Electronic Supplementary Information

Catalytic acceptorless dehydrogenative borylation of styrenes enabled by a molecularly defined manganese complex

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1. General Information

All the reactions were conducted under the Ar and N_2 atmosphere unless otherwise mentioned. The glassware was dried in an oven. Solvents were dried under the standard protocol. All the solvents were degassed and stored over activated molecular sieves (4 Å). The chemicals were purchased from Avra Synthesis, Sigma-Aldrich, TCI, Alfa Aeser, Spectrochem, BLDpharm, and Combi-Blocks and used without further purification unless otherwise mentioned. Ligands and metal complexes were prepared according to our published procedures. ^{1}H, ^{13}C NMR spectra were collected using BRUKER (^{1}H: 500 MHz, ^{13}C: 126 MHz, ^{11}B: 161 MHz, and ^{19}F{^{1}H}:471 MHz) and JEOL (^{1}H: 400 MHz, ^{13}C{^{1}H}: 100 MHz) instrument. NMR data was taken in the ppm unit and referenced against the solvent residual peaks. Coupling constants (*J*) are reported in Hertz (Hz). Coupling patterns are indicated as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), td (triplet of doublet), or m (multiplet). FT-IR spectra were recorded by BRUKER FT–IR Spectrometer. GS-MS was performed on a Thermo Scientific ISQ QD Mass Spectrometer attached with Thermo Scientific TRACE 1300 gas chromatograph using an DB-5MS capillary column (30 m × 0.25 mm × 0.25 µm, Agilent Technologies) with helium as the carrier gas. Mass spectral analyses were done in Bruker micrOTOF-Q II Spectrometer. For thin-layer chromatography (TLC) analysis, Merck precoated TLC plates (silica gel 60 F254/ 0.25 mm) were used. Visualization was accomplished by UV light (254 nm) and an aqueous $KMnO_4$ stain. All the kinetics study has been done by GC-MS analysis using an appropriate internal standard.

2. Synthesis of ligands and Mn(I)-complexes

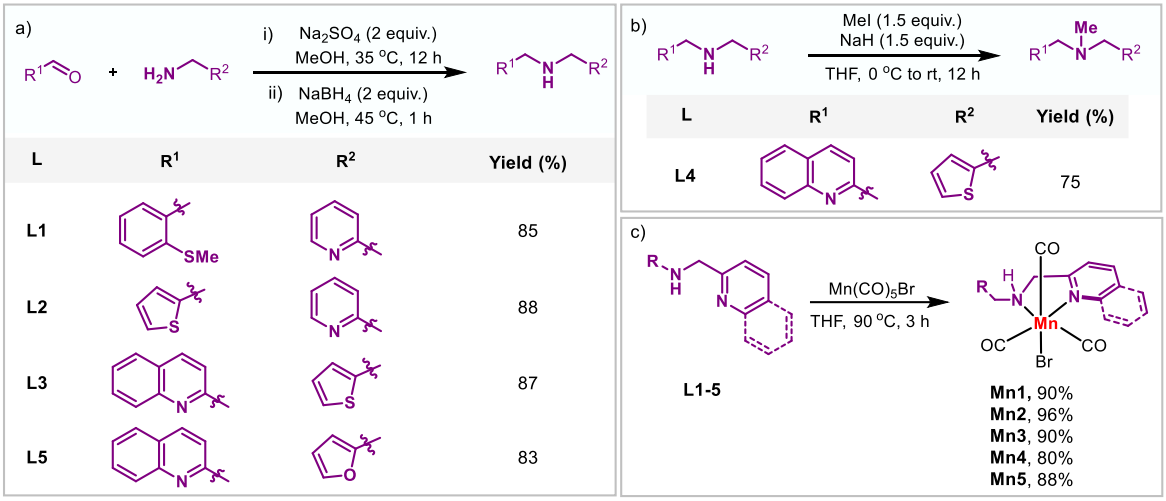


Fig. S1. Ligands **L1-5** and Mn complexes **Mn1-5**.

The ligands **L1-5** and the complexes **Mn1-5** were prepared following a modified procedure known in the literature.[1]

2.1. Synthesis of the ligands

N-(2-(methylthio)benzyl)-1-(pyridin-2-yl)methanamine (L1) and 1-(pyridin-2-yl)-N-(thiophen-2-ylmethyl)methanamine (L2):[1] The ligands were prepared according to the following modified procedures. Aldehyde (2.0 mmol) and 2-(aminomethyl)pyridine (2.1 mmol)

are mixed in methanol, and then sodium sulfate (4.0 mmol) was added. The reaction mixture was stirred at 35 °C for 12 h and then filtered. To the filtrate was added $NaBH_4$ (4.0 mmol) and heated at 45 °C for 1 h. The solvent was removed under a vacuum resulting in a white paste. The organic part was extracted with DCM and purified using flash column chromatography. The ligands were obtained as yellow oil. The spectral data resembles that reported in the literature.

N-(2-(methylthio)benzyl)-1-(pyridin-2-yl)methanamine (L1):[1b] Yield: 85% (1.70 mmol, 415.4 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.55 (d, *J* = 3.8 Hz, 1H), 7.67 - 7.60 (m, 1H), 7.36 (t, *J* = 8.1 Hz, 2H), 7.26 – 7.20 (m, 2H), 7.18 – 7.08 (m, 2H), 3.95 (s, 2H), 3.92 (s, 2H), 2.47 (s, 3H), 2.04 (br s, 1H).

1-(pyridin-2-yl)-N-(thiophen-2-ylmethyl)methanamine (L2):[1a] Yield: 88% (1.76 mmol, 360.0 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.52 (d, J = 4.3 Hz, 1H), 7.61 (td, J = 7.7, 1.6 Hz, 1H), 7.29 (d, J = 7.7 Hz, 1H), 7.18 (dd, J = 4.4, 2.1 Hz, 1H), 7.13 (dd, J = 7.4, 4.8 Hz, 1H), 6.95 – 6.89 (m, 2H), 4.01 (s, 2H), 3.92 (s, 2H), 2.13 (s, 1H).

1-(quinolin-2-yl)-N-(thiophen-2-ylmethyl)methanamine (L3): Quinoline-2-carbaldehyde (2.0 mmol) and thiophen-2-ylmethanamine (2.1 mmol) are mixed in methanol, and then sodium sulfate (2.5 mmol) was added. The reaction mixture was stirred at 35 °C for 12 h and then filtered. To the filtrate was added $NaBH_4$ (4.0 mmol) and heated at 45 °C for 1 h. The solvent was removed under a vacuum resulting in a white paste. The organic part was extracted with DCM and purified using flash column chromatography. The ligands were obtained as yellow oil. Yield: 87%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 (d, J = 8.5 Hz, 1H), 8.06 (d, J = 8.5 Hz, 1H), 7.80 (d, J = 8.2 Hz, 1H), 7.70 (t, J = 7.6 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.46 (d, J = 8.4 Hz, 1H), 7.24 (d, J = 4.9 Hz, 1H), 7.01 – 6.93 (m, 2H), 4.16 (s, 2H), 4.13 (s, 2H), 2.41 (br s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.7, 147.9, 143.7, 136.6, 129.7, 129.1, 127.7, 127.5, 126.8, 126.3, 125.5, 124.8, 120.7, 54.7, 48.2. **Selected IR** (ATR, cm^{-1}): 3062, 2918, 2835, 1614, 1598, 1501, 1423, 1110, 826, 745, 694. **HRMS (ESI) m/z:** $[M+H]^+$ Calculated for $[C_{15}H_{15}N_2S^+]$ 255.0950, found 255.0956.

N-methyl-1-(quinolin-2-yl)-N-(thiophen-2-ylmethyl)methanamine (L4): A solution of 1-(quinolin-2-yl)-N-(thiophen-2-ylmethyl)methanamine (**L3**) (0.5 mmol) in dry THF (3 ml) was cooled to 0 °C and NaH (1.5 equiv.) was added in one portion. The resulting mixture was stirred at that temperature for 30 min, and methyl iodide (1.5 equiv.) was added dropwise. The solution was warmed to room temperature and stirred overnight. The reaction was quenched with water. The organic part was extracted with EtOAc and purified using flash column chromatography. Yield: 75%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15 (d, J = 8.4 Hz, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.69 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.25 (s, 1H), 7.03 – 6.91 (m, 2H), 3.89 (d, J = 7.0 Hz, 4H), 2.35 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.5, 147.7, 142.7, 136.6, 129.4, 129.1, 127.64, 127.57, 126.6, 126.2, 126.0, 125.1, 121.1, 63.6, 56.6, 42.6. **Selected IR** (ATR, cm^{-1}): 2919, 2835, 1613, 1590, 1410, 1100, 810, 682. **GC-MS (ESI) m/z:** [M] Calculated for $[C_{16}H_{16}N_2S]$ 268.10, found 268.24.

1-(furan-2-yl)-N-(quinolin-2-ylmethyl)methanamine (L5): Quinoline-2-carbaldehyde (2.0 mmol) and furan-2-ylmethanamine (2.1 mmol) are mixed in methanol, and then sodium sulfate (2.5 mmol) was added. The reaction mixture was stirred at 35 °C for 12 h and then filtered. To the filtrate was added $NaBH_4$ (4.0 mmol) and heated at 45 °C for 1 h. The solvent was removed

under a vacuum, resulting in a white paste. The organic part was extracted with DCM and purified using flash column chromatography. The ligands were obtained as a yellow oil. Yield: 83%. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 – 8.03 (m, 2H), 7.78 (d, J = 8.2 Hz, 1H), 7.75 – 7.57 (m, 2H), 7.50 (t, J = 7.5 Hz, 1H), 7.42 (s, 1H), 7.38 – 7.24 (m, 1H), 6.34 – 6.20 (m, 1H), 4.11 (s, 2H), 3.91 (s, 2H), 3.00 (br s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.8, 153.7, 147.8, 142.1, 136.6, 129.6, 129.1, 127.7, 127.4, 126.2, 120.7, 110.3, 107.4, 54.6, 45.9. **Selected IR** (ATR, cm^{-1}): 3051, 2924, 2850, 2364, 1618, 1598, 1505, 1425, 1147, 1011, 826, 729. **HRMS (ESI) m/z:** $[M+H]^+$ Calculated for $[C_{15}H_{15}N_2O^+]$ 239.1179, found 239.1188.

2.2. Synthesis of the Mn(I)-complexes

Mn1-3, 5: To a solution of the ligand (0.20 mmol) in dry THF (2 mL) was added $Mn(CO)_5Br$ (0.21 mmol, 57.7 mg) under argon atmosphere. The resulting yellow-colored solution was heated at 90 ^{o}C for 3h, during which time the color changed to dark orange or brown. The solution was cooled to ambient temperature, and the solvent was removed under a vacuum. The resulting orange or yellow residue was washed with hexane and dried under vacuum to yield the complexes as orange or yellow-colored solid. The crystal suitable for the single crystal XRD was obtained by the slow diffusion of Et_2O into a saturated solution of **Mn3** in THF.

Mn4: To a solution of the ligand **L4** (0.10 mmol) in dry THF (0.3 mL) was added $Mn(CO)_5Br$ (0.11 mmol, 30.2 mg) under argon atmosphere. The resulting yellow-colored solution was heated at 85 ^{o}C for 3h. The solution was cooled to ambient temperature, and the solvent was removed under a vacuum. The resulting orange or yellow residue was washed with hexane and dried under vacuum to yield the complexes as orange-colored solid. A saturated solution of the complex was prepared in chloroform and a few drops of methanol was added. The resulting mixture was kept for crystallization under room temperature to yield orange colored block type crystals suitable for single crystal XRD.

Mn1:[1b] Yield: 90% (0.18 mmol, 83.4 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.00 (s, 1H), 7.73 (br s, 1H), 7.53 – 6.93 (m, 6H), 5.10 – 4.72 (m, 1H), 4.69 – 4.35 (m, 1H), 4.17 (br s, 1H), 3.97 (s, 1H), 2.53 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 222.9, 221.4, 221.1, 158.9, 153.8, 138.4, 138.2, 133.6, 130.8, 129.8, 127.1, 125.7, 124.7, 121.3, 58.6, 56.9, 16.2.

Mn2:[1a] Yield: 96% (0.19 mmol, 81.2 mg). **^{1}H NMR** (500 MHz, CDCl3) δ 9.02 (s, 1H), 8.10 – 7.60 (s, 1H), 7.56 – 6.69 (m, 5H), 4.94 (s, 1H), 4.58 – 3.46 (m, 4H). **^{13}C NMR** (126 MHz, CDCl3) δ 222.7, 221.2, 221.0, 158.4, 154.0, 138.3, 137.7, 128.8, 127.7, 126.9, 124.9, 121.4, 57.3, 53.6

Mn3: Yield: 90% (85 mg, 0.18 mmol). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.18 (d, *J* = 8.7 Hz, 1H), 8.19 (d, *J* = 8.1 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 8.2 Hz, 1H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.38 (br s, 1H), 7.25 (br s, 1H), 7.20 – 7.14 (m, 1H), 7.08 (br s, 1H), 5.04 (d, J = 14.5 Hz, 1H), 4.45 (dd, *J* = 16.4, 3.9 Hz, 1H), 4.34 (t, *J* = 13.2 Hz, 2H), 4.00 (m, *J* = 12.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 222.3, 221.3, 220.4, 160.6, 148.6, 139.6, 137.8, 131.8, 130.0, 128.9, 128.8, 128.6, 127.9, 127.9, 127.1, 117.9, 59.3, 53.1. Selected **IR** (ATR, cm^{-1}): 3212 (s, ν_{NH}), 2018 (s, ν_{CO}), 1936 (s, ν_{CO}), 1907 (s, ν_{CO}), 1602, 1513, 1433, 1005, 951, 830. **HRMS (ESI) m/z:** Calculated for $[C_{18}H_{14}MnN_2O_3S; [M – Br]^+]$ 393.0106, found 393.0105.

Mn4: Yield: 80% (78 mg, 0.16 mmol). **^{1}H NMR** (500 MHz, $CDCl_3$) (500 MHz, $CDCl_3$) δ 222.5, 8.88 (s, 1H), 8.31 (d, *J* = 8.3 Hz, 1H), 7.96 (t, *J* = 8.6 Hz, 2H), 7.72 (s, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.10 – 7.04 (m, 1H), 6.89 (s, 1H), 5.16 (d, *J* = 16.3 Hz, 1H), 4.59 (d, *J* = 14.4 Hz, 1H), 4.22 (d, *J* = 14.7 Hz, 1H), 4.10 (d, *J* = 16.2 Hz, 1H), 3.15 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.8, 149.2, 140.0, 132.4, 132.2, 131.6, 129.3, 128.6, 128.4, 127.9, 127.8, 127.6, 119.3, 63.1, 60.9, 48.2. Selected **IR** (ATR, cm^{-1}): 2014 (ν_{CO}), 1917 (ν_{CO}), 1905 (ν_{CO}), 1598, 1513, 1038, 844, 782, 684. **HRMS (ESI) m/z:** Calculated for $[C_{19}H_{16}MnN_2O_3S; [M - Br]^+]$ 407.0262, found 407.0253.

Mn5: Yield: 88% (80.5 mg, 0.17 mmol). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.17 (d, *J* = 8.7 Hz, 1H), 8.21 (d, *J* = 7.6 Hz, 1H), 7.98 – 7.81 (m, 2H), 7.65 (t, *J* = 7.1 Hz, 1H), 7.49 (s, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 6.61 – 6.34 (m, 2H), 4.69 (d, *J* = 10.9 Hz, 1H), 4.47 (s, 2H), 4.23 (d, *J* = 9.0 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 222.4, 221.2, 220.5, 160.8, 149.5, 148.6, 143.6, 139.6, 131.8, 129.9, 128.8, 128.7, 127.8, 117.8, 111.2, 110.9, 59.8, 51.1. Selected **IR** (ATR, cm^{-1}): 2020 (s, ν_{CO}), 1931 (s, ν_{CO}), 1892 (s, ν_{CO}), 1604, 1513, 1433, 1147, 820 747, 630. **HRMS (ESI) m/z:** Calculated for $[C_{18}H_{14}MnN_2O_4; [M - Br]^+]$ 377.0334, found 377.0305.

2.3 Crystal data for Mn3.

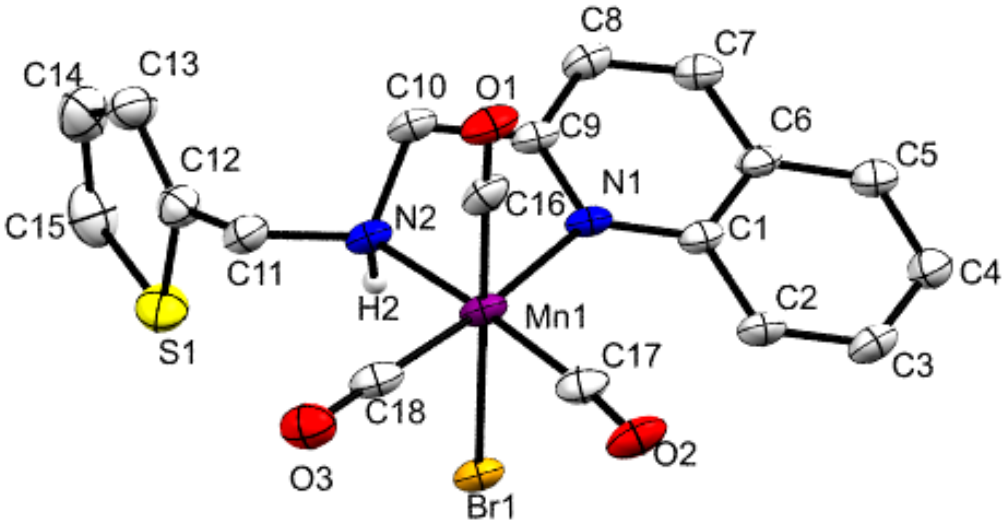


Fig. S2. ORTEP diagram of **Mn3** (CCDC = 2192558; 50% probability ellipsoids).[2]

Table S1. Crystal data and structure refinement for **Mn3**.

Empirical formula	$C_{18}H_{14}BrMnN_2O_3S$
Formula weight	473.22
Temperature/K	100.00(13)
Crystal system	triclinic
Space group	P-1
a/Å	7.6734(2)
b/Å	11.8500(3)
c/Å	13.3321(3)
α/°	104.364(2)
β/°	97.514(2)
γ/°	93.655(2)
Volume/Å^3	1158.45(5)
Z	2
ρ_{calc}g/cm^3	1.357
μ/mm^{-1}	7.640
F(000)	472.0

Crystal size/mm^3	0.1 × 0.05 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.924 to 136.522
Index ranges	-9 ≤ h ≤ 9, -12 ≤ k ≤ 14, -16 ≤ l ≤ 15
Reflections collected	16706
Independent reflections	4196 [R_{int} = 0.0582, R_{sigma} = 0.0413]
Data/restraints/parameters	4196/0/235
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0398, wR_2 = 0.1099
Final R indexes [all data]	R_1 = 0.0426, wR_2 = 0.1128
Largest diff. peak/hole / e Å^{-3}	1.23/-0.66

Table S2. Selected bond lengths and bond angles of **Mn3**.

Interatomic distances (Å)			
Mn(1)-Br(1)	2.5397(5)	Mn(1)-C(18)	1.799(3)
Mn(1)-N(1)	2.138(2)	Mn(1)-C(17)	1.812(3)
Mn(1)-N(2)	2.082(2)	Mn(1)-C(16)	1.802(3)
Bond angles(°)			
N(1)-Mn(1)-Br(1)	89.19(6)	C(17)-Mn(1)-Br(1)	90.15(9)
N(2)-Mn(1)-Br(1)	84.86(6)	C(17)-Mn(1)-N(1)	103.43(11)
N(1)-Mn(1)-N(2)	77.11(8)	C(17)-Mn(1)-N(2)	174.97(11)
C(18)-Mn(1)-Br(1)	87.94(9)	C(16)-Mn(1)-Br(1)	178.89(9)
C(18)-Mn(1)-N(1)	170.47(11)	C(16)-Mn(1)-N(1)	91.87(11)
C(18)-Mn(1)-N(2)	93.58(11)	C(16)-Mn(1)-N(2)	95.71(10)
C(18)-Mn(1)-C(17)	85.66(13)	C(16)-Mn(1)-C(17)	89.27(12)
C(18)-Mn(1)-C(16)	91.07(13)		

2.4. Crystal data for Mn4.

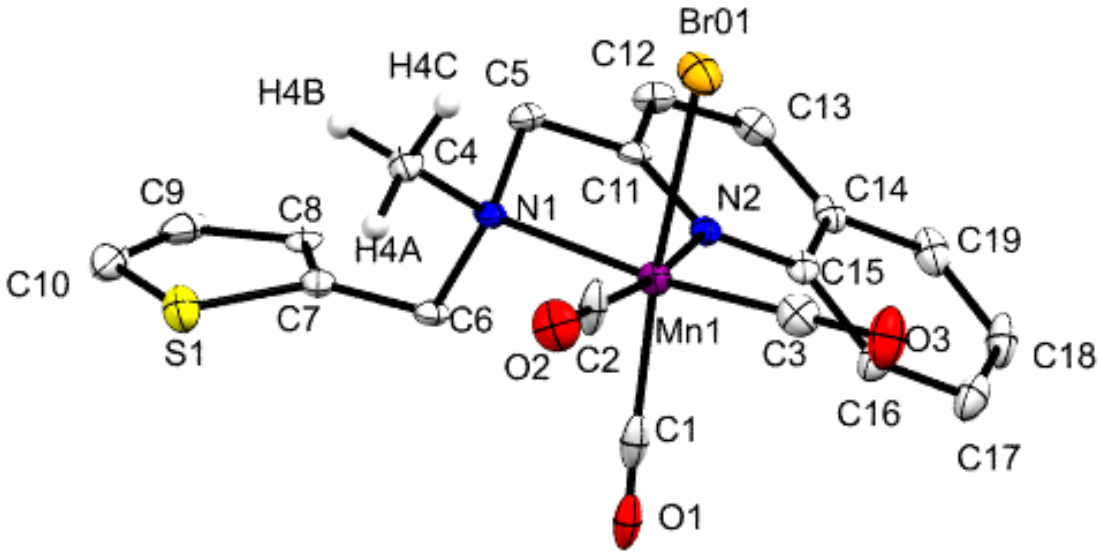


Fig. S3. ORTEP diagram of **Mn4** (CCDC = 2297411; 50% probability ellipsoids).[3]

Table S3. Crystal data and structure refinement for **Mn4**.

Empirical formula	$C_{19}H_{16}BrMnN_2O_3S$
Formula weight	487.25
Temperature/K	106(9)

Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.2068(4)
b/Å	15.5782(5)
c/Å	9.4496(3)
α/°	90
β/°	98.364(3)
γ/°	90
Volume/Å^3	1923.46(11)
Z	4
ρ_{calc}g/cm^3	1.683
μ/mm^{-1}	2.894
F(000)	976.0
Crystal size/mm^3	0.002 × 0.002 × 0.001
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.068 to 54.164
Index ranges	-16 ≤ h ≤ 16, -19 ≤ k ≤ 19, -12 ≤ l ≤ 11
Reflections collected	24716
Independent reflections	4053 [R_{int} = 0.0989, R_{sigma} = 0.0501]
Data/restraints/parameters	4053/0/233
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0504, wR_2 = 0.1353
Final R indexes [all data]	R_1 = 0.0586, wR_2 = 0.1398
Largest diff. peak/hole / e Å^{-3}	1.63/-1.02

Table S4. Selected bond lengths and bond angles of **Mn4**.

Interatomic distances (Å)			
Mn(1)-Br(1)	2.5289(7)	Mn(1)-C(1)	1.905(5)
Mn(1)-N(1)	2.153(3)	Mn(1)-C(2)	1.804(4)
Mn(1)-N(2)	2.107(3)	Mn(1)-C(3)	1.812(4)
Bond angles(°)			
N(1)-Mn(1)-Br(1)	90.03(8)	C(2)-Mn(1)-Br(1)	85.56(15)
N(2)-Mn(1)-Br(1)	92.20(9)	C(2)-Mn(1)-N(1)	94.20(15)
N(1)-Mn(1)-N(2)	78.30(12)	C(2)-Mn(1)-N(2)	172.19(15)
C(1)-Mn(1)-Br(1)	171.34(12)	C(3)-Mn(1)-Br(1)	83.83(13)
C(1)-Mn(1)-N(1)	97.59(14)	C(3)-Mn(1)-N(1)	173.34(16)
C(1)-Mn(1)-N(2)	93.38(15)	C(3)-Mn(1)-N(2)	99.33(15)
C(1)-Mn(1)-C(2)	89.75(19)	C(3)-Mn(1)-C(2)	87.88(17)
C(1)-Mn(1)-C(3)	88.73(18)		

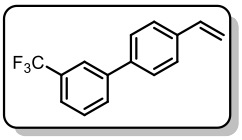
3. Synthesis of starting materials

3.1. General procedure A

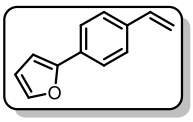
In an oven-dried 25 mL Schlenk tube was added $Pd(OAc)_2$ (0.15 mmol, 34 mg), PPh_3 (0.30 mmol, 79.0 mg), boronic acid (6 mmol), 4-bromostyrene (3 mmol, 393 μL), Na_2CO_3 (12 mmol, 1.9 g), PhMe (15 mL), EtOH (4.5 mL), H_2O (4.5 mL) under nitrogen atmosphere and the tube was sealed. The mixture was transferred to a pre-heated oil bath at 100 °C. After 24 h, the reaction mixture was cooled, and water (2.0 mL) was added. The mixture was filtered and extracted with EtOAc. The combined organic layer was dried over Na_2SO_4, and the solvent

was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography with hexane/EtOAc as eluent.

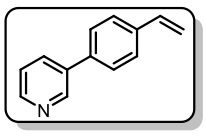
3-(trifluoromethyl)-4'-vinyl-1,1'-biphenyl: Yield: 80% (2.40 mmol, 596 mg). **^{1}H NMR** (500 MHz, CDCl3) δ 7.86 (s, 1H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.66 – 7.45 (m, 6H), 6.78 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.84 (d, *J* = 17.5 Hz, 1H), 5.33 (d, *J* = 11.0 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.7, 139.2, 137.5, 136.3, 131.4 (q, *J* = 31.9 Hz), 130.3, 129.4, 127.4, 127.0, 124.4 (q, *J* = 272.2 Hz), 124.1 (q, *J* = 4.0 Hz), 123.8 (q, *J* = 4.2 Hz), 114.6. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -62.59. Selected **IR** (ATR, cm^{-1}): 3037, 2932, 1630, 1485, 1441, 1326, 1253, 1155, 1114, 914, 799. **GC-MS (ESI) m/z:** [M] Calculated for [$C_{15}H_{11}F_3$] 248.08, found 247.95.



2-(4-vinylphenyl)furan: Yield: 75% (2.25 mmol, 383 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.50 – 7.38 (m, 3H), 6.72 (dd, *J* = 17.5, 10.8 Hz, 1H), 6.66 (d, *J* = 3.7 Hz, 1H), 6.48 (dd, *J* = 3.4, 1.8 Hz, 1H), 5.77 (d, *J* = 17.7 Hz, 1H), 5.26 (d, *J* = 11.0 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.0, 142.3, 136.7, 136.6, 130.4, 126.7, 124.0, 113.9, 111.9, 105.3. Selected **IR** (ATR, cm^{-1}): 2924, 1622, 1600, 1406, 1151, 1120, 1007, 900, 842, 799. **HRMS (ESI) m/z:** $[M+H]^+$ Calculated for [$C_{12}H_{11}O^+$] 171.0804, found 171.0785.



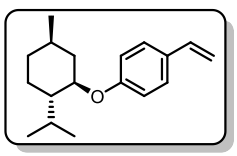
3-(4-vinylphenyl)pyridine: Yield: 60% (1.80 mmol, 326 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.86 (d, *J* = 2.7 Hz, 1H), 8.58 (dd, *J* = 4.9, 1.5 Hz, 1H), 7.90 – 7.82 (m, 1H), 7.60 – 7.44 (m, 4H), 7.35 (dd, *J* = 7.9, 4.9 Hz, 1H), 6.76 (dd, *J* = 17.7, 11.0 Hz, 1H), 5.81 (d, *J* = 17.7 Hz, 1H), 5.31 (d, *J* = 11.0 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.6, 148.3, 137.6, 137.2, 136.3, 136.3, 134.2, 127.4, 127.0, 123.7, 114.7. Selected **IR** (ATR, cm^{-1}): 3031, 2924, 1629, 1575, 1474, 1394, 992, 908, 846, 803. **GC-MS (ESI) m/z:** [M] Calculated for [$C_{13}H_{11}N$] 181.09, found 181.02.



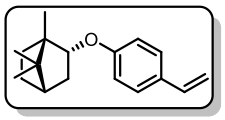
3.2. General procedure B

To an oven-dried 25 mL Schlenk round-bottomed flask was added 4-hydroxystyrene (3 mmol, 360 mg), alcohol (3 mmol), PPh_3 (3 mmol, 787 mg), and THF (12 mL) under N_2 atmosphere. The mixture was cooled at 0 °C, and to this, diisopropyl azodicarboxylate (DIAD, 3 mmol, 590 µL) was added. The reaction was allowed to warm to room temperature and stirred for 30 h. The resulting solution was diluted with H_2O (15 mL) and extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4 and purified by silica gel column chromatography with hexane/EtOAc (98:2) as eluent.

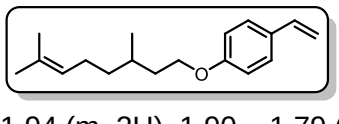
1-(((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)-4-vinylbenzene: Yield: 30% (0.90 mmol, 233 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 8.2 Hz, 2H), 6.66 (dd, *J* = 17.7, 10.7 Hz, 1H), 5.60 (d, *J* = 17.7 Hz, 1H), 5.11 (d, *J* = 11.0 Hz, 1H), 4.63 (s, 1H), 2.09 (d, *J* = 14.0 Hz, 1H), 1.82 – 1.56 (m, 5H), 1.09 – 0.97 (m, 2H), 0.93 (d, *J* = 6.7 Hz, 3H), 0.86 (d, *J* = 6.7 Hz, 3H), 0.82 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.3, 136.5, 130.0, 127.6, 115.7, 111.3, 73.5, 48.0, 37.8, 35.2, 29.4, 26.3, 25.00, 22.4, 21.2, 21.0. Selected **IR** (ATR, cm^{-1}): 2958, 2870, 1604, 1507, 1456, 1242, 1172, 1015, 829, 789. **GC-MS (ESI) m/z:** [M] Calculated for [$C_{18}H_{26}O$] 258.20, found 258.48.



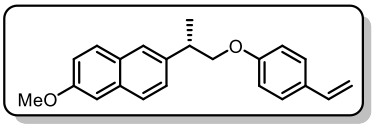
(1S,2R,4S)-1,7,7-trimethyl-2-(4-vinylphenoxy)bicyclo[2.2.1]heptane: Yield: 32% (0.96, mmol, 246 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.6 Hz, 2H), 6.81 (d, *J* = 8.5 Hz, 2H), 6.65 (dd, *J* = 17.6, 10.8 Hz, 1H), 5.59 (d, *J* = 17.6 Hz, 1H), 5.10 (d, *J* = 10.9 Hz, 1H), 4.09 – 4.02 (m, 1H), 1.87 – 1.80 (m, 2H), 1.78 – 1.72 (m, 2H), 1.64 – 1.58 (m, 1H), 1.15 – 1.10 (m, 2H), 1.06 (s, 3H), 0.99 (s, 3H), 0.88 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.9, 136.5, 130.0, 127.4, 115.5, 111.2, 84.7, 49.3, 47.1, 45.4, 39.6, 34.3, 27.5, 20.4, 20.2, 11.9. Selected **IR** (ATR, cm^{-1}): 2950, 2925, 2876, 1629, 1606, 1507, 1453, 1244, 1062, 1009, 831. **GC-MS (ESI) m/z:** [M] Calculated for [$C_{18}H_{24}O$] 256.18, found 255.91.



