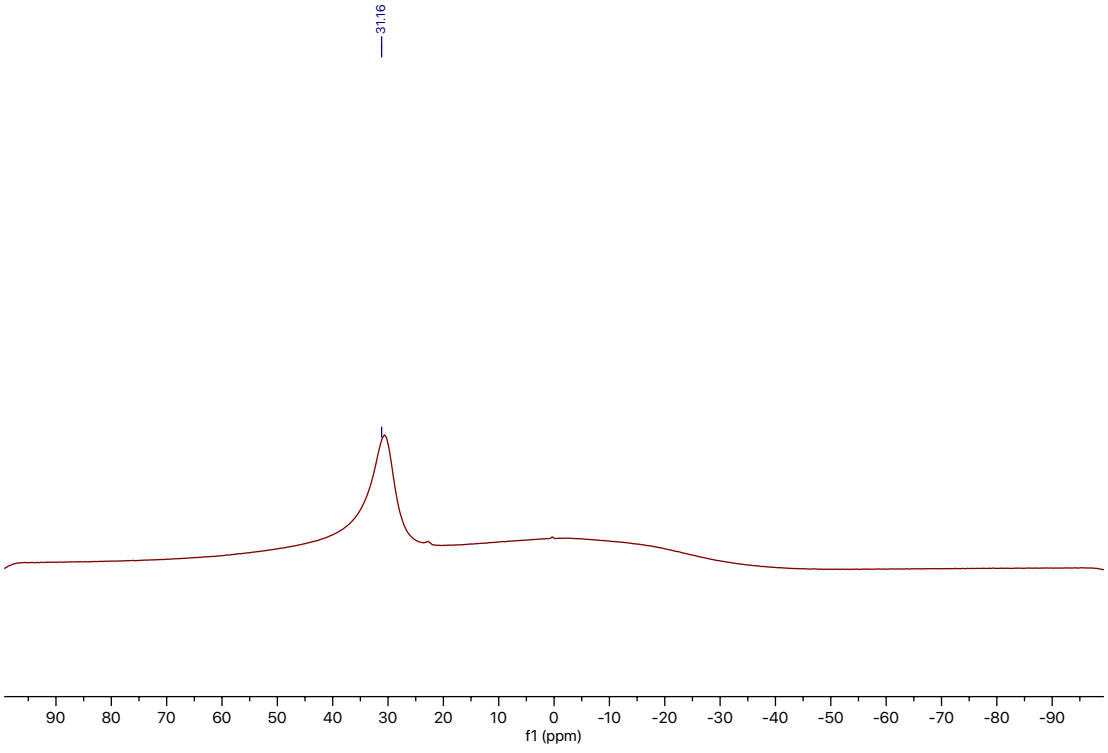




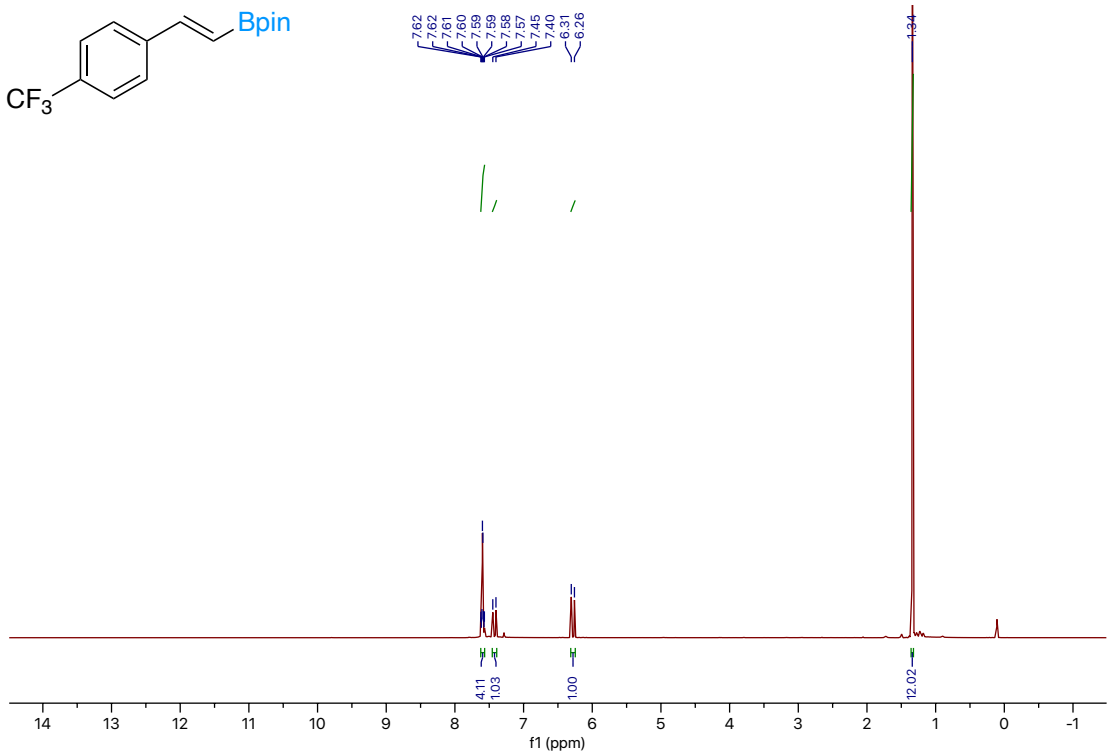
(*E*)-4,4,5,5-tetramethyl-2-(2-(phenanthren-9-yl)vinyl)-1,3,2-dioxaborolane (4f): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

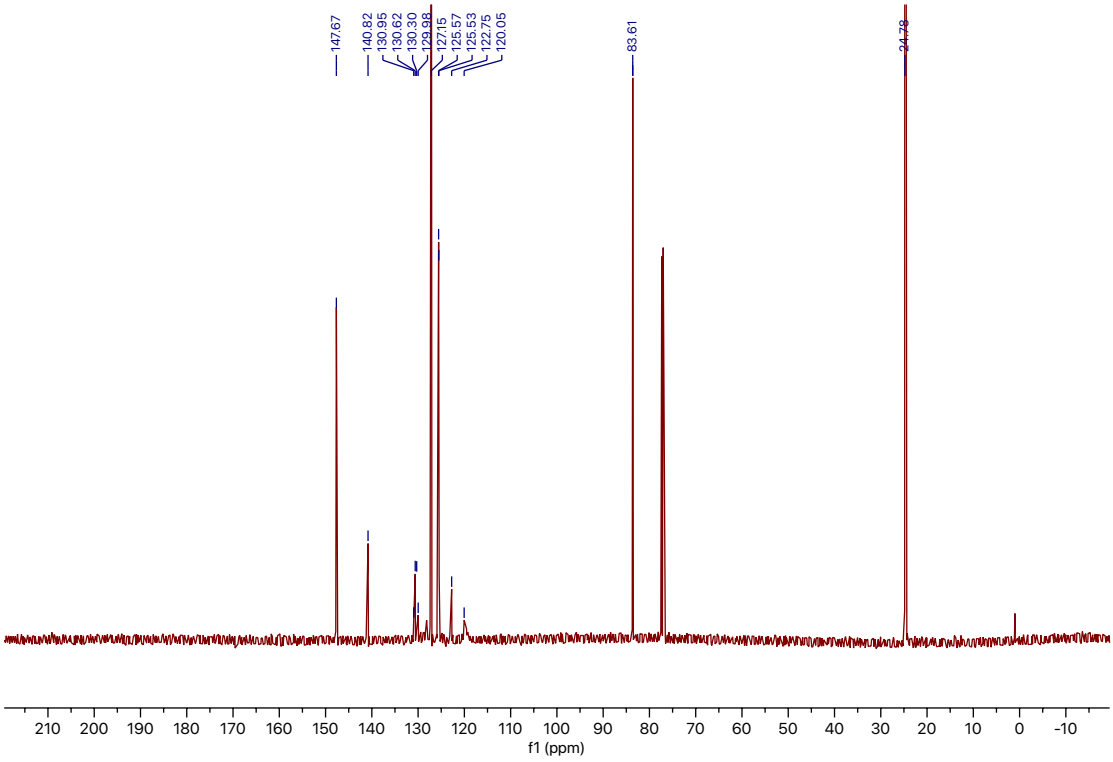


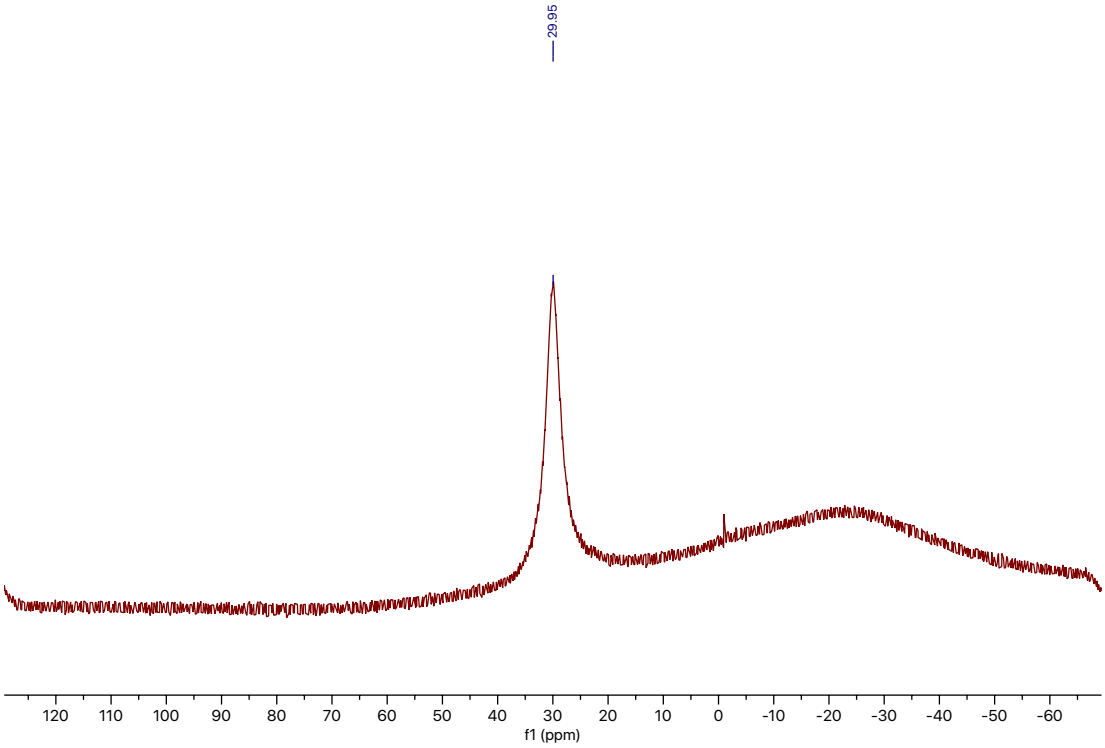

147.28
134.61
131.68
130.67
130.39
130.34
129.09
126.46
126.40
126.72
125.45
125.23
124.71
123.30
122.57
83.54
77.47
77.15
76.84
24.98
f1 (ppm)

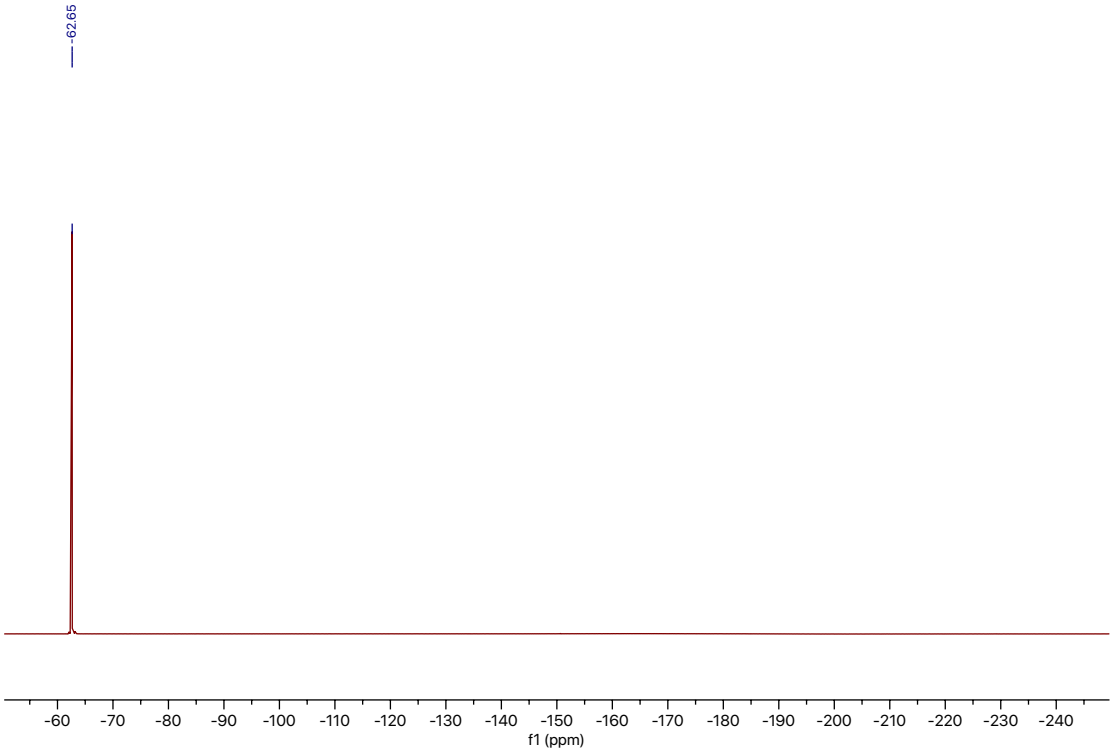

31.16
f1 (ppm)

(*E*)-4,4,5,5-tetramethyl-2-(4-(trifluoromethyl)styryl)-1,3,2-dioxaborolane (4g): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$), ^{19}F NMR (376 MHz, $CDCl_3$).

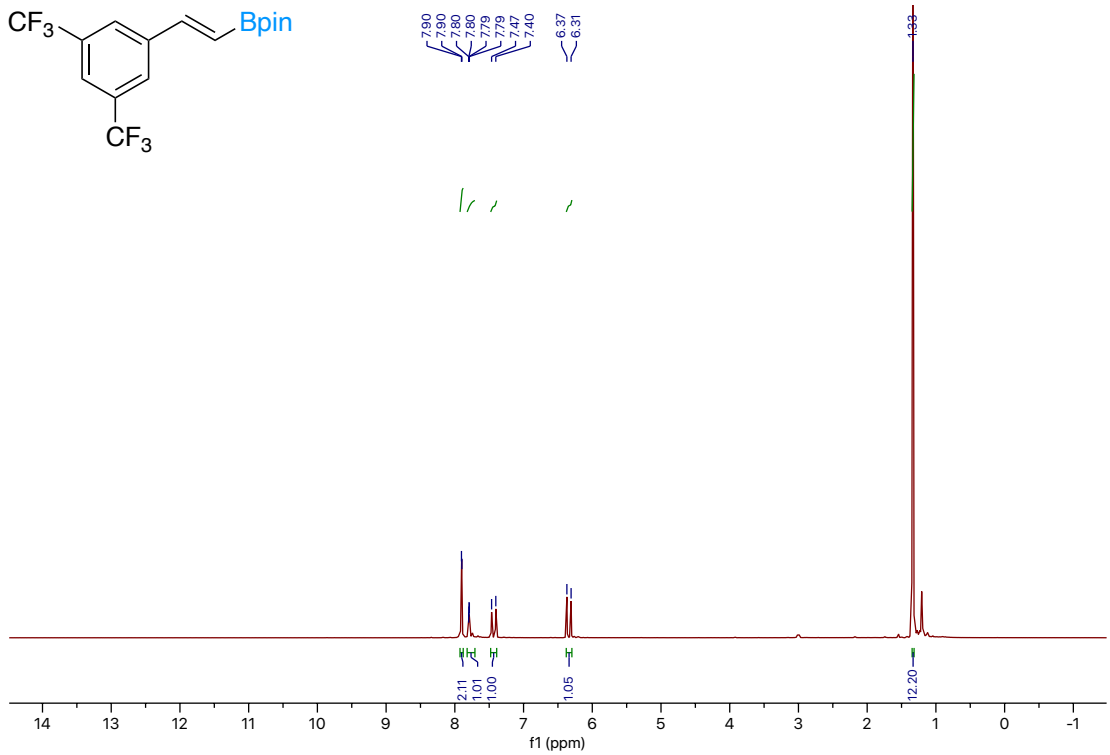


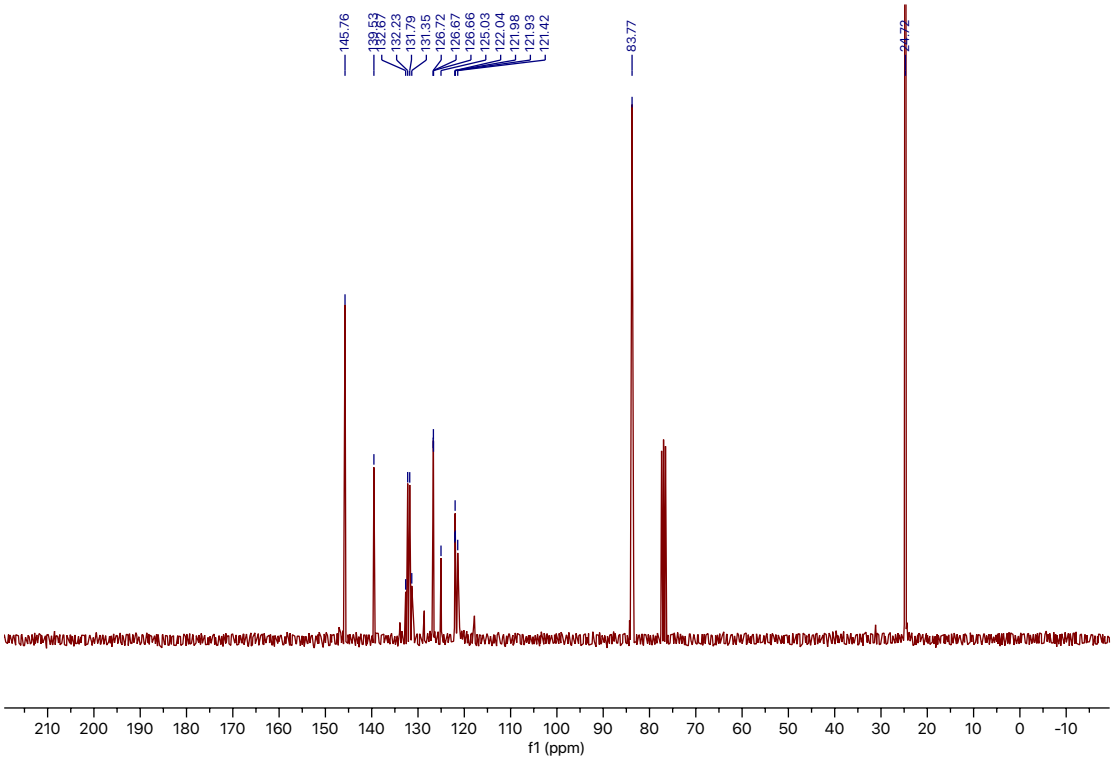


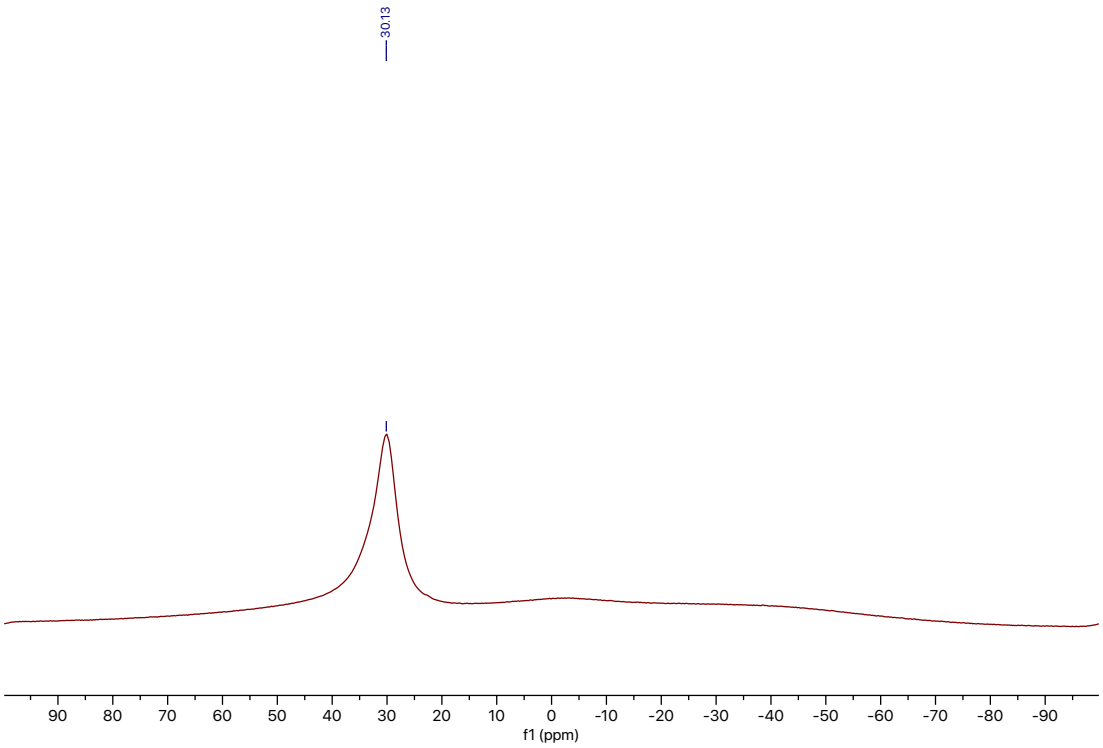

29.95
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60
f1 (ppm)

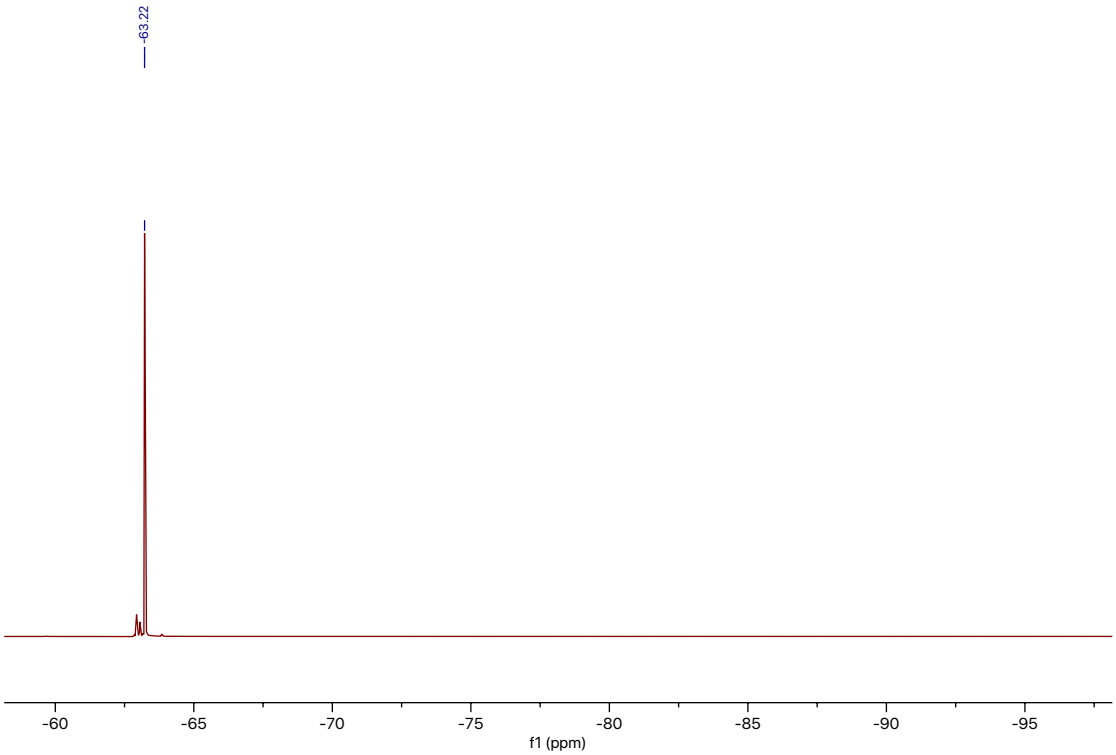

-62.65
-60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

(*E*)-2-(3,5-bis(trifluoromethyl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4h): ^{1}H NMR (300 MHz, $CDCl_3$); ^{13}C NMR (76 MHz, $CDCl_3$); ^{11}B NMR (96 MHz, $CDCl_3$); ^{19}F NMR (283 MHz, $CDCl_3$).

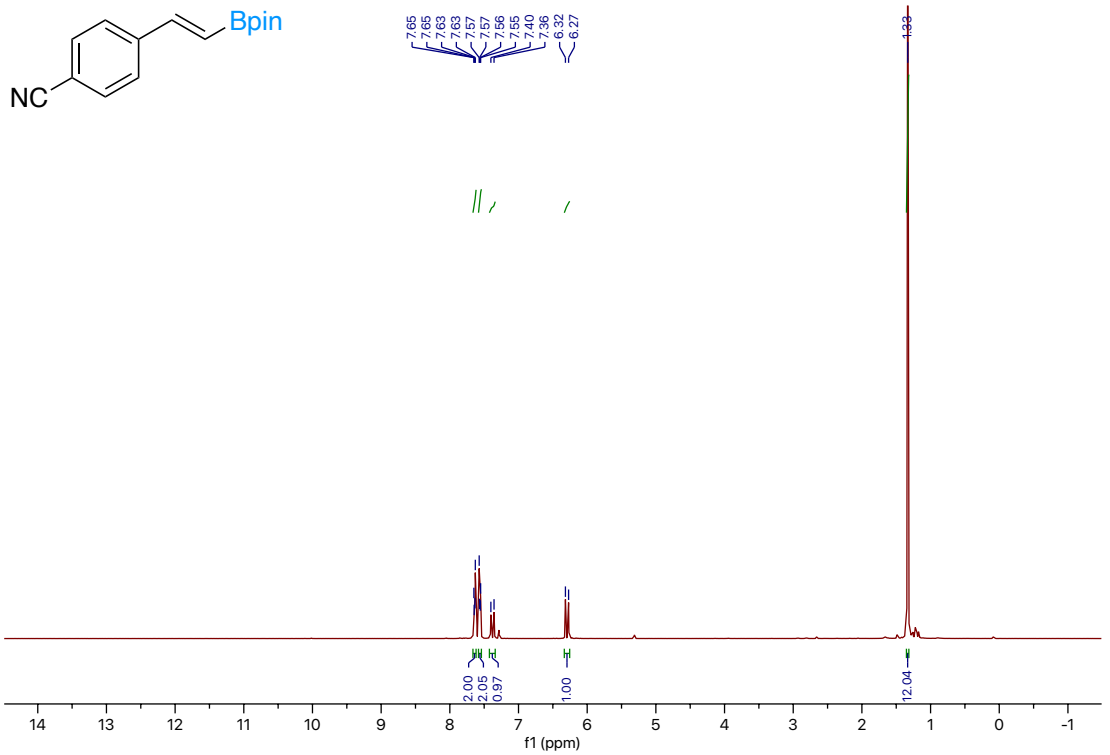


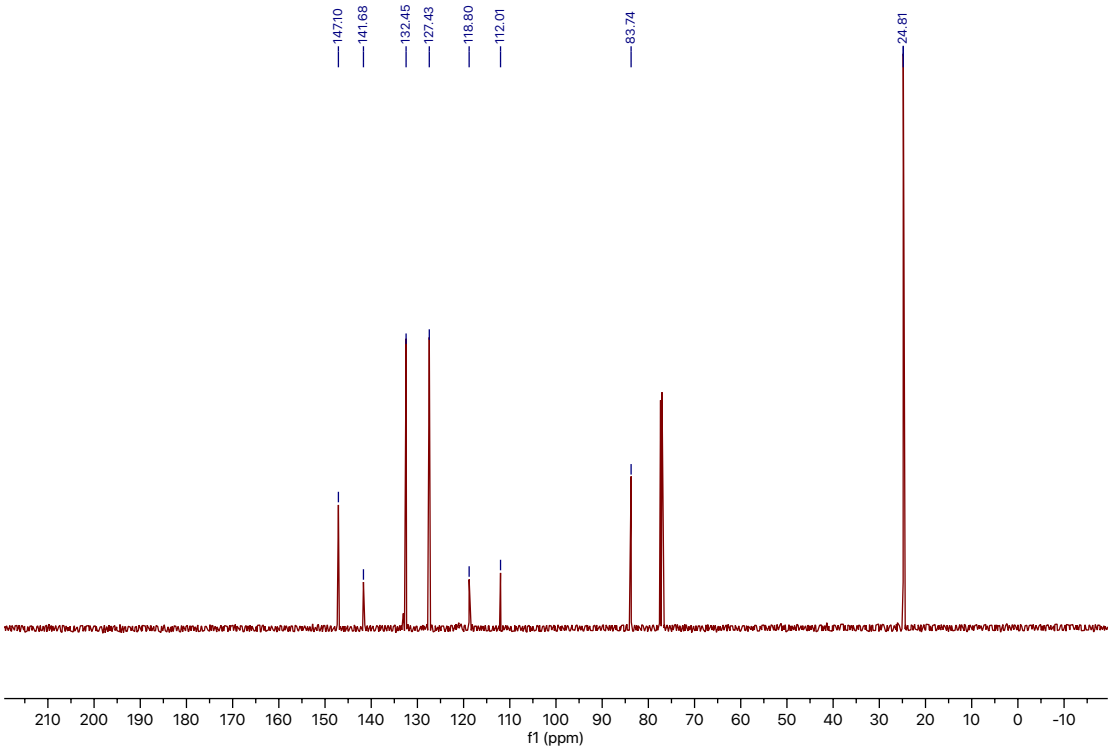


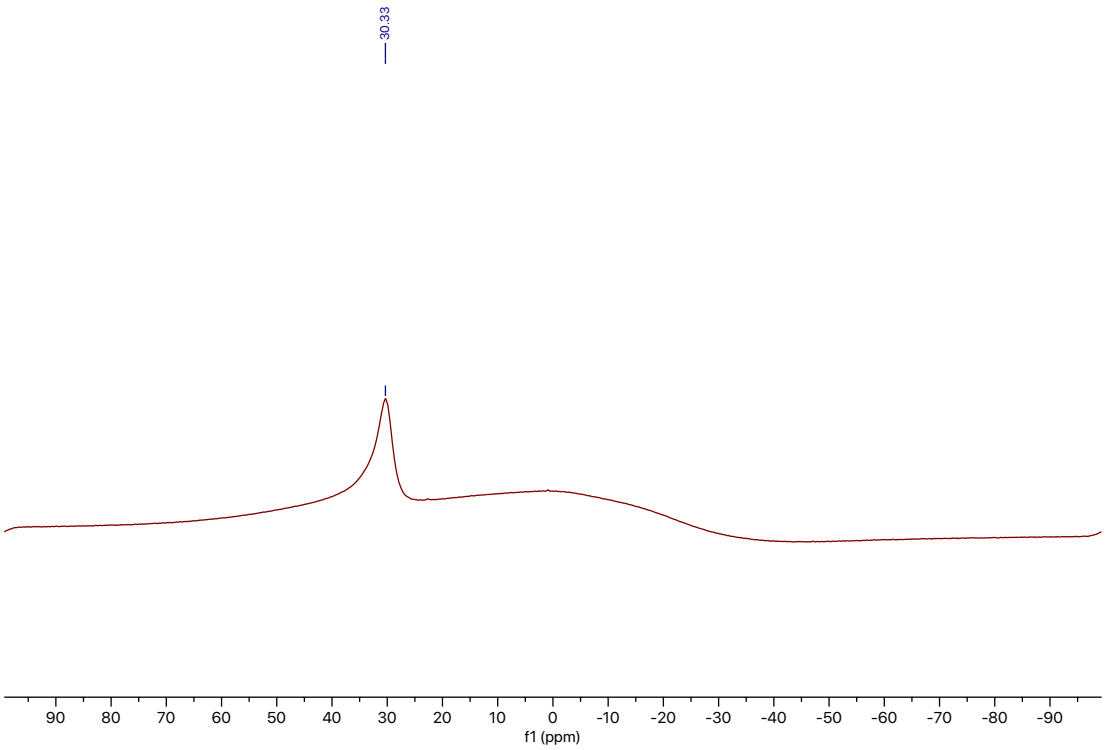

30.13
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)


-63.22
-60 -65 -70 -75 -80 -85 -90 -95
f1 (ppm)

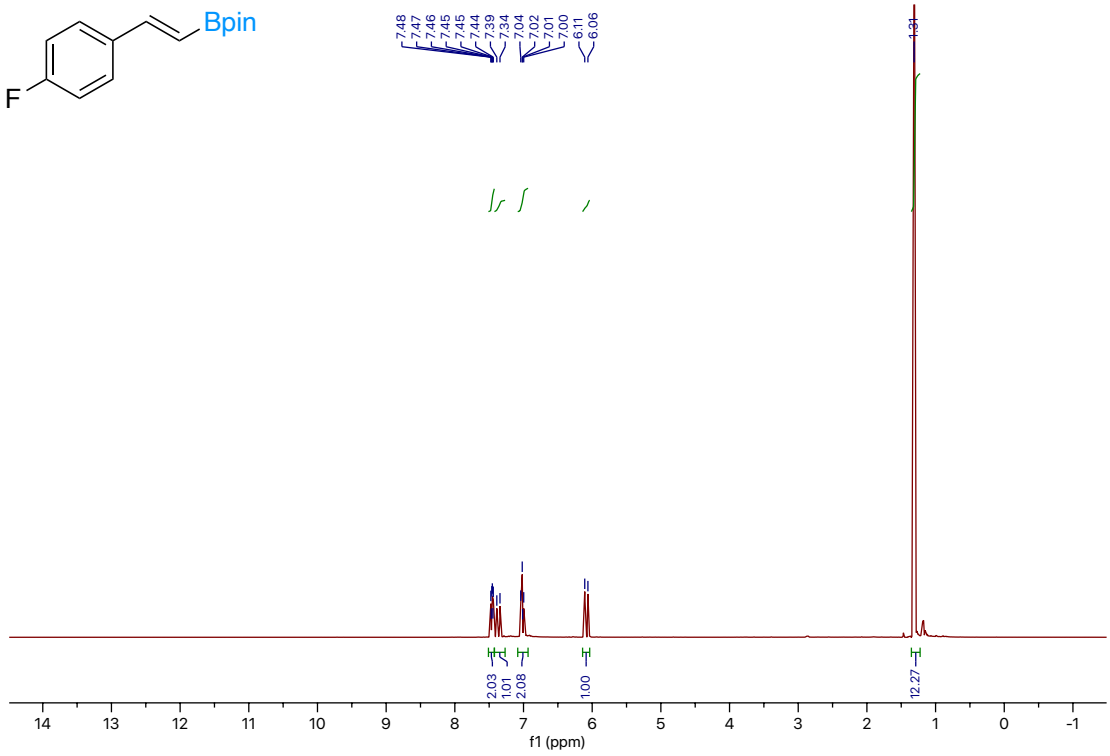
(*E*)-2-(4-isocyanostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4i): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

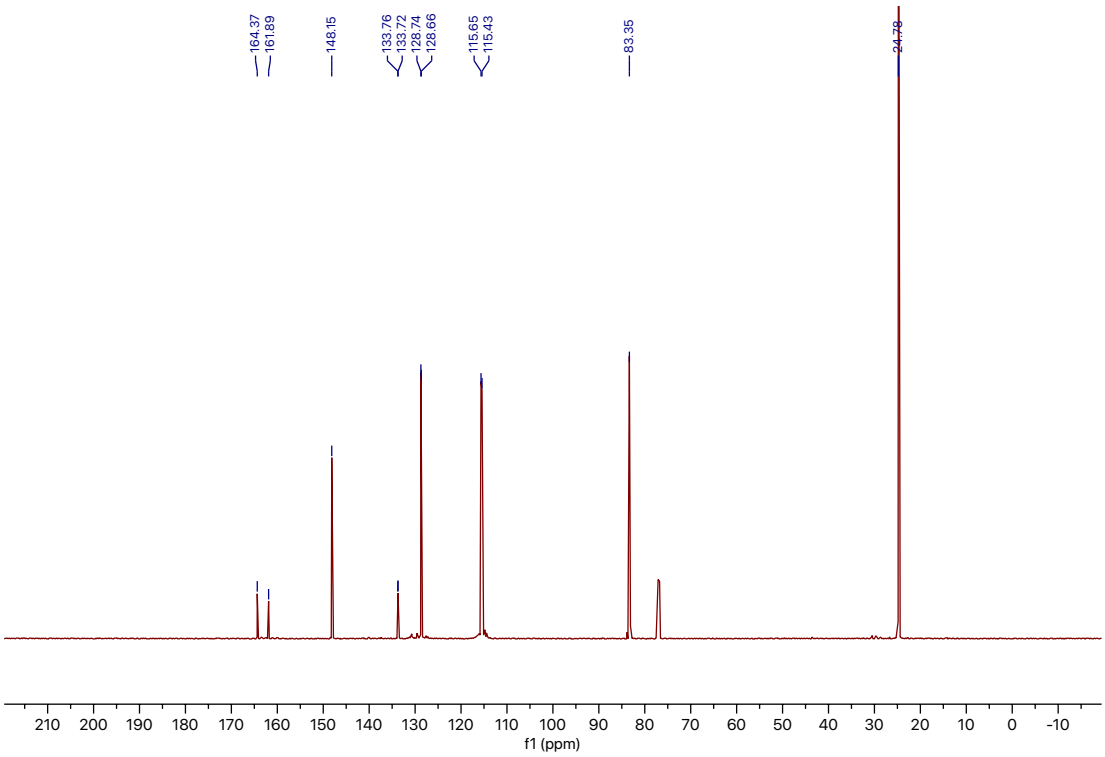


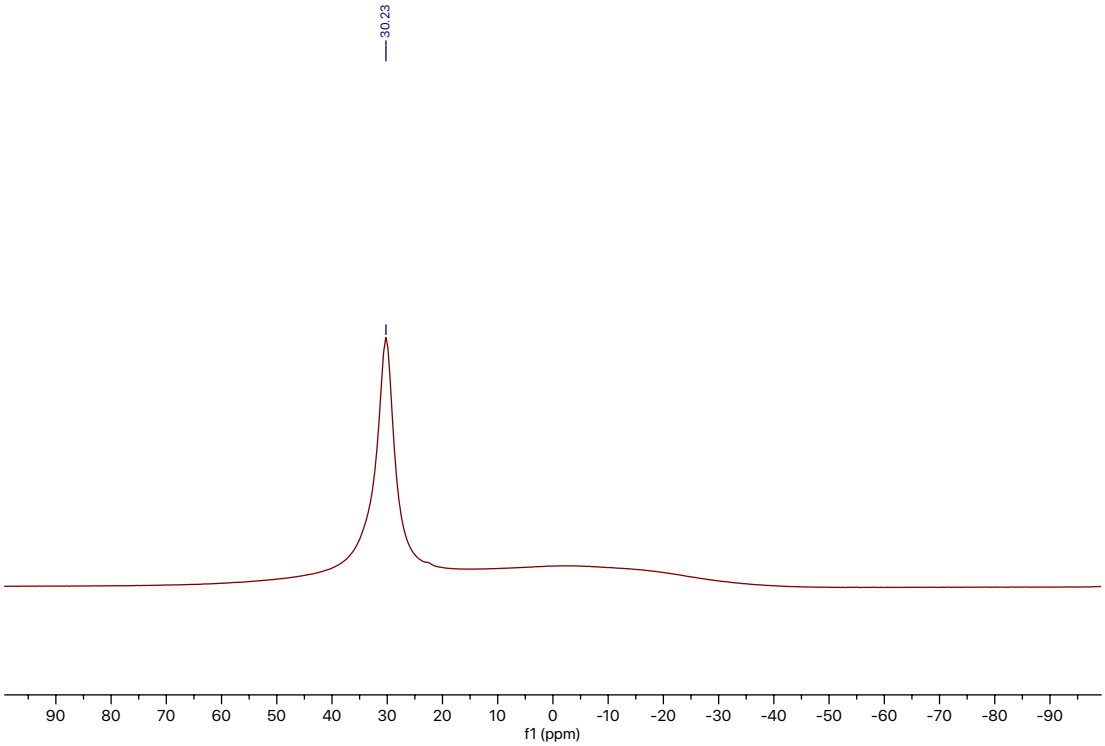


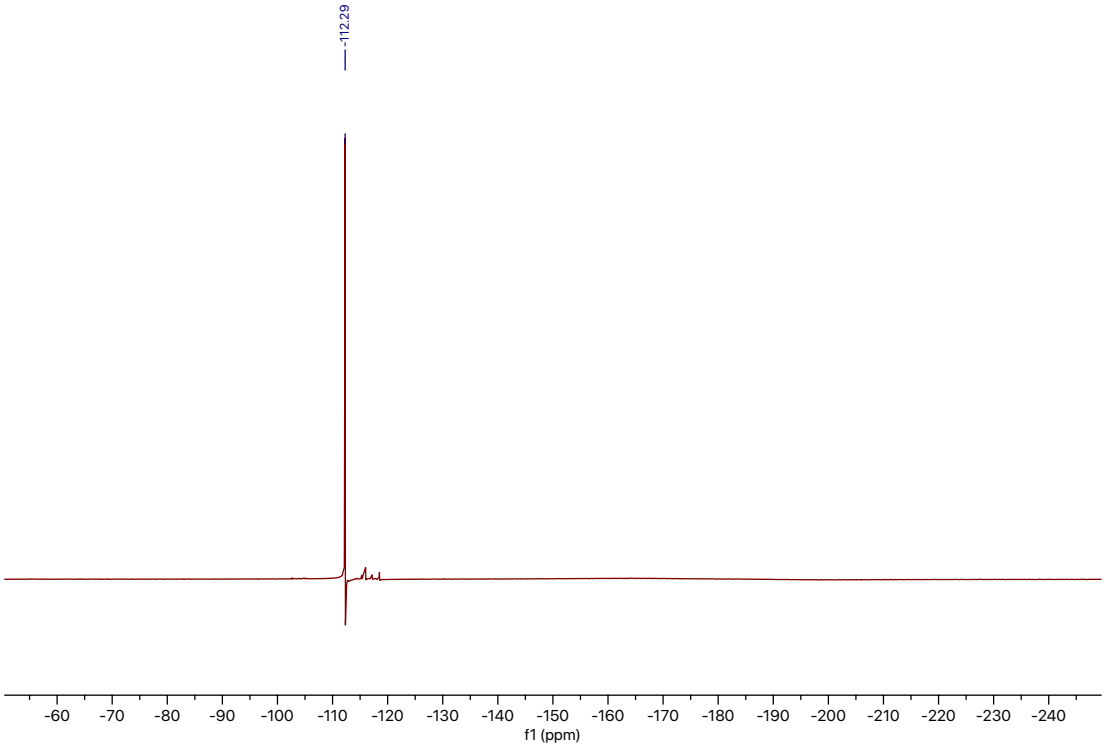


(*E*)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4j): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$), ^{19}F NMR (376 MHz, $CDCl_3$).

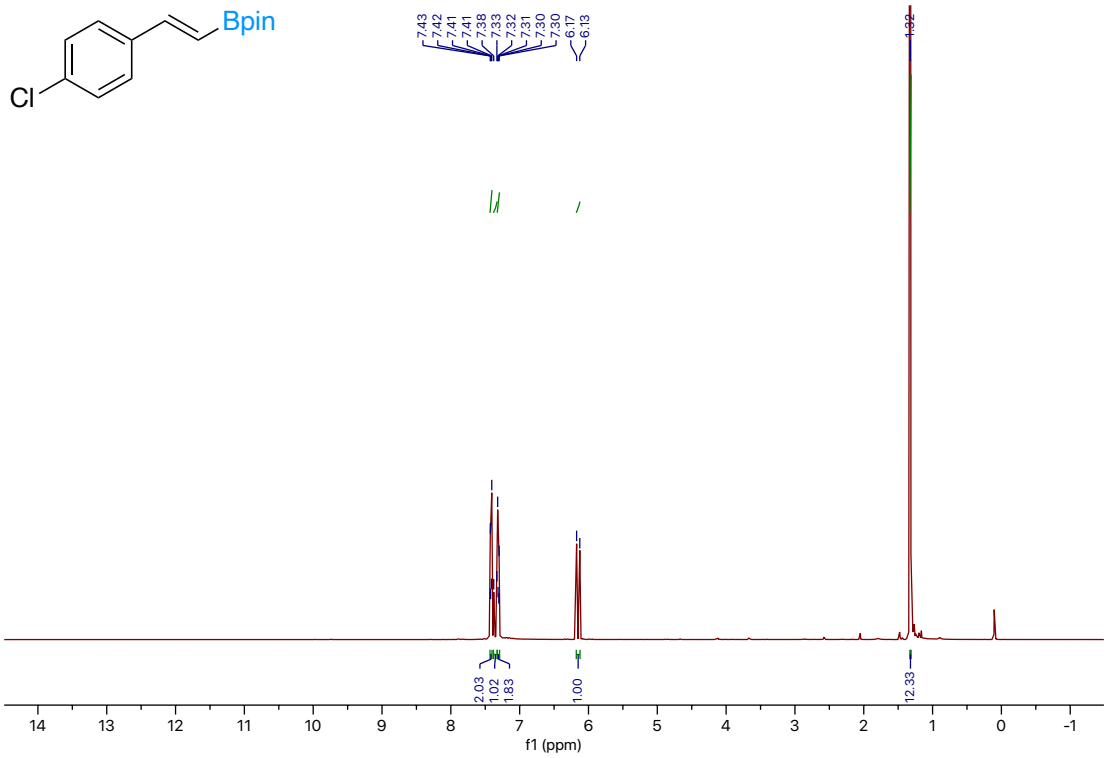


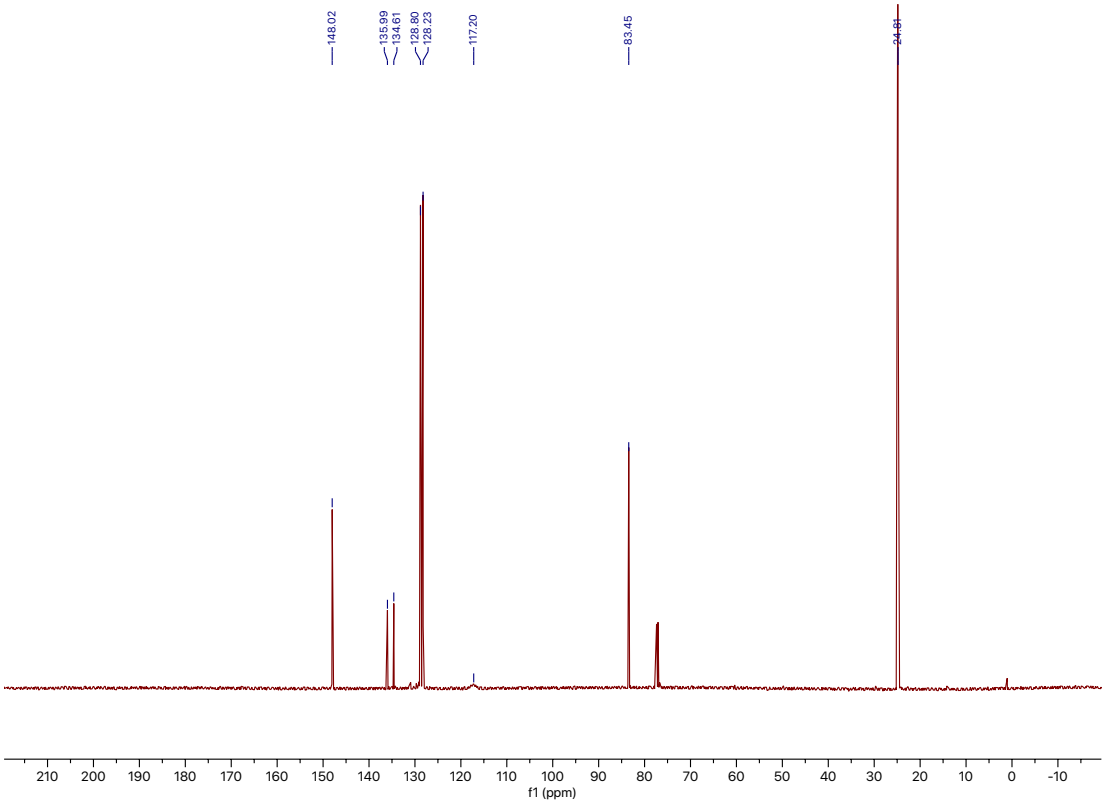

164.37
161.89
148.15
133.76
133.72
128.74
128.66
115.65
115.43
83.35
24.78
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

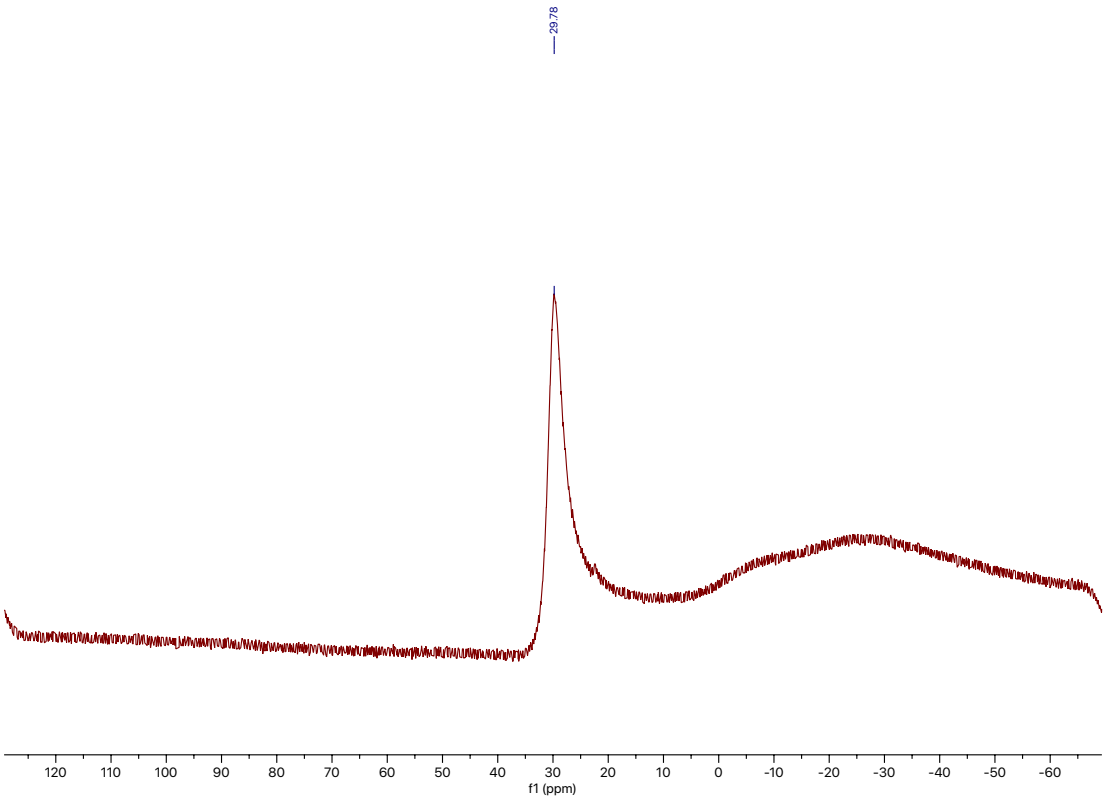

30.23
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)



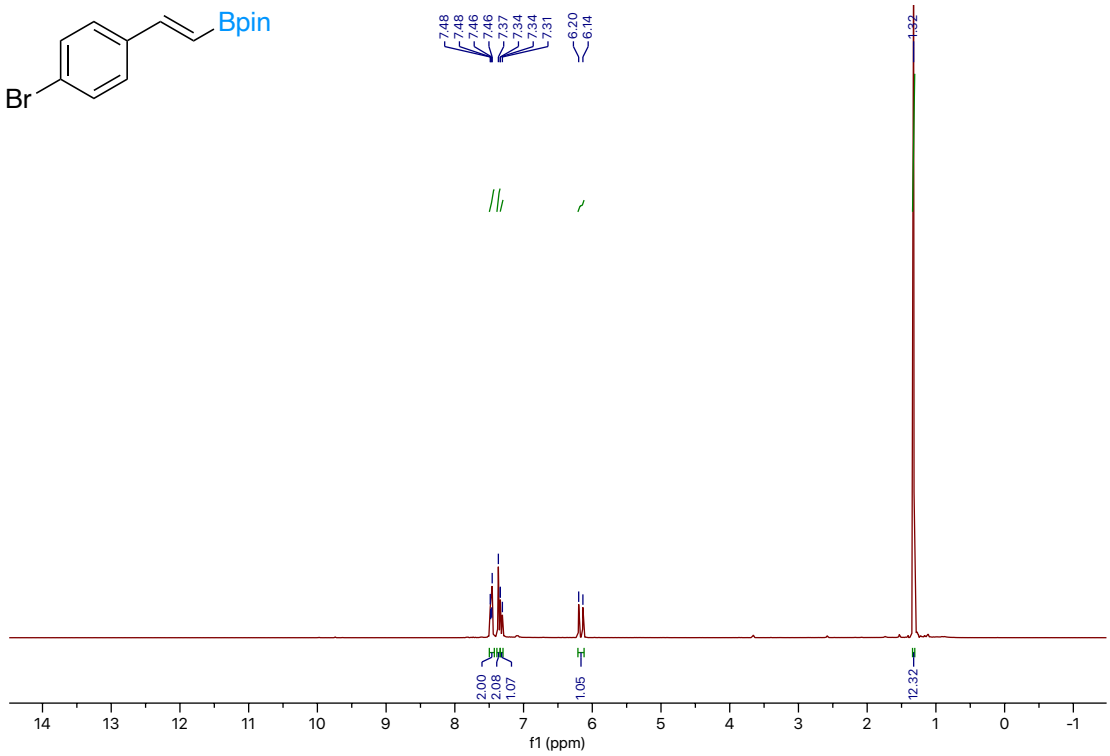
(*E*)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4k): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

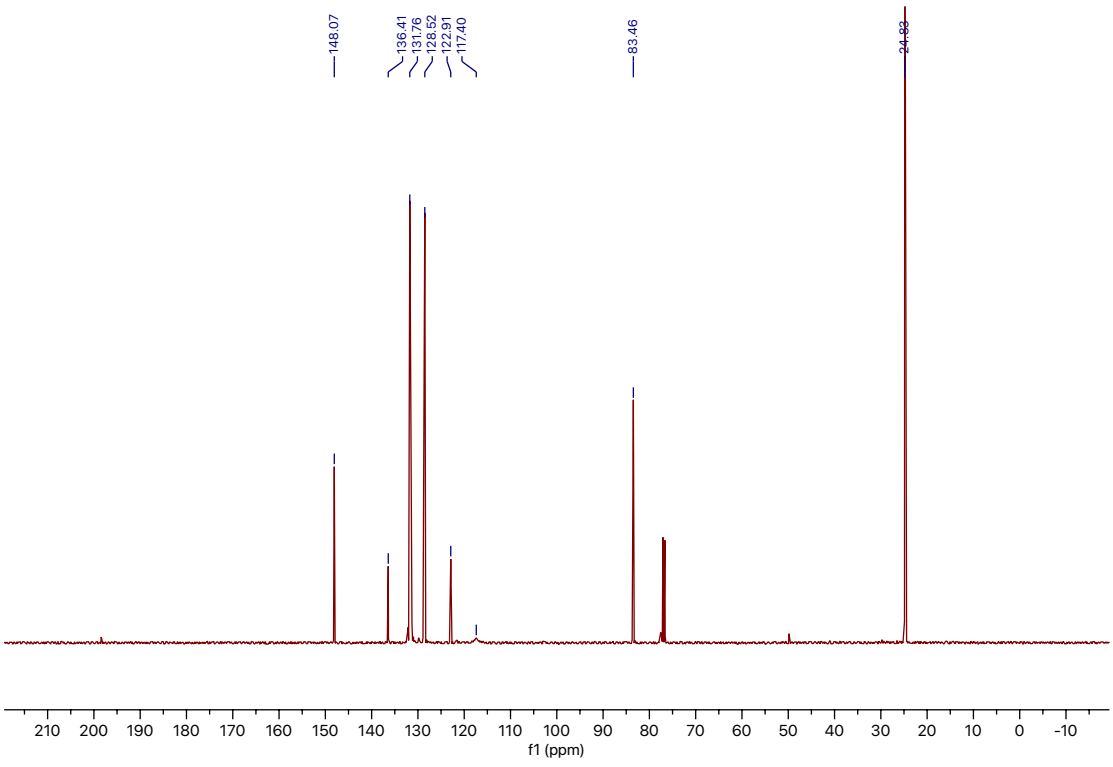


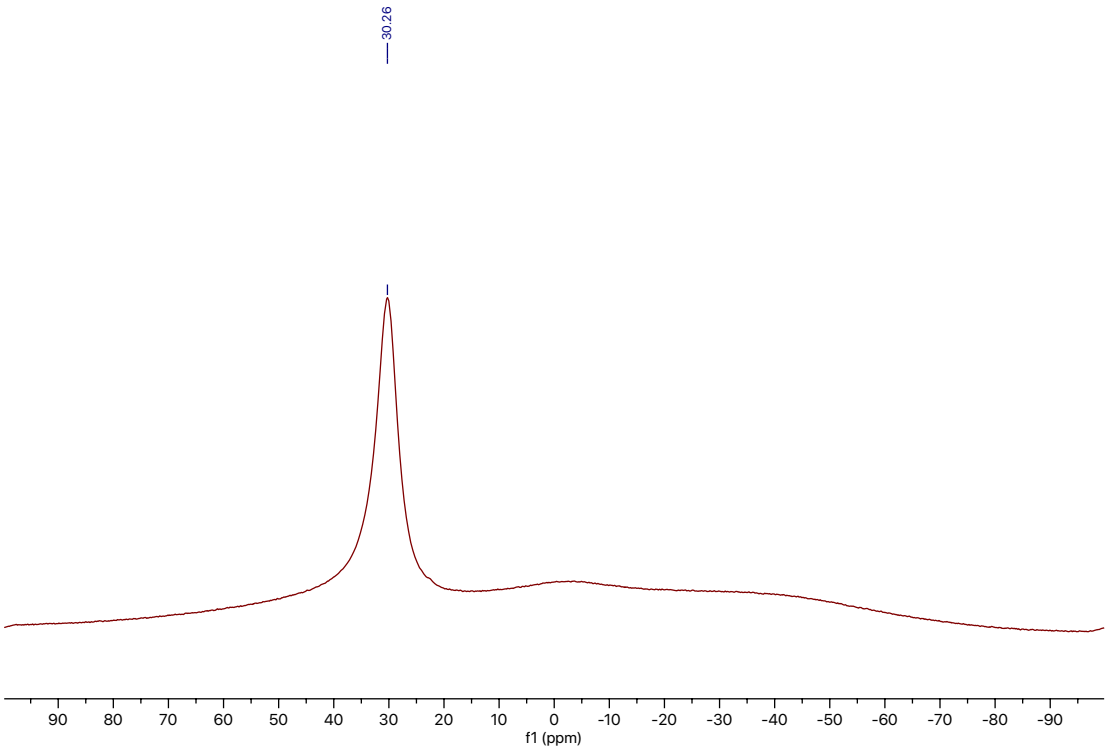

148.02
135.99
134.61
128.80
128.23
117.20
83.45
24.81
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


29.78
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60
f1 (ppm)

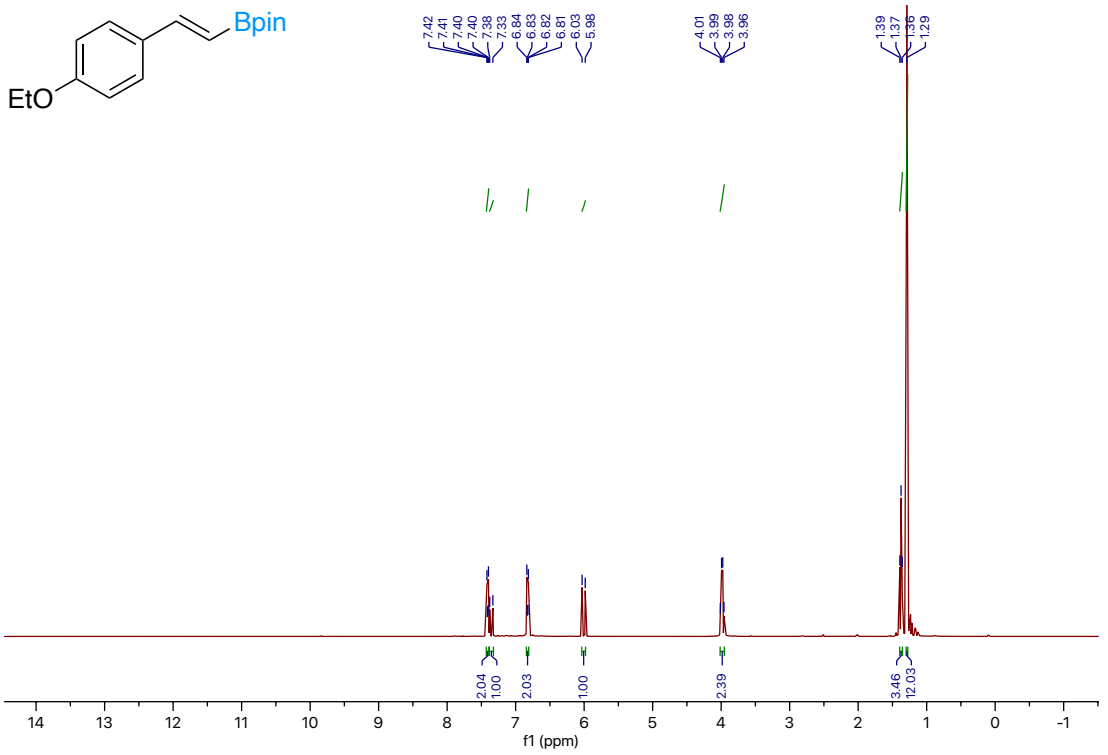
(*E*)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4l): ^{1}H NMR (300 MHz, $CDCl_3$); ^{13}C NMR (76 MHz, $CDCl_3$); ^{11}B NMR (96 MHz, $CDCl_3$).