1-((3,7-dimethyloct-6-en-1-yl)oxy)-4-vinylbenzene: Yield: 40% (1.20 mmol, 310 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.3 Hz, 2H), 6.86 (d, *J* = 8.3 Hz, 2H), 6.66 (dd, *J* = 17.5, 10.9 Hz, 1H), 5.60 (d, *J* = 17.6 Hz, 1H), 5.12 (d, *J* = 10.5 Hz, 2H), 4.06 – 3.93 (m, 2H), 2.09 – 1.94 (m, 2H), 1.90 – 1.79 (m, 1H), 1.69 (s, 3H), 1.62 (s, 3H), 1.61 – 1.56 (m, 1H), 1.46 – 1.36 (m, 1H), 1.33 – 1.15 (m, 2H), 0.96 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.1, 136.4, 131.4, 130.4, 127.5, 124.8, 114.7, 111.5, 66.5, 37.3, 36.3, 29.7, 25.9, 25.6, 19.7, 17.8. Selected **IR** (ATR, cm^{-1}): 2961, 2916, 1740, 1606, 1509, 1246, 1174, 988, 898, 832. **GC-MS (ESI) m/z:** [M] Calculated for [$C_{18}H_{26}O$] 258.20, found 258.48.



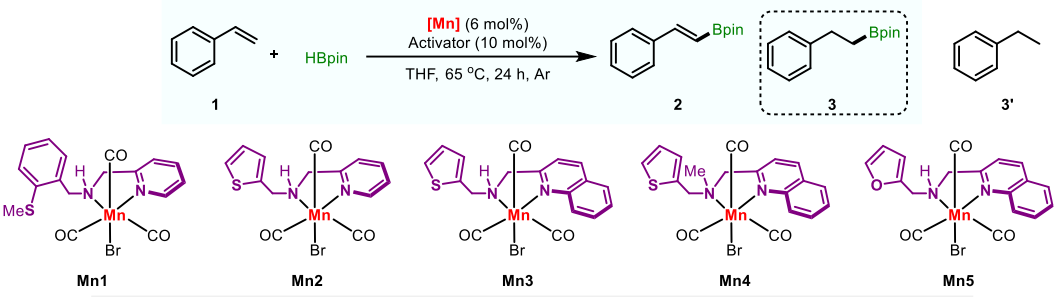
(S)-2-methoxy-6-(1-(4-vinylphenoxy)ethyl)naphthalene: Yield: 80% (2.40 mmol, 764 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.60 (s, 1H), 7.35 (d, *J* = 8.5 Hz, 1H), 7.27 (d, *J* = 8.9 Hz, 2H), 7.13 – 7.05 (m, 2H), 6.80 (d, *J* = 8.6 Hz, 2H), 6.60 (dd, *J* = 17.6, 10.9 **Hz, 1H), 5.55 (d, *J* = 17.5 Hz, 1H), 5.06 (d, *J* = 10.9 Hz, 1H),** 4.12 (dd, *J* = 9.2, 5.9 Hz, 1H), 3.98 (dd, *J* = 9.2, 7.8 Hz, 1H), 3.86 (s, 3H), 3.37 – 3.27 (m, 1H), 1.44 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.0, 157.6, 138.9, 136.4, 133.6, 130.6, 129.3, 129.2, 127.5, 127.1, 126.6, 125.7, 119.0, 114.8, 111.6, 105.8, 73.7, 55.4, 39.6, 18.4. Selected **IR** (ATR, cm^{-1}): 2961, 2909, 2858, 1629, 1602, 1507, 1482, 1388, 1237, 1165, 1023, 836. **HRMS (ESI) m/z:** $[M+H]^+$ Calculated for [$C_{22}H_{23}O_2^+$] 319.1693, found 319.1690.



4. Detailed optimization of the Mn(I)-catalyzed dehydrogenative borylation of styrene

General procedure: In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar, **[Mn]** (0.006 mmol), base (0.01 mmol), solvent (33 µL), alkene (0.1 mmol) and HBpin (0.15 mmol) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 ^{o}C in a preheated oil bath. After 24 h the reaction was cooled to room temperature 1 mL of $CHCl_3$ was added. The mixture was filtered through a short plug of silica. The combined organic layer was evaporated, and mesitylene (0.1 mmol, 14 µL) was added. The yield and selectivity of the products were measured by ^{1}H NMR analysis.

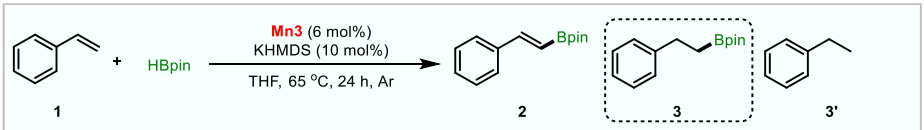
Table S5. Screening of Mn(I)-catalyst and base[a]



Entry	[Mn]	Activator	Yield of 2 (%)	Yield of 3 (%)	Selectivity 2:3:3'
1	**Mn1**	KO^{t}Bu	30	5	86:14:0
2	**Mn2**	KO^{t}Bu	37	8	83:17:0
3	**Mn3**	KO^{t}Bu	46	7	88:12:0
4	**Mn3**	KHMDS	76	6	93:7:0
5	**Mn4**	KHMDS	20[b]	-	-
6	**Mn4**	-	n.d.	n.d.	-
7	**Mn5**	KHMDS	37	7	84:16:0
8	**Mn3**	LiHMDS	62	6	91:9:0
9	**Mn3**	LiEt$_3$BH	29	19	60:40:0
10	**Mn3**	KOMe	23	8	74:26:0
11	**Mn3**	KH	33	7	82:18:0

[a]Reaction conditions: **1** (0.1 mmol), HBpin (0.15 mmol), [**Mn**] (6 mol%), activator (10 mol%), THF (33 μL), 65 °C, 24 h, Ar. Yields were determined by ^{1}H NMR using mesitylene as the internal standard, n.d. = not detected. [b]Isolated yield.

Table S6. Screening of solvent[a]



Entry	Solvent	Yield of 2 (%)	Yield of 3 (%)	Selectivity 2:3:3'
1	THF	76	6	93:7:0
2	1,4-dioxane	40	10	80:20:0
3	CH_2Cl_2	<10	<10	-
4	PhMe	<10	<10	-
5	Benzene	<10	<10	-
6	CH_3CN	41	10	80:20:0

[a]Reaction conditions: **1** (0.1 mmol), HBpin (0.15 mmol), **Mn3** (6 mol%), KHMDS(10 mol%), solvent (33 μL), 65 °C, 24 h, Ar. Yields were determined by ^{1}H NMR using mesitylene as the internal standard.

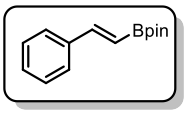
5. General procedure for the dehydrogenative borylation of alkenes

In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.006 mmol, 5.7 mg), KHMDS (0.02 mmol, 4 mg), THF (66 µL), alkene (0.2 mmol) and HBpin (0.3 mmol, 43.6 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 °C in a preheated oil bath. After 24 h the reaction was cooled to room temperature and diluted with 1 mL of CH_2Cl_2. The selectivity of the products was measured by ^{1}H NMR analysis. The crude mixture was then purified by silica gel column chromatography using hexane/EtOAc as eluent.

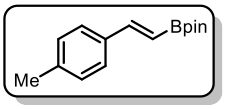
6. Analytical data for the products and unsuccessful substrates

6.1 Analytical data for the products

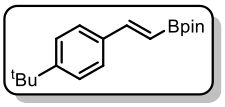
(*E*)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane (2):[4] Yield: 72% (0.144 mmol, 33.0 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.49 (d, *J* = 7.2 Hz, 2H), 7.40 (d, *J* = 18.4 Hz, 1H), 7.37 – 7.27 (m, 3H), 6.17 (d, *J* = 18.4 Hz, 1H), 1.32 (s, 12H). **^{13}C NMR** (126 MHz, CDCl3) δ 149.7, 137.7, 129.0, 128.7, 127.2, 83.5, 25.0.



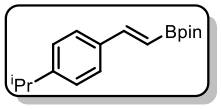
(*E*)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane (4):[4] Yield: 64% (0.128 mmol, 31.2 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.42 – 7.33 (m, 3H), 7.14 (d, *J* = 7.9 Hz, 2H), 6.12 (d, *J* = 18.4 Hz, 1H), 2.35 (s, 3H), 1.32 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 149.6, 139.1, 134.9, 129.4, 127.2, 83.4, 24.9, 21.5. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.0.



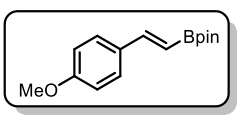
(*E*)-2-(4-(tert-butyl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (5):[4] Yield: 78% (0.156 mmol, 44.6 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 – 7.35 (m, 5H), 6.13 (d, *J* = 18.4 Hz, 1H), 1.32 (s, 21H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 152.3, 149.5, 134.9, 127.0, 125.6, 83.4, 34.8, 31.4, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.1.



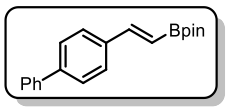
(*E*)-2-(4-isopropylstyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (6):[5] Yield: 60% (0.120 mmol, 32.6 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.45 – 7.34 (m, 3H), 7.20 (d, *J* = 8.0 Hz, 2H), 6.12 (d, *J* = 18.4 Hz, 1H), 2.94 – 2.86 (m, 1H), 1.31 (s, 12H), 1.25 (d, *J* = 6.9 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.0, 149.6, 135.3, 127.2, 126.8, 83.4, 34.1, 25.0, 24.00. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.2.



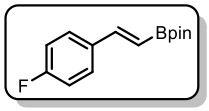
(*E*)-2-(4-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (7):[6] Yield: 75% (0.150 mmol, 39.0 mg). **^{1}H NMR** (400 MHz, CDCl3) δ 7.46 – 7.40 (m, 2H), 7.39 – 7.31 (m, 1H), 6.86 (d, *J* = 8.6 Hz, 2H), 6.06 – 5.95 (m, 1H), 3.81 (s, 3H), 1.31 (s, 12H). **^{13}C NMR** (101 MHz, CDCl3) δ 160.43, 149.20, 130.55, 128.60, 114.10, 83.35, 55.41, 24.94. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.0.



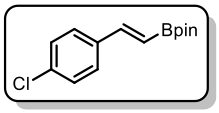
(*E*)-2-(2-([1,1'-biphenyl]-4-yl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (8):[4] Yield: 78% (0.156 mmol, 47.8 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 – 7.56 (m, 6H), 7.48 – 7.42 (m, 3H), 7.38 – 7.32 (m, 1H), 6.22 (d, *J* = 18.4 Hz, 1H), 1.33 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 149.1, 141.8, 140.7, 136.7, 128.9, 127.7, 127.6, 127.4, 127.1, 83.5, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.4.



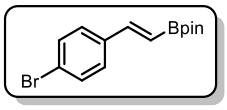
(*E*)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (9):[4] Yield: 70% (0.140 mmol, 35 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 – 7.42 (m, 2H), 7.35 (d, *J* = 18.4 Hz, 1H), 7.02 (t, *J* = 8.5 Hz, 2H), 6.07 (d, *J* = 18.4 Hz, 1H), 1.31 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.3 (d, *J* = 248.2 Hz), 148.3, 133.9, 128.9 (d, *J* = 8.3 Hz), 115.7 (d, *J* = 21.4 Hz), 83.5, 24.9. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.5. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -112.41.



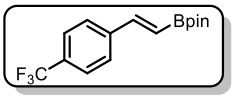
(*E*)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (10):[4] Yield: 61% (0.122 mmol, 32.0 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.4 Hz, 2H), 7.32 (t, *J* = 13.4 Hz, 3H), 6.13 (d, *J* = 18.4 Hz, 1H), 1.31 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.2, 136.1, 134.8, 128.9, 128.4, 83.6, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 29.8.



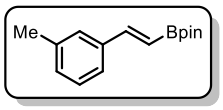
(*E*)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (11):[4] Yield: 63% (0.126 mmol, 39.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.9 Hz, 2H), 7.37 (d, *J* = 7.0 Hz, 2H), 7.31 (d, *J* = 19.5 Hz, 1H), 6.17 (d, *J* = 18.4 Hz, 1H), 1.34 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.2, 136.6, 131.9, 128.7, 123.1, 83.6, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.2.



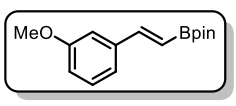
(*E*)-4,4,5,5-tetramethyl-2-(4-(trifluoromethyl)styryl)-1,3,2-dioxaborolane (12):[4] Yield: 50% (0.10 mmol, 30 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 – 7.54 (m, 4H), 7.40 (d, *J* = 18.4 Hz, 1H), 6.26 (d, *J* = 18.5 Hz, 1H), 1.32 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 147.8, 141.0, 130.6 (q, *J* = 32.2 Hz), 127.3, 125.7 (q, *J* = 4.1 Hz), 125.3, 123.1, 83.8, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 29.9. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -62.65.



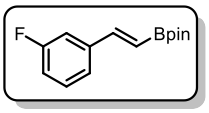
(*E*)-4,4,5,5-tetramethyl-2-(3-methylstyryl)-1,3,2-dioxaborolane (13):[6] Yield: 60% (0.12 mmol, 29 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 18.4 Hz, 1H), 7.30 (d, *J* = 6.2 Hz, 2H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 7.4 Hz, 1H), 6.16 (d, *J* = 18.4 Hz, 1H), 2.35 (s, 3H), 1.32 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 149.8, 138.2, 137.6, 129.8, 128.6, 127.9, 124.4, 83.4, 24.9, 21.5. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.2.



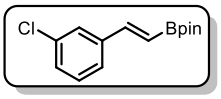
(*E*)-2-(3-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (14):[6] Yield: 71% (0.142 mmol, 37.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 18.3 Hz, 1H), 7.27 (t, *J* = 6.9 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 7.06 (s, 1H), 6.87 (d, *J* = 7.9 Hz, 1H), 6.18 (d, *J* = 18.3 Hz, 1H), 3.83 (s, 3H), 1.34 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.9, 149.5, 139.1, 129.7, 120.0, 114.9, 112.1, 83.5, 55.3, 24.9. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.3.



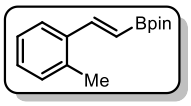
(*E*)-2-(3-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (15):[4] Yield: 66% (0.132 mmol, 32.7 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 1H), 7.33 – 7.25 (m, 2H), 7.20 (d, *J* = 10.0 Hz, 1H), 7.04 – 6.97 (m, 1H), 6.19 (d, *J* = 18.4 Hz, 1H), 1.34 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.2 (d, *J* = 245.7 Hz), 148.20 (d, *J* = 2.1 Hz), 140.02 (d, *J* = 7.2 Hz), 130.16 (d, *J* = 8.3 Hz), 123.13 (d, *J* = 2.6 Hz), 115.8 (d, *J* = 21.4 Hz), 113.4 (d, *J* = 21.4 Hz), 83.6, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -113.5.



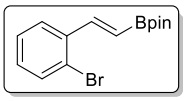
(*E*)-2-(3-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (16):[4] Yield: 50% (0.10 mmol, 26.4 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.42 – 7.34 (m, 2H), 7.31 (d, *J* = 5.2 Hz, 2H), 6.22 (d, *J* = 18.4 Hz, 1H), 1.37 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.0, 139.5, 134.7, 129.9, 128.9, 127.1, 125.3, 83.6, 24.9. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 29.9.



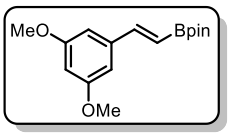
(*E*)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane (17):[7] Yield: 58% (0.116 mmol, 28.3 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 18.0 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.20 – 7.12 (m, 3H), 6.09 (d, *J* = 18.4 Hz, 1H), 2.42 (s, 3H), 1.32 (s, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 147.3, 136.8, 136.4, 130.5, 128.7, 126.2, 125.9, 83.4, 25.0, 20.0. **^{11}B NMR** (128 MHz, $CDCl_3$) δ 29.0.



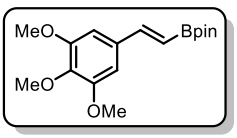
(*E*)-2-(2-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (18):[8] Yield: 51% (0.102 mmol, 31.5 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.47 – 7.44 (m, 2H), 7.36 – 7.33 (m, 3H), 6.15 (d, *J* = 18.4 Hz, 1H), 1.31 (s, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 148.2, 131.9, 131.3, 130.0, 128.7, 123.1, 83.6, 25.0. **^{11}B NMR** (128 MHz, $CDCl_3$) δ 29.6.



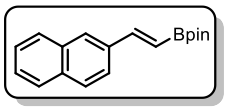
(*E*)-2-(3,5-dimethoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (19):[9] Yield: 74% (0.148 mmol, 43.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 (d, *J* = 18.4 Hz, 1H), 6.65 (d, *J* = 2.2 Hz, 2H), 6.42 (t, *J* = 2.2 Hz, 1H), 6.14 (d, *J* = 18.4 Hz, 1H), 3.78 (s, 6H), 1.31 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.0, 149.5, 139.7, 105.1, 101.5, 83.5, 55.4, 24.9. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.2.



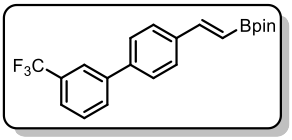
(*E*)-4,4,5,5-tetramethyl-2-(3,4,5-trimethoxystyryl)-1,3,2-dioxaborolane (20):[10] Yield: 78% (0.156 mmol, 50 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30 (d, *J* = 18.3 Hz, 1H), 6.72 (s, 2H), 6.05 (d, *J* = 18.3 Hz, 1H), 3.84 (s, 9H), 1.29 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.4, 149.4, 139.0, 133.3, 104.2, 83.5, 61.0, 56.1, 24.9. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.0.



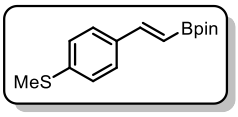
(*E*)-4,4,5,5-tetramethyl-2-(2-(naphthalen-2-yl)vinyl)-1,3,2-dioxaborolane (21):[4] Yield: 50% (0.10 mmol, 28.0 mg) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 – 7.79 (m, 4H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 18.4 Hz, 1H), 7.50 – 7.44 (m, 2H), 6.29 (d, *J* = 18.4 Hz, 1H), 1.34 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 149.7, 135.2, 133.9, 133.6, 128.6, 128.4, 128.2, 127.8, 126.5, 126.4, 123.6, 83.5, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.6.



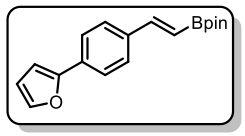
(E)-4,4,5,5-tetramethyl-2-(2-(3'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)vinyl)-1,3,2-dioxaborolane (22): Yield: 71% (0.142 mmol, 53.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.63 – 7.53 (m, 6H), 7.45 (d, *J* = 18.5 Hz, 1H), 6.24 (d, *J* = 18.5 Hz, 1H), 1.33 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.8, 141.5, 140.1, 137.4, 131.6 (q, *J* = 31.5 Hz), 130.4, 129.4, 127.8, 127.5, 124.3 (q, *J* = 273.4 Hz), 124.2 (q, *J* = 3.8 Hz), 123.9 (q, *J* = 3.8 Hz), 83.6, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 29.9. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -62.62. Selected **IR** (ATR, cm^{-1}): 2979, 2934, 1622, 1484, 1351, 1326, 1258, 1113, 797.



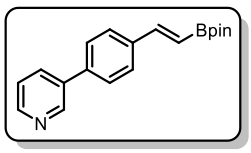
(*E*)-4,4,5,5-tetramethyl-2-(4-(methylthio)styryl)-1,3,2-dioxaborolane (23):[11] Yield: 75% (0.150 mmol, 41.4 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 18.4 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 2H), 6.11 (d, *J* = 18.3 Hz, 1H), 2.48 (s, 3H), 1.31 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.9, 139.8, 134.4, 127.6, 126.3, 83.4, 24.9, 15.6. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.4.



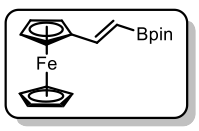
(*E*)-2-(4-(furan-2-yl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (24): Yield: 60% (0.120 mmol, 35.5 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.53 – 7.46 (m, 3H), 7.40 (d, *J* = 18.5 Hz, 1H), 6.69 – 6.65 (m, 1H), 6.50 – 6.46 (m, 1H), 6.18 (d, *J* = 18.4 Hz, 1H), 1.32 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.8, 149.1, 142.5, 136.5, 131.3, 127.6, 124.0, 111.9, 105.7, 83.5, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.0. Selected **IR** (ATR, cm^{-1}): 2979, 2939, 1620, 1603, 1513, 1346, 1322, 1141, 997, 850. **HRMS (ESI) m/z:** Calculated for $[C_{18}H_{22}BO_3^+$; $[M+H]^+]$ 297.1657, found 297.1660.



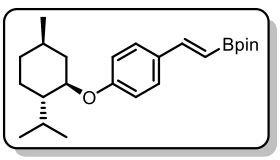
(*E*)-3-(4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)phenyl)pyridine (25): Yield: 50% (0.10 mmol, 30.7 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.87 (br s, 1H), 8.59 (br s, 1H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.61 – 7.54 (m, 4H), 7.43 (d, *J* = 18.2 Hz, 1H), 6.23 (d, *J* = 18.4 Hz, 1H), 1.32 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.7, 138.2, 137.5, 136.3, 134.4, 128.9, 127.9, 127.4, 127.1, 123.8, 83.6, 25.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 29.7. Selected **IR** (ATR, cm^{-1}): 2924, 2852, 1620, 1470, 1371, 1334, 1264, 1136, 1001, 971, 848. **HRMS (ESI) m/z:** Calculated for $[C_{19}H_{23}BNO_2^+$; $[M+H]^+]$ 308.1816, found 308.1825.



[(1*E*)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]-ferrocene (26):[4] Yield: 63% (0.126 mmol, 42.3 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.21 (d, *J* = 18.2 Hz, 1H), 5.72 (d, *J* = 18.2 Hz, 1H), 4.42 (t, *J* = 2.1 Hz, 2H), 4.27 (t, *J* = 2.1 Hz, 2H), 4.10 (s, 5H), 1.30 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 149.6, 83.2, 82.9, 69.7, 69.6, 67.7, 25.00. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.0.

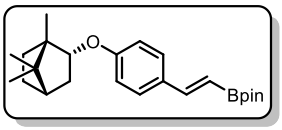


2-((*E*)-4-(((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (27): Yield: 68% (0.136 mmol, 52.3 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 18.4 Hz, 1H), 6.85 (d, *J* = 8.8 Hz, 2H), 5.99 (d, *J* = 18.2 Hz, 1H), 4.65 – 4.62 (m, 1H), 2.11 – 2.06 (m, 1H), 1.77 – 1.65 (m, 4H), 1.62 – 1.55 (m, 2H), 1.31 (s, 12H), 1.08 – 0.98 (m, 2H), 0.92 (d, *J* = 6.7 Hz, 3H), 0.85 (d, *J* = 6.7 Hz, 3H), 0.81 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.3, 149.4, 130.0,

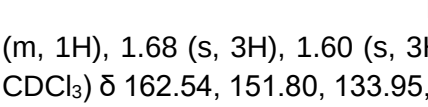


128.7, 115.7, 83.3, 73.5, 47.9, 37.9, 35.1, 29.4, 26.3, 25.0, 22.4, 21.2, 21.0. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.2. Selected **IR** (ATR, cm^{-1}):2950, 2921, 2870, 1620, 1600, 1507, 1369, 1246, 1137, 964, 805. **HRMS (ESI) m/z:** Calculated for $[C_{24}H_{38}BO_3^+]$; $[M+H]^+$] 385.2909, found 385.2926. $[\alpha]^{25}_D$ = +32.00 (*c* = 0.01 g/ml, $CHCl_3$).

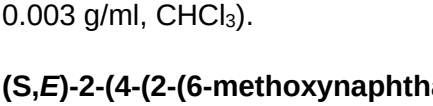
4,4,5,5-tetramethyl-2-((*E*)-4-(((1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)styryl)-1,3,2-dioxaborolane (28): Yield: 80% (0.160 mmol, 61.2 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.6 Hz, 2H), 7.34 (d, *J* = 18.4 Hz, 1H), 6.81 (d, *J* = 8.6 Hz, 2H), 5.99 (d, *J* = 18.4 Hz, 1H), 4.05 (t, *J* = 5.4 Hz, 1H), 1.86 – 1.74 (m, 4H), 1.64 – 1.59 (m, 1H), 1.31 (s, 12H), 1.15 – 1.09 (m, 2H), 1.05 (s, 3H), 0.98 (s, 3H), 0.87 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.9, 149.4, 130.0, 128.5, 115.5, 84.7, 83.3, 49.4, 47.2, 45.4, 39.7, 34.3, 27.5, 25.0, 20.5, 20.2, 11.9. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.0. Selected **IR** (ATR, ν cm^{-1}): 2953, 2930, 2879, 1616, 1602, 1571, 1505, 1353, 1246, 1139, 1060, 813. **HRMS (ESI) m/z:** Calculated for $[C_{24}H_{35}BNaO_3^+]$; $[M+H]^+$] 405.2571, found 405.2558. $[\alpha]^{25}_D$ = +110.00 (*c* = 0.01 g/ml, $CHCl_3$).



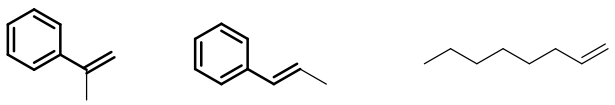
(E)-2-(4-((3,7-dimethyloct-6-en-1-yl)oxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (29): Yield: 66% (0.132 mmol, 50.7 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.9 Hz, 2H), 7.38 – 7.32 (m, 1H), 6.85 (d, *J* = 8.9 Hz, 2H), 6.00 (d, *J* = 18.4 Hz, 1H), 5.10 (t, *J* = 7.3 Hz, 1H), 4.02 – 3.97 (m, 2H), 2.05 – 1.94 (m, 3H), 1.84 – 1.79 (m, 1H), 1.68 (s, 3H), 1.60 (s, 3H), 1.43 – 1.34 (m, 2H), 1.31 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.54, 151.80, 133.95, 132.85, 131.08, 127.28, 117.17, 85.83, 68.97, 39.76, 38.72, 32.16, 28.34, 28.08, 27.44, 22.19, 20.30. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.2. Selected **IR** (ATR, ν cm^{-1}): 2962, 2925, 2874, 1622, 1604, 1575, 1509, 1353, 1248, 1143, 970, 815. **HRMS (ESI) m/z:** Calculated for $[C_{24}H_{38}BO_3^+]$; $[M+H]^+$] 385.2909, found 385.2926. $[\alpha]^{25}_D$ = -1.66 (*c* = 0.003 g/ml, $CHCl_3$).



(S,*E*)-2-(4-(2-(6-methoxynaphthalen-2-yl)propoxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (30): Yield: 50% (0.10 mmol, 22.2 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 – 7.61 (m, 4H), 7.44 – 7.41 (m, 2H), 7.38 – 7.33 (m, 1H), 7.16 – 7.13 (m, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.02 (d, *J* = 18.4 Hz, 1H), 4.21 – 4.15 (m, 1H), 4.07 – 4.02 (m, 1H), 3.92 (s, 3H), 3.42 – 3.34 (m, 1H), 1.49 (d, *J* = 7.0 Hz, 3H), 1.32 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.9, 157.6, 149.2, 138.8, 133.6, 130.6, 129.3, 129.0, 128.6, 127.1, 126.6, 125.7, 119.0, 114.8, 105.8, 83.3, 73.6, 55.4, 39.6, 24.9, 18.4. **^{11}B NMR** (161 MHz, $CDCl_3$) δ 30.2. Selected **IR** (ATR, ν cm^{-1}): 2975, 2930, 2872, 1620, 1604, 1506, 1353, 1252, 1213, 1141, 848, 809. **HRMS (ESI) m/z:** Calculated for $[C_{28}H_{34}BO_4^+]$; $[M+H]^+$] 445.2545, found 445.2564. $[\alpha]^{25}_D$ = -11.00 (*c* = 0.001 g/ml, $CHCl_3$).



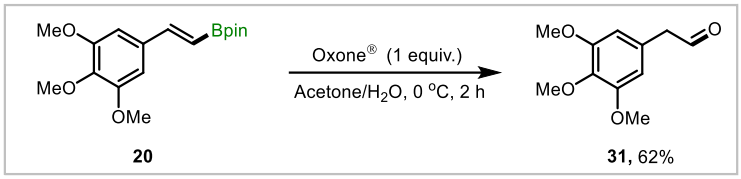
6.2 Unsuccessful substrates



no product | no product | inseperable mixture of hydroboration and ABD products

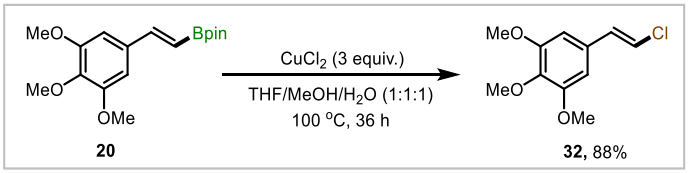
7. Synthetic applications

7.1. Synthesis of 2-(3,4,5-trimethoxyphenyl)acetaldehyde (31):[12]



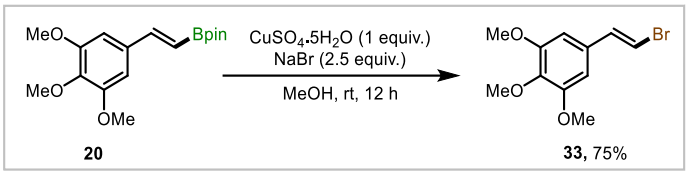
To a 15 mL oven-dried reaction tube were added **20** (0.20 mmol, 64 mg) and acetone (0.4 mL). While stirring at 0 °C, Oxone® solution (0.2 mmol in 0.4 mL H_2O) was added dropwise and the mixture was stirred for 2 h. The reaction was quenched with 1M HCl and extracted with DCM upon completion. The combined organic layers were washed with brine and dried over Na_2SO_4. The crude mixture was purified by flash column chromatography with hexane/EtOAc (80:20) as eluent. Yield: 62% (0.124 mmol, 26.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.73 (t, *J* = 2.4 Hz, 1H), 6.42 (s, 2H), 3.86 (s, 6H), 3.84 (s, 3H), 3.61 (d, *J* = 2.4 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 199.3, 153.8, 137.6, 127.4, 106.8, 61.0, 56.3, 50.9.

7.2. Synthesis of (*E*)-5-(2-chlorovinyl)-1,2,3-trimethoxybenzene (32):[13]



An oven-dried 15 mL reaction tube was charged with **20** (0.2 mmol, 64.0 mg), $CuCl_2$ (0.6 mmol, 80 mg), THF (1.0 mL), MeOH (1.0 mL) and H_2O (1.0 mL) under N_2 atmosphere. The mixture was heated at 100 °C. After 36 h the reaction was cooled to room temperature. The reaction mixture was diluted with water and extracted with Et_2O. The organic phase was washed with brine and dried over Na_2SO_4. The crude mixture was purified by flash column chromatography using hexane/EtOAc (95:5) as eluent. Yield: 88% (0.176 mmol, 40.4 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.75 (d, *J* = 13.4 Hz, 1H), 6.56 (d, *J* = 13.7 Hz, 1H), 6.50 (s, 2H), 3.86 (s, 6H), 3.84 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.58, 138.45, 133.34, 130.68, 118.25, 103.50, 61.03, 56.25.

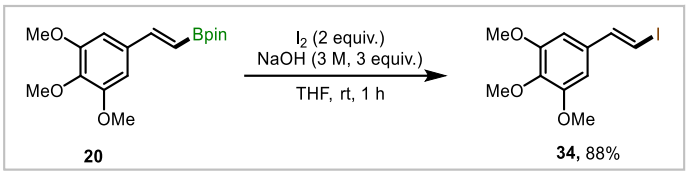
7.3. Synthesis of (*E*)-5-(2-bromovinyl)-1,2,3-trimethoxybenzene (33):[14]



An oven-dried 15 mL reaction tube was charged with **20** (0.2 mmol, 64.0 mg), $CuSO_4.5H_2O$ (0.2 mmol, 50 mg), NaBr (0.5 mmol, 52 mg), and MeOH (1.6 mL) under N_2 atmosphere. The mixture was heated at 50 °C. After 12 h the reaction was cooled to room temperature. The reaction mixture was diluted with water and extracted with Et_2O. The organic phase was washed with brine and dried over Na_2SO_4. The crude mixture was purified by flash column chromatography using hexane/EtOAc (95:5) as eluent. Yield: 75% (0.150 mmol, 41 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.02 (d, *J* = 13.9 Hz, 1H), 6.68 (d, *J* = 14.0 Hz, 1H), 6.50 (s, 2H),

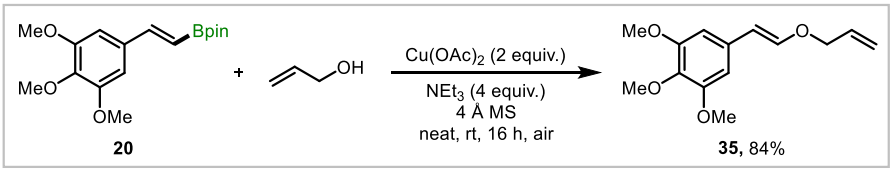
3.86 (s, 6H), 3.84 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.6, 138.6, 137.2, 131.7, 106.0, 103.5, 61.0, 56.3.

7.4. Synthesis of (*E*)-5-(2-iodovinyl)-1,2,3-trimethoxybenzene (34):[13]



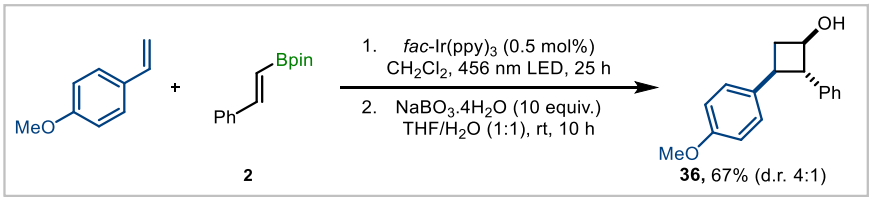
To a solution of **20** (0.2 mmol, 64.0 mg) in THF (2 mL) were added 3.0 M solution of NaOH (0.6 mmol, 0.2 mL) at 0 °C. After 10 min, I_2 (0.4 mmol, 52 mg) was added, and the reaction mixture was stirred at room temperature for 1 h. The reaction mixture was diluted with CH_2Cl_2 and the organic phase was washed with a saturated solution of $Na_2S_2O_3$ and brine. The organic layers were dried over Na_2SO_4, and the crude mixture was purified by silica gel column chromatography with hexane/EtOAc (95:5) as eluent. Yield: 88% (0.176 mmol, 56.4 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 15.0 Hz, 1H), 6.73 (d, *J* = 14.6 Hz, 1H), 6.50 (s, 2H), 3.86 (s, 6H), 3.84 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.5, 144.9, 138.7, 133.6, 103.4, 75.8, 61.0, 56.3.

7.5. Synthesis of (*E*)-5-(2-(allyloxy)vinyl)-1,2,3-trimethoxybenzene (35):



To a 15 mL oven-dried reaction tube were added **20** (0.2 mmol, 64 mg), allyl alcohol (1.2 mL), $Cu(OAc)_2$ (0.4 mmol, 72.6 mg), triethyl amine (0.8 mmol, 112 µL) and 4 Å molecular sieves (50 mg). The tube was sealed under air and stirred at room temperature for 16 h. The reaction mixture was diluted with CH_2Cl_2. The organic layer was washed with brine and dried over Na_2SO_4. The crude mixture was purified using silica gel column chromatography employing hexane/EtOAc (95:5 to 92:8) as eluent. Yield: 84% (0.168 mmol, 42 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.91 (d, *J* = 12.8 Hz, 1H), 6.43 (s, 2H), 5.99 (ddt, *J* = 15.9, 10.7, 5.5 Hz, 1H), 5.84 (d, *J* = 12.8 Hz, 1H), 5.38 (d, *J* = 17.2 Hz, 1H), 5.28 (d, *J* = 10.7 Hz, 1H), 4.37 (d, *J* = 5.4 Hz, 2H), 3.85 (s, 6H), 3.82 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.5, 147.4, 136.7, 133.3, 132.2, 118.0, 107.0, 102.5, 71.0, 61.1, 56.2. **HRMS (ESI) m/z:** Calculated for $[C_{14}H_{19}O_4^+]$; $[M+H]^+$] 251.1278, found 251.1270.

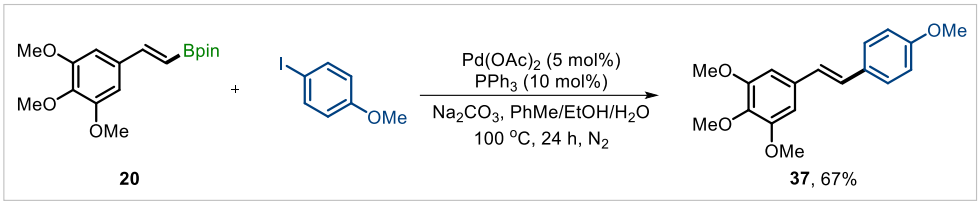
7.6. Synthesis of (1R,2S,3S)-3-(4-methoxyphenyl)-2-phenylcyclobutan-1-ol (36):[15]



In an argon-filled glovebox, to a 15 mL oven-dried reaction tube were added alkenylboronate **2** (0.2 mmol, 46 mg), *fac*-Ir(ppy)$_3$ (0.001 mmol, 0.7 mg). To this dry CH_2Cl_2 (0.25 mL), and

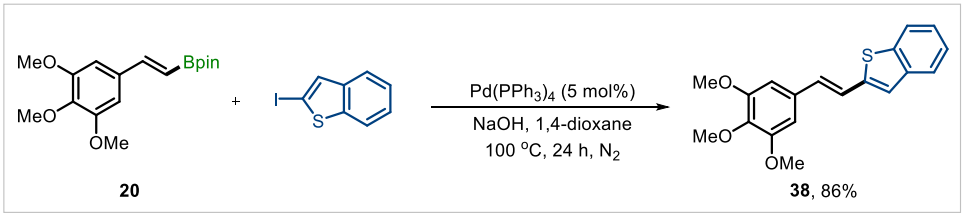
alkene (1.0 mmol, 134 µL) were added dropwise. The tube was sealed and stirred at room temperature under the irradiation of 456 nm blue LED for 25 h. Upon completion, the volatiles was removed under reduced pressure. The crude mixture was dissolved in THF (1.5 mL), to which $NaBO_3.4H_2O$ (2.00 mmol, 306 mg) was added, followed by H_2O (1.5 mL). The resulting mixture was stirred for 10 h and quenched by adding H_2O (2.0 mL). The mixture was extracted with EtOAc (3 x 3.00 mL). The combined organic parts were dried over sodium sulfate, and the crude mixture was purified by silica gel column chromatography using hexane/EtOAc (80:20) as eluent. Yield: 67% (0.134 mmol, 34.2 mg, d.r. 4:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 – 7.29 (m, 1.6H), 7.28 – 7.21 (m, 2.4H), 7.16 (d, *J* = 8.7 Hz, 1.6H), 7.13 – 7.04 (m, 0.6H), 6.89 – 6.86 (m, 0.8H), 6.84 (d, *J* = 8.7 Hz, 1.6H), 6.69 (d, *J* = 8.7 Hz, 0.4H), 4.83 (dd, *J* = 7.7, 6.2 Hz, 0.2H), 4.24 (dd, *J* = 7.7, 6.2 Hz, 0.8H), 3.79 (s, 2.4H), 3.77 – 3.73 (m, 0.4H) 3.72 (s, 0.6H), 3.30 (dd, *J* = 10.1, 7.6 Hz, 0.8H), 3.03 (td, *J* = 10.1, 7.6 Hz, 0.8H), 2.76 (dt, *J* = 10.5, 7.2 Hz, 0.8H), 2.68 (ddd, *J* = 11.9, 7.9, 1.9 Hz, 0.2H), 2.49 – 2.39 (m, 0.2H), 2.17 (s, 1H), 2.04 – 1.98 (m, 0.8H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.3, 157.8, 141.7, 139.0, 135.5, 132.6, 129.5, 128.6, 128.0, 127.9, 127.9, 126.9, 126.7, 126.2, 114.0, 113.5, 70.3, 70.0, 59.3, 55.6, 55.4, 55.3, 37.6, 36.8, 36.7, 34.8.

7.7. Synthesis of (*E*)-1,2,3-trimethoxy-5-(4-methoxystyryl)benzene (37)[16]



In an oven-dried 15 mL reaction tube were added $Pd(OAc)_2$ (0.01 mmol, 2.2 mg), PPh_3 (0.02 mmol, 5.2 mg), **20** (0.2 mmol, 64 mg), 4-iodoanisole (0.32 mmol, 75 mg), Na_2CO_3 (0.8 mmol, 84.8 mg), PhMe (1.0 mL), EtOH (0.2 mL) and water (0.2 mL) under nitrogen atmosphere. The mixture was transferred to a pre-heated oil bath at 100 °C. After 24 h, the reaction mixture was cooled, and water (0.5 mL) was added. The mixture was filtered and extracted with EtOAc. The combined organic layer was dried over Na_2SO_4, and the solvent was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography with hexane/EtOAc (95:5) as eluent. Yield: 67%, (0.134 mmol, 39.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.9 Hz, 2H), 7.00 – 6.88 (m, 4H), 6.72 (s, 2H), 3.91 (s, 6H), 3.87 (s, 3H), 3.83 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.4, 153.5, 137.8, 133.6, 130.2, 127.9, 127.8, 126.67, 114.3, 103.5, 61.1, 56.3, 55.5.

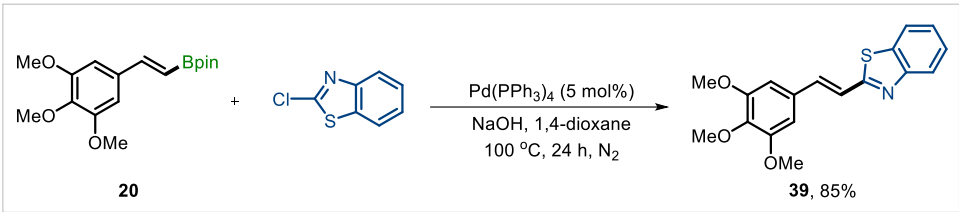
7.8. Synthesis of (*E*)-2-(3,4,5-trimethoxystyryl)benzo[b]thiophene (38)[17]



In an oven-dried 15 mL reaction tube were added $Pd(PPh_3)_4$ (0.01 mmol, 23 mg), **20** (0.2 mmol, 64 mg), 2-iodobenzothiophene (0.32 mmol, 84 mg), NaOH (0.4 mmol, 16 mg), 1,4-dioxane (0.8 mL) under nitrogen atmosphere. The mixture was transferred to a pre-heated oil

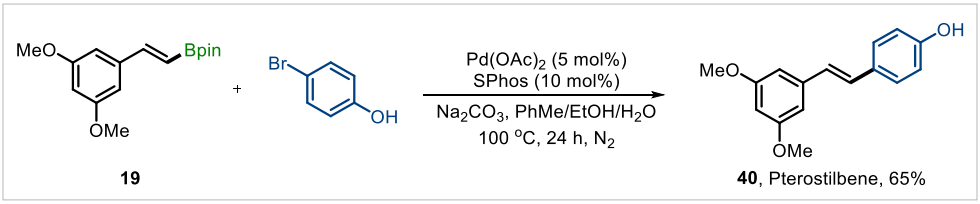
bath at 100 °C. After 24 h, the reaction mixture was cooled and quenched with water (0.5 mL). The mixture was filtered and extracted with EtOAc. The combined organic layer was dried over Na_2SO_4, and the solvent was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography with hexane/EtOAc (90:10-80:20) as eluent. Yield: 86% (0.172 mmol, 56.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.80 – 7.74 (m, 1H), 7.72 – 7.67 (m, 1H), 7.36 – 7.27 (m, 2H), 7.27 – 7.19 (m, 2H), 6.92 (d, J = 15.9 Hz, 1H), 6.73 (s, 2H), 3.92 (s, 6H), 3.88 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.6, 142.9, 140.3, 139.0, 138.5, 132.4, 130.9, 124.9, 124.7, 123.5, 123.3, 122.3, 121.9, 103.8, 61.1, 56.3.

7.9. Synthesis of (*E*)-2-(3,4,5-trimethoxystyryl)benzo[d]thiazole (39)[17]



In an oven-dried 15 mL reaction tube were added $Pd(PPh_3)_4$ (0.01 mmol, 23 mg), **20** (0.2 mmol, 64 mg), 2-chlorobenzothiazole (0.32 mmol, 84 mg), NaOH (0.4 mmol, 16 mg), 1,4-dioxane (0.8 mL) under nitrogen atmosphere. The mixture was transferred to a pre-heated oil bath at 100 °C. After 24 h, the reaction mixture was cooled and quenched with water (0.5 mL). The mixture was filtered and extracted with EtOAc. The combined organic layer was dried over Na_2SO_4, and the solvent was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography with hexane/EtOAc (90:10-80:20) as eluent. Yield: 85% (0.170 mmol, 56.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.49 – 7.40 (m, 2H), 7.38 – 7.30 (m, 2H), 6.81 (s, 2H), 3.91 (s, 6H), 3.89 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.0, 153.9, 153.6, 139.6, 137.6, 134.4, 131.1, 126.5, 125.5, 123.0, 121.7, 121.6, 104.6, 61.1, 56.3.

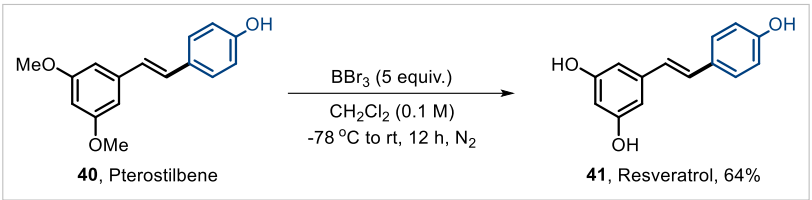
7.10. Synthesis of Pterostilbene (40)[16]



In an oven-dried 15 mL reaction tube were added $Pd(OAc)_2$ (0.01 mmol, 2.2 mg), SPhos (0.02 mmol, 7.6 mg), **19** (0.2 mmol, 58 mg), 4-bromophenol (0.32 mmol, 55.4 mg), Na_2CO_3 (0.8 mmol, 84.8 mg), PhMe (1.0 mL), EtOH (0.2 mL) and water (0.2 mL) under nitrogen atmosphere. The mixture was transferred to a pre-heated oil bath at 100 °C. After 24 h, the reaction mixture was cooled, and water (0.5 mL) was added. The mixture was filtered and extracted with EtOAc. The combined organic layer was dried over Na_2SO_4, and the solvent was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography with hexane/EtOAc (95:5 to 90:10) as eluent. Yield: 65%, (0.130 mmol, 33.3 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.6 Hz, 2H), 7.03 (d, *J* = 16.2 Hz, 1H), 6.89 (d, *J* = 16.2 Hz, 1H), 6.83 (d, *J* = 8.6 Hz, 2H), 6.66 (d, *J* = 2.2 Hz, 2H), 6.40 (t, *J* = 2.2 Hz, 1H),

3.83 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.0, 155.6, 139.8, 130.1, 128.9, 128.1, 126.6, 115.8, 104.6, 99.8, 55.5.

7.11. Synthesis of Resveratrol (41)[18]



40, Pterostilbene — **41**, Resveratrol, 64%

In an oven-dried 10 mL Schlenk tube were added **40** (0.2 mmol, 51.3 mg) containing a stirring bar. The flask was sealed with a rubber septum and evacuated by a high vacuum. The flask was backfilled with N_2, and 2 mL of dry CH_2Cl_2 was added. The flask was immersed in a cold reaction bath at -78 °C, and neat BBr_3 (1.0 mmol, 0.1 mL) was added over 10 min *via* a syringe. The mixture was stirred at -78 °C for another 30 min. After that, the mixture was allowed slowly to reach room temperature and stirred for 12 h. The reaction was neutralized by adding saturated $NaHCO_3$ solution and extracted with EtOAc. The combined organic layers were evaporated under reduced pressure, and the crude mixture was purified by flash silica gel column chromatography using hexane/ EtOAc (60:40-50:50) as eluent. Yield: 64% (0.128 mmol, 29.2 mg). **^{1}H NMR** (500 MHz, DMSO-*d6*) δ 9.49 (s, 1H), 9.14 (d, *J* = 2.3 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 6.88 (d, *J* = 16.3 Hz, 1H), 6.76 (d, *J* = 16.3 Hz, 1H), 6.70 (d, *J* = 8.1 Hz, 2H), 6.34 (s, 2H), 6.10 – 6.03 (m, 1H). **^{13}C NMR** (126 MHz, DMSO-*d6*) δ 158.5, 157.2, 139.3, 128.1, 127.9, 127.9, 125.7, 115.5, 104.3, 101.8.

8. Mechanistic studies

8.1. H_2 gas detection

In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.006 mmol, 2.8 mg), KHMDS (0.01 mmol, 2 mg), THF (33 µL), 4-phenylstyrene (**42**, 0.1 mmol, 18.0 mg), and HBpin (0.15 mmol, 21.8 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 °C in a preheated oil bath. After 24 h the H_2 gas was detected by the headspace analysis of the reaction mixture by GC.

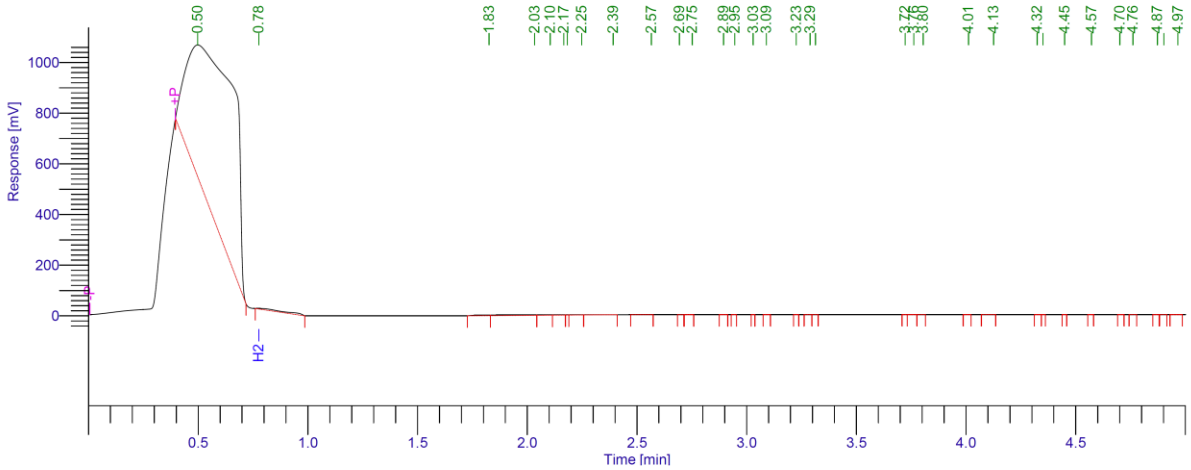


Fig. S4. GC of pure H_2 gas.

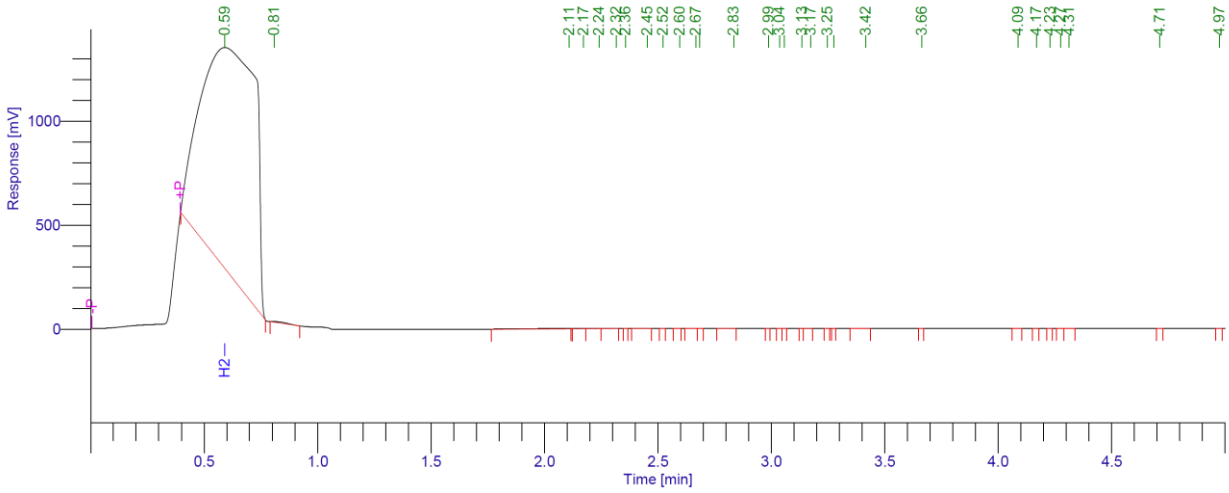
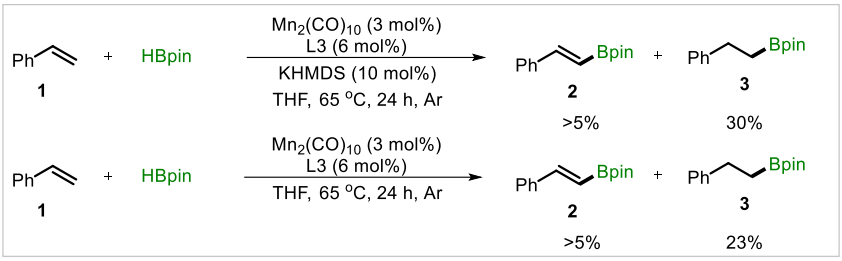


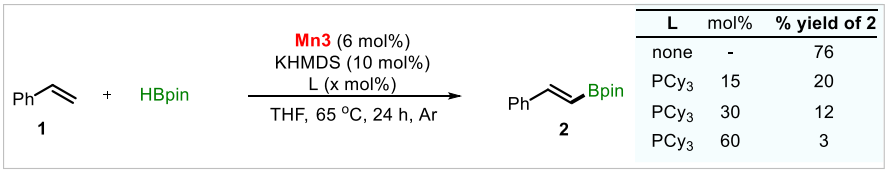
Fig. S5. GC sample of the gas phase for the standard dehydrogenative borylation.

8.2. Control experiments to eliminate Mn(0) catalyzed dehydrogenative borylation pathway.



In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **$Mn_2(CO)_{10}$** (0.006 mmol, 2.3 mg), **L3** (0.012 mmol, 3.1 mg), KHMDS (0.02 mmol, 4 mg), THF (66 µL), **1** (0.2 mmol, 22.8 µL) and HBpin (0.3 mmol, 43.6 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 °C in a preheated oil bath. After 24 h the reaction was cooled to room temperature and mesitylene (0.2 mmol, 27.8 µL) was added. The yield of the unsaturated product was detected by GC-FID and the isolated yields of the saturated product was reported.

8.3. Effect of exogenous ligands:

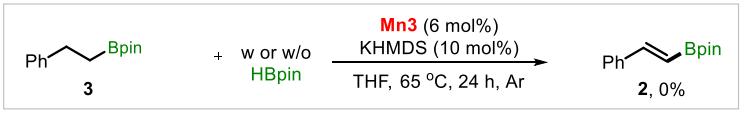


L	mol%	% yield of 2
none	-	76
PCy_3	15	20
PCy_3	30	12
PCy_3	60	3

In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.006 mmol, 2.8 mg), KHMDS (0.01 mmol, 2 mg), **L**, THF (33 µL), **1** (0.1 mmol, 11.4 µL) and HBpin (0.15 mmol, 21.8 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 °C in a preheated oil bath. After 24 h the reaction was cooled to room temperature 1 mL of $CHCl_3$ was added. The mixture was filtered through a short plug of silica. The combined organic layer was evaporated, and mesitylene (0.1 mmol, 14 µL) was added. The yield of the product was measured by ^1H NMR analysis.

In the absence of an exogenous ligand, 76% yield of **2** was obtained. The addition of ligands resulted in lower yields (20, 12 and 3% with 15, 30 and 60 mol% of PCy_3) of **2**.

8.4. Control experiment to exclude hydroboration/dehydrogenation pathway:



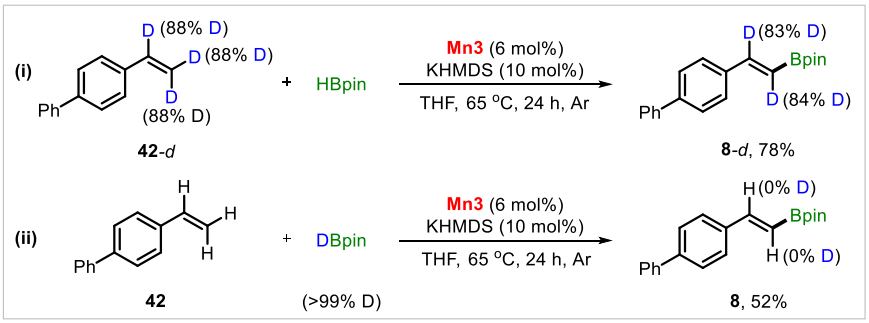
Without HBpin. In an argon-filled glovebox, to a 15 mL oven dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.006 mmol, 2.8 mg), KHMDS (0.01 mmol, 2 mg), THF (33 µL), **3** (0.1 mmol, 23.2 mg) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 °C in a preheated oil bath. After 24 h, the reaction was cooled to room temperature 1 mL of $CHCl_3$ was added. The mixture

was filtered through a short plug of silica. The combined organic layer was evaporated, and mesitylene (0.1 mmol, 14 µL) was added. The yield of the product was measured by ^{1}H NMR analysis.

With HBpin. In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.006 mmol, 2.8 mg), KHMDS (0.01 mmol, 2 mg), THF (33 µL), **3** (0.1 mmol, 23.2 mg) and HBpin (0.15 mmol, 21.8 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 ^{o}C in a preheated oil bath. After 24 h the reaction was cooled to room temperature 1 mL of $CHCl_3$ was added. The mixture was filtered through a short plug of silica. The combined organic layer was evaporated, and mesitylene (0.1 mmol, 14 µL) was added. The yield of the product was measured by ^{1}H NMR analysis.

In both cases, the alkenyl boronate ester product **2** was not detected by ^{1}H NMR analysis.

8.5. Deuterium labelling experiment:



Equation (i): In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.012 mmol, 5.6 mg), KHMDS (0.02 mmol, 4 mg), THF (66 µL), **42-***d* (0.2 mmol, 36.6 mg) and HBpin (0.3 mmol, 43.6 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 ^{o}C in a preheated oil bath. After 24 h the reaction was cooled to room temperature 1 mL of CH_2Cl_2 was added. The solvent was removed under reduced pressure, and the crude mixture was purified by silica gel column chromatography using hexane/EtOAc (98:2) as eluent. Yield: 78% (0.16 mmol, 48.0 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.65 – 7.55 (m, 6H), 7.46 – 7.41 (m, 2.17 H), 7.34 (t, *J* = 7.2 Hz, 1H), 6.20 (s, 0.16 H) 1.33 (s, 12H).

Equation (ii): In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.012 mmol, 5.6 mg), KHMDS (0.02 mmol, 4 mg), THF (66 µL), **42** (0.2 mmol, 36.0 mg) and DBpin (0.3 mmol, 44.0 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 ^{o}C in a preheated oil bath. After 24 h the reaction was cooled to room temperature 1 mL of CH_2Cl_2 was added. The solvent was removed under reduced pressure, and the crude mixture was purified by silica gel column chromatography using hexane/EtOAc (98:2) as eluent. Yield: 52% (0.1 mmol, 32.0 mg). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.62 – 7.56 (m, 6H), 7.47 – 7.42 (m, 3H), 7.35 (t, *J* = 7.4 Hz, 1H), 6.21 (d, *J* = 18.4 Hz, 1H), 1.33 (s, 12H).

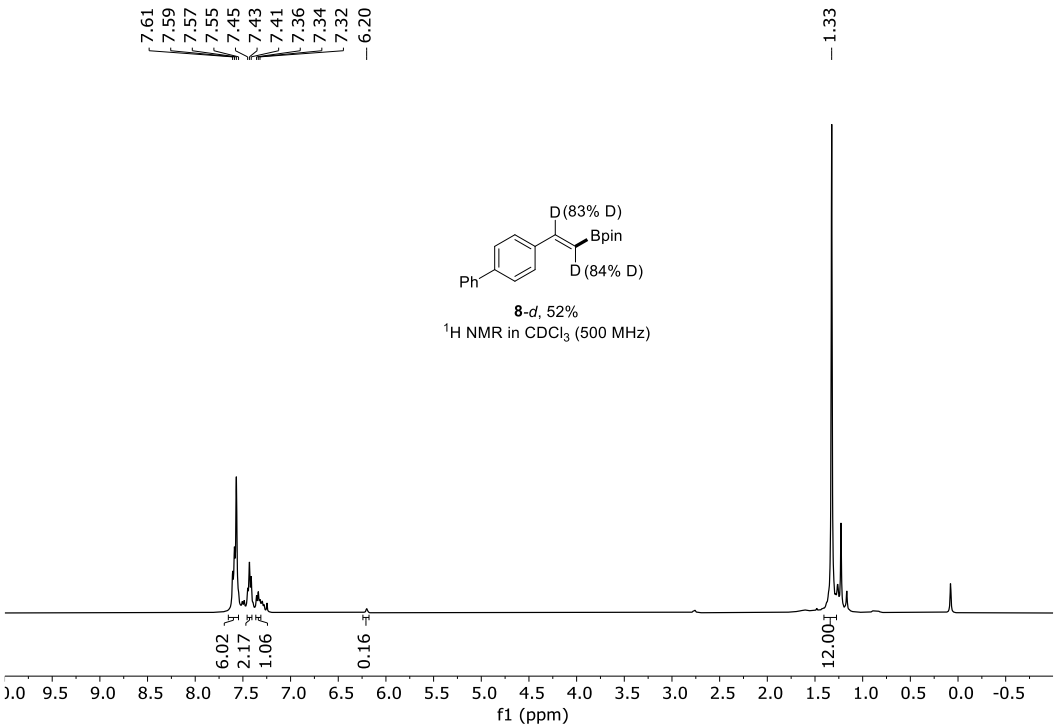


Fig. S6: ^{1}H NMR of **8-*d***.