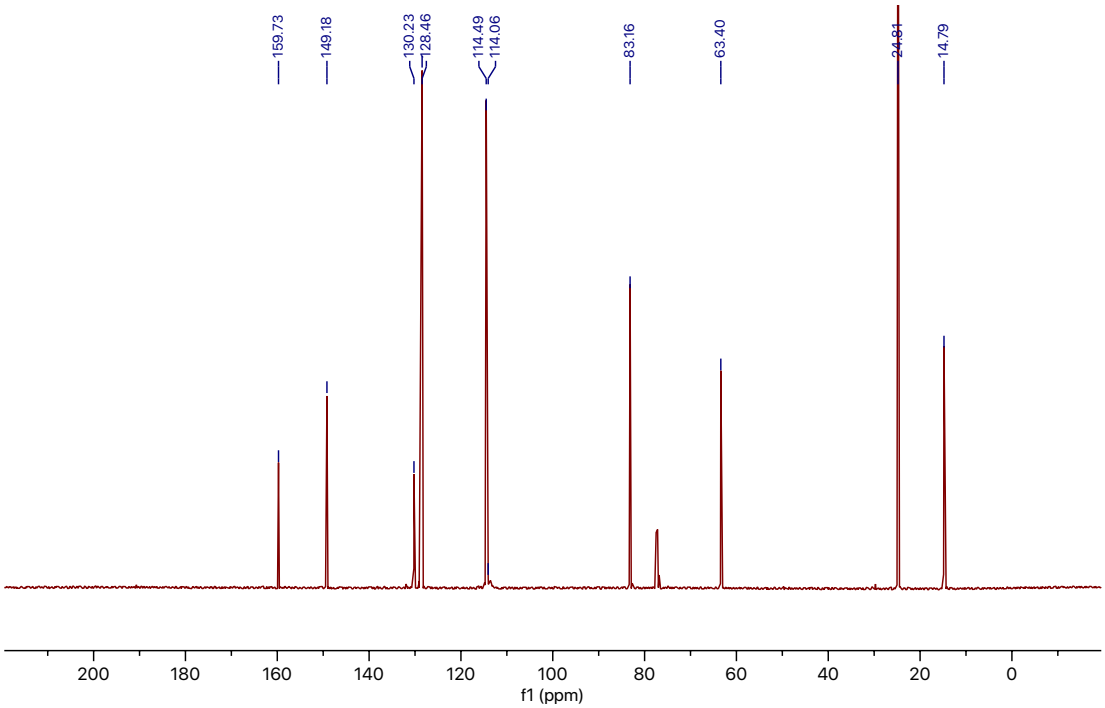


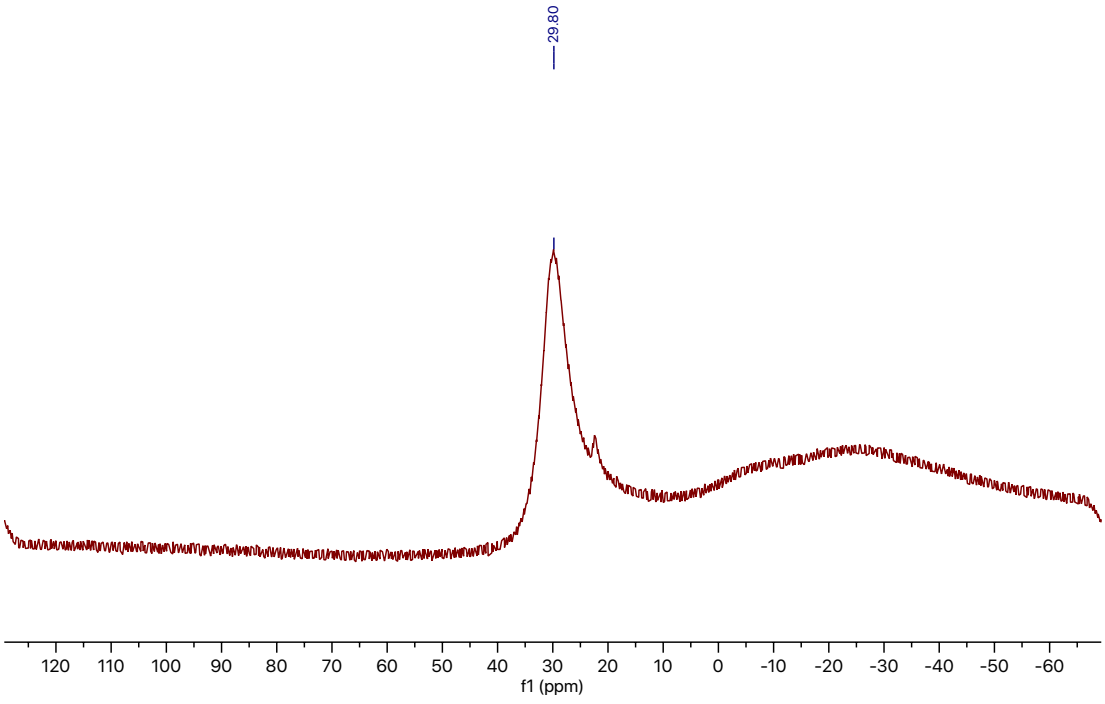




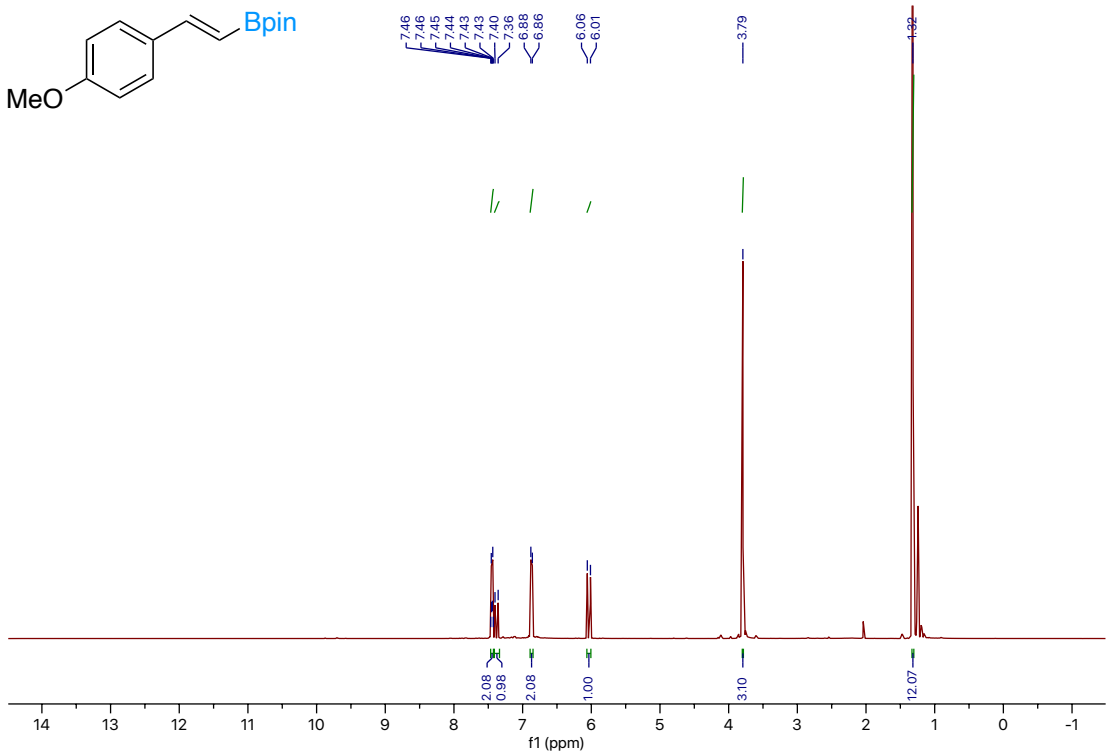
(*E*)-2-(4-ethoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4m): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

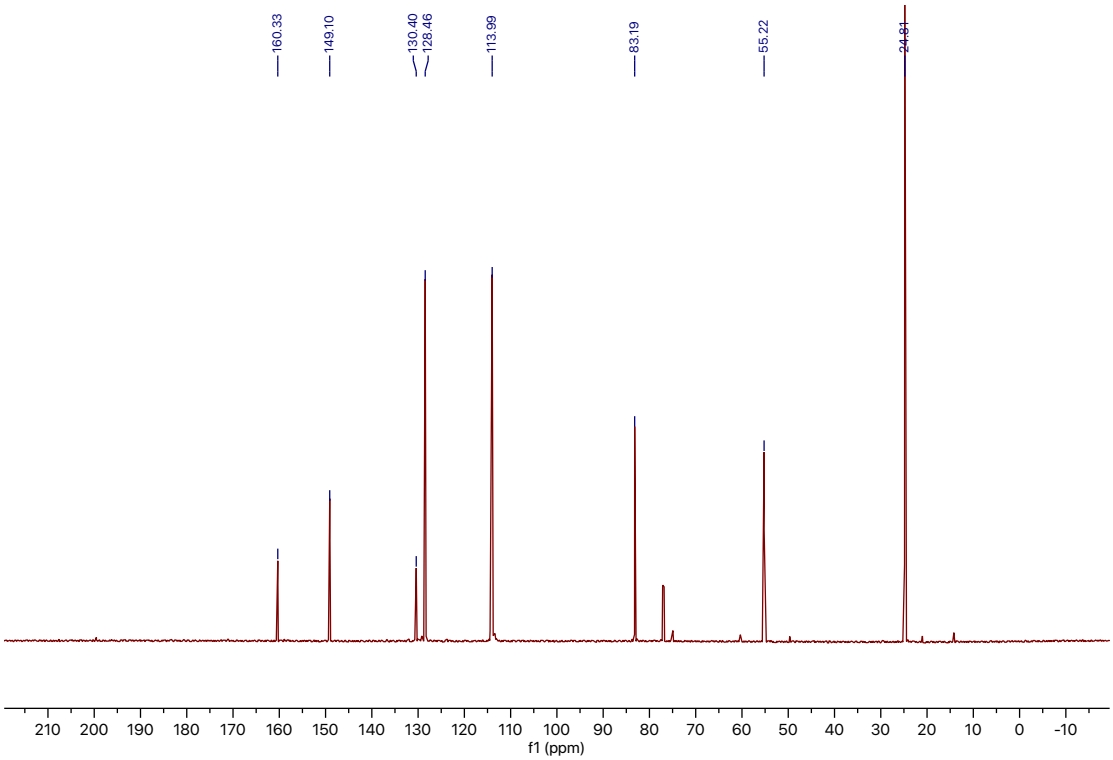


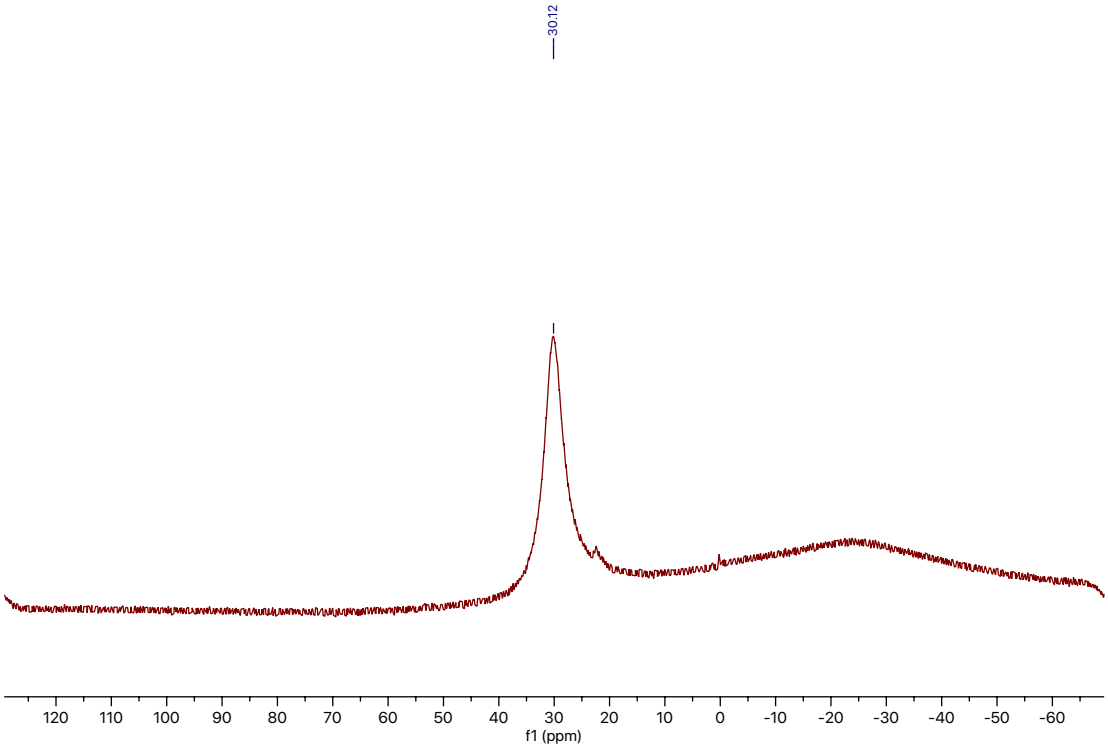

159.73
149.18
130.23
128.46
114.49
114.06
83.16
63.40
24.81
14.79
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


29.80
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
f1 (ppm)

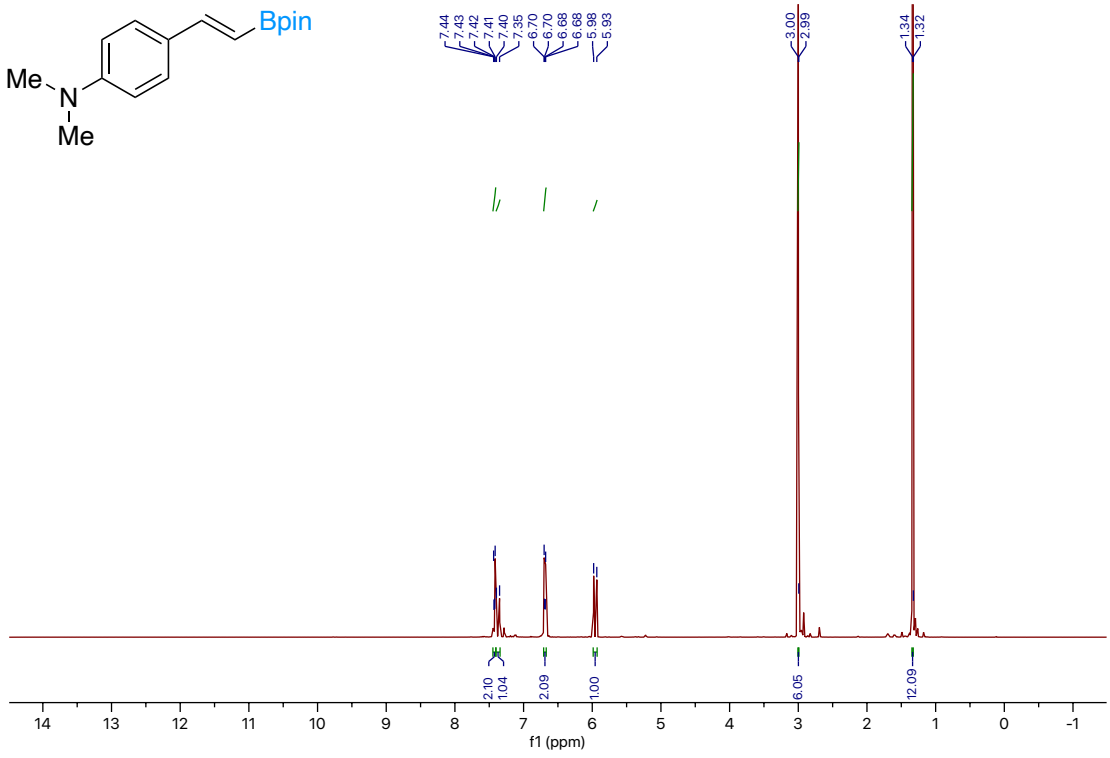
(*E*)-2-(4-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4n): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

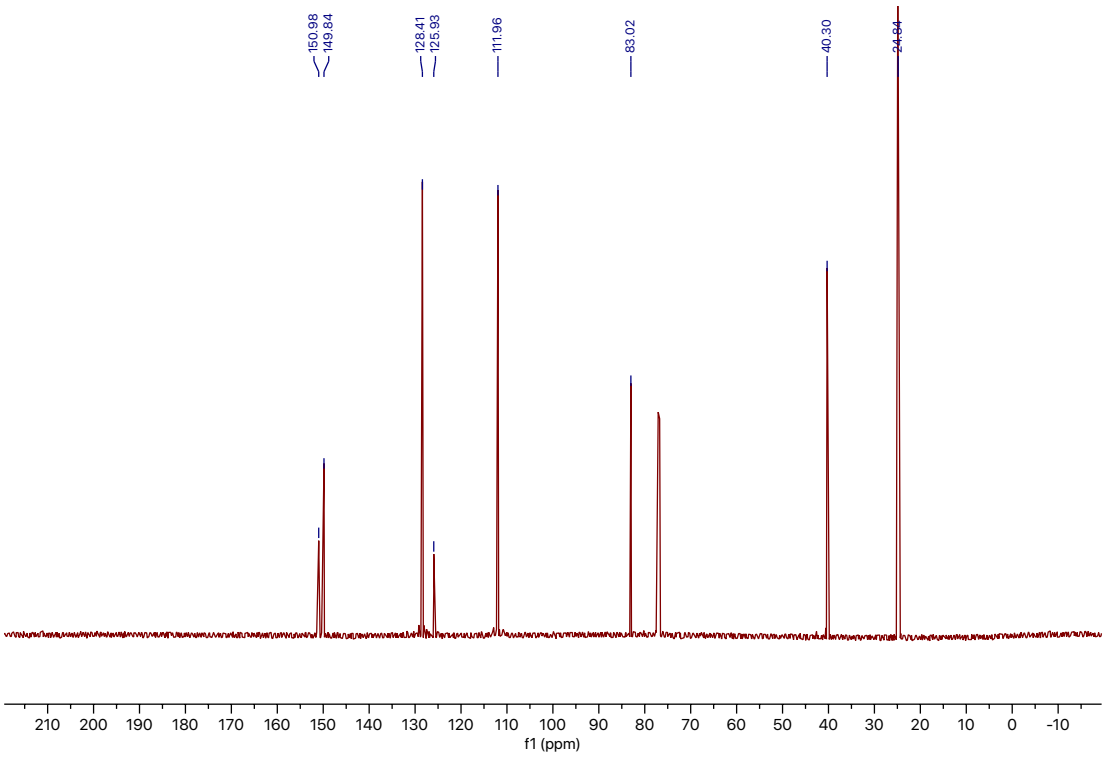


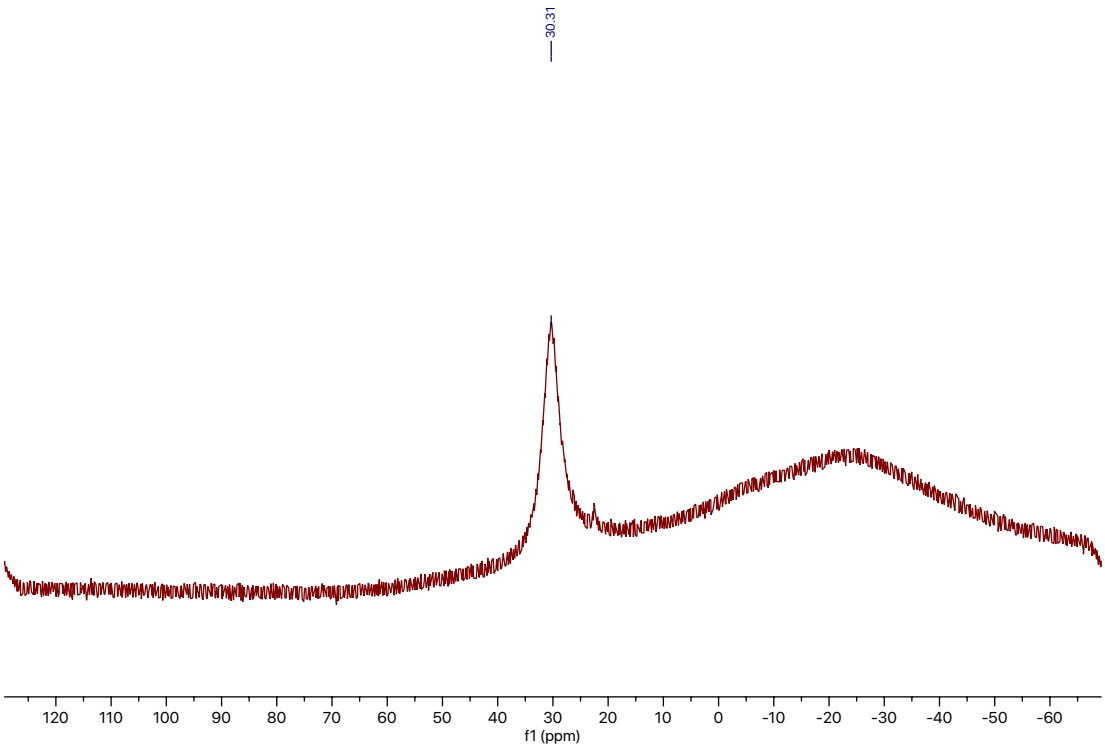




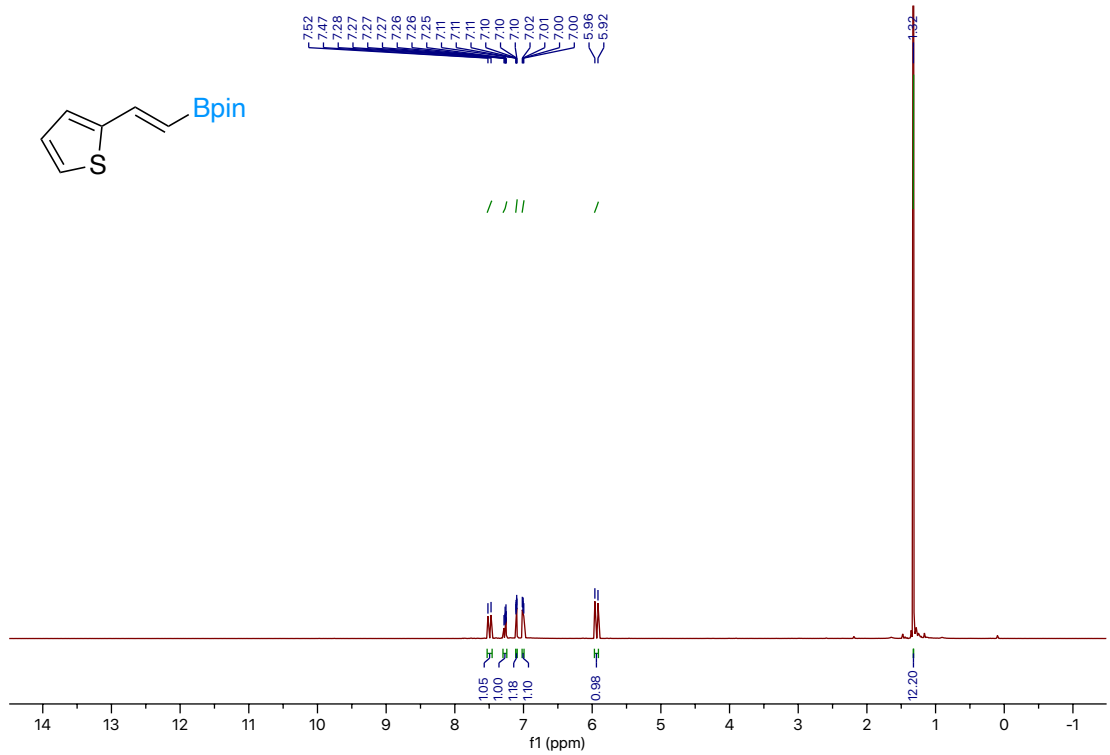
(*E*)-*N*,*N*-dimethyl-4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)aniline (4o): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

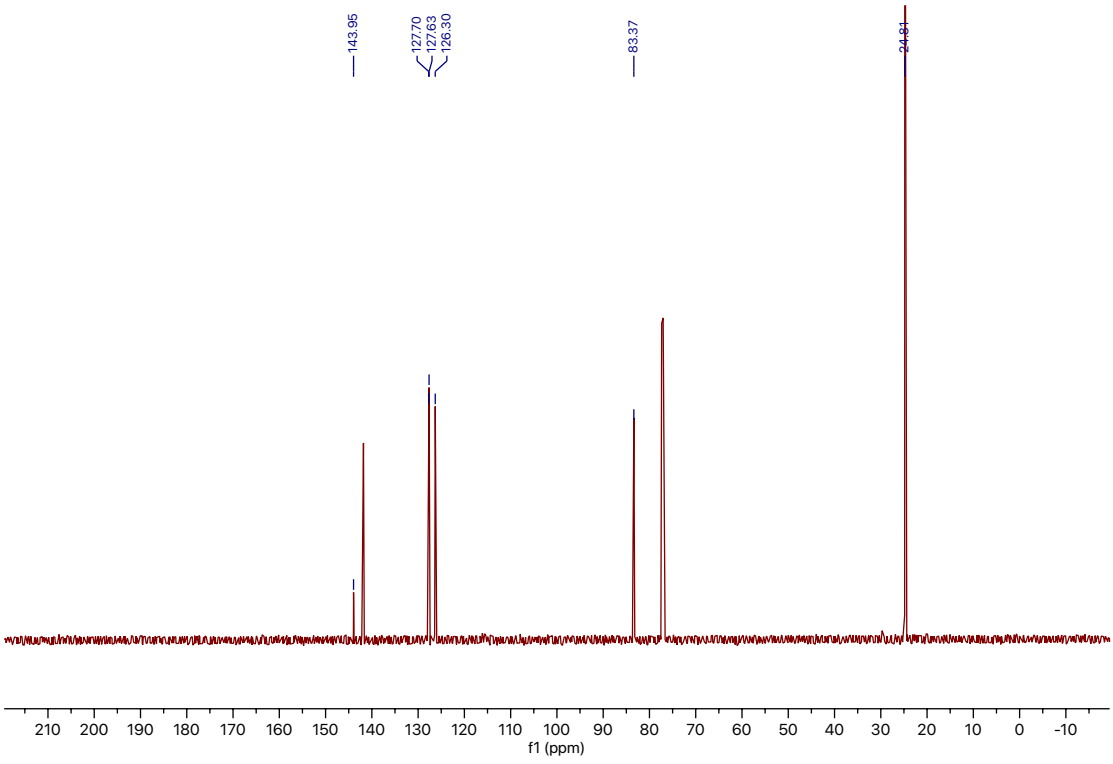


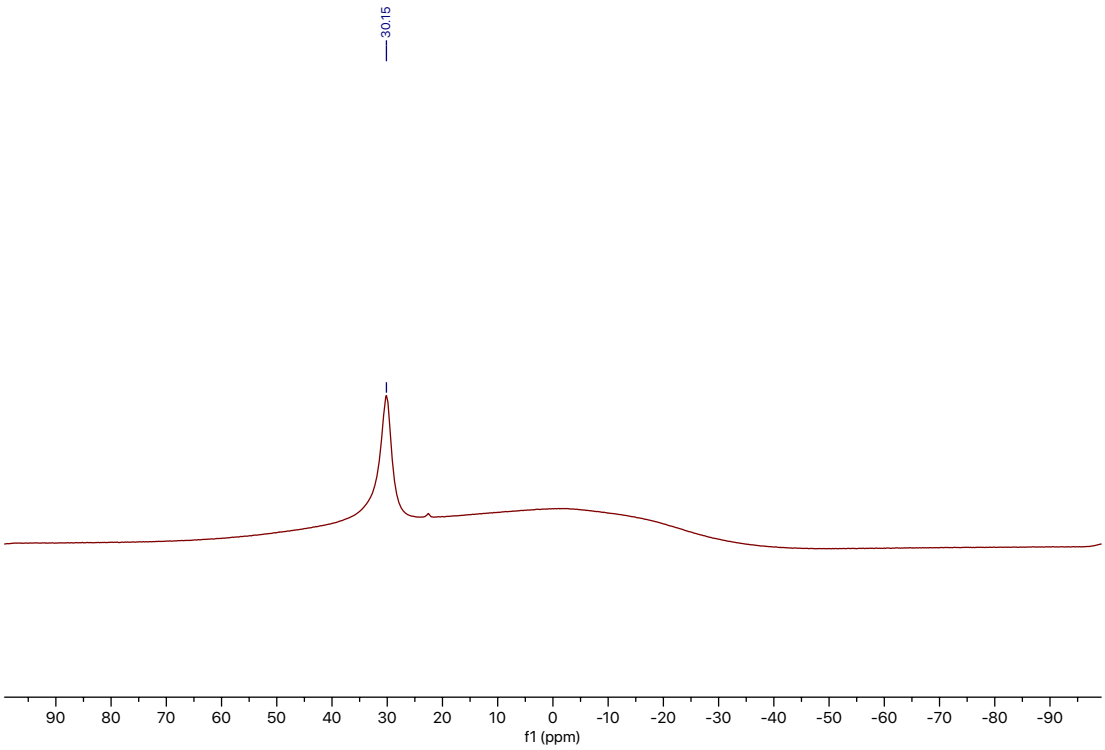

150.98
149.84
128.41
125.93
111.96
83.02
40.30
24.84
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


30.31
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60
f1 (ppm)

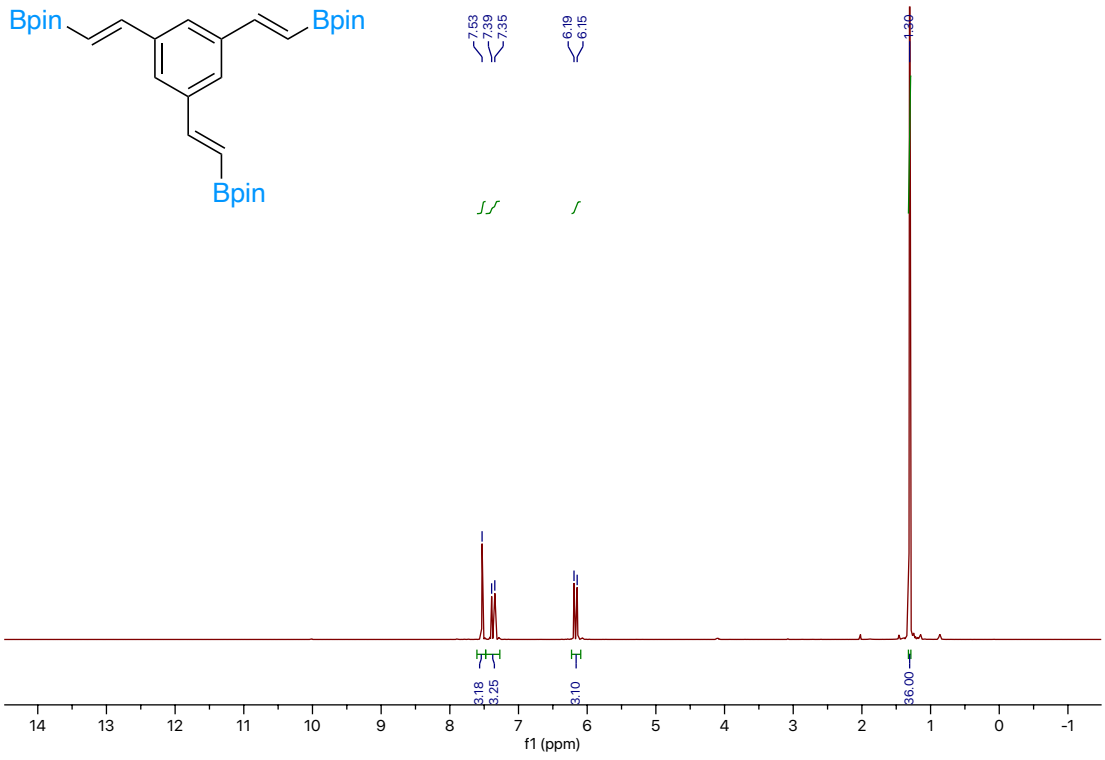
(*E*)-4,4,5,5-tetramethyl-2-(2-(thiophen-2-yl)vinyl)-1,3,2-dioxaborolane (4p): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

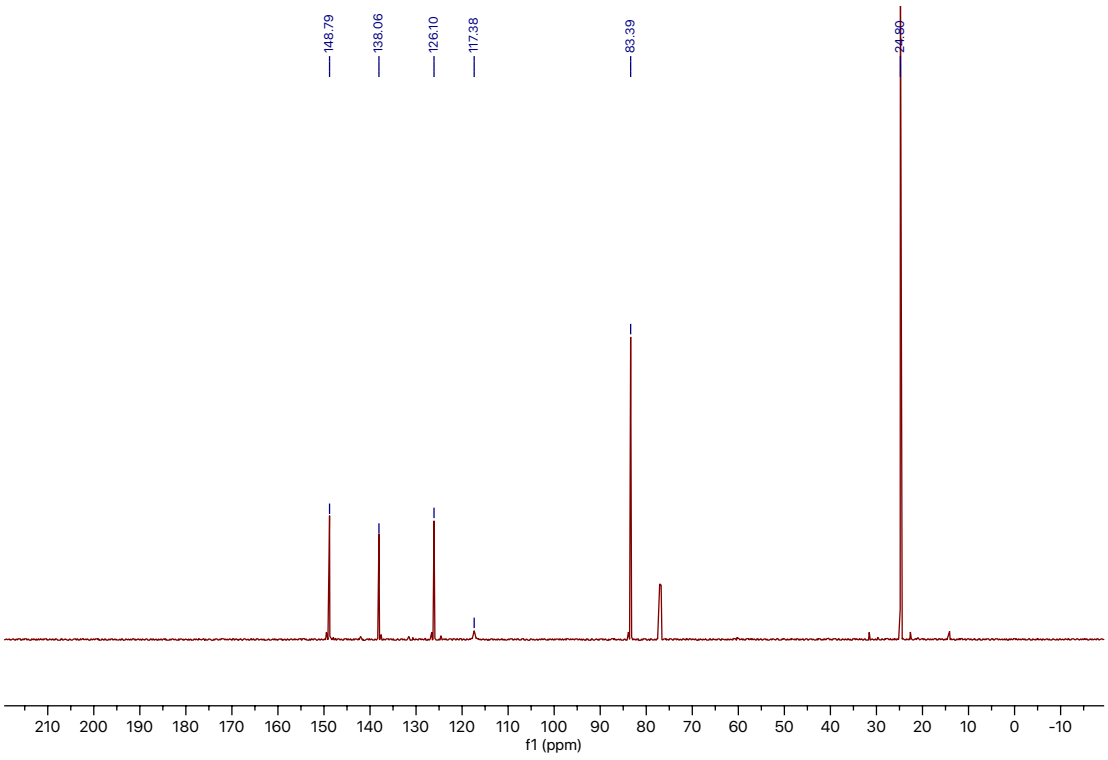


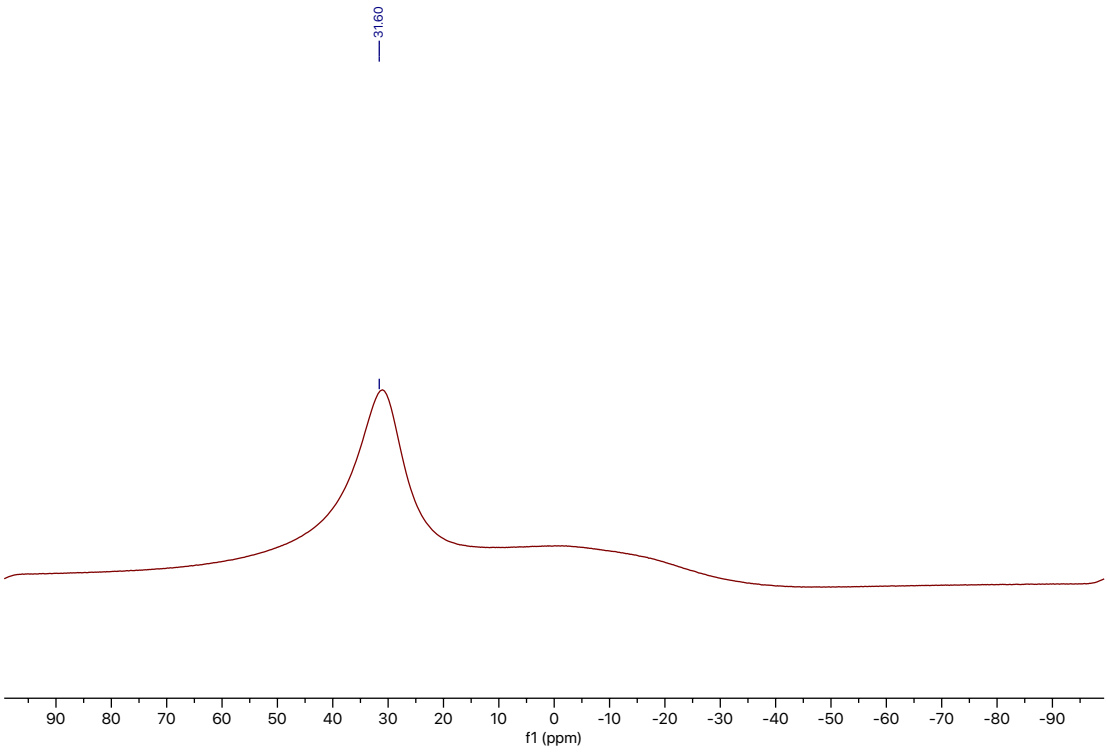




1,3,5-tris((*E*)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)benzene (4q): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

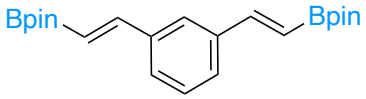


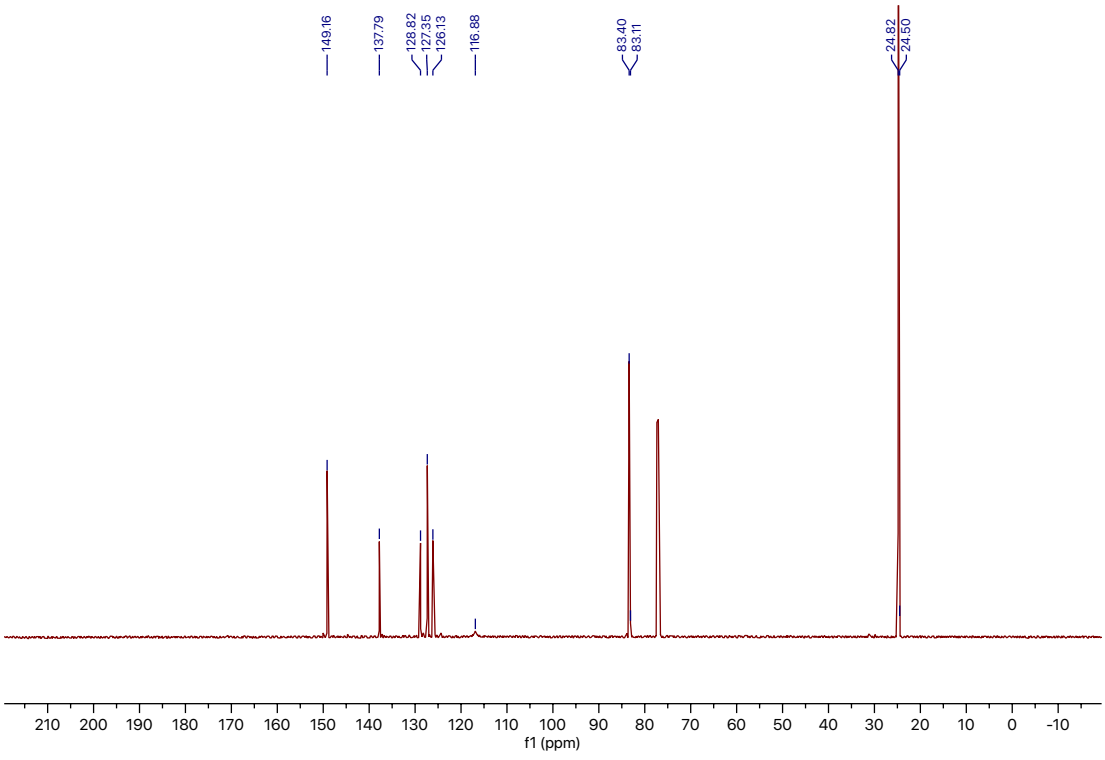

148.79
138.06
126.10
117.38
83.39
24.80
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

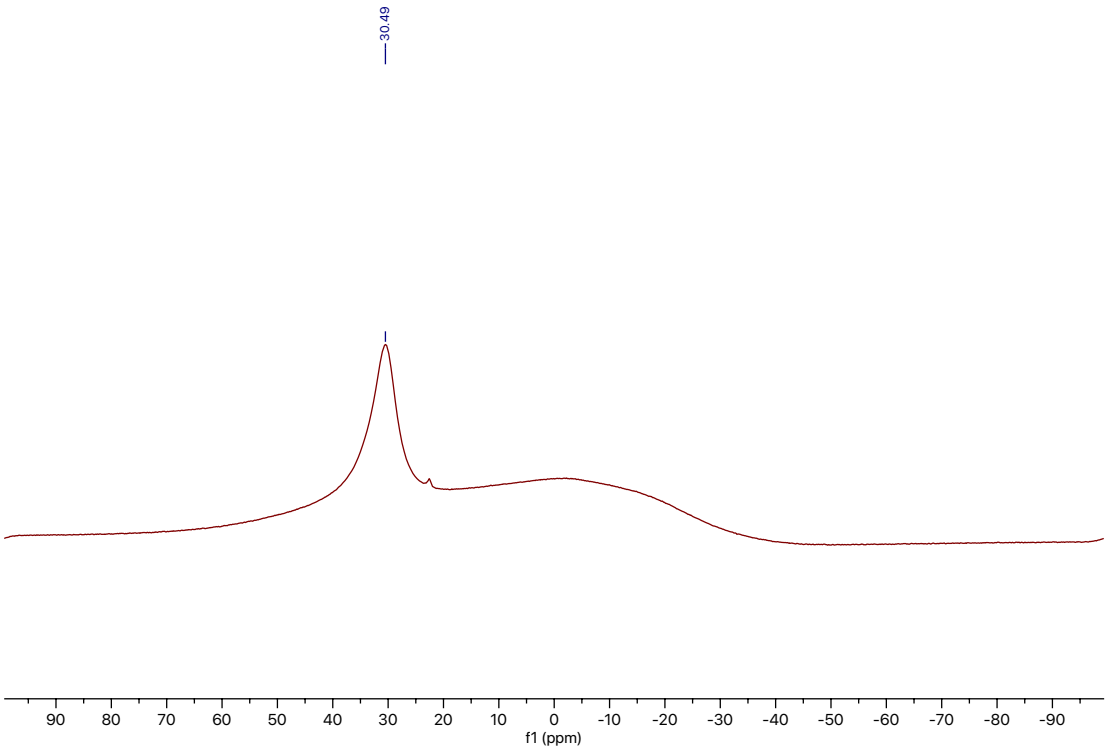

31.60
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

1,3-bis((*E*)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)benzene (4r):

^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

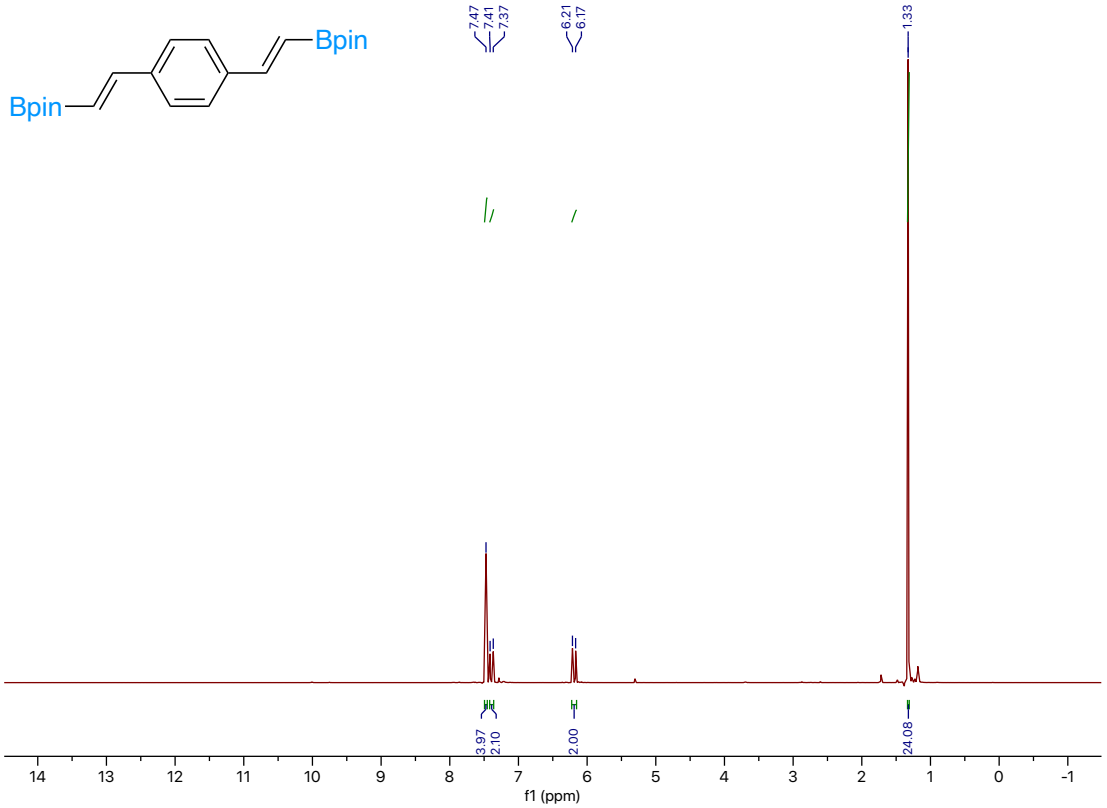


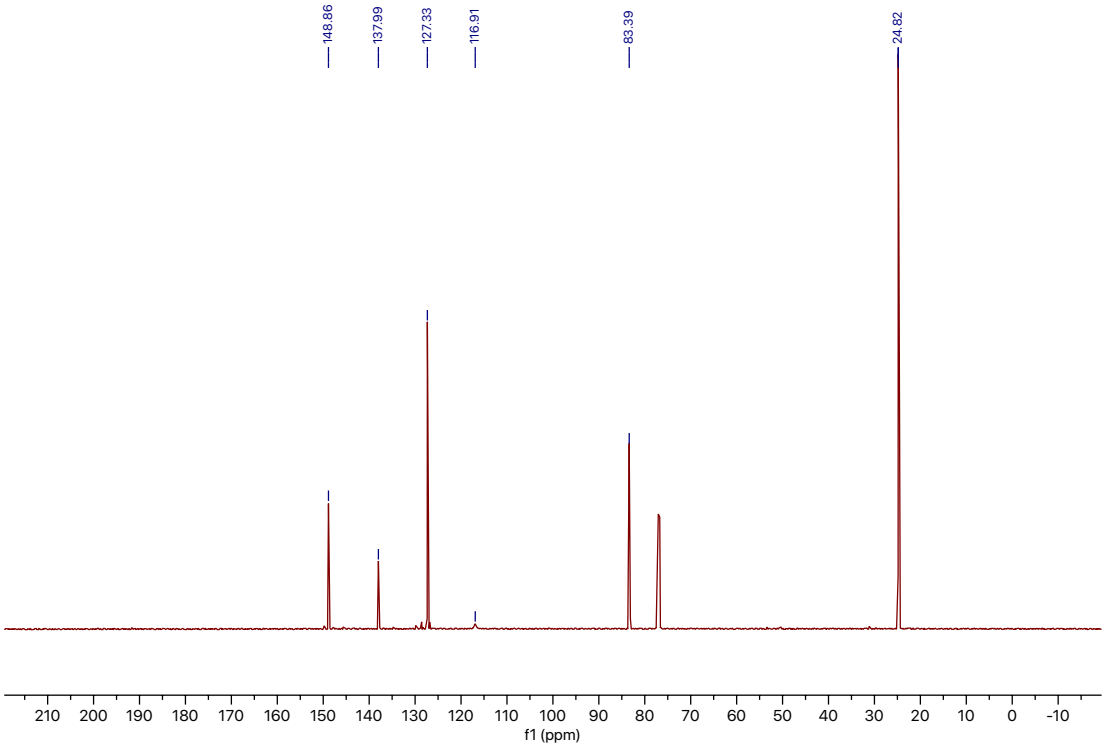


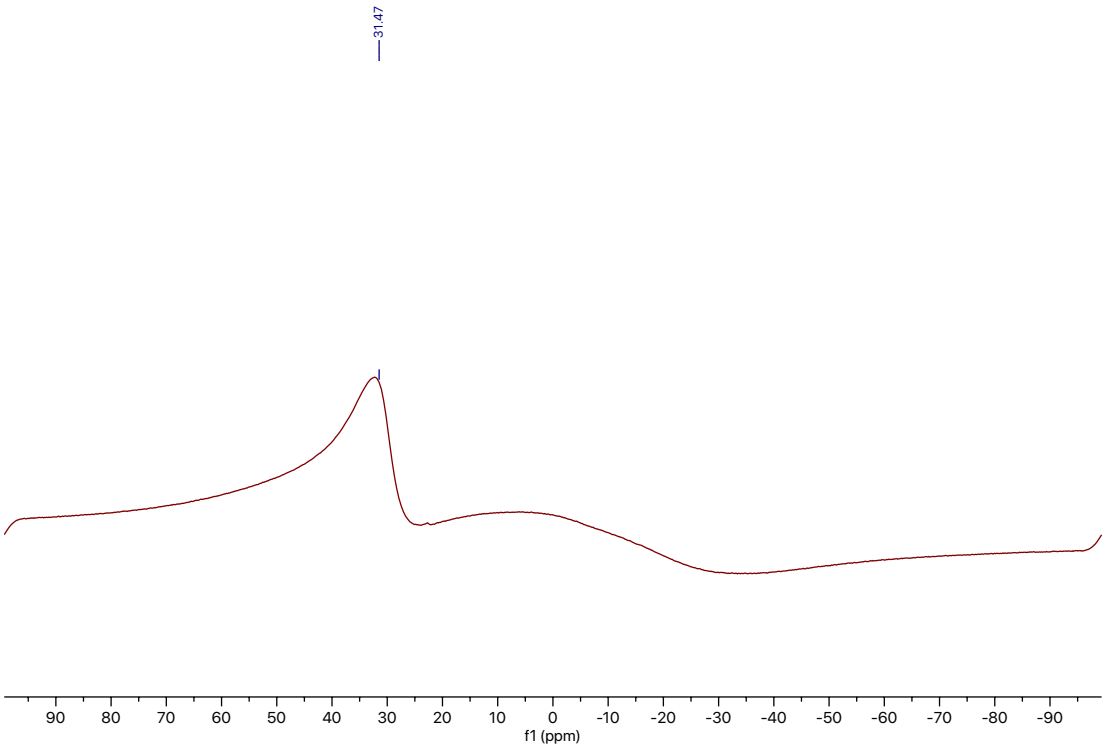


1,4-bis((*E*)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)benzene (4s):

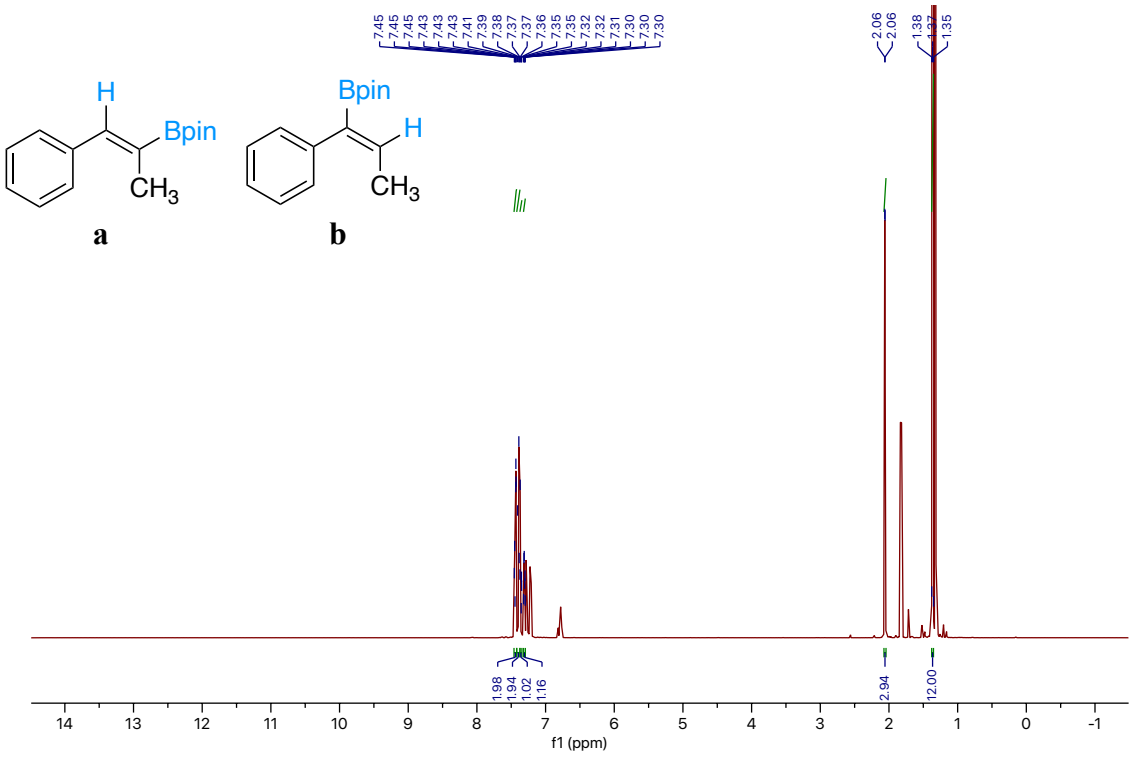
^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

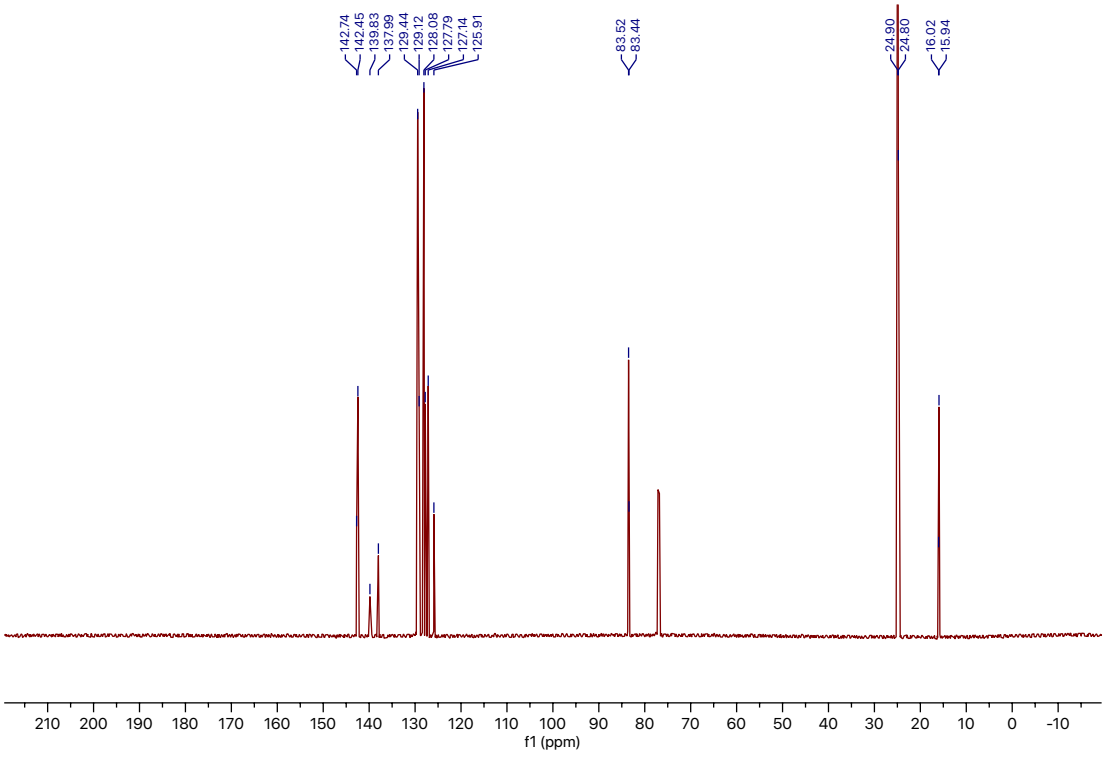


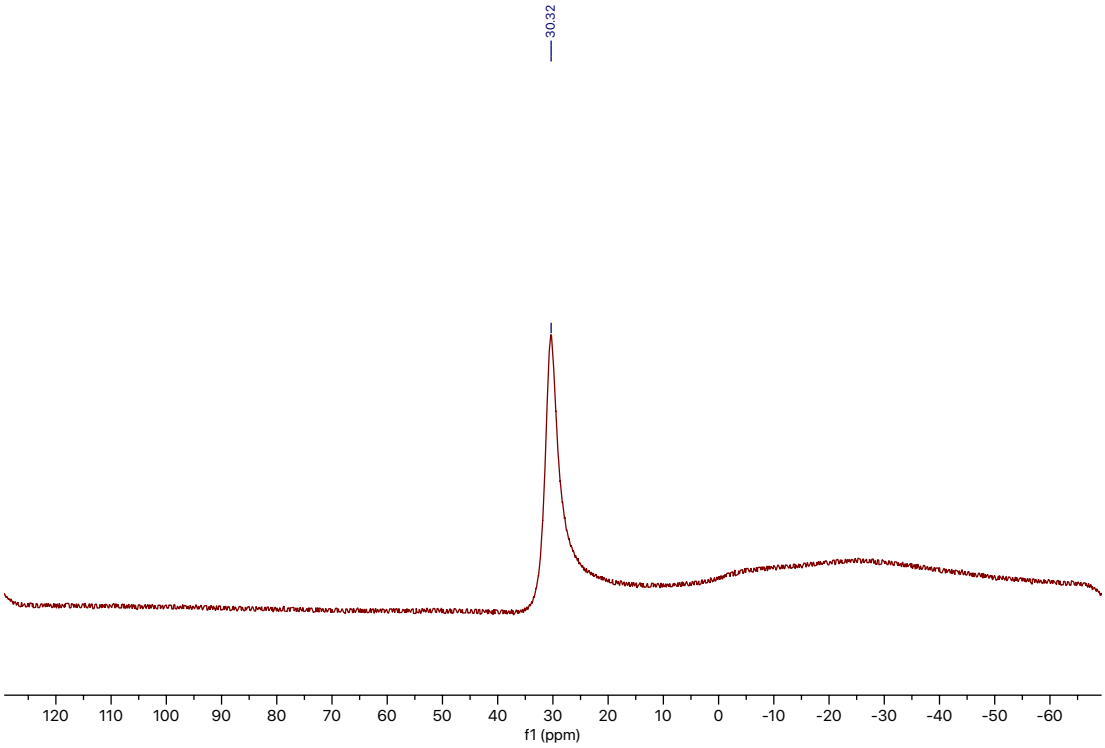

148.86
137.99
127.33
116.91
83.39
24.82
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


31.47
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

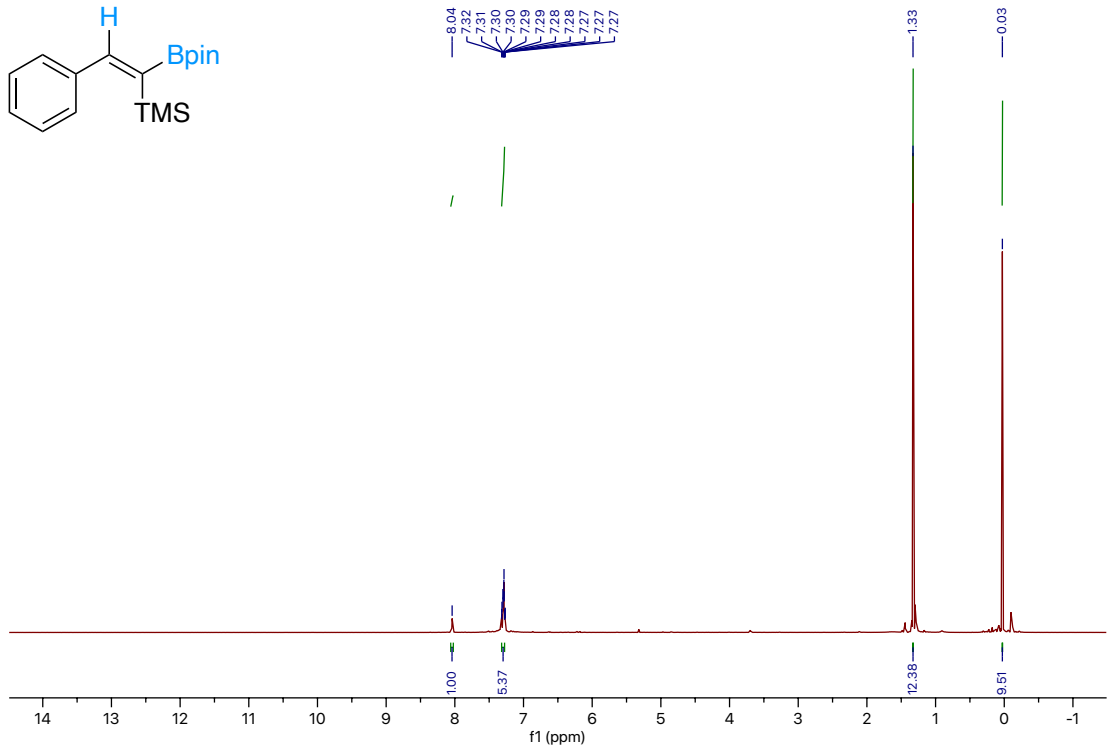
(*Z*)-4,4,5,5-Tetramethyl-2-(1-phenyl(prop-1-en)-2-yl)-1,3,2-dioxa-borolane (4t): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

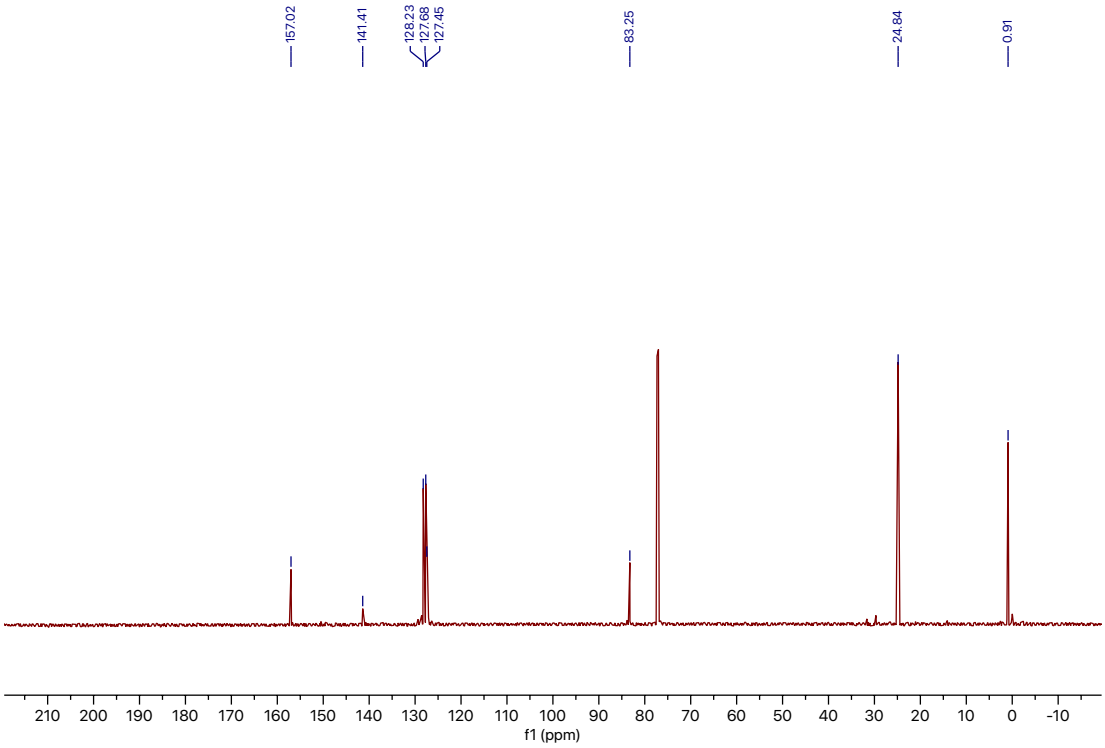


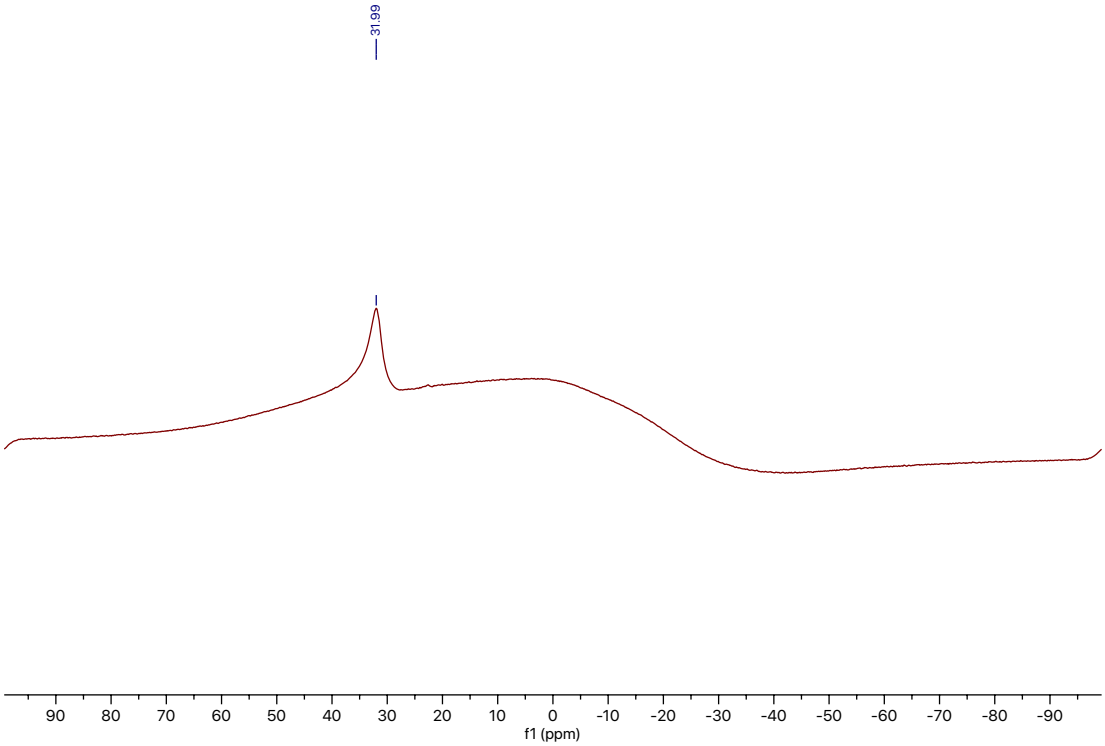




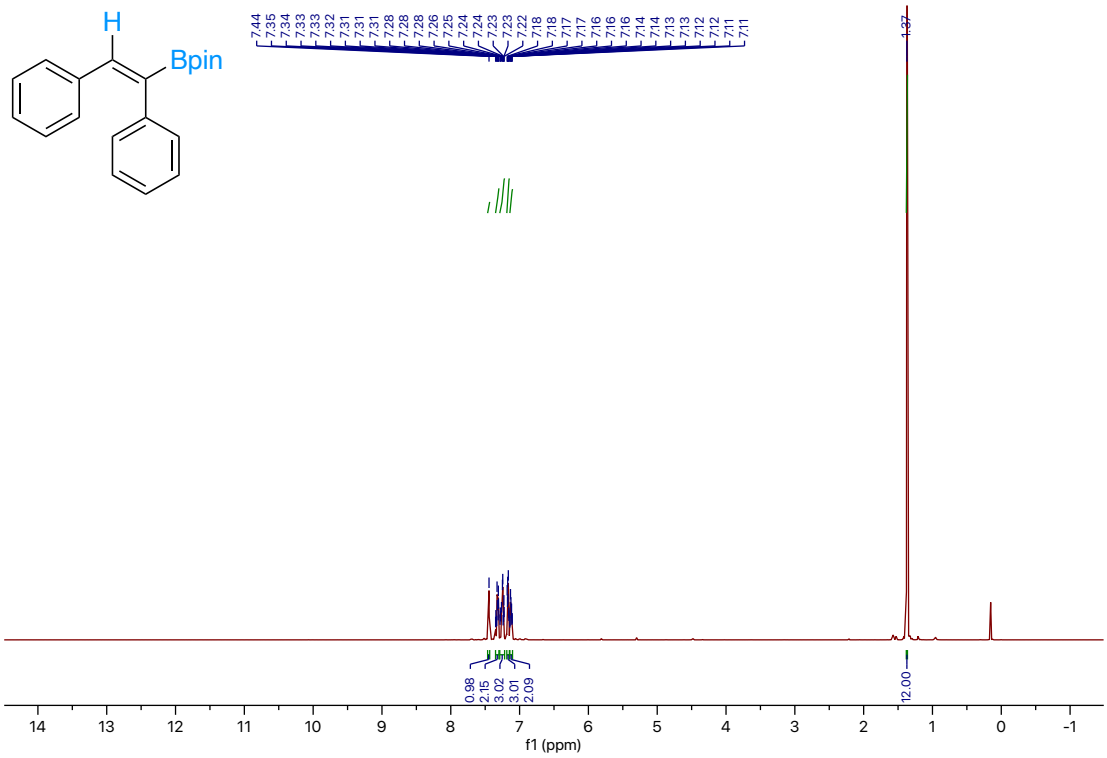
(*Z*)-trimethyl(2-phenyl-1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)silane (4u): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