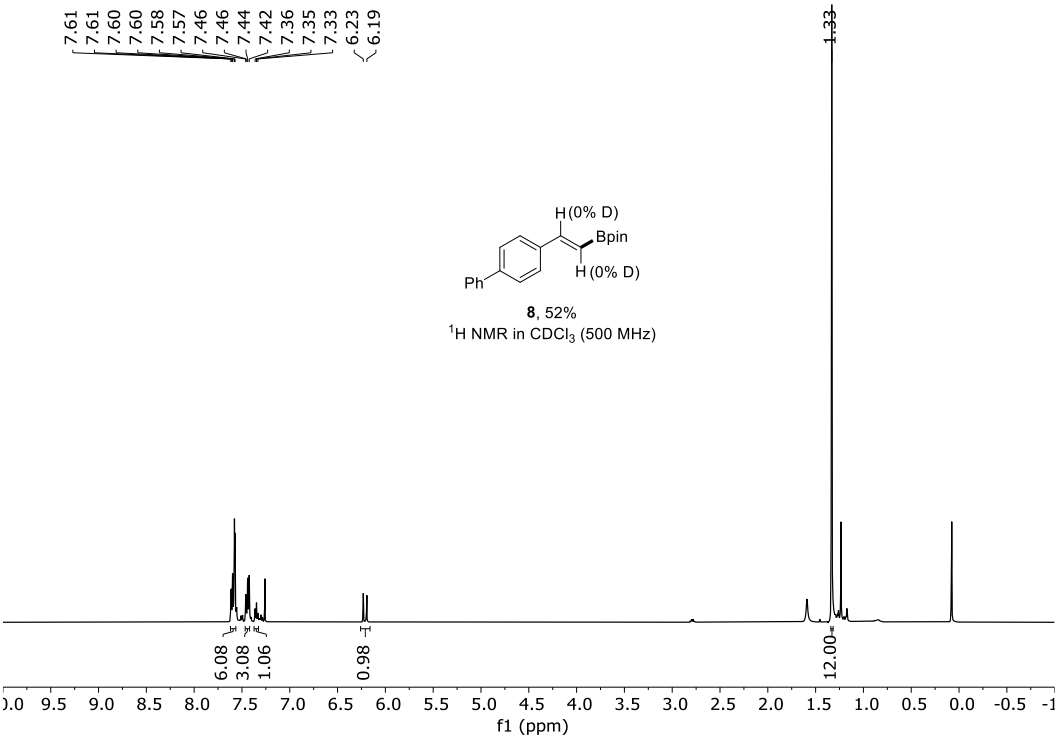


Fig. S7: ^{1}H NMR of **8**.

8.6. Determination of kinetic isotope effect

In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.006 mmol, 2.8 mg), KHMDS (0.01 mmol, 2 mg), THF (80 µL), **42** (0.1 mmol, 18 mg) and HBpin (0.15 mmol, 21.8 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 °C in a preheated oil bath. After certain time intervals, the reaction was cooled to room temperature, and 1 mL of EtOAc and mesitylene (0.1 mmol, 14 µL) was added. The yield of the product was measured by GC-MS analysis. The same is repeated at different times.

From the plot of the yield of **8** *vs* time, the initial rate was determined. The initial rate $k_{H\ (\mathbf{40}/HBpin)} = 9.13 \times 10^{-3}$ M/min.

The same procedure was followed for **42**-*d* (0.1 mmol, 18.3 mg). The initial rate $k_{D\ (\mathbf{40}\text{-}\mathbf{\mathit{d}}/HBpin)} = 5.26 \times 10^{-3}$ M/min.

KIE = $k_{H\ (\mathbf{40}/HBpin)}$ **/** $k_{D\ (\mathbf{40}\text{-}\mathbf{\mathit{d}}/HBpin)}$ **= 1.74**.

Following the same procedure for DBpin (0.15 mmol, 22.0 µL) the initial rate was measured, $k_{D\ (\mathbf{40}/DBpin)} = 3.82 \times 10^{-3}$ M/min.

KIE = $k_{H\ (\mathbf{40}/HBpin)}$ **/** $k_{D\ (\mathbf{40}/DBpin)}$ **= 2.39**.

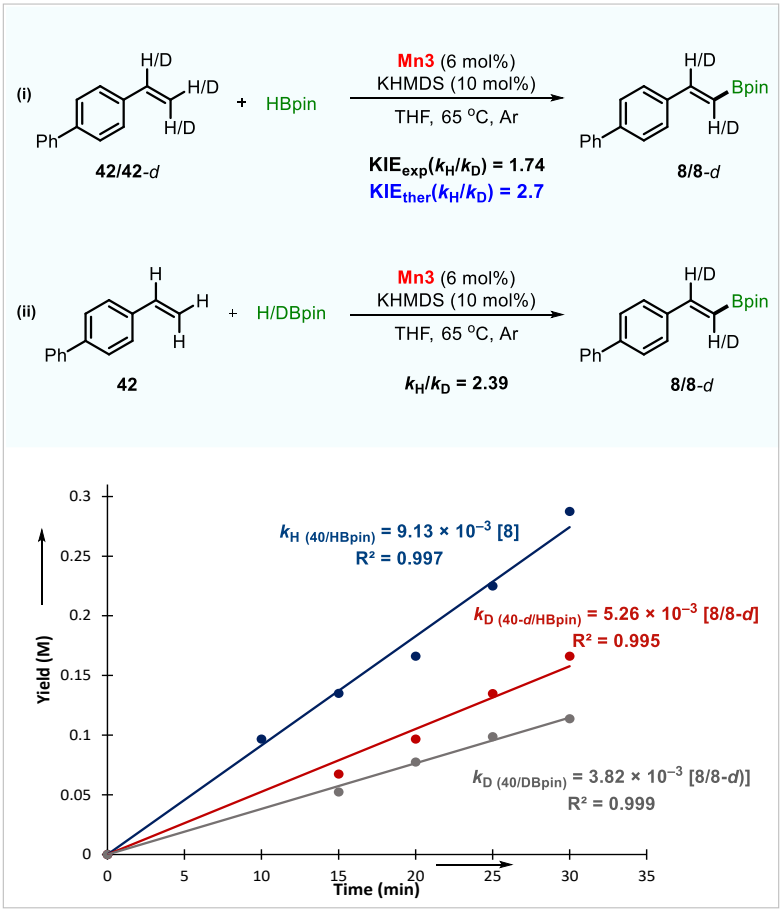


Fig. S8. Yield *vs* time plot for determination of kinetic isotope effect.

8.7. Hammet correlation study:

In an argon-filled glovebox, to a 15 mL oven-dried reaction tube equipped with a magnetic stirrer bar **Mn3** (0.006 mmol, 2.8 mg), KHMDS (0.01 mmol, 2 mg), THF (80 µL), alkene (0.1 mmol) and HBpin (0.15 mmol, 21.8 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at 65 °C in a preheated oil bath. After 45 min time interval, the reaction was cooled to room temperature, and 1 mL of EtOAc and mesitylene (0.1 mmol, 14 µL) was added. The yield of the product was measured by GC-MS analysis. The same is repeated for different substrates. The k_X/k_H was determined, and a plot of **log (k_X/k_H)** vs Hammett **σ** was found to be linear. From the slop of such plot **ρ** was determined to be –0.60.

X	k_X/k_H	σ	log (k_X/k_H)
H	1.000	0	0
OMe	1.229	-0.268	0.0894
^{t}Bu	1.086	-0.200	0.0357
Cl	0.629	0.227	-0.2016
CF_3	0.400	0.54	-0.3979

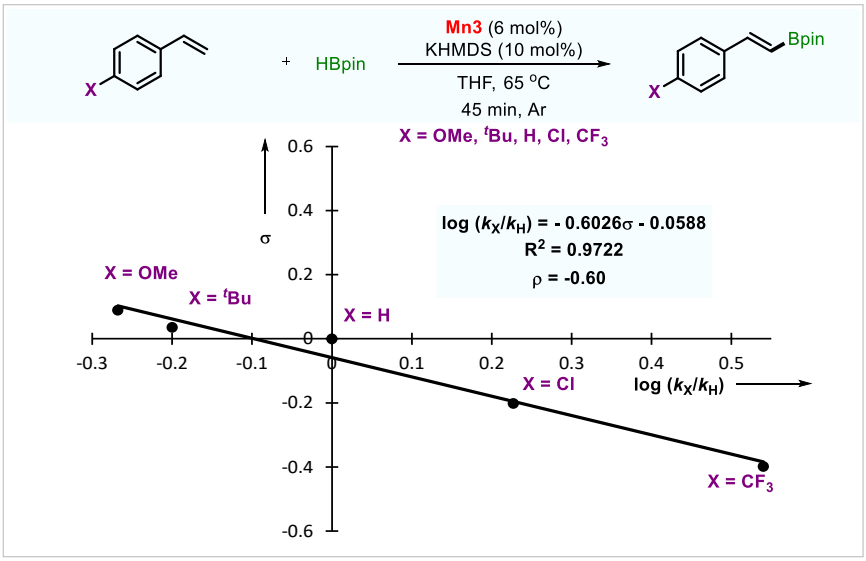


Fig. S9: log (k_X/k_H) vs σ plot for Hammet correlation study.

8.8. Eyring analysis:

In an argon-filled glovebox, to 15 mL oven-dried reaction tubes each equipped with a magnetic stirrer bar **Mn3** (0.006 mmol, 2.8 mg), KHMDS (0.01 mmol, 2 mg), THF (80 µL), **42** (0.1 mmol, 18 mg) and HBpin (0.15 mmol, 21.8 µL) were added at room temperature. The reaction tube was sealed and taken out of the glovebox. The mixture was heated at different temperatures 50 °C, 55 °C, 60 °C, 65 °C and 70 °C in a preheated oil bath. After 25 min time interval, the reaction was cooled to room temperature, and 1 mL of EtOAc and mesitylene (0.1 mmol, 14 µL) was added. The yield of the product was measured by GC-MS analysis

***k* [M/min]**	**T(K)**	**1/T**	**ln(*k*/T)**
1.4×10^{-3}	323	0.003096	-12.349
3.15×10^{-3}	328	0.003049	-11.553
6.00×10^{-3}	333	0.003003	-10.924
8.95×10^{-3}	338	0.002959	-10.539
1.65×10^{-2}	343	0.002915	-9.942

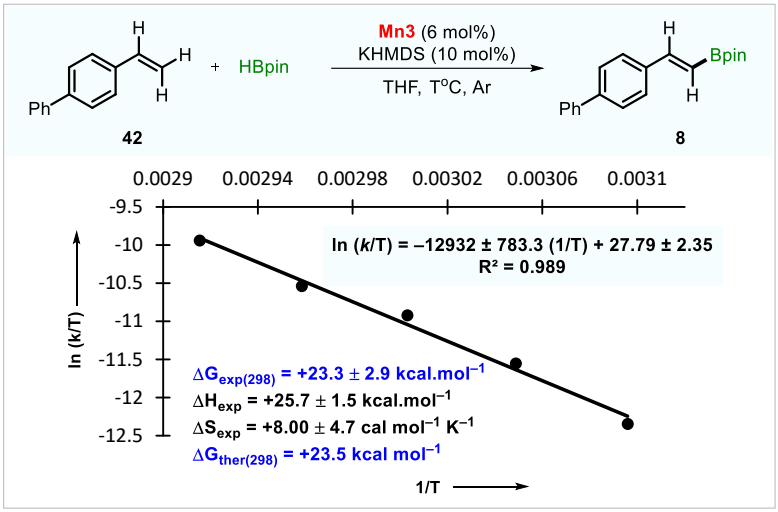


Fig. S10: ln (*k*/T) *vs* 1/T plot for Eyring analysis.

8.9. IR analysis

A solid-state ATR of **Mn3** was taken. It shows three sharp CO stretching frequencies at 2018, 1938, and 1907 cm^{-1}.

In the second experiment, **Mn3** (0.03 mmol, 14 mg) was treated with KHMDS (0.06 mmol, 12 mg) in 2 mL THF solution. The color of the solution instantly changed from orange to prussian blue. The mixture was stirred for 2 h at room temperature. The solution was filtered through a syringe filter under Ar atmosphere. The solvent was evaporated under vacuum, and solid-state ATR was measured for the remaining dark blue solid.

In the third experiment, **Mn3** (0.03 mmol, 14 mg) was treated with KHMDS (0.06 mmol, 12 mg) and HBpin (0.06 mmol, 9 µL) in 2 mL THF solution. The mixture was stirred for 2 h at room temperature. The solution was filtered through a syringe filter under Ar atmosphere. The solvent was evaporated under vacuum, and solid-state ATR was measured for the remaining solid.

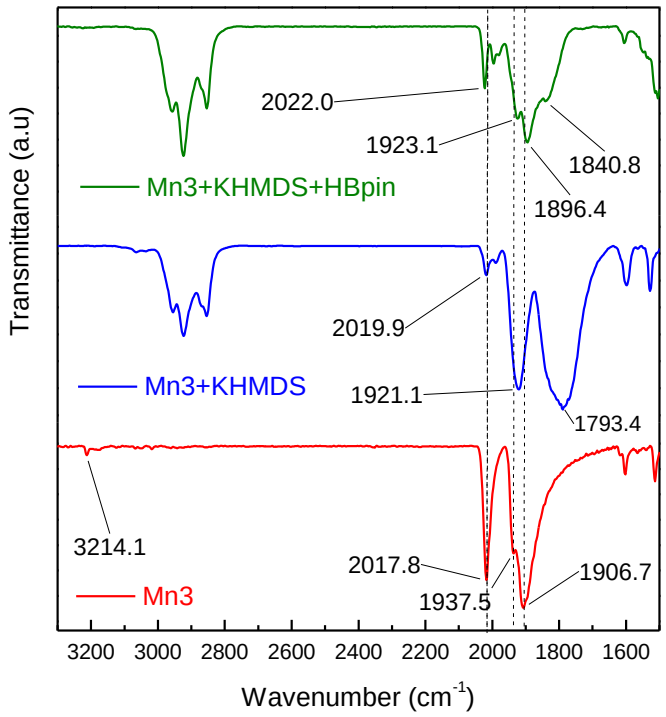


Fig. S11. IR spectrum for a) **Mn3** catalyst; b) **Mn3** catalyst after treatment with KHMDS; c) **Mn3** catalyst after treatment with KHMDS and HBpin.

8.10. ^{1}H and ^{11}B NMR experiment with stoichiometric Mn3, KHMDS and HBpin

In an Ar-filled glove box, **Mn3** (0.03 mmol, 14 mg) were taken in an oven-dried NMR tube, and 0.5 mL of THF-*d8* was added to it followed by the addition of KHMDS (0.06 mmol, 12 mg) and HBpin (0.036 mmol, 6 µL). The NMR tube was sealed and heated at 60 °C for 30 mins. The ^{1}H and ^{11}B NMR of the resulting mixture was measured.

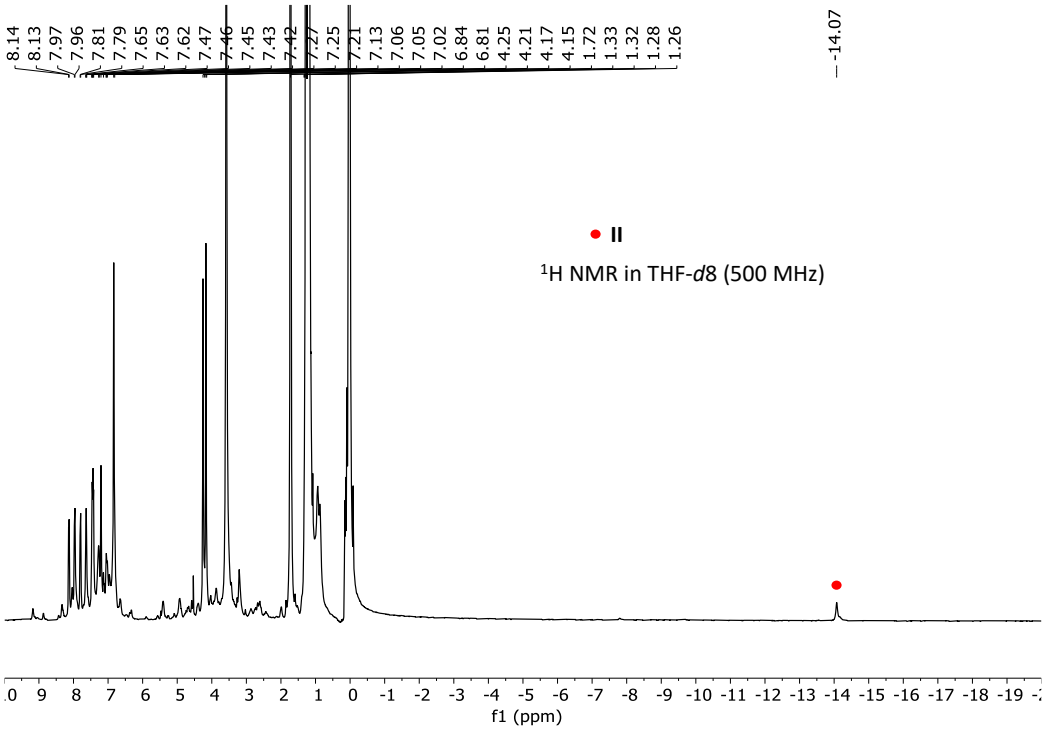


Fig. S12. ^{1}H NMR spectra of **Mn3** after treatment with KHMDS and HBpin.

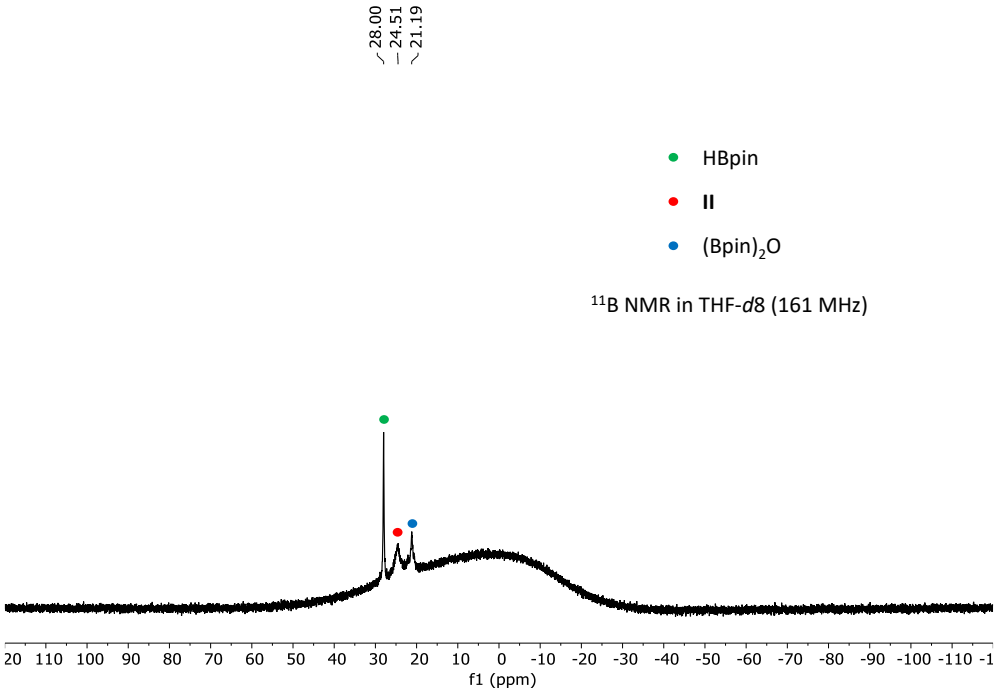


Fig. S13. ^{11}B NMR spectra of **Mn3** after treatment with KHMDS and HBpin.

9. Computational details:

All calculations were carried out using Density Functional Theory as implemented in the Gaussian16[19] quantum chemistry programs. The geometries of stationary points and transition states (TS) were optimized with B3LYP-D3BJ functional.[20] We used double-ζ basis set with the relativistic effective core potential of Hay and Wadt (LANL2DZ)[21] for the manganese and bromine atom and 6-31G* basis set for other elements (H, C, O, S, B, N, Si and K). The geometries were optimized without any symmetry constraints. Harmonic force constants were computed at the optimized geometries to characterize the stationary points as minima or saddle points. The zero-point vibrational corrections were determined from the harmonic vibrational frequencies to convert the total energies E^e to E^0. The rigid-rotor harmonic oscillator approximation was applied for evaluating the thermal and entropic contribution that were necessary to obtain the enthalpies, H_{298} and Gibbs free energies, G_{298} at 298 K. To get accurate energies, optimized structures were re-evaluated by additional single point energy calculations using 6-311G* triple-ζ basis set[22] for light atoms (H, C, O, S, B, N, Si and K). The solvent correction was done using the polarized continuum model.[23]

9.1. Regioselectivity for dehydrogenative borylation

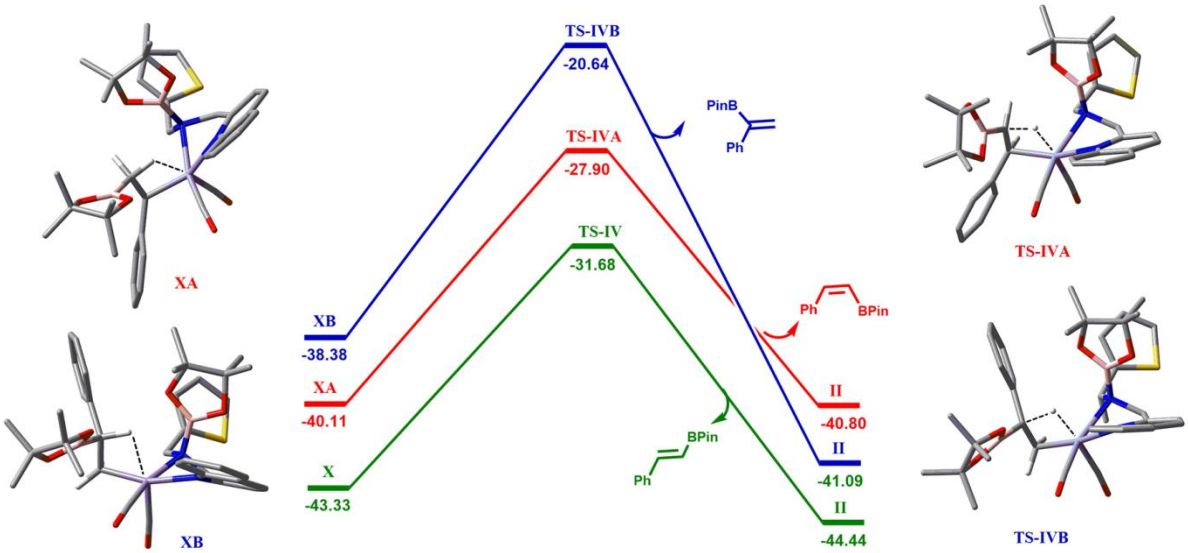


Fig. S14. Potential energy surface to compare the formation of different regioisomers.

To shed light on the regioselectivity towards formation of trans-borylated product, we analysed the energy profiles of the intermediate **X**, its other isomers (**XA**, **XB**) and corresponding transition states (**TS-IV**, **TS-IVA**, **TS-IVB**) that leads to corresponding regioisomers (Fig. S13). Potential energy surface analysis discloses that formation of the trans regioisomer (green line) is energetically more favourable than that of the other two regioisomers (red and blue lines).

9.2. Alternate pathways for dehydrogenative borylation

We also investigated other alternative pathways for the dehydrogenative borylation via computational studies. In this alternative proposal, first few steps till the formation of intermediate **III** are common to the major pathway depicted in the main text. As described earlier as a result of detachment of the thiophene arm, intermediate **III** possesses a vacant site for the incoming substrate (see Fig. S13). The styrene (model olefin) binds to the vacant

site leading to the formation of □-bound intermediate **XI**. Upon binding the olefinic protons becomes sufficiently acidic to be deprotonated by the base KHMDS and leads to intermediate **XII** via concerted metalation deprotonation (CMD) process. This process is thermodynamically downhill by 11.16 kcal mol^{-1} from the previous intermediate **XII**. To probe the influence of metal-binding on the acidity of olefinic proton, we investigated the thermodynamics of the direct deprotonation of unbound styrene with KHMDS. Not surprisingly, direct deprotonation of styrene without any prior activation is significantly uphill process to generate a species 40.90 kcal mol^{-1} higher in energy.

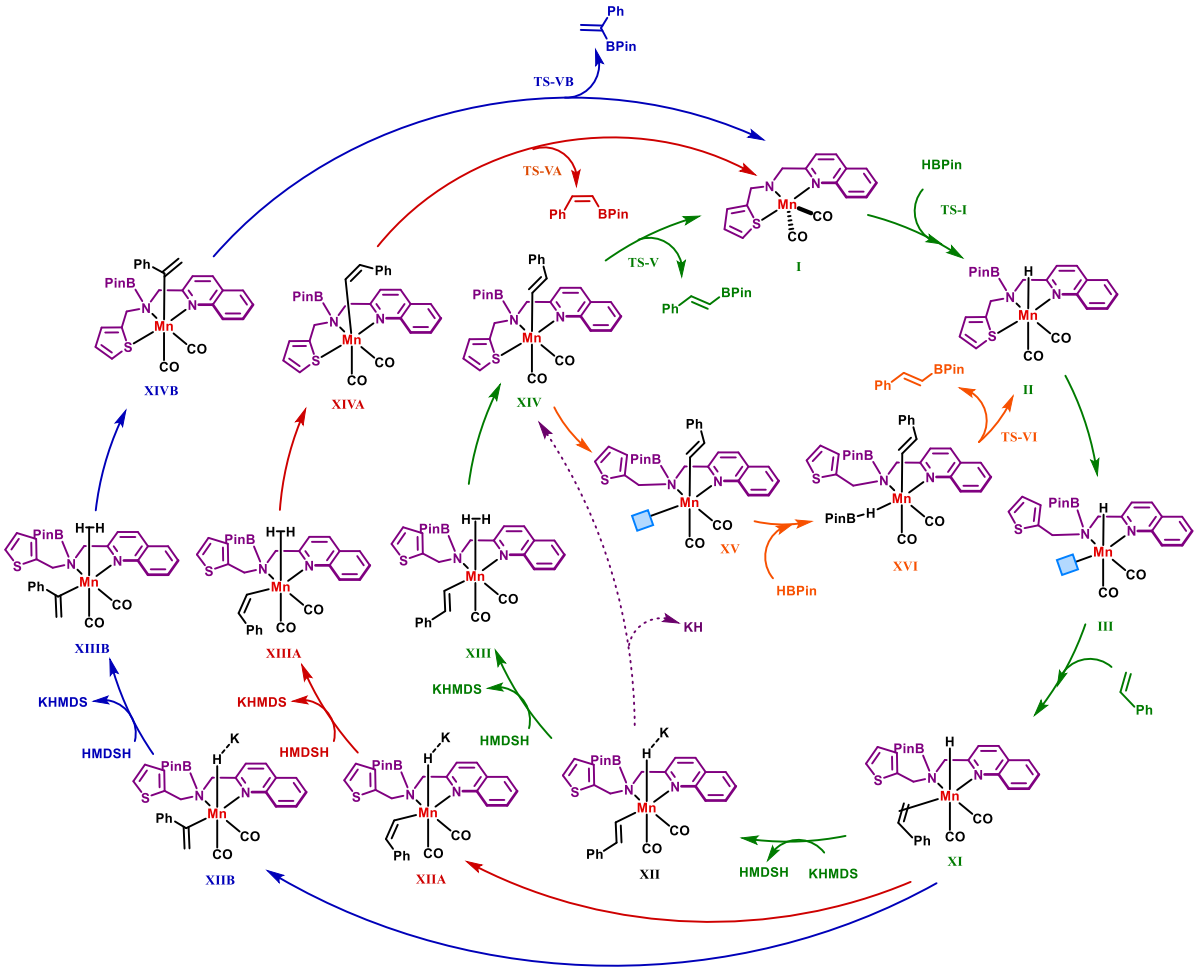


Fig. S15. Proposed alternative pathway for catalytic dehydrogenative borylation of olefins.

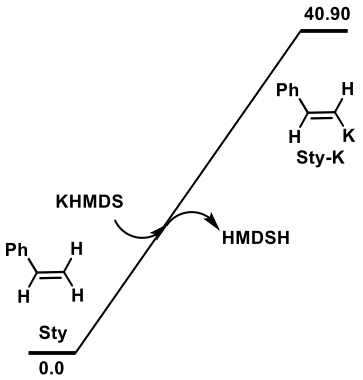


Fig. S16. Potential energy surface of deprotonation of unbound styrene.

Then Mn-hydride in intermediate **XIII** abstracts proton from the silyl amine produced via CMD process and a high energy □□□dihydrogen bound intermediate **XIV** is formed. To confirm the feasibility of this process, we calculated the pk_a of that Mn-hydride intermediate to be 32, following the protocol given by Morris.[24] The known pk_a value of that silyl amine is 26.[25] These values indicates that the Mn-hydride in intermediate **XIV** is sufficiently hydridic to deprotonate that silyl amine. Later release of H_2 leads to intermediate **XV**. An alternative path towards formation of intermediate **XIV** upon direct release of KH (dotted violet line, fig. S13), seems to be an unfavourable process as it is energetically uphill by 28.43 kcal mol^{-1}. From intermediate **XIV** two possible pathways can be sketched towards formation of the desired product. In one of them (marked in green, fig. S15), direct release of dehydrogenative borylation product via **TS-V** possesses an energy barrier of 14.2 kcal mol^{-1} and leads to intermediate **I**, where amido nitrogen center is engaged in □-donation. In other alternative pathway (marked in orange), detachment of the hemilabile thiophene arm leads to intermediate **XV**, followed by HBpin binding to the vacant site in □^{1}-fashion to give intermediate **XVI**. Then a □-complex assisted metathesis (□-CAM) prompts the generation of the desired dehydrogenative borylation product via **TS-VI** posing a transition barrier of 27.12 kcal mol^{-1} and give rise to intermediate **II**. Due to higher energy barrier, this □-CAM pathway seems to be less-favourable than the former pathway via **TS-V**.

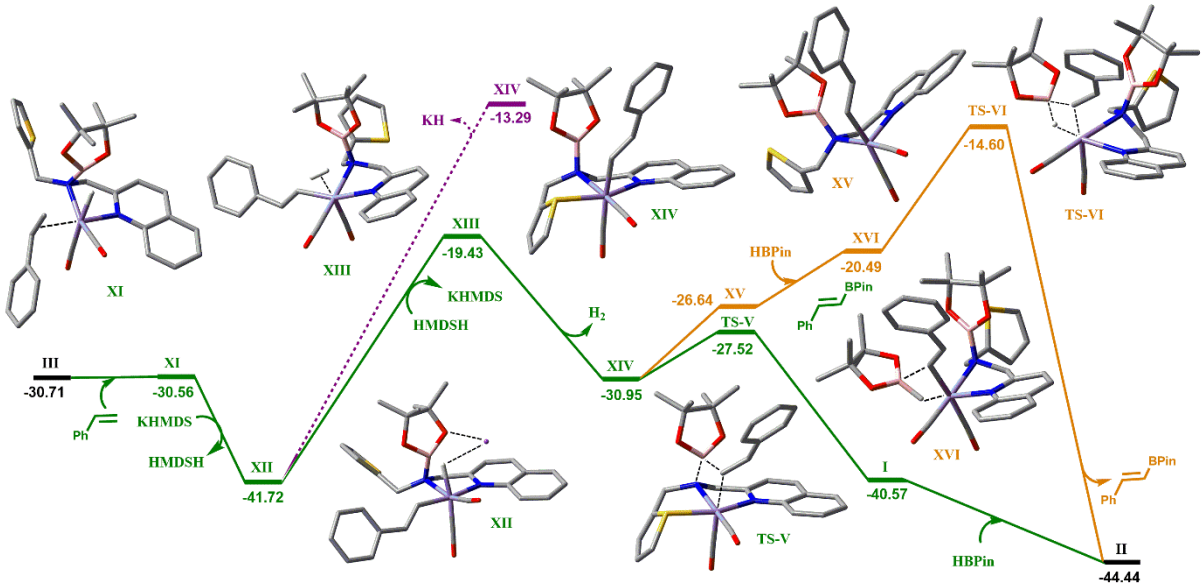


Fig. S17. Potential energy surface of alternate pathway for catalytic dehydrogenative borylation of olefins.