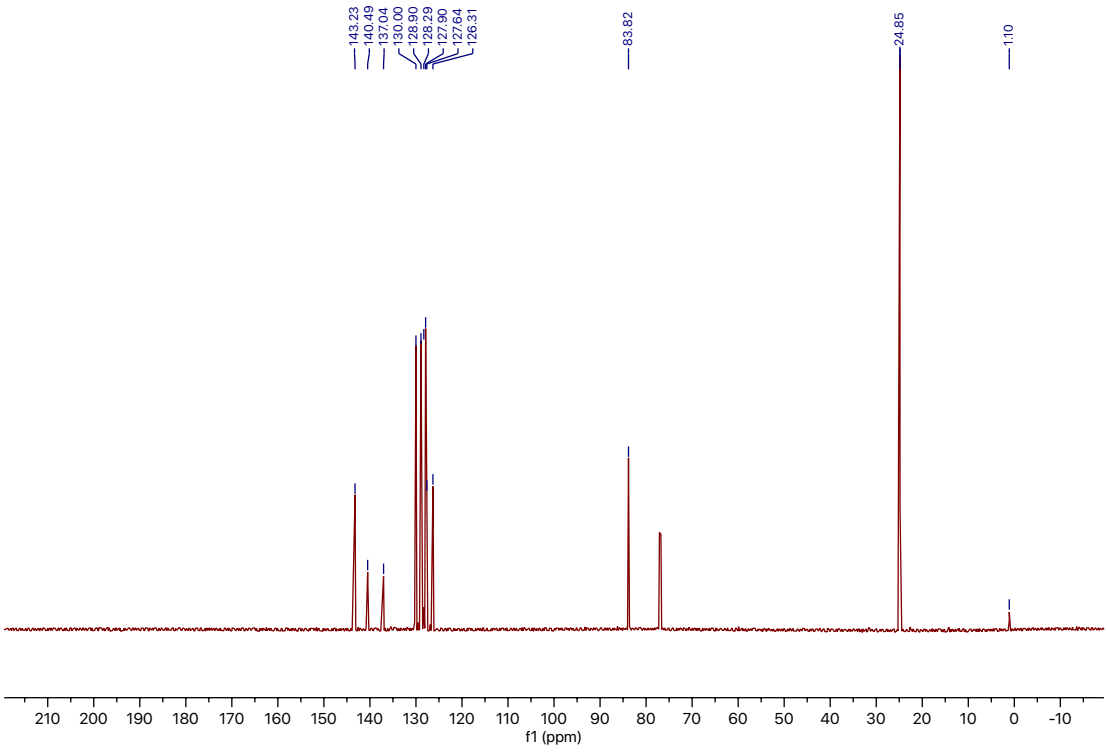


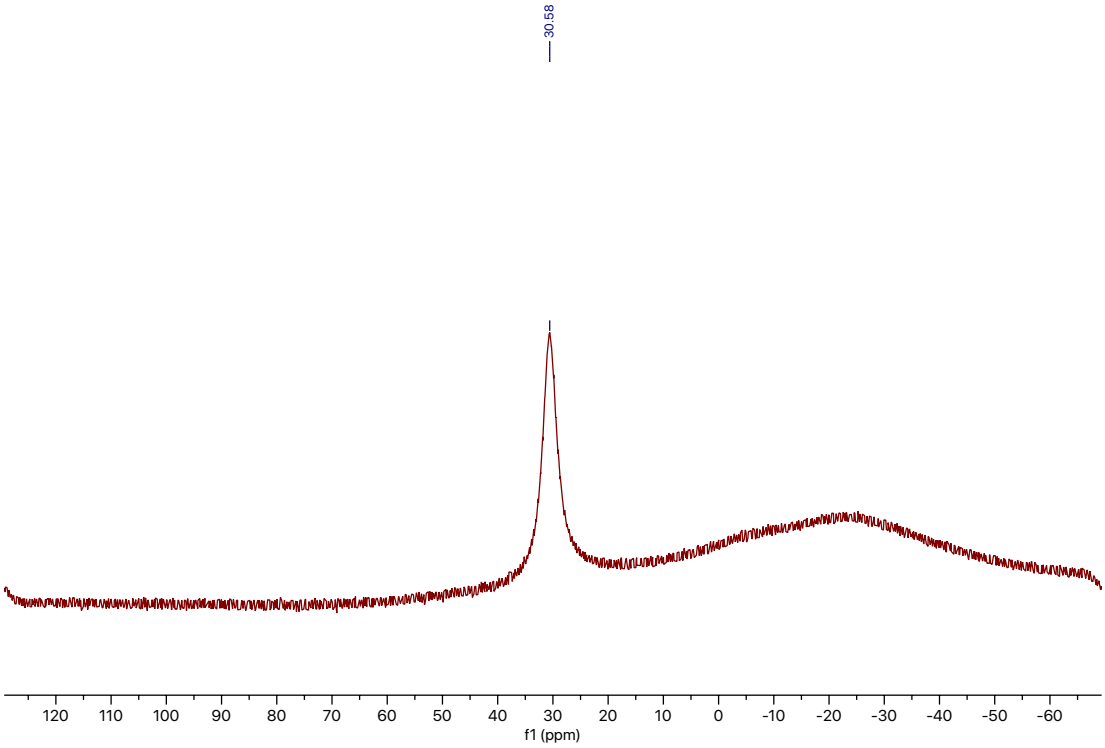

157.02
141.41
128.23
127.68
127.45
83.25
24.84
0.91
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


31.99
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

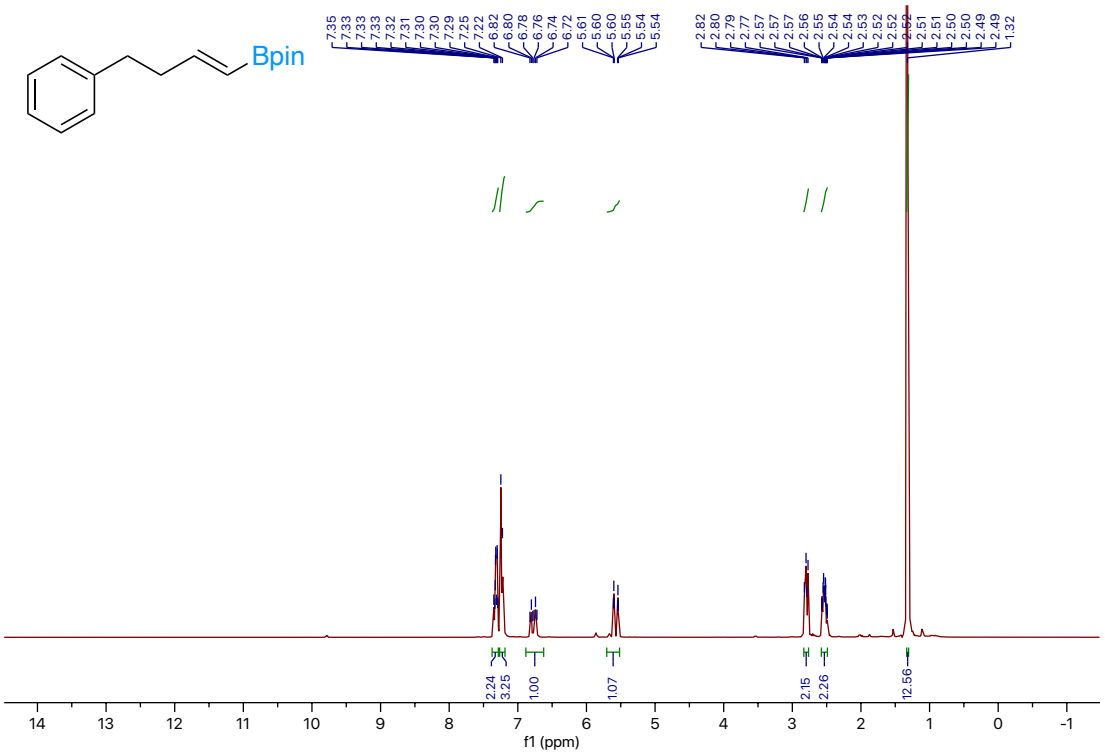
(*Z*)-2-(1,2-diphenylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4v): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

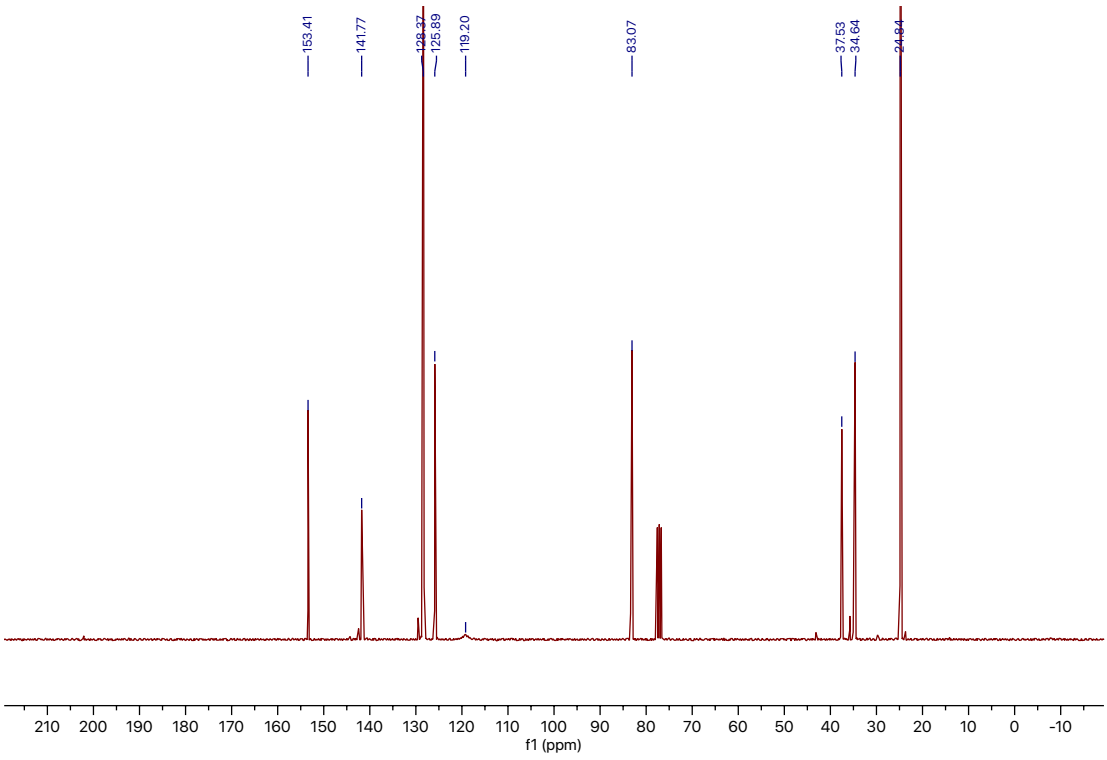


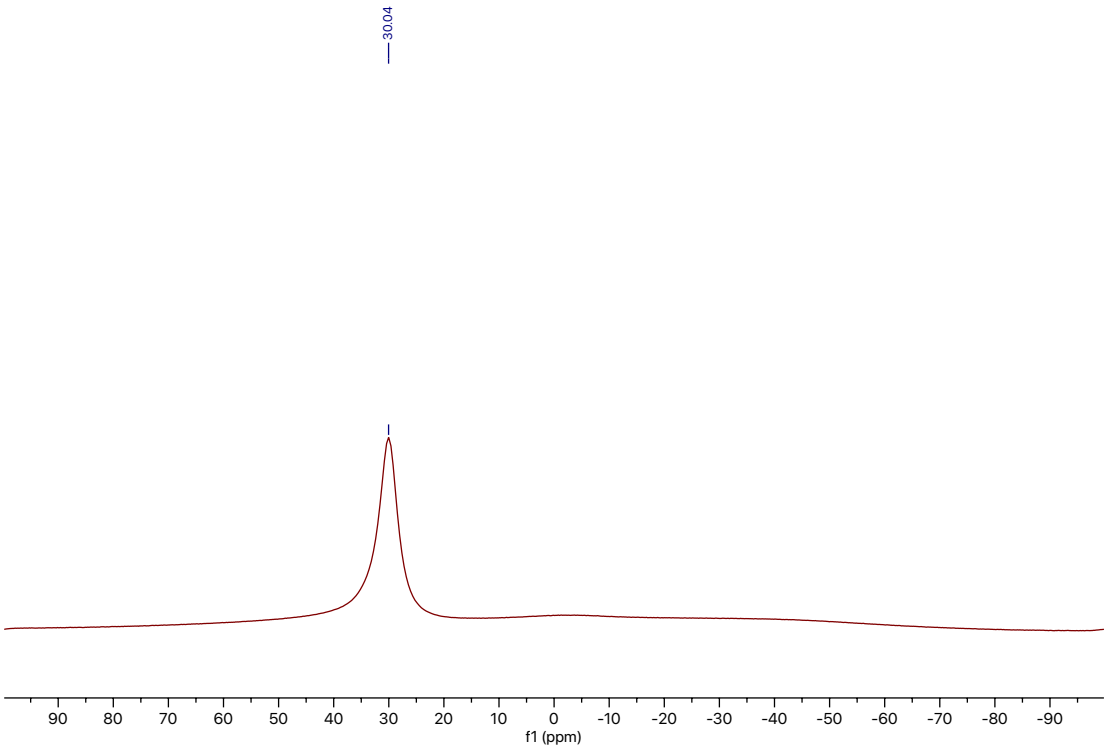




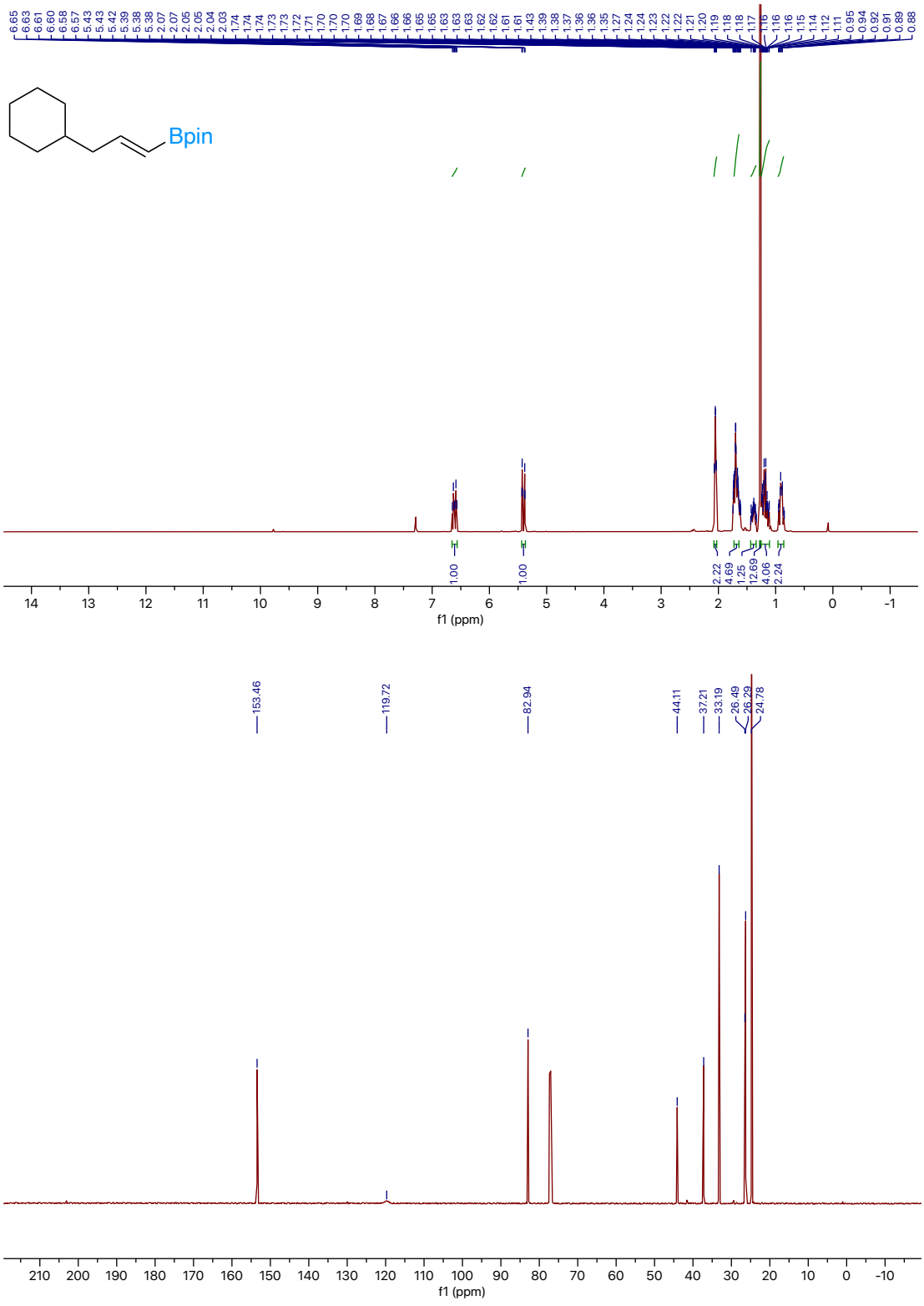
(*E*)-4,4,5,5-tetramethyl-2-(4-phenylbut-1-en-1-yl)-1,3,2-dioxaborolane (4w): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

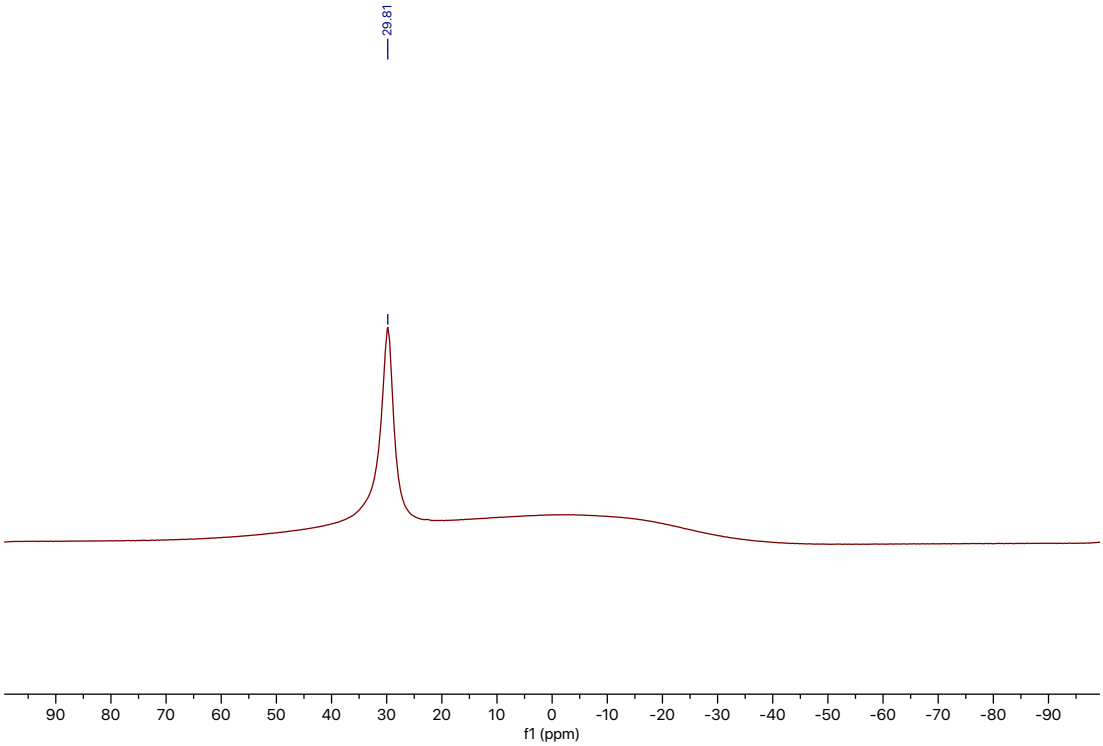



153.41
141.77
128.37
125.89
119.20
83.07
37.53
34.64
24.84
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

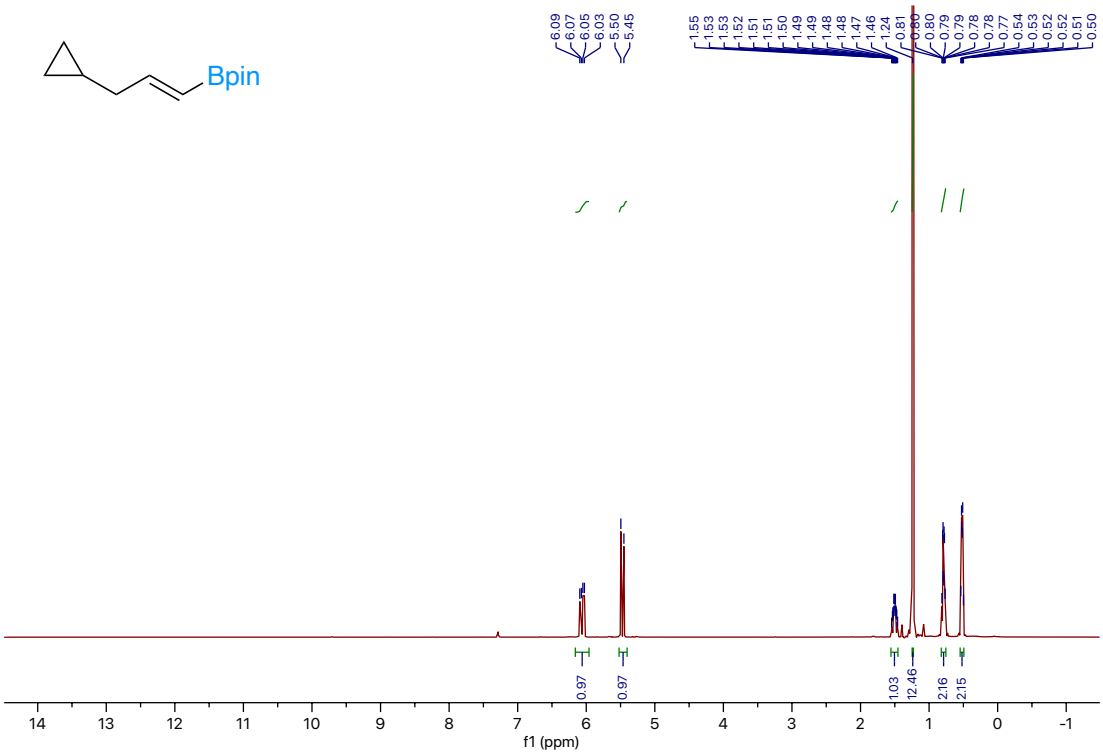

30.04
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

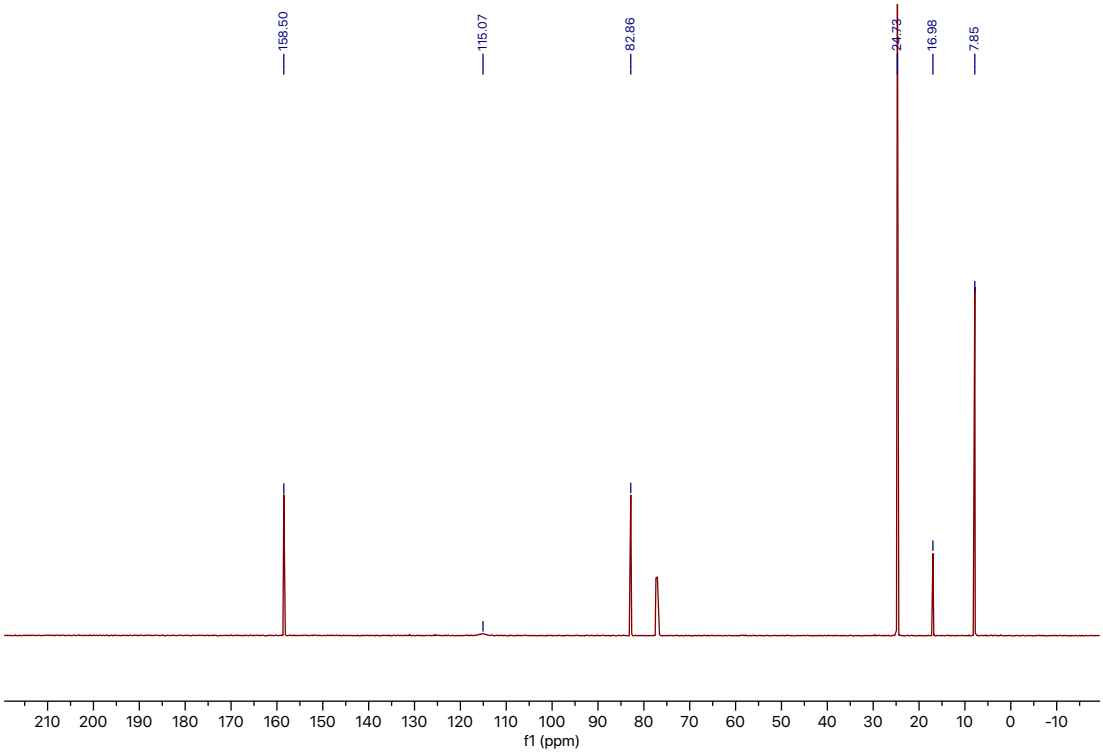
(*E*)-2-(3-cyclohexylprop-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4x): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

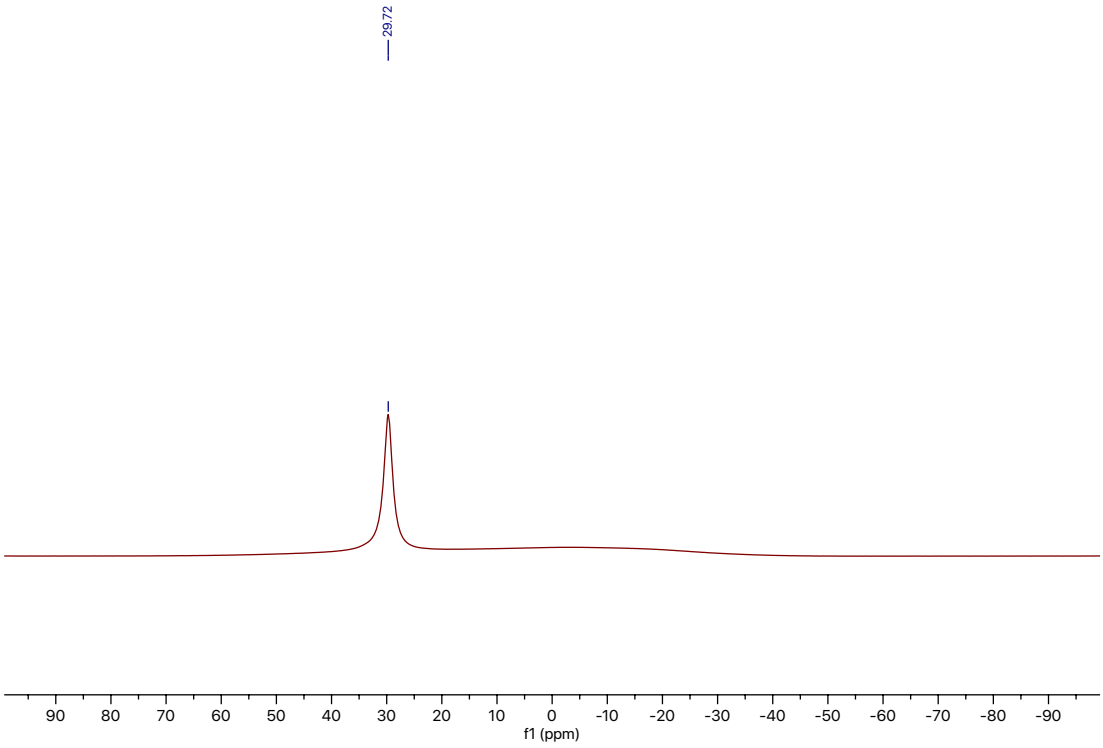




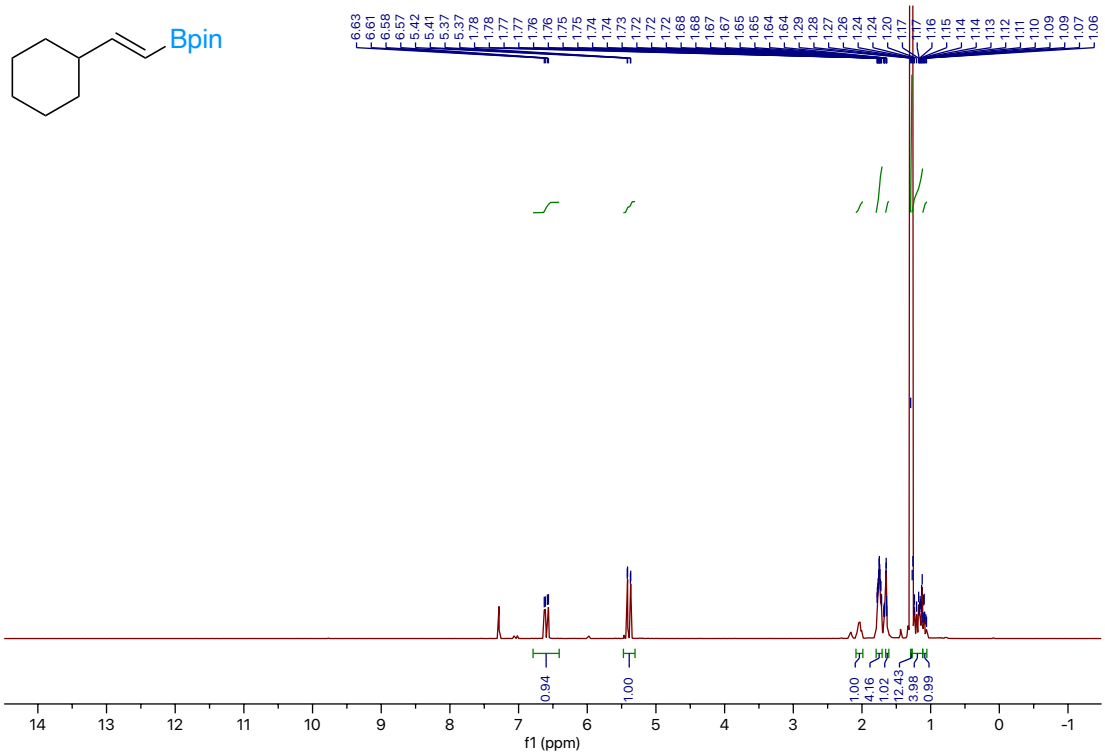
(*E*)-2-(3-cyclopropylprop-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4y): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

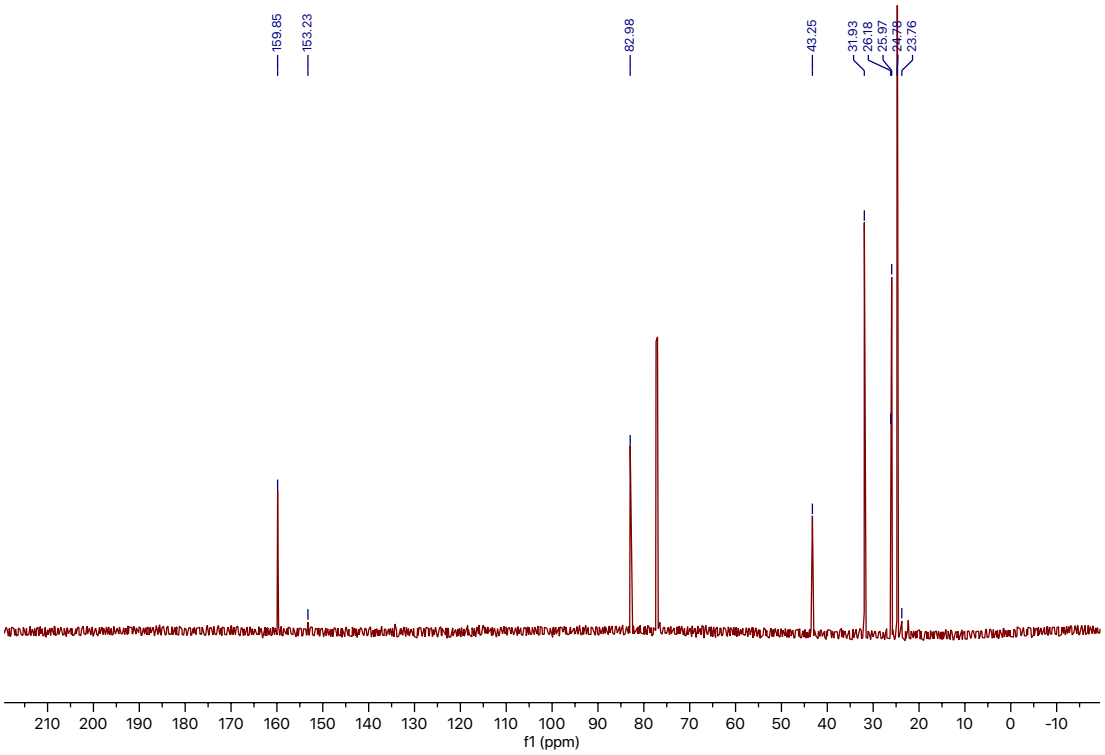


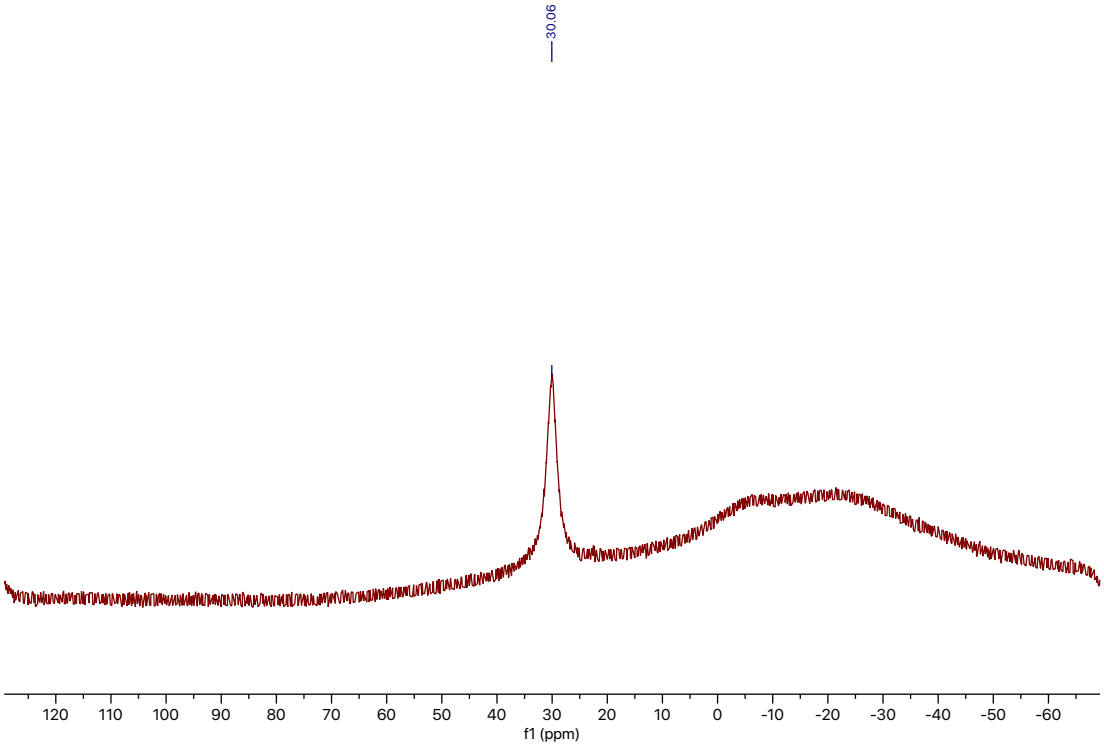

158.50
115.07
82.86
24.73
16.98
7.85
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


29.72
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

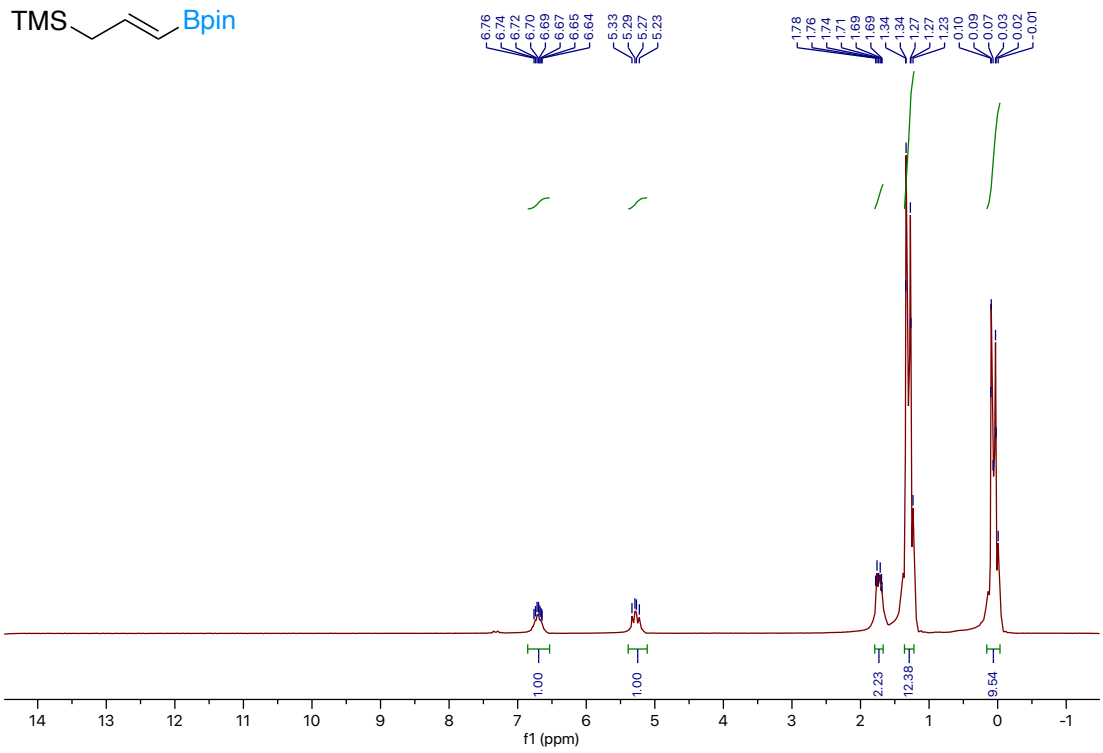
(*E*)-2-(2-cyclohexylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4z): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

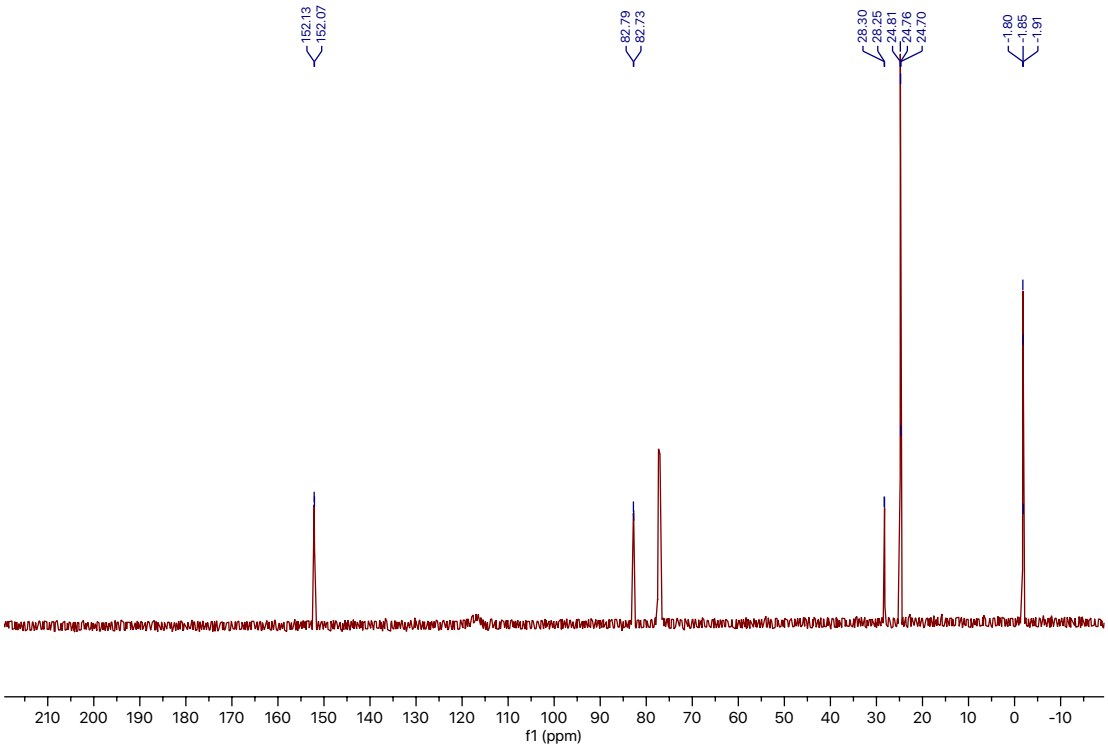


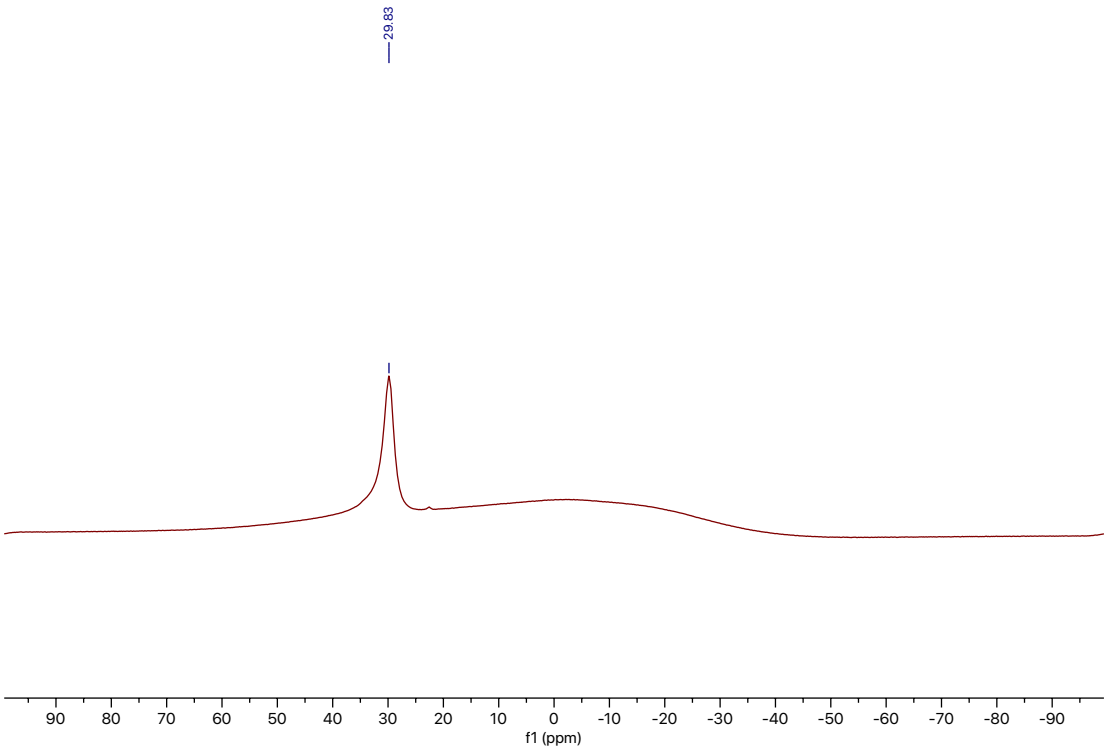




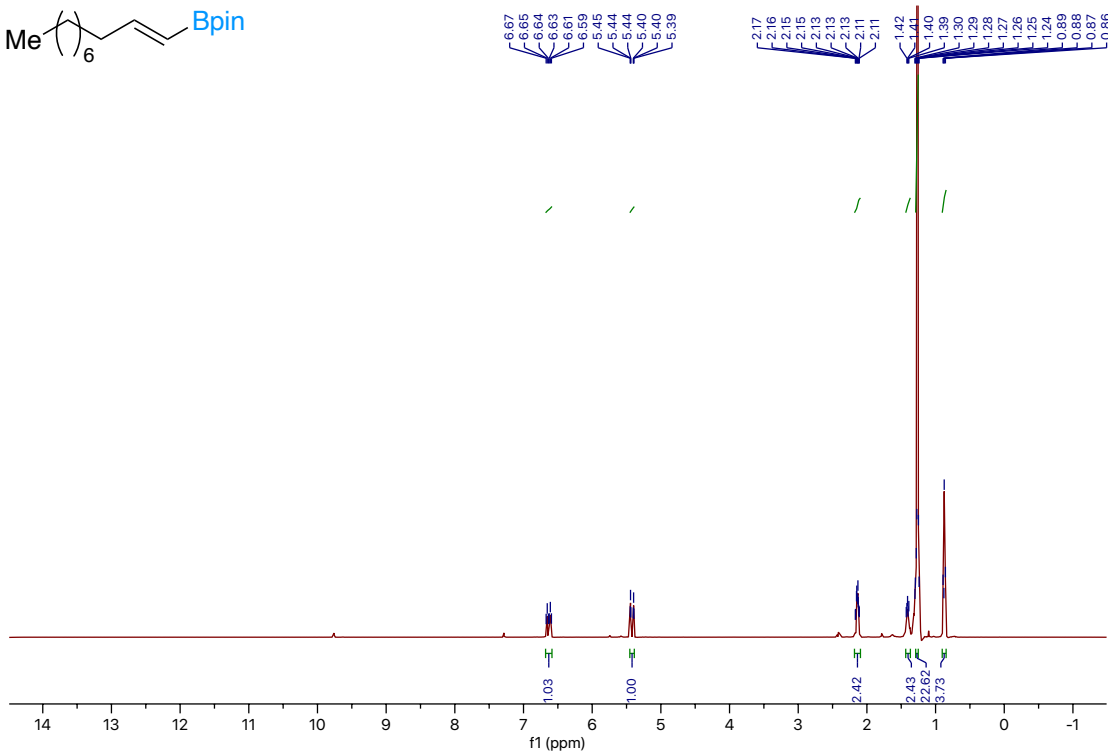
(*E*)-trimethyl(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)allyl)silane (4aa): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

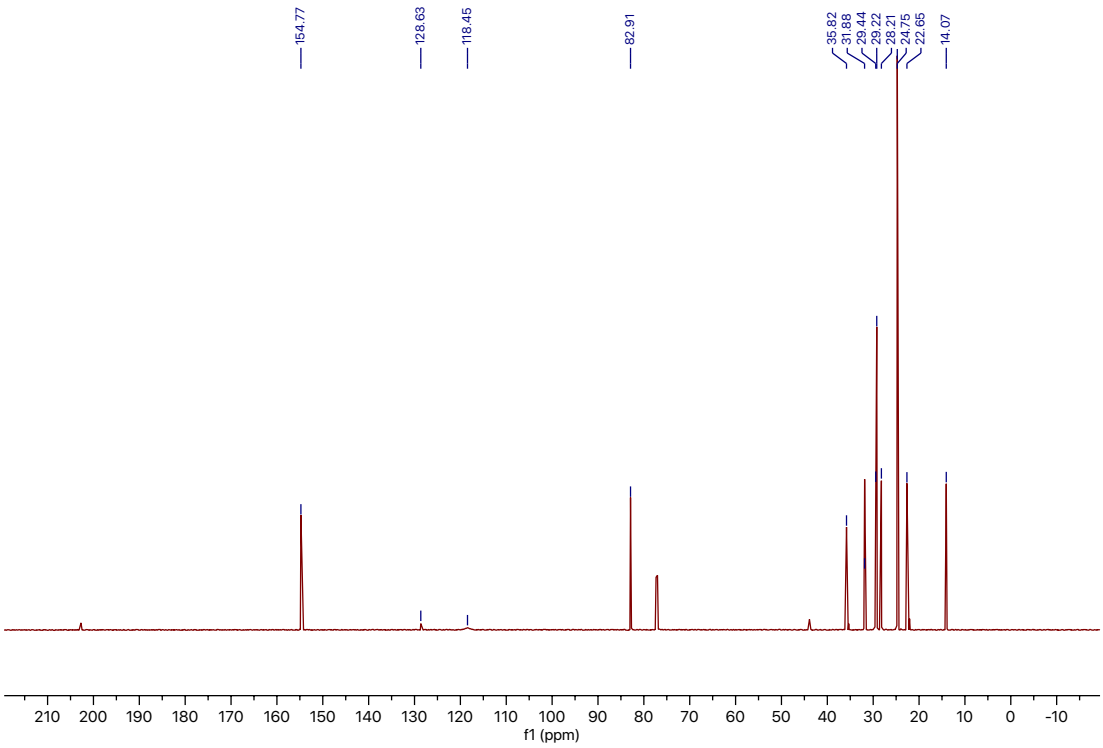


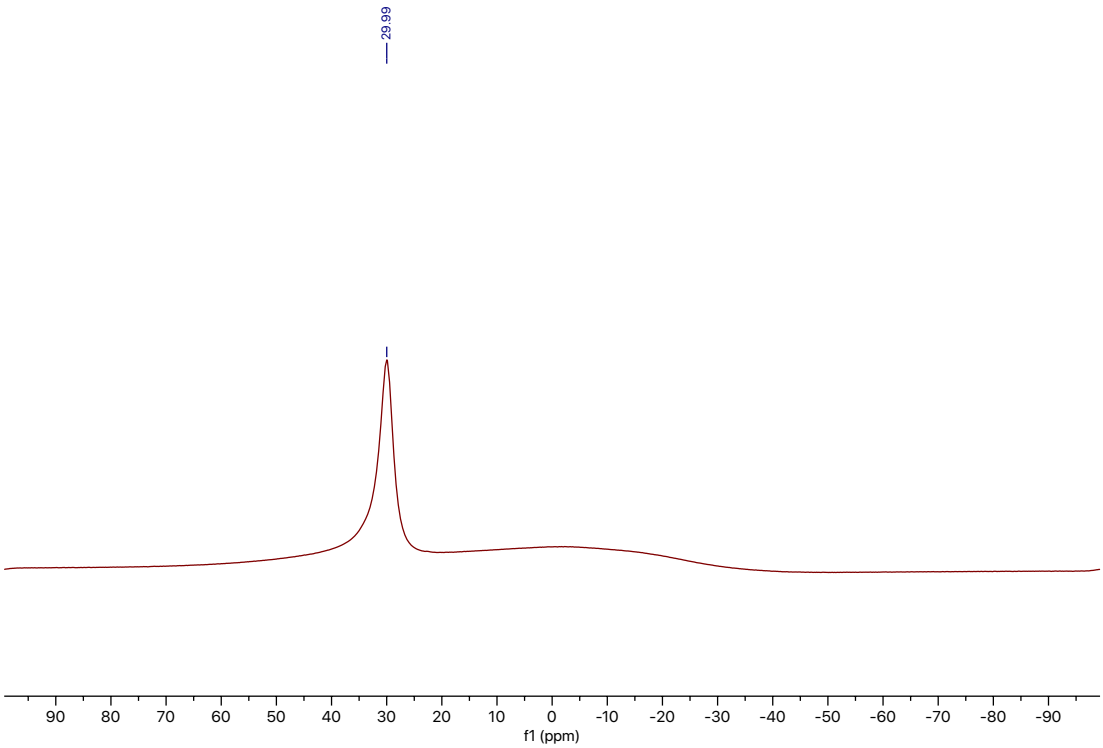

152.13
152.07
82.79
82.73
28.30
28.25
24.81
24.76
24.70
-1.80
-1.85
-1.91
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


29.83
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

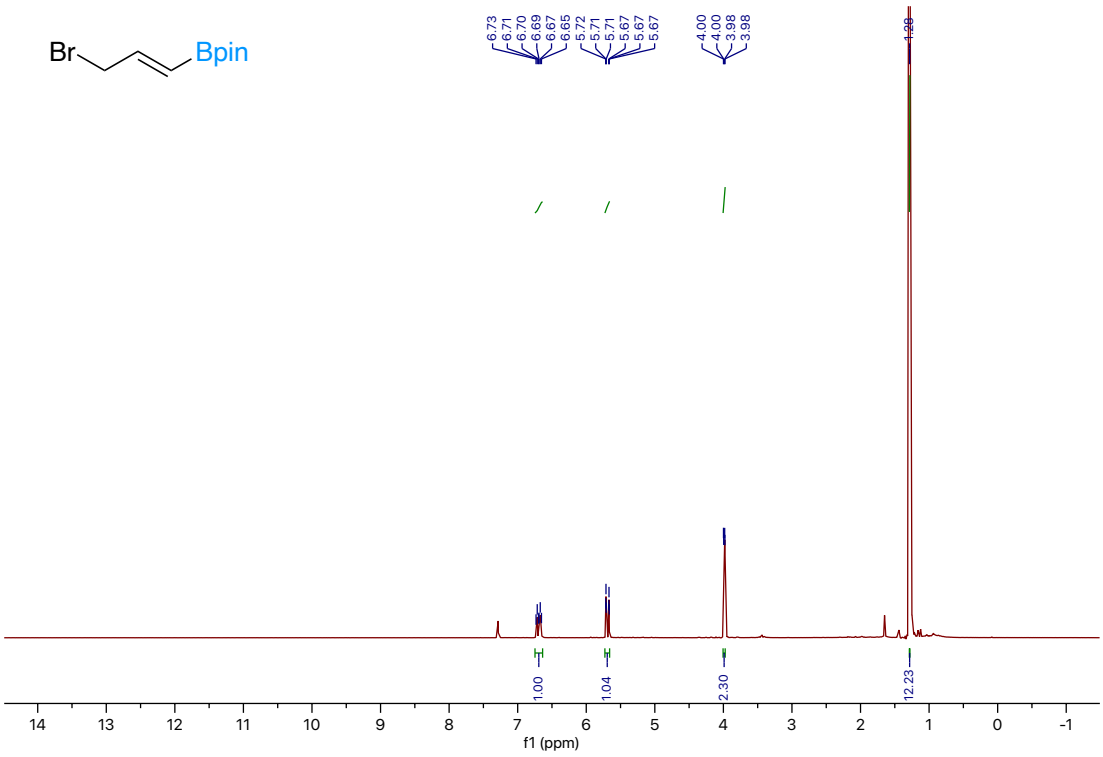
(*E*)-2-(dec-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4bb): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

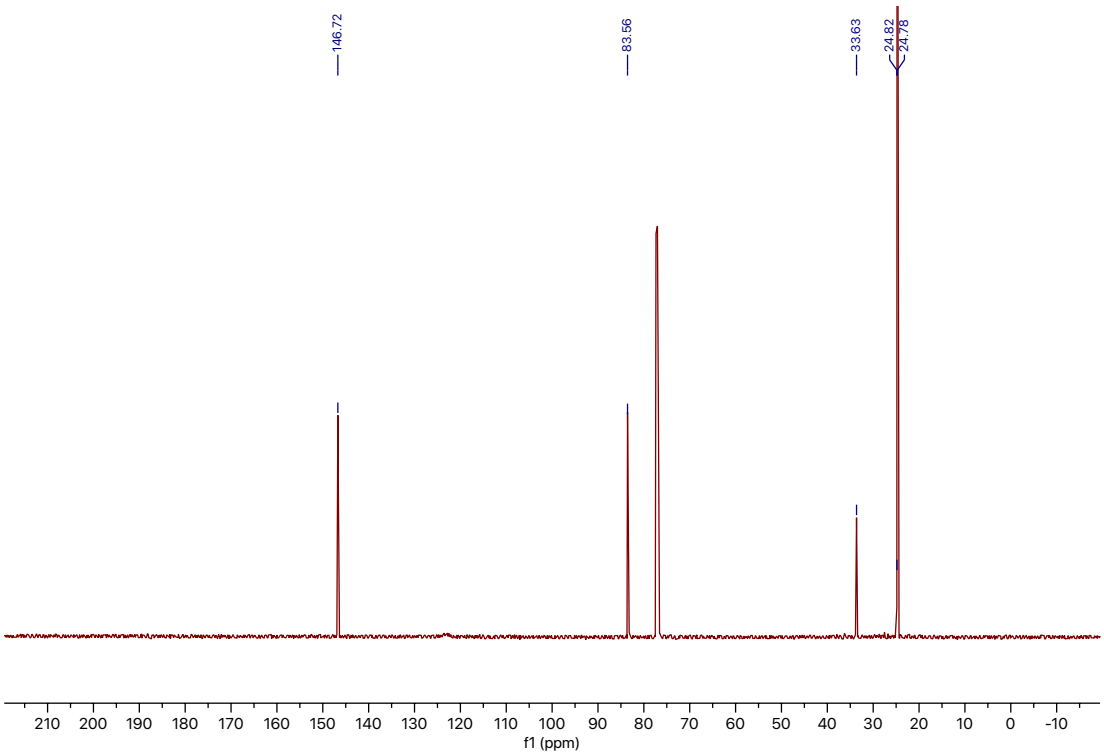


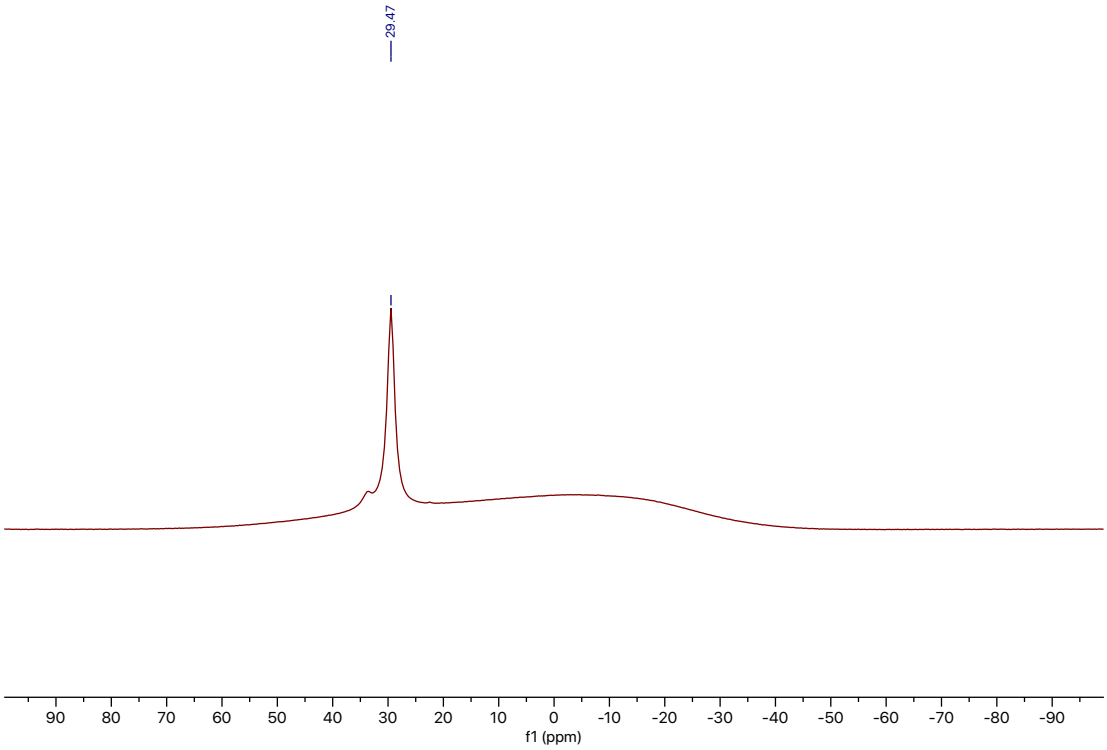




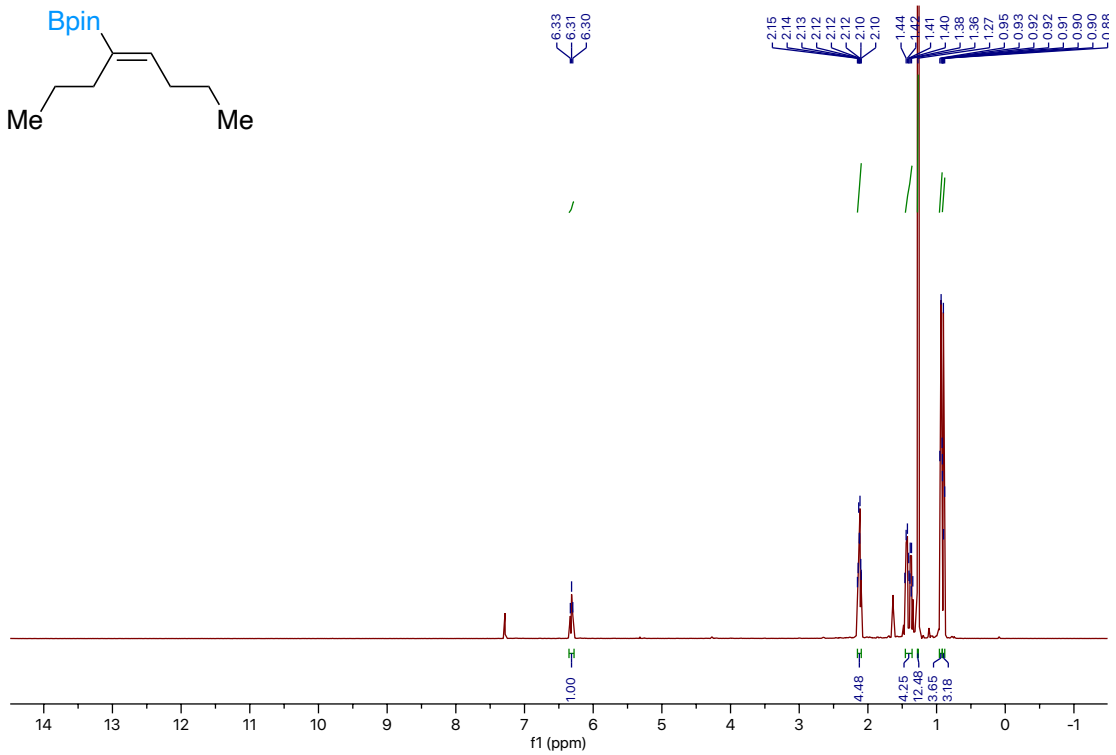
(*E*)-2-(3-bromoprop-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4cc): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

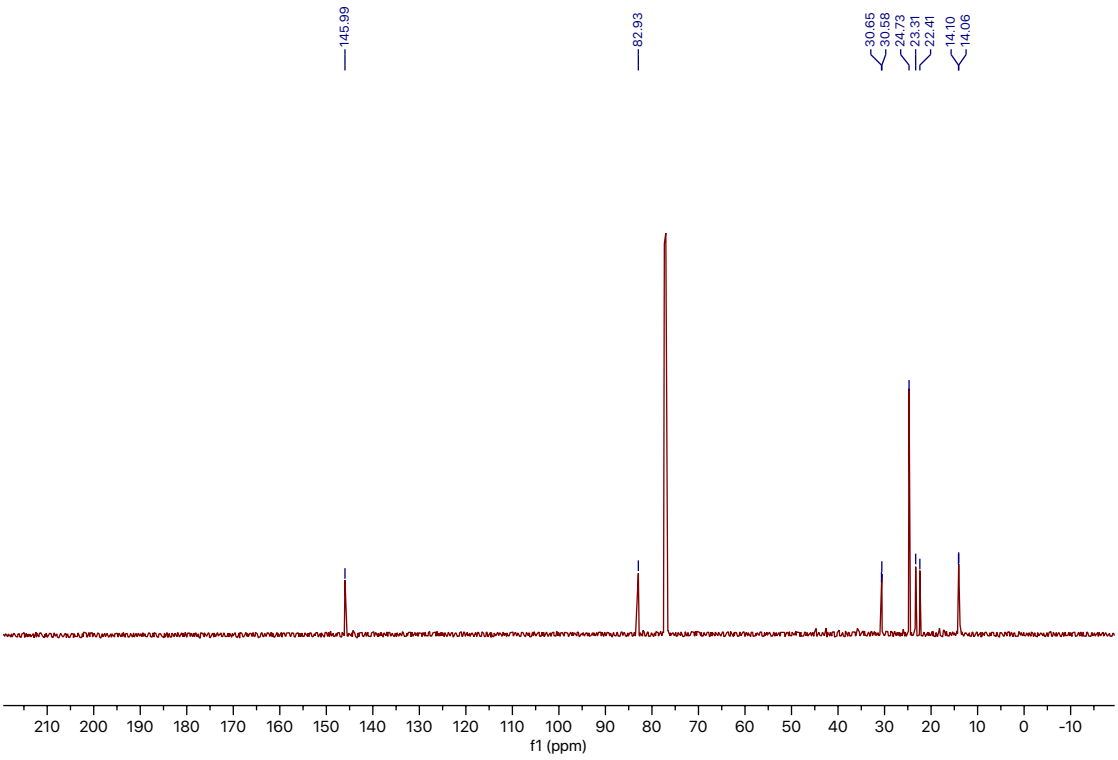


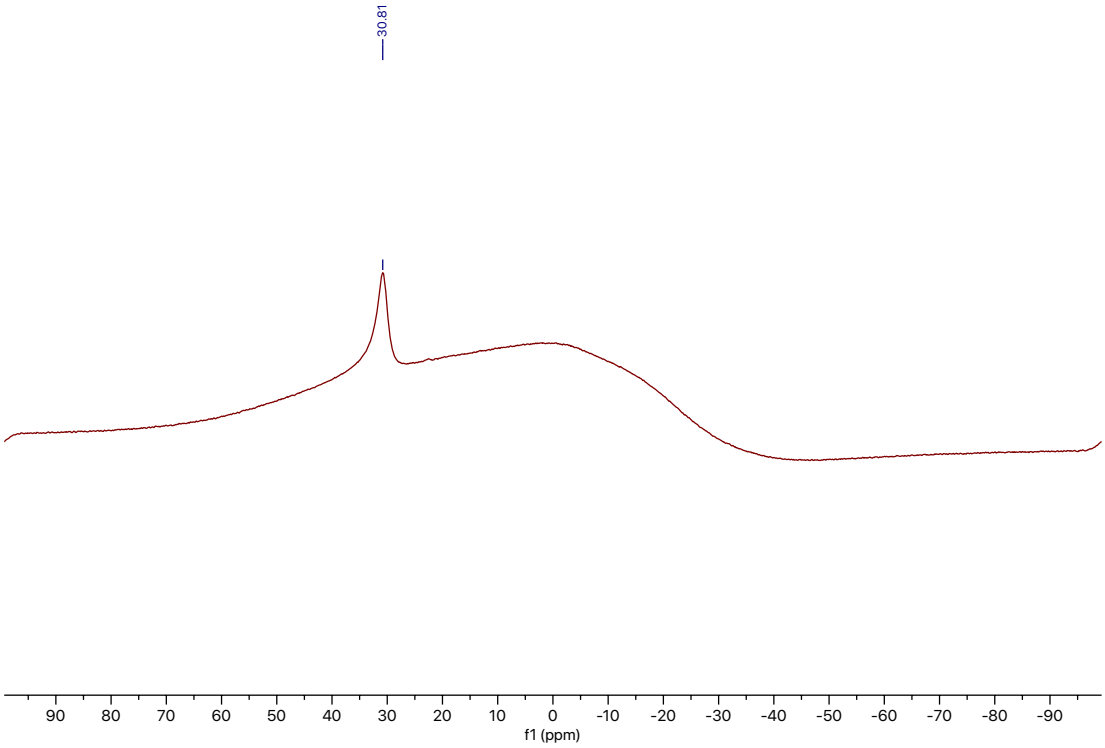

146.72
83.56
33.63
24.82
24.78
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


29.47
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

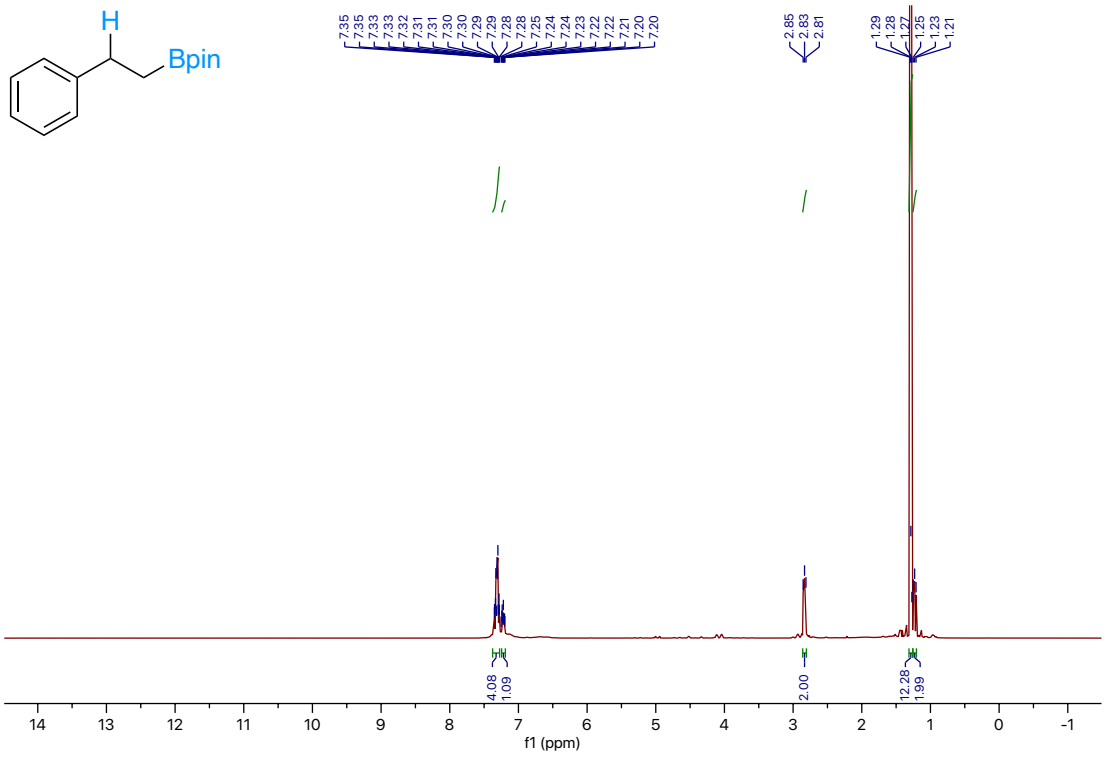
(*Z*)-4,4,5,5-tetramethyl-2-(oct-4-en-4-yl)-1,3,2-dioxaborolane (4dd): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

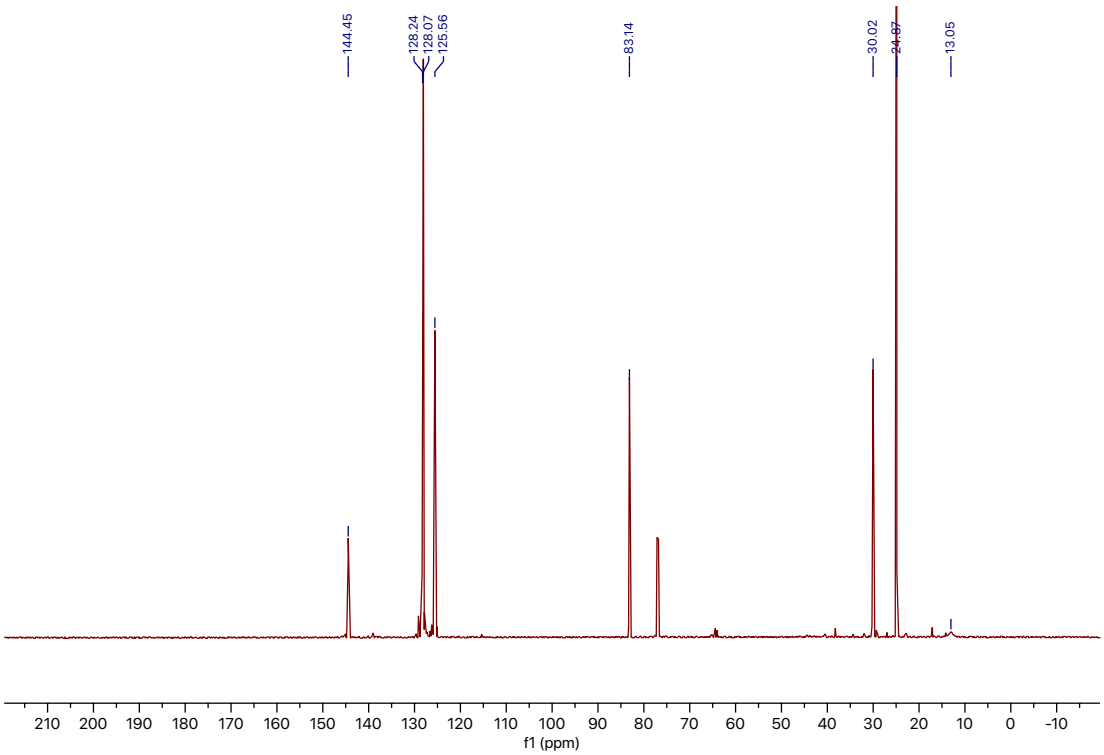


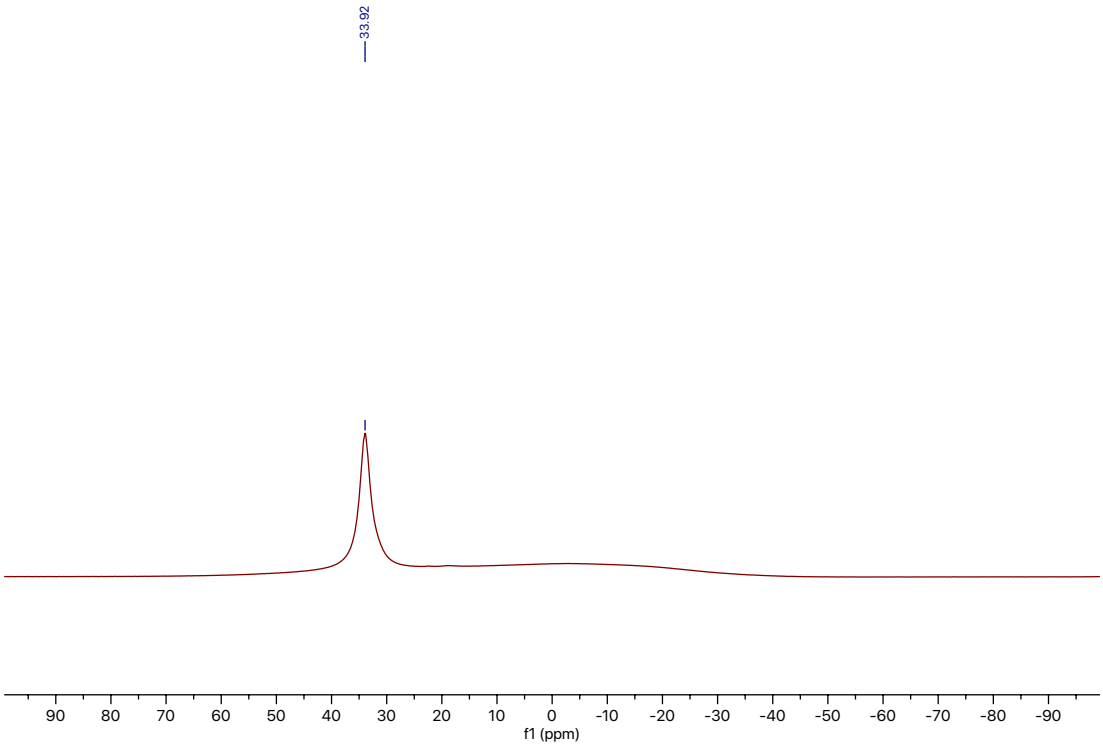




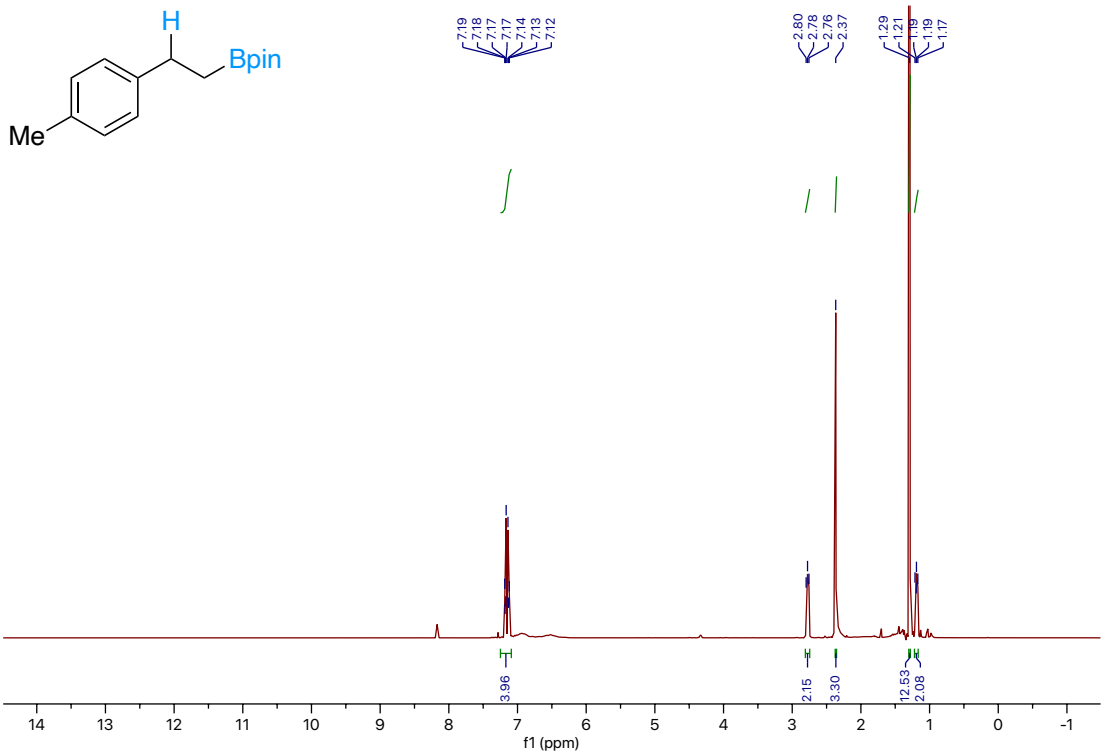
4,4,5,5-tetramethyl-2-phenethyl-1,3,2-dioxaborolane (14a): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

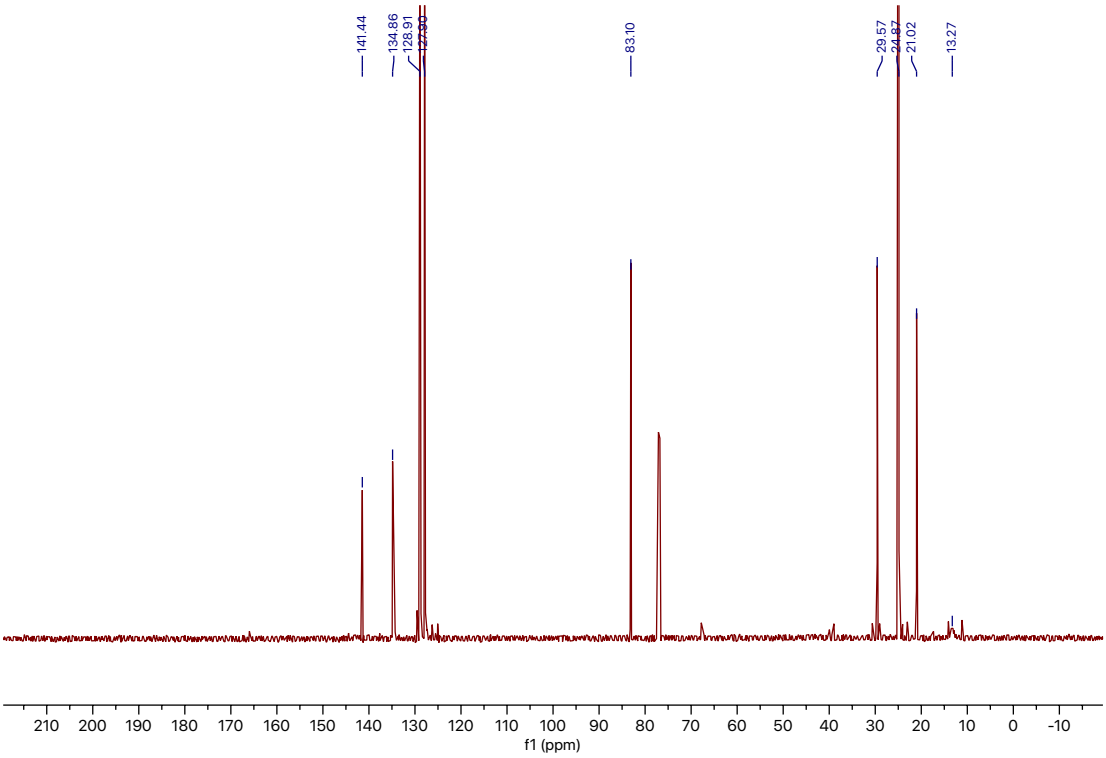


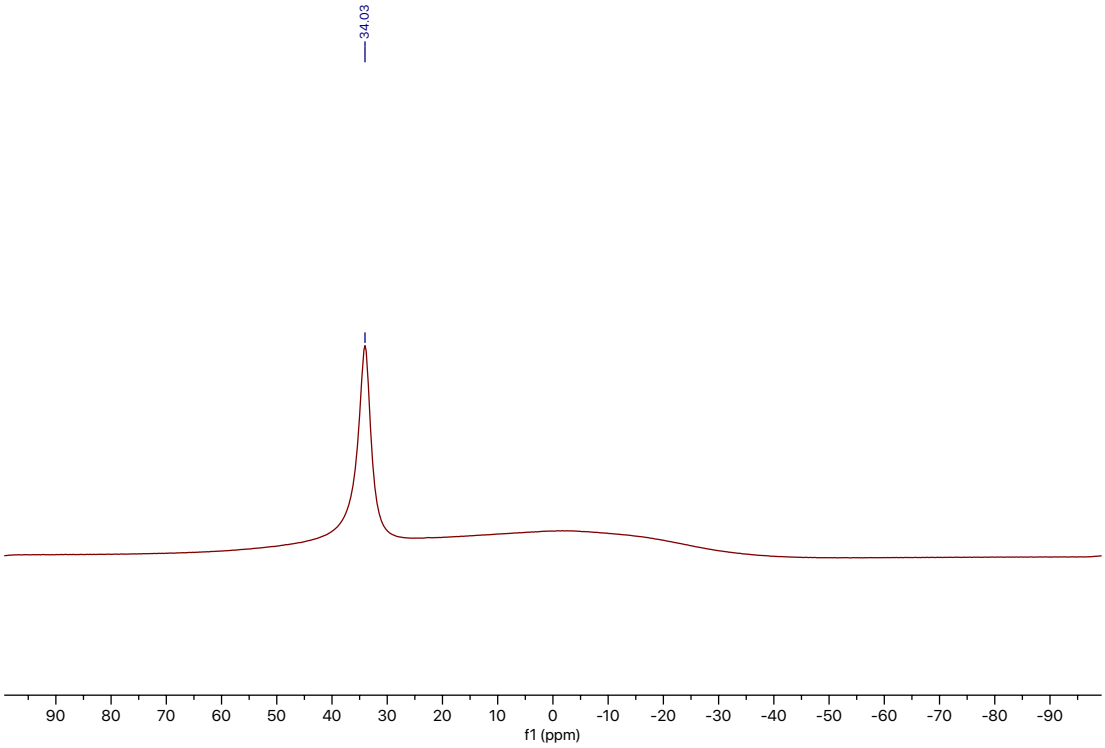

144.45
128.24
128.07
125.56
83.14
30.02
24.87
13.05
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


33.92
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

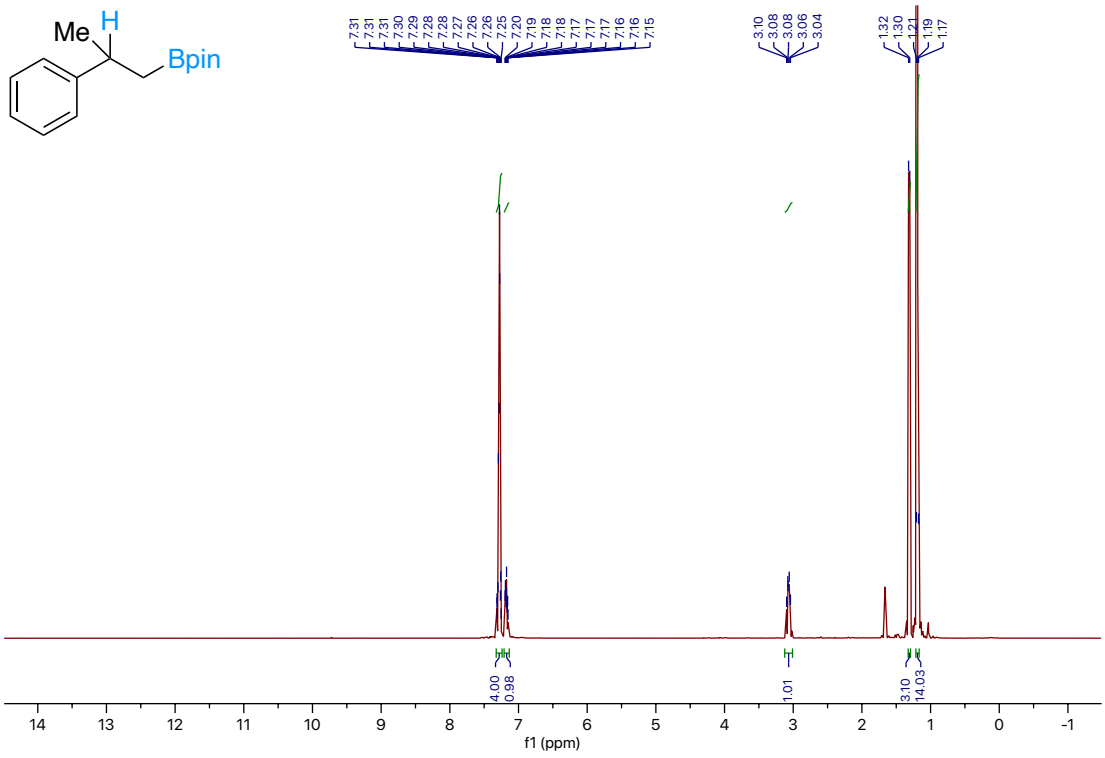
4,4,5,5-tetramethyl-2-(4-methylphenethyl)-1,3,2-dioxaborolane (14b): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

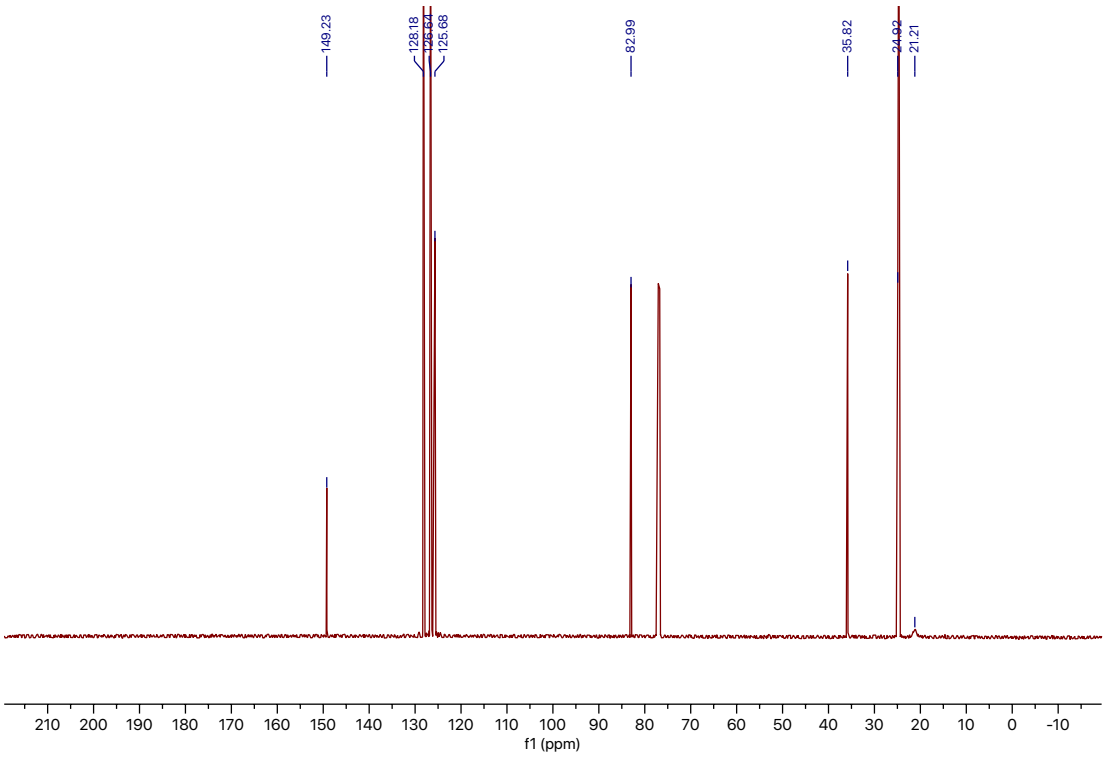


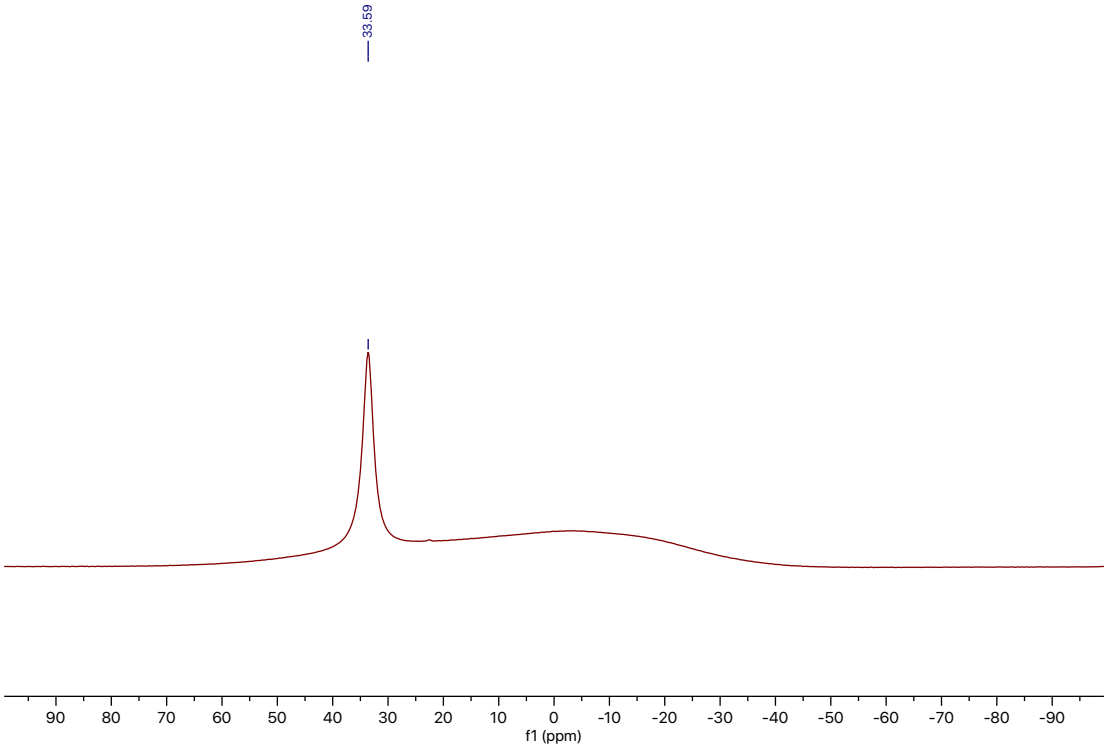




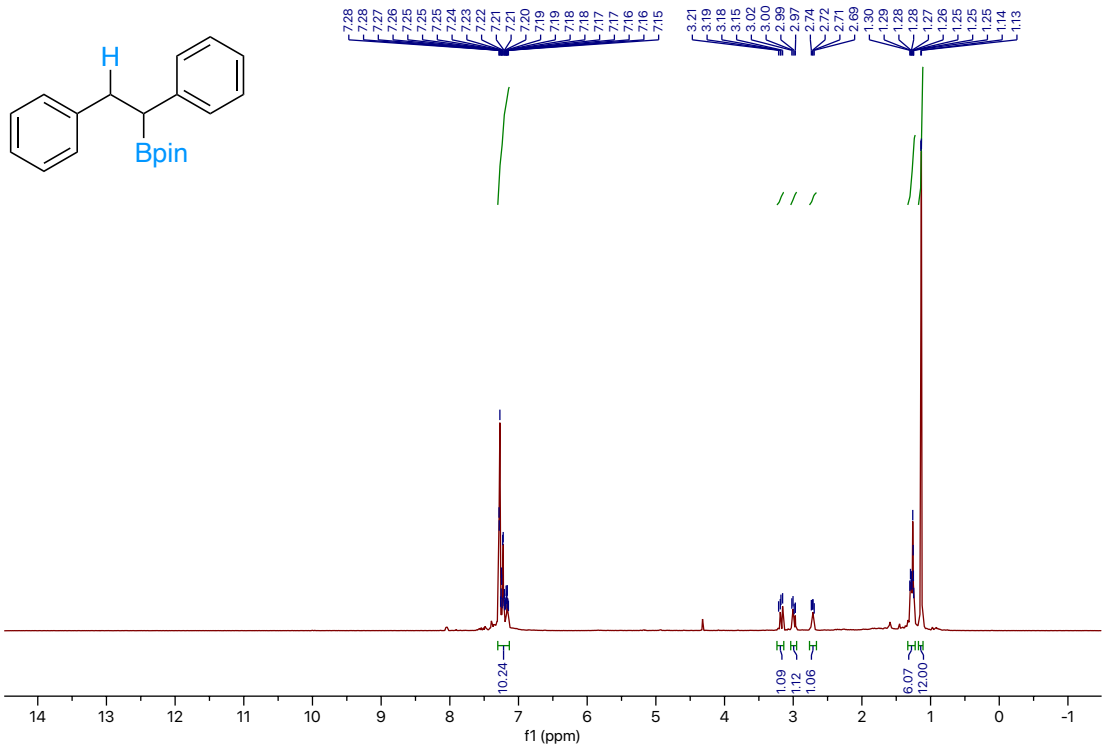
4,4,5,5-tetramethyl-2-(2-phenylpropyl)-1,3,2-dioxaborolane (14c): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

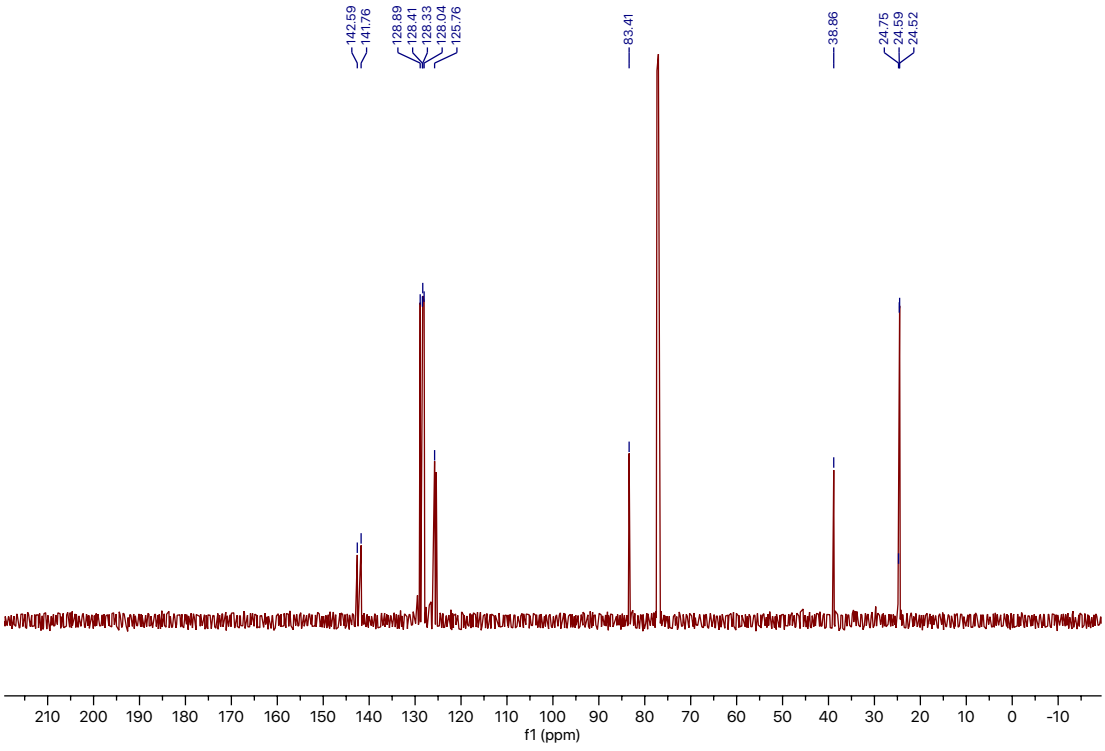


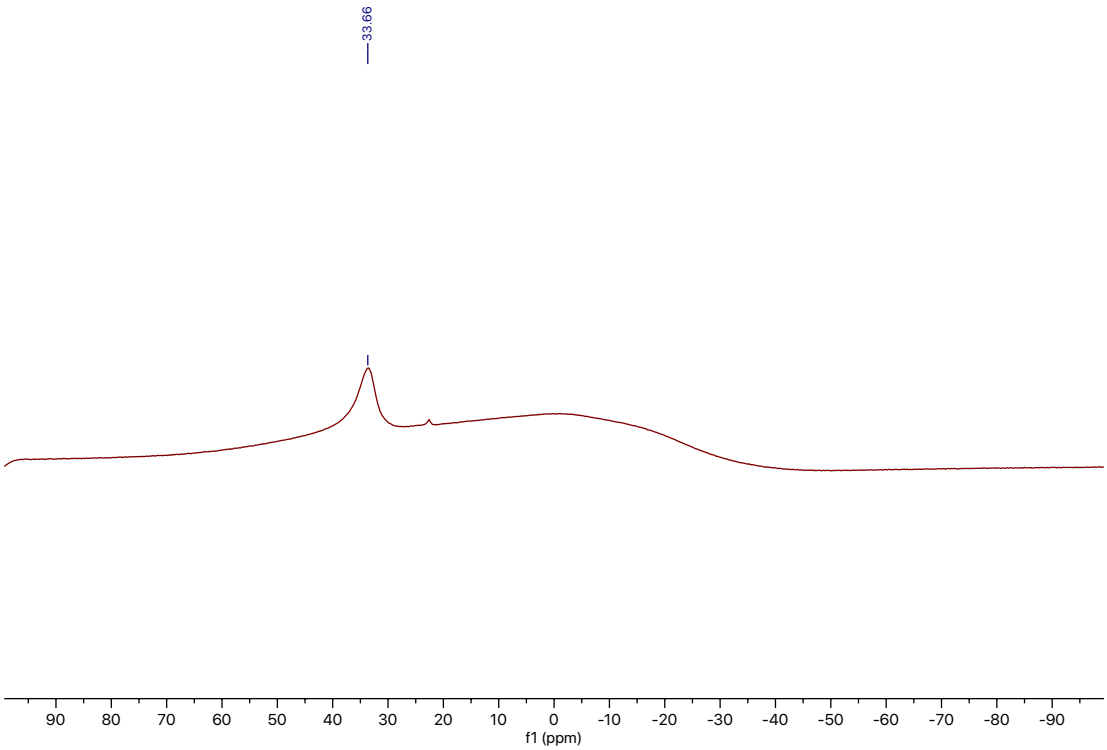

149.23
128.18
125.68
82.99
35.82
24.92
21.21
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


33.59
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

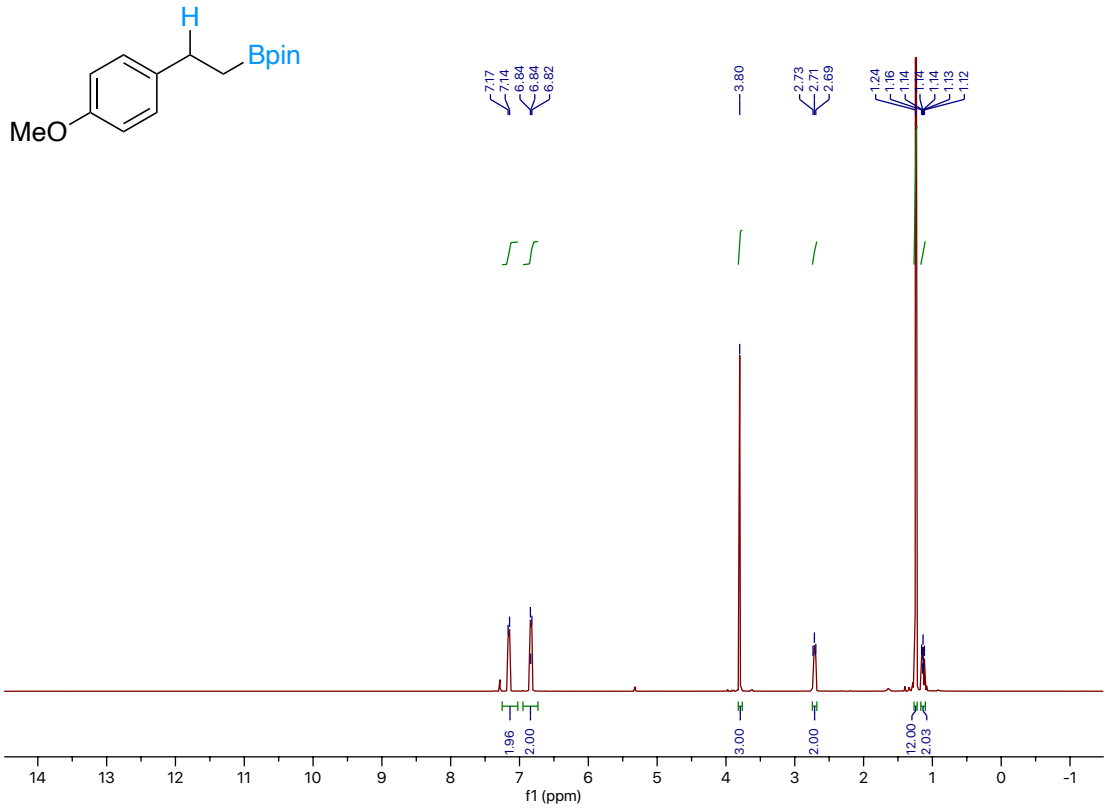
(*R*)-2-(2-(4-Methoxyphenyl)-1-phenylethyl)-4,4,5,5-tetramethyl1,3,2-dioxaborolane (14d): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

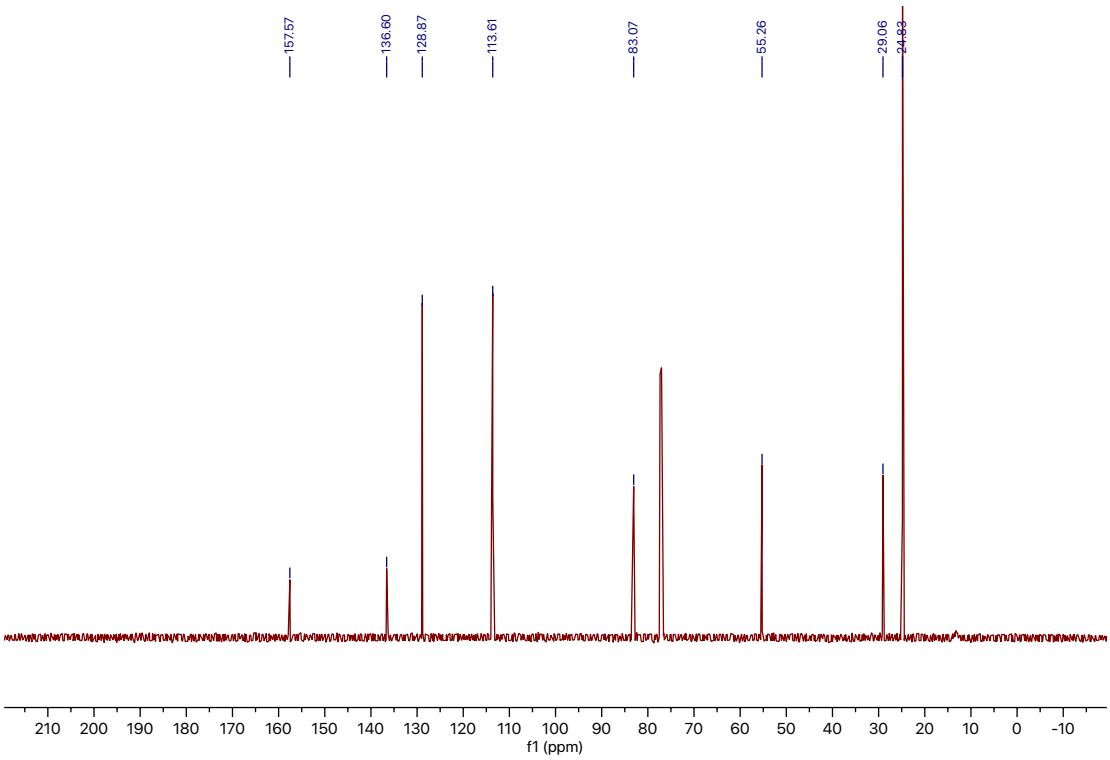






2-(4-methoxyphenethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (14e): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).




157.57
136.60
128.87
113.61
83.07
55.26
29.06
24.83
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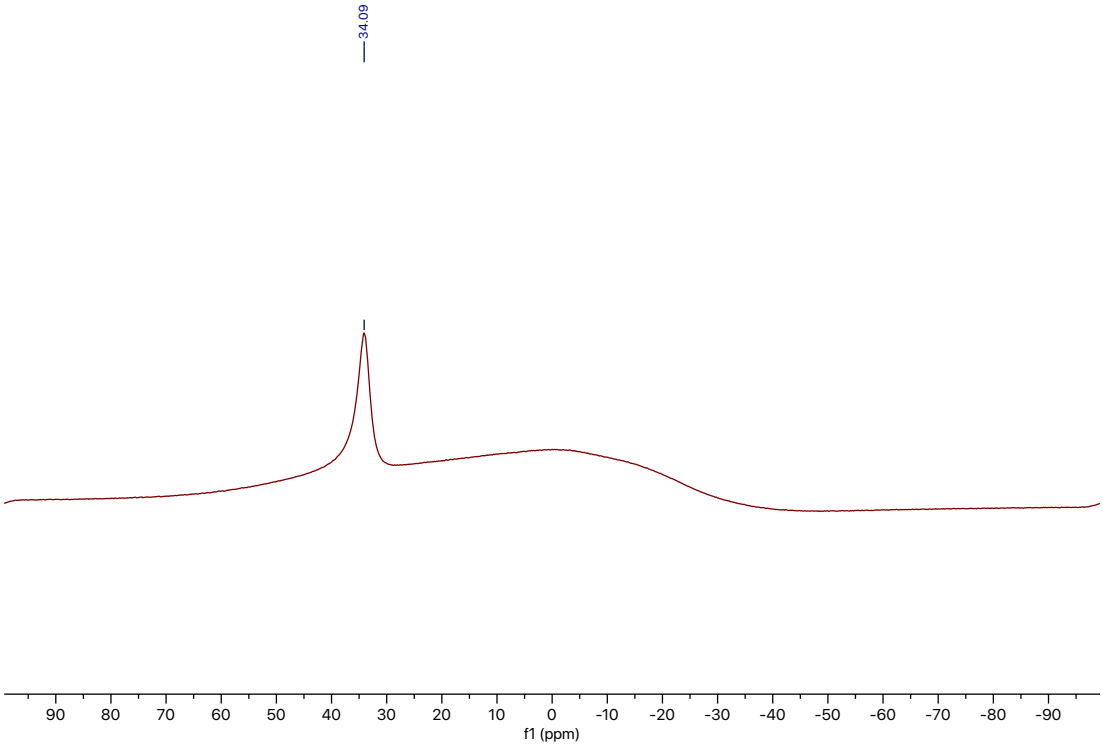
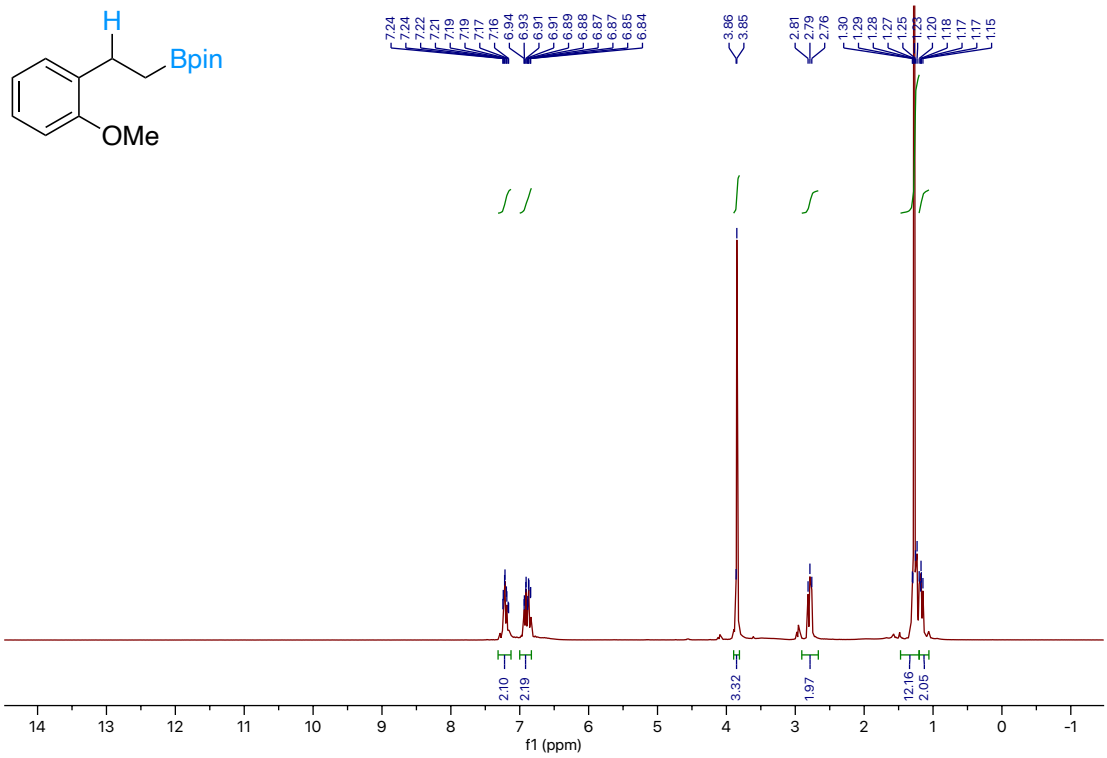
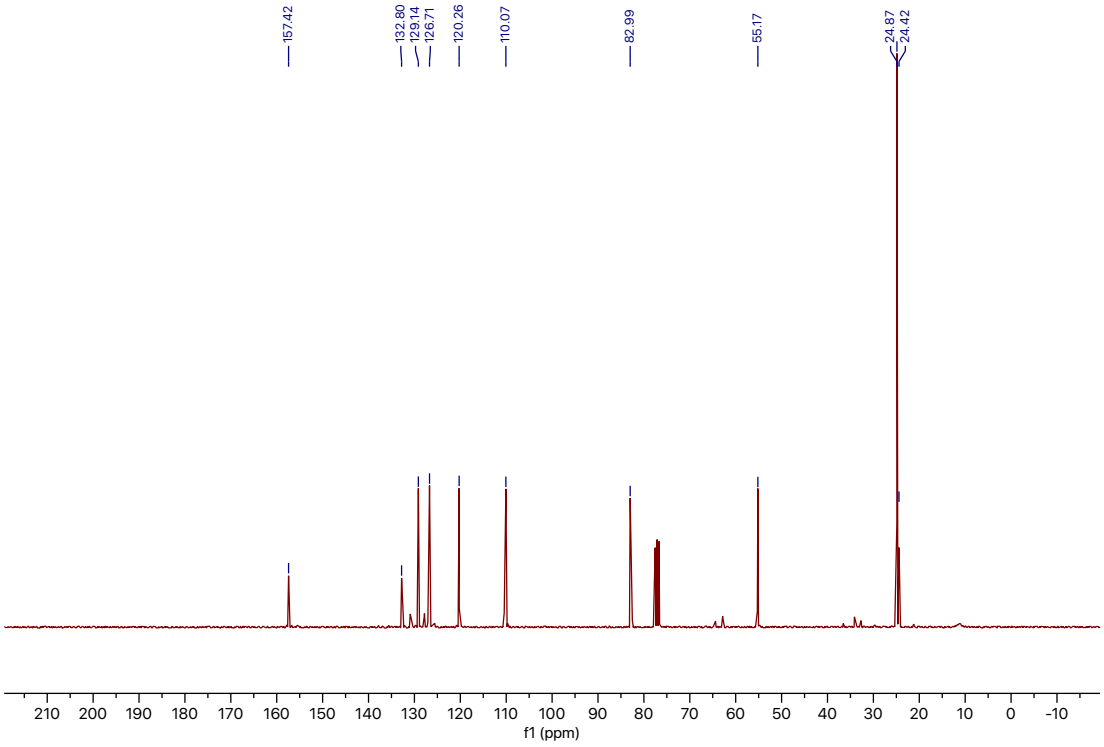
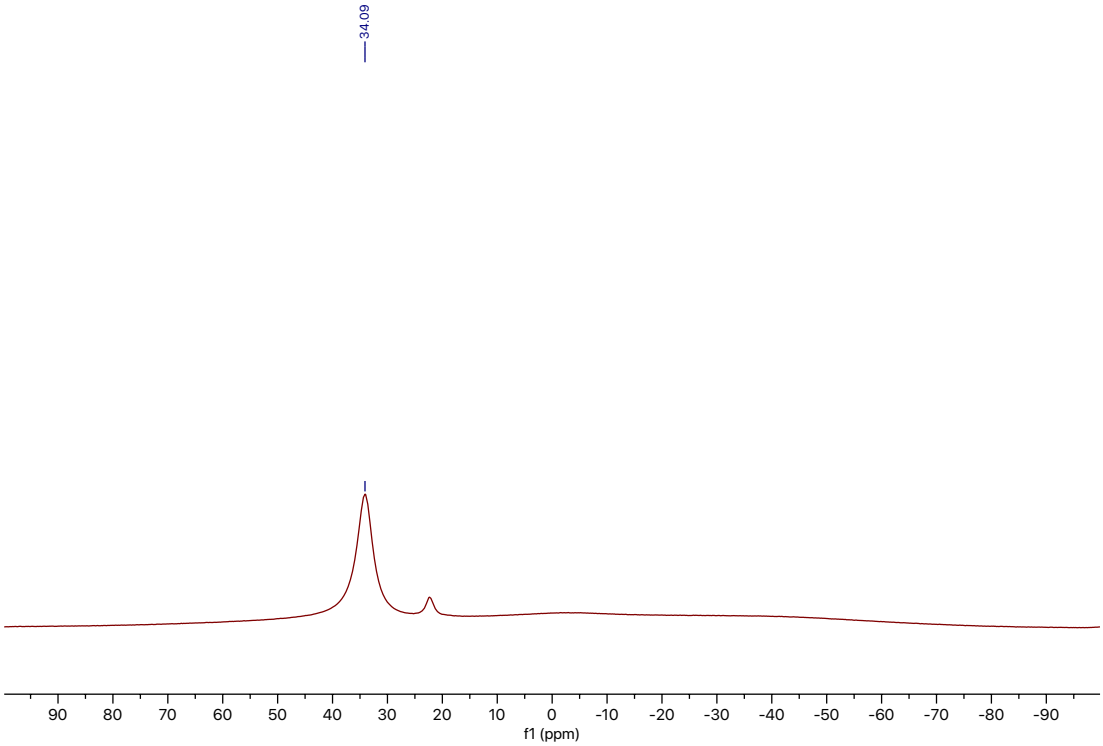
f1 (ppm)


34.09
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

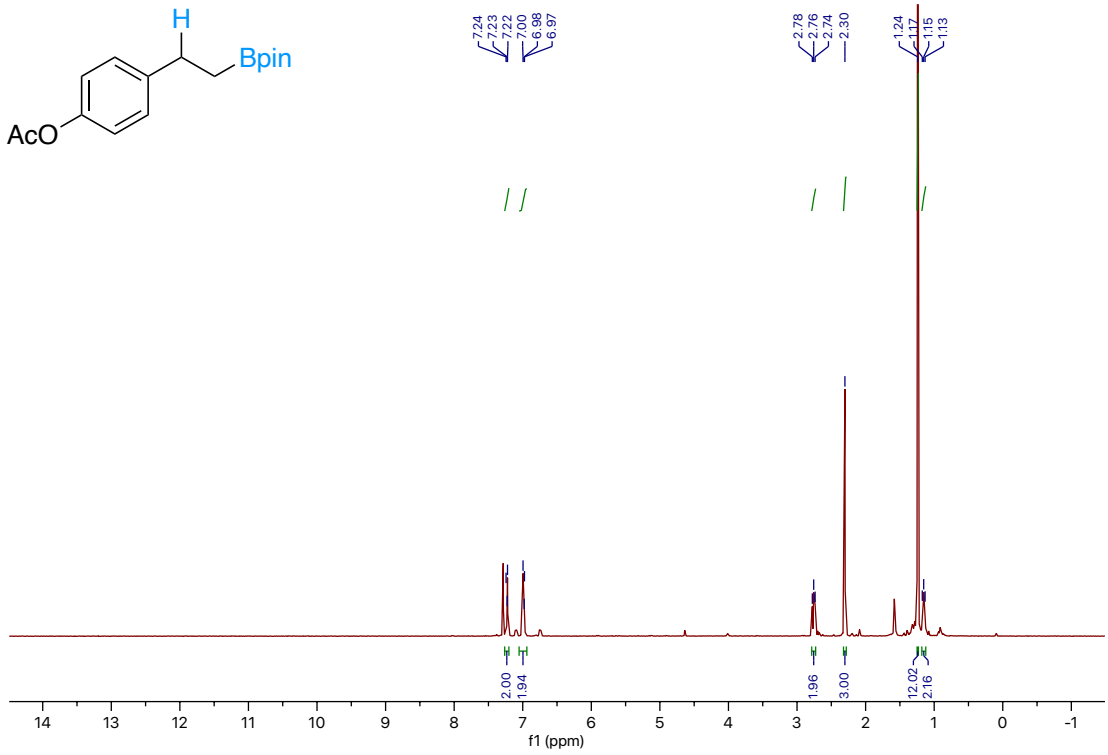
2-(2-methoxyphenethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (14f): ^{1}H NMR (300 MHz, $CDCl_3$), ^{13}C NMR (76 MHz, $CDCl_3$), ^{11}B NMR (96 MHz, $CDCl_3$).

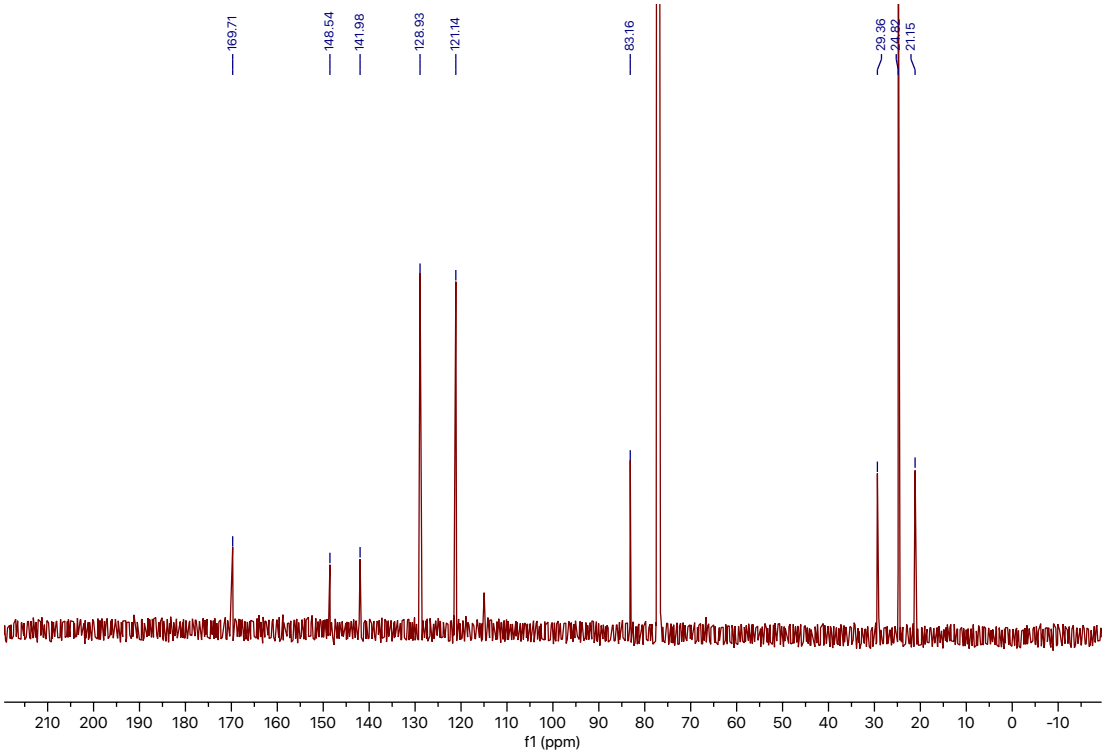


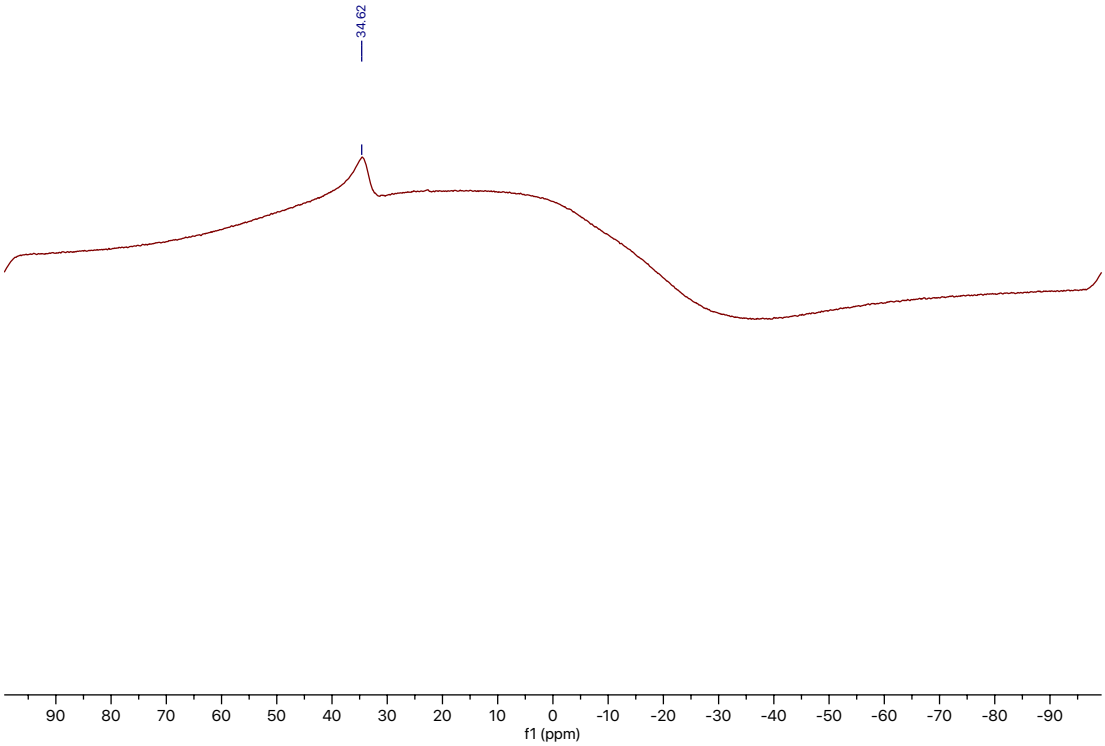




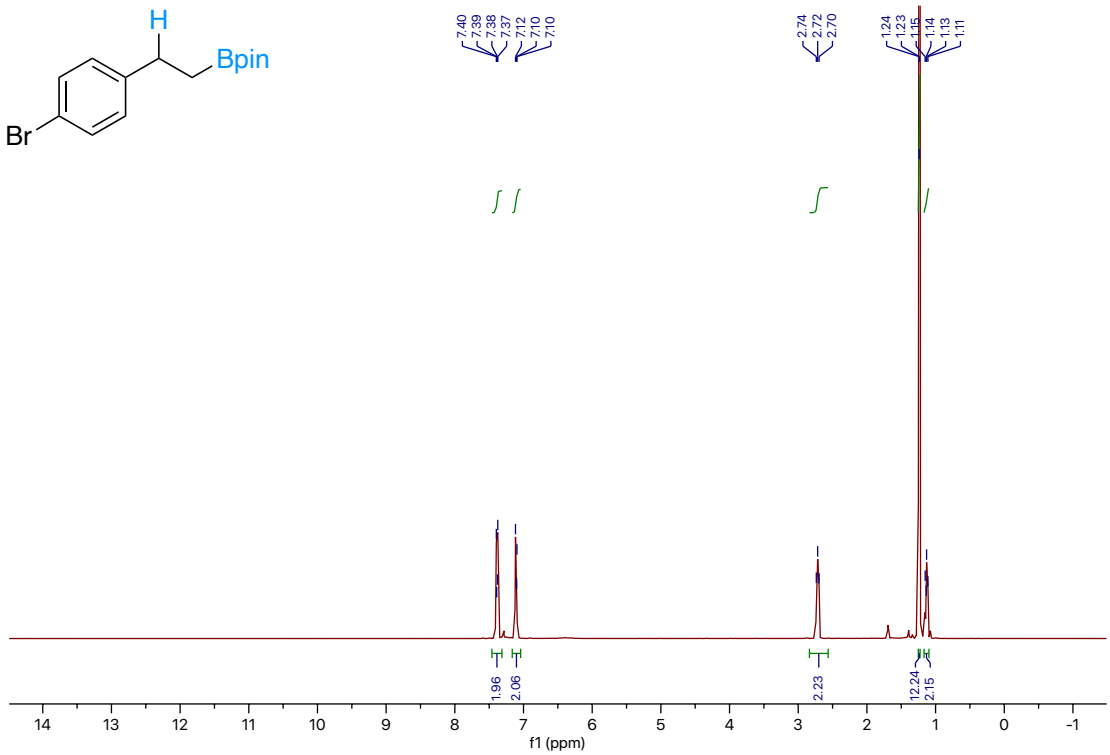
4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)phenyl acetate (14g): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

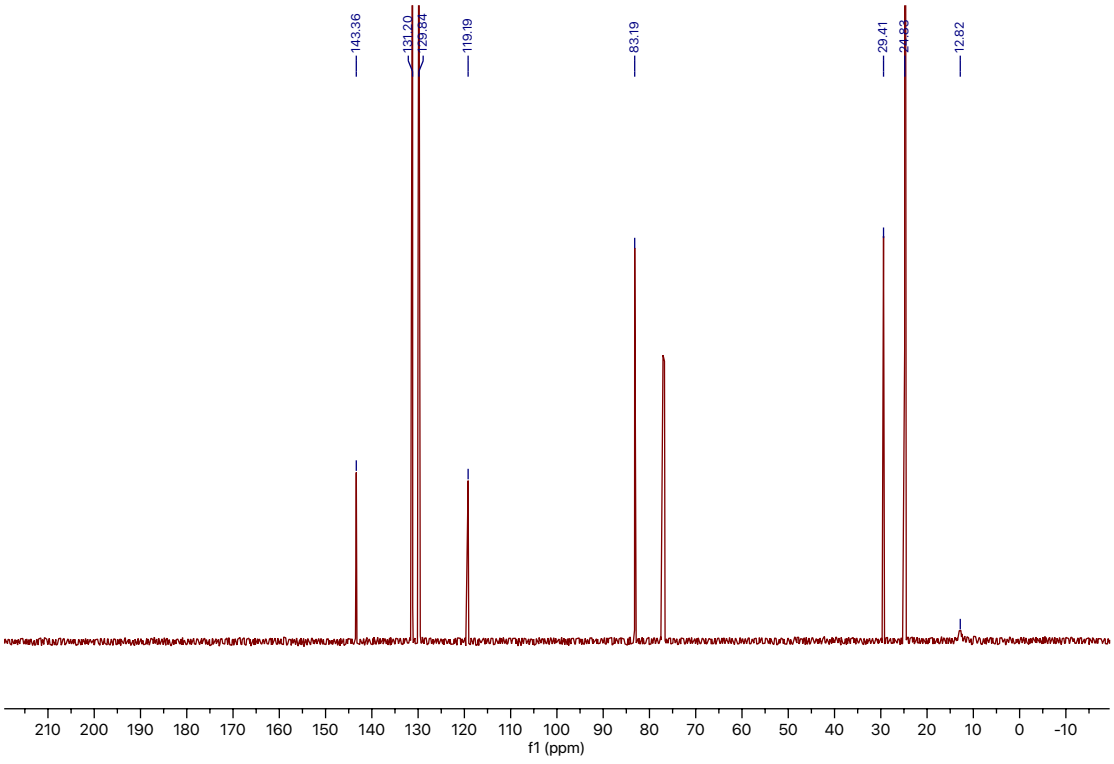


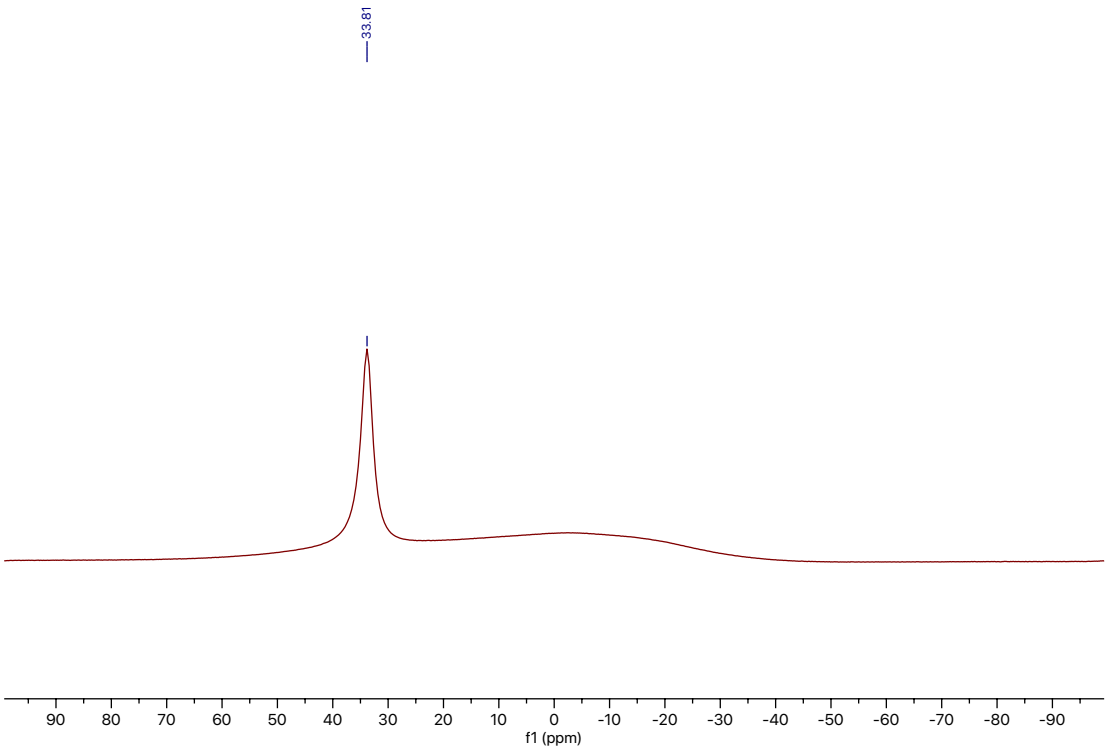

169.71
148.54
141.98
128.93
121.14
83.16
29.36
24.82
21.15
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