To acquire information regarding the regioselective nature of this reaction towards formation of trans-borylated product, we compared into the energy profiles of the intermediates and transition states (Fig. S17). Scrutiny of the potential energy surface reveals that the pathway towards trans regioisomer (green line) is a lower energy pathway than that of the other two regioisomers (red and blue lines).

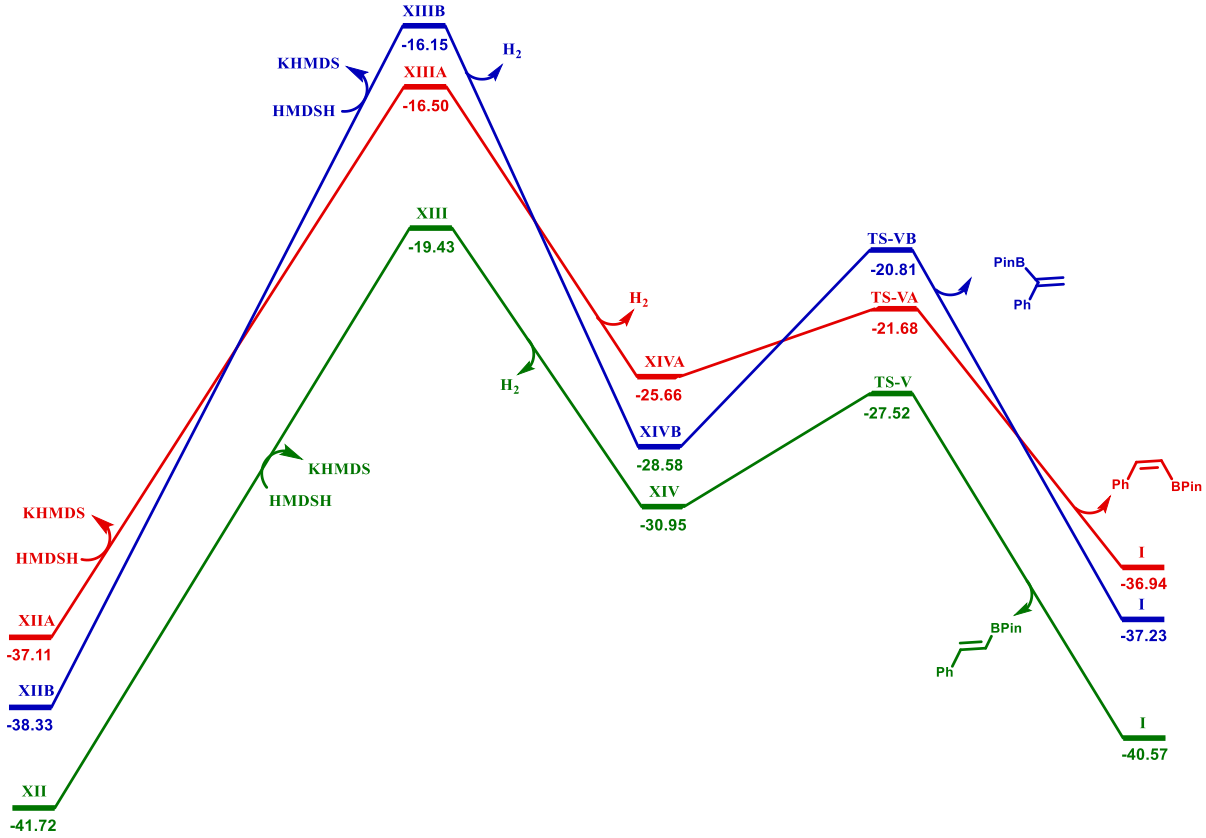


Fig. S18. Potential energy surface for the formation of different regioisomers in the alternate pathway.

9.3. Computational probation for hemilability:

The hemilability of the thiophene arm in the catalyst **Mn3** plays a preeminent role in dictating the substrate binding. Some substrate scope studies even strongly suggest the importance of the vacant site in the Mn-coordination sphere. For example, 4-cyano styrene failed as a substrate to give desired product under the optimized reaction conditions. This can be explained by the binding preference between olefin (π-donor) and nitrile (N-donor) (Fig. S17). An energy comparison between olefin (π-donor) bound intermediate (**VIII-CN-1**) and nitrile (N-donor) (**VIII-CN-2**) reveals that **VIII-CN-2** is more stable than **VIII-CN-1** by about 13.61 kcal mol^{-1}. Therefore, the nitrile binding prohibits the catalyst from reacting further and thus behaves as a catalyst poison. Given this fact, this is also completely unsurprising that the reaction remains unproductive in acetonitrile solvent.

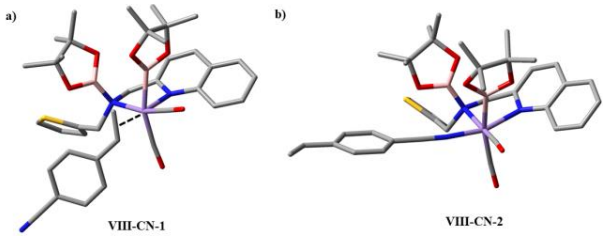


Figure S19. Optimized geometries for (a) π-bound (**VIII-CN-1**) and (b) nitrile bound (**VIII-CN-2**) intermediates while 4-cyano styrene was used as substrate.

10. Cartesian Coordinates for Optimized geometries of intermediates and Transition States:

I

0 1

Mn	-0.70429200	1.17997200	0.09651000
S	1.21014600	2.58918900	0.51489500
O	-2.64825200	3.37023700	-0.20629400
O	-1.09815800	0.68879300	2.97916500
C	0.03371600	-0.75042900	-1.86507300
H	0.73962100	-1.58369200	-1.67859300
H	0.00763000	-0.63143600	-2.96651000
C	1.69545600	0.98737300	-1.66110800
H	2.54241900	0.35254900	-1.34131300
H	1.73666000	1.03218500	-2.76246400
C	1.72609500	4.69964900	-0.86160500
H	1.86796300	5.73334500	-1.15846200
C	-1.90502800	2.49088000	-0.03478400
C	1.81411500	2.37786300	-1.12150100
C	-0.97482200	0.92171200	1.84527100
C	1.21330600	4.33356200	0.34348100
H	0.91829800	4.96075200	1.17312800
N	0.42133100	0.45721900	-1.19941500
C	2.04132700	3.57974600	-1.71359700
H	2.37125900	3.68355100	-2.74177900
C	-1.33038200	-1.15975800	-1.40016200
C	-1.94090200	-2.32589500	-1.91706200
C	-3.19241900	-2.67751500	-1.48960300
C	-3.18325800	-0.69174000	-0.05753500
C	-3.85465500	-1.85909200	-0.54153100
C	-3.85830000	0.12634200	0.87952600
C	-5.15494100	-2.16899200	-0.07067200
C	-5.12472000	-0.20016100	1.31663900
H	-3.37024600	1.01510400	1.24726900
C	-5.78323300	-1.35650000	0.84462900
H	-5.62073700	0.44575500	2.03484800
H	-1.39993800	-2.92136400	-2.64566100
H	-3.68848700	-3.56844500	-1.86493800
H	-5.64351600	-3.06207100	-0.45123300
H	-6.77967900	-1.59848700	1.20154900
N	-1.90878500	-0.36712200	-0.49744000

II

0 1

Mn	1.54799200	1.19108400	1.14791400
S	1.42623600	-1.25121600	0.85458300
O	-0.24699500	1.24455000	3.49859200
O	-0.54387800	1.49095100	-0.90609100
C	3.85525900	1.80634300	2.79842700
H	4.95159300	1.81756300	2.86571500
H	3.45636800	1.69040000	3.81755300
C	3.51856900	-0.62520600	2.58765500
H	4.37017400	-1.14351900	2.13471900
H	3.70575700	-0.51551700	3.66069100
C	0.15500900	-2.37347600	2.79653700
H	-0.60583200	-2.88159700	3.37889800
C	0.44939400	1.20658000	2.57113200
C	2.24588100	-1.39551600	2.40923800
C	0.26104400	1.44200100	-0.06736700
C	-0.02449000	-1.98418800	1.50627500
H	-0.88309600	-2.13800600	0.86712500
N	3.36885900	0.71401300	1.96995800
C	1.44526300	-2.00920400	3.32198700
H	1.73167800	-2.14996200	4.35887400
B	3.77425900	0.82838200	0.46647500
O	4.22124500	-0.42155700	-0.07580700
O	4.73477700	1.84776200	0.14127700
C	5.20288400	-0.10448900	-1.07264800
C	5.85162400	1.19875400	-0.48249100
C	6.44762400	2.14368900	-1.52240500
H	6.87023100	3.02300600	-1.02451900
H	7.24982100	1.65376900	-2.08678600
H	5.68395700	2.48856000	-2.22273400
C	6.89279700	0.89229300	0.60452700
H	7.81802200	0.47906400	0.18836300
H	7.13752000	1.82256100	1.12796400
H	6.49530300	0.18106800	1.33573000
C	4.48036700	0.15013900	-2.40318600
H	5.18497100	0.31112300	-3.22612800
H	3.86482600	-0.72341900	-2.63967500
H	3.82227600	1.02086600	-2.33262900
C	6.15311300	-1.28990200	-1.21182800
H	5.61258100	-2.15004800	-1.62034100
H	6.97902900	-1.05245000	-1.89228000
H	6.56890300	-1.58157100	-0.24437500
H	2.64685300	1.19615300	-0.14348300
C	3.37135800	3.12537800	2.26147300
C	4.12973700	4.29107900	2.51222200
C	3.67455500	5.50025500	2.06252700
C	1.69960000	4.34679000	1.19618400
C	2.42739300	5.56344900	1.39726200
C	0.41266400	4.43275000	0.61480300
C	1.88065500	6.79377000	0.95367600
C	-0.10063800	5.64573700	0.20833300
H	-0.17617900	3.53603700	0.51563400
C	0.64027100	6.83864900	0.36134600
H	-1.09309200	5.68133500	-0.23094300
H	5.07481400	4.19803900	3.03599200
H	4.24606000	6.41168000	2.21567700
H	2.45971400	7.70089400	1.10500600
H	0.22408200	7.78399600	0.02683900
N	2.22012800	3.12789700	1.59168400

III

0 1

Mn	1.56960000	1.34106200	1.02080200
S	5.17737000	0.20333200	5.00034900
O	-0.69872200	1.25890200	2.92535100
O	-0.02658900	1.31156100	-1.46679400
C	3.46280900	2.28833600	2.96537800
H	4.53369500	2.39405100	3.16785300
H	2.93775500	2.25641800	3.93242000
C	3.10891600	-0.15101200	3.06849500
H	2.36529800	0.02757100	3.85560600
H	2.73223400	-0.96234400	2.43990100
C	6.35337300	-1.86761500	4.02938400
H	7.06959700	-2.66377200	3.85941800
C	0.19014900	1.26505300	2.17914000
C	4.41185800	-0.61374600	3.65723000
C	0.56263700	1.37723800	-0.46878100
C	6.50277200	-0.91599100	5.00071400
H	7.30729800	-0.80357400	5.71451600
N	3.17229500	1.06226400	2.23008500
C	5.16019600	-1.69226400	3.26470200
H	4.86868200	-2.31894800	2.43105900
B	3.88830000	0.97392800	0.86274000
O	4.28352200	-0.34581800	0.49442000
O	4.95192200	1.89440500	0.62167600
C	5.39748500	-0.18296100	-0.40245900
C	6.07207700	1.13721900	0.13128800
C	6.78399400	1.95968900	-0.94052500
H	7.21679300	2.85776100	-0.48726800
H	7.59731400	1.38638800	-1.40083100
H	6.09111500	2.27752300	-1.72260600
C	7.01920400	0.88887900	1.31291000
H	7.94535400	0.39415500	0.99972200
H	7.28160400	1.85486100	1.75675400
H	6.54014200	0.27834800	2.08101000
C	4.84772600	-0.03347500	-1.82839200
H	5.65013500	0.01535700	-2.57188200
H	4.21946700	-0.90104900	-2.05400200
H	4.23106800	0.86468500	-1.92347600
C	6.27901800	-1.42508500	-0.31371500
H	5.72445600	-2.29724600	-0.67627200
H	7.17502600	-1.31096800	-0.93459000

H	6.58959800	-1.61996300	0.71450200
H	2.90658400	1.38053100	-0.00204300
C	2.96655000	3.49769600	2.21828800
C	3.59141200	4.74723000	2.42498000
C	3.10262000	5.85876500	1.79131800
C	1.34849100	4.45152900	0.83344100
C	1.94516000	5.74352000	0.98559100
C	0.13477300	4.35486500	0.11242600
C	1.35523500	6.86723700	0.35344200
C	-0.42519800	5.46896200	-0.47444400
H	-0.36370400	3.40010400	0.05416800
C	0.19443400	6.73508200	-0.37222200
H	-1.36054800	5.37047000	-1.01702500
H	4.46525300	4.79475400	3.06528200
H	3.57823300	6.82866400	1.90815600
H	1.83403100	7.83596700	0.46807700
H	-0.25594700	7.59946600	-0.85035700
N	1.91909400	3.33344300	1.40967700

IV

0 1

Mn	2.09760000	0.98739100	1.17632400
S	6.89662200	-1.29921500	2.86544800
O	0.35007500	0.46398500	3.52055400
O	-0.20767700	1.63731000	-0.53232300
C	3.95586700	1.39661300	3.36417300
H	4.93636000	1.46360900	3.85171200
H	3.25630700	0.97504300	4.09781500
C	4.07849300	-0.93516600	2.61232100
H	3.16618500	-1.19538100	3.15339400
H	4.09438600	-1.52997300	1.69983800
C	6.54798100	-1.71667800	5.38487700
H	6.73230500	-1.92747700	6.43245900
C	1.06873300	0.65202700	2.61925300
C	5.26074700	-1.24365600	3.48366600
C	0.69822600	1.40304900	0.15852200
C	7.53551400	-1.64358400	4.44204500
H	8.60043100	-1.77710100	4.57760400
N	3.98746700	0.49196500	2.20441100
C	5.25056200	-1.48522700	4.83335100
H	4.33273100	-1.50024200	5.41242000
B	4.89034800	0.86999700	1.11076000
O	5.45443600	-0.07699700	0.29042500
O	5.44167600	2.11996800	0.98929900
C	6.23686100	0.64526600	-0.70119900
C	6.51664100	2.02723300	0.01816700
C	6.43223900	3.24615700	-0.89430300
H	6.61065400	4.15298300	-0.30778900
H	7.18908800	3.19625200	-1.68506800
H	5.44507500	3.32777900	-1.35295300
C	7.82195800	2.04865300	0.81847600
H	8.69870600	2.03119800	0.16305500
H	7.85372500	2.96690000	1.41310500
H	7.87715200	1.19895800	1.50466500
C	5.36678500	0.77028700	-1.95434100
H	5.90046000	1.28327900	-2.76096500
H	5.10274300	-0.23451500	-2.29837200
H	4.43721400	1.30072000	-1.73533700
C	7.48478200	-0.17646600	-1.00578100
H	7.19112000	-1.12593100	-1.46374500
H	8.13444900	0.35462600	-1.71037700
H	8.05371200	-0.39840100	-0.10090100
C	3.49963400	2.77382000	2.96595000
C	3.93624000	3.88778600	3.71590200
C	3.52410900	5.14389900	3.35658700
C	2.36941600	4.12970300	1.45489200
C	2.74064100	5.30168600	2.18958000
C	1.69516500	4.29890500	0.22230700
C	2.35290200	6.58041500	1.71459100
C	1.34988900	5.55634100	-0.22332300
H	1.49295500	3.42941600	-0.38051800
C	1.65981000	6.70918800	0.53381200
H	0.83911100	5.66030900	-1.17603500
H	4.58632600	3.72460900	4.56914000
H	3.81636100	6.02022000	3.92886100
H	2.63098700	7.45506800	2.29679200
H	1.36957400	7.69090100	0.17163400
N	2.69074200	2.86879400	1.91366500
O	0.25259000	-1.59268700	-0.10671400
B	1.31882200	-1.40946000	0.71891000
O	1.36801900	-2.26887700	1.77988700
C	0.26531300	-3.21331000	1.61871500
C	-0.67770900	-2.46956500	0.59708500
C	-0.34736000	-3.45904600	2.99214000
H	-1.23883600	-4.09072900	2.91101900
H	0.37729000	-3.97345400	3.63122200
H	-0.62117500	-2.51945900	3.47575400
C	0.87898000	-4.49877100	1.06003100
H	1.65995800	-4.84509800	1.74350700
H	0.12976100	-5.29054300	0.96014100
H	1.33631500	-4.32530700	0.08125500
C	-1.35371700	-3.37226800	-0.42745700
H	-2.01428100	-4.09153100	0.06944900
H	-1.96014300	-2.76347800	-1.10462200
H	-0.62407400	-3.92140900	-1.02611100
C	-1.70971700	-1.55675800	1.26585600
H	-2.16395000	-0.92330800	0.49863300
H	-2.49909500	-2.13919600	1.75195200
H	-1.24833200	-0.90408200	2.01037100
H	2.27312400	-0.71911500	0.37485200
H	2.98766000	1.31600100	-0.14940800

V

0 1

Mn	1.65938100	1.36140200	2.01614000
S	6.43732500	-1.46178300	3.15321500
O	0.68620500	0.72894000	4.70622300
O	-1.14481800	1.68332300	1.23765000
C	4.15330600	1.84362800	3.54316600
H	5.22456000	1.81751700	3.77383400
H	3.61582100	1.71638500	4.49151800
C	3.73694200	-0.56780700	3.42054500
H	2.97855900	-0.49406600	4.20118200
H	3.40458200	-1.33970600	2.73360800
C	6.69827100	-1.21084500	5.70444000
H	7.11383200	-1.21489700	6.70595300
C	1.07937300	0.99533600	3.64055700
C	5.04738200	-0.91141300	4.06574500
C	-0.01676300	1.61659700	1.54370700
C	7.40533600	-1.56798300	4.59042000
H	8.43433200	-1.89573100	4.52749100
N	3.75896500	0.72297300	2.66924000
C	5.35392300	-0.83482700	5.39991800
H	4.62769900	-0.52235600	6.14340400
B	4.44371900	0.63454300	1.39124600
O	4.62517400	-0.55615100	0.74024500
O	4.99714700	1.71384300	0.75650800
C	5.21726000	-0.25509500	-0.55713100
C	5.81213600	1.19165600	-0.33364500
C	5.67080000	2.13108000	-1.52484900
H	6.07663700	3.11374200	-1.26568400
H	6.22696100	1.74839300	-2.38750900
H	4.62542400	2.26007600	-1.81210300
C	7.25577100	1.18729500	0.17567300
H	7.95404300	0.85320100	-0.59803800
H	7.52762900	2.20535900	0.47044600
H	7.36444900	0.53974700	1.05049100
C	4.09205700	-0.30783100	-1.59137700
H	4.48278900	-0.16179300	-2.60347400
H	3.60667200	-1.28459000	-1.54000600
H	3.32351800	0.44244600	-1.40101800
C	6.25381500	-1.33160800	-0.85913000
H	5.75225900	-2.29846600	-0.96324400
H	6.77363800	-1.11448500	-1.79865700
H	6.99106100	-1.41740700	-0.05906000
C	3.77840700	3.17967500	2.96930100
C	4.64088300	4.28164300	3.16833800
C	4.28037400	5.51379200	2.68994900
C	2.22893900	4.49410300	1.83779000
C	3.05131200	5.65454500	2.00364800

C	0.99990800	4.63644100	1.14952900
C	2.62427600	6.89971000	1.47631700
C	0.61153800	5.86056800	0.64955900
H	0.36857500	3.76851200	1.03570000
C	1.42639400	7.00477300	0.80878100
H	-0.33805000	5.94525300	0.12953400
H	5.57993500	4.12821000	3.68914700
H	4.92314300	6.38021600	2.82070300
H	3.26481600	7.76711600	1.61259700
H	1.10354200	7.96074200	0.40760700
N	2.61454000	3.26231200	2.33049000
O	1.04972700	-0.89384100	0.08466700
B	1.20045000	-0.53615800	1.43166400
O	1.00844900	-1.65886200	2.23358900
C	0.91485200	-2.83215700	1.38883000
C	0.46481000	-2.21671800	0.02326500
C	-0.07558800	-3.80675100	2.01624600
H	-0.23363700	-4.67629500	1.36723500
H	0.31553000	-4.16357400	2.97452800
H	-1.03921200	-3.32832900	2.20291200
C	2.31328900	-3.46026400	1.33111500
H	2.64127100	-3.68813800	2.35068400
H	2.31717700	-4.39307400	0.75691100
H	3.03619600	-2.76915800	0.88690500
C	0.98791000	-2.93653600	-1.21475500
H	0.59453600	-3.95849700	-1.26734800
H	0.66603900	-2.40202600	-2.11444500
H	2.07904700	-2.98606300	-1.22118700
C	-1.05289000	-2.02370000	-0.07979600
H	-1.27053400	-1.40594700	-0.95633000
H	-1.58034100	-2.97782500	-0.18621600
H	-1.43930400	-1.50171000	0.80033000
H	2.07882900	1.15392100	0.22679900
H	2.25973600	1.91029800	0.30276000

VI

0 1

Mn	1.53444000	1.00908400	1.21796200
S	0.88539500	-1.35546100	1.10988500
O	-0.47648000	1.48261100	3.36380600
O	-0.39669900	2.01111100	-0.73067600
C	3.19089800	1.14867400	3.57864200
H	4.03892100	1.06052000	4.27365200
H	2.27024600	0.92749800	4.12911400
C	3.04828800	-1.22890300	2.84569000
H	3.66397200	-1.85372900	2.19376500
H	3.37329600	-1.40603300	3.87926200
C	-0.65874000	-2.00751200	3.07997300
H	-1.53398500	-2.26391400	3.66675200
C	0.37993900	1.27257300	2.60281300
C	1.60564500	-1.58422800	2.70053100
C	0.37158300	1.62606500	0.06757500
C	-0.70684000	-1.69196200	1.75814000
H	-1.56642800	-1.65765400	1.10296200
N	3.30532900	0.18766700	2.46553300
C	0.67061700	-1.92994700	3.62680500
H	0.90116900	-2.08448300	4.67590900
B	4.52157100	0.38240200	1.67920200
O	5.02105200	-0.51548100	0.76888600
O	5.37383100	1.41842000	1.96003800
C	6.43033000	-0.17089300	0.59321900
C	6.46828100	1.34686000	1.00671400
C	6.13272900	2.31234500	-0.13108200
H	6.00059000	3.31294000	0.29329700
H	6.94337200	2.35604100	-0.86646900
H	5.20232600	2.03658100	-0.63257900
C	7.74491200	1.78074400	1.71807900
H	8.61139200	1.66741500	1.05725300
H	7.66540400	2.83644700	1.99463800
H	7.92045500	1.20307600	2.62833500
C	6.83887900	-0.44095100	-0.84574800
H	7.88578100	-0.15773100	-1.00204200
H	6.73543500	-1.50661700	-1.07172900
H	6.21842600	0.12191600	-1.54150800
C	7.21190600	-1.07840100	1.54849100
H	6.97644800	-2.12147300	1.31678600
H	8.29231300	-0.93686300	1.44693400
H	6.93442600	-0.88890000	2.59051500
C	3.15082400	2.55720000	3.03091200
C	3.71821800	3.60993900	3.77626500
C	3.70260400	4.88336800	3.26671600
C	2.62526600	3.98118500	1.26642700
C	3.16880600	5.10076700	1.97550200
C	2.15161000	4.18313300	-0.05159400
C	3.17460600	6.38049400	1.36303100
C	2.18278800	5.43571700	-0.62290500
H	1.80887200	3.33196300	-0.61262100
C	2.68514100	6.54966800	0.08907100
H	1.82071500	5.56476500	-1.63872300
H	4.16276100	3.39125000	4.74157700
H	4.11523900	5.71959200	3.82460600
H	3.58079600	7.22017600	1.92103100
H	2.69385500	7.53132300	-0.37545100
N	2.57652800	2.72718300	1.83868700
O	3.22988900	1.51113600	-1.44375600
O	1.87209500	-0.31308800	-1.52346300
B	2.36710300	0.69830600	-0.69929600
C	2.53157600	-0.26901100	-2.80724000
C	4.38436100	1.39864900	-3.57931500
H	4.27948300	1.15933000	-4.64396000
H	4.70120100	2.44334300	-3.49555500
H	5.17397200	0.76975500	-3.16530800
C	2.02493800	2.20081700	-3.39454200
H	2.39429200	3.21639000	-3.21721200
H	1.86496700	2.07674000	-4.47084600
H	1.06541600	2.09388300	-2.88134500
C	3.05840700	1.20414600	-2.85344900
C	1.51334200	-0.61816900	-3.88857800
H	1.95305300	-0.52183800	-4.88851300
H	1.18411000	-1.65438400	-3.76079400
H	0.63312300	0.02518400	-3.82753300
C	3.64571400	-1.31997700	-2.76768600
H	3.19587100	-2.29809600	-2.57049200
H	4.19474700	-1.37683900	-3.71410800
H	4.34505800	-1.10655400	-1.95678700

VII

0 1

Mn	1.90462000	1.61182200	0.83327900
S	3.64131200	-1.77853900	4.85406900
O	-0.63793400	1.13999800	2.30780000
O	0.34895800	2.99525300	-1.23271800
C	2.96293500	1.31705200	3.45248200
H	3.71759300	1.08533600	4.21410600
H	1.98089300	1.02928300	3.85058100
C	2.78167200	-0.87214800	2.29373300
H	1.75963000	-0.90035800	2.68500300
H	2.75038100	-1.24963400	1.27126500
C	5.42918400	-3.20787600	3.67957400
H	6.25192000	-3.89169500	3.50242600
C	0.40218600	1.36022200	1.83167600
C	3.70558200	-1.73107800	3.10672200
C	0.97455700	2.47922800	-0.39128500
C	4.97112100	-2.89021000	4.92905600
H	5.32814500	-3.24588700	5.88592300
N	3.18277700	0.55521100	2.20878300
C	4.70545500	-2.54576300	2.64208600
H	4.91666200	-2.64795500	1.58470100
B	4.46955700	0.81854900	1.55373700
O	5.09696800	-0.03338200	0.66869300
O	5.27196400	1.84965800	1.97898200
C	6.47407200	0.42963000	0.53565000
C	6.40354000	1.90981600	1.07382600
C	6.06791200	2.94613000	-0.00265700
H	5.83918100	3.89672500	0.48852600
H	6.91271100	3.10093500	-0.68179600
H	5.19552000	2.65086000	-0.58793000
C	7.62186800	2.35756100	1.87364400
H	8.52174600	2.34594900	1.24886500
H	7.46668100	3.38178800	2.22660000

H	7.78980600	1.71964200	2.74404000
C	6.88436700	0.31559800	-0.92698900
H	7.88653000	0.73217800	-1.07808100
H	6.91086900	-0.73861500	-1.22287200
H	6.17775200	0.83797500	-1.57231000
C	7.32823700	-0.49118100	1.41044000
H	7.20265100	-1.52305900	1.06999100
H	8.39019600	-0.23438800	1.34284000
H	7.01792900	-0.44485700	2.45807100
C	2.98753900	2.79480700	3.16326100
C	3.37492700	3.70791500	4.16364100
C	3.42430900	5.04725200	3.86972300
C	2.82725200	4.47929100	1.56699500
C	3.18153200	5.46746500	2.54050500
C	2.72639700	4.87333900	0.21135100
C	3.32252100	6.82115500	2.14074000
C	2.89523400	6.19273500	-0.14864100
H	2.56325800	4.11391800	-0.53737600
C	3.17167400	7.18276600	0.82223000
H	2.82588600	6.47126300	-1.19591800
H	3.62369700	3.33293100	5.15105900
H	3.68711600	5.78233400	4.62538300
H	3.57150300	7.56117800	2.89681100
H	3.28804600	8.21964900	0.52134100
N	2.63899000	3.16096000	1.92973000
O	3.65938000	1.30834700	-1.98441200
O	2.31661300	-0.10191000	-0.77703300
B	3.00406000	1.12458200	-0.78937300
C	2.56026100	-0.80959900	-2.02688300
C	4.30514600	-0.11335800	-3.83839600
H	3.96633800	-0.86338200	-4.56220400
H	4.68444100	0.74877900	-4.39585700
H	5.12946600	-0.53507900	-3.26089000
C	2.09321500	1.05666800	-3.77596200
H	2.55893400	1.92375900	-4.25399600
H	1.68181100	0.41069900	-4.55860900
H	1.27427100	1.42212500	-3.15150300
C	3.15357900	0.32952100	-2.94242300
C	1.24259100	-1.40128400	-2.51351200
H	1.36973300	-1.89427700	-3.48429700
H	0.89224900	-2.14990300	-1.79585100
H	0.47057200	-0.63509800	-2.60715500
C	3.55888300	-1.92371000	-1.70195200
H	3.11038300	-2.59481900	-0.96179300
H	3.80712300	-2.51468200	-2.58982200
H	4.47208900	-1.51062100	-1.27024600

VIII

0 1

Mn	1.99314300	2.29237900	1.22942300
S	5.65731100	-0.23949400	4.85097400
O	0.11773100	2.99179400	3.42112700
O	0.03648000	2.71525400	-0.89536500
C	4.43277600	3.27797900	2.80506000
H	5.52338300	3.24330800	2.88309400
H	4.05974700	3.60651300	3.78196500
C	3.47538800	1.27298900	3.82236700
H	2.66827800	1.86301000	4.26053000
H	3.06435000	0.30316200	3.57302000
C	5.91485700	1.50652400	6.72559800
H	6.26471400	2.03242400	7.60696400
C	0.89645900	2.65803900	2.62094000
C	4.56543400	1.12637500	4.84433400
C	0.80893100	2.61014000	-0.02183800
C	6.46049500	0.33560900	6.27567500
H	7.28563300	-0.22253400	6.69741400
N	3.86836400	1.93848400	2.54126100
C	4.83009800	1.94985700	5.91038700
H	4.24611000	2.84119500	6.11635000
B	4.74128800	1.13144300	1.69664300
O	4.78481300	-0.23817000	1.78638100
O	5.73615400	1.66423600	0.90978700
C	5.81570100	-0.70253300	0.86450700
C	6.69393900	0.58892200	0.67342700
C	7.29102600	0.74018900	-0.71738000
H	7.84893900	1.67918400	-0.78355800
H	7.98408300	-0.08289200	-0.92394900
H	6.51602500	0.74333700	-1.48197500
C	7.78889300	0.74983500	1.73291100
H	8.58985700	0.01645000	1.59568300
H	8.22031100	1.75138300	1.64086800
H	7.38696600	0.64148300	2.74387700
C	5.11760900	-1.15810800	-0.41868500
H	5.84091700	-1.56883800	-1.13098500
H	4.40472300	-1.95095600	-0.17023100
H	4.57064900	-0.34140700	-0.89583900
C	6.54136500	-1.87374600	1.51625000
H	5.84398900	-2.70698500	1.64678200
H	7.36346400	-2.21651900	0.87820500
H	6.94109500	-1.60931600	2.49604700
C	4.01577500	4.33714800	1.82920400
C	4.90940300	5.38249800	1.51154100
C	4.47134900	6.42588700	0.73527000
C	2.26184400	5.39245300	0.73915800
C	3.11129900	6.47850000	0.35658300
C	0.87633800	5.49667400	0.47122700
C	2.57001100	7.56867100	-0.37058000
C	0.37478700	6.58121800	-0.21393700
H	0.21484600	4.72649300	0.83829200
C	1.22735700	7.61560600	-0.66515700
H	-0.69252800	6.64406700	-0.40376800
H	5.93391700	5.32537300	1.86313600
H	5.14379100	7.22444700	0.43277600
H	3.23606700	8.37253200	-0.67343000
H	0.81548900	8.45442500	-1.21815500
N	2.76738100	4.28749900	1.38586600
O	3.32484600	3.68137600	-1.14828800
O	3.35517000	1.45687900	-1.58876600
B	3.04218200	2.42334300	-0.63114900
C	3.55393700	2.11710600	-2.86906300
C	5.46999200	3.73436100	-2.19041100
H	6.04683200	3.67799800	-3.11997000
H	5.63962400	4.71527700	-1.73554900
H	5.83399600	2.97921700	-1.49136500
C	3.44467800	4.68426900	-3.32769200
H	3.74074300	5.65130200	-2.90870900
H	3.85796400	4.60658100	-4.34015800
H	2.35469700	4.66766700	-3.38846900
C	3.96722900	3.56372600	-2.43301700
C	2.20574900	2.06621100	-3.59752700
H	2.26963300	2.50881900	-4.59724300
H	1.90289800	1.01952700	-3.70252600
H	1.42856700	2.58373500	-3.02972300
C	4.60100800	1.35778000	-3.67450900
H	4.25485900	0.33578500	-3.85948800
H	4.76366300	1.84177000	-4.64448000
H	5.55933000	1.30538900	-3.15607100
C	0.88624000	0.20640900	1.52914900
C	1.83531500	0.18209500	0.51759000
H	2.77969000	-0.31608200	0.68283200
H	1.54027000	0.26121100	-0.51887400
H	-0.12629500	0.50773700	1.27246900
C	0.98372100	-0.53585800	2.80525900
C	0.08874500	-0.26301100	3.85369600
C	1.92812800	-1.56171100	2.99461400
C	0.17050200	-0.94684200	5.06423300
H	-0.65829200	0.51327900	3.72301500
C	2.01355900	-2.24291000	4.20774600
H	2.61792100	-1.80615000	2.19548600
C	1.14142000	-1.93345500	5.25284000
H	-0.52369500	-0.70589600	5.86476800
H	2.76361100	-3.01874200	4.33484400
H	1.20931000	-2.46263300	6.19904200