34.62
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

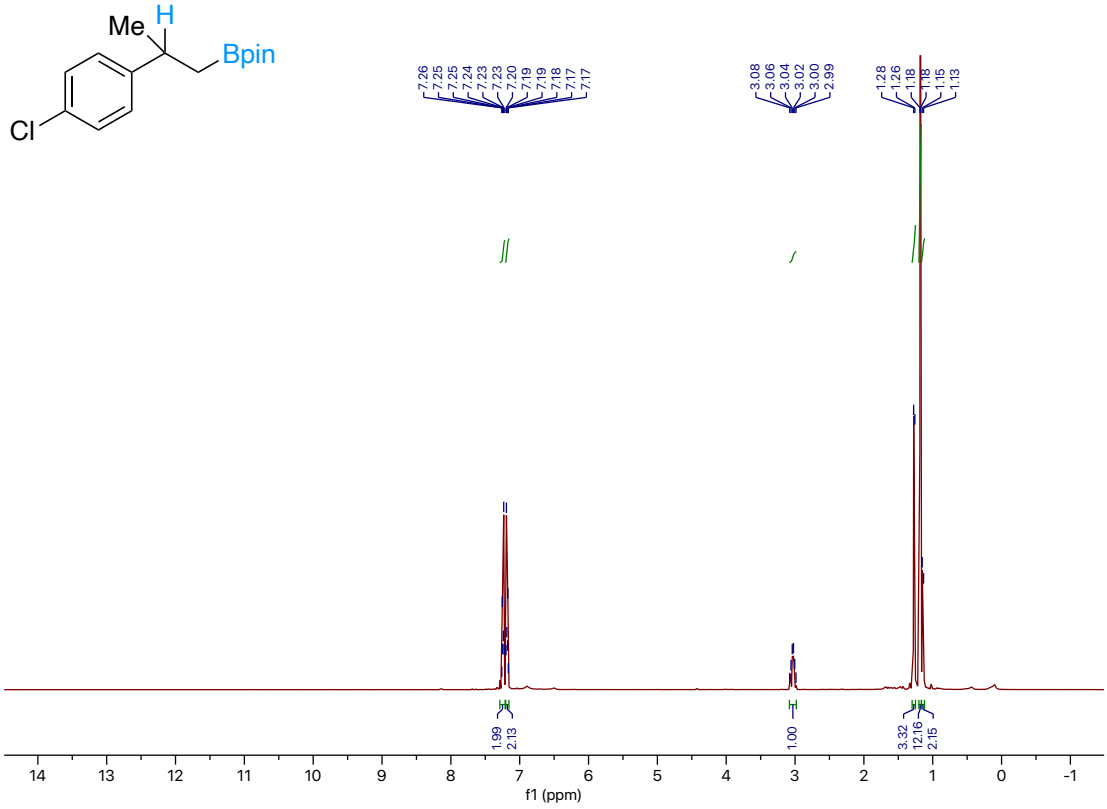
2-(4-bromophenethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (14h): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

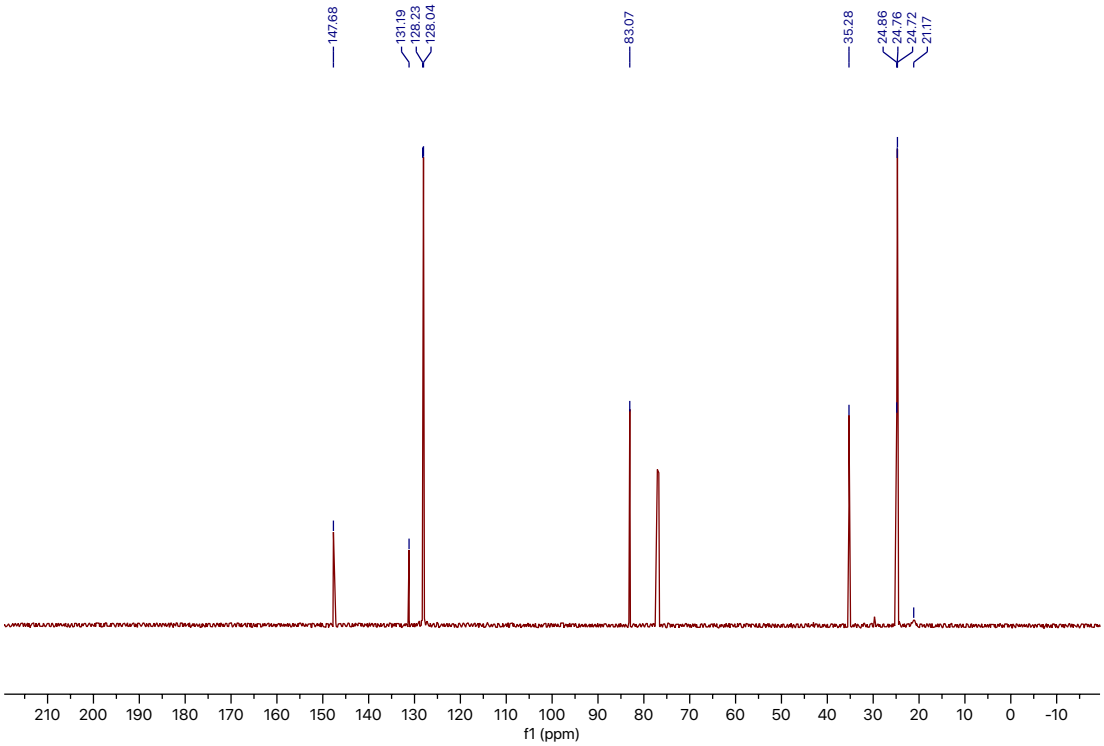


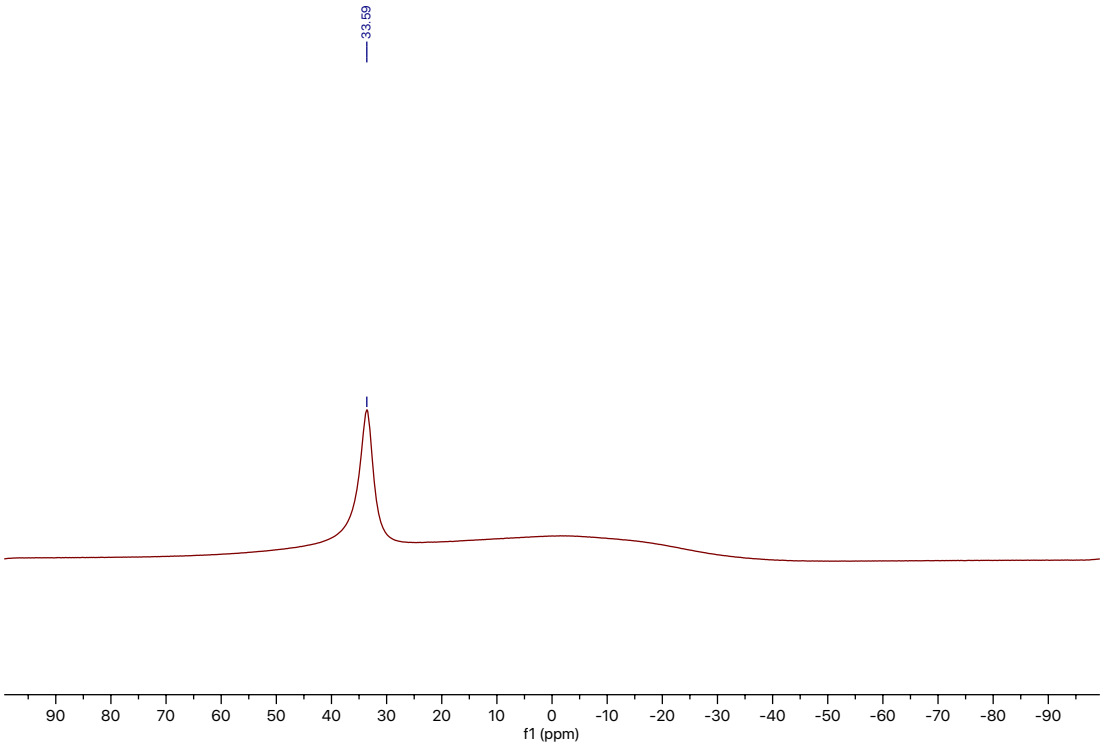




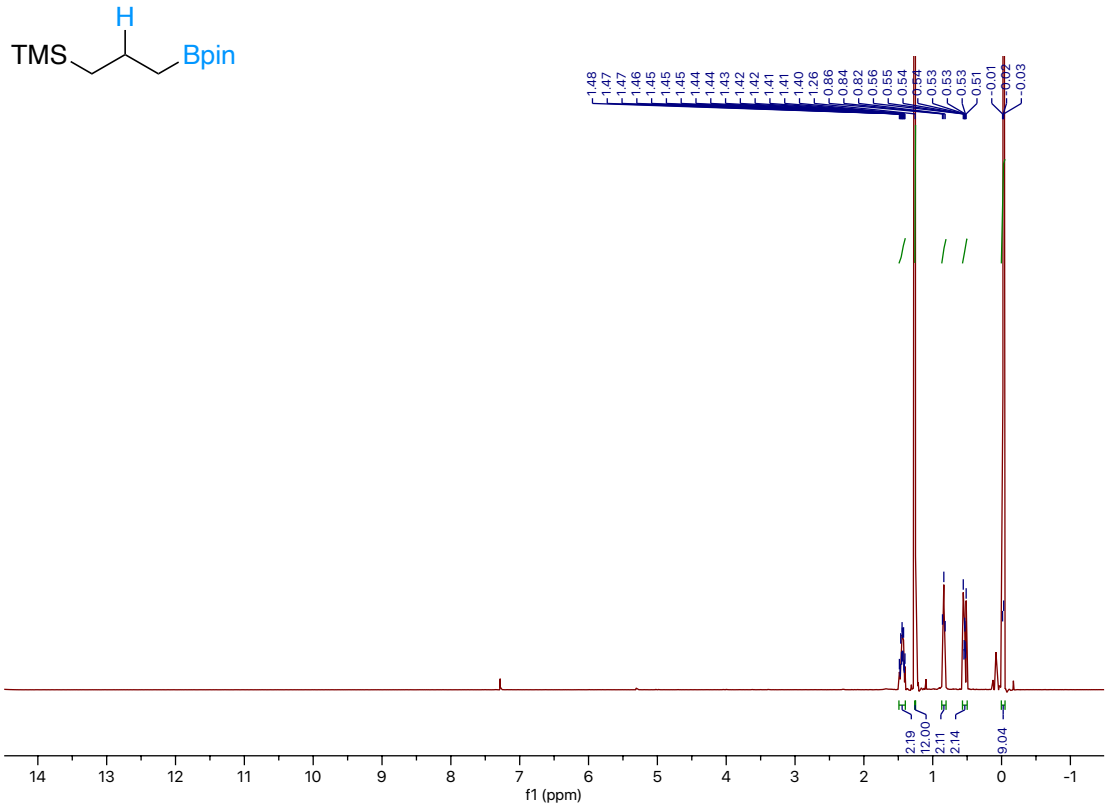
2-(2-(4-chlorophenyl)propyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (14i): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

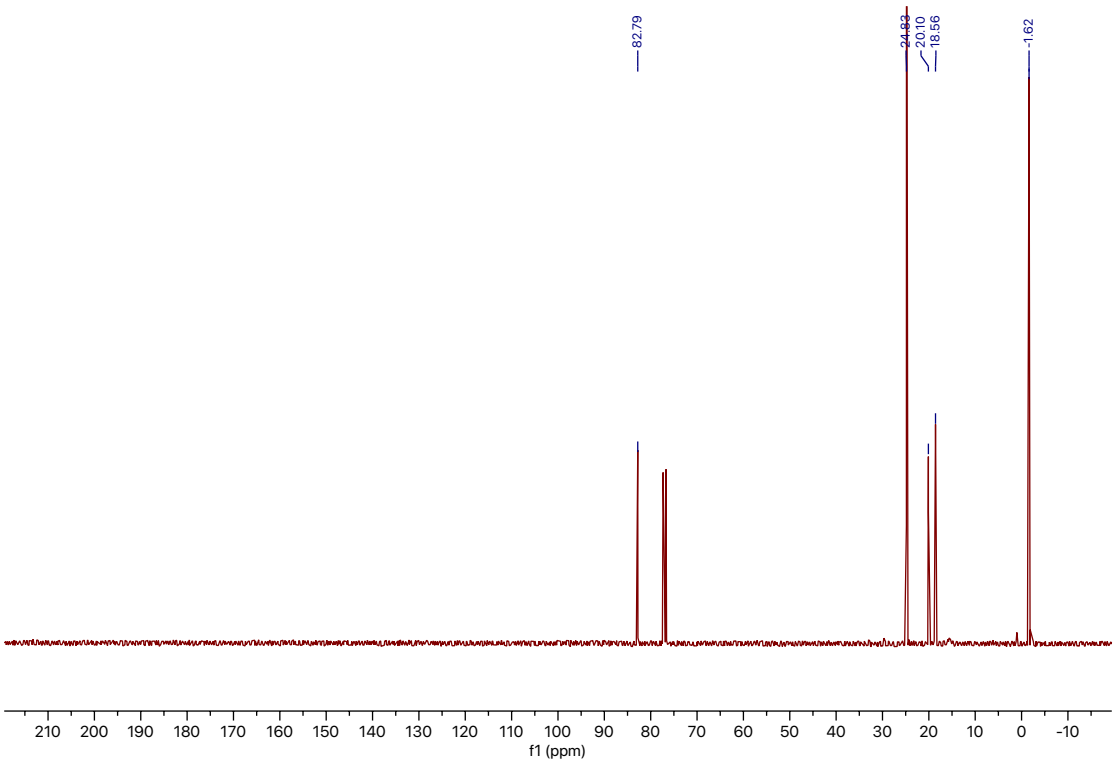


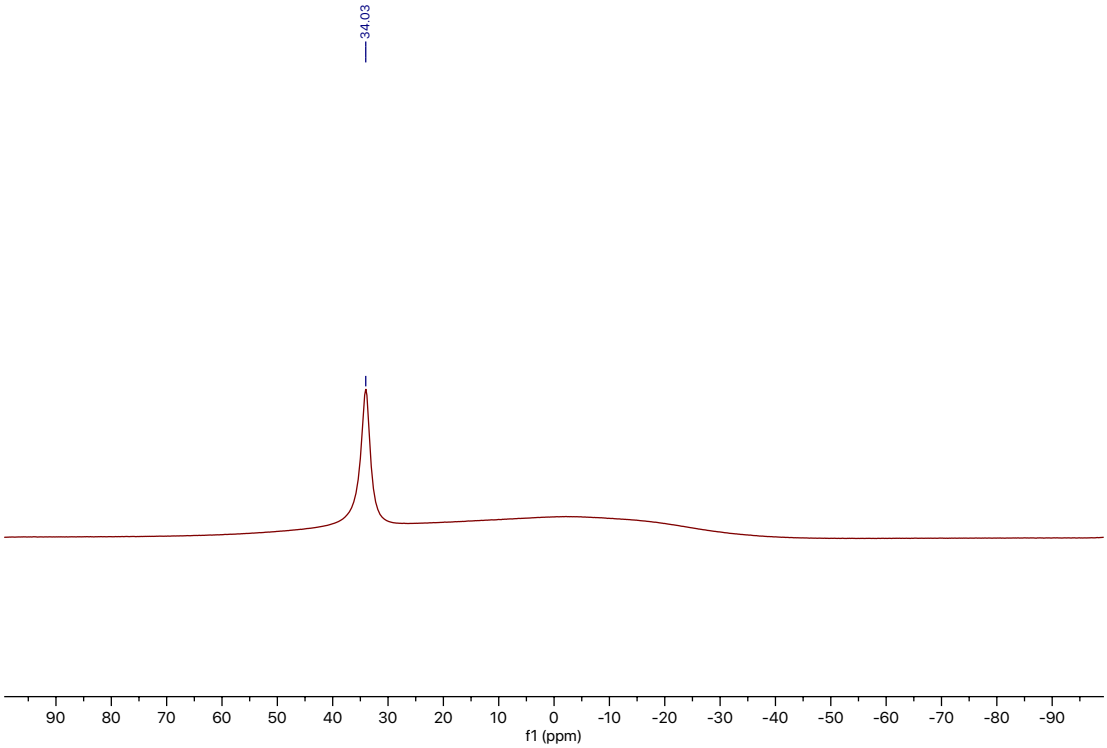

147.68
131.19
128.23
128.04
83.07
35.28
24.86
24.76
24.72
21.17
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


33.59
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

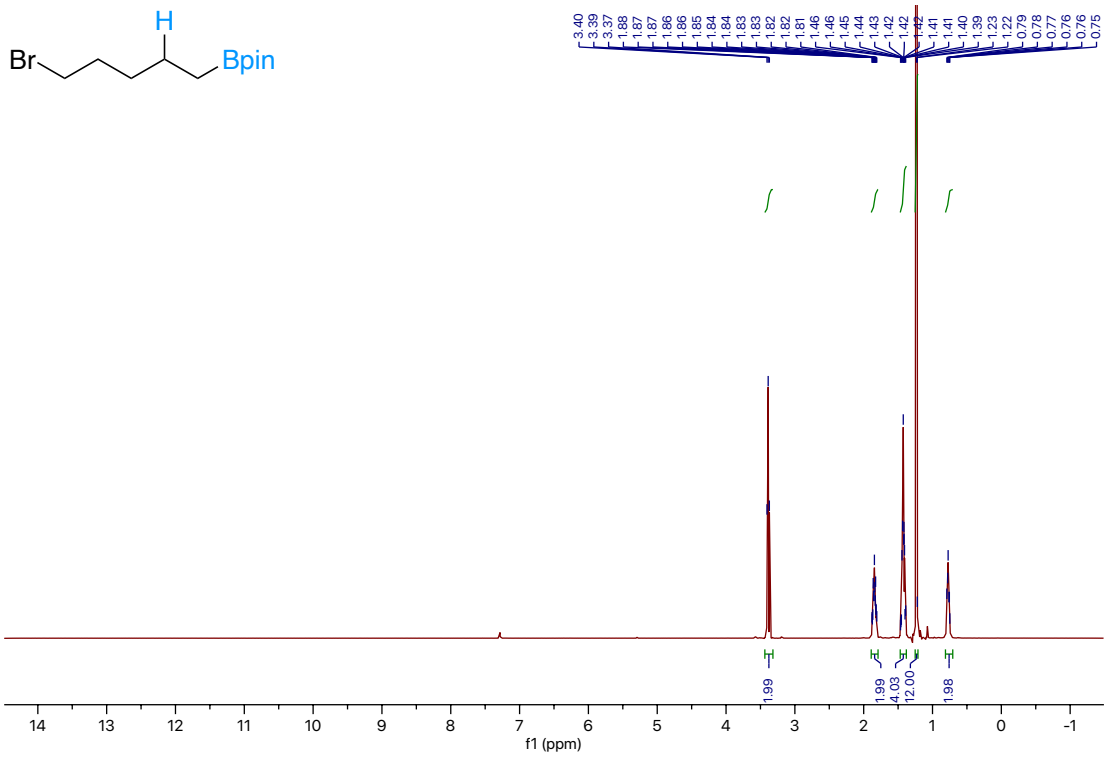
trimethyl(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propyl)silane (14j): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).

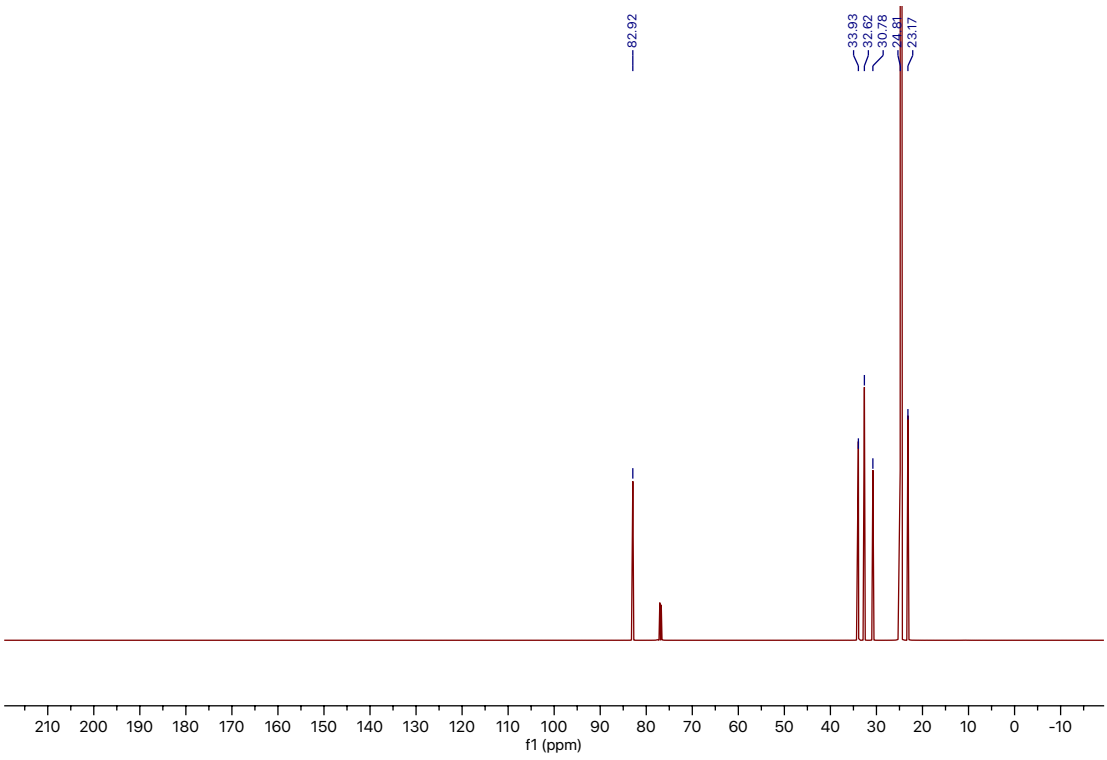


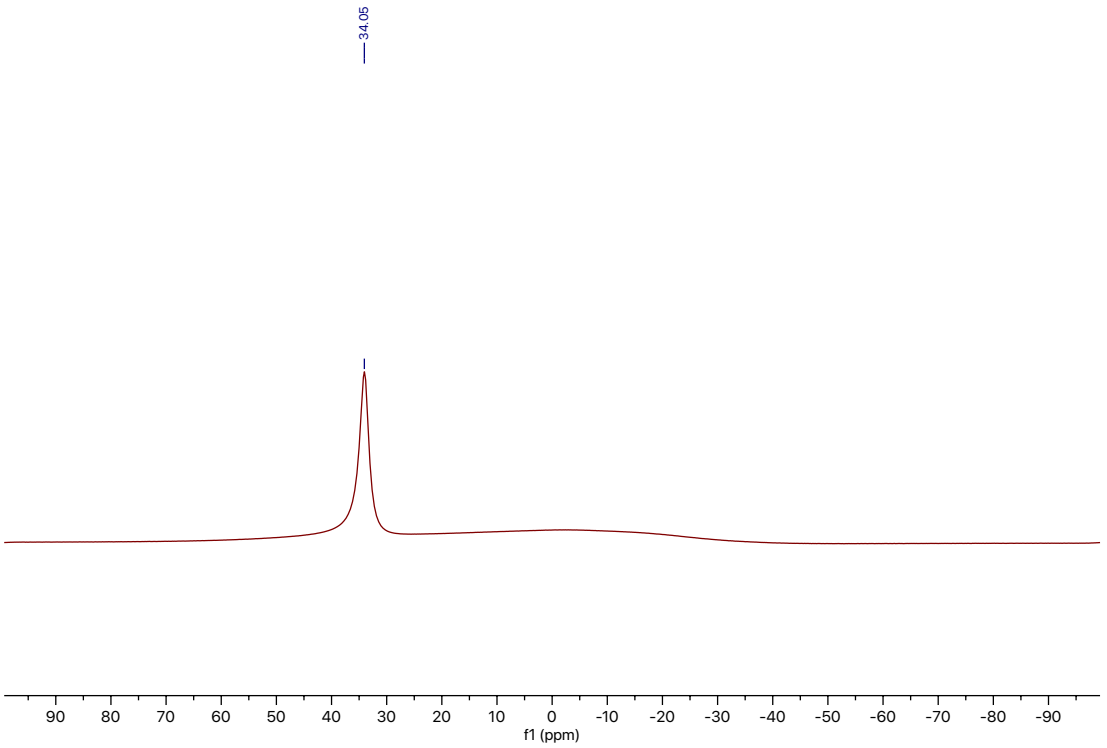




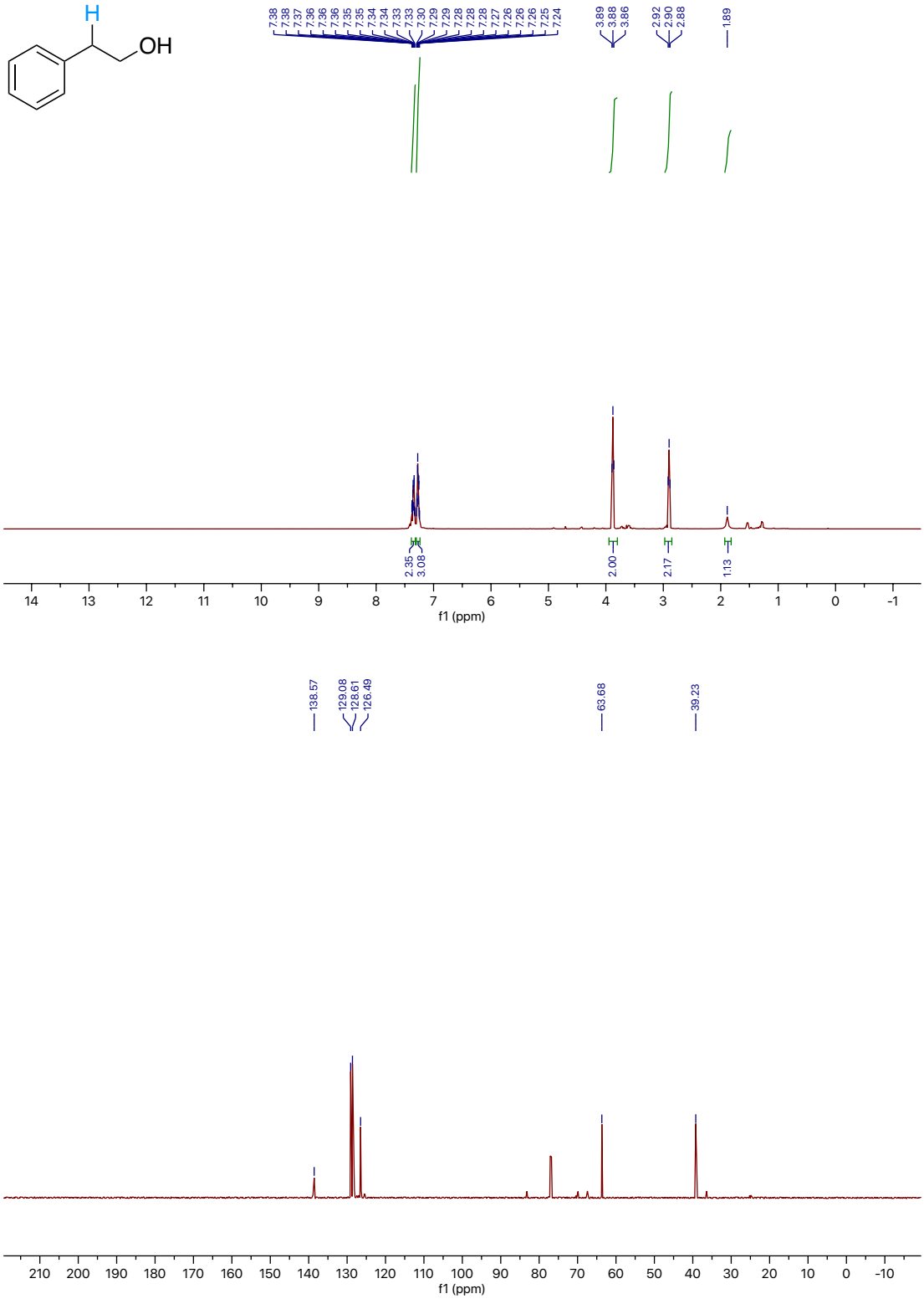
2-(5-bromopentyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (14k): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$), ^{11}B NMR (128 MHz, $CDCl_3$).



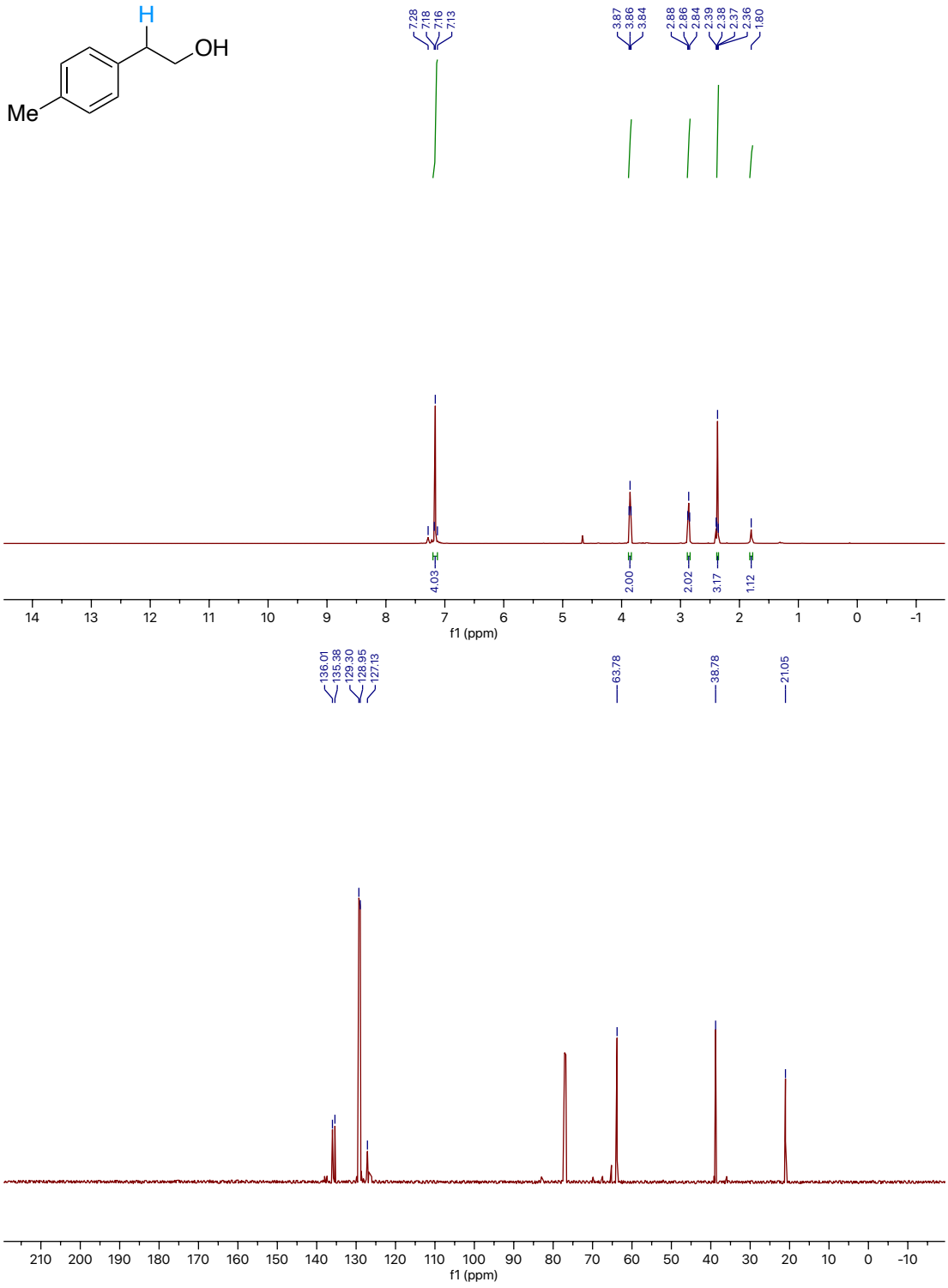

82.92
33.93
32.62
30.78
24.81
23.17
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


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

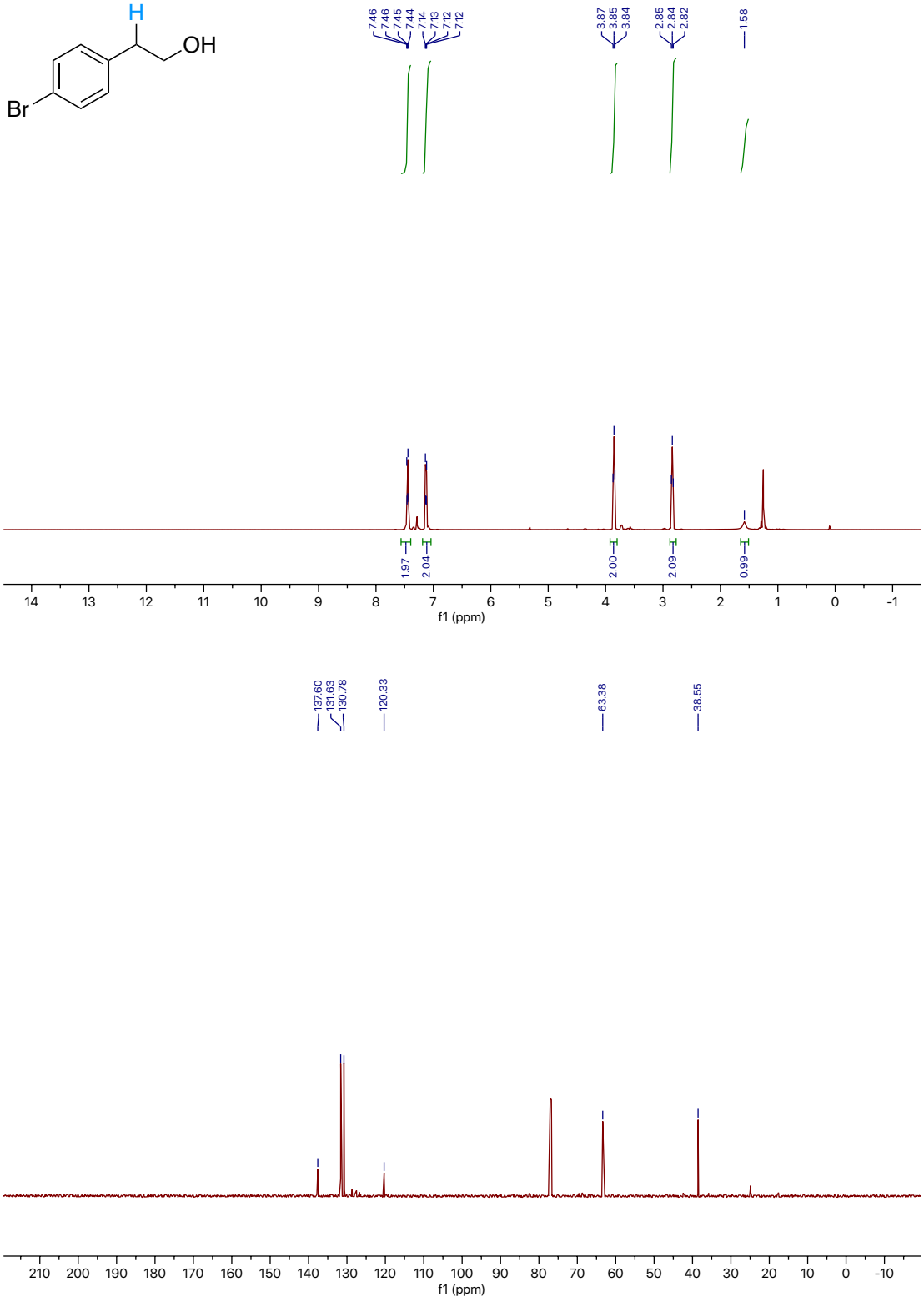
2-phenylethan-1-ol (17a): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$).



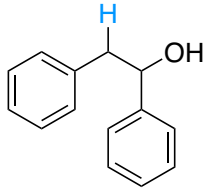
2-(*p*-tolyl)ethan-1-ol (17b): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$).



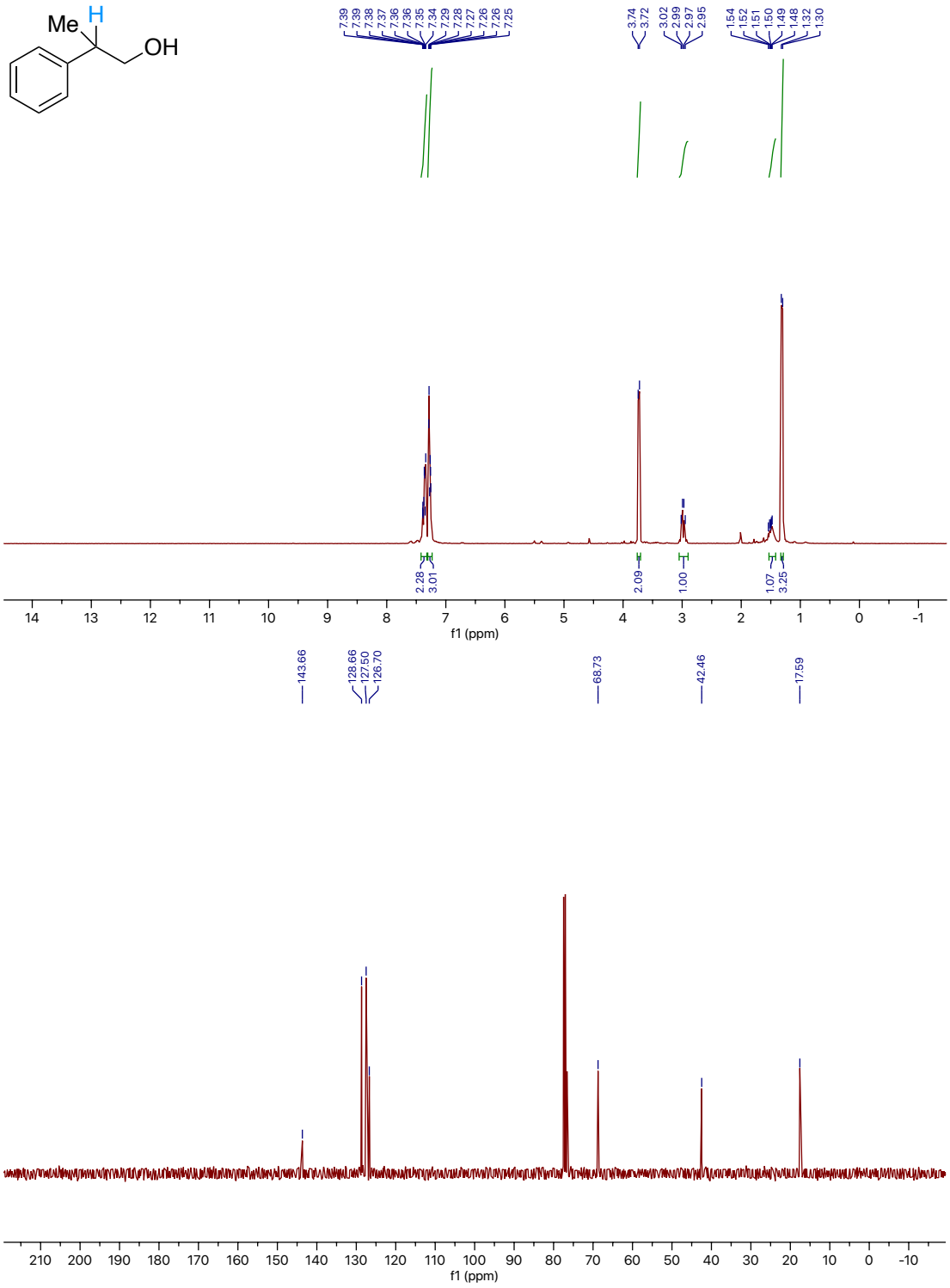
2-(4-bromophenyl)ethan-1-ol (17c): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$).



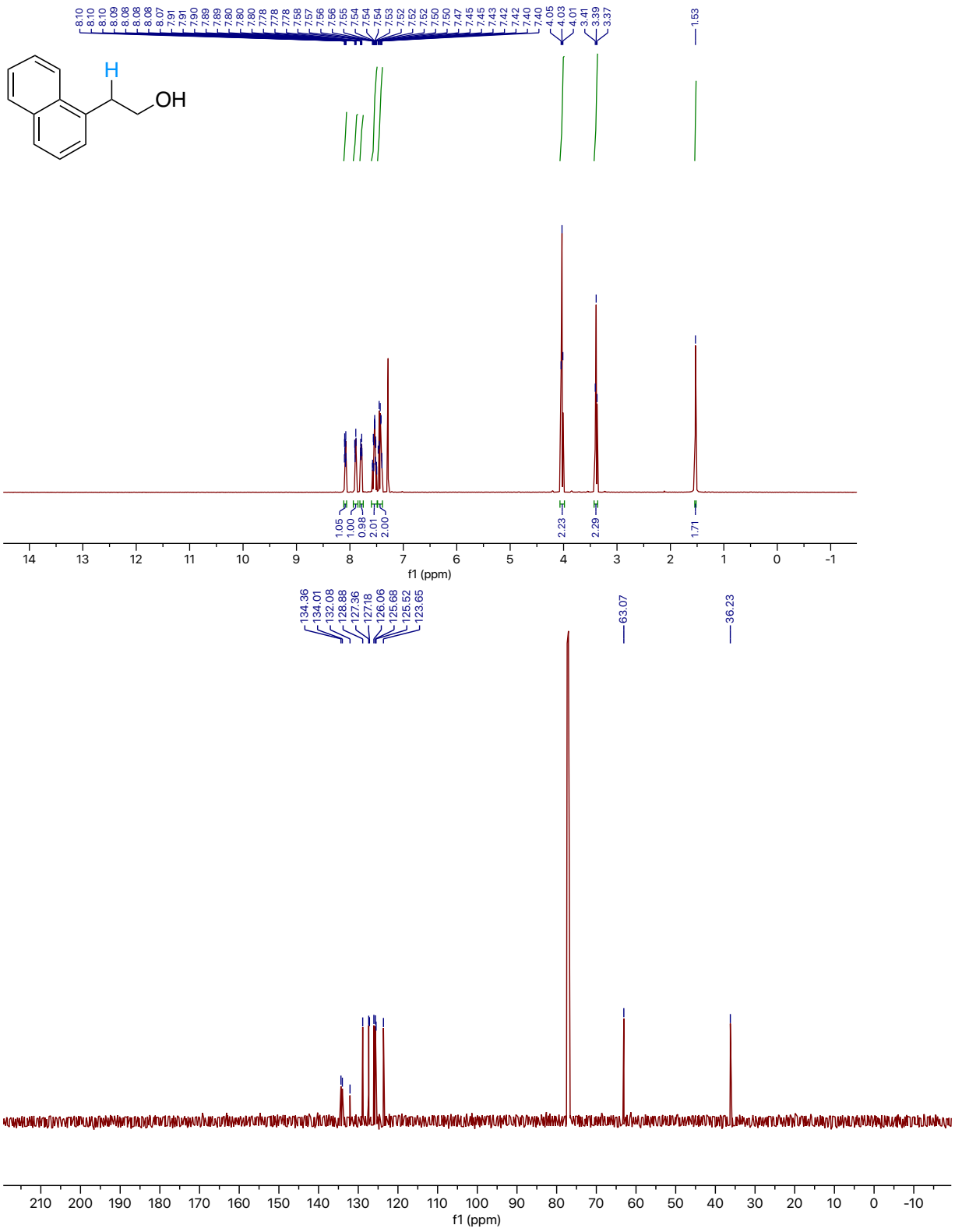
1,2-diphenylethan-1-ol (17d): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$).



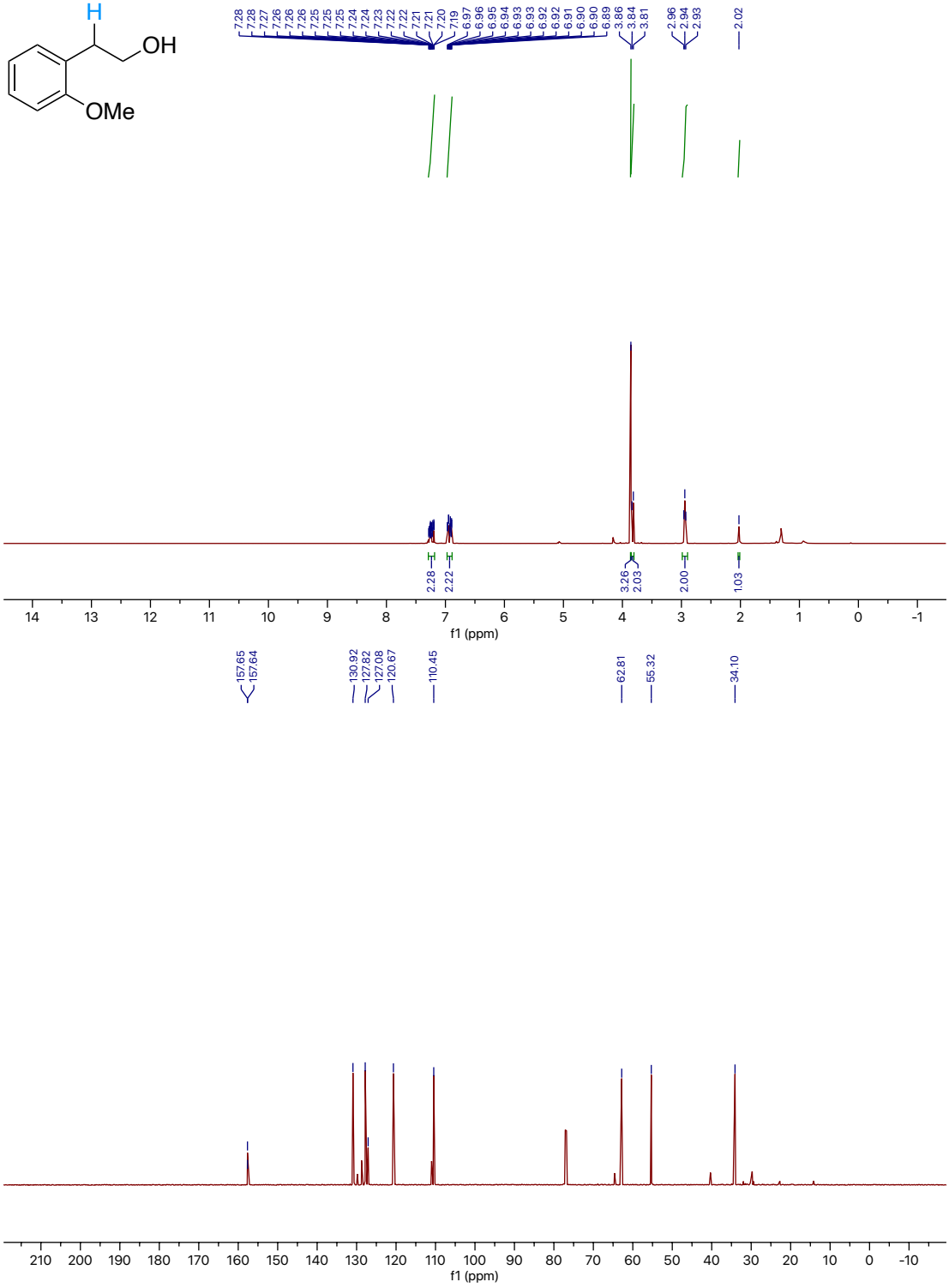
2-phenylpropan-1-ol (17e): ^{1}H NMR (300 MHz, $CDCl_3$), ^{13}C NMR (76 MHz, $CDCl_3$).



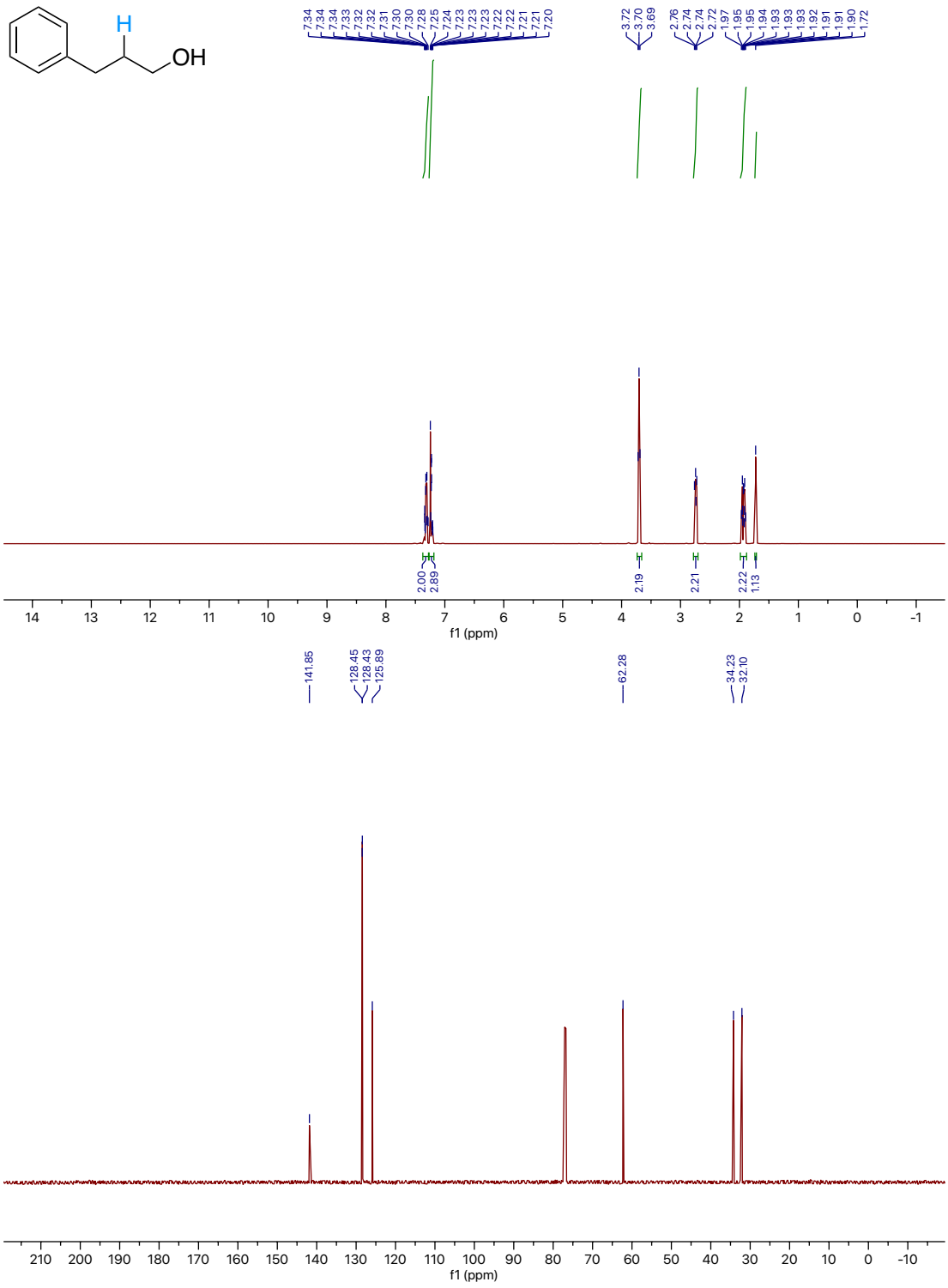
2-(naphthalen-1-yl)ethan-1-ol (17f): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$).



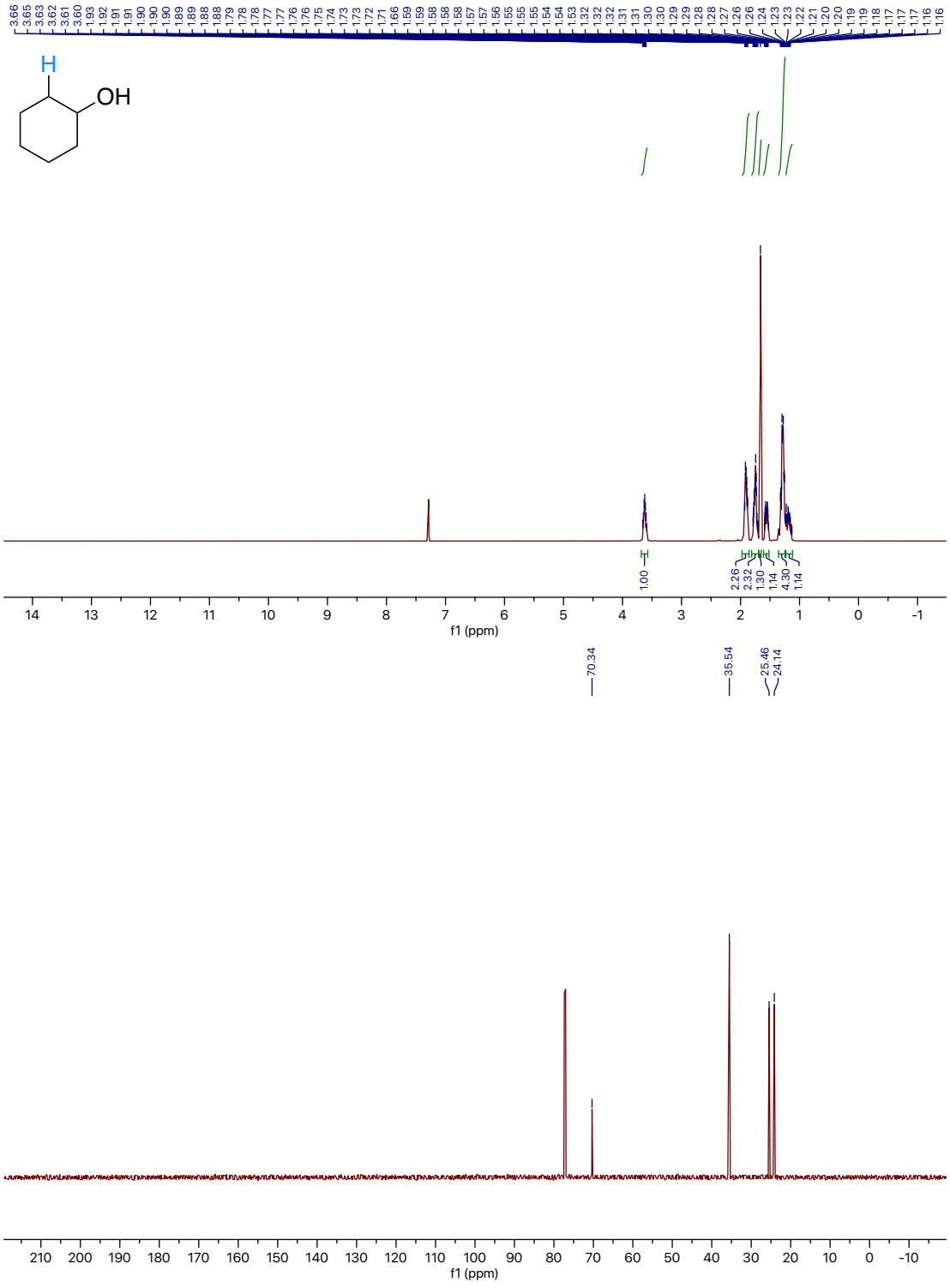
2-(2-methoxyphenyl)ethan-1-ol (17g): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$).



3-phenylpropan-1-ol (17h): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$).



cyclohexanol (17i): ^{1}H NMR (400 MHz, $CDCl_3$), ^{13}C NMR (101 MHz, $CDCl_3$).



Tropylium Promoted Hydroboration Reactions: Mechanistic Insights via Experimental and Computational Studies

Supporting Information: Part 2 - Computational

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Computational Methods

DFT calculations were carried out using the *Gaussian 16* program.[1] Geometries of all stationary points were fully optimized using the M06-2X functional[2] with 6-31+G(d,p) basis set. Vibrational frequency calculations at the same level of theory of the geometry optimization were performed at 298.15 K to confirm if each structure is a local minimum or a transition state. To obtain higher accuracy for the electronic energies, single-point energy calculations were carried out using the MN15 functional[3] and 6-311+G(2d,2p) basis set. Solvation energy corrections were calculated using the PCM solvation model[4] in geometry optimizations and single-point energy calculations. To mimic the neat condition, phenylacetylene was used as solvent. Since the solvent parameters for phenylacetylene are not available in *Gaussian 16*, the solvent parameters of toluene were used and the dielectric constant was modified to the value of phenylacetylene ($\varepsilon \approx 2.99$). To account for the standard state change from a 1 atm ideal gas to a 1 M solution, a term of $RT \times \ln(V)$ was added to the free energies of all species.[5]

Born-Oppenheimer molecular dynamics (BOMD)[6] trajectory simulations were carried out using *Gaussian 16* program. BOMD trajectories were propagated using the classical equations of motion with energies and forces computed at the PCM/M06-2X/6-31G(d) level of theory to reduce computational cost. The initial geometries and velocities for BOMD simulations were generated from the normal mode sampling of transition states at 298 K. An initial kinetic energy of 0.6 kcal/mol was added along the transition vector. A time step of about 0.8 fs was used in the trajectory propagation. The Hessian was updated every 12 steps.

Intrinsic reaction coordinate (IRC)[7] calculations were performed at PCM/M06-2X/6-31+G(d,p) level of theory. The stepsize was set to 0.2 $amu^{1/2}$Bohr. Hessian was computed analytically every 10 steps.

Natural of bonding was analyzed by using intrinsic bond orbital (IBO) analysis[8] at MN15/def2-TZVPP level of theory.

References

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Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16 Rev. C.01*, Wallingford, CT, 2016.

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(8) (a) Knizia, G. *J. Chem. Theory Comput.* **2013**, *9*, 4834-4843; (b) Knizia, G.; Klein, J. E. M. N. *Angew. Chem. Int. Ed.* **2015**, *54*, 5518-5522.

Energy profile for the hydroboration of alkyne

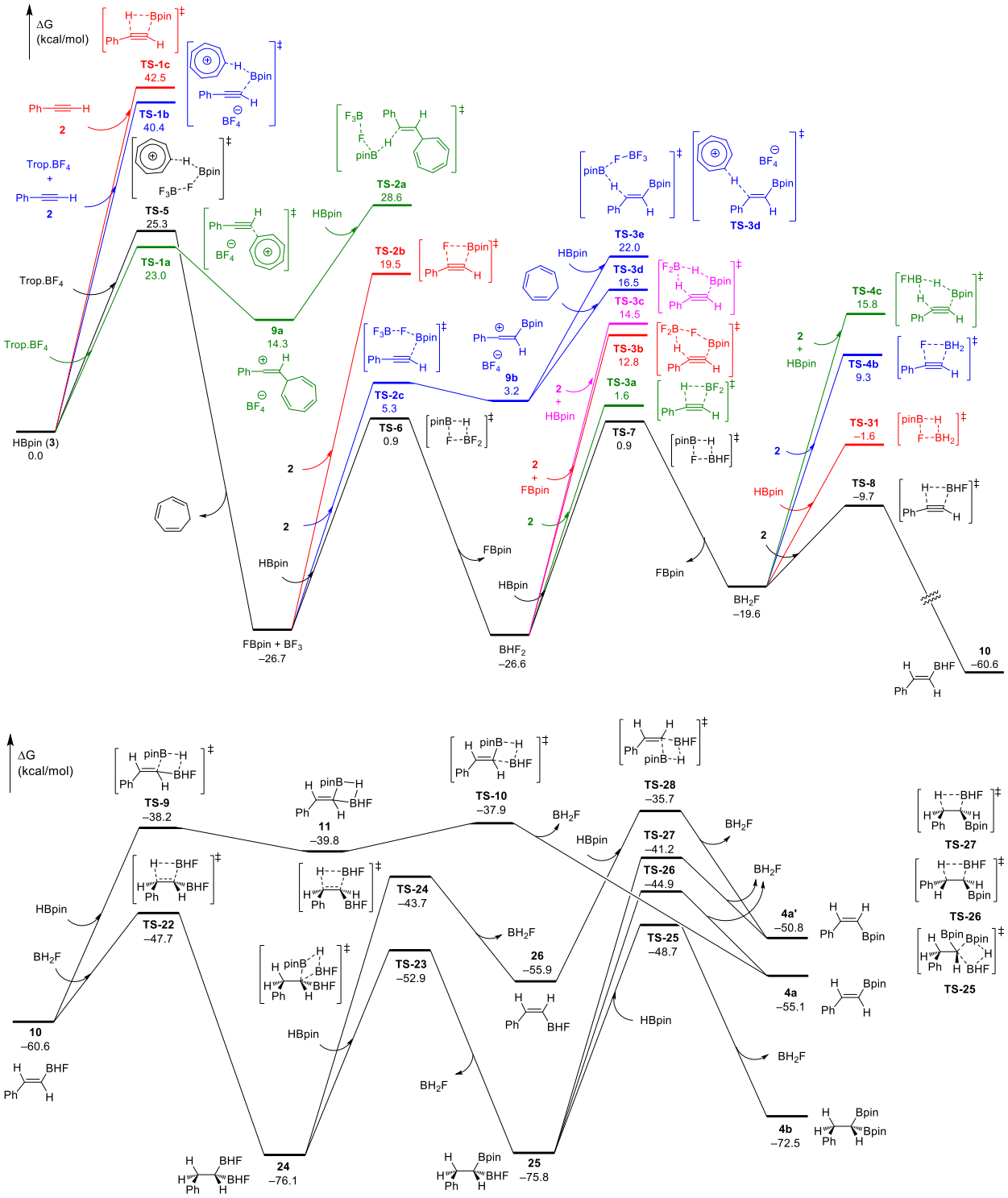

Figure S1. Full computed free energy profile (kcal/mol) for the hydroboration of alkyne **2**. It is important to mention that from **10**, a 1,2-*syn*-addition between **10** and BH_2F can take place giving

intermediate **24** with the activation barrier is calculated to be 9.8 kcal/mol lower in energy than that of **TS-10**. From intermediate **24**, two transborylation steps are found to occur giving *gem*-diboron alkane product **4b**. However, considering the extremely low concentration of the *in situ* BH_2F species, the pathway that forms *gem*-diboron alkane **4b** is considered to be unfavorable. Our assumption is supported by experimental findings that in the hydroboration of alkyne, no boron alkyne product is observed; whereas, with the same reaction condition, the hydroboration of alkene can occur efficiently (see main text). See Figure S8 for the reaction mechanism of the hydroboration of alkene catalyzed by BH_2F species.

BOMD simulations for the formation of 7 from TS-2

Four trajectories are carried out to confirm the formation of carbocation **7** from **TS-2**. Selected snapshots of a representative BOMD trajectory is shown in Figure S2. From the hydride transfer transition state **TS-2**, the associated pair **6** is formed quickly after 27 fs. At 75 fs after **TS-2**, because of the highly reactive of borenium cation $^{+}$Bpin, it reacts with C–C double bond giving carbocation **7'**, which has a positive charge at C1 atom. At 240 fs after **TS-2**, Bpin moiety migrates from C2 atom to C1 atom to form a more stable carbocation **7**, where the positive charge is stabilized by the phenyl group. Our BOMD simulations clearly indicate that from **TS-2**, the carbocation **7** can be formed rapidly after 248 fs (average over four trajectories) without crossing any transition state.

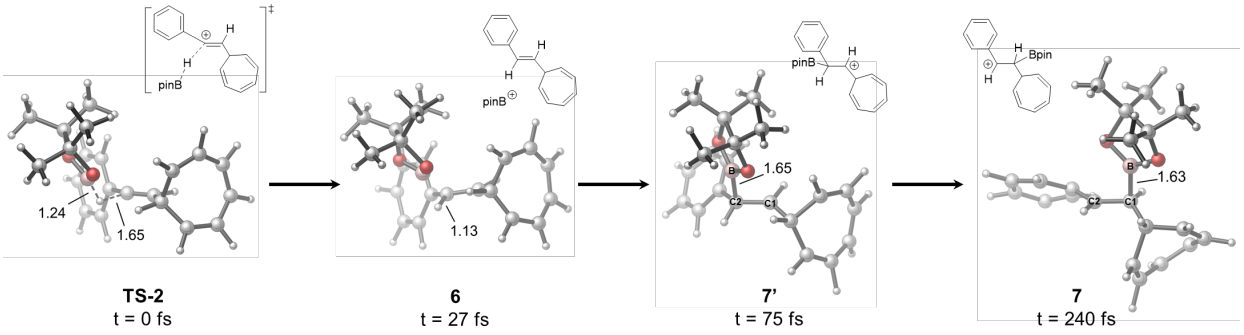

Figure S2. Selected snapshots of a representative BOMD trajectory for the formation of carbocation **7** from **TS-2**. Distances are in Å.

IBO analysis for transient μ-H bridged species 11

IBO analysis shows that the transient μ-H bridged species **11** involves three-center two-electron bonds ("3c-2e", *aka* banana bond). The first 3c-2e bond utilizes the sp^2 hybrid orbital of bridging carbon atom, while the second one employs the 1*s* orbital of bridging hydrogen atom.

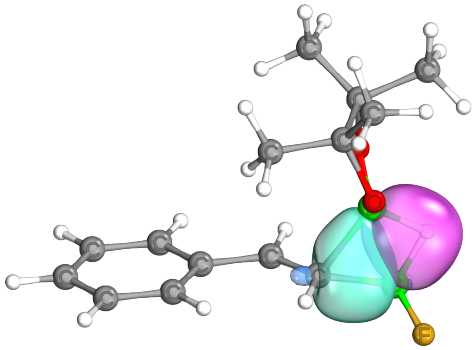

Figure S3. IBO analysis for the transient μ-H bridged intermediate **11**.

Catalytic cycle for the hydroboration of alkyne catalyzed by BHF_2

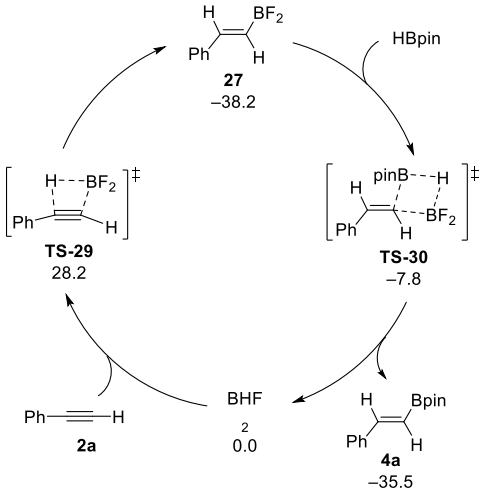

Figure S4. Catalytic cycle for the hydroboration of alkyne catalyzed by BHF_2. All energy values (kcal/mol) are relative to BHF_2. The transborylation of this reaction occurs via a concerted manner rather than a stepwise one. No transient μ-H bridged species in the transborylation could be located during optimization.

Energy profile for the hydroboration of alkyne catalyzed by BH_3

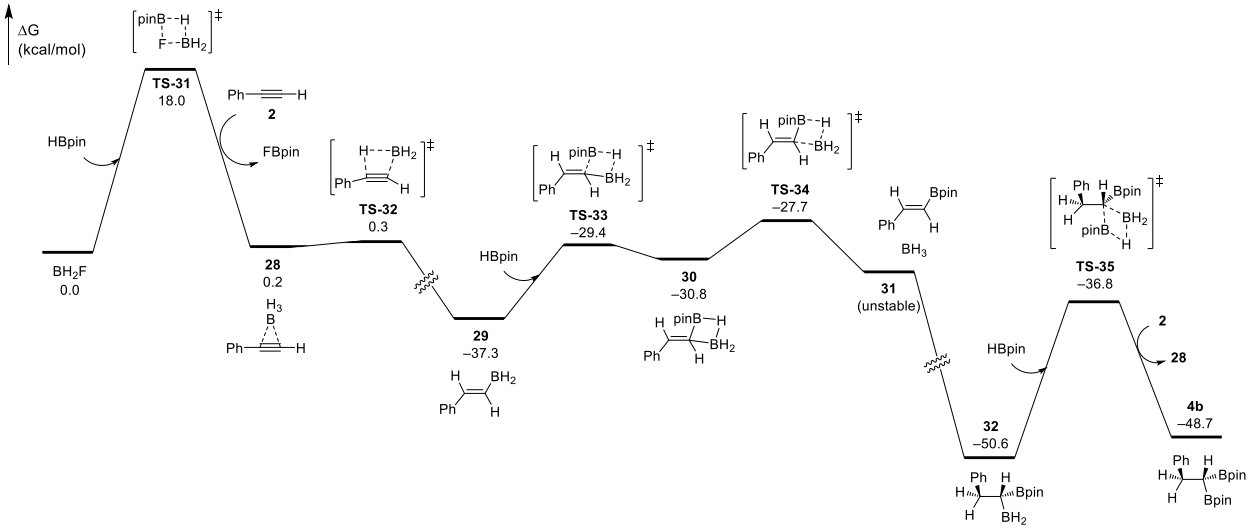

Figure S5. Free energy profile (kcal/mol) for the hydroboration of alkyne catalyzed by BH_3. See Figure S6 and Figure S7 for the formation of **32** from **TS-34** suggested from IRC calculation and BOMD simulations.

IRC calculation for the formation of intermediate 32 from TS-34

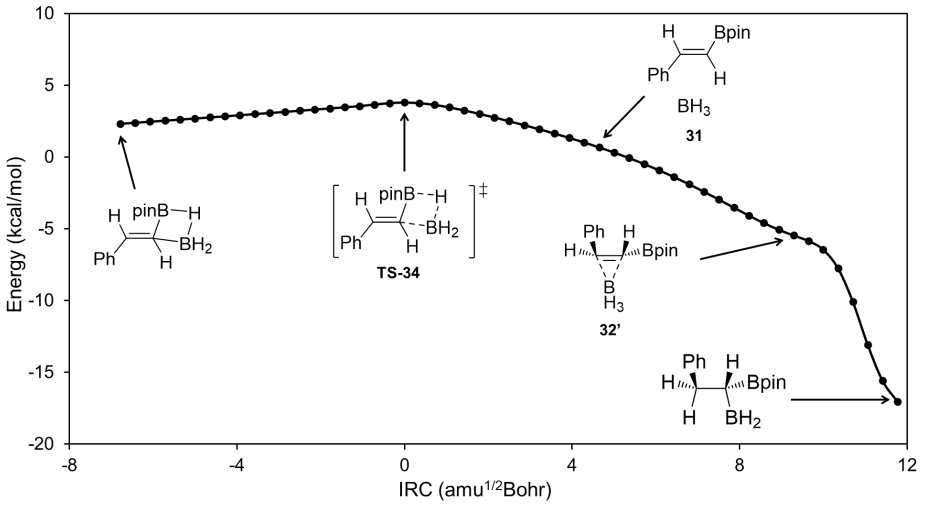

Figure S6. Potential energy surface from IRC calculation at PCM/M06-2X/6-31+G(d,p) level of theory. All energy values (kca/mol) are relative to intermediate **30**. IRC calculation indicates that intermediate **32** is formed from **TS-34** without crossing any barrier.

BOMD simulations for the formation of intermediate 32 from TS-34

Four trajectories are carried out to unravel the formation of alkane intermediate **32** from **TS-34**. Selected snapshots of a representative BOMD trajectory is shown in Figure S7. From the transborylation transition state **TS-34**, the associated pair between **4a** and BH_3 is quickly formed after 75 fs. At 255 fs after **TS-34**, the **4a**–BH_3 complex intemediate **32'** is formed, which rapidly transform to alkane intermediate **32** after only 20 fs. Our BOMD simulations clearly indicate that from **TS-34**, the alkane intermediate **32** can be formed rapidly after 271 fs (average over four trajectories) without crossing any transition state.

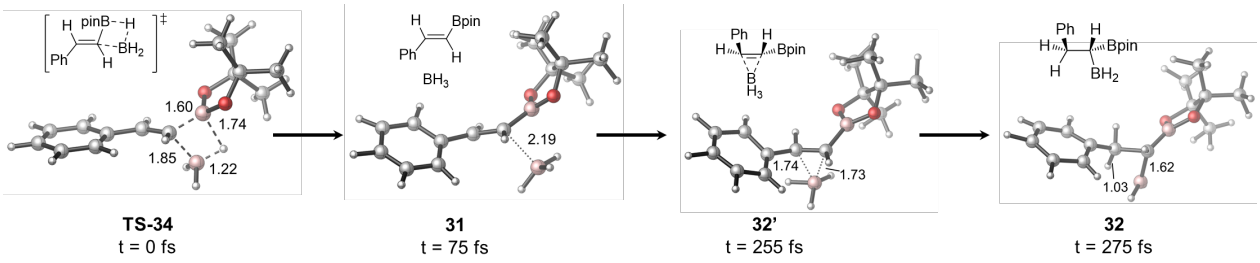

Figure S7. Selected snapshots of a representative BOMD trajectory for the formation of carbocation **32** from **TS-34**. Distances are in Å.

Catalytic cycle for the hydroboration of alkene

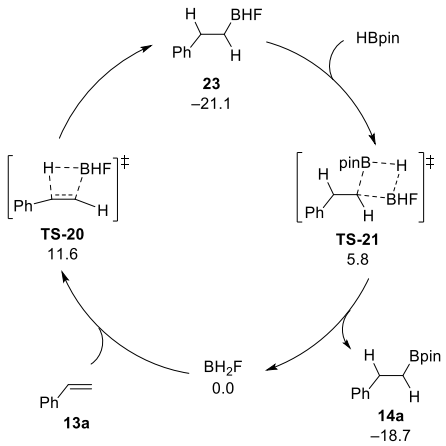

Figure S8. Catalytic cycle for the hydroboration of alkene catalyzed by BH_2F. All energy values (kcal/mol) are relative to BH_2F. The transborylation of this reaction occurs in a concerted manner

rather than a stepwise one. No transient μ-H bridged species in the transborylation could be located during optimization.

The formation of BH_2F and B_2pin_3 from FBpin for the reaction with Trop.BF_4

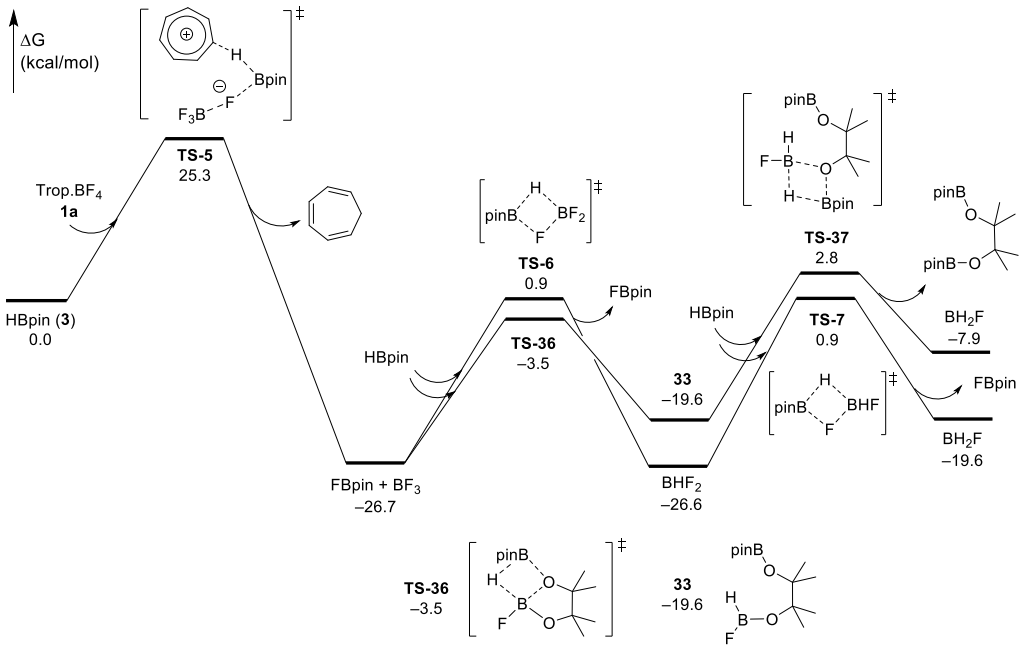

Figure S9. For the reaction with Trop.BF_4 **1a**, it is also possible to form BH_2F via an alternative pathway, i.e. with production B_2pin_3. However, the activation barrier to form B_2pin_3 is 29.5 kcal/mol relative to FBpin (+BF_3). This barrier is 1.9 kcal/mol higher in energy than the formation of BH_2F as depicted in Figure 3a (in the main text).

Energy and Cartesian Coordinates

HBpin

M06-2X/6-31+G(d,p) SCF energy (au)	-411.71507595
M06-2X/6-31+G(d,p) enthalpy (au)	-411.51266395
M06-2X/6-31+G(d,p) free energy (au)	-411.55566995
MN15/6-311+G(2d,2p) SCF energy (au)	-411.52019312
MN15/6-311+G(2d,2p) enthalpy (au)	-411.31778112
MN15/6-311+G(2d,2p) free energy (au)	-411.36078712

Cartesian coordinates

ATOM	X	Y	Z
O	-0.791938	0.305245	0.260865
C	-0.578402	1.739659	0.205035
C	-1.907297	2.247685	-0.445935
O	-2.859335	1.232778	-0.033438
B	-2.143788	0.100431	0.241676
H	-2.645990	-0.955052	0.443144
C	-0.399369	2.214163	1.645747
H	0.434391	1.667859	2.093805
H	-0.177040	3.284139	1.685311
H	-1.297169	2.019792	2.240012
C	0.675626	2.021956	-0.605528
H	0.806827	3.100914	-0.737433
H	1.547952	1.633006	-0.073976
H	0.631722	1.548992	-1.587948
C	-2.381663	3.602843	0.052003
H	-1.632222	4.370809	-0.165802
H	-3.309225	3.874524	-0.458581
H	-2.571134	3.589667	1.126582
C	-1.872031	2.222946	-1.972731
H	-2.883055	2.396401	-2.349782
H	-1.214066	3.002623	-2.366527
H	-1.528106	1.252886	-2.343898

Alkyne 2

M06-2X/6-31+G(d,p) SCF energy (au)	-308.27700745
M06-2X/6-31+G(d,p) enthalpy (au)	-308.15914545
M06-2X/6-31+G(d,p) free energy (au)	-308.19685545
MN15/6-311+G(2d,2p) SCF energy (au)	-308.08773081
MN15/6-311+G(2d,2p) enthalpy (au)	-307.96986881
MN15/6-311+G(2d,2p) free energy (au)	-308.00757881

Cartesian coordinates

ATOM	X	Y	Z
C	-2.200083	-0.293040	0.000041
C	-0.808451	-0.297333	0.000634
C	-0.102469	0.914695	0.000158
C	-0.808399	2.126756	-0.000922
C	-2.200029	2.122524	-0.001509
C	-2.898377	0.914756	-0.001031
H	-2.740227	-1.234283	0.000415
H	-0.258913	-1.232951	0.001470
H	-0.258816	3.062349	-0.001285
H	-2.740136	3.063788	-0.002341

H	-3.983678	0.914781	-0.001487
C	1.334809	0.914666	0.000781
C	2.543936	0.914624	0.001329
H	3.612093	0.914461	0.001858

Trop.BF_4

M06-2X/6-31+G(d,p) SCF energy (au)	-695.13030169
M06-2X/6-31+G(d,p) enthalpy (au)	-694.98262869
M06-2X/6-31+G(d,p) free energy (au)	-695.03431269
MN15/6-311+G(2d,2p) SCF energy (au)	-694.89977532
MN15/6-311+G(2d,2p) enthalpy (au)	-694.75210232
MN15/6-311+G(2d,2p) free energy (au)	-694.80378632

Cartesian coordinates

ATOM	X	Y	Z
C	1.571832	1.348757	0.213466
C	1.060121	0.628970	1.291608
C	0.924034	1.736609	-0.957981
C	-0.226350	0.122039	1.465161
C	-0.397082	1.509716	-1.336480
H	1.525208	2.304743	-1.662080
C	-1.318519	0.209916	0.603707
H	-0.405130	-0.390182	2.405368
C	-1.396006	0.830721	-0.640707
H	-0.689563	1.923142	-2.297451
H	-2.234713	-0.254836	0.956660
H	-2.364320	0.785083	-1.131065
H	2.605726	1.665315	0.309509
H	1.745458	0.466790	2.117853
B	0.010375	3.345788	2.486969
F	-0.689449	3.170540	1.272919
F	-0.369392	4.540676	3.093452
F	-0.275220	2.253100	3.334138
F	1.395278	3.354978	2.211691

Trop.Br

M06-2X/6-31+G(d,p) SCF energy (au)	-2842.60656921
M06-2X/6-31+G(d,p) enthalpy (au)	-2842.47872821
M06-2X/6-31+G(d,p) free energy (au)	-2842.51914821
MN15/6-311+G(2d,2p) SCF energy (au)	-2845.18563096
MN15/6-311+G(2d,2p) enthalpy (au)	-2845.05778996
MN15/6-311+G(2d,2p) free energy (au)	-2845.09820996

Cartesian coordinates

ATOM	X	Y	Z
C	1.143073	1.935658	0.554087
C	0.920622	0.701503	1.348441
C	0.824094	1.805419	-0.889896
C	-0.216752	-0.024366	1.359836
C	-0.335498	1.333505	-1.393081
H	1.587965	2.155751	-1.579316
C	-1.404793	0.221545	0.576292
H	-0.268660	-0.858338	2.055902
C	-1.457370	0.822338	-0.640887
H	-0.463865	1.375014	-2.472218
H	-2.327080	-0.208080	0.959518

H	-2.418214	0.832805	-1.149556
H	2.161577	2.290551	0.684970
H	1.741805	0.395326	1.991495
Br	0.095861	3.476663	1.359181

Cycloheptatriene

M06-2X/6-31+G(d,p) SCF energy (au)	-271.39840998
M06-2X/6-31+G(d,p) enthalpy (au)	-271.26267398
M06-2X/6-31+G(d,p) free energy (au)	-271.29838498
MN15/6-311+G(2d,2p) SCF energy (au)	-271.23256872
MN15/6-311+G(2d,2p) enthalpy (au)	-271.09683272
MN15/6-311+G(2d,2p) free energy (au)	-271.13254372

Cartesian coordinates

ATOM	X	Y	Z
H	-1.547314	1.471190	2.530998
C	-0.712050	0.840120	2.866225
C	-0.527186	1.014452	4.350025
C	-1.051640	-0.603634	2.609640
C	-1.564138	0.899050	5.202945
C	-2.222027	-1.131151	3.019563
H	-0.340723	-1.223896	2.068975
C	-2.896913	0.460219	4.829173
H	-1.406958	1.130151	6.254606
C	-3.189983	-0.444486	3.856294
H	-2.469785	-2.149462	2.726915
H	-3.714639	0.789480	5.466931
H	-4.222616	-0.778818	3.781235
H	0.183716	1.138323	2.319324
H	0.462423	1.252104	4.733119

4a

M06-2X/6-31+G(d,p) SCF energy (au)	-720.07104564
M06-2X/6-31+G(d,p) enthalpy (au)	-719.74536364
M06-2X/6-31+G(d,p) free energy (au)	-719.80716964
MN15/6-311+G(2d,2p) SCF energy (au)	-719.68579036
MN15/6-311+G(2d,2p) enthalpy (au)	-719.36010836
MN15/6-311+G(2d,2p) free energy (au)	-719.42191436

Cartesian coordinates

ATOM	X	Y	Z
C	-1.370351	1.485334	-2.347972
C	-0.328310	0.817849	-1.707520
C	0.694198	1.525735	-1.061101
C	0.647817	2.928514	-1.075363
C	-0.390437	3.596676	-1.714372
C	-1.404457	2.878259	-2.353007
H	-2.152997	0.918327	-2.842158
H	-0.302519	-0.268875	-1.704670
H	1.429228	3.501894	-0.586472
H	-0.410647	4.682067	-1.716774
H	-2.213306	3.403379	-2.851157
C	1.769860	0.768686	-0.397046
C	2.808222	1.260465	0.301607
H	2.917084	2.336683	0.426873
H	1.690888	-0.314985	-0.497239

O	4.910577	0.751964	1.708664
C	5.786017	-0.381719	1.919822
C	4.813136	-1.590342	1.720071
O	3.845151	-1.051648	0.788723
B	3.860560	0.316908	0.935970
C	4.051445	-1.956186	2.992788
H	3.257590	-2.662049	2.735455
H	4.710332	-2.425447	3.728842
H	3.592409	-1.071966	3.445405
C	5.453067	-2.827011	1.111123
H	6.259359	-3.194383	1.754472
H	4.703229	-3.617004	1.016905
H	5.859572	-2.618336	0.120027
C	6.401043	-0.282555	3.306112
H	6.990153	-1.178873	3.526503
H	7.066557	0.583732	3.348684
H	5.634889	-0.166038	4.074571
C	6.872274	-0.309741	0.848097
H	7.381911	0.653768	0.929435
H	7.610271	-1.106578	0.976843
H	6.441816	-0.388213	-0.154814

4a'

M06-2X/6-31+G(d,p) SCF energy (au)	-720.06515150
M06-2X/6-31+G(d,p) enthalpy (au)	-719.73963550
M06-2X/6-31+G(d,p) free energy (au)	-719.80021650
MN15/6-311+G(2d,2p) SCF energy (au)	-719.67999095
MN15/6-311+G(2d,2p) enthalpy (au)	-719.35447495
MN15/6-311+G(2d,2p) free energy (au)	-719.41505595

Cartesian coordinates

ATOM	X	Y	Z
C	0.842071	-2.905909	0.148588
C	1.315086	-1.608630	0.321767
C	1.424362	-0.735292	-0.767871
C	1.007441	-1.182271	-2.029287
C	0.540406	-2.482333	-2.207209
C	0.459854	-3.349868	-1.117948
H	0.760761	-3.568613	1.005008
H	1.586409	-1.259252	1.313352
H	1.064360	-0.505775	-2.878312
H	0.233970	-2.816194	-3.193664
H	0.088443	-4.360982	-1.252338
C	1.922140	0.647089	-0.615985
C	2.898789	1.073461	0.204176
H	3.077176	2.148729	0.215463
H	1.418492	1.378528	-1.249754
O	4.430243	0.723063	2.234657
C	5.471874	-0.199060	2.636940
C	5.007647	-1.531857	1.963535
O	4.287567	-1.051896	0.804488
B	3.856922	0.220203	1.089758
C	5.539565	-0.241530	4.154794
H	6.254904	-1.003030	4.482445
H	5.874984	0.728070	4.532365
H	4.564332	-0.462004	4.592313

C	4.008457	-2.313197	2.815970
H	3.563810	-3.099560	2.199653
H	4.497642	-2.776330	3.677651
H	3.205565	-1.663909	3.179846
C	6.135120	-2.441400	1.503765
H	6.756529	-2.738723	2.354887
H	5.713846	-3.344314	1.053943
H	6.765263	-1.949274	0.760973
C	6.782260	0.332937	2.059653
H	6.939216	1.350879	2.425534
H	7.631001	-0.283660	2.368880
H	6.748232	0.360614	0.966349

4b

M06-2X/6-31+G(d,p) SCF energy (au)	-1131.83557296
M06-2X/6-31+G(d,p) enthalpy (au)	-1131.30343396
M06-2X/6-31+G(d,p) free energy (au)	-1131.38790096
MN15/6-311+G(2d,2p) SCF energy (au)	-1131.25500338
MN15/6-311+G(2d,2p) enthalpy (au)	-1130.72286438
MN15/6-311+G(2d,2p) free energy (au)	-1130.80733138

Cartesian coordinates

ATOM	X	Y	Z
C	-3.295377	1.318814	1.393626
C	-2.265447	2.423992	1.072238
H	-4.154030	1.404967	0.717984
C	-3.769531	1.384870	2.826106
C	-3.205309	0.564191	3.807755
C	-4.749498	2.307492	3.211574
C	-3.605667	0.662638	5.140816
H	-2.440169	-0.152333	3.519153
C	-5.154975	2.408563	4.540723
H	-5.199201	2.951065	2.458349
C	-4.581913	1.585784	5.511900
H	-3.154697	0.016471	5.888664
H	-5.919141	3.127935	4.819737
H	-4.897004	1.662621	6.547923
H	-2.696697	3.420955	1.230828
H	-2.841017	0.340892	1.203606
B	-0.966410	2.328396	1.949571
O	-0.305386	3.404194	2.488186
O	-0.304510	1.140325	2.167157
C	1.017007	2.947033	2.858316
C	0.785859	1.416094	3.079593
C	1.931244	3.243174	1.670086
C	1.479832	3.705705	4.090876
C	1.969034	0.535521	2.711975
C	0.290760	1.088368	4.486649
H	1.885543	4.313064	1.451306
H	2.968252	2.971404	1.887383
H	1.600341	2.702431	0.777183
H	2.435883	3.307695	4.447022
H	1.620159	4.760131	3.838686
H	0.747070	3.639090	4.896959
H	2.842603	0.797391	3.318001
H	1.719468	-0.511284	2.904900

H	2.228391	0.638553	1.656520
H	-0.030154	0.043135	4.512895
H	1.084192	1.226901	5.226823
H	-0.564228	1.714659	4.759622
O	-0.834688	3.250774	-0.924306
C	-0.649903	2.915538	-2.320008
C	-1.027463	1.398879	-2.343043
O	-1.991367	1.309000	-1.265274
B	-1.719939	2.338625	-0.396630
C	-1.618844	3.782287	-3.121786
H	-1.419461	4.832811	-2.895467
H	-1.493439	3.626982	-4.197139
H	-2.656942	3.562922	-2.854356
C	0.786136	3.219777	-2.714265
H	0.981331	2.879636	-3.736676
H	0.954873	4.299123	-2.672821
H	1.494831	2.735211	-2.040065
C	-1.673656	0.922412	-3.632883
H	-0.993206	1.073906	-4.477321
H	-1.895051	-0.145495	-3.558367
H	-2.605765	1.454345	-3.831250
C	0.141549	0.492460	-1.960243
H	-0.236369	-0.520971	-1.803557
H	0.900293	0.466625	-2.747544
H	0.609292	0.829012	-1.028686

TS-1

M06-2X/6-31+G(d,p) SCF energy (au)	-578.85994414
M06-2X/6-31+G(d,p) enthalpy (au)	-578.61543214
M06-2X/6-31+G(d,p) free energy (au)	-578.66972614
MN15/6-311+G(2d,2p) SCF energy (au)	-578.50556919
MN15/6-311+G(2d,2p) enthalpy (au)	-578.26105719
MN15/6-311+G(2d,2p) free energy (au)	-578.31535119

Cartesian coordinates

ATOM	X	Y	Z
C	-2.27349900	-2.09986400	3.61805200
C	-1.64197900	-1.73554300	2.43825700
C	-1.80279400	-0.42475800	1.94207800
C	-2.59486700	0.51056400	2.64038700
C	-3.22154300	0.12994200	3.81752600
C	-3.06124900	-1.17073100	4.30370900
H	-2.15375800	-3.10443900	4.00797700
H	-1.02200600	-2.44054200	1.89468200
H	-2.70121000	1.51738400	2.25077000
H	-3.83325300	0.84215400	4.35977600
H	-3.55212900	-1.46223700	5.22651800
C	-1.16805900	-0.04748100	0.74139200
C	-0.74360500	0.23232900	-0.38523000
H	0.04274100	0.61353700	-1.01568600
C	-2.18851900	-0.24432900	-1.65201600
C	-2.51589800	1.04173800	-2.22370600
C	-1.56534500	-1.28993000	-2.43074100
C	-1.76088600	1.74923900	-3.11413000
C	-0.58850900	-1.12808500	-3.37035700
H	-1.86551300	-2.30386400	-2.18229800

C	-0.51916600	1.36255200	-3.69754700
H	-2.11988900	2.73988200	-3.37915500
C	-0.00295200	0.09449000	-3.81087300
H	-0.17438200	-2.03411000	-3.80399000
H	0.03280000	2.15391800	-4.19704200
H	0.91124700	-0.00346100	-4.38971300
H	-2.94066800	-0.61143800	-0.96093500
H	-3.41933800	1.50965700	-1.84309700

5

M06-2X/6-31+G(d,p) SCF energy (au)	-578.87126762
M06-2X/6-31+G(d,p) enthalpy (au)	-578.62526262
M06-2X/6-31+G(d,p) free energy (au)	-578.67825762
MN15/6-311+G(2d,2p) SCF energy (au)	-578.51848297
MN15/6-311+G(2d,2p) enthalpy (au)	-578.27247797
MN15/6-311+G(2d,2p) free energy (au)	-578.32547297

Cartesian coordinates

ATOM	X	Y	Z
C	-2.07836200	-2.03835600	3.73952700
C	-1.70670000	-1.77720400	2.43672000
C	-1.98881700	-0.49733700	1.87626500
C	-2.64290400	0.50511600	2.65009000
C	-3.00503600	0.22236700	3.95098600
C	-2.72280200	-1.04233400	4.48777100
H	-1.87371900	-3.00499300	4.18436000
H	-1.20320900	-2.52149400	1.82924400
H	-2.84263800	1.47243800	2.20171000
H	-3.50345500	0.96992600	4.55667500
H	-3.00996900	-1.25578400	5.51267000
C	-1.62429800	-0.22494800	0.58117100
C	-1.33066200	0.01142000	-0.63741700
H	-0.36674400	0.43794100	-0.92887500
C	-2.32501600	-0.29248700	-1.80228800
C	-2.64450800	0.98316600	-2.52730100
C	-1.70483400	-1.29579400	-2.73210500
C	-1.71573100	1.74459700	-3.14340000
C	-0.54899300	-1.08292900	-3.39608600
H	-2.20843800	-2.25347000	-2.82686200
C	-0.32212900	1.41071100	-3.32903400
H	-2.03514600	2.70183800	-3.54791100
C	0.19657300	0.15416700	-3.44068600
H	-0.13059000	-1.91295200	-3.95990000
H	0.34899300	2.24281300	-3.52586200
H	1.24429000	0.07398800	-3.71871900
H	-3.23501500	-0.70594800	-1.36815900
H	-3.67936800	1.31211500	-2.50797700

TS-2

M06-2X/6-31+G(d,p) SCF energy (au)	-990.58139877
M06-2X/6-31+G(d,p) enthalpy (au)	-990.13272577
M06-2X/6-31+G(d,p) free energy (au)	-990.20959677
MN15/6-311+G(2d,2p) SCF energy (au)	-990.03506384
MN15/6-311+G(2d,2p) enthalpy (au)	-989.58639084
MN15/6-311+G(2d,2p) free energy (au)	-989.66326184

Cartesian coordinates

ATOM	X	Y	Z
C	-0.01089900	-1.39196400	2.51345400
C	-0.23787500	-0.65660600	1.36156700
C	-1.24383900	0.33362400	1.36188000
C	-2.03537800	0.55875900	2.50988500
C	-1.80021000	-0.18903600	3.65156800
C	-0.79141200	-1.15882800	3.65007400
H	0.76656700	-2.14709500	2.53238900
H	0.34529500	-0.82070100	0.46206900
H	-2.80893400	1.31931800	2.48644300
H	-2.39385100	-0.02217300	4.54303600
H	-0.61199800	-1.74162100	4.54790900
C	-1.43652000	1.13793400	0.21754900
C	-1.20508600	2.17825600	-0.52346000
H	-0.42072100	2.81493900	-0.09460300
C	-1.81144500	2.63910500	-1.83871800
C	-2.18384500	4.10055400	-1.77013500
C	-0.84566700	2.42154500	-2.97905900
C	-1.29208100	5.08590800	-1.54588100
C	0.37144700	2.99764800	-3.04085100
H	-1.16745100	1.73546100	-3.75791400
C	0.14771700	4.93974600	-1.47875900
H	-1.67630200	6.09417500	-1.41087900
C	0.88771100	4.00907700	-2.14122000
H	1.03301500	2.69681300	-3.85006000
H	0.68731700	5.72071300	-0.94898300
H	1.96929500	4.10866100	-2.09668100
H	-2.70996800	2.04758500	-2.01931900
H	-3.23597000	4.34405900	-1.88338300
O	-1.87505700	-1.63695600	-1.07596000
C	-1.49624200	-2.27093900	-2.34807300
C	-2.45349600	-1.56456800	-3.36910700
O	-2.66926300	-0.25555100	-2.73162300
B	-2.42155600	-0.45732200	-1.42214600
H	-2.68835400	0.40769500	-0.57860400
C	-0.02615900	-1.92729400	-2.56579300
H	0.55615100	-2.31231400	-1.72493900
H	0.35125800	-2.38710000	-3.48242100
H	0.12596900	-0.84398600	-2.63002300
C	-1.69526500	-3.76942300	-2.22915700
H	-1.50014800	-4.24594200	-3.19493700
H	-0.99226500	-4.17606000	-1.49844500
H	-2.70910000	-4.01642900	-1.91146200
C	-1.85607500	-1.33800100	-4.74467800
H	-1.61366800	-2.30031200	-5.20637600
H	-2.58433400	-0.82805400	-5.37964500
H	-0.94897800	-0.73298700	-4.69646300
C	-3.82306500	-2.22540900	-3.46941500
H	-4.49020100	-1.57234700	-4.03667900
H	-3.75304200	-3.18488300	-3.98810700
H	-4.25985300	-2.39421100	-2.48078200

7

M06-2X/6-31+G(d,p) SCF energy (au)	-990.66259971
M06-2X/6-31+G(d,p) enthalpy (au)	-990.20869371

M06-2X/6-31+G(d,p) free energy (au)	-990.28313871
MN15/6-311+G(2d,2p) SCF energy (au)	-990.11345647
MN15/6-311+G(2d,2p) enthalpy (au)	-989.65955047
MN15/6-311+G(2d,2p) free energy (au)	-989.73399547

Cartesian coordinates

ATOM	X	Y	Z
C	-1.01312300	-0.96332100	3.73275800
C	-1.64443300	-0.63060800	2.54815500
C	-0.91685600	-0.00117200	1.50383000
C	0.46186500	0.29173200	1.68407900
C	1.08243900	-0.04797000	2.86904100
C	0.34627000	-0.67225100	3.88778900
H	-1.56327200	-1.44362300	4.53329200
H	-2.69844200	-0.84978900	2.40411300
H	1.02550600	0.78205000	0.89781100
H	2.13333800	0.17077200	3.01787300
H	0.84260500	-0.93109900	4.81795400
C	-1.60460200	0.30290000	0.31015400
C	-1.06197500	0.79827500	-0.91751100
H	-0.11494400	1.33336200	-0.81032800
C	-2.06672600	1.50533200	-1.85772500
C	-2.46642400	2.86511900	-1.33215300
C	-1.49964400	1.67027600	-3.24864500
C	-1.59538900	3.87565100	-1.13561200
C	-0.38514600	2.38106800	-3.51619500
H	-2.01197800	1.15861900	-4.05938000
C	-0.20297600	3.90357000	-1.53833300
H	-1.96829800	4.77742700	-0.65487600
C	0.33590100	3.23688800	-2.59371800
H	0.00579400	2.34385400	-4.53085900
H	0.43376400	4.61757800	-1.02176100
H	1.36905400	3.45851000	-2.84965500
H	-2.95578800	0.87122600	-1.92042700
H	-3.51559500	3.01589500	-1.08938900
O	0.63244800	-1.08219600	-1.56766700
C	0.66773000	-2.22144000	-2.49234000
C	-0.83475800	-2.66685900	-2.52020800
O	-1.53493500	-1.40698100	-2.24816400
B	-0.63611800	-0.62098600	-1.61204800
H	-2.66926100	0.05358200	0.29769300
C	1.15379200	-1.67258000	-3.82907600
H	2.13273000	-1.20907500	-3.68623200
H	1.25150100	-2.47298300	-4.56670100
H	0.46710100	-0.91510900	-4.22010200
C	1.62967100	-3.25899000	-1.94379000
H	1.60488800	-4.16068400	-2.56338600
H	2.64628100	-2.85914900	-1.96424800
H	1.38395700	-3.53028400	-0.91575300
C	-1.31387500	-3.21219900	-3.85250000
H	-0.74169400	-4.10531800	-4.12175800
H	-2.36711000	-3.49224700	-3.77354800
H	-1.20965100	-2.47340500	-4.64869400
C	-1.20217300	-3.60794000	-1.37774200
H	-2.28837400	-3.72390000	-1.35154000
H	-0.75127900	-4.59312400	-1.52082600

H	-0.87143000	-3.20781800	-0.41318100

TS-3

M06-2X/6-31+G(d,p) SCF energy (au)	-990.65918552
M06-2X/6-31+G(d,p) enthalpy (au)	-990.20627852
M06-2X/6-31+G(d,p) free energy (au)	-990.27984052
MN15/6-311+G(2d,2p) SCF energy (au)	-990.10900988
MN15/6-311+G(2d,2p) enthalpy (au)	-989.65610288
MN15/6-311+G(2d,2p) free energy (au)	-989.72966488

Cartesian coordinates

ATOM	X	Y	Z
C	-1.38535400	0.50483600	4.12024400
C	-1.83452300	0.11698000	2.86910000
C	-0.96958700	0.16542200	1.75059300
C	0.36697300	0.59242000	1.93082100
C	0.81182100	0.97220400	3.18837800
C	-0.06266800	0.93388600	4.27781600
H	-2.05220300	0.47255900	4.97454500
H	-2.85821200	-0.22041600	2.73355300
H	1.05649500	0.59365600	1.09337100
H	1.83934200	1.28917300	3.32853400
H	0.29235100	1.22913800	5.26001800
C	-1.49166900	-0.18701600	0.46824800
C	-0.88730300	0.03848900	-0.77126200
H	0.18231400	0.25097400	-0.77846500
C	-1.52462600	1.83746000	-1.11550700
C	-0.85086900	2.72762100	-0.17917100
C	-1.27490500	2.02322500	-2.54366000
C	0.45711900	3.10407900	-0.22188700
C	-0.06825000	2.21441300	-3.13789800
H	-2.14875800	1.92665000	-3.18334800
C	1.43597000	2.76408800	-1.21009600
H	0.81451300	3.70838200	0.60844300
C	1.20426900	2.36403100	-2.49705700
H	-0.05709600	2.23935700	-4.22473700
H	2.47111000	2.94461500	-0.93315800
H	2.07355000	2.25394000	-3.13946800
H	-2.58367700	1.71741000	-0.90422000
H	-1.44421400	3.07097600	0.66445200
O	-0.65840900	-1.36869800	-2.92348400
C	-1.53678400	-1.86514400	-3.97624400
C	-2.92339500	-1.94709200	-3.24674800
O	-2.78981200	-0.92721700	-2.21086500
B	-1.45129000	-0.76795900	-1.99771500
H	-2.51007300	-0.58063700	0.45717600
C	-1.50552900	-0.83172500	-5.09787300
H	-0.46829900	-0.67892300	-5.40717300
H	-2.08101100	-1.17293800	-5.96246900
H	-1.91292300	0.12802400	-4.76794900
C	-1.00093100	-3.19839300	-4.46880600
H	-1.69606200	-3.64189600	-5.18819900
H	-0.04237000	-3.04286000	-4.96994900
H	-0.85099100	-3.89873700	-3.64572300
C	-4.12144100	-1.60781500	-4.11590400
H	-4.19553900	-2.31306400	-4.94955200

H	-5.03556400	-1.68445300	-3.52187600
H	-4.05372200	-0.59518300	-4.51723400
C	-3.14201900	-3.27339400	-2.52438500
H	-4.03386000	-3.19190700	-1.89812100
H	-3.29275200	-4.08843100	-3.23702000
H	-2.29061800	-3.52322500	-1.88378900

TS-4

M06-2X/6-31+G(d,p) SCF energy (au)	-990.64865762
M06-2X/6-31+G(d,p) enthalpy (au)	-990.19581462
M06-2X/6-31+G(d,p) free energy (au)	-990.26998462
MN15/6-311+G(2d,2p) SCF energy (au)	-990.09808953
MN15/6-311+G(2d,2p) enthalpy (au)	-989.64524653
MN15/6-311+G(2d,2p) free energy (au)	-989.71941653

Cartesian coordinates

ATOM	X	Y	Z
C	-1.70714700	-1.59636100	3.69468200
C	-2.08363900	-1.06606000	2.47014800
C	-1.17155200	-0.30690400	1.70085200
C	0.14429400	-0.12155000	2.18529800
C	0.51664000	-0.66621900	3.40353100
C	-0.40638700	-1.39558800	4.16164900
H	-2.41683700	-2.16671800	4.28319200
H	-3.09211300	-1.22052000	2.09736000
H	0.86978400	0.43085000	1.59920200
H	1.52811800	-0.52651400	3.76951500
H	-0.10679400	-1.81368400	5.11728300
C	-1.64729700	0.21350500	0.45149900
C	-1.01924700	1.02109100	-0.50196400
H	-1.71846300	1.35627300	-1.27192100
C	-0.06564100	-0.31354900	-1.58771600
C	-1.02489400	-1.27593400	-2.10997600
C	0.69518900	0.48694500	-2.54099500
C	-1.89552600	-1.08986500	-3.13621000
C	0.21687700	1.09532000	-3.65965500
H	1.73329000	0.66267800	-2.27139400
C	-2.04383800	0.07081200	-3.96574100
H	-2.59455000	-1.89868400	-3.33228600
C	-1.11186600	1.04206600	-4.19347200
H	0.91758700	1.71977100	-4.20873000
H	-2.96203900	0.12465900	-4.54401900
H	-1.35608000	1.79618400	-4.93620600
H	0.55562600	-0.71180300	-0.78782000
H	-1.09217700	-2.21231200	-1.55995900
O	-0.19546700	3.42827400	-0.28789700
C	1.07149300	4.14850800	-0.25226100
C	2.02424500	3.11148500	0.43321200
O	1.41075100	1.84112800	0.05713200
B	0.09685200	2.10242900	-0.21345400
H	-2.64072200	-0.14988400	0.18258200
C	1.44506600	4.43712100	-1.70306000
H	0.63741600	5.00779500	-2.16777700
H	2.36622000	5.02222100	-1.76432700
H	1.58061800	3.50911800	-2.26765300
C	0.87794800	5.44175100	0.51992200

H	1.83443600	5.96115700	0.63383500
H	0.19776500	6.09567400	-0.03121300
H	0.45540600	5.25900500	1.50912600
C	3.45656600	3.12808500	-0.07087000
H	3.91245400	4.10509900	0.11708800
H	4.04008100	2.37199300	0.46052500
H	3.50793200	2.91660000	-1.14044500
C	1.98683600	3.17758300	1.95741200
H	2.52070700	2.31366300	2.36329300
H	2.47433000	4.08505100	2.32260600
H	0.95867000	3.15758000	2.33302200

TS-5

M06-2X/6-31+G(d,p) SCF energy (au)	-1106.82021665
M06-2X/6-31+G(d,p) enthalpy (au)	-1106.47131965
M06-2X/6-31+G(d,p) free energy (au)	-1106.54546765
MN15/6-311+G(2d,2p) SCF energy (au)	-1106.39603128
MN15/6-311+G(2d,2p) enthalpy (au)	-1106.04713428
MN15/6-311+G(2d,2p) free energy (au)	-1106.12128228

Cartesian coordinates

ATOM	X	Y	Z
O	-2.195287	-0.794362	-2.186495
C	-3.112430	-0.930428	-3.285938
C	-4.454190	-0.413561	-2.667731
O	-4.330830	-0.834526	-1.294396
B	-2.956169	-0.883570	-1.013893
H	-2.698185	-1.867999	-0.237724
C	-3.505812	-2.777812	0.809526
C	-4.398173	-3.541179	-0.011902
C	-2.408124	-3.328290	1.545819
C	-4.119589	-4.700878	-0.683202
C	-1.672422	-4.439744	1.236167
H	-2.090849	-2.739724	2.401302
C	-2.908109	-5.443160	-0.705961
H	-4.917918	-5.093158	-1.308871
C	-1.833013	-5.328759	0.139666
H	-0.830940	-4.651654	1.890329
H	-2.862195	-6.243954	-1.438784
H	-1.031949	-6.049097	-0.000557
H	-3.949494	-1.896854	1.263854
H	-5.378845	-3.101406	-0.162003
C	-3.174836	-2.411017	-3.662398
H	-2.162121	-2.758848	-3.883091
H	-3.568858	-3.003414	-2.829938
H	-3.803137	-2.577550	-4.542561
C	-2.599210	-0.110280	-4.459847
H	-1.669162	-0.548172	-4.832620
H	-3.330072	-0.109677	-5.275620
H	-2.398019	0.920424	-4.163160
C	-4.557696	1.111326	-2.686052
H	-4.723517	1.487470	-3.700043
H	-5.401635	1.413016	-2.060069
H	-3.649929	1.570316	-2.284094
C	-5.707533	-1.039228	-3.258685
H	-5.721236	-2.119897	-3.098238

H	-6.592386	-0.608355	-2.781695
H	-5.767657	-0.841391	-4.334142
B	-1.691067	0.158295	1.224881
F	-2.538716	0.304153	-0.068236
F	-2.582377	-0.300263	2.172707
F	-0.723624	-0.765735	0.924469
F	-1.224981	1.414024	1.467394

FBpin

M06-2X/6-31+G(d,p) SCF energy (au)	-511.00358367
M06-2X/6-31+G(d,p) enthalpy (au)	-510.80651867
M06-2X/6-31+G(d,p) free energy (au)	-510.85166467
MN15/6-311+G(2d,2p) SCF energy (au)	-510.79669097
MN15/6-311+G(2d,2p) enthalpy (au)	-510.59962597
MN15/6-311+G(2d,2p) free energy (au)	-510.64477197

Cartesian coordinates

ATOM	X	Y	Z
O	-2.157981	-1.045906	-2.518439
C	-3.188521	-0.483470	-3.374389
C	-4.418135	-0.402532	-2.403116
O	-3.777777	-0.227018	-1.110937
B	-2.521863	-0.739031	-1.241711
C	-3.386535	-1.396041	-4.571984
H	-2.486505	-1.384452	-5.191989
H	-3.579377	-2.424565	-4.262710
H	-4.226750	-1.045302	-5.179767
C	-2.691856	0.889226	-3.820485
H	-1.730066	0.767746	-4.324751
H	-3.394429	1.355788	-4.516292
H	-2.550974	1.557406	-2.965438
C	-5.348540	0.770961	-2.654990
H	-5.766947	0.712007	-3.664845
H	-6.174357	0.741392	-1.939583
H	-4.828759	1.723817	-2.542719
C	-5.206090	-1.707832	-2.332556
H	-4.544624	-2.562084	-2.159011
H	-5.914016	-1.646171	-1.502424
H	-5.765049	-1.880610	-3.256209
F	-1.712592	-0.925337	-0.201973

BF_3

M06-2X/6-31+G(d,p) SCF energy (au)	-324.47137693
M06-2X/6-31+G(d,p) enthalpy (au)	-324.45455893
M06-2X/6-31+G(d,p) free energy (au)	-324.48519293
MN15/6-311+G(2d,2p) SCF energy (au)	-324.41897177
MN15/6-311+G(2d,2p) enthalpy (au)	-324.40215377
MN15/6-311+G(2d,2p) free energy (au)	-324.43278777

Cartesian coordinates

ATOM	X	Y	Z
B	-4.534274	0.655423	0.384711
F	-3.604232	0.138937	1.160205
F	-4.346855	1.834845	-0.169568
F	-5.651794	-0.005083	0.165691

TS-6

M06-2X/6-31+G(d,p) SCF energy (au)	-736.15721966
M06-2X/6-31+G(d,p) enthalpy (au)	-735.93740766
M06-2X/6-31+G(d,p) free energy (au)	-735.99007366
MN15/6-311+G(2d,2p) SCF energy (au)	-735.91367745
MN15/6-311+G(2d,2p) enthalpy (au)	-735.69386545
MN15/6-311+G(2d,2p) free energy (au)	-735.74653145

Cartesian coordinates

ATOM	X	Y	Z
O	-0.837693	0.321462	0.232730
C	-0.599142	1.760440	0.249432
C	-1.912749	2.314362	-0.401056
O	-2.904680	1.341822	0.039704
B	-2.198334	0.193430	0.271602
H	-2.600243	-0.867458	-0.458242
C	-0.439591	2.175260	1.709610
H	0.371016	1.592102	2.153228
H	-0.191100	3.236920	1.791769
H	-1.354117	1.984870	2.279502
C	0.667574	2.048498	-0.535707
H	0.814364	3.129062	-0.631563
H	1.527935	1.631119	-0.006553
H	0.627320	1.606818	-1.532682
C	-2.331501	3.688337	0.091133
H	-1.552875	4.423854	-0.135189
H	-3.249775	3.993652	-0.416876
H	-2.515723	3.686992	1.166570
C	-1.883656	2.269769	-1.926099
H	-2.889836	2.469650	-2.302520
H	-1.203840	3.025062	-2.329649
H	-1.567320	1.286470	-2.287759
B	-3.079050	-1.588673	0.574423
F	-4.399603	-1.720294	0.405484
F	-2.753061	-0.566687	1.598033
F	-2.322561	-2.684204	0.704861

BHF_2

M06-2X/6-31+G(d,p) SCF energy (au)	-225.18216234
M06-2X/6-31+G(d,p) enthalpy (au)	-225.16007134
M06-2X/6-31+G(d,p) free energy (au)	-225.18851734
MN15/6-311+G(2d,2p) SCF energy (au)	-225.14240817
MN15/6-311+G(2d,2p) enthalpy (au)	-225.12031717
MN15/6-311+G(2d,2p) free energy (au)	-225.14876317

Cartesian coordinates

ATOM	X	Y	Z
B	-3.140312	-1.653172	0.790398
F	-4.372751	-1.746752	0.320348
F	-2.339115	-2.690200	0.613584
H	-2.768655	-0.678396	1.349478

TS-7

M06-2X/6-31+G(d,p) SCF energy (au)	-636.86870985
M06-2X/6-31+G(d,p) enthalpy (au)	-636.64324985
M06-2X/6-31+G(d,p) free energy (au)	-636.69376785

MN15/6-311+G(2d,2p) SCF energy (au)	-636.63762978
MN15/6-311+G(2d,2p) enthalpy (au)	-636.41216978
MN15/6-311+G(2d,2p) free energy (au)	-636.46268778

Cartesian coordinates

ATOM	X	Y	Z
O	-0.819716	0.315085	0.187135
C	-0.597268	1.752629	0.233445
C	-1.911577	2.304530	-0.415873
O	-2.896407	1.320089	0.001907
B	-2.184349	0.167777	0.233904
H	-2.576864	-0.892659	-0.436104
C	-0.453199	2.145617	1.701982
H	0.359039	1.562389	2.142869
H	-0.214949	3.207994	1.804144
H	-1.370642	1.937685	2.260837
C	0.672689	2.070497	-0.535657
H	0.807998	3.154186	-0.611950
H	1.533954	1.654118	-0.006836
H	0.645809	1.645672	-1.540481
C	-2.343356	3.669133	0.092728
H	-1.569104	4.414274	-0.117085
H	-3.260598	3.974879	-0.417126
H	-2.535677	3.650639	1.166662
C	-1.870174	2.285045	-1.941728
H	-2.875645	2.481085	-2.322312
H	-1.194662	3.052732	-2.329209
H	-1.542655	1.309871	-2.315185
B	-3.089446	-1.578331	0.637904
F	-4.422609	-1.609896	0.466141
F	-2.701174	-0.535922	1.621957
H	-2.456848	-2.577322	0.726738

BH_2F

M06-2X/6-31+G(d,p) SCF energy (au)	-125.88299547
M06-2X/6-31+G(d,p) enthalpy (au)	-125.85626447
M06-2X/6-31+G(d,p) free energy (au)	-125.88220047
MN15/6-311+G(2d,2p) SCF energy (au)	-125.85441172
MN15/6-311+G(2d,2p) enthalpy (au)	-125.82768072
MN15/6-311+G(2d,2p) free energy (au)	-125.85361672

Cartesian coordinates

ATOM	X	Y	Z
B	-3.157800	-1.645369	0.788001
F	-2.331443	-2.674155	0.622993
H	-2.735988	-0.687425	1.356574
H	-4.262931	-1.751498	0.356840

TS-8

M06-2X/6-31+G(d,p) SCF energy (au)	-434.15866096
M06-2X/6-31+G(d,p) enthalpy (au)	-434.01328696
M06-2X/6-31+G(d,p) free energy (au)	-434.05725896
MN15/6-311+G(2d,2p) SCF energy (au)	-433.94368255
MN15/6-311+G(2d,2p) enthalpy (au)	-433.79830855
MN15/6-311+G(2d,2p) free energy (au)	-433.84228055

Cartesian coordinates

ATOM	X	Y	Z
C	-0.788124	0.920915	0.125336
C	0.153561	1.712688	0.343375
H	0.624304	2.632275	0.631489
B	0.862552	0.192295	0.039366
H	0.002006	-0.483442	-0.538230
C	-2.149501	0.419667	0.052264
C	-2.460145	-0.916398	-0.211521
C	-3.176900	1.349839	0.271842
C	-3.791980	-1.319549	-0.259850
H	-1.664460	-1.637013	-0.370909
C	-4.503721	0.939483	0.215977
H	-2.927166	2.385112	0.481147
C	-4.813919	-0.395417	-0.049329
H	-4.029337	-2.358680	-0.461619
H	-5.296220	1.661761	0.381285
H	-5.850459	-0.713836	-0.089676
F	1.318135	-0.407147	1.218393
H	1.656586	0.414638	-0.830513

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M06-2X/6-31+G(d,p) SCF energy (au)	-434.24575538
M06-2X/6-31+G(d,p) enthalpy (au)	-434.09518538
M06-2X/6-31+G(d,p) free energy (au)	-434.14032038
MN15/6-311+G(2d,2p) SCF energy (au)	-434.02883092
MN15/6-311+G(2d,2p) enthalpy (au)	-433.87826092
MN15/6-311+G(2d,2p) free energy (au)	-433.92339592

Cartesian coordinates

ATOM	X	Y	Z
B	-2.740889	-0.182814	-1.115762
C	-1.222693	0.253144	4.930355
C	-1.937127	0.055562	3.751180
C	-1.321939	0.213889	2.501353
C	0.033619	0.576725	2.459526
C	0.747706	0.774141	3.635282
C	0.122328	0.613208	4.874507
H	-1.714752	0.126297	5.889263
H	-2.986247	-0.225398	3.794032
H	0.532786	0.704962	1.504359
H	1.795201	1.054357	3.588684
H	0.683603	0.768146	5.790487
C	-2.121988	-0.006738	1.288327
C	-1.725567	0.096024	0.002073
H	-0.698277	0.373390	-0.231473
H	-3.159878	-0.286569	1.478838
F	-2.370874	-0.087353	-2.402044
H	-3.876406	-0.489583	-0.900440

TS-9

M06-2X/6-31+G(d,p) SCF energy (au)	-845.94343944
M06-2X/6-31+G(d,p) enthalpy (au)	-845.58935144
M06-2X/6-31+G(d,p) free energy (au)	-845.65457044
MN15/6-311+G(2d,2p) SCF energy (au)	-845.53442222
MN15/6-311+G(2d,2p) enthalpy (au)	-845.18033422

MN15/6-311+G(2d,2p) free energy (au)	-845.24555322

Cartesian coordinates

ATOM	X	Y	Z
B	-2.78928500	-0.39419500	-0.97857400
C	-0.81717000	0.14502500	5.05705900
C	-1.65487400	0.03646800	3.95046800
C	-1.14570500	0.16432300	2.64923800
C	0.22704500	0.41327800	2.47992900
C	1.06237000	0.52246800	3.58432800
C	0.54327900	0.38763100	4.87511700
H	-1.22458300	0.04189100	6.05741600
H	-2.71644700	-0.15082800	4.08797600
H	0.64125900	0.52601800	1.48287700
H	2.12084800	0.71502400	3.44256100
H	1.19989100	0.47406400	5.73501400
C	-2.07209200	0.04489700	1.52264000
C	-1.77953100	0.12406400	0.20572000
H	-0.74708700	0.26197500	-0.11279800
H	-3.11897100	-0.07965900	1.80359900
F	-2.08430400	-0.85572900	-2.07389800
H	-3.73230300	-1.02255600	-0.59450100
O	-1.94037600	2.35143800	-1.25490500
C	-2.05236200	3.59423000	-0.52067800
C	-3.52343100	3.52799700	0.00941200
O	-3.71602700	2.10831000	0.21571000
B	-2.80964900	1.47040200	-0.62918200
H	-3.42598800	0.69066100	-1.47043800
C	-1.01610700	3.56875800	0.60337300
H	-0.03036400	3.38731800	0.16575600
H	-0.99019500	4.52306500	1.13721100
H	-1.22520800	2.77307300	1.32473300
C	-1.77265800	4.74461200	-1.47339800
H	-1.96392700	5.70266700	-0.97893500
H	-0.72316200	4.71962000	-1.77857100
H	-2.39335400	4.67786800	-2.36850700
C	-3.75036300	4.24760600	1.32907800
H	-3.50789900	5.31097300	1.23101700
H	-4.80179800	4.16134000	1.61614400
H	-3.13937200	3.81720100	2.12498500
C	-4.54436700	3.98167700	-1.03240100
H	-5.54509700	3.72170700	-0.67800300
H	-4.50055000	5.06328400	-1.18941800
H	-4.37606200	3.48089400	-1.99076300

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M06-2X/6-31+G(d,p) SCF energy (au)	-845.94344278
M06-2X/6-31+G(d,p) enthalpy (au)	-845.58842178
M06-2X/6-31+G(d,p) free energy (au)	-845.65698178
MN15/6-311+G(2d,2p) SCF energy (au)	-845.53456626
MN15/6-311+G(2d,2p) enthalpy (au)	-845.17954526
MN15/6-311+G(2d,2p) free energy (au)	-845.24810526

Cartesian coordinates

ATOM	X	Y	Z
B	-2.79448100	-0.38209600	-0.93815700

C	-0.76758500	0.03266600	5.09040900
C	-1.61867400	-0.02601400	3.99043100
C	-1.12016000	0.13254800	2.68834500
C	0.25461100	0.36448300	2.51136600
C	1.10294700	0.42537300	3.60951500
C	0.59490000	0.25781500	4.90088100
H	-1.16603700	-0.09504900	6.09150900
H	-2.68190000	-0.19894800	4.13364000
H	0.65965100	0.50366100	1.51393500
H	2.16279000	0.60600300	3.46259400
H	1.26182600	0.30611000	5.75583200
C	-2.05878000	0.06041500	1.56877200
C	-1.77219100	0.14111000	0.25008100
H	-0.73753100	0.24024700	-0.07484100
H	-3.10770300	-0.02833700	1.85547000
F	-2.07843600	-0.87539800	-2.01288300
H	-3.73571000	-1.00196200	-0.53759100
O	-1.90257400	2.34452000	-1.21657900
C	-2.04017400	3.60193700	-0.51409600
C	-3.51599300	3.52738800	-0.00097100
O	-3.68169100	2.11330100	0.25492000
B	-2.76446200	1.46303200	-0.57418300
H	-3.40093900	0.69740500	-1.43648200
C	-1.01956200	3.61585700	0.62469300
H	-0.02512600	3.44009500	0.20489200
H	-1.01500700	4.58085100	1.13962000
H	-1.22818200	2.83104600	1.35855700
C	-1.76383800	4.73398900	-1.48944700
H	-1.97467900	5.70051600	-1.01998500
H	-0.71031300	4.71687800	-1.78108200
H	-2.37214300	4.63760300	-2.39039800
C	-3.77405200	4.28982200	1.28852300
H	-3.54824300	5.35305500	1.15547700
H	-4.82779400	4.19564100	1.56453900
H	-3.16703200	3.89894100	2.10749800
C	-4.53016200	3.92476900	-1.07221900
H	-5.53061800	3.65564900	-0.72384800
H	-4.50633800	5.00126500	-1.26490200
H	-4.33691000	3.39642400	-2.01095300

TS-10

M06-2X/6-31+G(d,p) SCF energy (au)	-845.94185564
M06-2X/6-31+G(d,p) enthalpy (au)	-845.58825764
M06-2X/6-31+G(d,p) free energy (au)	-845.65443764
MN15/6-311+G(2d,2p) SCF energy (au)	-845.53250362
MN15/6-311+G(2d,2p) enthalpy (au)	-845.17890562
MN15/6-311+G(2d,2p) free energy (au)	-845.24508562

Cartesian coordinates

ATOM	X	Y	Z
B	-2.673784	-0.062375	-0.602589
C	-0.610277	-0.705920	5.283110
C	-1.427346	-0.258743	4.249348
C	-0.909646	-0.070953	2.958068
C	0.448716	-0.342541	2.720547
C	1.262653	-0.789827	3.752498

C	0.735384	-0.971820	5.034593
H	-1.020742	-0.847845	6.277248
H	-2.477555	-0.051142	4.435635
H	0.866443	-0.205676	1.728606
H	2.310044	-0.999042	3.561882
H	1.376184	-1.321958	5.837652
C	-1.812871	0.396949	1.912108
C	-1.518361	0.655027	0.612744
H	-0.504219	0.509024	0.247287
H	-2.842917	0.560963	2.232372
F	-1.852708	-0.797615	-1.431813
H	-3.554357	-0.621432	-0.021450
O	-1.652864	2.705895	-0.982412
C	-2.183915	4.025384	-0.721920
C	-3.617083	3.709792	-0.180342
O	-3.402078	2.463085	0.519197
B	-2.353872	1.832711	-0.151591
H	-3.109464	0.938258	-1.194458
C	-1.288893	4.674187	0.333218
H	-0.260004	4.678526	-0.035883
H	-1.591246	5.705962	0.534871
H	-1.317865	4.108544	1.269827
C	-2.157718	4.830208	-2.011245
H	-2.646836	5.799308	-1.866349
H	-1.121144	5.010657	-2.308323
H	-2.659375	4.298138	-2.821397
C	-4.161694	4.731079	0.804621
H	-4.219364	5.719595	0.337094
H	-5.169038	4.439688	1.114455
H	-3.532633	4.796818	1.694254
C	-4.626948	3.459276	-1.300095
H	-5.533087	3.029130	-0.865290
H	-4.892153	4.391070	-1.807900
H	-4.235663	2.760229	-2.045296

TS-11

M06-2X/6-31+G(d,p) SCF energy (au)	-3254.30075620
M06-2X/6-31+G(d,p) enthalpy (au)	-3253.97148020
M06-2X/6-31+G(d,p) free energy (au)	-3254.03564820
MN15/6-311+G(2d,2p) SCF energy (au)	-3256.68649138
MN15/6-311+G(2d,2p) enthalpy (au)	-3256.35721538
MN15/6-311+G(2d,2p) free energy (au)	-3256.42138338

Cartesian coordinates

ATOM	X	Y	Z
O	-2.326553	-0.922671	-2.148369
C	-3.089305	-0.266587	-3.171367
C	-4.552361	-0.629339	-2.764045
O	-4.476115	-0.640425	-1.331448
B	-3.131486	-0.935091	-0.987222
H	-3.008514	-2.001796	-0.310126
C	-3.790821	-3.083304	0.777717
C	-3.502918	-2.400573	1.988845
C	-5.077432	-3.247554	0.195126
C	-4.269072	-1.458325	2.629817
C	-6.219966	-2.527159	0.437321

H	-5.140963	-4.004973	-0.581606
C	-5.568001	-0.992095	2.312532
H	-3.803378	-0.982400	3.488561
C	-6.426421	-1.464311	1.350110
H	-7.082638	-2.792859	-0.168368
H	-5.935013	-0.176902	2.929337
H	-7.399504	-0.984453	1.295720
H	-3.048630	-3.814188	0.470388
H	-2.514182	-2.578000	2.401524
C	-2.654776	-0.804727	-4.526501
H	-1.629607	-0.485063	-4.734019
H	-2.683110	-1.896229	-4.546078
H	-3.301613	-0.418171	-5.321843
C	-2.817276	1.237361	-3.089976
H	-1.737196	1.397883	-3.148696
H	-3.297665	1.773698	-3.914764
H	-3.171340	1.650482	-2.141635
C	-5.602080	0.382211	-3.199888
H	-5.606321	0.489277	-4.290183
H	-6.593728	0.042094	-2.886009
H	-5.415545	1.358564	-2.748824
C	-4.949073	-2.035030	-3.222681
H	-4.188819	-2.764801	-2.924376
H	-5.896968	-2.303962	-2.746208
H	-5.080837	-2.087812	-4.307819
Br	-2.461023	0.415629	0.535755

BrBpin

M06-2X/6-31+G(d,p) SCF energy (au)	-2982.96430446
M06-2X/6-31+G(d,p) enthalpy (au)	-2982.76883546
M06-2X/6-31+G(d,p) free energy (au)	-2982.81681846
MN15/6-311+G(2d,2p) SCF energy (au)	-2985.51686770
MN15/6-311+G(2d,2p) enthalpy (au)	-2985.32139870
MN15/6-311+G(2d,2p) free energy (au)	-2985.36938170

Cartesian coordinates

ATOM	X	Y	Z
O	-2.098985	-0.839645	-2.533762
C	-3.189928	-0.425718	-3.409554
C	-4.361387	-0.210033	-2.393981
O	-3.646784	0.175295	-1.181605
B	-2.397097	-0.338750	-1.308313
C	-3.431535	-1.516800	-4.436945
H	-2.564221	-1.594465	-5.097258
H	-3.592067	-2.485536	-3.961290
H	-4.306783	-1.272002	-5.047105
C	-2.739755	0.865724	-4.085863
H	-1.803510	0.676878	-4.616441
H	-3.485945	1.211882	-4.806213
H	-2.566802	1.658669	-3.352060
C	-5.327606	0.900544	-2.765026
H	-5.805683	0.679316	-3.724774
H	-6.107291	0.975710	-2.002963
H	-4.820420	1.863875	-2.837070
C	-5.113071	-1.496627	-2.066294
H	-4.422522	-2.303309	-1.802547

H	-5.770134	-1.312336	-1.213006
H	-5.723401	-1.821426	-2.913370
Br	-1.145627	-0.356756	0.137101

TS-12

M06-2X/6-31+G(d,p) SCF energy (au)	-3394.65765419
M06-2X/6-31+G(d,p) enthalpy (au)	-3394.25957519
M06-2X/6-31+G(d,p) free energy (au)	-3394.32796519
MN15/6-311+G(2d,2p) SCF energy (au)	-3397.01507588
MN15/6-311+G(2d,2p) enthalpy (au)	-3396.61699688
MN15/6-311+G(2d,2p) free energy (au)	-3396.68538688

Cartesian coordinates

ATOM	X	Y	Z
O	-4.181743	-0.936302	-1.018359
C	-4.594788	0.109785	-1.983342
C	-3.231037	0.779979	-2.356676
O	-2.290438	-0.312347	-2.202972
B	-2.810610	-1.231415	-1.343286
C	-5.609856	1.045568	-1.355296
H	-6.538182	0.505448	-1.149441
H	-5.239337	1.483443	-0.429159
H	-5.837926	1.844199	-2.068925
C	-5.212156	-0.674920	-3.136113
H	-6.038340	-1.275706	-2.748721
H	-5.600212	0.003588	-3.900170
H	-4.482301	-1.346845	-3.597312
C	-3.162691	1.257761	-3.799529
H	-3.944650	1.999480	-3.990881
H	-2.192955	1.729029	-3.976746
H	-3.277854	0.430137	-4.500928
C	-2.815034	1.903210	-1.410833
H	-2.891798	1.614287	-0.360784
H	-1.777523	2.167765	-1.629826
H	-3.438711	2.787666	-1.570239
Br	-2.167681	-3.060149	-1.394428
O	-3.905500	-1.915075	1.326284
C	-4.954126	-1.493619	2.221119
C	-4.586750	0.007065	2.469918
O	-3.983352	0.392294	1.212826
B	-3.536385	-0.783995	0.608004
C	-4.915352	-2.368253	3.463878
H	-5.192512	-3.391662	3.197001
H	-3.916394	-2.386957	3.903070
H	-5.626492	-2.003165	4.212454
C	-6.288906	-1.663929	1.495159
H	-6.378398	-2.704102	1.171497
H	-7.132446	-1.424826	2.149417
H	-6.337889	-1.026239	0.608118
C	-5.776885	0.915324	2.736167
H	-6.314553	0.588377	3.632407
H	-5.427275	1.938416	2.900939
H	-6.470283	0.919083	1.892352
C	-3.525710	0.181652	3.554448
H	-2.673597	-0.480233	3.373524
H	-3.171028	1.215490	3.535090

H	-3.931324	-0.029094	4.548233
H	-2.357219	-0.816816	0.165004

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M06-2X/6-31+G(d,p) SCF energy (au)	-3394.69509968
M06-2X/6-31+G(d,p) enthalpy (au)	-3394.29508368
M06-2X/6-31+G(d,p) free energy (au)	-3394.36576068
MN15/6-311+G(2d,2p) SCF energy (au)	-3397.04733484
MN15/6-311+G(2d,2p) enthalpy (au)	-3396.64731884
MN15/6-311+G(2d,2p) free energy (au)	-3396.71799584