IX

0 1

Mn	1.80359700	2.27528700	1.64901400
S	3.90515900	1.23842500	6.65133200
O	0.15611300	2.37324700	4.04730900
O	-0.66644900	2.97529200	0.25559700

C	3.80586000	2.93944900	3.66086800
H	4.72426300	2.94056400	4.25831600
H	2.96991000	3.07046600	4.35807400
C	3.27014200	0.57397400	3.97059200
H	2.26144700	0.76816500	4.33491300
H	3.23709600	-0.37068900	3.43642100
C	6.09727900	-0.08587000	6.42897700
H	7.04962400	-0.55237300	6.65682100
C	0.81964700	2.36523200	3.08266200
C	4.23524200	0.46419600	5.11829400
C	0.35784300	2.76089500	0.77085500
C	5.39277600	0.66522200	7.33090500
H	5.65060200	0.90022200	8.35462600
N	3.61481700	1.64210900	2.97264000
C	5.43518000	-0.20196300	5.16937300
H	5.81179600	-0.76667600	4.32663800
B	4.76416900	1.29925400	2.13809600
O	5.29972700	0.04373300	2.05189200
O	5.45647500	2.24665700	1.43265600
C	6.46173800	0.10669500	1.17122000
C	6.74202700	1.66027800	1.08254200
C	7.13363200	2.15762700	-0.30226800
H	7.27725600	3.24253000	-0.27235500
H	8.07335700	1.69771600	-0.62718800
H	6.35317600	1.93331700	-1.02995800
C	7.72821400	2.16460500	2.14086600
H	8.74763000	1.81913700	1.94359600
H	7.72402100	3.25869800	2.12943900
H	7.43579000	1.83508200	3.14333800
C	6.08021400	-0.53529900	-0.16352500
H	6.96135800	-0.63599300	-0.80614400
H	5.68381500	-1.53668400	0.03089000
H	5.32766300	0.03820900	-0.70452100
C	7.57773300	-0.70255300	1.82696200
H	7.28193300	-1.75509400	1.87459300
H	8.49937700	-0.63592700	1.23884500
H	7.78630100	-0.36112900	2.84281700
C	3.81337200	4.10105100	2.71690500
C	4.73845800	5.14750600	2.92970200
C	4.71343600	6.24382700	2.11077600
C	2.83715000	5.21230100	0.92379600
C	3.74607800	6.30945800	1.08105400
C	1.85347500	5.31181500	-0.09001000
C	3.65145300	7.43673500	0.22621300
C	1.76774900	6.43505400	-0.88573200
H	1.16665500	4.49602200	-0.23952400
C	2.67574900	7.50650000	-0.73993700
H	0.98863500	6.48969700	-1.63998900
H	5.45861200	5.05584500	3.73536500
H	5.41438200	7.06400600	2.24035400
H	4.35954200	8.24963400	0.36381600
H	2.59774400	8.37796500	-1.38277000
N	2.90166800	4.09969800	1.74739100
O	3.92283400	1.53383700	-1.85274800
O	1.69579000	2.05561400	-1.86295700
B	2.69964300	1.36347400	-1.23322000
C	2.20486300	2.46488100	-3.16349900
C	4.60611200	2.06946700	-4.10758300
H	4.44992500	2.73658300	-4.96266800
H	5.66604200	2.10992300	-3.83662500
H	4.37353800	1.04756700	-4.41389400
C	4.25229200	3.85327200	-2.38294300
H	5.29894300	3.75632500	-2.08229100
H	4.18407400	4.63748600	-3.14365500
H	3.67780600	4.16731200	-1.51007000
C	3.75679800	2.50849400	-2.91963800
C	1.57316000	3.79578700	-3.54614800
H	1.95404000	4.13720500	-4.51539200
H	0.48849900	3.67529400	-3.62706500
H	1.77786200	4.56380200	-2.80094200
C	1.77913300	1.37393400	-4.15198600
H	0.69130700	1.26802200	-4.11199800
H	2.06754600	1.62407000	-5.17788400
H	2.22281400	0.40777600	-3.89155400
C	1.37200900	0.38086300	0.93248600
C	2.52580000	0.31429600	-0.07792200
H	3.48086700	0.17618800	0.43301500
H	0.42478000	0.41322700	0.38405300
H	2.43273900	-0.61515500	-0.68020700
C	1.30081300	-0.78117300	1.86707600
C	0.23434900	-0.85960400	2.78606300
C	2.25139900	-1.81756800	1.90486700
C	0.14517600	-1.88887400	3.71564900
H	-0.51718100	-0.07539000	2.77677900
C	2.16682100	-2.85292300	2.84153100
H	3.08649700	-1.80883900	1.21292000
C	1.12033600	-2.89289900	3.75948900
H	-0.68492500	-1.90689000	4.41764800
H	2.92888200	-3.62902800	2.85002700
H	1.05716300	-3.69210900	4.49267700

X

0 1

Mn	1.97135500	1.67263700	1.34967600
S	4.60587700	1.91406300	6.45042000
O	-0.15642400	2.10010900	3.30065300
O	-0.05876100	2.26113100	-0.67773600
C	3.32505300	3.13065800	3.50826900
H	4.08795800	3.43160500	4.23613200
H	2.34232200	3.26502200	3.97401200
C	3.09360400	0.80671200	4.27467000
H	2.15768500	1.17904800	4.69828400
H	2.89380800	-0.17954300	3.87034000
C	5.97119700	-0.26564400	6.49258300
H	6.69854200	-1.02328100	6.76294800
C	0.70536700	1.99703200	2.51387700
C	4.17603600	0.66156800	5.30572400
C	0.78343500	2.02964700	0.09761000
C	5.88818500	0.95202000	7.11246500
H	6.49405600	1.33702800	7.92138300
N	3.45961200	1.70419700	3.13594800
C	4.99501100	-0.42828200	5.46310200
H	4.88695900	-1.31330700	4.84794600
B	4.76958200	1.39551900	2.56723100
O	5.20465700	0.12943200	2.28822800
O	5.70123700	2.37066500	2.31778700
C	6.51453900	0.25620400	1.66123300
C	6.97173900	1.69182500	2.11726200
C	7.77388200	2.47393900	1.08496200
H	8.02240300	3.46059800	1.48769900
H	8.71032400	1.95714900	0.84776700
H	7.20685400	2.61776700	0.16295200
C	7.68287900	1.69926200	3.47395400
H	8.68181000	1.25676400	3.40501000
H	7.78680700	2.73523200	3.80993800
H	7.10908700	1.15529400	4.22973000
C	6.31273800	0.14729600	0.14758700
H	7.26847200	0.20490200	-0.38228800
H	5.85118400	-0.81555100	-0.08773700
H	5.65788700	0.93861500	-0.22863500
C	7.38722600	-0.88571500	2.16732200
H	6.97680900	-1.84016300	1.82309000
H	8.40837700	-0.79465300	1.78104300
H	7.42254200	-0.90448400	3.25824900
C	3.43562900	4.01054600	2.29631100
C	3.94055500	5.32444300	2.41297400
C	4.06915100	6.09545900	1.28655000
C	3.27062300	4.19016300	-0.01726700
C	3.76172400	5.53309300	0.02343300
C	3.05304600	3.58445000	-1.27767500
C	3.95800600	6.24144200	-1.18908800
C	3.27702500	4.29285900	-2.43851900
H	2.74276200	2.55140200	-1.33213900
C	3.71536800	5.63620800	-2.40109600
H	3.12058300	3.80292600	-3.39521800
H	4.21900800	5.69834400	3.39273800
H	4.43672200	7.11660000	1.34195200
H	4.31849900	7.26560800	-1.13987900
H	3.87460500	6.18112300	-3.32684100
N	3.04882800	3.47793100	1.14335900

O	2.81721400	0.50825900	-2.35930800
O	1.70146400	-1.43070100	-1.87559500
B	2.42954900	-0.38225000	-1.38275200
C	1.76205900	-1.36477700	-3.32640000
C	3.05319500	0.39651500	-4.76280600
H	2.58906900	0.07248900	-5.70088200
H	3.26392300	1.46797800	-4.84204800
H	4.00407000	-0.12689300	-4.64314600
C	0.88881200	1.05218800	-3.67950000
H	1.21097500	2.09775600	-3.66412100
H	0.33594000	0.87557500	-4.60767000
H	0.21606100	0.90683800	-2.83156800
C	2.11871600	0.14615800	-3.58484600
C	0.41743600	-1.81223100	-3.88690600
H	0.39954200	-1.71256400	-4.97805400
H	0.24782300	-2.86402800	-3.63714000
H	-0.40337600	-1.22759900	-3.46717500
C	2.86916900	-2.33054900	-3.76018300
H	2.64214700	-3.32653700	-3.36900300
H	2.94552100	-2.39425100	-4.85039200
H	3.84045700	-2.02246600	-3.36029800
C	1.62254700	-0.34263100	1.09575100
C	2.78421700	-0.19533400	0.13062900
H	3.26889600	0.84363300	0.18826400
H	0.66845500	-0.48619900	0.58787900
H	3.63232200	-0.82089200	0.41794700
C	1.71456800	-1.30558600	2.22159500
C	0.60827600	-1.41732800	3.09106900
C	2.83167600	-2.11093200	2.50722300
C	0.63072300	-2.25515900	4.19970700
H	-0.26382600	-0.79820200	2.89915700
C	2.85511400	-2.95702000	3.61979300
H	3.71190100	-2.06286400	1.87736100
C	1.76146900	-3.03111700	4.48018400
H	-0.23535100	-2.30010400	4.85529900
H	3.73823700	-3.56377600	3.80872900
H	1.78327400	-3.68284000	5.34891400

XA

0 1

Mn	1.79175600	1.84106800	1.46489400
S	4.06780700	1.33822400	6.64253100
O	-0.10882700	2.33449300	3.62384700
O	-0.22864400	2.95123800	-0.34385400
C	3.48497100	2.92232000	3.60215700
H	4.31344400	3.09314600	4.29972500
H	2.54852500	3.07687200	4.14916500
C	3.08988300	0.52322300	4.09550900
H	2.10510600	0.80155300	4.47835000
H	2.98007100	-0.42845400	3.57580400
C	5.94097600	-0.41131000	6.42316800
H	6.80841900	-1.02700300	6.63394300
C	0.66485800	2.20745600	2.75385500
C	4.09090200	0.34757600	5.20378900
C	0.57882900	2.46458200	0.34120800
C	5.48299100	0.55951400	7.27233200
H	5.88326800	0.85453300	8.23269900
N	3.48897100	1.53540600	3.08020400
C	5.14521500	-0.53176900	5.24375100
H	5.33486200	-1.23891500	4.44486800
B	4.71567000	1.19324300	2.37142100
O	5.07229500	-0.09065500	2.04493700
O	5.64737700	2.13139000	2.01123300
C	6.27186000	0.00175400	1.21671400
C	6.84755500	1.40820800	1.62241800
C	7.52434800	2.18011500	0.49685200
H	7.87001000	3.14715100	0.87450800
H	8.39325500	1.63171200	0.11683500
H	6.83530000	2.36754100	-0.32908100
C	7.74540100	1.36061500	2.86232700
H	8.70403700	0.87864400	2.64605200
H	7.94092300	2.38454900	3.19430300
H	7.25914700	0.82652400	3.68450300
C	5.83525200	-0.06135000	-0.25035800
H	6.70409700	-0.04040100	-0.91556000
H	5.28943200	-0.99100200	-0.43123200
H	5.18073400	0.77557000	-0.51072200
C	7.16866000	-1.18297400	1.55199300
H	6.66931100	-2.11321500	1.26435800
H	8.11382200	-1.11940000	1.00181200
H	7.38901900	-1.22950700	2.62041200
C	3.59118900	3.89968900	2.46069900
C	4.27170400	5.12518200	2.62491800
C	4.43031900	5.95413600	1.54320500
C	3.29744100	4.27313800	0.18078200
C	3.97505200	5.52973100	0.27096900
C	2.92243900	3.79092200	-1.09800000
C	4.20043800	6.28620900	-0.90711800
C	3.17870400	4.54073200	-2.22560600
H	2.45509700	2.82006200	-1.19144600
C	3.80667000	5.80441900	-2.13455400
H	2.89483200	4.14828700	-3.19773400
H	4.66440800	5.38589800	3.60227600
H	4.93520300	6.91175200	1.63776500
H	4.70411000	7.24544700	-0.82052300
H	3.98824800	6.38507900	-3.03410200
N	3.05190900	3.51818300	1.30749500
O	2.08998700	0.59565800	-2.22278300
O	2.33224600	-1.64543300	-1.82400200
B	2.23137300	-0.39463200	-1.27605500
C	2.48145100	-1.48332500	-3.26142200
C	2.61126300	0.77956700	-4.56914100
H	2.55731200	0.29297100	-5.54924400
H	2.13445200	1.76168900	-4.65221200
H	3.66131400	0.93275000	-4.31052800
C	0.38133200	-0.05399800	-3.79050800
H	0.00293700	0.97013900	-3.71639800
H	0.16788000	-0.43171600	-4.79570200
H	-0.15764700	-0.66725000	-3.06517300
C	1.88671500	-0.04673200	-3.51171100
C	1.74008900	-2.61782200	-3.95835900
H	1.77322900	-2.49228200	-5.04646700
H	2.21427500	-3.57241500	-3.71037300
H	0.69690400	-2.66664100	-3.64100300
C	3.98366000	-1.57225300	-3.55139300
H	4.36134600	-2.52518200	-3.16892000
H	4.19215600	-1.52218000	-4.62490200
H	4.53018100	-0.76571900	-3.05238800
C	1.30292800	-0.12046900	1.26704200
C	2.43745600	-0.07101300	0.24330600
H	1.61986400	-0.67999100	2.15024500
H	2.90389400	0.97992700	0.17048200
H	3.27500700	-0.65794500	0.62285100
C	-0.05655900	-0.56948600	0.88343600
C	-0.81753700	-1.32068100	1.79722600
C	-0.65998100	-0.26208900	-0.34903600
C	-2.11096900	-1.74418200	1.49820300
H	-0.37880200	-1.57285800	2.76048600
C	-1.94840700	-0.69237700	-0.65707800
H	-0.12916300	0.35433700	-1.06260400
C	-2.68676600	-1.43913100	0.26329600
H	-2.66927000	-2.32144300	2.23132300
H	-2.38283200	-0.42869300	-1.61878100
H	-3.69339500	-1.77135000	0.02536600

XB

0 1

Mn	1.86987000	1.66405000	1.28945700
S	4.70983500	0.92815100	6.17904100
O	-0.21777800	2.05539700	3.27718900
O	-0.15470200	2.52960500	-0.63962900
C	3.26290200	2.79483500	3.56346100
H	4.03849100	2.99402700	4.31324700
H	2.28832700	2.82733900	4.06034300
C	3.15623600	0.32206000	3.85257300
H	2.22978700	0.54294600	4.39032000
H	2.97051900	-0.55293500	3.23358400
C	6.20754200	-1.08341200	5.60041200
H	6.99576900	-1.82724500	5.63485700
C	0.63312300	1.97556900	2.47558000

C	4.29596000	-0.01718900	4.76924500
C	0.68744100	2.16735700	0.08726700
C	6.08201100	-0.07682600	6.51931200
H	6.70579300	0.12960600	7.37830200
N	3.42921900	1.46132100	2.93413200
C	5.18944800	-1.04571800	4.59959400
H	5.12092100	-1.73597700	3.76568600
B	4.75437500	1.35966500	2.30231400
O	5.18299900	0.27742500	1.59768200
O	5.67349600	2.37011700	2.39582300
C	6.42754100	0.67754900	0.94256400
C	6.92510100	1.85404500	1.85956700
C	7.62926600	2.98961400	1.12691100
H	7.92056400	3.76252400	1.84490700
H	8.53571900	2.62691300	0.63002500
H	6.97752100	3.44844600	0.38066600
C	7.75307700	1.38796600	3.05874500
H	8.74039300	1.03255700	2.74687900
H	7.88887200	2.23048100	3.74352100
H	7.24644100	0.58851400	3.60544900
C	6.05514800	1.14809200	-0.46527400
H	6.94477000	1.43282200	-1.03570300
H	5.55326900	0.33464400	-0.98987400
H	5.37409500	2.00398800	-0.43342400
C	7.34180700	-0.53743700	0.88779500
H	6.87697700	-1.31387100	0.27485700
H	8.30810400	-0.27220100	0.44413800
H	7.51432300	-0.94923100	1.88444600
C	3.34952800	3.83811700	2.47668800
C	3.83321400	5.13685800	2.73832200
C	3.99924100	6.01280100	1.69388200
C	3.25512100	4.24531400	0.18409300
C	3.74637000	5.57491000	0.37019200
C	3.07813400	3.75320900	-1.13256700
C	3.99256200	6.38770800	-0.76560100
C	3.35115100	4.56240200	-2.21418700
H	2.75506900	2.72978200	-1.27870700
C	3.79585300	5.89333900	-2.03496900
H	3.22763700	4.16889100	-3.21863300
H	4.07927200	5.41608100	3.75756200
H	4.36009800	7.02393800	1.86165100
H	4.35273600	7.40166200	-0.61265100
H	3.99353200	6.51774300	-2.90113700
N	2.99905200	3.42858300	1.26063200
O	2.38039900	0.48168100	-2.42995300
O	0.61405400	-0.84460700	-1.82510700
B	1.76145700	-0.22645800	-1.42170700
C	0.55144400	-0.76916000	-3.27356900
C	2.42925900	0.18939500	-4.82342900
H	1.83206300	0.08999400	-5.73656000
H	3.10085200	1.04474300	-4.94870500
H	3.04107100	-0.70778200	-4.70776000
C	0.83235000	1.77869300	-3.73658900
H	1.59163400	2.56228400	-3.82360000
H	0.20198100	1.81707300	-4.63085600
H	0.22213800	2.00090300	-2.86026000
C	1.53098400	0.42366300	-3.61220700
C	-0.90021600	-0.53827900	-3.67758000
H	-0.98977700	-0.42466900	-4.76378900
H	-1.50354500	-1.39896800	-3.37337200
H	-1.30954900	0.35072000	-3.19395000
C	1.04092200	-2.12671600	-3.78856500
H	0.39986900	-2.91075400	-3.37532400
H	1.00129900	-2.18473300	-4.88102200
H	2.06570200	-2.32804200	-3.46114900
C	1.33757500	-0.26442100	1.11601900
C	2.38670400	-0.37246300	0.01615400
H	1.54472200	-0.86285000	2.00561000
H	3.10092600	0.51437400	0.09605700
H	0.33259400	-0.51044300	0.77081100
C	3.33429700	-1.58141600	0.01728600
C	4.18280300	-1.80061000	-1.08109200
C	3.38882600	-2.50350000	1.06851600
C	5.06900100	-2.87761800	-1.11464300
H	4.14573800	-1.11577100	-1.92285200
C	4.28109600	-3.57696300	1.04619900
H	2.71843200	-2.39566400	1.91241400
C	5.13140900	-3.76943900	-0.04280800
H	5.70926900	-3.01937800	-1.98180200
H	4.29937500	-4.27359900	1.88066200
H	5.82089300	-4.60876800	-0.06280400

XI

0 1

Mn	1.33658800	1.10646800	1.04753900
S	5.04733000	0.07752500	5.15466900
O	-0.78297800	1.67403500	3.03428000
O	-0.17226000	1.35956400	-1.46524800
C	3.30139300	2.00728000	3.00635000
H	4.35813200	2.06908000	3.28567100
H	2.71204800	1.99666600	3.93729500
C	3.11461000	-0.41074900	3.10217700
H	2.35773700	-0.32100700	3.89264900
H	2.85491100	-1.27475000	2.49448300
C	6.55775300	-1.69142700	4.05876700
H	7.39134000	-2.35398700	3.85375900
C	0.02418200	1.40504100	2.24631100
C	4.46300400	-0.70528500	3.70362700
C	0.37139100	1.32192700	-0.43850200
C	6.52560100	-0.82882300	5.12039800
H	7.27670900	-0.67138600	5.88234400
N	3.01465200	0.79156900	2.25056200
C	5.37978100	-1.62082200	3.25552400
H	5.21215000	-2.20263200	2.35817000
B	3.69986900	0.77936800	0.86234500
O	4.32699600	-0.45785400	0.50715300
O	4.60591700	1.85557000	0.58195500
C	5.39618100	-0.12741200	-0.39557900
C	5.84012800	1.28974300	0.11998100
C	6.42036100	2.20267900	-0.95799600
H	6.69221100	3.16671700	-0.51518800
H	7.32308800	1.76594600	-1.40128300
H	5.69334200	2.39004700	-1.75112800
C	6.80094900	1.21739700	1.31523900
H	7.80026400	0.87786800	1.02077200
H	6.89489800	2.22027800	1.74514800
H	6.41868900	0.54710500	2.08852400
C	4.82424500	-0.08741800	-1.82030400
H	5.60411100	0.08635100	-2.56910900
H	4.34901800	-1.05016700	-2.03475700
H	4.06645500	0.69497500	-1.91963100
C	6.47128000	-1.20549400	-0.29794400
H	6.06627400	-2.16357600	-0.64146800
H	7.33051600	-0.95498200	-0.93055800
H	6.82012500	-1.32969400	0.72895800
H	2.65710500	1.00423000	0.01764900
C	2.92303700	3.23289200	2.23161900
C	3.63286100	4.43609000	2.45133400
C	3.26904700	5.56253500	1.76724200
C	1.44272900	4.27579800	0.77119300
C	2.14086700	5.51767700	0.91299600
C	0.23531200	4.27673600	0.03403200
C	1.67108900	6.67196200	0.23833600
C	-0.21069200	5.42127400	-0.59230300
H	-0.35904400	3.37894900	-0.00202100
C	0.52018300	6.62688300	-0.51384100
H	-1.14456000	5.39280100	-1.14564800
H	4.47631500	4.42866000	3.13265900
H	3.81602600	6.49454400	1.88133400
H	2.23111200	7.59708000	0.34602000
H	0.16068800	7.51530300	-1.02389900
N	1.90669700	3.12528900	1.38379600
C	0.40165500	-1.13910900	1.37943900
H	0.76822400	-1.32548700	2.38424700
C	-1.06823400	-1.20032700	1.25943600
C	-1.83354100	-1.31826900	2.43080400
C	-1.73988900	-1.16947900	0.02572700
C	-3.22332000	-1.39422600	2.37819700
H	-1.32793000	-1.33930400	3.39274900
C	-3.12872000	-1.24032000	-0.02780600

H	-1.17785000	-1.08193900	-0.89686300
C	-3.87779000	-1.35210800	1.14677400
H	-3.79385400	-1.48174300	3.29839900
H	-3.62916500	-1.21097200	-0.99160400
H	-4.96158700	-1.40829600	1.10053800
C	1.30730100	-1.11723300	0.34880700
H	0.97758000	-1.14070600	-0.68466100
H	2.35221500	-1.35750600	0.49427800

XII

0 1

Mn	1.35645200	1.57702500	1.17735800
S	5.30468000	0.43838500	5.01268800
O	-0.72784900	2.00305100	3.21497900
O	-0.34405600	1.62893900	-1.19653000
C	3.60942600	2.41315600	2.90259200
H	4.69536100	2.40302300	3.05554900
H	3.14917400	2.50209300	3.89993700
C	3.09081000	0.06132800	3.23695200
H	2.43505600	0.35396000	4.06608100
H	2.60263100	-0.77562600	2.74156500
C	6.36161800	-1.69410400	4.04220800
H	7.04114500	-2.51950900	3.85933000
C	0.09760200	1.85981200	2.40744400
C	4.42627800	-0.40278500	3.75101300
C	0.27611400	1.65498500	-0.19462400
C	6.60232900	-0.71240000	4.96464000
H	7.45362600	-0.60113600	5.62231200
N	3.11958700	1.19113300	2.28035900
C	5.12173700	-1.51611500	3.35623300
H	4.75030300	-2.17125400	2.57853300
B	3.61645600	0.92597400	0.84762200
O	4.16878700	-0.37628300	0.61585300
O	4.55887900	1.90847100	0.26728900
C	5.24102300	-0.25594400	-0.31425200
C	5.77169000	1.19651300	-0.03811500
C	6.44645900	1.87250200	-1.22999400
H	6.74097400	2.89347600	-0.96172000
H	7.34844300	1.32979500	-1.53274000
H	5.78452600	1.92263100	-2.10224700
C	6.69332400	1.26387900	1.18596600
H	7.67668200	0.82777500	0.98150100
H	6.83492600	2.31443300	1.46172700
H	6.25334600	0.73802200	2.03623500
C	4.67450200	-0.43149600	-1.73407500
H	5.45500100	-0.42214900	-2.50235700
H	4.14611800	-1.38756500	-1.78178100
H	3.94145900	0.34707000	-1.97657800
C	6.26399500	-1.35789900	-0.04510600
H	5.80735700	-2.33551800	-0.23115800
H	7.13298700	-1.25698300	-0.70597500
H	6.60373100	-1.33527100	0.99118500
H	2.55946800	1.07830400	0.08625900
C	3.22747700	3.64074000	2.13464900
C	4.00015500	4.81687500	2.28220300
C	3.63859800	5.95936900	1.61826000
C	1.69587400	4.73898800	0.76663200
C	2.45278400	5.95347500	0.84051200
C	0.46564700	4.75790400	0.06056300
C	1.99472100	7.10630400	0.15343900
C	0.04412800	5.90003800	-0.59209300
H	-0.14369500	3.86616000	0.06672900
C	0.81803200	7.08218600	-0.56184600
H	-0.90613300	5.89081300	-1.11779600
H	4.88717300	4.78143000	2.90601600
H	4.22958500	6.86834900	1.68992100
H	2.58740600	8.01529500	0.21685300
H	0.47199400	7.97170200	-1.07938400
N	2.14027300	3.56440000	1.36360900
C	-0.04063400	-1.12487100	1.72030200
H	-0.84481100	-0.62857300	2.26777100
C	-0.15693200	-2.59290300	1.70426900
C	-1.33176200	-3.20023100	2.18566700
C	0.86825800	-3.44463600	1.24498500
C	-1.48817900	-4.58512100	2.19352200
H	-2.13417500	-2.56419500	2.55340700
C	0.71397600	-4.82734100	1.25085300
H	1.79898400	-3.01112400	0.88965500
C	-0.46608700	-5.41080300	1.72300500
H	-2.41116700	-5.02068700	2.56898200
H	1.52369300	-5.45850500	0.89123700
H	-0.58218600	-6.49125800	1.72964100
C	0.93546800	-0.38718400	1.15035600
H	1.67483500	-0.96776900	0.58581500
K	2.84763300	2.90821400	-1.50401600

XIIA

0 1

Mn	1.54143700	1.26967500	1.42023000
S	5.81240700	0.44387600	4.99045000
O	-0.18533500	1.77673400	3.75751700
O	-0.32268700	1.24016200	-0.82363500
C	3.83848300	2.27983900	2.98746000
H	4.92917300	2.35512900	3.07203600
H	3.43686300	2.32575700	4.01257900
C	3.54798700	-0.10516000	3.33078600
H	2.92878400	0.12643000	4.20583900
H	3.10407300	-0.98134100	2.86305500
C	7.02747300	-1.53050800	3.88083200
H	7.77810600	-2.27161000	3.62805900
C	0.44249100	1.54635200	2.80863700
C	4.95291900	-0.44552900	3.74936900
C	0.36048100	1.28932600	0.13886800
C	7.21828200	-0.55913600	4.82576700
H	8.09099100	-0.37882900	5.43855900
N	3.40929600	1.02514300	2.38457800
C	5.73685600	-1.46436200	3.27304100
H	5.39154800	-2.12744400	2.49022400
B	3.81901400	0.81794600	0.91403600
O	4.48745700	-0.41816600	0.62758300
O	4.61046500	1.89508800	0.27786700
C	5.47024600	-0.18177400	-0.37593000
C	5.86583200	1.31609600	-0.11904700
C	6.38174700	2.06566400	-1.34577000
H	6.58641700	3.11031000	-1.08513400
H	7.31185600	1.62209100	-1.71716600
H	5.65842600	2.05125200	-2.16916900
C	6.85934200	1.47216700	1.03923500
H	7.86644200	1.14465200	0.76078100
H	6.90824800	2.52986800	1.31962700
H	6.53849300	0.89614600	1.91028800
C	4.82349000	-0.40638200	-1.75399900
H	5.54140100	-0.31098900	-2.57566700
H	4.39468600	-1.41191300	-1.77696100
H	3.99849200	0.29333100	-1.93250100
C	6.61949300	-1.17209800	-0.19692800
H	6.25516000	-2.19118700	-0.36319100
H	7.42207600	-0.97613100	-0.91772400
H	7.03104500	-1.12035900	0.81196800
H	2.69587100	0.85945500	0.23659700
C	3.31220500	3.47677200	2.25875900
C	3.99864700	4.70912100	2.36555700
C	3.50495700	5.82198000	1.73734200
C	1.60789200	4.45668800	1.01191100
C	2.27190700	5.72615400	1.04354700
C	0.33120000	4.38376500	0.39806900
C	1.67825200	6.84239400	0.40136700
C	-0.22307800	5.49223300	-0.21220500
H	-0.20743200	3.44885700	0.44207400
C	0.45838100	6.73007900	-0.22809600
H	-1.20630200	5.41172000	-0.66633500
H	4.92600400	4.74098500	2.92787200
H	4.02696600	6.77415500	1.77621200
H	2.20215400	7.79435600	0.43087100
H	0.00864800	7.59210900	-0.71131000
N	2.18516500	3.31757100	1.56186000
C	0.36022100	-1.61073600	1.91162500
C	1.26258000	-0.73386000	1.41923100
H	2.11579900	-1.24858900	0.95897000
K	2.68286100	2.72984900	-1.35342200