Cartesian coordinates

ATOM	X	Y	Z
O	-3.749152	-0.321565	-0.889199
C	-4.082423	0.757572	-1.865114
C	-2.941161	0.484447	-2.887100
O	-2.901382	-0.936577	-2.967244
B	-3.090255	-1.543237	-1.709531
C	-4.004852	2.096084	-1.154077
H	-4.873888	2.237418	-0.507647
H	-3.094400	2.180105	-0.556508
H	-4.000908	2.893271	-1.903544
C	-5.467178	0.486152	-2.434176
H	-6.195528	0.416987	-1.623545
H	-5.753156	1.318500	-3.083442
H	-5.480643	-0.440819	-3.009855
C	-3.247878	1.038510	-4.270429
H	-3.415389	2.119687	-4.231739
H	-2.394956	0.847288	-4.926219
H	-4.125824	0.552769	-4.699087
C	-1.586814	0.998586	-2.391372
H	-1.375215	0.651230	-1.375549
H	-0.810852	0.607774	-3.053765
H	-1.541111	2.091233	-2.408427
Br	-4.586156	-2.974180	-1.761269
O	-3.845490	-1.343050	1.273640
C	-4.873791	-1.505239	2.293467
C	-5.727248	-0.202882	2.109046
O	-5.555515	0.075909	0.685523
B	-4.392514	-0.532407	0.337818
C	-4.198010	-1.631016	3.646921
H	-3.636577	-2.567657	3.686839
H	-3.506971	-0.805945	3.827925
H	-4.949093	-1.646485	4.443007
C	-5.642544	-2.776209	1.947678
H	-4.931357	-3.601859	1.866160
H	-6.374920	-3.012619	2.724718
H	-6.157232	-2.682642	0.987278
C	-7.208446	-0.367842	2.395981
H	-7.357460	-0.674944	3.436009
H	-7.719275	0.586383	2.243912
H	-7.660854	-1.112748	1.739790
C	-5.158101	0.999079	2.856637
H	-4.089375	1.122540	2.654842
H	-5.679826	1.900198	2.524068
H	-5.298839	0.893710	3.935632

H	-2.176601	-1.970439	-1.070137

TS-13

M06-2X/6-31+G(d,p) SCF energy (au)	-3806.38646598
M06-2X/6-31+G(d,p) enthalpy (au)	-3805.78316598
M06-2X/6-31+G(d,p) free energy (au)	-3805.87678898
MN15/6-311+G(2d,2p) SCF energy (au)	-3808.54458346
MN15/6-311+G(2d,2p) enthalpy (au)	-3807.94128346
MN15/6-311+G(2d,2p) free energy (au)	-3808.03490646

Cartesian coordinates

ATOM	X	Y	Z
O	-1.125341	-0.524368	0.104713
C	-0.698701	-1.917184	0.097469
C	0.741774	-1.892850	-0.502008
O	1.451630	-1.039446	0.406204
B	-0.597574	0.406891	1.018414
C	-0.735192	-2.494827	1.511468
H	-1.692628	-2.236838	1.973416
H	0.080114	-2.114078	2.128015
H	-0.661965	-3.584681	1.467109
C	-1.693510	-2.654222	-0.786936
H	-1.762180	-2.199385	-1.776458
H	-2.677144	-2.619847	-0.310377
H	-1.403002	-3.701680	-0.899781
C	0.746009	-1.295023	-1.909692
H	0.253736	-1.974471	-2.610223
H	1.774333	-1.152880	-2.245191
H	0.227834	-0.332988	-1.921251
C	1.401595	-3.270285	-0.490412
H	1.482831	-3.656540	0.528473
H	2.408315	-3.182350	-0.909089
H	0.841404	-3.983872	-1.100253
Br	0.141004	2.041493	0.186063
O	-3.253602	1.270290	-0.140852
C	-4.491508	0.674765	-0.598864
C	-4.883805	-0.250075	0.608023
O	-3.596040	-0.580845	1.193714
B	-2.737277	0.421128	0.798869
C	-5.486424	1.788261	-0.885245
H	-5.134490	2.379312	-1.734628
H	-5.601271	2.453032	-0.027686
H	-6.464148	1.367039	-1.141587
C	-4.178911	-0.094451	-1.878075
H	-3.457818	-0.890693	-1.686710
H	-3.739013	0.597381	-2.600920
H	-5.083372	-0.530090	-2.312262
C	-5.589865	-1.535897	0.211424
H	-6.536150	-1.307470	-0.289911
H	-5.808873	-2.123947	1.106654
H	-4.977343	-2.141084	-0.459473
C	-5.680451	0.482418	1.685798
H	-5.181243	1.410011	1.981662
H	-5.754559	-0.163055	2.564688
H	-6.690631	0.721674	1.342194
H	-1.934188	0.932936	1.590433

H	-0.178339	0.142161	2.092575
B	2.689541	-0.511622	0.244436
O	3.237881	0.285778	1.221787
O	3.533403	-0.709288	-0.828173
C	4.424331	0.877454	0.648771
C	4.822368	-0.173920	-0.440105
C	5.457033	1.076124	1.745581
C	4.016445	2.220293	0.045889
C	5.636344	-1.335178	0.126841
C	5.505000	0.406182	-1.667330
H	5.099379	1.832752	2.448871
H	6.404114	1.423650	1.319872
H	5.634712	0.150828	2.296689
H	3.534364	2.819389	0.822790
H	3.299547	2.084821	-0.770068
H	4.886043	2.764648	-0.333896
H	5.157968	-1.753263	1.018066
H	6.649219	-1.017774	0.390168
H	5.703363	-2.120690	-0.630557
H	4.860016	1.121972	-2.179613
H	5.750321	-0.399324	-2.364804
H	6.435271	0.908523	-1.382603

BpinOCH$_2$CH$_2$OBpin

M06-2X/6-31+G(d,p) SCF energy (au)	-1208.53751264
M06-2X/6-31+G(d,p) enthalpy (au)	-1207.96228264
M06-2X/6-31+G(d,p) free energy (au)	-1208.04875764
MN15/6-311+G(2d,2p) SCF energy (au)	-1207.96545782
MN15/6-311+G(2d,2p) enthalpy (au)	-1207.39022782
MN15/6-311+G(2d,2p) free energy (au)	-1207.47670282

Cartesian coordinates

ATOM	X	Y	Z
O	-1.389031	-0.752891	-0.498967
C	-0.818718	-1.906558	0.140008
C	0.673182	-1.912022	-0.318719
O	1.242353	-0.743068	0.294327
C	-0.941120	-1.745339	1.657001
H	-0.447474	-0.827785	1.980459
H	-0.490075	-2.593284	2.178219
H	-1.998422	-1.706377	1.929796
C	-1.564342	-3.161970	-0.318465
H	-2.614993	-3.075334	-0.033289
H	-1.157155	-4.054811	0.161786
H	-1.510357	-3.286878	-1.402977
C	0.796766	-1.787137	-1.839100
H	0.335174	-2.641477	-2.340324
H	1.853938	-1.765954	-2.113846
H	0.312889	-0.871829	-2.183038
C	1.419031	-3.155012	0.170940
H	1.345820	-3.267802	1.255531
H	2.474141	-3.065150	-0.096611
H	1.026601	-4.056200	-0.306148
O	-3.061352	0.881723	-0.903360
C	-4.498030	0.937464	-0.783996
C	-4.767452	-0.015619	0.427674

O	-3.684048	-0.966996	0.309542
B	-2.659412	-0.318107	-0.354608
C	-4.921084	2.379898	-0.558410
H	-4.704304	2.967592	-1.454398
H	-4.384368	2.824217	0.281606
H	-5.996951	2.436341	-0.362553
C	-5.083323	0.408123	-2.092366
H	-4.691400	1.007072	-2.918341
H	-6.174862	0.477820	-2.097604
H	-4.797566	-0.635392	-2.258002
C	-6.089832	-0.761663	0.370526
H	-6.925569	-0.054481	0.354433
H	-6.192597	-1.392734	1.257433
H	-6.149348	-1.398015	-0.514215
C	-4.603769	0.682048	1.776867
H	-3.658498	1.231833	1.823302
H	-4.600855	-0.075450	2.565245
H	-5.424480	1.379557	1.966801
B	2.513297	-0.311574	0.144023
O	3.533697	-0.963263	-0.523765
O	2.920631	0.887025	0.691216
C	4.619820	-0.015848	-0.644980
C	4.357303	0.938463	0.567436
C	4.455264	0.681570	-1.994287
C	5.939883	-0.766477	-0.590685
C	4.784891	2.379475	0.341254
C	4.944694	0.406945	1.873948
H	4.448934	-0.076350	-2.782239
H	5.277295	1.376894	-2.186251
H	3.511182	1.233545	-2.039282
H	6.777995	-0.062064	-0.577783
H	6.037963	-1.398904	-1.477188
H	5.999707	-1.402002	0.294657
H	5.860192	2.432112	0.141187
H	4.573820	2.967274	1.238516
H	4.246558	2.826415	-0.496294
H	4.655638	-0.635520	2.040210
H	4.557125	1.007234	2.701025
H	6.036456	0.472584	1.876139

BH_2Br

M06-2X/6-31+G(d,p) SCF energy (au)	-2597.84259859
M06-2X/6-31+G(d,p) enthalpy (au)	-2597.81756859
M06-2X/6-31+G(d,p) free energy (au)	-2597.84611159
MN15/6-311+G(2d,2p) SCF energy (au)	-2600.57764829
MN15/6-311+G(2d,2p) enthalpy (au)	-2600.55261829
MN15/6-311+G(2d,2p) free energy (au)	-2600.58116129

Cartesian coordinates

ATOM	X	Y	Z
B	-2.053247	-0.534407	0.000002
H	-2.602674	0.513348	-0.000001
H	-2.602674	-1.582162	-0.000001
Br	-0.159092	-0.534407	0.000000

TS-14

M06-2X/6-31+G(d,p) SCF energy (au)	-2906.13532465
M06-2X/6-31+G(d,p) enthalpy (au)	-2905.99108265
M06-2X/6-31+G(d,p) free energy (au)	-2906.03745265
MN15/6-311+G(2d,2p) SCF energy (au)	-2908.67868456
MN15/6-311+G(2d,2p) enthalpy (au)	-2908.53444256
MN15/6-311+G(2d,2p) free energy (au)	-2908.58081256

Cartesian coordinates

ATOM	X	Y	Z
C	-0.790536	0.913012	0.131724
C	0.157801	1.698887	0.349358
H	0.624517	2.621392	0.637226
B	0.853184	0.209012	0.036250
H	0.018190	-0.521322	-0.472027
C	-2.137403	0.386889	0.044470
C	-2.411138	-0.982287	-0.011672
C	-3.184107	1.320427	0.033192
C	-3.731936	-1.415834	-0.079667
H	-1.597595	-1.701040	0.009167
C	-4.498933	0.876253	-0.041675
H	-2.959793	2.381304	0.077730
C	-4.774984	-0.490929	-0.097229
H	-3.944826	-2.478754	-0.118266
H	-5.308900	1.597785	-0.057533
H	-5.802672	-0.834294	-0.154487
H	1.650941	0.376943	-0.833595
Br	1.545677	-0.667188	1.714023

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M06-2X/6-31+G(d,p) SCF energy (au)	-2906.21087428
M06-2X/6-31+G(d,p) enthalpy (au)	-2906.06143728
M06-2X/6-31+G(d,p) free energy (au)	-2906.10776428
MN15/6-311+G(2d,2p) SCF energy (au)	-2908.75354731
MN15/6-311+G(2d,2p) enthalpy (au)	-2908.60411031
MN15/6-311+G(2d,2p) free energy (au)	-2908.65043731

Cartesian coordinates

ATOM	X	Y	Z
B	-2.726619	-0.179146	-1.111170
C	-1.226379	0.251519	4.923050
C	-1.940467	0.054370	3.744102
C	-1.323742	0.213713	2.494682
C	0.032126	0.577118	2.452312
C	0.745238	0.773946	3.628197
C	0.118727	0.611965	4.866916
H	-1.718018	0.124276	5.882027
H	-2.989507	-0.226798	3.785689
H	0.531634	0.706158	1.497584
H	1.792591	1.054521	3.582713
H	0.679660	0.766583	5.783145
C	-2.121653	-0.006149	1.284070
C	-1.719864	0.096498	-0.004496
H	-0.691660	0.372511	-0.232145
H	-3.160121	-0.284632	1.470672
H	-3.856195	-0.482937	-0.905584
Br	-2.200144	-0.043881	-2.953292

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M06-2X/6-31+G(d,p) SCF energy (au)	-3317.92110224
M06-2X/6-31+G(d,p) enthalpy (au)	-3317.56793724
M06-2X/6-31+G(d,p) free energy (au)	-3317.63646424
MN15/6-311+G(2d,2p) SCF energy (au)	-3320.26743542
MN15/6-311+G(2d,2p) enthalpy (au)	-3319.91427042
MN15/6-311+G(2d,2p) free energy (au)	-3319.98279742

Cartesian coordinates

ATOM	X	Y	Z
B	-2.66037300	-0.38031200	-1.03148600
C	-1.04117600	0.64565600	4.99095000
C	-1.78903500	0.33072900	3.85887700
C	-1.20007600	0.32556000	2.58615800
C	0.16575600	0.63412300	2.47460200
C	0.91348900	0.94295400	3.60459000
C	0.31253000	0.95266700	4.86616100
H	-1.51346700	0.64763200	5.96808700
H	-2.84407800	0.08792300	3.95522500
H	0.64773600	0.62150900	1.50172400
H	1.96931300	1.17387400	3.50487200
H	0.90024500	1.19355200	5.74626800
C	-2.03831500	0.00830900	1.42345900
C	-1.70205300	0.12735600	0.12393300
H	-0.70620100	0.47665600	-0.14615500
H	-3.05061300	-0.31852900	1.66517600
H	-3.62165300	-1.01156300	-0.72334300
O	-2.03049000	2.45878000	-1.45149900
C	-2.12055000	3.66512200	-0.63824900
C	-3.59676400	3.60005300	-0.10664800
O	-3.86821100	2.16776800	-0.08686100
B	-2.95830500	1.60861500	-0.93429100
H	-3.35455100	0.64825200	-1.64964600
C	-1.07662000	3.54558900	0.46972600
H	-0.09683700	3.38226300	0.01242300
H	-1.03434400	4.46303000	1.06341600
H	-1.28945800	2.70899500	1.14011800
C	-1.82008000	4.86383100	-1.52147800
H	-1.98748500	5.79197300	-0.96576700
H	-0.77228700	4.83378400	-1.83084000
H	-2.44500300	4.86907700	-2.41580800
C	-3.78438500	4.14801800	1.29777700
H	-3.49779100	5.20403900	1.33368600
H	-4.83684200	4.06855300	1.58156900
H	-3.18698400	3.59436800	2.02478200
C	-4.60624200	4.21873400	-1.06925500
H	-5.61421800	3.97114100	-0.72751400
H	-4.50602500	5.30710800	-1.10049600
H	-4.47859600	3.82463800	-2.08178000
Br	-1.67604900	-1.04824500	-2.62698500

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M06-2X/6-31+G(d,p) SCF energy (au)	-3317.92320728
M06-2X/6-31+G(d,p) enthalpy (au)	-3317.56921428
M06-2X/6-31+G(d,p) free energy (au)	-3317.63897228

MN15/6-311+G(2d,2p) SCF energy (au)	-3320.26944139
MN15/6-311+G(2d,2p) enthalpy (au)	-3319.91544839
MN15/6-311+G(2d,2p) free energy (au)	-3319.98520639

Cartesian coordinates

ATOM	X	Y	Z
B	-2.69853800	-0.28998400	-0.85680700
C	-0.78675500	0.10163900	5.18959400
C	-1.61216400	0.05968200	4.07002000
C	-1.06947700	0.12979700	2.77728500
C	0.32365000	0.24472100	2.62741000
C	1.14571800	0.28707800	3.74545700
C	0.59313200	0.21537100	5.02769800
H	-1.21753900	0.04621800	6.18375300
H	-2.68861000	-0.02764700	4.18976300
H	0.76390100	0.29879200	1.63708800
H	2.22012500	0.37414800	3.62191600
H	1.24069600	0.24764300	5.89814500
C	-1.98330400	0.09796900	1.64060100
C	-1.66514900	0.23531300	0.32929900
H	-0.62438800	0.35117000	0.03790900
H	-3.03828800	0.00024000	1.89900000
H	-3.62518600	-0.90867300	-0.44241500
O	-1.75919000	2.40151100	-1.14229000
C	-2.02773400	3.69941400	-0.56084200
C	-3.51843600	3.55115600	-0.11390900
O	-3.57580600	2.15926400	0.28067000
B	-2.58886900	1.51591800	-0.46511800
H	-3.21547000	0.71698600	-1.42808200
C	-1.07522600	3.88120500	0.62125600
H	-0.04870600	3.76265300	0.26409500
H	-1.17718300	4.87588200	1.06437600
H	-1.25982500	3.13183300	1.39843200
C	-1.78395100	4.76540300	-1.61525700
H	-2.08862900	5.74785600	-1.23976300
H	-0.71827400	4.80541900	-1.85591800
H	-2.33598600	4.54891300	-2.53143700
C	-3.90964300	4.41008500	1.07694100
H	-3.76406800	5.47055000	0.84620900
H	-4.96597200	4.25267000	1.31094700
H	-3.31907200	4.15575700	1.95912400
C	-4.49958500	3.74953600	-1.26787800
H	-5.49181900	3.42505300	-0.94403600
H	-4.55691600	4.80053500	-1.56531500
H	-4.20858000	3.15623900	-2.14042300
Br	-1.63674500	-1.15147600	-2.30447400

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M06-2X/6-31+G(d,p) SCF energy (au)	-3317.92138676
M06-2X/6-31+G(d,p) enthalpy (au)	-3317.56883876
M06-2X/6-31+G(d,p) free energy (au)	-3317.63744476
MN15/6-311+G(2d,2p) SCF energy (au)	-3320.26755413
MN15/6-311+G(2d,2p) enthalpy (au)	-3319.91500613
MN15/6-311+G(2d,2p) free energy (au)	-3319.98361213

Cartesian coordinates

ATOM	X	Y	Z
B	-2.633015	-0.016675	-0.545805
C	-0.696598	-0.697083	5.315030
C	-1.504210	-0.291988	4.258380
C	-0.947765	-0.025627	2.995547
C	0.439821	-0.169030	2.811783
C	1.242957	-0.575931	3.867359
C	0.676745	-0.839858	5.118552
H	-1.133890	-0.902922	6.286089
H	-2.575716	-0.181495	4.400476
H	0.886047	0.030027	1.843272
H	2.311748	-0.689557	3.720792
H	1.310164	-1.158782	5.940251
C	-1.838051	0.384575	1.925367
C	-1.507236	0.678782	0.632872
H	-0.467816	0.614361	0.323769
H	-2.890195	0.463388	2.201947
H	-3.496696	-0.613681	0.013738
O	-1.586329	2.735459	-0.934760
C	-2.152768	4.060078	-0.778403
C	-3.586362	3.749342	-0.232888
O	-3.357525	2.541870	0.536859
B	-2.283573	1.914504	-0.068626
H	-3.076567	0.894475	-1.214257
C	-1.283362	4.800420	0.236361
H	-0.251368	4.802728	-0.123698
H	-1.611289	5.836231	0.362311
H	-1.308512	4.302291	1.210597
C	-2.126684	4.767843	-2.122902
H	-2.638130	5.733701	-2.054629
H	-1.090283	4.948791	-2.419705
H	-2.606141	4.167151	-2.897591
C	-4.157311	4.811114	0.691804
H	-4.229771	5.770985	0.170029
H	-5.161526	4.517611	1.009252
H	-3.537129	4.938185	1.580931
C	-4.582211	3.416395	-1.342542
H	-5.482292	2.992132	-0.890003
H	-4.862003	4.314763	-1.900114
H	-4.172909	2.686518	-2.046690
Br	-1.470112	-1.135252	-1.727730

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M06-2X/6-31+G(d,p) SCF energy (au)	-384.70546954
M06-2X/6-31+G(d,p) enthalpy (au)	-384.55706454
M06-2X/6-31+G(d,p) free energy (au)	-384.59725854
MN15/6-311+G(2d,2p) SCF energy (au)	-384.49401897
MN15/6-311+G(2d,2p) enthalpy (au)	-384.34561397
MN15/6-311+G(2d,2p) free energy (au)	-384.38580797

Cartesian coordinates

ATOM	X	Y	Z
C	-0.585838	0.347930	0.089648
C	0.478429	1.364801	-0.013084
O	-0.752830	1.512609	-0.707680
H	-0.461069	-0.571038	-0.481704

H	1.345697	1.177632	-0.641271
H	0.620064	2.048375	0.821844
C	-1.435196	0.237323	1.309444
C	-1.615390	-1.006693	1.918084
C	-2.042600	1.368500	1.861836
C	-2.382138	-1.118837	3.076977
H	-1.155356	-1.890210	1.482666
C	-2.811788	1.254961	3.017584
H	-1.919773	2.329828	1.370964
C	-2.981342	0.012286	3.629812
H	-2.516278	-2.089724	3.543572
H	-3.284536	2.136735	3.438956
H	-3.582496	-0.074431	4.529356

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M06-2X/6-31+G(d,p) SCF energy (au)	-510.61349275
M06-2X/6-31+G(d,p) enthalpy (au)	-510.43510275
M06-2X/6-31+G(d,p) free energy (au)	-510.48306775
MN15/6-311+G(2d,2p) SCF energy (au)	-510.37543265
MN15/6-311+G(2d,2p) enthalpy (au)	-510.19704265
MN15/6-311+G(2d,2p) free energy (au)	-510.24500765

Cartesian coordinates

ATOM	X	Y	Z
C	-0.428558	1.026773	0.005501
C	0.793102	1.590008	0.607974
O	0.039913	2.355684	-0.357498
H	-1.332497	1.067615	0.608581
H	1.760329	1.278678	0.227833
H	0.750305	1.997177	1.613241
C	-0.389402	0.014109	-1.081329
C	-1.246863	-1.085019	-1.011432
C	0.503452	0.135872	-2.149575
C	-1.201372	-2.069079	-1.997600
H	-1.950959	-1.170219	-0.188272
C	0.539784	-0.843781	-3.137551
H	1.150752	1.005609	-2.218020
C	-0.308447	-1.949604	-3.060816
H	-1.869318	-2.922152	-1.938686
H	1.227135	-0.742293	-3.971037
H	-0.277940	-2.711684	-3.832790
B	-0.808950	3.660105	0.195402
H	-1.153240	3.314889	1.306943
H	0.006894	4.544616	0.122741
F	-1.857237	3.746745	-0.711811

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M06-2X/6-31+G(d,p) SCF energy (au)	-510.57232321
M06-2X/6-31+G(d,p) enthalpy (au)	-510.39699421
M06-2X/6-31+G(d,p) free energy (au)	-510.44257221
MN15/6-311+G(2d,2p) SCF energy (au)	-510.34365911
MN15/6-311+G(2d,2p) enthalpy (au)	-510.16833011
MN15/6-311+G(2d,2p) free energy (au)	-510.21390811

Cartesian coordinates

ATOM	X	Y	Z

C	-0.533856	1.085121	-0.575200
C	0.390862	2.217419	-0.372478
O	-0.435383	3.328846	-0.442032
H	-1.491334	1.226119	-0.075285
H	1.166812	2.263380	-1.145319
H	0.907738	2.121488	0.603061
C	-0.366014	-0.057163	-1.374200
C	-1.430052	-0.997261	-1.428613
C	0.842535	-0.327047	-2.072167
C	-1.284554	-2.173381	-2.141068
H	-2.351004	-0.780242	-0.895727
C	0.978150	-1.505100	-2.779274
H	1.652344	0.393954	-2.055671
C	-0.082779	-2.422150	-2.812732
H	-2.092474	-2.894510	-2.183482
H	1.895812	-1.719760	-3.314664
H	0.030024	-3.342286	-3.377863
B	-0.910176	3.722850	0.921144
H	-1.442030	2.734137	1.458530
H	0.085225	4.050192	1.579876
F	-1.832963	4.779443	0.764965

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M06-2X/6-31+G(d,p) SCF energy (au)	-510.57177141
M06-2X/6-31+G(d,p) enthalpy (au)	-510.39622241
M06-2X/6-31+G(d,p) free energy (au)	-510.44502041
MN15/6-311+G(2d,2p) SCF energy (au)	-510.34048143
MN15/6-311+G(2d,2p) enthalpy (au)	-510.16493243
MN15/6-311+G(2d,2p) free energy (au)	-510.21373043

Cartesian coordinates

ATOM	X	Y	Z
C	-0.411053	1.134317	-0.607684
C	0.515740	2.260570	-0.571138
O	0.201763	3.168474	0.398550
H	-1.326539	1.279520	-0.030665
H	0.424413	2.697232	-1.604034
H	1.565846	1.913860	-0.536716
C	-0.279516	-0.065100	-1.324287
C	-1.363169	-0.982767	-1.295704
C	0.884630	-0.373771	-2.081609
C	-1.290886	-2.166349	-2.008038
H	-2.246428	-0.739684	-0.712635
C	0.943960	-1.554351	-2.791551
H	1.722491	0.315485	-2.095678
C	-0.140741	-2.445624	-2.752428
H	-2.114599	-2.870290	-1.990884
H	1.825475	-1.800223	-3.372087
H	-0.081225	-3.375369	-3.309941
B	0.946294	4.459714	0.227278
H	0.710211	4.897029	-0.906183
H	0.605715	5.208147	1.125457
F	2.360251	4.157101	0.306822

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M06-2X/6-31+G(d,p) SCF energy (au)	-510.57035909

M06-2X/6-31+G(d,p) enthalpy (au)	-510.39570109
M06-2X/6-31+G(d,p) free energy (au)	-510.44316809
MN15/6-311+G(2d,2p) SCF energy (au)	-510.33894312
MN15/6-311+G(2d,2p) enthalpy (au)	-510.16428512
MN15/6-311+G(2d,2p) free energy (au)	-510.21175212

Cartesian coordinates

ATOM	X	Y	Z
C	-0.193183	1.149753	-0.600753
C	0.866889	2.150228	-0.468036
O	0.667462	2.992866	0.592258
H	-1.126826	1.423984	-0.105964
H	0.794661	2.678894	-1.454154
H	1.871206	1.696035	-0.488428
C	-0.166004	-0.057628	-1.315206
C	-1.368237	-0.809841	-1.403185
C	1.006668	-0.526496	-1.970048
C	-1.401160	-1.985218	-2.131008
H	-2.257513	-0.445493	-0.897409
C	0.960703	-1.697032	-2.698191
H	1.933257	0.032125	-1.893453
C	-0.239196	-2.421795	-2.775457
H	-2.315166	-2.562929	-2.202922
H	1.847290	-2.063144	-3.202668
H	-0.262869	-3.345853	-3.344903
B	0.652367	4.447001	0.217814
H	-0.247135	4.631450	-0.611878
H	0.513443	5.089899	1.242711
F	1.915977	4.741115	-0.422277

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M06-2X/6-31+G(d,p) SCF energy (au)	-510.71182942
M06-2X/6-31+G(d,p) enthalpy (au)	-510.53065042
M06-2X/6-31+G(d,p) free energy (au)	-510.58060742
MN15/6-311+G(2d,2p) SCF energy (au)	-510.47317463
MN15/6-311+G(2d,2p) enthalpy (au)	-510.29199563
MN15/6-311+G(2d,2p) free energy (au)	-510.34195263

Cartesian coordinates

ATOM	X	Y	Z
C	-0.941728	1.003293	-0.163643
C	-0.516455	2.308193	-0.830485
O	-0.934120	3.420093	-0.040561
H	-2.022297	1.035891	0.009584
H	-0.995051	2.408771	-1.808646
H	0.570594	2.329325	-0.972087
C	-0.577664	-0.177869	-1.029969
C	-1.448326	-0.618833	-2.032007
C	0.655888	-0.819788	-0.882427
C	-1.096498	-1.678143	-2.866897
H	-2.412431	-0.130389	-2.153983
C	1.012008	-1.880261	-1.714709
H	1.339976	-0.488985	-0.104354
C	0.135922	-2.312100	-2.709888
H	-1.785956	-2.011004	-3.636610
H	1.971426	-2.371082	-1.583362

H	0.410145	-3.139455	-3.356709
B	-0.052927	4.176800	0.630032
H	-0.450681	0.927666	0.812746
H	1.124822	3.994395	0.606472
F	-0.539763	5.187530	1.359303

TS-19

M06-2X/6-31+G(d,p) SCF energy (au)	-922.40797150
M06-2X/6-31+G(d,p) enthalpy (au)	-922.02370350
M06-2X/6-31+G(d,p) free energy (au)	-922.09419750
MN15/6-311+G(2d,2p) SCF energy (au)	-921.97635279
MN15/6-311+G(2d,2p) enthalpy (au)	-921.59208479
MN15/6-311+G(2d,2p) free energy (au)	-921.66257879

Cartesian coordinates

ATOM	X	Y	Z
C	-0.857432	-0.077908	1.471545
B	1.181987	0.004249	2.830612
H	-1.056639	-0.134315	0.399118
F	2.141045	0.862745	3.212859
H	0.650309	-0.694116	3.636315
H	-0.999429	-1.078303	1.894283
O	2.702997	-0.192599	0.199756
C	2.308034	-0.404741	-1.174147
C	1.597066	-1.799948	-1.101847
O	1.047077	-1.807753	0.237581
B	1.781204	-0.880314	0.966481
C	1.362809	0.729054	-1.571399
H	1.873029	1.681403	-1.406767
H	1.080594	0.658973	-2.625819
H	0.454417	0.723705	-0.963295
C	3.552754	-0.375923	-2.047021
H	3.302040	-0.640876	-3.079524
H	3.975592	0.632269	-2.044634
H	4.311864	-1.067833	-1.678443
C	0.463279	-1.983358	-2.097989
H	0.836671	-1.892998	-3.123462
H	0.029152	-2.979553	-1.977789
H	-0.325771	-1.244064	-1.945399
C	2.577923	-2.967482	-1.189612
H	2.047863	-3.889392	-0.936718
H	2.990624	-3.067668	-2.197548
H	3.402501	-2.838378	-0.482335
O	0.519925	0.319834	1.616561
C	-1.758934	0.946444	2.149517
H	-1.507086	0.997651	3.215395
H	-1.563873	1.931943	1.714877
C	-3.208920	0.563087	1.975497
C	-3.944575	1.032480	0.883027
C	-3.825933	-0.309464	2.877724
C	-5.269786	0.641492	0.696344
H	-3.476281	1.714788	0.177354
C	-5.150453	-0.703148	2.694817
H	-3.264099	-0.678178	3.732982
C	-5.875981	-0.227989	1.602541
H	-5.829416	1.018899	-0.153908

H	-5.616712	-1.377337	3.406565
H	-6.908512	-0.530880	1.460446
H	2.124239	-1.156719	2.124921

16a

M06-2X/6-31+G(d,p) SCF energy (au)	-796.52870164
M06-2X/6-31+G(d,p) enthalpy (au)	-796.17278264
M06-2X/6-31+G(d,p) free energy (au)	-796.23913664
MN15/6-311+G(2d,2p) SCF energy (au)	-796.12176251
MN15/6-311+G(2d,2p) enthalpy (au)	-795.76584351
MN15/6-311+G(2d,2p) free energy (au)	-795.83219751

Cartesian coordinates

ATOM	X	Y	Z
C	-1.046016	0.564834	-0.924913
C	0.230734	-0.146574	-0.494388
O	1.198402	0.837672	-0.137015
H	-0.812499	1.225683	-1.766181
H	0.614727	-0.768157	-1.312250
H	0.031132	-0.802278	0.361681
C	-2.109543	-0.432368	-1.314667
C	-2.203638	-0.898499	-2.630053
C	-2.990124	-0.947048	-0.357553
C	-3.155698	-1.853947	-2.982964
H	-1.526994	-0.503877	-3.384585
C	-3.944090	-1.902555	-0.705061
H	-2.929326	-0.590378	0.668112
C	-4.029335	-2.358746	-2.020212
H	-3.217628	-2.201119	-4.009821
H	-4.622730	-2.287660	0.049882
H	-4.773567	-3.100107	-2.293651
O	2.825578	-0.882150	0.344545
C	4.078828	-0.894089	1.069755
C	4.607799	0.562664	0.837599
O	3.381685	1.319223	0.712433
B	2.419601	0.433173	0.289150
H	-1.393175	1.192793	-0.097749
C	3.745874	-1.176294	2.533364
H	3.200313	-2.121532	2.593280
H	4.653322	-1.258610	3.138027
H	3.115918	-0.386244	2.953655
C	4.967012	-1.990063	0.505343
H	5.958374	-1.952617	0.968534
H	4.524613	-2.966200	0.721347
H	5.078907	-1.894301	-0.576042
C	5.424060	1.130079	1.986997
H	6.309664	0.512029	2.167422
H	5.756830	2.140119	1.733761
H	4.835994	1.181782	2.904904
C	5.366110	0.712280	-0.480123
H	5.528120	1.775925	-0.672049
H	6.338118	0.212834	-0.438316
H	4.793815	0.295166	-1.314536

13a

M06-2X/6-31+G(d,p) SCF energy (au)	-309.52220657

M06-2X/6-31+G(d,p) enthalpy (au)	-309.38011957
M06-2X/6-31+G(d,p) free energy (au)	-309.41942357
MN15/6-311+G(2d,2p) SCF energy (au)	-309.33267816
MN15/6-311+G(2d,2p) enthalpy (au)	-309.19059116
MN15/6-311+G(2d,2p) free energy (au)	-309.22989516

Cartesian coordinates

ATOM	X	Y	Z
C	-1.102895	0.976037	0.418497
C	-0.068191	1.805322	0.584157
C	-2.043385	0.955796	-0.719100
C	-3.180420	0.140730	-0.643449
C	-1.846844	1.718458	-1.880382
C	-4.103455	0.095184	-1.686790
H	-3.342220	-0.461016	0.247308
C	-2.766215	1.674665	-2.922873
H	-0.964738	2.344267	-1.975219
C	-3.900224	0.864190	-2.830585
H	-4.978956	-0.541452	-1.605503
H	-2.596604	2.270673	-3.814297
H	-4.614934	0.830691	-3.646730
H	0.181862	2.579365	-0.135455
H	-1.303833	0.235368	1.191534
H	0.562657	1.733581	1.463360

TS-20

M06-2X/6-31+G(d,p) SCF energy (au)	-435.40381151
M06-2X/6-31+G(d,p) enthalpy (au)	-435.23355851
M06-2X/6-31+G(d,p) free energy (au)	-435.27741951
MN15/6-311+G(2d,2p) SCF energy (au)	-435.18838103
MN15/6-311+G(2d,2p) enthalpy (au)	-435.01812803
MN15/6-311+G(2d,2p) free energy (au)	-435.06198903

Cartesian coordinates

ATOM	X	Y	Z
C	-0.967234	0.795194	0.313461
C	-0.045462	1.829845	0.569540
B	0.830481	0.495902	-0.065987
H	0.000700	-0.312535	-0.531255
C	-1.972284	0.843970	-0.781640
C	-3.154019	0.109675	-0.648930
C	-1.764660	1.614125	-1.931109
C	-4.127535	0.157783	-1.644647
H	-3.313381	-0.496909	0.238458
C	-2.731981	1.649849	-2.931118
H	-0.842784	2.175106	-2.054321
C	-3.917105	0.926551	-2.787966
H	-5.045799	-0.408705	-1.528773
H	-2.561433	2.243439	-3.823385
H	-4.671819	0.960716	-3.567032
F	1.557574	-0.118888	0.957091
H	1.374325	0.898286	-1.056170
H	-0.058203	2.715303	-0.053711
H	-1.189292	0.099050	1.119163
H	0.322921	1.952096	1.581468

23

M06-2X/6-31+G(d,p) SCF energy (au)	-435.46002161
M06-2X/6-31+G(d,p) enthalpy (au)	-435.28647561
M06-2X/6-31+G(d,p) free energy (au)	-435.33402661
MN15/6-311+G(2d,2p) SCF energy (au)	-435.24061442
MN15/6-311+G(2d,2p) enthalpy (au)	-435.06706842
MN15/6-311+G(2d,2p) free energy (au)	-435.11461942

Cartesian coordinates

ATOM	X	Y	Z
C	-1.665824	0.875426	0.647371
C	-0.180211	1.196152	0.880636
B	0.810572	0.661003	-0.201531
H	-1.979192	1.285546	-0.318843
C	-2.546943	1.428110	1.741780
C	-2.812246	0.678551	2.892633
C	-3.075967	2.719720	1.651031
C	-3.584353	1.204445	3.927652
H	-2.411564	-0.329383	2.975543
C	-3.848946	3.251081	2.682753
H	-2.882223	3.312992	0.760061
C	-4.105422	2.494143	3.825747
H	-3.782762	0.605642	4.811477
H	-4.254531	4.254247	2.592099
H	-4.709606	2.904454	4.628773
F	0.340133	-0.030821	-1.247353
H	1.993665	0.825265	-0.168685
H	-0.032319	2.283560	0.966239
H	-1.797718	-0.210136	0.582773
H	0.146227	0.808457	1.857829

TS-21

M06-2X/6-31+G(d,p) SCF energy (au)	-847.14893507
M06-2X/6-31+G(d,p) enthalpy (au)	-846.77190507
M06-2X/6-31+G(d,p) free energy (au)	-846.84064507
MN15/6-311+G(2d,2p) SCF energy (au)	-846.73736046
MN15/6-311+G(2d,2p) enthalpy (au)	-846.36033046
MN15/6-311+G(2d,2p) free energy (au)	-846.42907046

Cartesian coordinates

ATOM	X	Y	Z
C	-2.036167	0.182868	1.442043
C	-0.850815	1.041964	0.974795
B	0.602050	-0.007612	0.059621
H	-2.909416	0.416050	0.827710
C	-2.345335	0.424091	2.900635
C	-1.665571	-0.283012	3.898235
C	-3.281071	1.389922	3.283253
C	-1.913378	-0.030931	5.246500
H	-0.938719	-1.040921	3.613244
C	-3.532833	1.646005	4.630786
H	-3.819980	1.942463	2.516659
C	-2.848616	0.935835	5.616653
H	-1.379702	-0.591509	6.007945
H	-4.265598	2.396831	4.910441
H	-3.045057	1.131525	6.666073

F	1.775562	0.629254	0.323353
H	0.365132	-1.048714	0.584952
H	-1.084146	2.113504	1.087684
H	-1.807912	-0.875502	1.280689
O	-0.169156	2.365958	-1.230004
C	-1.058768	2.844225	-2.266434
C	-1.856834	1.553329	-2.641632
O	-1.909142	0.857463	-1.371847
B	-0.776211	1.245457	-0.675798
C	-1.945346	3.919407	-1.639209
H	-1.305651	4.694896	-1.210173
H	-2.600984	4.380248	-2.383599
H	-2.566168	3.501236	-0.839957
C	-0.231318	3.430160	-3.398307
H	-0.876227	3.705383	-4.239423
H	0.279318	4.331328	-3.048671
H	0.522526	2.722000	-3.746521
C	-3.278530	1.798476	-3.118387
H	-3.276134	2.427047	-4.014850
H	-3.749785	0.844595	-3.369969
H	-3.877270	2.285931	-2.346905
C	-1.107846	0.663974	-3.632577
H	-1.604699	-0.308679	-3.678191
H	-1.110594	1.103775	-4.633874
H	-0.068088	0.509129	-3.329131
H	-0.016872	0.949250	1.678350
H	0.266810	0.064915	-1.114186

14a

M06-2X/6-31+G(d,p) SCF energy (au)	-721.28884204
M06-2X/6-31+G(d,p) enthalpy (au)	-720.93980704
M06-2X/6-31+G(d,p) free energy (au)	-721.00439904
MN15/6-311+G(2d,2p) SCF energy (au)	-720.90189547
MN15/6-311+G(2d,2p) enthalpy (au)	-720.55286047
MN15/6-311+G(2d,2p) free energy (au)	-720.61745247

Cartesian coordinates

ATOM	X	Y	Z
C	-2.505777	0.622983	1.536467
C	-1.583954	1.772046	1.093149
H	-3.525466	0.821103	1.188501
C	-2.507626	0.435604	3.034311
C	-1.561475	-0.388385	3.653321
C	-3.423215	1.119272	3.841157
C	-1.528306	-0.526018	5.040322
H	-0.844993	-0.929367	3.038929
C	-3.395415	0.985930	5.228931
H	-4.167296	1.760920	3.374263
C	-2.446438	0.161921	5.833614
H	-0.788418	-1.173367	5.501575
H	-4.117152	1.522334	5.837726
H	-2.424734	0.054003	6.913543
H	-1.889937	2.702501	1.591730
H	-2.186971	-0.306177	1.050914
O	-0.671958	2.856023	-1.085715
C	-1.123946	3.022132	-2.451064

C	-1.973206	1.728128	-2.676616
O	-2.439631	1.431962	-1.337637
B	-1.563685	2.019404	-0.456816
C	-1.962747	4.298371	-2.489994
H	-1.351384	5.130715	-2.132094
H	-2.297497	4.523107	-3.506641
H	-2.840877	4.213042	-1.842631
C	0.085603	3.156308	-3.361750
H	-0.228264	3.187259	-4.410294
H	0.611607	4.087214	-3.134038
H	0.781075	2.326306	-3.225976
C	-3.173191	1.905137	-3.592407
H	-2.848434	2.224366	-4.588121
H	-3.699132	0.952014	-3.692809
H	-3.872102	2.643641	-3.195964
C	-1.132136	0.534834	-3.126163
H	-1.745846	-0.367835	-3.069728
H	-0.786866	0.657978	-4.156564
H	-0.260793	0.400186	-2.478041
H	-0.558907	1.587520	1.440720

TS-1a

M06-2X/6-31+G(d,p) SCF energy (au)	-1003.38888671
M06-2X/6-31+G(d,p) enthalpy (au)	-1003.12269471
M06-2X/6-31+G(d,p) free energy (au)	-1003.19223971
MN15/6-311+G(2d,2p) SCF energy (au)	-1002.96834147
MN15/6-311+G(2d,2p) enthalpy (au)	-1002.70214947
MN15/6-311+G(2d,2p) free energy (au)	-1002.77169447

Cartesian coordinates

ATOM	X	Y	Z
C	-1.451877	-2.301821	3.880030
C	-1.060781	-1.721663	2.682433
C	-1.801832	-0.644824	2.156045
C	-2.930971	-0.155064	2.839622
C	-3.308833	-0.744752	4.037187
C	-2.574373	-1.814187	4.554600
H	-0.889847	-3.134807	4.288164
H	-0.193516	-2.087093	2.142123
H	-3.506632	0.650696	2.400614
H	-4.185912	-0.382437	4.561933
H	-2.881533	-2.274985	5.488134
C	-1.398497	-0.067401	0.932444
C	-1.077696	0.331379	-0.190100
H	-0.512283	0.979538	-0.836277
B	-5.009159	-1.114667	0.218585
F	-4.072097	-2.076258	0.655270
F	-6.150362	-1.152746	1.012407
F	-4.404627	0.164433	0.292266
F	-5.321301	-1.369685	-1.130292
C	-2.094673	-0.815778	-1.498671
C	-2.828070	0.179732	-2.244689
C	-1.015710	-1.572755	-2.085386
C	-2.313990	1.046338	-3.167210
C	-0.076398	-1.113986	-2.964701
H	-0.912955	-2.592930	-1.725210

C	-0.964686	1.143773	-3.613142
H	-3.000842	1.781396	-3.577921
C	0.022705	0.192349	-3.523494
H	0.715154	-1.806367	-3.238741
H	-0.716842	2.040703	-4.174768
H	0.961014	0.422754	-4.020758
H	-2.711711	-1.378235	-0.804513
H	-3.876833	0.262416	-1.975916

9a

M06-2X/6-31+G(d,p) SCF energy (au)	-1003.40358600
M06-2X/6-31+G(d,p) enthalpy (au)	-1003.13611300
M06-2X/6-31+G(d,p) free energy (au)	-1003.20491700
MN15/6-311+G(2d,2p) SCF energy (au)	-1002.98401315
MN15/6-311+G(2d,2p) enthalpy (au)	-1002.71654015
MN15/6-311+G(2d,2p) free energy (au)	-1002.78534415

Cartesian coordinates

ATOM	X	Y	Z
C	-1.564586	-1.827645	4.003853
C	-1.307882	-1.608004	2.666311
C	-1.870167	-0.466974	2.031016
C	-2.711057	0.425351	2.750848
C	-2.956297	0.187021	4.087331
C	-2.384533	-0.933489	4.704061
H	-1.151761	-2.694248	4.506686
H	-0.701449	-2.290125	2.080983
H	-3.155003	1.265956	2.229271
H	-3.599857	0.849814	4.653688
H	-2.591177	-1.119669	5.753683
C	-1.631391	-0.248492	0.698374
C	-1.378141	-0.029302	-0.535399
H	-0.505134	0.573346	-0.802384
B	-4.330437	-2.149610	0.888295
F	-3.107650	-2.663383	0.384982
F	-4.310681	-2.198531	2.287223
F	-4.431438	-0.798260	0.469717
F	-5.397603	-2.884673	0.379070
C	-2.231445	-0.567520	-1.708760
C	-2.754283	0.584184	-2.521690
C	-1.395568	-1.481527	-2.561000
C	-1.968011	1.473311	-3.163245
C	-0.279689	-1.093416	-3.212668
H	-1.705954	-2.522029	-2.600366
C	-0.529523	1.398787	-3.302011
H	-2.448219	2.329947	-3.630686
C	0.218877	0.260530	-3.324163
H	0.308823	-1.860358	-3.711007
H	-0.019595	2.331442	-3.531558
H	1.273054	0.365692	-3.569575
H	-3.058247	-1.119717	-1.272926
H	-3.833264	0.710921	-2.540857

TS-2a

M06-2X/6-31+G(d,p) SCF energy (au)	-1415.10986493
M06-2X/6-31+G(d,p) enthalpy (au)	-1414.64045393

M06-2X/6-31+G(d,p) free energy (au)	-1414.73088893
MN15/6-311+G(2d,2p) SCF energy (au)	-1414.49944960
MN15/6-311+G(2d,2p) enthalpy (au)	-1414.03003860
MN15/6-311+G(2d,2p) free energy (au)	-1414.12047360

Cartesian coordinates

ATOM	X	Y	Z
C	-0.770825	-1.199302	4.532662
C	-0.811382	-1.184595	3.147275
C	-1.533194	-0.161762	2.490654
C	-2.242833	0.815024	3.229119
C	-2.194826	0.782858	4.609814
C	-1.459283	-0.222193	5.254680
H	-0.222353	-1.976333	5.052738
H	-0.326451	-1.948915	2.549827
H	-2.811097	1.573157	2.699438
H	-2.727036	1.526071	5.193231
H	-1.432735	-0.244678	6.340024
C	-1.565247	-0.154409	1.098780
C	-1.252929	-0.024456	-0.141807
H	-0.382284	0.622206	-0.310396
O	-3.619777	-2.206093	2.693951
C	-4.813160	-2.674851	3.356057
C	-5.925817	-1.821534	2.660050
O	-5.389199	-1.622630	1.336778
B	-4.007890	-1.785931	1.429195
H	-3.268644	-1.003065	0.846749
C	-4.664112	-2.426037	4.849377
H	-3.868889	-3.064414	5.245477
H	-4.401781	-1.385104	5.052392
H	-5.593871	-2.668395	5.375305
C	-4.953788	-4.171218	3.080825
H	-4.042246	-4.674230	3.412888
H	-5.806472	-4.591925	3.622578
H	-5.074770	-4.369047	2.013099
C	-7.276977	-2.511236	2.551536
H	-7.662840	-2.756721	3.546882
H	-7.990725	-1.842382	2.062402
H	-7.205692	-3.427880	1.963818
C	-6.086742	-0.439647	3.294582
H	-5.113607	0.052311	3.397755
H	-6.717514	0.173113	2.644959
H	-6.555642	-0.501061	4.281328
B	-2.403699	-3.851819	0.180028
F	-3.701024	-3.145432	0.315748
F	-2.255971	-4.114126	-1.173024
F	-1.418154	-2.975904	0.629699
F	-2.467853	-4.998359	0.937442
C	-1.877554	-0.652664	-1.386089
C	-2.489545	0.399322	-2.274724
C	-0.825772	-1.419791	-2.147684
C	-1.792206	1.411481	-2.829265
C	0.273389	-0.848932	-2.681171
H	-0.969981	-2.494622	-2.205516
C	-0.353568	1.574095	-2.803570
H	-2.349709	2.178447	-3.362368

C	0.562597	0.568535	-2.742439
H	1.024178	-1.507350	-3.112049
H	0.021672	2.580234	-2.975110
H	1.607845	0.841356	-2.868316
H	-2.647727	-1.345130	-1.048382
H	-3.562809	0.338854	-2.432857

TS-1b

M06-2X/6-31+G(d,p) SCF energy (au)	-1415.08759063
M06-2X/6-31+G(d,p) enthalpy (au)	-1414.62006363
M06-2X/6-31+G(d,p) free energy (au)	-1414.71393463
MN15/6-311+G(2d,2p) SCF energy (au)	-1414.47544817
MN15/6-311+G(2d,2p) enthalpy (au)	-1414.00792117
MN15/6-311+G(2d,2p) free energy (au)	-1414.10179217

Cartesian coordinates

ATOM	X	Y	Z
O	-2.634722	-0.713477	-2.553352
C	-3.893483	-0.087034	-2.903239
C	-4.877545	-0.743778	-1.880194
O	-4.028766	-0.948998	-0.725846
B	-2.732331	-1.059528	-1.211921
H	-2.131266	-2.181281	-0.913048
C	-1.891305	-3.439620	-0.164857
C	-2.902605	-3.451312	0.860946
C	-1.769087	-4.441405	-1.192176
C	-4.123443	-4.059181	0.836950
C	-2.730141	-5.279986	-1.677903
H	-0.785940	-4.509690	-1.649396
C	-4.699506	-4.886833	-0.172051
H	-4.745787	-3.897743	1.713465
C	-4.090754	-5.421727	-1.273292
H	-2.419324	-5.936382	-2.486937
H	-5.736321	-5.168829	-0.008029
H	-4.694548	-6.082757	-1.889042
H	-0.947586	-3.023973	0.182902
H	-2.649008	-2.884416	1.753234
C	-3.641182	-0.004468	4.056350
C	-2.775373	-0.263976	3.000776
C	-2.891941	0.491311	1.819338
C	-3.863688	1.502587	1.704007
C	-4.726352	1.742895	2.763846
C	-4.613682	0.990374	3.936938
H	-3.556123	-0.580809	4.971343
H	-2.012519	-1.032973	3.074546
H	-3.930165	2.079277	0.787231
H	-5.482722	2.516164	2.683085
H	-5.287904	1.185411	4.765108
C	-2.024759	0.224344	0.733727
C	-1.393913	-0.099220	-0.274930
H	-0.494850	-0.088838	-0.863546
C	-4.199394	-0.387568	-4.361098
H	-3.470550	0.118143	-4.999904
H	-4.150590	-1.458800	-4.563913
H	-5.197640	-0.021752	-4.623460
C	-3.732543	1.417194	-2.690022

H	-2.888554	1.769210	-3.288799
H	-4.630537	1.959886	-2.999009
H	-3.526552	1.646333	-1.640063
C	-6.047605	0.135687	-1.471397
H	-6.657077	0.391096	-2.344495
H	-6.676919	-0.402533	-0.757582
H	-5.704533	1.057624	-0.998042
C	-5.370000	-2.114562	-2.336691
H	-4.530679	-2.753488	-2.631807
H	-5.887952	-2.595888	-1.502727
H	-6.063583	-2.031206	-3.178341
B	-0.244745	-3.171472	2.935938
F	-0.317151	-4.349775	2.173897
F	-1.375843	-3.083701	3.774725
F	0.923740	-3.140709	3.689274
F	-0.279263	-2.063724	2.047249

TS-1c

M06-2X/6-31+G(d,p) SCF energy (au)	-719.93879484
M06-2X/6-31+G(d,p) enthalpy (au)	-719.61936784
M06-2X/6-31+G(d,p) free energy (au)	-719.68080084
MN15/6-311+G(2d,2p) SCF energy (au)	-719.55564846
MN15/6-311+G(2d,2p) enthalpy (au)	-719.23622146
MN15/6-311+G(2d,2p) free energy (au)	-719.29765446

Cartesian coordinates

ATOM	X	Y	Z
C	-0.807869	0.907077	0.183470
C	0.109466	1.726519	0.369688
H	0.600914	2.654073	0.584739
B	0.892563	0.196152	0.027243
H	-0.062054	-0.589289	-0.172245
O	1.719082	0.271363	-1.148606
O	1.700834	-0.161515	1.165255
C	3.072880	0.192577	-0.689265
C	2.932819	-0.648007	0.622273
C	2.776350	-2.142316	0.328873
H	3.713654	-2.586457	-0.019968
H	2.472411	-2.649190	1.249017
H	2.006596	-2.310565	-0.431285
C	4.042319	-0.424933	1.639302
H	3.875112	-1.064726	2.510643
H	5.017516	-0.678986	1.209858
H	4.064080	0.613267	1.976594
C	3.918594	-0.461403	-1.772529
H	3.987523	0.205089	-2.637310
H	4.933144	-0.655522	-1.407771
H	3.473934	-1.402913	-2.100920
C	3.583815	1.608479	-0.408569
H	4.650690	1.609693	-0.164398
H	3.431100	2.219699	-1.302597
H	3.041419	2.064343	0.425354
C	-2.167716	0.398995	0.073727
C	-2.488163	-0.922641	-0.239872
C	-3.187338	1.334304	0.306121
C	-3.823879	-1.307855	-0.320610

H	-1.697904	-1.644245	-0.419351
C	-4.517691	0.940246	0.222993
H	-2.928964	2.359960	0.549819
C	-4.839158	-0.381315	-0.090410
H	-4.069105	-2.336136	-0.564389
H	-5.303832	1.665865	0.403452
H	-5.878356	-0.686933	-0.154494

TS-2b

M06-2X/6-31+G(d,p) SCF energy (au)	-819.21812063
M06-2X/6-31+G(d,p) enthalpy (au)	-818.90383863
M06-2X/6-31+G(d,p) free energy (au)	-818.96742863
MN15/6-311+G(2d,2p) SCF energy (au)	-818.82638226
MN15/6-311+G(2d,2p) enthalpy (au)	-818.51210026
MN15/6-311+G(2d,2p) free energy (au)	-818.57569026

Cartesian coordinates

ATOM	X	Y	Z
C	-0.947608	0.750687	0.486845
C	0.090724	1.376838	0.895404
H	0.148021	2.272983	1.497255
B	1.212575	0.366738	0.198742
O	2.004029	0.867124	-0.858532
O	2.015150	-0.366193	1.098063
C	3.375622	0.615448	-0.520588
C	3.260206	-0.621640	0.427984
C	3.126959	-1.936521	-0.343341
H	4.071145	-2.220118	-0.818629
H	2.839958	-2.724768	0.358058
H	2.351434	-1.860972	-1.111061
C	4.367993	-0.730824	1.464632
H	4.216944	-1.629706	2.069233
H	5.345733	-0.806980	0.976588
H	4.372244	0.134080	2.130935
C	4.164238	0.362748	-1.797020
H	4.206845	1.281276	-2.389358
H	5.189975	0.058199	-1.562098
H	3.694098	-0.414311	-2.402605
C	3.918443	1.852060	0.198799
H	4.984999	1.753845	0.422909
H	3.777532	2.722547	-0.447934
H	3.377850	2.024515	1.134823
C	-2.302311	0.348064	0.250659
C	-2.972532	-0.420123	1.214741
C	-2.955954	0.750251	-0.924541
C	-4.300103	-0.774674	1.003899
H	-2.446806	-0.727332	2.112734
C	-4.281534	0.387002	-1.126929
H	-2.417386	1.337777	-1.660724
C	-4.950170	-0.372497	-0.164069
H	-4.826949	-1.365324	1.745427
H	-4.794990	0.693812	-2.031679
H	-5.986092	-0.653156	-0.326019
F	0.051838	-0.504988	-0.401284

TS-2c

M06-2X/6-31+G(d,p) SCF energy (au)	-1143.73800028
M06-2X/6-31+G(d,p) enthalpy (au)	-1143.40544628
M06-2X/6-31+G(d,p) free energy (au)	-1143.47907228
MN15/6-311+G(2d,2p) SCF energy (au)	-1143.29011942
MN15/6-311+G(2d,2p) enthalpy (au)	-1142.95756542
MN15/6-311+G(2d,2p) free energy (au)	-1143.03119142

Cartesian coordinates

ATOM	X	Y	Z
O	-1.894682	0.466233	-3.218975
C	-0.795531	1.020190	-3.975954
C	-0.945760	2.552864	-3.698254
O	-1.458133	2.561939	-2.342248
B	-2.192995	1.383344	-2.219468
C	-6.046389	-0.264498	1.438737
C	-4.814629	-0.360320	0.808277
C	-3.975829	0.769913	0.759436
C	-4.377423	1.989544	1.339381
C	-5.616364	2.073181	1.956249
C	-6.445171	0.948523	2.004947
H	-6.703025	-1.126356	1.478739
H	-4.492532	-1.282006	0.337383
H	-3.717617	2.849006	1.284376
H	-5.941787	3.009065	2.396575
H	-7.414962	1.020423	2.487252
C	-2.724516	0.683212	0.115334
C	-1.702490	0.663899	-0.582136
H	-0.654878	0.420403	-0.594698
C	-0.969121	0.619993	-5.432198
H	-0.827017	-0.459293	-5.533670
H	-1.969160	0.869422	-5.790561
H	-0.226909	1.125743	-6.058677
C	0.506983	0.445954	-3.420184
H	0.439445	-0.645136	-3.420605
H	1.361733	0.742769	-4.034880
H	0.692411	0.786771	-2.397261
C	0.353877	3.337961	-3.739457
H	0.815898	3.256539	-4.728914
H	0.149322	4.394010	-3.543848
H	1.060809	2.979487	-2.988975
C	-1.997825	3.207166	-4.593551
H	-2.929147	2.633030	-4.593813
H	-2.208732	4.208987	-4.210469
H	-1.639789	3.295896	-5.623411
B	-4.868791	0.628751	-2.612161
F	-5.921863	1.146283	-1.931135
F	-3.656142	1.638729	-2.110878
F	-4.443216	-0.588194	-2.183468
F	-4.888444	0.813742	-3.952644

9b

M06-2X/6-31+G(d,p) SCF energy (au)	-1143.73838100
M06-2X/6-31+G(d,p) enthalpy (au)	-1143.40359000
M06-2X/6-31+G(d,p) free energy (au)	-1143.48182800
MN15/6-311+G(2d,2p) SCF energy (au)	-1143.29107984
MN15/6-311+G(2d,2p) enthalpy (au)	-1142.95628884

MN15/6-311+G(2d,2p) free energy (au)	-1143.03452684

Cartesian coordinates

ATOM	X	Y	Z
O	-2.596466	1.005262	-2.057465
C	-3.591613	0.476881	-2.985582
C	-3.856096	-0.955178	-2.407511
O	-3.574894	-0.770051	-0.987344
B	-2.746953	0.305972	-0.906061
C	-1.659143	-2.584988	4.006424
C	-1.465343	-1.830244	2.868663
C	-2.366127	-0.767428	2.586985
C	-3.440902	-0.462266	3.465251
C	-3.619885	-1.235593	4.594217
C	-2.730908	-2.284471	4.859004
H	-0.981823	-3.395045	4.249495
H	-0.637368	-2.015655	2.193300
H	-4.080909	0.383306	3.241225
H	-4.427730	-1.020097	5.283366
H	-2.869548	-2.877621	5.757882
C	-2.155208	0.020948	1.487691
C	-2.007230	0.720943	0.427205
H	-1.365943	1.602206	0.493121
C	-5.283124	-1.449483	-2.563370
H	-5.545636	-1.511690	-3.624175
H	-5.371502	-2.448876	-2.130070
H	-5.993009	-0.790048	-2.061788
C	-2.865226	-1.998811	-2.914771
H	-2.986543	-2.913181	-2.328864
H	-3.047587	-2.233290	-3.966859
H	-1.832715	-1.653128	-2.807328
C	-4.805192	1.396673	-2.888806
H	-4.491959	2.417449	-3.120335
H	-5.579599	1.099616	-3.600982
H	-5.232871	1.387237	-1.881770
C	-3.010205	0.498840	-4.388034
H	-3.702936	0.023559	-5.089764
H	-2.860006	1.534300	-4.703011
H	-2.050744	-0.018669	-4.432786
B	-0.768885	1.772130	3.735709
F	-0.908648	0.768135	4.706488
F	-2.051725	2.184348	3.305996
F	-0.056899	2.854708	4.242115
F	-0.093884	1.230524	2.610833

TS-3d

M06-2X/6-31+G(d,p) SCF energy (au)	-1415.13584142
M06-2X/6-31+G(d,p) enthalpy (au)	-1414.66579542
M06-2X/6-31+G(d,p) free energy (au)	-1414.75759342
MN15/6-311+G(2d,2p) SCF energy (au)	-1414.52108971
MN15/6-311+G(2d,2p) enthalpy (au)	-1414.05104371
MN15/6-311+G(2d,2p) free energy (au)	-1414.14284171

Cartesian coordinates

ATOM	X	Y	Z
O	-2.322531	0.967438	-2.234525

C	-2.860303	0.515731	-3.506849
C	-4.180464	-0.216201	-3.079474
O	-3.869979	-0.640022	-1.721413
B	-2.905954	0.208405	-1.268985
C	-2.135912	-2.542874	4.181931
C	-2.054412	-2.033589	2.903618
C	-2.871358	-0.926586	2.546145
C	-3.782865	-0.361902	3.475352
C	-3.840696	-0.889593	4.756592
C	-3.035077	-1.977149	5.099968
H	-1.515658	-3.382044	4.477090
H	-1.372727	-2.447920	2.168454
H	-4.390109	0.480343	3.158434
H	-4.522939	-0.465831	5.485193
H	-3.095519	-2.387932	6.103425
C	-2.780475	-0.408340	1.260640
C	-2.368696	0.220060	0.212816
H	-1.543915	0.909392	0.433726
C	-5.384322	0.716066	-2.981136
H	-5.706360	1.045641	-3.972945
H	-6.208255	0.172435	-2.510500
H	-5.156631	1.587085	-2.362016
C	-4.520592	-1.448574	-3.900993
H	-5.443331	-1.894011	-3.518810
H	-4.683484	-1.173491	-4.947991
H	-3.728074	-2.197708	-3.852839
C	-3.072379	1.724722	-4.402137
H	-2.104537	2.168298	-4.649750
H	-3.562210	1.425325	-5.334430
H	-3.682941	2.480974	-3.906501
C	-1.819779	-0.424920	-4.109318
H	-2.127585	-0.772801	-5.099320
H	-0.874368	0.114400	-4.208148
H	-1.654494	-1.295256	-3.466941
B	-4.906651	2.175920	0.855412
F	-4.029783	2.381259	1.937418
F	-4.189027	2.276020	-0.356653
F	-5.440929	0.870876	0.957134
F	-5.935677	3.114537	0.878992
H	-4.244478	-1.295779	0.712194
C	-5.075817	-2.082090	0.599863
C	-4.429845	-3.412824	0.467596
C	-6.067720	-1.842835	1.678664
C	-4.220004	-4.370339	1.397978
C	-6.219397	-2.462942	2.869509
H	-6.737637	-1.012442	1.475671
C	-4.637760	-4.417328	2.786692
H	-3.672510	-5.248199	1.061007
C	-5.498298	-3.591533	3.424821
H	-7.004938	-2.067423	3.510379
H	-4.227175	-5.242224	3.364401
H	-5.720123	-3.819047	4.464991
H	-5.481329	-1.759820	-0.362107
H	-4.036508	-3.612638	-0.528214

TS-3e

M06-2X/6-31+G(d,p) SCF energy (au)	-1555.44184537
M06-2X/6-31+G(d,p) enthalpy (au)	-1554.90511137
M06-2X/6-31+G(d,p) free energy (au)	-1555.00036337
MN15/6-311+G(2d,2p) SCF energy (au)	-1554.80384343
MN15/6-311+G(2d,2p) enthalpy (au)	-1554.26710943
MN15/6-311+G(2d,2p) free energy (au)	-1554.36236143

Cartesian coordinates

ATOM	X	Y	Z
O	-2.785044	0.502724	-2.009538
C	-3.775793	-0.275691	-2.752993
C	-3.161067	-1.721111	-2.728222
O	-2.338146	-1.692231	-1.528992
B	-2.128345	-0.395541	-1.228438
C	-0.743522	-1.455490	4.604435
C	-0.738107	-1.378776	3.221396
C	-1.407053	-0.302910	2.592300
C	-2.108444	0.664318	3.354624
C	-2.108459	0.565832	4.732263
C	-1.426694	-0.492128	5.350037
H	-0.236661	-2.272971	5.104027
H	-0.259213	-2.131949	2.606552
H	-2.632558	1.465575	2.843546
H	-2.637112	1.297433	5.333121
H	-1.437648	-0.567386	6.433300
C	-1.412041	-0.203105	1.207415
C	-1.202280	0.075130	-0.029458
H	-0.334666	0.717083	-0.213060
C	-4.177862	-2.840036	-2.577674
H	-4.849871	-2.858108	-3.442301
H	-3.648927	-3.793878	-2.516213
H	-4.765227	-2.723268	-1.665254
C	-2.214778	-2.000695	-3.891569
H	-1.698283	-2.944136	-3.698057
H	-2.763117	-2.087704	-4.833663
H	-1.464883	-1.210076	-3.993040
C	-5.079409	-0.165464	-1.967949
H	-5.343866	0.891554	-1.876161
H	-5.890772	-0.683411	-2.487140
H	-4.985835	-0.591972	-0.963576
C	-3.926542	0.327725	-4.138214
H	-4.606201	-0.282907	-4.741045
H	-4.351259	1.331466	-4.054674
H	-2.966855	0.398133	-4.652975
O	-3.592482	-2.239825	2.778406
C	-4.850980	-2.619559	3.361733
C	-5.867426	-1.840084	2.463945
O	-5.220617	-1.850912	1.181056
B	-3.836031	-1.997237	1.417904
H	-3.078611	-1.181910	0.901063
C	-4.849764	-2.205528	4.825757
H	-4.116117	-2.806253	5.371903
H	-4.579811	-1.152625	4.935835
H	-5.834326	-2.370775	5.276761
C	-5.004009	-4.136157	3.240476
H	-4.137693	-4.613648	3.705218