H	0.60084400	-2.67978600	1.87886100
C	-0.93346800	-1.33704200	2.56917600
C	-1.29066000	-2.05717300	3.72360800
C	-1.86229400	-0.40933600	2.06778600
C	-2.49946100	-1.82912000	4.37747600
H	-0.59501300	-2.79656900	4.11504100
C	-3.07379200	-0.17994100	2.71796000
H	-1.63301100	0.12065400	1.15175200
C	-3.39762200	-0.88147100	3.88036200
H	-2.74253900	-2.39120400	5.27609900
H	-3.77291500	0.54590500	2.30897000
H	-4.34248700	-0.70176800	4.38653400

XIIB

0 1

Mn	1.50086300	1.24861300	1.35027000
S	5.57112200	0.33489600	5.08788500
O	-0.22534000	2.03793500	3.60953400
O	-0.48644800	1.20794500	-0.79052500
C	3.77210800	2.20750000	2.94780600
H	4.85701800	2.26574500	3.09546800
H	3.31551300	2.24130400	3.95034700
C	3.48974900	-0.19550900	3.19997900
H	2.79468300	-0.04849700	4.03492500
H	3.14004700	-1.05983000	2.63938100
C	6.99927800	-1.45933100	3.92704400
H	7.81427200	-2.13156700	3.68095700
C	0.42293800	1.68665500	2.71171400
C	4.87723900	-0.48693600	3.70473200
C	0.26643500	1.26655700	0.11607900
C	7.04734300	-0.56797100	4.96448700
H	7.85203500	-0.39525500	5.66615900
N	3.35965000	0.97206000	2.29873900
C	5.76230000	-1.41275200	3.21489800
H	5.52203400	-2.02455900	2.35517200
B	3.78785900	0.78741900	0.82864800
O	4.54704300	-0.39794100	0.54407100
O	4.51325300	1.91262600	0.19536100
C	5.53451500	-0.09284100	-0.43459000
C	5.81601700	1.42723800	-0.16904200
C	6.30767500	2.21682600	-1.38035700
H	6.42974800	3.27240500	-1.11214000
H	7.27612100	1.84260900	-1.72942900
H	5.60774900	2.15441000	-2.22152100
C	6.76678500	1.64887200	1.01470700
H	7.80222100	1.40119500	0.75851900
H	6.72791000	2.70476800	1.30330300
H	6.47040300	1.04109100	1.87336000
C	4.94119000	-0.36115100	-1.82892700
H	5.66974100	-0.20790300	-2.63229200
H	4.59128300	-1.39637600	-1.86540400
H	4.06995300	0.27449100	-2.02653000
C	6.74614400	-1.00039700	-0.22818600
H	6.45851800	-2.04225400	-0.40327300
H	7.55009600	-0.74707200	-0.92934900
H	7.12927200	-0.92229600	0.79014400
H	2.65098500	0.74515900	0.16933200
C	3.30829400	3.42342400	2.20760300
C	4.01358600	4.63957400	2.37006800
C	3.58787100	5.76619900	1.71891500
C	1.72043600	4.44688400	0.85183700
C	2.40989900	5.69956700	0.93332200
C	0.50093700	4.40203700	0.12809700
C	1.89727800	6.82798700	0.24484500
C	0.02624200	5.52049000	-0.52957200
H	-0.06638300	3.48283100	0.12765100
C	0.73332200	6.74315100	-0.48619000
H	-0.91595100	5.46024300	-1.06656500
H	4.90116300	4.64720800	2.99396300
H	4.12582200	6.70665900	1.80136200
H	2.43971800	7.76715900	0.31692700
H	0.34629300	7.61417200	-1.00602600
N	2.22096500	3.29862200	1.44728600
C	1.58854900	-1.69288400	0.61808400
C	1.03506600	-0.75279800	1.40947700
K	2.57070400	2.58760400	-1.47777300
H	1.31216100	-2.74783100	0.69887700
H	2.34511600	-1.46113700	-0.12600300
C	0.04179300	-1.22835800	2.40698600
C	-1.29740100	-0.79656700	2.38110300
C	0.41247700	-2.12919700	3.42176800
C	-2.21977000	-1.24254200	3.32399900
H	-1.61151800	-0.10603400	1.60395000
C	-0.50658000	-2.56630900	4.37718200
H	1.43737300	-2.48787400	3.45489600
C	-1.82903200	-2.12464700	4.33522800
H	-3.24969100	-0.89726400	3.27241000
H	-0.18728800	-3.25758200	5.15388300
H	-2.54684300	-2.46314600	5.07770300

XIII

0 1

Mn	0.39555100	-1.61967600	-0.37264200
S	-0.85171900	3.23717400	-2.98895800
O	-0.34601800	-2.14475500	-3.15630500
O	0.37816000	-4.53180600	-0.05191300
C	1.24629800	0.89447900	-1.64544600
H	1.41568500	1.97177600	-1.74827400
H	0.98841000	0.50832400	-2.63994900
C	-1.20490100	0.88889800	-1.41087100
H	-1.22378400	0.34274800	-2.35634300
H	-1.98412400	0.45688600	-0.78599500
C	-2.23729300	4.53962000	-1.25788600
H	-2.76435400	5.33735200	-0.74619600
C	-0.02421700	-1.92519900	-2.05869500
C	-1.47289800	2.35305900	-1.61233100
C	0.45498800	-3.37480700	-0.16574600
C	-1.55593400	4.71988800	-2.43110800
H	-1.43641700	5.62824900	-3.00572000
N	0.10962200	0.60262200	-0.75185800
C	-2.19077100	3.19009400	-0.79420200
H	-2.66704500	2.83610700	0.11155600
B	0.20968500	1.19531400	0.57368200
O	-0.87617400	1.39936800	1.38003700
O	1.39474700	1.63152700	1.10758700
C	-0.37975800	1.90922700	2.65056300
C	1.04206500	2.46058000	2.25567800
C	2.11648200	2.29281600	3.32107800
H	3.06894100	2.68014400	2.94668000
H	1.85292900	2.85159400	4.22567000
H	2.25765400	1.24318200	3.58677200
C	1.00683600	3.90359100	1.74292400
H	0.80593900	4.61287800	2.55178900
H	1.97999200	4.14554600	1.30544700
H	0.24437300	4.03092900	0.96772600
C	-0.33280700	0.72954900	3.62372300
H	-0.05582300	1.05638700	4.63084400
H	-1.32312700	0.26730000	3.66785800
H	0.38053500	-0.03184200	3.30053100
C	-1.35896200	2.96478800	3.15095000
H	-2.32114900	2.49343200	3.37363200
H	-0.98825900	3.43144600	4.07006800
H	-1.52528800	3.74358800	2.40425100
H	1.03185000	-1.15978000	1.37393100
C	2.51515500	0.22807200	-1.19518000
C	3.74708600	0.87967200	-1.42812900
C	4.91415400	0.26614600	-1.05711500
C	3.57341500	-1.59670100	-0.21427200
C	4.85747500	-0.99875700	-0.42638000
C	3.52166300	-2.84964900	0.44251400
C	6.02784300	-1.67124600	0.00769300
C	4.67680200	-3.47767900	0.85615500
H	2.56124900	-3.31229400	0.60706900
C	5.94365300	-2.89051200	0.63830400
H	4.60891500	-4.44048100	1.35372300
H	3.74418900	1.85970400	-1.89292300
H	5.87825900	0.73878700	-1.22391600
H	6.99096500	-1.19923100	-0.16737500
H	6.84281700	-3.40149500	0.96874500
N	2.41119300	-0.97087000	-0.62748800

C	-2.62412500	-2.27130300	-0.26799600
H	-2.54377700	-2.99077800	-1.08614600
C	-4.00052300	-2.05302900	0.20739300
C	-5.02618800	-2.92254300	-0.20614900
C	-4.35895800	-0.98298500	1.05225900
C	-6.34269600	-2.75008900	0.21747000
H	-4.77468700	-3.74990100	-0.86590800
C	-5.67260200	-0.80976300	1.47716400
H	-3.59693600	-0.27432300	1.36580100
C	-6.67556900	-1.69298300	1.06583300
H	-7.11102400	-3.44307300	-0.11645900
H	-5.92070200	0.02617200	2.12735900
H	-7.70128400	-1.55311500	1.39588500
C	-1.51033800	-1.67095600	0.19860000
H	-1.68776400	-0.99071300	1.04383800
H	0.44990700	-1.64631700	1.49993000

XIIIA

0 1

Mn	1.23468400	1.59749300	1.13315600
S	4.31025200	0.16279700	5.61658900
O	-0.08923800	1.84993500	3.73661700
O	-1.40468300	1.82492400	-0.11543500
C	3.35547900	2.29641500	3.07505300
H	4.36895900	2.31889900	3.48989300
H	2.66161400	2.28603200	3.92444300
C	2.90245800	-0.12430700	3.16812300
H	2.02795800	0.06925600	3.79144800
H	2.64031300	-0.95036200	2.51062500
C	6.15039900	-1.37722100	4.69319900
H	7.05288300	-1.97296000	4.61022000
C	0.40406100	1.67317600	2.69811500
C	4.10087500	-0.47635500	4.00234800
C	-0.33771500	1.80214600	0.35711700
C	5.82909700	-0.65033800	5.80766300
H	6.38417400	-0.55716600	6.73114700
N	3.11645700	1.06985300	2.29101100
C	5.16382200	-1.27889600	3.66583100
H	5.22087400	-1.78208700	2.70878700
B	4.08833800	0.83273300	1.23554800
O	4.38569400	-0.41052400	0.74972400
O	4.82293500	1.84502600	0.66775000
C	5.29334800	-0.22629200	-0.37296600
C	5.89132300	1.20245900	-0.08747700
C	6.17828400	2.03955300	-1.32639300
H	6.56258700	3.01949100	-1.02728200
H	6.93339200	1.55390800	-1.95410600
H	5.27630500	2.19585200	-1.92162400
C	7.10934300	1.17091900	0.84065800
H	7.98784500	0.75274900	0.33957400
H	7.34250600	2.19396800	1.15049200
H	6.90486400	0.58175500	1.74047400
C	4.45227400	-0.29740100	-1.64942000
H	5.08118100	-0.24782200	-2.54381700
H	3.90510700	-1.24404200	-1.65876600
H	3.72010800	0.51228600	-1.69697000
C	6.31152300	-1.36055800	-0.35264600
H	5.80155600	-2.31247300	-0.52892600
H	7.05859900	-1.22332900	-1.14203300
H	6.82621600	-1.42231000	0.60834700
H	1.71180000	1.82412400	-0.66306300
C	3.10732000	3.54617300	2.27775400
C	3.90426000	4.68501700	2.53292300
C	3.66716200	5.84234100	1.83997800
C	1.85859400	4.68059800	0.67569600
C	2.62869400	5.87086100	0.88008400
C	0.81653500	4.71775300	-0.28211000
C	2.34116300	7.03495600	0.12325500
C	0.55919200	5.86523300	-1.00103100
H	0.21364800	3.83530400	-0.42836100
C	1.32610200	7.03594600	-0.80457900
H	-0.25050300	5.86819700	-1.72466700
H	4.69898400	4.61669900	3.26788600
H	4.26590600	6.73350300	2.00778000
H	2.94022300	7.92522800	0.29544500
H	1.10878900	7.93033500	-1.38048900
N	2.11724500	3.52504300	1.38897600
C	0.50389900	-1.44600600	1.20713400
C	1.03986200	-0.33637900	0.65875000
H	1.63216100	-0.57017200	-0.23821300
H	0.75415700	-2.42618800	0.78591100
C	-0.35339500	-1.51610300	2.40853900
C	-0.04360600	-2.41959800	3.44062900
C	-1.49799200	-0.71700500	2.55548800
C	-0.82162300	-2.49224200	4.59463600
H	0.82879100	-3.06134500	3.33465100
C	-2.27995600	-0.78894300	3.70748200
H	-1.77241000	-0.04275700	1.75196200
C	-1.94329200	-1.67112900	4.73534700
H	-0.55363400	-3.18919100	5.38494900
H	-3.15760600	-0.15456800	3.80077300
H	-2.55288900	-1.72580100	5.63329200
H	2.41449000	1.69977400	-0.37449900

XIIIB

0 1

Mn	1.31814400	1.36160600	1.39428800
S	4.87434200	0.17282100	5.53790600
O	0.18807800	1.76740700	4.07152800
O	-1.36681800	1.77148000	0.29488300
C	3.54873600	2.22764900	3.10368100
H	4.58026300	2.33445500	3.45788900
H	2.91034500	2.16136800	3.99240400
C	3.33901500	-0.23159200	3.18177700
H	2.48632900	-0.14560200	3.85810500
H	3.13598400	-1.06886300	2.51760100
C	6.78751300	-1.17290700	4.46946600
H	7.73567100	-1.67679600	4.31693600
C	0.62835900	1.58258000	3.01145300
C	4.61769800	-0.47119000	3.93310900
C	-0.28806900	1.64549300	0.72023600
C	6.47455500	-0.48949700	5.61340700
H	7.08034800	-0.34908200	6.49821900
N	3.36736500	0.98893600	2.32001800
C	5.72740000	-1.16332700	3.51303000
H	5.76624800	-1.65176900	2.54727000
B	4.29674200	0.87264800	1.20345800
O	4.66850900	-0.32042300	0.64957700
O	4.91941100	1.96245700	0.64857000
C	5.52301300	-0.01675700	-0.49085200
C	6.01302900	1.44245100	-0.16153300
C	6.19321200	2.35144300	-1.36977100
H	6.50747400	3.34553100	-1.03744700
H	6.96465200	1.95582900	-2.03940800
H	5.26337200	2.46035300	-1.93171300
C	7.25807900	1.47418400	0.73021800
H	8.15140500	1.15129900	0.18670600
H	7.41658500	2.49969600	1.07690900
H	7.13157900	0.83455500	1.60960500
C	4.65221300	-0.09743300	-1.74614800
H	5.24953400	0.04071600	-2.65274100
H	4.17960600	-1.08251500	-1.78767800
H	3.86208000	0.65738000	-1.73616600
C	6.62691300	-1.06596500	-0.54888700
H	6.18749500	-2.04791700	-0.74872000
H	7.33380300	-0.83860000	-1.35430500
H	7.17724600	-1.12368600	0.39240100
H	1.76795800	0.83896500	-0.35087700
C	3.16715300	3.44576900	2.30873200
C	3.81840600	4.67141700	2.57424500
C	3.47561500	5.78500700	1.85400400
C	1.89469700	4.39733000	0.60999500
C	2.50588700	5.67318200	0.82947200
C	0.96421800	4.27439200	-0.44983200
C	2.14518200	6.77488000	0.01333200
C	0.64065000	5.36172100	-1.23265800
H	0.50774700	3.31465300	-0.63603200
C	1.22667500	6.62655800	-0.99980200
H	-0.07758600	5.24212800	-2.03823000
H	4.58197900	4.70583300	3.34408000

H	3.94981500	6.74494000	2.03952800
H	2.61584200	7.73596700	0.20268300
H	0.95461900	7.47317500	-1.62268300
N	2.21354800	3.30577100	1.39303100
C	1.47305000	-1.48355200	0.41777400
C	0.92349500	-0.65412700	1.33078100
H	1.28616000	-2.56042800	0.42617600
H	2.13721200	-1.14575200	-0.37530100
C	0.09302100	-1.30661300	2.38058400
C	-1.21170200	-0.87342600	2.68052000
C	0.60145100	-2.38445000	3.13074200
C	-1.96938200	-1.48901200	3.67385200
H	-1.64089400	-0.05168900	2.11831900
C	-0.14885600	-2.99262500	4.13767000
H	1.60421400	-2.74394000	2.91787400
C	-1.44118200	-2.54813700	4.41605700
H	-2.97782200	-1.13514500	3.87325500
H	0.27944800	-3.81570200	4.70488200
H	-2.02836000	-3.01721600	5.20089600
H	2.20094200	1.47072800	-0.28542800

H	4.68248900	3.98879300	3.84549700
H	4.09794100	6.26119100	2.98083600
H	2.73072900	7.63792700	1.45563100
H	1.00662800	7.80089700	-0.32390400
N	2.27093700	3.05820600	1.67631700
C	2.41289900	1.27611200	-0.69280300
H	2.20640800	0.44012700	-1.37619100
C	3.05132100	2.31753800	-1.27075500
H	3.31989500	3.17878700	-0.66111800
C	3.47075800	2.47086100	-2.67292400
C	3.21348600	1.51516100	-3.67571800
C	4.17516700	3.63038200	-3.05093100
C	3.65375400	1.70465700	-4.98179900
H	2.66004300	0.61616200	-3.42141100
C	4.61561900	3.82384500	-4.35895000
H	4.37470200	4.38671800	-2.29470700
C	4.36077700	2.85873200	-5.33433000
H	3.44142900	0.94863300	-5.73376600
H	5.15812500	4.73000300	-4.61709600
H	4.70183900	3.00399600	-6.35557800

XIV

0 1

Mn	1.52092300	1.16057600	1.15812900
S	1.47406100	-1.28294700	0.83711200
O	-0.11602500	1.11771100	3.64515900
O	-0.91188600	1.54431400	-0.42410300
C	3.52139500	1.65331000	3.23042200
H	4.49836400	1.70131100	3.73057100
H	2.76269300	1.45638000	3.99667000
C	3.31960100	-0.79596600	2.88356900
H	4.17494900	-1.41389300	2.59750100
H	3.33997400	-0.68676800	3.97230900
C	-0.08402900	-2.44243700	2.53674600
H	-0.93291400	-2.94587300	2.98617800
C	0.56477400	1.10560500	2.70077300
C	2.03647500	-1.46142100	2.49527000
C	0.04794300	1.44771000	0.23057700
C	-0.05377500	-2.03740600	1.23905800
H	-0.80862500	-2.15614200	0.47412100
N	3.47104400	0.55301200	2.25303600
C	1.10908800	-2.09676400	3.26221500
H	1.23286000	-2.26047600	4.32742700
B	4.52810300	0.59343200	1.24082600
O	4.98084900	-0.55685600	0.65594300
O	5.29152400	1.69911000	1.00004600
C	6.09970700	-0.20348100	-0.20763200
C	6.48660500	1.25107300	0.29600400
C	6.79680900	2.24467200	-0.81606600
H	6.99482200	3.22852900	-0.37850400
H	7.68917700	1.93341200	-1.37059100
H	5.96727100	2.34386600	-1.51560500
C	7.60667900	1.26013400	1.34122200
H	8.56872400	0.97041000	0.90752800
H	7.70112800	2.27222800	1.74617300
H	7.38194200	0.58325700	2.17176700
C	5.59296000	-0.25394100	-1.64688300
H	6.39305500	-0.03226500	-2.35996300
H	5.21760400	-1.26163300	-1.85113300
H	4.77824000	0.44948100	-1.80115700
C	7.18810900	-1.25438400	-0.00350000
H	6.81695400	-2.22762800	-0.33852200
H	8.07727100	-1.00901200	-0.59428000
H	7.47905600	-1.34518200	1.04537700
C	3.21919000	2.99537600	2.61142300
C	3.90795700	4.12691500	3.09889400
C	3.58988200	5.37075400	2.62069600
C	1.94864500	4.29910900	1.15942300
C	2.59152900	5.49041800	1.62813200
C	0.98124400	4.42438100	0.13321000
C	2.23125100	6.74868600	1.08027900
C	0.65529200	5.65927400	-0.38130400
H	0.52282800	3.53509200	-0.26234700
C	1.27758900	6.83628200	0.09460400
H	-0.08567000	5.72465400	-1.17219500

XIVA

0 1

Mn	1.54880500	0.93852800	1.06863900
S	1.37955200	-1.56351200	1.21980700
O	-0.12416300	1.25812600	3.50760400
O	-0.83815800	1.08433800	-0.62149300
C	3.54622800	1.66393700	3.05082400
H	4.53733600	1.79807800	3.50659100
H	2.83133600	1.47127200	3.86014100
C	3.46766000	-0.80251300	2.89606000
H	4.23295600	-1.46200500	2.48154900
H	3.71669300	-0.63170800	3.94904400
C	-0.01264700	-2.27396400	3.27070900
H	-0.82191300	-2.63026200	3.89830400
C	0.56802800	1.09977700	2.58537300
C	2.12225800	-1.44538100	2.80907300
C	0.10120900	1.08924000	0.06807300
C	-0.11618500	-2.13719700	1.92138500
H	-0.95783500	-2.36037500	1.28046500
N	3.52283800	0.49737800	2.15328700
C	1.26701800	-1.86087500	3.78265700
H	1.50969200	-1.82630600	4.83938100
B	4.55290500	0.51269700	1.10995700
O	5.08750700	-0.64968700	0.62408600
O	5.24832000	1.64053400	0.76654400
C	6.20109900	-0.30528400	-0.24825100
C	6.48258700	1.21191000	0.12079700
C	6.75113900	2.11390400	-1.07796600
H	6.88785800	3.14512400	-0.73822300
H	7.66583600	1.79988900	-1.59285100
H	5.92271600	2.10373700	-1.78632900
C	7.58004100	1.39588200	1.17383800
H	8.56730300	1.13313900	0.78172200
H	7.59850100	2.44574000	1.48130300
H	7.38563400	0.78679900	2.06240800
C	5.74307300	-0.52455300	-1.68917800
H	6.55672600	-0.32963200	-2.39523600
H	5.43104500	-1.56750300	-1.80221500
H	4.89163600	0.11075300	-1.93139200
C	7.34926400	-1.25799400	0.07771200
H	7.05068600	-2.28072200	-0.17136600
H	8.23750800	-1.01062600	-0.51358200
H	7.61514800	-1.23109500	1.13675700
C	3.13392700	2.94943700	2.37892900
C	3.68727100	4.15433400	2.86064100
C	3.20799700	5.35162900	2.39448300
C	1.71889200	4.09067200	0.92376700
C	2.19557600	5.35012700	1.41076500
C	0.76710100	4.09853700	-0.12289200
C	1.67823300	6.55586000	0.87066900
C	0.29521800	5.28351100	-0.63766700
H	0.45081900	3.16213700	-0.54704400
C	0.74175200	6.52671000	-0.13342800
H	-0.41556500	5.25870600	-1.45724400

H	4.47323300	4.11108200	3.60718600
H	3.60003800	6.29697700	2.75985400
H	2.05156900	7.49915500	1.26063300
H	0.35632000	7.45144500	-0.55225700
N	2.19146400	2.89825500	1.43631400
C	2.44032000	0.63078200	-0.79286400
H	2.45740900	-0.44784400	-1.00547500
C	2.72127900	1.30870000	-1.93122600
H	2.86428500	0.73542300	-2.85627300
C	2.85378500	2.76145400	-2.16358800
C	2.26778800	3.33936000	-3.30420400
C	3.61457200	3.59287400	-1.32553500
C	2.39698400	4.70015900	-3.57288000
H	1.68926800	2.70749800	-3.97432400
C	3.76331200	4.95081900	-1.60432600
H	4.09137800	3.15730900	-0.45767800
C	3.14708100	5.51545300	-2.72089200
H	1.91684100	5.12578200	-4.45064900
H	4.35329100	5.57267700	-0.93592900
H	3.25410100	6.57638900	-2.93019500

XIVB

0 1

Mn	1.50673600	1.14278100	0.90503400
S	1.02086600	-1.27414200	0.72418900
O	-0.22183300	1.33509200	3.31684000
O	-0.80425800	1.95189500	-0.70149400
C	3.37832500	1.31377300	3.11217700
H	4.30612000	1.27269600	3.70123700
H	2.55455600	1.01425000	3.76940600
C	3.24444500	-1.05271500	2.38088300
H	3.87917800	-1.65852700	1.73151500
H	3.59873200	-1.19669600	3.40937900
C	-0.39395200	-2.08034000	2.72785200
H	-1.22457600	-2.41735600	3.33803300
C	0.49179600	1.21094300	2.40571900
C	1.82107600	-1.49175300	2.27693800
C	0.11292000	1.66452000	-0.04188600
C	-0.51909500	-1.72662800	1.42043300
H	-1.40285400	-1.73816800	0.79752000
N	3.42287200	0.37474100	1.97569600
C	0.94790900	-1.92783900	3.22560300
H	1.22932000	-2.09481900	4.26012600
B	4.59484000	0.58712800	1.11876100
O	5.21889700	-0.43779400	0.46249500
O	5.28895000	1.76199200	1.11808800
C	6.41898600	0.08999600	-0.17562700
C	6.57896900	1.52534700	0.49350700
C	6.84158600	2.66053900	-0.49092200
H	6.86907300	3.60948100	0.05374800
H	7.80594500	2.52594600	-0.99261200
H	6.05493100	2.72310100	-1.24324600
C	7.60481700	1.57022000	1.62996300
H	8.62506700	1.42500600	1.26172600
H	7.54872200	2.54930200	2.11519100
H	7.39556300	0.80738200	2.38604800
C	6.16855600	0.12363900	-1.68260900
H	7.04484800	0.50735300	-2.21493700
H	5.97038300	-0.89209300	-2.03589800
H	5.30004100	0.73496900	-1.92463300
C	7.55541200	-0.88328800	0.13188400
H	7.32724600	-1.85396900	-0.31833000
H	8.49915800	-0.52572200	-0.29353400
H	7.68928600	-1.03137800	1.20569300
C	3.15329000	2.73465100	2.65223200
C	3.72492200	3.78784300	3.39693800
C	3.47027600	5.08594000	3.03708500
C	2.15484300	4.22512200	1.16637500
C	2.67381000	5.34158200	1.89760100
C	1.40766500	4.48000300	-0.00935700
C	2.39188700	6.66074600	1.45828700
C	1.15626500	5.77257300	-0.41296500
H	1.07565600	3.64535200	-0.60391900
C	1.63987600	6.87603200	0.32771200
H	0.58424400	5.94344500	-1.31997400

H	4.35367000	3.54948700	4.24832400
H	3.88003000	5.91856100	3.60243200
H	2.78731900	7.49391200	2.03329400
H	1.42616200	7.88749000	-0.00463600
N	2.38060700	2.92913800	1.58388700
C	2.51203300	1.17334100	-0.94439100
C	3.28777100	2.18547200	-1.37365200
H	3.56350200	3.02216800	-0.73907100
C	2.20569000	0.10190800	-1.92728200
C	2.87563600	-1.13494000	-1.90063300
C	1.19788700	0.27772000	-2.89144000
C	2.55958800	-2.14715200	-2.80618700
H	3.64872400	-1.29582500	-1.15683900
C	0.87378500	-0.73865900	-3.79102700
H	0.66153800	1.22103700	-2.92244300
C	1.55338500	-1.95788500	-3.75573000
H	3.09849900	-3.09114400	-2.76591800
H	0.08941800	-0.57422200	-4.52609300
H	1.30242200	-2.74860300	-4.45762600
H	3.68711800	2.22288800	-2.39252400

XV

0 1

Mn	1.69342100	1.18832500	1.14591800
S	6.05181400	-1.67867900	3.22129100
O	0.07914000	0.62594100	3.59114200
O	-0.83918600	1.73686800	-0.23639300
C	3.65997600	1.47538000	3.18204500
H	4.65311800	1.45589100	3.64482300
H	2.93591400	1.19272100	3.95563300
C	3.37374000	-0.89956600	2.57810100
H	2.38730800	-0.97031000	3.04257100
H	3.38264100	-1.55041400	1.70142800
C	5.31729100	-1.86031100	5.68544400
H	5.32767100	-2.02346100	6.75723600
C	0.76063400	0.86097300	2.67567000
C	4.38128300	-1.33206200	3.60242800
C	0.16360100	1.57284200	0.32983500
C	6.41715900	-2.00433300	4.88631100
H	7.42020800	-2.28991000	5.17366700
N	3.55336600	0.49740700	2.08217500
C	4.15697500	-1.47319800	4.94840300
H	3.18173400	-1.30676500	5.39478600
B	4.63058200	0.61837600	1.08812700
O	5.13511100	-0.48105700	0.45123600
O	5.34292000	1.76570000	0.90704100
C	6.24346700	-0.03728600	-0.38978800
C	6.54731500	1.42098600	0.16298600
C	6.75923000	2.47388800	-0.91835200
H	6.89477700	3.45278600	-0.44735300
H	7.65868200	2.24978300	-1.50244000
H	5.90859700	2.53550500	-1.59711200
C	7.68997700	1.47014600	1.18156100
H	8.65598000	1.25275300	0.71528700
H	7.73313000	2.47576700	1.61105300
H	7.52588900	0.76020500	1.99747800
C	5.74927800	-0.07268200	-1.83348200
H	6.53715600	0.22453700	-2.53252100
H	5.44382600	-1.09553700	-2.07539700
H	4.89149600	0.57935400	-1.97518800
C	7.39065500	-1.02967500	-0.21849700
H	7.06516500	-2.01771100	-0.55751900
H	8.24875100	-0.72741800	-0.82867300
H	7.71229900	-1.11709400	0.81973100
C	3.34743200	2.86809600	2.70798000
C	4.03616300	3.95555600	3.28361100
C	3.72161400	5.23311300	2.90151900
C	2.09362100	4.28125900	1.34117700
C	2.73804300	5.42999000	1.90599200
C	1.15268000	4.49049400	0.30409400
C	2.39553500	6.72774800	1.44657400
C	0.84643400	5.76311400	-0.12520900
H	0.70017900	3.63976900	-0.17462500
C	1.46228700	6.89674500	0.45181800
H	0.12618500	5.89149600	-0.92742000

H	4.80616100	3.75618900	4.02098100
H	4.22460500	6.09286000	3.33547600
H	2.89422500	7.58243500	1.89580500
H	1.20545700	7.89193300	0.10178600
N	2.39380900	3.00522400	1.78419400
C	2.47917400	1.25308200	-0.69666100
H	2.30687900	0.32395400	-1.26892900
C	2.99665700	2.28023200	-1.40377800
H	3.20503000	3.21374400	-0.88009200
C	3.34729800	2.33462600	-2.83091200
C	3.05171500	1.30258200	-3.74269100
C	4.02129600	3.46638400	-3.32766400
C	3.43318000	1.39103600	-5.07762100
H	2.51444200	0.42548800	-3.39411200
C	4.40306300	3.55828400	-4.66496400
H	4.24622500	4.28119400	-2.64276600
C	4.11493400	2.51761400	-5.54900500
H	3.19268100	0.57879400	-5.75897400
H	4.92536200	4.44419700	-5.01734300
H	4.40936000	2.58444800	-6.59258700