H	-5.911832	-4.483320	3.743976
H	-5.036408	-4.446153	2.192869
C	-7.235339	-2.494141	2.339663
H	-7.707499	-2.589217	3.323627
H	-7.880863	-1.876511	1.708411
H	-7.157899	-3.484376	1.887224
C	-6.017357	-0.378885	2.893091
H	-5.033333	0.085921	3.019045
H	-6.558586	0.162034	2.111775
H	-6.572722	-0.286518	3.831616
B	-2.086421	-4.032692	0.545103
F	-3.430050	-3.340495	0.554402
F	-1.989484	-4.626217	-0.690915
F	-1.128988	-3.054606	0.755745
F	-2.119527	-4.949123	1.573719

TS-3a

M06-2X/6-31+G(d,p) SCF energy (au)	-533.42923646
M06-2X/6-31+G(d,p) enthalpy (au)	-533.28916046
M06-2X/6-31+G(d,p) free energy (au)	-533.33589946
MN15/6-311+G(2d,2p) SCF energy (au)	-533.20160016
MN15/6-311+G(2d,2p) enthalpy (au)	-533.06152416
MN15/6-311+G(2d,2p) free energy (au)	-533.10826316

Cartesian coordinates

ATOM	X	Y	Z
C	-0.804302	0.903566	0.204171
C	0.140323	1.694749	0.401145
H	0.602955	2.632822	0.643175
B	0.902317	0.208245	0.007243
H	-0.046648	-0.578921	-0.190885
C	-2.160189	0.395745	0.082597
C	-2.478300	-0.931344	-0.210641
C	-3.177866	1.339849	0.288156
C	-3.813883	-1.313952	-0.298225
H	-1.689099	-1.659034	-0.369015
C	-4.507759	0.946241	0.198255
H	-2.920771	2.369474	0.515213
C	-4.828273	-0.380026	-0.094921
H	-4.059495	-2.345574	-0.526112
H	-5.293936	1.676705	0.356627
H	-5.867441	-0.684082	-0.164833
F	1.629158	0.367979	-1.162572
F	1.646655	-0.221465	1.095247

TS-3b

M06-2X/6-31+G(d,p) SCF energy (au)	-1044.43107317
M06-2X/6-31+G(d,p) enthalpy (au)	-1044.09314617
M06-2X/6-31+G(d,p) free energy (au)	-1044.16406017
MN15/6-311+G(2d,2p) SCF energy (au)	-1043.99923825
MN15/6-311+G(2d,2p) enthalpy (au)	-1043.66131125
MN15/6-311+G(2d,2p) free energy (au)	-1043.73222525

Cartesian coordinates

ATOM	X	Y	Z
O	-2.863437	0.292945	-1.621550

C	-3.349562	0.043396	-2.957869
C	-2.346197	-1.045369	-3.463365
O	-2.041748	-1.771540	-2.254951
B	-2.308000	-0.912322	-1.183593
C	-0.913903	-0.602621	4.823161
C	-1.137979	-0.968733	3.505260
C	-1.058714	0.014917	2.496133
C	-0.772306	1.359752	2.815241
C	-0.547428	1.707673	4.137194
C	-0.620253	0.728629	5.133935
H	-0.971846	-1.345446	5.610614
H	-1.386157	-1.988572	3.232514
H	-0.731987	2.098260	2.021668
H	-0.321314	2.735251	4.398508
H	-0.448906	1.008746	6.168570
C	-1.241409	-0.356719	1.153696
C	-1.116038	-0.737867	-0.058320
H	-0.092695	-0.949799	-0.383044
C	-2.922608	-2.007545	-4.489977
H	-3.256888	-1.462823	-5.379472
H	-2.153091	-2.722161	-4.795175
H	-3.765895	-2.565081	-4.078810
C	-1.038319	-0.442127	-3.976129
H	-0.312720	-1.247776	-4.117159
H	-1.179444	0.070390	-4.932321
H	-0.629117	0.271498	-3.253785
C	-4.784058	-0.477406	-2.858738
H	-5.379254	0.244045	-2.292726
H	-5.228265	-0.596259	-3.851604
H	-4.825639	-1.436225	-2.335940
C	-3.316923	1.347747	-3.738466
H	-3.563429	1.170087	-4.790666
H	-4.057303	2.038402	-3.325432
H	-2.334703	1.820621	-3.680507
B	-3.910593	-1.084270	1.020912
H	-3.162402	-0.114986	1.188141
F	-3.439846	-1.704712	-0.276969
F	-5.219797	-0.722648	0.838290
F	-3.731829	-2.048708	1.991977

TS-3c

M06-2X/6-31+G(d,p) SCF energy (au)	-945.13227935
M06-2X/6-31+G(d,p) enthalpy (au)	-944.78939335
M06-2X/6-31+G(d,p) free energy (au)	-944.85955335
MN15/6-311+G(2d,2p) SCF energy (au)	-944.71830181
MN15/6-311+G(2d,2p) enthalpy (au)	-944.37541581
MN15/6-311+G(2d,2p) free energy (au)	-944.44557581

Cartesian coordinates

ATOM	X	Y	Z
O	-2.817107	0.312037	-1.587899
C	-3.343354	0.068398	-2.908191
C	-2.373484	-1.035913	-3.439400
O	-2.065909	-1.775801	-2.240221
B	-2.283935	-0.910254	-1.156453
C	-1.018148	-0.495605	4.837160

C	-1.192854	-0.896962	3.521829
C	-1.044214	0.051198	2.487601
C	-0.736645	1.396083	2.779337
C	-0.564474	1.780671	4.100380
C	-0.705369	0.837208	5.122504
H	-1.128715	-1.213010	5.642573
H	-1.454075	-1.919026	3.268283
H	-0.638754	2.108491	1.967172
H	-0.324482	2.810717	4.339212
H	-0.572519	1.145312	6.154800
C	-1.173018	-0.361993	1.147826
C	-1.041746	-0.751653	-0.054806
H	-0.046719	-0.989636	-0.434614
C	-2.987936	-1.979894	-4.460753
H	-3.330399	-1.422995	-5.339549
H	-2.238428	-2.706572	-4.786563
H	-3.832860	-2.524841	-4.036039
C	-1.062300	-0.456098	-3.970470
H	-0.354478	-1.274847	-4.125829
H	-1.209016	0.061797	-4.923050
H	-0.628467	0.247642	-3.252827
C	-4.779589	-0.434543	-2.759251
H	-5.348109	0.296937	-2.179143
H	-5.258941	-0.559854	-3.734694
H	-4.814202	-1.389069	-2.225830
C	-3.315504	1.369352	-3.694012
H	-3.594428	1.191712	-4.738089
H	-4.033519	2.072265	-3.262611
H	-2.325132	1.827850	-3.665805
B	-3.753335	-1.325262	0.838302
H	-3.144510	-0.300429	1.165355
F	-5.095732	-1.162640	0.627888
F	-3.438839	-2.413073	1.626552
H	-3.200185	-1.586545	-0.352617

TS-4b

M06-2X/6-31+G(d,p) SCF energy (au)	-434.12315474
M06-2X/6-31+G(d,p) enthalpy (au)	-433.97770174
M06-2X/6-31+G(d,p) free energy (au)	-434.02240674
MN15/6-311+G(2d,2p) SCF energy (au)	-433.91285014
MN15/6-311+G(2d,2p) enthalpy (au)	-433.76739714
MN15/6-311+G(2d,2p) free energy (au)	-433.81210214

Cartesian coordinates

ATOM	X	Y	Z
C	-0.936602	0.746215	0.474463
C	0.112546	1.383063	0.859180
H	0.136240	2.304993	1.425247
B	1.206377	0.354408	0.214818
C	-2.293891	0.351225	0.247654
C	-2.959018	-0.431812	1.204633
C	-2.956244	0.766433	-0.918861
C	-4.286228	-0.787508	0.996330
H	-2.427932	-0.749018	2.096018
C	-4.282380	0.403612	-1.119399
H	-2.423135	1.365479	-1.649755

C	-4.943234	-0.370555	-0.163066
H	-4.808347	-1.389375	1.732112
H	-4.801972	0.721268	-2.016840
H	-5.979419	-0.651506	-0.323107
F	0.057524	-0.551072	-0.338563
H	1.837828	-0.268978	1.026529
H	1.826351	0.807672	-0.710567

TS-4c

M06-2X/6-31+G(d,p) SCF energy (au)	-845.84016998
M06-2X/6-31+G(d,p) enthalpy (au)	-845.49235098
M06-2X/6-31+G(d,p) free energy (au)	-845.56053298
MN15/6-311+G(2d,2p) SCF energy (au)	-845.43906517
MN15/6-311+G(2d,2p) enthalpy (au)	-845.09124617
MN15/6-311+G(2d,2p) free energy (au)	-845.15942817

Cartesian coordinates

ATOM	X	Y	Z
O	-2.830099	0.311537	-1.574047
C	-3.333478	0.093004	-2.904995
C	-2.386268	-1.036339	-3.423308
O	-2.137015	-1.798345	-2.227088
B	-2.348747	-0.934205	-1.132990
C	-0.909069	-0.463434	4.848382
C	-1.109231	-0.905548	3.550320
C	-1.063952	0.022997	2.490143
C	-0.831498	1.390438	2.740893
C	-0.636541	1.818576	4.045974
C	-0.675381	0.893959	5.092897
H	-0.938865	-1.167363	5.672533
H	-1.306196	-1.950122	3.333040
H	-0.811093	2.087420	1.909882
H	-0.456795	2.867786	4.251975
H	-0.524545	1.234673	6.112380
C	-1.207881	-0.421449	1.160345
C	-1.083259	-0.791344	-0.048539
H	-0.089683	-0.995729	-0.450536
C	-3.003137	-1.947907	-4.472735
H	-3.307362	-1.369962	-5.352124
H	-2.268045	-2.692901	-4.790276
H	-3.874017	-2.472479	-4.075476
C	-1.044050	-0.491869	-3.914107
H	-0.356635	-1.330287	-4.057033
H	-1.148496	0.037839	-4.865866
H	-0.609675	0.193331	-3.179008
C	-4.787443	-0.368011	-2.791770
H	-5.347542	0.379458	-2.223849
H	-5.248471	-0.478821	-3.777828
H	-4.861518	-1.321230	-2.259522
C	-3.250738	1.397435	-3.681713
H	-3.513925	1.235340	-4.732472
H	-3.955556	2.119264	-3.259735
H	-2.247702	1.825507	-3.630611
B	-3.780776	-1.428194	0.850978
H	-3.191485	-0.399413	1.196549
F	-5.144941	-1.260996	0.695412

H	-3.262468	-1.598647	-0.362842
H	-3.433373	-2.435360	1.420729

TS-22

M06-2X/6-31+G(d,p) SCF energy (au)	-560.12563124
M06-2X/6-31+G(d,p) enthalpy (au)	-559.94717024
M06-2X/6-31+G(d,p) free energy (au)	-559.99732724
MN15/6-311+G(2d,2p) SCF energy (au)	-559.88175874
MN15/6-311+G(2d,2p) enthalpy (au)	-559.70329774
MN15/6-311+G(2d,2p) free energy (au)	-559.75345474

Cartesian coordinates

ATOM	X	Y	Z
C	-0.995061	0.830440	0.323396
C	-0.069335	1.856877	0.592030
B	0.834509	0.479226	-0.055828
H	0.018249	-0.304459	-0.560215
C	-2.001365	0.867478	-0.764586
C	-3.157316	0.090889	-0.637617
C	-1.826018	1.664837	-1.901262
C	-4.137790	0.123583	-1.626257
H	-3.289861	-0.535779	0.240160
C	-2.799658	1.684491	-2.894899
H	-0.924534	2.258285	-2.020690
C	-3.958952	0.919240	-2.756735
H	-5.036126	-0.474768	-1.515803
H	-2.655064	2.298206	-3.777919
H	-4.718908	0.941463	-3.531119
F	1.558067	-0.144609	0.963103
H	1.406794	0.967467	-0.988555
H	-0.035648	2.700284	-0.092074
H	-1.201325	0.118898	1.122879
B	0.494310	2.039116	2.023082
H	0.284972	1.283073	2.919227
F	1.234458	3.120605	2.277478

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M06-2X/6-31+G(d,p) SCF energy (au)	-560.17447981
M06-2X/6-31+G(d,p) enthalpy (au)	-559.99285581
M06-2X/6-31+G(d,p) free energy (au)	-560.04560781
MN15/6-311+G(2d,2p) SCF energy (au)	-559.92766033
MN15/6-311+G(2d,2p) enthalpy (au)	-559.74603633
MN15/6-311+G(2d,2p) free energy (au)	-559.79878833

Cartesian coordinates

ATOM	X	Y	Z
C	-0.751538	0.826572	-0.303505
C	0.125818	1.708801	0.612955
B	1.655620	1.596997	0.292538
H	-0.490563	1.005431	-1.352700
C	-2.229063	1.079909	-0.107118
C	-3.022721	0.204444	0.639822
C	-2.824316	2.227504	-0.644604
C	-4.376933	0.468823	0.849489
H	-2.576977	-0.694142	1.059332
C	-4.175606	2.495826	-0.438650

H	-2.221460	2.915036	-1.234262
C	-4.957057	1.615930	0.311757
H	-4.977581	-0.224153	1.430670
H	-4.620368	3.389235	-0.866246
H	-6.010432	1.822400	0.472472
F	2.503322	2.460702	0.859091
H	2.129375	0.779089	-0.438421
H	-0.100434	2.780616	0.478871
H	-0.532906	-0.228147	-0.102522
B	-0.098573	1.429687	2.137564
H	-0.543304	0.409349	2.571821
F	0.258416	2.358076	3.029445

TS-23

M06-2X/6-31+G(d,p) SCF energy (au)	-971.86957384
M06-2X/6-31+G(d,p) enthalpy (au)	-971.48443484
M06-2X/6-31+G(d,p) free energy (au)	-971.55732984
MN15/6-311+G(2d,2p) SCF energy (au)	-971.43170898
MN15/6-311+G(2d,2p) enthalpy (au)	-971.04656998
MN15/6-311+G(2d,2p) free energy (au)	-971.11946498

Cartesian coordinates

ATOM	X	Y	Z
C	-1.971145	0.225757	-1.392916
C	-0.750611	1.081625	-0.994884
B	0.743350	0.042568	-0.103427
H	-2.866832	0.656346	-0.934712
C	-2.130462	0.164728	-2.894100
C	-1.351349	-0.721327	-3.647173
C	-3.016494	1.014680	-3.562072
C	-1.455386	-0.757138	-5.035928
H	-0.662570	-1.390371	-3.135116
C	-3.122906	0.982628	-4.953305
H	-3.632821	1.702599	-2.987841
C	-2.341965	0.097075	-5.693594
H	-0.847767	-1.453737	-5.605395
H	-3.818493	1.647193	-5.456604
H	-2.425067	0.069270	-6.775459
F	0.423205	-1.238692	-0.428974
H	1.751182	0.530159	-0.508473
H	0.097793	0.844623	-1.653456
H	-1.860641	-0.784416	-0.987179
B	-0.885972	2.635918	-1.274014
O	-0.278549	2.519014	1.098618
C	-0.795364	2.651571	2.447166
C	-2.075296	1.750945	2.394445
O	-1.712239	0.739762	1.423279
B	-0.694882	1.266949	0.642537
C	-1.062770	4.122116	2.717735
H	-0.115442	4.666585	2.747505
H	-1.561776	4.246351	3.684185
H	-1.688341	4.560723	1.937991
C	0.270683	2.115340	3.400589
H	-0.030158	2.254541	4.442605
H	1.201515	2.661970	3.230000
H	0.459797	1.049853	3.238266

C	-3.295408	2.484035	1.840198
H	-3.673845	3.223433	2.551723
H	-4.083721	1.752074	1.645549
H	-3.058124	2.992406	0.900638
C	-2.419609	1.069287	3.708959
H	-3.325951	0.471465	3.582583
H	-2.606953	1.815872	4.487703
H	-1.615635	0.408989	4.038251
H	0.510415	0.312920	1.071100
F	0.199897	3.321108	-1.626898
H	-1.933197	3.206086	-1.248153

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M06-2X/6-31+G(d,p) SCF energy (au)	-846.00506651
M06-2X/6-31+G(d,p) enthalpy (au)	-845.64801851
M06-2X/6-31+G(d,p) free energy (au)	-845.71806351
MN15/6-311+G(2d,2p) SCF energy (au)	-845.59101936
MN15/6-311+G(2d,2p) enthalpy (au)	-845.23397136
MN15/6-311+G(2d,2p) free energy (au)	-845.30401636

Cartesian coordinates

ATOM	X	Y	Z
C	-1.366462	0.796694	0.591894
C	-0.230458	1.838483	0.678645
B	0.963642	1.589216	-0.291839
H	-0.946737	-0.205977	0.721805
C	-2.114636	0.868997	-0.719720
C	-3.063071	1.876806	-0.932914
C	-1.861603	-0.036792	-1.754259
C	-3.738651	1.980630	-2.146888
H	-3.276417	2.584178	-0.134029
C	-2.535911	0.062249	-2.972057
H	-1.127322	-0.823616	-1.603062
C	-3.475481	1.071977	-3.172910
H	-4.473274	2.767142	-2.291433
H	-2.327112	-0.651861	-3.762992
H	-4.001753	1.149019	-4.119212
F	1.162810	0.356683	-0.782536
H	1.768794	2.415812	-0.598326
H	-0.599725	2.854187	0.468492
H	-2.069925	0.949245	1.417893
B	0.397191	1.942598	2.122133
O	1.210889	2.972400	2.524750
O	0.203116	1.003331	3.101352
C	1.792920	2.583964	3.794911
C	0.751611	1.546393	4.330148
C	3.151532	1.958571	3.484484
C	1.962307	3.821008	4.660816
C	1.345316	0.412438	5.149086
C	-0.407939	2.197951	5.080579
H	3.754377	2.685081	2.933811
H	3.682683	1.687338	4.401128
H	3.042072	1.062285	2.865683
H	2.314459	3.541496	5.659059
H	2.705245	4.483088	4.208475
H	1.024975	4.371273	4.758635

H	1.849872	0.808173	6.036522
H	0.545885	-0.256043	5.479144
H	2.061417	-0.168991	4.565923
H	-1.185539	1.447612	5.244345
H	-0.085071	2.583256	6.051752
H	-0.839064	3.021122	4.502614

TS-24

M06-2X/6-31+G(d,p) SCF energy (au)	-1257.69576206
M06-2X/6-31+G(d,p) enthalpy (au)	-1257.13571106
M06-2X/6-31+G(d,p) free energy (au)	-1257.22443606
MN15/6-311+G(2d,2p) SCF energy (au)	-1257.09126809
MN15/6-311+G(2d,2p) enthalpy (au)	-1256.53121709
MN15/6-311+G(2d,2p) free energy (au)	-1256.61994209

Cartesian coordinates

ATOM	X	Y	Z
C	-1.790168	0.007128	1.521836
C	-0.825304	1.113884	1.030833
B	0.701300	0.133706	0.139237
H	-2.177708	-0.551854	0.664403
C	-2.938506	0.588928	2.310976
C	-2.901450	0.629850	3.707172
C	-4.037250	1.149185	1.648718
C	-3.937966	1.222434	4.429583
H	-2.050188	0.194996	4.225023
C	-5.075108	1.739834	2.366249
H	-4.069841	1.114494	0.561558
C	-5.026941	1.779617	3.761013
H	-3.895282	1.246003	5.514590
H	-5.923529	2.166022	1.839189
H	-5.835240	2.238625	4.321633
F	1.834576	0.885411	0.298040
H	0.581000	-0.842284	0.811068
H	-1.403680	2.063028	0.960134
H	-1.231116	-0.692681	2.147823
B	0.179731	1.629856	2.141215
O	0.649381	2.911593	2.181870
O	0.557783	0.871907	3.214921
C	1.621396	2.971754	3.257552
C	1.181188	1.774340	4.167651
C	2.999235	2.772811	2.631375
C	1.531364	4.336250	3.921065
C	2.324632	1.049271	4.857093
C	0.104179	2.158640	5.179697
H	3.146211	3.536550	1.863456
H	3.788260	2.873728	3.382229
H	3.078324	1.793292	2.154364
H	2.181873	4.373117	4.801117
H	1.862686	5.104245	3.217390
H	0.509205	4.566251	4.226852
H	2.867165	1.737175	5.513860
H	1.925565	0.235092	5.467826
H	3.023210	0.627616	4.132709
H	-0.272159	1.249632	5.656994
H	0.507999	2.815206	5.955419

H	-0.736050	2.662608	4.691482
O	-0.250448	2.466347	-1.152722
C	-0.737489	2.539842	-2.514952
C	-2.117850	1.808798	-2.408013
O	-1.885509	0.855968	-1.338851
B	-0.831815	1.351085	-0.593681
C	-0.823709	4.002176	-2.919634
H	0.183453	4.423183	-2.976032
H	-1.292556	4.097845	-3.904515
H	-1.398491	4.581615	-2.195131
C	0.260853	1.801652	-3.404877
H	-0.009207	1.896673	-4.460442
H	1.250943	2.239546	-3.255376
H	0.314517	0.738098	-3.156034
C	-3.242400	2.732351	-1.943607
H	-3.506156	3.458522	-2.717613
H	-4.125976	2.127210	-1.723107
H	-2.959250	3.276022	-1.036253
C	-2.533698	1.054308	-3.659775
H	-3.505039	0.580298	-3.495488
H	-2.627040	1.744002	-4.505088
H	-1.810628	0.278056	-3.915690
H	0.323436	0.043039	-1.008810

TS-25

M06-2X/6-31+G(d,p) SCF energy (au)	-845.95406886
M06-2X/6-31+G(d,p) enthalpy (au)	-845.60056586
M06-2X/6-31+G(d,p) free energy (au)	-845.66679286
MN15/6-311+G(2d,2p) SCF energy (au)	-845.54347120
MN15/6-311+G(2d,2p) enthalpy (au)	-845.18996820
MN15/6-311+G(2d,2p) free energy (au)	-845.25619520

Cartesian coordinates

ATOM	X	Y	Z
C	-1.097792	0.919792	0.393768
C	-0.097499	1.888492	0.629920
B	0.670151	0.482223	-0.078374
H	-0.143842	-0.459985	0.013175
C	-2.046213	0.910221	-0.748912
C	-3.185302	0.103084	-0.654285
C	-1.852747	1.693104	-1.892307
C	-4.125828	0.084139	-1.680670
H	-3.334836	-0.509733	0.230873
C	-2.789296	1.666921	-2.921441
H	-0.966264	2.310235	-1.988080
C	-3.927489	0.866275	-2.817576
H	-5.008678	-0.540718	-1.593646
H	-2.629875	2.272877	-3.807373
H	-4.656598	0.851813	-3.621462
F	0.972940	0.745370	-1.412815
H	1.547589	0.154077	0.671157
H	0.034570	2.673173	-0.109595
H	-1.423678	0.337696	1.254276
B	0.443237	2.092198	2.064584
O	1.295352	3.098083	2.437308
O	0.129884	1.240015	3.096910

C	1.418382	3.035178	3.880887
C	1.046359	1.544891	4.178856
C	2.832966	3.427363	4.273542
C	0.409142	4.026149	4.456815
C	2.234563	0.596651	4.032975
C	0.340652	1.317769	5.504886
H	2.998715	4.481119	4.034537
H	2.979616	3.292531	5.350210
H	3.574674	2.832220	3.738291
H	0.484298	4.079906	5.546507
H	0.615426	5.016903	4.044106
H	-0.614455	3.747194	4.188866
H	2.947853	0.726179	4.851776
H	1.866495	-0.432394	4.049433
H	2.755284	0.759733	3.084345
H	0.125872	0.252716	5.626165
H	0.980417	1.634846	6.334870
H	-0.600771	1.867641	5.555280

TS-26

M06-2X/6-31+G(d,p) SCF energy (au)	-845.94709784
M06-2X/6-31+G(d,p) enthalpy (au)	-845.59333884
M06-2X/6-31+G(d,p) free energy (au)	-845.66187084
MN15/6-311+G(2d,2p) SCF energy (au)	-845.53552705
MN15/6-311+G(2d,2p) enthalpy (au)	-845.18176805
MN15/6-311+G(2d,2p) free energy (au)	-845.25030005

Cartesian coordinates

ATOM	X	Y	Z
C	-1.004385	0.823598	0.339524
C	-0.046779	1.830889	0.613361
B	0.806349	0.451883	-0.021896
H	-0.047646	-0.279035	-0.567496
C	-1.683677	-0.130107	1.257498
C	-2.979958	-0.521619	0.896320
C	-1.117431	-0.642906	2.430878
C	-3.713597	-1.387815	1.702187
H	-3.419872	-0.139456	-0.021243
C	-1.849383	-1.520619	3.226567
H	-0.113136	-0.361951	2.717194
C	-3.146617	-1.891140	2.871542
H	-4.719775	-1.673214	1.412766
H	-1.400610	-1.917826	4.131514
H	-3.710352	-2.572684	3.500835
F	1.470649	-0.237798	0.995309
H	1.436179	0.877722	-0.946600
H	-0.015598	2.610824	-0.143272
H	-1.565566	0.966200	-0.582033
B	0.623870	2.285809	1.944024
O	1.449137	3.384991	1.921522
O	0.510947	1.736987	3.193255
C	2.143522	3.418586	3.191947
C	1.155199	2.645018	4.122831
C	3.467019	2.682965	2.990033
C	2.389786	4.864763	3.587712
C	1.818418	1.831715	5.221829

C	0.059373	3.536526	4.702632
H	4.019798	3.171663	2.183675
H	4.077657	2.708268	3.897041
H	3.296309	1.639738	2.706624
H	2.826609	4.914349	4.590523
H	3.092493	5.320578	2.885272
H	1.465533	5.445023	3.576339
H	2.395712	2.486250	5.883036
H	1.051236	1.332000	5.819347
H	2.483225	1.071784	4.807806
H	-0.700458	2.902452	5.166398
H	0.461009	4.213008	5.462316
H	-0.419433	4.132256	3.919696

TS-27

M06-2X/6-31+G(d,p) SCF energy (au)	-560.11965178
M06-2X/6-31+G(d,p) enthalpy (au)	-559.94108378
M06-2X/6-31+G(d,p) free energy (au)	-559.99079078
MN15/6-311+G(2d,2p) SCF energy (au)	-559.87596948
MN15/6-311+G(2d,2p) enthalpy (au)	-559.69740148
MN15/6-311+G(2d,2p) free energy (au)	-559.74710848

Cartesian coordinates

ATOM	X	Y	Z
C	-0.874924	0.850966	-0.000217
C	0.063004	1.830997	0.361637
B	0.900045	0.246189	0.167151
H	0.201215	-0.485145	-0.544304
C	-1.776165	0.136315	0.953751
C	-1.964791	-1.247812	0.891376
C	-2.523318	0.888353	1.864984
C	-2.876494	-1.870512	1.737825
H	-1.378999	-1.840455	0.194729
C	-3.443003	0.264700	2.706605
H	-2.396620	1.966218	1.904223
C	-3.618617	-1.115671	2.647230
H	-3.003702	-2.947138	1.691529
H	-4.017980	0.859692	3.408597
H	-4.328448	-1.603271	3.307611
F	1.155699	-0.325588	1.409810
H	1.814696	0.573298	-0.530663
H	0.390193	2.493237	-0.435572
H	-1.199834	0.831404	-1.038894
B	0.418403	2.261137	1.813284
H	0.086950	1.710188	2.811135
F	1.168321	3.362006	1.933779

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M06-2X/6-31+G(d,p) SCF energy (au)	-434.23960002
M06-2X/6-31+G(d,p) enthalpy (au)	-434.08912202
M06-2X/6-31+G(d,p) free energy (au)	-434.13351502
MN15/6-311+G(2d,2p) SCF energy (au)	-434.02202173
MN15/6-311+G(2d,2p) enthalpy (au)	-433.87154373
MN15/6-311+G(2d,2p) free energy (au)	-433.91593673

Cartesian coordinates

ATOM	X	Y	Z
B	-2.445256	-0.769591	-1.138182
C	-5.143157	-1.994628	2.109743
C	-3.954205	-1.515243	1.565178
C	-3.574548	-0.177987	1.747316
C	-4.391647	0.653683	2.528633
C	-5.583574	0.177939	3.065579
C	-5.964553	-1.148020	2.853176
H	-5.421162	-3.033695	1.964890
H	-3.296836	-2.189040	1.024633
H	-4.092799	1.684736	2.698537
H	-6.212317	0.837642	3.655043
H	-6.889081	-1.523623	3.280006
C	-2.332659	0.371435	1.176511
C	-1.785206	0.065839	-0.019179
H	-0.825771	0.532185	-0.245362
H	-1.828922	1.101378	1.812170
F	-1.685736	-1.124444	-2.187508
H	-3.595125	-1.079929	-1.187018

TS-28

M06-2X/6-31+G(d,p) SCF energy (au)	-845.93926940
M06-2X/6-31+G(d,p) enthalpy (au)	-845.58561940
M06-2X/6-31+G(d,p) free energy (au)	-845.65093040
MN15/6-311+G(2d,2p) SCF energy (au)	-845.52978226
MN15/6-311+G(2d,2p) enthalpy (au)	-845.17613226
MN15/6-311+G(2d,2p) free energy (au)	-845.24144326

Cartesian coordinates

ATOM	X	Y	Z
B	-2.332722	0.015295	-0.400689
C	-4.228875	-0.297822	4.933878
C	-3.069920	0.031248	4.242454
C	-3.113311	0.382297	2.879655
C	-4.358467	0.394367	2.223306
C	-5.515751	0.060478	2.917178
C	-5.455320	-0.284752	4.268509
H	-4.178334	-0.565875	5.983871
H	-2.111579	0.015131	4.754583
H	-4.426468	0.684588	1.183206
H	-6.471108	0.073175	2.403076
H	-6.364520	-0.542382	4.802800
C	-1.843911	0.674021	2.231422
C	-1.555302	0.990401	0.935814
H	-0.494050	1.086168	0.713588
H	-0.990529	0.584243	2.905795
F	-1.275822	-0.357476	-1.204546
H	-2.966029	-0.841259	0.142112
O	-1.683228	2.744040	-0.945309
C	-2.295639	4.052041	-0.981864
C	-3.755108	3.749124	-0.511118
O	-3.549206	2.652658	0.411146
B	-2.411794	1.989021	-0.032238
H	-3.070238	0.825270	-0.975563
C	-1.532893	4.936595	0.003571
H	-0.475903	4.939604	-0.275038

H	-1.901477	5.966296	-0.016144
H	-1.620726	4.550161	1.023770
C	-2.187629	4.610029	-2.391671
H	-2.731515	5.557366	-2.469303
H	-1.137361	4.797296	-2.630498
H	-2.587313	3.910329	-3.127647
C	-4.432936	4.886824	0.233846
H	-4.496996	5.774660	-0.403858
H	-5.448151	4.589855	0.510678
H	-3.888603	5.143307	1.144345
C	-4.647970	3.246471	-1.644882
H	-5.571704	2.849682	-1.214901
H	-4.904804	4.057224	-2.332618
H	-4.161035	2.450494	-2.216137

TS-29

M06-2X/6-31+G(d,p) SCF energy (au)	-533.42923646
M06-2X/6-31+G(d,p) enthalpy (au)	-533.28916046
M06-2X/6-31+G(d,p) free energy (au)	-533.33589946
MN15/6-311+G(2d,2p) SCF energy (au)	-533.20160016
MN15/6-311+G(2d,2p) enthalpy (au)	-533.06152416
MN15/6-311+G(2d,2p) free energy (au)	-533.10826316

Cartesian coordinates

ATOM	X	Y	Z
C	-0.80430200	0.90356600	0.20417100
C	0.14032300	1.69474900	0.40114500
H	0.60295500	2.63282200	0.64317500
B	0.90231700	0.20824500	0.00724300
H	-0.04664800	-0.57892100	-0.19088500
C	-2.16018900	0.39574500	0.08259700
C	-2.47830000	-0.93134400	-0.21064100
C	-3.17786600	1.33984900	0.28815600
C	-3.81388300	-1.31395200	-0.29822500
H	-1.68909900	-1.65903400	-0.36901500
C	-4.50775900	0.94624100	0.19825500
H	-2.92077100	2.36947400	0.51521300
C	-4.82827300	-0.38002600	-0.09492100
H	-4.05949500	-2.34557400	-0.52611200
H	-5.29393600	1.67670500	0.35662700
H	-5.86744100	-0.68408200	-0.16483300
F	1.62915800	0.36797900	-1.16257200
F	1.64665500	-0.22146500	1.09524700

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M06-2X/6-31+G(d,p) SCF energy (au)	-533.54137051
M06-2X/6-31+G(d,p) enthalpy (au)	-533.39589451
M06-2X/6-31+G(d,p) free energy (au)	-533.44803351
MN15/6-311+G(2d,2p) SCF energy (au)	-533.31251473
MN15/6-311+G(2d,2p) enthalpy (au)	-533.16703873
MN15/6-311+G(2d,2p) free energy (au)	-533.21415773

Cartesian coordinates

ATOM	X	Y	Z
B	-2.74062500	-0.18125300	-1.12388800
C	-1.21949700	0.25877200	4.93485100

C	-1.94027300	0.05668200	3.76019900
C	-1.33096600	0.20876000	2.50696300
C	0.02490800	0.56855200	2.45635300
C	0.74528000	0.76991200	3.62751900
C	0.12571400	0.61614500	4.87060000
H	-1.70708600	0.13724600	5.89669400
H	-2.98954800	-0.22242300	3.80963400
H	0.52059900	0.69060600	1.49853700
H	1.79319000	1.04729600	3.57429200
H	0.69193200	0.77422000	5.78296800
C	-2.13937800	-0.01581900	1.30015900
C	-1.74732900	0.09447200	0.01591600
H	-0.72631300	0.38074300	-0.22546800
H	-3.17339100	-0.30312000	1.49573200
F	-2.39481500	-0.07782200	-2.40684500
F	-4.00470900	-0.53936500	-0.88808900

TS-30

M06-2X/6-31+G(d,p) SCF energy (au)	-945.22619734
M06-2X/6-31+G(d,p) enthalpy (au)	-944.87776434
M06-2X/6-31+G(d,p) free energy (au)	-945.13286034
MN15/6-311+G(2d,2p) SCF energy (au)	-944.80521716
MN15/6-311+G(2d,2p) enthalpy (au)	-944.45678416
MN15/6-311+G(2d,2p) free energy (au)	-944.52340216

Cartesian coordinates

ATOM	X	Y	Z
B	-2.74624900	-0.20989600	-0.72921800
C	-0.66873900	-0.41252200	5.19783500
C	-1.51597900	-0.20190500	4.11431200
C	-0.99320800	0.00591400	2.82825100
C	0.40059100	0.00331100	2.64743600
C	1.24476200	-0.20542000	3.72960400
C	0.71195100	-0.41458000	5.00533900
H	-1.08278600	-0.57426600	6.18741500
H	-2.59313500	-0.19848700	4.25676100
H	0.82256400	0.16664300	1.66111900
H	2.31985000	-0.20611600	3.58386500
H	1.37636100	-0.57829900	5.84789200
C	-1.92701300	0.22133500	1.72889700
C	-1.63657400	0.41153400	0.41822100
H	-0.60646700	0.40133000	0.07050100
H	-2.97984600	0.24020500	2.01414800
O	-1.79548000	2.51381200	-1.12756800
C	-2.13898500	3.83636400	-0.65134100
C	-3.59562000	3.62768300	-0.12368700
O	-3.53204000	2.28117700	0.40065700
B	-2.56413200	1.62910700	-0.36829700
H	-3.23981700	0.83215400	-1.31413700
C	-1.15714400	4.19266800	0.46459200
H	-0.13945500	4.11475500	0.07302000
H	-1.31455600	5.21363600	0.82418900
H	-1.25715100	3.50303500	1.30912300
C	-2.01816100	4.81746200	-1.80552700
H	-2.37945000	5.80628300	-1.50386800
H	-0.96920700	4.91080200	-2.09927100

H	-2.58954200	4.48098100	-2.67244600
C	-4.00239300	4.56659800	0.99963800
H	-3.94215500	5.60810300	0.66684200
H	-5.03503400	4.36019300	1.29365400
H	-3.36206100	4.43679300	1.87407100
C	-4.63373500	3.64922900	-1.24476300
H	-5.58443100	3.28292400	-0.84890000
H	-4.78312200	4.66245100	-1.62866900
H	-4.33348600	3.00414200	-2.07658300
F	-2.04528900	-0.90412700	-1.67644700
F	-3.80002400	-0.85996600	-0.14286600

TS-31

M06-2X/6-31+G(d,p) SCF energy (au)	-537.58325990
M06-2X/6-31+G(d,p) enthalpy (au)	-537.35229490
M06-2X/6-31+G(d,p) free energy (au)	-537.40124690
MN15/6-311+G(2d,2p) SCF energy (au)	-537.36469212
MN15/6-311+G(2d,2p) enthalpy (au)	-537.13372712
MN15/6-311+G(2d,2p) free energy (au)	-537.18267912

Cartesian coordinates

ATOM	X	Y	Z
O	-0.830556	0.290741	0.085438
C	-0.609463	1.726444	0.189793
C	-1.909938	2.304366	-0.466911
O	-2.902045	1.290931	-0.139007
B	-2.189796	0.148536	0.108426
H	-2.635169	-0.941981	-0.373464
C	-0.494462	2.062586	1.674926
H	0.308981	1.461708	2.108208
H	-0.256796	3.120025	1.820464
H	-1.421298	1.833904	2.208575
C	0.676671	2.070966	-0.540026
H	0.814133	3.156560	-0.572799
H	1.525827	1.633907	-0.008386
H	0.671308	1.683943	-1.560323
C	-2.366652	3.636520	0.102569
H	-1.592978	4.396969	-0.045571
H	-3.271831	3.963161	-0.415831
H	-2.588210	3.559377	1.168185
C	-1.826979	2.369012	-1.989512
H	-2.822343	2.584061	-2.386104
H	-1.144023	3.158579	-2.315010
H	-1.486522	1.416476	-2.406512
B	-3.064896	-1.520016	0.819829
F	-2.691267	-0.442289	1.723020
H	-2.359315	-2.475588	0.890067
H	-4.236651	-1.603241	0.629786

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M06-2X/6-31+G(d,p) SCF energy (au)	-334.88575990
M06-2X/6-31+G(d,p) enthalpy (au)	-334.73416790
M06-2X/6-31+G(d,p) free energy (au)	-334.77693190
MN15/6-311+G(2d,2p) SCF energy (au)	-334.68274155
MN15/6-311+G(2d,2p) enthalpy (au)	-334.53114955
MN15/6-311+G(2d,2p) free energy (au)	-334.57391355

Cartesian coordinates

ATOM	X	Y	Z
C	-0.87069900	0.69717200	0.71580300
C	0.35560700	0.77185500	0.76801300
H	1.41972400	0.70334700	0.68960700
B	-0.48439200	2.02320500	1.93961900
H	-1.02255500	2.94829600	1.39101600
C	-2.23015800	0.32999000	0.39451300
C	-2.43762200	-0.69160600	-0.54598200
C	-3.32311200	0.96448500	0.99453100
C	-3.73227300	-1.07107800	-0.87917900
H	-1.58277300	-1.17719800	-1.00551900
C	-4.61650700	0.57678400	0.65343500
H	-3.15016200	1.75189700	1.71914700
C	-4.82307300	-0.43756000	-0.28001200
H	-3.89145700	-1.86080200	-1.60595800
H	-5.46387600	1.06904100	1.11898800
H	-5.83309900	-0.73600600	-0.54205400
H	-1.00509400	1.53864000	2.90941800
H	0.67619100	2.27292700	2.15900300

TS-32

M06-2X/6-31+G(d,p) SCF energy (au)	-334.88340365
M06-2X/6-31+G(d,p) enthalpy (au)	-334.73319865
M06-2X/6-31+G(d,p) free energy (au)	-334.77457565
MN15/6-311+G(2d,2p) SCF energy (au)	-334.68066750
MN15/6-311+G(2d,2p) enthalpy (au)	-334.53046250
MN15/6-311+G(2d,2p) free energy (au)	-334.57368950

Cartesian coordinates

ATOM	X	Y	Z
C	-0.81633700	0.94622500	0.19989000
C	0.13766300	1.71451000	0.37770600
H	0.70264500	2.60048100	0.58625600
B	0.88429600	0.16598000	0.00424500
H	0.07148100	-0.71257000	-0.20537200
C	-2.16398400	0.42969800	0.08541500
C	-2.46946500	-0.89932900	-0.22082800
C	-3.20204300	1.35127700	0.30378000
C	-3.80008300	-1.30177400	-0.30759000
H	-1.67248000	-1.61451100	-0.38997500
C	-4.52633900	0.94022500	0.21483500
H	-2.96011400	2.38225600	0.54130100
C	-4.82914200	-0.38772000	-0.09110200
H	-4.03004700	-2.33502300	-0.54544900
H	-5.32277400	1.65724200	0.38453700
H	-5.86384700	-0.70726000	-0.16007500
H	1.47323800	0.37508400	-1.02167000
H	1.48124700	-0.11378800	1.00840900

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M06-2X/6-31+G(d,p) SCF energy (au)	-334.95206871
M06-2X/6-31+G(d,p) enthalpy (au)	-334.79686271
M06-2X/6-31+G(d,p) free energy (au)	-334.84324071
MN15/6-311+G(2d,2p) SCF energy (au)	-334.74623801

MN15/6-311+G(2d,2p) enthalpy (au)	-334.59103201
MN15/6-311+G(2d,2p) free energy (au)	-334.63354601

Cartesian coordinates

ATOM	X	Y	Z
B	-2.73010900	-0.18009900	-1.13393400
C	-1.22385200	0.25261100	4.92961800
C	-1.93785100	0.05526300	3.75036900
C	-1.32266100	0.21380600	2.49991400
C	0.03345500	0.57694100	2.45873300
C	0.74704700	0.77413000	3.63469400
C	0.12125500	0.61283400	4.87377100
H	-1.71581100	0.12560700	5.88855700
H	-2.98695800	-0.22579200	3.79255300
H	0.53257700	0.70541300	1.50374400
H	1.79454000	1.05448800	3.58874900
H	0.68238000	0.76766700	5.78989500
C	-2.12361300	-0.00694700	1.28862500
C	-1.73020700	0.09450100	-0.00337900
H	-0.69793700	0.37272000	-0.21404500
H	-3.16140400	-0.28627100	1.47917500
H	-2.41883200	-0.10058900	-2.28367200
H	-3.85306300	-0.48236000	-0.85252000

TS-33

M06-2X/6-31+G(d,p) SCF energy (au)	-746.66976851
M06-2X/6-31+G(d,p) enthalpy (au)	-746.31069951
M06-2X/6-31+G(d,p) free energy (au)	-746.56094051
MN15/6-311+G(2d,2p) SCF energy (au)	-746.27197610
MN15/6-311+G(2d,2p) enthalpy (au)	-745.91290710
MN15/6-311+G(2d,2p) free energy (au)	-745.97883910

Cartesian coordinates

ATOM	X	Y	Z
B	-3.00075000	-0.40049100	-1.05022200
C	-1.07122500	0.97929500	4.80145100
C	-1.87587400	0.62763000	3.71949700
C	-1.32708200	0.42915500	2.44440900
C	0.05939200	0.58405900	2.28300900
C	0.86424000	0.93236100	3.36192600
C	0.30251500	1.13369800	4.62537700
H	-1.51638200	1.13020700	5.77991900
H	-2.94744400	0.50669900	3.85770600
H	0.51221000	0.42295400	1.30935300
H	1.93478400	1.04407400	3.22041100
H	0.93423900	1.40394400	5.46563400
C	-2.22930100	0.09243700	1.32965600
C	-1.92822000	0.03561100	0.01806000
H	-0.90557300	0.25615500	-0.29225900
H	-3.26275100	-0.09833300	1.62468700
O	-2.24154700	2.68017100	-1.64584900
C	-2.27805900	3.82323000	-0.74164500
C	-3.75569300	3.78448800	-0.20282600
O	-4.12619000	2.38600600	-0.36765000
B	-3.25400800	1.86175600	-1.26363300
H	-3.47167600	0.82762200	-1.87524700

C	-1.23061700	3.56582700	0.33759200
H	-0.26029000	3.41869500	-0.14467500
H	-1.15533300	4.41671900	1.02041400
H	-1.46376700	2.67051000	0.91816100
C	-1.92586700	5.07337000	-1.53088400
H	-2.02607200	5.96053400	-0.89741100
H	-0.88790400	5.00828700	-1.86709100
H	-2.56575400	5.19102700	-2.40679400
C	-3.89937100	4.14841300	1.26563100
H	-3.54922900	5.17079800	1.44035500
H	-4.95285700	4.09241200	1.55140000
H	-3.33137700	3.46624300	1.90171800
C	-4.73073300	4.59091500	-1.05590300
H	-5.74886800	4.37505000	-0.72277500
H	-4.55046500	5.66453800	-0.95440300
H	-4.65039700	4.31880400	-2.11238200
H	-2.62637700	-0.88913400	-2.07805000
H	-4.09519600	-0.68136600	-0.65161700

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M06-2X/6-31+G(d,p) SCF energy (au)	-746.67331241
M06-2X/6-31+G(d,p) enthalpy (au)	-746.31301741
M06-2X/6-31+G(d,p) free energy (au)	-746.56448441
MN15/6-311+G(2d,2p) SCF energy (au)	-746.27645803
MN15/6-311+G(2d,2p) enthalpy (au)	-745.91616303
MN15/6-311+G(2d,2p) free energy (au)	-745.98105903

Cartesian coordinates

ATOM	X	Y	Z
B	-2.85670800	-0.33000200	-0.88047200
C	-0.70247700	0.01244800	5.09559400
C	-1.56737800	-0.00896600	4.00468400
C	-1.07736700	0.11967200	2.69629100
C	0.30530100	0.28112600	2.50465300
C	1.16785100	0.30539700	3.59350700
C	0.66729600	0.16927000	4.89133300
H	-1.09633900	-0.09122900	6.10137100
H	-2.63622400	-0.12840600	4.16047900
H	0.70694300	0.39295200	1.50251500
H	2.23378700	0.43169100	3.43367000
H	1.34522900	0.18788600	5.73878000
C	-2.03429600	0.09552000	1.58762500
C	-1.76130900	0.16871800	0.26583500
H	-0.72632900	0.24643400	-0.05746400
H	-3.08255900	0.04699200	1.88482200
O	-1.86291300	2.36608000	-1.17106900
C	-2.05113500	3.62797100	-0.49326100
C	-3.54489000	3.53220800	-0.04110700
O	-3.69503400	2.12081100	0.22505800
B	-2.73174700	1.46868500	-0.54903700
H	-3.29196500	0.70026800	-1.51526500
C	-1.07964800	3.67434600	0.68740700
H	-0.06479900	3.51690500	0.31140900
H	-1.11711600	4.64317500	1.19376300
H	-1.30169300	2.89029600	1.41820000
C	-1.75410800	4.75437200	-1.46938300

H	-2.00047800	5.72225200	-1.02030400
H	-0.68924700	4.75290000	-1.71751700
H	-2.32317800	4.63794200	-2.39341000
C	-3.87147500	4.30755100	1.22523600
H	-3.65964500	5.37306700	1.08699100
H	-4.93412500	4.19716800	1.45788700
H	-3.29317900	3.93916300	2.07481800
C	-4.52016700	3.89774900	-1.15931300
H	-5.52928900	3.61357700	-0.84996600
H	-4.50833700	4.97205800	-1.36532200
H	-4.27750000	3.36116600	-2.08182700
H	-2.27344700	-0.89389200	-1.75806800
H	-3.84080300	-0.81214600	-0.40427400

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M06-2X/6-31+G(d,p) SCF energy (au)	-746.66725437
M06-2X/6-31+G(d,p) enthalpy (au)	-746.30890037
M06-2X/6-31+G(d,p) free energy (au)	-746.55842637
MN15/6-311+G(2d,2p) SCF energy (au)	-746.27030107
MN15/6-311+G(2d,2p) enthalpy (au)	-745.91194707
MN15/6-311+G(2d,2p) free energy (au)	-745.97615507

Cartesian coordinates

ATOM	X	Y	Z
B	-2.53534300	0.02167100	-0.39545800
C	-0.69563100	-1.01659700	5.27763300
C	-1.44753600	-0.41128200	4.27585200
C	-0.88672200	-0.16030600	3.01335300
C	0.44445200	-0.53938700	2.76876200
C	1.19281500	-1.14621700	3.76840400
C	0.62522400	-1.38385900	5.02381300
H	-1.13739000	-1.20408100	6.25056500
H	-2.47860400	-0.12509100	4.46470400
H	0.88978000	-0.36550700	1.79474000
H	2.21907400	-1.43883000	3.57283900
H	1.21444400	-1.85920100	5.80163400
C	-1.71674200	0.48498500	2.00323400
C	-1.35623600	0.86949400	0.74729400
H	-0.32707500	0.74088500	0.42534400
H	-2.74887500	0.67062000	2.30206800
O	-1.56786400	2.85492700	-0.90643600
C	-2.19557000	4.15076600	-0.78347000
C	-3.58826000	3.79459600	-0.16506900
O	-3.27208200	2.63411700	0.63561700
B	-2.18848600	2.02250800	0.01771800
H	-2.95505800	0.92764400	-1.09727500
C	-1.32865700	4.98331200	0.16052700
H	-0.31310500	5.02430500	-0.24195700
H	-1.70756200	6.00514500	0.25531600
H	-1.28771200	4.52890400	1.15530400
C	-2.26059000	4.80144900	-2.15606800
H	-2.81823000	5.74270200	-2.10662600
H	-1.24768100	5.02122800	-2.50414300
H	-2.73922900	4.14468500	-2.88456600
C	-4.17189800	4.86624900	0.74155300
H	-4.31302300	5.80026100	0.18761800

H	-5.14641100	4.53836800	1.11370700
H	-3.52249100	5.05781700	1.59773700
C	-4.61362600	3.37691800	-1.21872700
H	-5.47648300	2.93663600	-0.71203000
H	-4.95235800	4.23874900	-1.80103800
H	-4.20241300	2.63293200	-1.90666900
H	-1.76828500	-0.68553900	-0.98345600
H	-3.41937400	-0.48693100	0.23034600

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M06-2X/6-31+G(d,p) SCF energy (au)	-746.71044635
M06-2X/6-31+G(d,p) enthalpy (au)	-746.34899635
M06-2X/6-31+G(d,p) free energy (au)	-746.60161835
MN15/6-311+G(2d,2p) SCF energy (au)	-746.30679667
MN15/6-311+G(2d,2p) enthalpy (au)	-745.94534667
MN15/6-311+G(2d,2p) free energy (au)	-746.01253767

Cartesian coordinates

ATOM	X	Y	Z
C	-1.50479700	0.96348300	0.65831200
C	-0.27594900	1.89695900	0.68503000
B	0.91642200	1.47554200	-0.21778900
H	-1.18333600	-0.05224900	0.91200100
C	-2.18493600	0.95757500	-0.69087400
C	-3.04937200	1.99776400	-1.05225300
C	-1.93827700	-0.05583100	-1.62258300
C	-3.64809500	2.02863800	-2.31007100
H	-3.25595300	2.79027700	-0.33597600
C	-2.53448600	-0.02982500	-2.88397300
H	-1.27458900	-0.87436900	-1.35533300
C	-3.39090400	1.01323700	-3.23225400
H	-4.31821600	2.84267400	-2.56989500
H	-2.33243300	-0.82767200	-3.59235700
H	-3.85770300	1.03373800	-4.21206200
H	1.76886500	2.26138700	-0.50464200
H	-0.54858700	2.93860300	0.46025400
H	-2.22754200	1.26595400	1.42553300
B	0.38148000	1.97484600	2.12105500
O	1.14987500	3.02505300	2.55675500
O	0.25674300	0.98240600	3.05994900
C	1.77841700	2.60856900	3.79490700
C	0.80071800	1.49814800	4.30203000
C	3.15805900	2.06468400	3.42811300
C	1.90793600	3.81113400	4.71466500
C	1.46611800	0.36180900	5.06015700
C	-0.37453700	2.05797100	5.10062100
H	3.71121000	2.84221500	2.89532000
H	3.72382500	1.78177900	4.32022000
H	3.07681400	1.19098000	2.77367300
H	2.29160600	3.50253400	5.69261900
H	2.61079400	4.52740700	4.28120500
H	0.94826800	4.31163700	4.85419100
H	1.96940400	0.74504800	5.95377700
H	0.70777100	-0.35908900	5.37662400
H	2.19752400	-0.15793300	4.43901400
H	-1.11086900	1.26332500	5.24508300

H	-0.05154600	2.41693400	6.08180400
H	-0.85728300	2.88257400	4.56719800
H	1.03854900	0.33787000	-0.56907300

TS-35

M06-2X/6-31+G(d,p) SCF energy (au)	-1158.41559720
M06-2X/6-31+G(d,p) enthalpy (au)	-1157.85139220
M06-2X/6-31+G(d,p) free energy (au)	-1158.30676920
MN15/6-311+G(2d,2p) SCF energy (au)	-1157.82475622
MN15/6-311+G(2d,2p) enthalpy (au)	-1157.26055122
MN15/6-311+G(2d,2p) free energy (au)	-1157.34832722

Cartesian coordinates

ATOM	X	Y	Z
C	-1.74765100	0.02771900	1.53904800
C	-0.87896900	1.22603900	1.08487600
B	0.86561800	0.24192000	0.18070000
H	-2.04163800	-0.56049400	0.66451100
C	-2.97901600	0.48470900	2.28322600
C	-2.96609900	0.61336300	3.67574100
C	-4.13398100	0.85189300	1.58277100
C	-4.08351000	1.09815100	4.35570300
H	-2.06803300	0.33321100	4.22083900
C	-5.25265500	1.33548500	2.25953200
H	-4.14467100	0.75510100	0.49915800
C	-5.23018200	1.46061800	3.64933300
H	-4.05994700	1.18978500	5.43768500
H	-6.14382000	1.61148400	1.70355200
H	-6.10146500	1.83503900	4.17767100
H	0.97376500	-0.52564500	1.08855300
H	-1.46298600	2.16302100	1.25628900
H	-1.14710500	-0.62021400	2.18329700
B	0.22065000	1.66858300	2.13406900
O	0.88827900	2.86348400	2.07730800
O	0.44242500	0.98243500	3.30090600
C	1.83868600	2.86223600	3.17152800
C	1.16861200	1.87493300	4.18318500
C	3.15965400	2.33456800	2.61606900
C	2.00198500	4.28383600	3.68215300
C	2.14320300	1.06011800	5.01700500
C	0.13196700	2.55192100	5.07755000
H	3.45668300	2.95804900	1.76875200
H	3.94886800	2.36989500	3.37250300
H	3.05506100	1.30463900	2.26178100
H	2.63489900	4.29728100	4.57557000
H	2.48203900	4.89386800	2.91251600
H	1.03716200	4.73260000	3.92523800
H	2.77080700	1.72192900	5.62283000
H	1.58705500	0.40348800	5.69134400
H	2.78572900	0.44276300	4.38705000
H	-0.42033800	1.78178700	5.62277700
H	0.60797200	3.21707400	5.80352900
H	-0.58255900	3.13094500	4.48378900
O	-0.41184700	2.66479500	-1.05177800
C	-0.83628600	2.68004700	-2.43727700
C	-2.18195800	1.88295800	-2.37606500

O	-1.96123700	0.99008700	-1.25564700
B	-0.99562300	1.57192000	-0.46849100
C	-0.97367600	4.12397300	-2.89103400
H	0.01254000	4.59516400	-2.90696900
H	-1.39150200	4.16685400	-3.90226100
H	-1.61642900	4.69418100	-2.21802300
C	0.24408200	1.96676700	-3.24722700
H	0.02031800	1.99828700	-4.31739700
H	1.19919800	2.46916500	-3.07358900
H	0.34635500	0.92240700	-2.93936400
C	-3.37692300	2.76086600	-2.00853500
H	-3.63853000	3.44020000	-2.82463900
H	-4.23653500	2.11689500	-1.80397900
H	-3.16945800	3.35335700	-1.11152600
C	-2.48767000	1.05698100	-3.61422800
H	-3.44203700	0.54027000	-3.48254800
H	-2.56672000	1.70479900	-4.49341600
H	-1.71314400	0.30962500	-3.79437500
H	0.32145700	-0.17122300	-0.80363900
H	1.64728300	1.13404800	0.05965400

TS-36

M06-2X/6-31+G(d,p) SCF energy (au)	-922.69595638
M06-2X/6-31+G(d,p) enthalpy (au)	-922.29639138
M06-2X/6-31+G(d,p) free energy (au)	-922.36192338
MN15/6-311+G(2d,2p) SCF energy (au)	-922.29656801
MN15/6-311+G(2d,2p) enthalpy (au)	-921.89700301
MN15/6-311+G(2d,2p) free energy (au)	-921.96253501

Cartesian coordinates

ATOM	X	Y	Z
O	-4.17265500	-0.94728000	-1.01800900
C	-4.58191200	0.09714700	-1.98964000
C	-3.21707400	0.78349700	-2.34008700
O	-2.26244800	-0.28366200	-2.16527000
B	-2.76538200	-1.22124400	-1.30212400
C	-5.62391700	1.01970600	-1.38631200
H	-6.54600100	0.46442100	-1.19335400
H	-5.27981500	1.47357300	-0.45818400
H	-5.85272600	1.80648200	-2.11268700
C	-5.16913800	-0.69569500	-3.15215200
H	-5.99539300	-1.30631400	-2.78080700
H	-5.55143500	-0.02004600	-3.92149000
H	-4.42387000	-1.35715600	-3.60296600
C	-3.13573300	1.25812200	-3.78441100
H	-3.92733400	1.98474200	-3.99298800
H	-2.17172300	1.74629200	-3.94699600
H	-3.22242700	0.42580200	-4.48439200
C	-2.84574300	1.92545300	-1.39637000
H	-2.93289100	1.64142200	-0.34576800
H	-1.81127000	2.21332100	-1.60013900
H	-3.48736600	2.79372400	-1.57297800
O	-3.97153500	-1.92792800	1.29131900
C	-4.98499100	-1.49447500	2.21751100
C	-4.58980600	-0.00007800	2.45428800
O	-4.04680900	0.38125600	1.17169300

B	-3.61631500	-0.79828600	0.54797600
C	-4.92106100	-2.36912600	3.45945000
H	-5.22354100	-3.38833800	3.20390400
H	-3.90864200	-2.40365300	3.86580300
H	-5.60133200	-1.99181700	4.23042700
C	-6.34573000	-1.64217800	1.53524800
H	-6.46068900	-2.67895800	1.20867900
H	-7.16474300	-1.39557100	2.21740100
H	-6.41502200	-0.99691200	0.65454500
C	-5.75608800	0.92007500	2.78016300
H	-6.25891000	0.59204100	3.69605000
H	-5.38759300	1.93766400	2.93786700
H	-6.48451900	0.93927600	1.96662900
C	-3.47807600	0.15681300	3.49011200
H	-2.64475500	-0.51733300	3.27084300
H	-3.10946400	1.18545300	3.45578700
H	-3.84124200	-0.04930800	4.50119700
H	-2.39363400	-0.82974700	0.17305800
F	-2.31630800	-2.48592500	-1.31724500

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M06-2X/6-31+G(d,p) SCF energy (au)	-922.72315556
M06-2X/6-31+G(d,p) enthalpy (au)	-922.32199956
M06-2X/6-31+G(d,p) free energy (au)	-922.39134856
MN15/6-311+G(2d,2p) SCF energy (au)	-922.32012002
MN15/6-311+G(2d,2p) enthalpy (au)	-921.91896402
MN15/6-311+G(2d,2p) free energy (au)	-921.98831302

Cartesian coordinates

ATOM	X	Y	Z
O	-3.77196500	-0.32077700	-0.88011100
C	-4.11375400	0.71656900	-1.87360800
C	-2.94768600	0.48056400	-2.88402800
O	-2.85231300	-0.93026800	-2.96741400
B	-2.89110900	-1.57258800	-1.70516400
C	-4.10524200	2.08499600	-1.21180300
H	-4.99056500	2.21611600	-0.58659900
H	-3.21202900	2.22382500	-0.59822200
H	-4.11325200	2.85623100	-1.98821600
C	-5.47739700	0.36927700	-2.45430800
H	-6.21997900	0.33503800	-1.65354500
H	-5.78342700	1.13649500	-3.17036600
H	-5.44206500	-0.59908000	-2.95896600
C	-3.26135800	1.02132500	-4.27246800
H	-3.48465700	2.09254800	-4.23874000
H	-2.39061200	0.87280200	-4.91621000
H	-4.10725300	0.49122400	-4.71381400
C	-1.62525700	1.06632100	-2.37639200
H	-1.41822500	0.76053800	-1.34701900
H	-0.82071300	0.68903700	-3.01266500
H	-1.62583200	2.15889800	-2.42713300
O	-3.89781400	-1.38872900	1.25181200
C	-4.92350700	-1.52143100	2.27350300
C	-5.69284900	-0.16234100	2.14498900
O	-5.52373300	0.15017200	0.73221800
B	-4.39607400	-0.51071400	0.34063700

C	-4.25101500	-1.74278800	3.61685500
H	-3.74658000	-2.71219000	3.61531400
H	-3.51050300	-0.96876400	3.82505500
H	-4.99722400	-1.74487700	4.41787400
C	-5.77612100	-2.72716600	1.88842900
H	-5.12659300	-3.60122900	1.80140400
H	-6.53808600	-2.92937400	2.64619000
H	-6.27017300	-2.57240200	0.92430200
C	-7.17747800	-0.24052200	2.45285600
H	-7.33191900	-0.57359500	3.48402500
H	-7.62709400	0.74962200	2.34195200
H	-7.68821600	-0.93052800	1.77929200
C	-5.03535300	0.97217600	2.92573300
H	-3.96327400	1.02970600	2.71292100
H	-5.49805800	1.91723800	2.62980300
H	-5.17066800	0.84031200	4.00256300
H	-1.89339000	-1.68667100	-1.04442400
F	-3.72754600	-2.66788400	-1.67333400

TS-37

M06-2X/6-31+G(d,p) SCF energy (au)	-1334.41780608
M06-2X/6-31+G(d,p) enthalpy (au)	-1333.81355908
M06-2X/6-31+G(d,p) free energy (au)	-1333.90545808
MN15/6-311+G(2d,2p) SCF energy (au)	-1333.82243084
MN15/6-311+G(2d,2p) enthalpy (au)	-1333.21818384
MN15/6-311+G(2d,2p) free energy (au)	-1333.31008284

Cartesian coordinates

ATOM	X	Y	Z
O	-1.12916800	-0.36709800	0.10683600
C	-0.73322300	-1.77193300	-0.07578200
C	0.70345700	-1.67255900	-0.66738900
O	1.34418300	-0.76254800	0.25035500
B	-0.35164800	0.49666000	0.96115200
C	-0.76658100	-2.48171100	1.27425400
H	-1.72974000	-2.28240200	1.74888200
H	0.04024100	-2.14492200	1.92871000
H	-0.66924100	-3.56014000	1.12346500
C	-1.72147000	-2.39445100	-1.04552500
H	-1.86997300	-1.75151700	-1.91502300
H	-2.67733400	-2.53983100	-0.53915700
H	-1.35055800	-3.36658600	-1.38137400
C	0.70509600	-1.06133000	-2.06642600
H	0.28207700	-1.76397200	-2.78889200
H	1.73333500	-0.84623700	-2.36469500
H	0.12248400	-0.13662600	-2.08603600
C	1.42819100	-3.01567500	-0.64451600
H	1.58254600	-3.35747400	0.38160600
H	2.40143200	-2.91094000	-1.12911500
H	0.85590100	-3.77373800	-1.18584200
O	-3.23886600	0.94278200	-0.54054500
C	-4.57096800	0.43011400	-0.66980200
C	-4.77871100	-0.35163200	0.67845000
O	-3.44575400	-0.74711400	1.02713100
B	-2.59603900	0.28547300	0.53937600
C	-5.52746600	1.60374400	-0.85845800

H	-5.32795000	2.08177700	-1.82190000
H	-5.39874500	2.35168300	-0.07421300
H	-6.56811900	1.26096500	-0.85543700
C	-4.64392600	-0.46569200	-1.90691600
H	-4.02971200	-1.35929300	-1.79597600
H	-4.27517100	0.10084300	-2.76690000
H	-5.67357600	-0.77622800	-2.11169500
C	-5.64869100	-1.59477700	0.56103500
H	-6.65311300	-1.33078700	0.21310900
H	-5.73944700	-2.07062500	1.54167000
H	-5.21710900	-2.31904400	-0.13337600
C	-5.30648000	0.54483800	1.80303700
H	-4.69465400	1.44608600	1.90780600
H	-5.25550700	-0.01247100	2.74243100
H	-6.34419500	0.84482900	1.63024700
H	-2.11271400	1.06943200	1.36809400
H	-0.11555000	0.23661400	2.08988000
B	2.64700900	-0.35886300	0.20363900
O	3.15772700	0.44866300	1.18487100
O	3.55640100	-0.69528900	-0.76847400
C	4.45070700	0.89579300	0.70879100
C	4.85035400	-0.24834700	-0.28330000
C	5.38484700	1.05806400	1.89579900
C	4.23037600	2.23559200	0.01011000
C	5.49689700	-1.44225600	0.41511900
C	5.69033600	0.20126200	-1.46608700
H	5.03316600	1.87917400	2.52563800
H	6.39689900	1.29723000	1.55331700
H	5.42143100	0.15081600	2.50133200
H	3.76309800	2.92565800	0.71672300
H	3.56507000	2.12745800	-0.85217800
H	5.17666400	2.66695000	-0.32808900
H	4.90268300	-1.76578600	1.27549200
H	6.50646600	-1.20122200	0.75903600
H	5.55972700	-2.27232500	-0.29343600
H	5.16047300	0.93727900	-2.07305900
H	5.92831400	-0.66032900	-2.09550100
H	6.63015000	0.64121800	-1.11734300
F	0.06108200	1.63977300	0.40497300