XVI

0 1

Mn	1.73687600	1.42399300	1.10608700
S	6.30592300	-1.23808800	3.31690000
O	0.25021700	1.16180300	3.67239900
O	-0.82437900	1.91920500	-0.24160900
C	3.76170000	1.93884900	3.14395600
H	4.75301100	2.00588100	3.60565400
H	3.05673400	1.66789400	3.93909500
C	3.61684000	-0.47511000	2.74509500
H	2.64775500	-0.53930900	3.24706400
H	3.62600300	-1.20579500	1.93924500
C	5.75975300	-1.04096300	5.82657300
H	5.84800500	-1.05160100	6.90724400
C	0.87513200	1.24454100	2.69320200
C	4.68100600	-0.76934800	3.76218500
C	0.18662400	1.76408500	0.31081800
C	6.79007500	-1.34321700	4.97985500
H	7.80326200	-1.62525600	5.23303200
N	3.71245700	0.87905100	2.11958600
C	4.55792500	-0.71449300	5.12735600
H	3.62425500	-0.45343000	5.61539100
B	4.78889500	0.98528600	1.13003500
O	5.30460700	-0.10193500	0.48038900
O	5.49216400	2.14296900	0.94579900
C	6.39178700	0.36901800	-0.36864300
C	6.71060400	1.80268700	0.22499600
C	6.97464500	2.87882400	-0.82085800
H	7.11661100	3.84211700	-0.32033000
H	7.88758200	2.65098500	-1.38245300
H	6.14805800	2.97971400	-1.52346400
C	7.82952500	1.80252300	1.27131400
H	8.80338800	1.59068900	0.81866100
H	7.87395400	2.79252400	1.73564800
H	7.63977600	1.06728400	2.05809300
C	5.86794400	0.39967100	-1.80426800
H	6.63750600	0.74343000	-2.50215100
H	5.57707600	-0.61439900	-2.09390800
H	4.99583000	1.04586200	-1.89141900
C	7.53797300	-0.63252300	-0.26023900
H	7.20238800	-1.60494800	-0.63371300
H	8.38892000	-0.30901500	-0.86975500
H	7.87231200	-0.76343800	0.76965200
C	3.36975400	3.28528400	2.60238100
C	3.98960800	4.43066100	3.14930400
C	3.59796200	5.67438000	2.73230500
C	2.03996400	4.58047600	1.19619800
C	2.60725600	5.78275000	1.73016100
C	1.10237600	4.70246900	0.14217200
C	2.19123600	7.04412000	1.23151000
C	0.72513800	5.94092300	-0.32784800
H	0.71640000	3.81270400	-0.32105400
C	1.26217100	7.12682900	0.22228900
H	0.01104100	6.00153000	-1.14344700
H	4.76839000	4.29953900	3.89269100
H	4.04675000	6.57538600	3.14179100
H	2.63208400	7.93996300	1.66081400
H	0.94984500	8.09379500	-0.16042600
N	2.41736200	3.33742300	1.67264000
C	2.51520000	1.72520800	-0.78122300
H	2.11652400	1.11361800	-1.59618500
C	3.26203300	2.77001200	-1.20359000
H	3.68881200	3.45186200	-0.47092100
C	3.58503200	3.15993800	-2.58563600
C	3.25911900	2.38625500	-3.71647700
C	4.26532000	4.37307200	-2.80695800
C	3.60396100	2.80215700	-4.99855200
H	2.72767000	1.45069400	-3.58195700
C	4.61067900	4.79319700	-4.09019100
H	4.51689100	4.99164300	-1.94826700
C	4.28478100	4.00759500	-5.19670700
H	3.34071800	2.18199500	-5.85203300
H	5.13435100	5.73619900	-4.22629600
H	4.55352000	4.32900700	-6.19911200
O	0.91144800	-1.10831600	-1.09914500
B	1.68681900	-0.95734400	0.00626600
O	2.69985900	-1.86243800	0.11774700
C	2.49179200	-2.86471500	-0.92237900
C	1.57459500	-2.09840100	-1.94813600
C	1.79206300	-4.04530500	-0.24419800
H	1.64407800	-4.87641100	-0.94077000
H	2.41193600	-4.39547000	0.58639500
H	0.81837900	-3.75020600	0.15846900
C	3.85352700	-3.28820300	-1.45675800
H	4.42055300	-3.78095400	-0.66113600
H	3.74091200	-3.99472700	-2.28640200
H	4.43128900	-2.42890900	-1.79859600
C	2.36780300	-1.32630000	-3.00266800
H	2.84275500	-2.00640100	-3.71695900
H	1.68337100	-0.67261200	-3.55088000
H	3.13856000	-0.70324300	-2.54428500
C	0.49867100	-2.94942900	-2.61083300
H	-0.09923200	-2.32425500	-3.28057100
H	0.95290600	-3.75012900	-3.20506600
H	-0.17304500	-3.39581700	-1.87501100
H	1.34363100	-0.32571500	0.98468000

HBpin

0 1

B	-0.68896800	-1.27936600	0.86846400
O	-1.21623700	-2.50557300	0.57526000
O	0.29488800	-1.30821300	1.81650200
C	-0.38113400	-3.49950800	1.24045400
C	0.31180500	-2.65630200	2.37337300
C	1.75636300	-3.04011400	2.67125200
H	2.15663600	-2.38533000	3.45121200
H	1.81503700	-4.07360400	3.03047400
H	2.38978500	-2.94027600	1.78767000
C	-0.50019800	-2.59999600	3.67059100
H	-0.48837500	-3.56120500	4.19413400
H	-0.06496600	-1.84166400	4.32780100
H	-1.54029600	-2.32229700	3.47493700
C	0.59928100	-4.01876500	0.18470500
H	1.22897100	-4.82157900	0.58115600
H	0.03080500	-4.41071700	-0.66360100
H	1.24681300	-3.21697700	-0.18279600
C	-1.27416900	-4.63193200	1.73337200
H	-1.72695800	-5.14127800	0.87730500
H	-0.68948100	-5.36726500	2.29730600
H	-2.07914500	-4.26145600	2.37107100
H	-1.05404500	-0.27583000	0.34483100

Styrene

0 1

C	0.38380500	-1.26183500	1.32151400
H	0.78158500	-1.31169300	2.33500700
C	-1.08211600	-1.33789300	1.23869900
C	-1.82262200	-1.47007400	2.42442800
C	-1.78586300	-1.28448200	0.02251700

C	-3.21400500	-1.54704500	2.40241900
H	-1.29472900	-1.51276700	3.37412100
C	-3.17419000	-1.36106200	-0.00192700
H	-1.24168900	-1.18178800	-0.91130200
C	-3.89650000	-1.49286400	1.18774700
H	-3.76382900	-1.64920200	3.33390000
H	-3.69784700	-1.31772200	-0.95300500
H	-4.98086900	-1.55231700	1.16504300
C	1.25067700	-1.14190900	0.30901300
H	0.93854200	-1.08623100	-0.73012900
H	2.31948200	-1.09513800	0.49228600

KHMDS

0 1

N	1.42731800	0.01696100	1.12218400
Si	0.64073500	1.06545300	0.06642900
Si	2.75920300	0.11921400	2.14599300
C	2.99700900	-1.59350300	2.99373300
H	2.12020800	-1.87613100	3.59870900
H	3.18922500	-2.39130100	2.25812200
H	3.85461700	-1.59282900	3.67760600
C	2.58893100	1.36618500	3.57115500
H	3.45350900	1.35046300	4.24759100
H	2.49143100	2.38638100	3.17938200
H	1.68963900	1.16162300	4.16577900
C	4.41349300	0.49029000	1.28533900
H	4.38519700	1.47840000	0.80924000
H	5.26092300	0.48127400	1.98324000
H	4.61750900	-0.24288700	0.49481700
C	-0.13767700	2.59761100	0.87979600
H	0.63833400	3.22779000	1.33204000
H	-0.69309000	3.21655300	0.16303400
H	-0.82693300	2.30818000	1.68308000
C	-0.82640100	0.11483700	-0.74105400
H	-0.48032800	-0.75656500	-1.32028200
H	-1.55483100	-0.22901700	0.01107000
H	-1.38403600	0.74785900	-1.44212300
C	1.69572200	1.69111300	-1.38650400
H	1.12193300	2.31713700	-2.08232500
H	2.53917700	2.28909600	-1.01939300
H	2.11805200	0.85258800	-1.95453600
K	0.37211100	-2.25897300	1.16254500

HMDSH

0 1

N	1.36944800	-0.10287100	1.12010000
Si	0.68572200	1.01109800	-0.04116000
Si	2.68257000	0.11004400	2.25457000
C	3.28266100	-1.60610100	2.76099500
H	2.47706800	-2.19478100	3.21736500
H	3.66079900	-2.16650100	1.89820300
H	4.09269300	-1.53767800	3.49684300
C	2.13177500	1.05519300	3.79426300
H	2.95660000	1.18171400	4.50677800
H	1.76167800	2.05298800	3.53179400
H	1.32031400	0.52820600	4.31005400
C	4.08033100	1.07271700	1.42883500
H	3.75070400	2.06417500	1.09664300
H	4.91645300	1.22335500	2.12247200
H	4.46020000	0.53799700	0.55103900
C	0.54746500	2.72627800	0.73449800
H	1.52545100	3.11318400	1.04413800
H	0.12274000	3.44612200	0.02431800
H	-0.09630100	2.70441000	1.62099400
C	-1.02590400	0.36769700	-0.50827800
H	-0.97288600	-0.64108300	-0.93641500
H	-1.68830400	0.32798600	0.36415000
H	-1.49764200	1.01480200	-1.25729200
C	1.74777500	1.13957400	-1.59743800
H	1.31338000	1.83585000	-2.32580000
H	2.75659100	1.49443300	-1.35725600
H	1.84969800	0.16309500	-2.08558700
H	0.93240000	-1.01889500	1.14060400

CO

0 1

C	-0.73541700	-1.20731600	0.82449100
O	0.40252300	-1.20731600	0.82449100

KBr

0 1

Br	2.55142100	0.93424300	-0.83764900
K	3.35252300	3.30898000	-2.32859300

H_2

0 1

H	-0.03022300	-1.20731600	0.82449100
H	-0.77301100	-1.20731600	0.82449100

Trans-borylated product

0 1

B	0.79380300	-2.93052900	0.37112400
O	-0.42935400	-3.55967600	0.37037300
O	1.33265800	-2.80470300	1.63347300
C	-0.64537100	-4.08188600	1.70913900
C	0.29390100	-3.17076500	2.58007400
C	0.94213900	-3.86579900	3.77156900
H	1.58941500	-3.16010300	4.30143300
H	0.18017500	-4.22214100	4.47384100
H	1.55291600	-4.71440600	3.45699100
C	-0.37626600	-1.86712000	3.02577300
H	-1.13278400	-2.04505000	3.79673500
H	0.38716400	-1.19982700	3.43643100
H	-0.85161000	-1.35964700	2.18087500
C	-0.20642800	-5.54946600	1.68438000
H	-0.39908800	-6.04441200	2.64161200
H	-0.76693500	-6.07296000	0.90433500
H	0.85960800	-5.63775600	1.45400600
C	-2.12977900	-3.97967900	2.03950400
H	-2.70099200	-4.63109800	1.37093100
H	-2.31997900	-4.29869500	3.07044400
H	-2.49898400	-2.95973500	1.91480000
C	1.48877600	-2.41622000	-0.90566500
H	1.01701500	-2.60160000	-1.87027200
C	2.65877900	-1.74824500	-0.85191300
H	3.09746800	-1.58105500	0.13224200
C	3.44022200	-1.20354200	-1.96668600
C	3.03995500	-1.31654700	-3.31065500
C	4.64512700	-0.53595300	-1.68852900
C	3.81672200	-0.78161800	-4.33213800
H	2.11369000	-1.82737900	-3.55438100
C	5.42498500	0.00053600	-2.71067400
H	4.96720800	-0.44112700	-0.65440000
C	5.01315900	-0.12036200	-4.03783900
H	3.49036300	-0.87921600	-5.36390400
H	6.35296200	0.51232700	-2.47137000
H	5.61763900	0.29626800	-4.83852600

Cis-borylated product

0 1

C	2.14925000	4.58786800	-0.42098600
C	3.32728000	4.49472100	-1.08121000
H	3.34535700	3.78290200	-1.90892000
B	1.62030200	5.42206000	0.76821600
O	0.29874500	5.29036400	1.13858200
O	2.29284600	6.32511100	1.56389400
C	0.11872700	5.99165800	2.39528300
C	1.30576500	7.01869300	2.37648500
C	0.96918300	8.31931800	1.64124700
H	0.27667900	8.93986000	2.21876300
H	1.89137400	8.88577400	1.48178300
H	0.52279100	8.11504500	0.66348900
C	1.92320400	7.32149900	3.73604700
H	2.75116100	8.02720200	3.61623900
H	1.18290900	7.77661500	4.40332700
H	2.31316100	6.41835700	4.20955100
C	-1.27161200	6.61623400	2.41343500
H	-2.02892200	5.82640900	2.40520500
H	-1.41494200	7.21633700	3.31898700
H	-1.43698500	7.25229400	1.54156500

C	0.24576200	4.94470800	3.50673100
H	0.05698700	5.37889000	4.49373400
H	-0.48733200	4.15224500	3.33045100
H	1.24157800	4.49119600	3.50916600
H	1.37554400	3.92702400	-0.81630600
C	4.62382100	5.16460800	-0.92491200
C	4.93155100	6.11274100	0.06912000
C	5.63302500	4.82380400	-1.84670600
C	6.19684000	6.68990100	0.12622900
H	4.18017800	6.39513200	0.79383800
C	6.89751000	5.40236900	-1.78817000
H	5.41346000	4.09200600	-2.62051800
C	7.18526300	6.34147300	-0.79753300
H	6.41460700	7.41944600	0.90192500
H	7.65604400	5.12045100	-2.51315900
H	8.17026600	6.79701100	-0.74428000

Gem-borylated product

0 1

C	0.23821200	-0.25646300	0.05482200
C	1.62595100	-0.17573000	-0.07337900
C	2.25738700	1.06560700	-0.07981100
C	1.51944800	2.25592300	0.03566100
C	0.12583900	2.15730900	0.18265300
C	-0.50716400	0.91583200	0.18521200
H	-0.25559400	-1.22421400	0.06382600
H	2.21927500	-1.08230300	-0.15828300
H	3.33988700	1.11825700	-0.15213100
H	-0.45986000	3.06211000	0.29744700
H	-1.58747300	0.86453800	0.29206700
C	2.19165400	3.57926800	-0.00973400
C	3.27749200	3.78685600	-0.77914700
H	3.68943300	3.01628200	-1.42788600
H	3.77729600	4.75074800	-0.79014200
B	1.67648500	4.78607300	0.83350300
O	0.63717600	4.72876600	1.72993900
O	2.24263200	6.03708500	0.75178800
C	0.34444000	6.09220000	2.14325600
C	1.69961900	6.82799200	1.84291400
C	1.55962500	8.27170400	1.37571400
H	1.08303500	8.88410300	2.14929000
H	2.55020700	8.69017400	1.17299400
H	0.96897900	8.34140000	0.46011900
C	2.70352800	6.73644200	2.99620400
H	3.68053400	7.07795300	2.64207200
H	2.40321900	7.36189300	3.84282900
H	2.81039300	5.70482600	3.34500300
C	-0.81299300	6.57669300	1.26485600
H	-1.65615200	5.88899600	1.37930800
H	-1.14378100	7.57984600	1.55171300
H	-0.52672400	6.59257300	0.20884100
C	-0.07243000	6.07678800	3.60869100
H	-0.23148800	7.09686400	3.97572000
H	-1.01099800	5.52499700	3.71823400
H	0.67955200	5.59216800	4.23440400

VIII-CN-1

0 1

Mn	1.99051500	2.28047800	1.24041900
S	5.68018200	-0.22730600	4.84652000
O	0.14960200	2.98006600	3.46404700
O	0.01681000	2.71724600	-0.86672300
C	4.49083000	3.29392600	2.73503500
H	5.58347100	3.25264400	2.73381700
H	4.19433200	3.63026400	3.73497800
C	3.52708400	1.33030600	3.82731600
H	2.74680800	1.95258900	4.26958500
H	3.08582900	0.36672400	3.61032500
C	6.02458000	1.54652700	6.68060300
H	6.40417900	2.07628300	7.54703500
C	0.91648500	2.65726900	2.64968400
C	4.63457100	1.17431200	4.82818000
C	0.79388000	2.60568300	0.00012300
C	6.52334200	0.34903000	6.24693800
H	7.33339000	-0.23006500	6.66945100
N	3.90357500	1.95406700	2.51945400
C	4.94249400	2.00972200	5.87322600
H	4.38967200	2.92220700	6.07271600
B	4.75698600	1.11649300	1.68320000
O	4.77945800	-0.25186600	1.79021000
O	5.74631300	1.62255900	0.87372700
C	5.79337400	-0.74447000	0.86107600
C	6.68801700	0.53072300	0.64324200
C	7.27311100	0.65581600	-0.75517100
H	7.84357200	1.58582800	-0.83838000
H	7.95265100	-0.17931600	-0.95779100
H	6.49113600	0.66047400	-1.51273000
C	7.79455100	0.69068300	1.69049000
H	8.58356900	-0.05585800	1.55582200
H	8.23958700	1.68442300	1.58089500
H	7.40076300	0.60145700	2.70654700
C	5.07403000	-1.20382100	-0.40893400
H	5.78338300	-1.63610600	-1.12227100
H	4.35012900	-1.98151700	-0.14488300
H	4.53772200	-0.38371900	-0.89247000
C	6.50831700	-1.91824900	1.51934100
H	5.80179400	-2.74132700	1.66468000
H	7.32009600	-2.27885900	0.87808300
H	6.92013000	-1.64854500	2.49263200
C	4.01387300	4.35276600	1.78651900
C	4.87971300	5.41511000	1.44630000
C	4.39917300	6.45569200	0.69269000
C	2.20672500	5.38899900	0.76606000
C	3.02619600	6.48941200	0.36038900
C	0.81123300	5.47593100	0.54872400
C	2.44452500	7.57676100	-0.33887800
C	0.27038900	6.55843700	-0.10980400
H	0.17213700	4.69587100	0.93420600
C	1.09143700	7.60751800	-0.58397800
H	-0.80391300	6.60787400	-0.25974000
H	5.91638800	5.37274800	1.76263400
H	5.04828000	7.26682600	0.37328800
H	3.08820800	8.39182700	-0.65935400
H	0.64828200	8.44446100	-1.11501800
N	2.75171400	4.28825300	1.38880000
O	3.31166700	3.67599800	-1.13813500
O	3.32977800	1.45240200	-1.58713200
B	3.02338400	2.41767700	-0.62906800
C	3.53362000	2.11754000	-2.86525200
C	5.46471400	3.70635500	-2.16789800
H	6.04522000	3.64969900	-3.09501300
H	5.64455000	4.68178800	-1.70535600
H	5.81570200	2.94113800	-1.47287400
C	3.45840500	4.68711000	-3.31372900
H	3.76392600	5.64877700	-2.88929300
H	3.87781600	4.60815000	-4.32346200
H	2.36879500	4.68414000	-3.38269300
C	3.96154600	3.55678100	-2.42095700
C	2.18380600	2.08432400	-3.59137800
H	2.25137000	2.52972200	-4.58948100
H	1.86878900	1.04166200	-3.69984800
H	1.41331500	2.60918200	-3.02105100
C	4.57212000	1.35236400	-3.67559000
H	4.21595200	0.33481300	-3.86569800
H	4.73802500	1.83992700	-4.64311500
H	5.53039300	1.28857000	-3.15856700
C	0.90793600	0.23894500	1.55410300
C	1.84300000	0.20577600	0.52206800
H	2.78621400	-0.29762200	0.67489100
H	1.52318100	0.25545200	-0.50915200
H	-0.11306500	0.52077800	1.30982600
C	1.02215100	-0.50408900	2.82454300
C	0.11354100	-0.25824300	3.87106300
C	1.99264500	-1.50731800	3.01775400
C	0.20397500	-0.93370500	5.07973100
H	-0.65466900	0.49608500	3.73886600
C	2.09627400	-2.18712300	4.22402000
H	2.69489200	-1.73108100	2.22498600
C	1.20778300	-1.89904300	5.27325600
H	-0.49301000	-0.71843000	5.88293100

H	2.86302500	-2.94187300	4.36359900
C	1.31922500	-2.58801800	6.52164900
N	1.41337600	-3.14813000	7.53749500

VIII-CN-2

0 1

Mn	1.88665700	2.58736500	1.37575900
S	5.28632000	-0.28179200	4.97813200
O	-0.00502400	3.32204600	3.55632100
O	-0.16757200	2.94025500	-0.67157000
C	4.28046800	3.32122600	3.07509500
H	5.33975700	3.22409700	3.33602300
H	3.76351000	3.68875500	3.97013100
C	3.15136200	1.31703100	3.93532100
H	2.36353400	1.94404700	4.35690300
H	2.68114600	0.39730800	3.59284400
C	5.34999800	1.27712600	7.02752700
H	5.61811500	1.72323200	7.97871300
C	0.79517600	2.99358700	2.77639300
C	4.15620300	1.05261200	5.02015800
C	0.65382700	2.85579800	0.15909400
C	5.95900800	0.16621800	6.51349800
H	6.76469000	-0.41419500	6.94274200
N	3.68410400	2.01864700	2.73253300
C	4.31987400	1.77685700	6.17411400
H	3.70390900	2.63868300	6.41021300
B	4.50731300	1.17833200	1.87420100
O	4.45915900	-0.19295600	1.96218700
O	5.52976700	1.64880400	1.08757500
C	5.44784400	-0.72349700	1.02874500
C	6.40703600	0.51053000	0.83232800
C	6.99252700	0.63141400	-0.56600700
H	7.59726700	1.54048300	-0.63893900
H	7.63784400	-0.22704300	-0.78314900
H	6.20828700	0.67620600	-1.31975100
C	7.52464700	0.59171100	1.87729600
H	8.27234400	-0.19366600	1.72767800
H	8.02134100	1.56236200	1.78377800
H	7.12836900	0.50687500	2.89296500
C	4.70411700	-1.13590700	-0.24148500
H	5.39607500	-1.55514200	-0.97973800
H	3.97458200	-1.90922200	0.01348000
H	4.16712000	-0.29511900	-0.68502600
C	6.10671100	-1.94064800	1.66930800
H	5.36154100	-2.73194800	1.79631600
H	6.90048400	-2.32755900	1.02068100
H	6.53261300	-1.71011800	2.64679700
C	4.10137300	4.37086800	2.01273900
C	5.15547100	5.26091000	1.72450900
C	4.94665400	6.29080100	0.83944800
C	2.62799200	5.55615000	0.66425000
C	3.65443900	6.48553000	0.30521500
C	1.30804300	5.80152900	0.21680300
C	3.34645100	7.56353100	-0.56481500
C	1.03473500	6.86948500	-0.60643200
H	0.51942200	5.14186400	0.54596600
C	2.06390800	7.74709200	-1.02471500
H	0.01498800	7.04136000	-0.93775500
H	6.12273000	5.09762900	2.18716500
H	5.75059300	6.96786600	0.56307000
H	4.14348200	8.24689700	-0.84652900
H	1.83232300	8.57526400	-1.68794000
N	2.90088900	4.45338100	1.44089400
O	3.13534500	3.64748600	-1.20786100
O	2.98946400	1.38751400	-1.38475500
B	2.81008700	2.47775000	-0.53369200
C	3.15701000	1.88184800	-2.74263100
C	5.19980100	3.45163200	-2.37930800
H	5.71171500	3.25109300	-3.32692300
H	5.44840700	4.46801200	-2.05785000
H	5.57002000	2.76526700	-1.61577600
C	3.15497800	4.38459900	-3.49212200
H	3.52133500	5.37378400	-3.19901900
H	3.50173800	4.17520800	-4.51100700
H	2.06382400	4.42035300	-3.49018200
C	3.67709100	3.34254200	-2.50646800
C	1.77079200	1.83107500	-3.39524800
H	1.80391000	2.15124200	-4.44226000
H	1.40518200	0.79990100	-3.36035200
H	1.05674900	2.45657900	-2.85393300
C	4.11486000	0.96838000	-3.49865300
H	3.69759600	-0.04242800	-3.55094700
H	4.26143200	1.32905500	-4.52343500
H	5.09172000	0.90788400	-3.01605600
C	1.44064000	-0.43804700	1.27975600
C	1.37889800	-1.85487000	1.26652200
C	2.23646600	-2.60131800	2.09759900
C	0.47369000	-2.52899700	0.42252300
C	2.17925900	-3.98761800	2.07498600
H	2.94944800	-2.08172800	2.72643700
C	0.43137200	-3.91390600	0.41388900
H	-0.18463500	-1.95317500	-0.21947400
C	1.28099700	-4.67617800	1.23894800
H	2.84469000	-4.55731300	2.71854200
H	-0.27174000	-4.41289400	-0.24488300
C	1.27118900	-6.14322500	1.26218300
H	1.98810600	-6.58979600	1.95049800
C	0.49060400	-6.96004100	0.54256500
H	-0.24975400	-6.59639800	-0.16431700
H	0.57041200	-8.03774300	0.64249700
N	1.54087100	0.72310500	1.32138900

TS-I

0 1

Mn	-0.53135300	1.06972000	0.18793500
S	1.53150000	2.29688600	0.67250200
O	-1.94027100	3.32004900	-1.03646200
O	-1.47036200	1.55077900	2.95587500
C	-0.02269000	-0.71331100	-2.00210100
H	0.58656100	-1.61535900	-2.16638300
H	-0.22655700	-0.29737100	-3.01146300
C	1.73739200	0.94089100	-1.73012900
H	2.67430900	0.36929700	-1.61737100
H	1.59795900	1.11195000	-2.81128100
C	1.65963300	4.55353100	-0.56002900
H	1.66910000	5.61653000	-0.77564800
C	-1.38853000	2.44156900	-0.50973100
C	1.85091900	2.27542500	-1.05928700
C	-1.15778700	1.36110300	1.85110300
C	1.39914300	4.04333100	0.67326100
H	1.21112600	4.57101400	1.59805700
N	0.60001600	0.25003500	-1.14111400
C	1.89063900	3.54012000	-1.55768700
H	2.01845800	3.75569400	-2.61307700
B	1.27706600	-1.18825000	0.81587200
O	2.53223500	-0.66601900	1.05162000
O	1.30946100	-2.45521900	0.27466000
C	3.48949200	-1.74078800	0.88958300
C	2.69691100	-2.80563200	0.02931200
C	2.89245400	-4.25485700	0.47167400
H	2.28502400	-4.91224900	-0.15839200
H	3.94057300	-4.55739300	0.36891700
H	2.58415600	-4.40373800	1.50810300
C	2.96321200	-2.70190400	-1.47491700
H	3.97928400	-3.02783700	-1.72043900
H	2.25933600	-3.35054100	-2.00578900
H	2.82944100	-1.68312600	-1.84081900
C	3.82457800	-2.23061600	2.30339000
H	4.58103800	-3.02197600	2.29263900
H	4.21107300	-1.38775200	2.88373800
H	2.93157500	-2.60629200	2.81154900
C	4.74499200	-1.18179600	0.22724400
H	5.19203600	-0.42493400	0.87892500
H	5.48562600	-1.97269200	0.06381000
H	4.52169200	-0.70950800	-0.73159200
H	0.29430100	-0.78129100	1.34951900
C	-1.34235800	-1.12732500	-1.42368300
C	-1.98532500	-2.30009100	-1.88485600
C	-3.21016300	-2.64281800	-1.38034900
C	-3.14606700	-0.60073100	-0.03640800

C	-3.83926400	-1.78260200	-0.44651300
C	-3.81925500	0.30826300	0.81312400
C	-5.13488600	-2.04889000	0.06221400
C	-5.08785900	0.03123500	1.27724300
H	-3.33577500	1.23783100	1.06988100
C	-5.74970700	-1.16325100	0.91726700
H	-5.58532600	0.74824900	1.92344000
H	-1.47987600	-2.91651200	-2.62074300
H	-3.71738200	-3.55062000	-1.69581400
H	-5.63638800	-2.96086900	-0.25077500
H	-6.74459100	-1.36965900	1.29998400
N	-1.86482500	-0.33173900	-0.48903700

TS-II

0 1

Mn	1.62765900	1.20896900	1.45481300
S	6.53017500	-1.36587300	3.30752200
O	0.31834000	0.37299800	3.95567600
O	-0.93996600	2.26100200	0.48491100
C	3.81471700	1.66472500	3.55109900
H	4.77941000	1.68074700	4.07340000
H	3.04920500	1.42466500	4.30028600
C	3.75309300	-0.75029800	3.12877300
H	2.85446600	-0.83274800	3.74535700
H	3.64119900	-1.46232700	2.31503900
C	6.30406800	-1.36766000	5.87423600
H	6.53315500	-1.43999600	6.93168400
C	0.84845900	0.76500600	2.99058400
C	4.94836300	-1.04795000	3.98780100
C	0.07952700	1.84482500	0.85286200
C	7.23303600	-1.53714400	4.88577600
H	8.28660400	-1.75978000	4.98875600
N	3.78283000	0.60829500	2.52843500
C	5.00189800	-1.08582300	5.35711000
H	4.12586200	-0.91963100	5.97593200
B	4.67186400	0.75082900	1.39186300
O	5.06305900	-0.32892000	0.64330100
O	5.25457300	1.93351600	1.02153500
C	5.82341000	0.18775900	-0.48474000
C	6.26104700	1.61980100	0.02047200
C	6.22418400	2.71138400	-1.04282800
H	6.51680800	3.66639600	-0.59543100
H	6.92281300	2.48677400	-1.85635300
H	5.22149800	2.82603700	-1.45909100
C	7.60824800	1.62512800	0.74809000
H	8.43964900	1.44654600	0.05882100
H	7.75096100	2.60411700	1.21567600
H	7.63405100	0.86628100	1.53543500
C	4.87194200	0.22550900	-1.68233900
H	5.38807000	0.54798800	-2.59231100
H	4.47403500	-0.78064500	-1.84599100
H	4.02669700	0.89269400	-1.49630100
C	6.97570600	-0.77282000	-0.75696900
H	6.57476100	-1.74209100	-1.06859500
H	7.61368400	-0.39286500	-1.56258400
H	7.58781700	-0.93010600	0.13308600
C	3.53427300	3.03171800	2.98436600
C	4.19804900	4.15191700	3.53857200
C	3.95094100	5.40038100	3.03086200
C	2.47575500	4.35347600	1.39297500
C	3.08854900	5.53561400	1.91719100
C	1.68816700	4.46476300	0.22167500
C	2.84229200	6.78665700	1.29671500
C	1.47931600	5.69234000	-0.36767600
H	1.28528700	3.56239100	-0.21375000
C	2.04489900	6.86798000	0.17876500
H	0.87606000	5.75572800	-1.26845500
H	4.89157700	4.00120900	4.35912000
H	4.42867400	6.28289600	3.44818400
H	3.30665200	7.67519300	1.71645100
H	1.86141200	7.82763400	-0.29505700
N	2.66465400	3.12762400	1.98783800
O	-0.23571600	-1.03368800	0.42825800
B	0.98893200	-0.73536300	0.99639000
O	1.64213500	-1.88885300	1.40366500
C	0.89359800	-3.03038300	0.91138800
C	-0.53729800	-2.42128600	0.72369800
C	0.99124200	-4.15268300	1.93778300
H	0.37031200	-5.00588500	1.64164300
H	2.02811700	-4.49653100	2.01193100
H	0.67394800	-3.81527000	2.92673300
C	1.55015000	-3.45035300	-0.40774900
H	2.61097100	-3.64888400	-0.22650400
H	1.09194600	-4.35554300	-0.81978500
H	1.47604300	-2.65076700	-1.15115100
C	-1.34129200	-3.00520500	-0.43167800
H	-1.52340900	-4.07500100	-0.27665400
H	-2.31020000	-2.50050000	-0.49648300
H	-0.82644600	-2.87178500	-1.38556000
C	-1.36734000	-2.42848100	2.01243200
H	-2.25673800	-1.80977300	1.86034100
H	-1.68942800	-3.44011500	2.28102400
H	-0.80266900	-2.00348800	2.84746900
H	1.84001800	0.28164500	0.15280300
H	2.36163100	1.26019800	-0.20757200

TS-III

0 1

Mn	1.83271300	2.64671800	1.46572400
S	5.54671600	-0.46465300	4.95065100
O	0.52464100	3.22919200	4.06239700
O	-0.70252500	3.61531000	0.38667400
C	4.25118300	3.17250900	3.13872100
H	5.24173000	3.11647100	3.60122600
H	3.55499700	3.54454200	3.90117100
C	3.37029400	1.04536200	3.92439000
H	2.51173700	1.53752200	4.38042900
H	3.04065600	0.07467200	3.57638300
C	5.76219300	1.23214500	6.87363400
H	6.09543600	1.73736500	7.77340400
C	1.11159100	3.03118000	3.07736500
C	4.43761500	0.88652800	4.96937200
C	0.34784100	3.29905600	0.77817100
C	6.32866200	0.08089900	6.39839300
H	7.15360700	-0.48021700	6.81637700
N	3.77423800	1.84386000	2.72068300
C	4.68060800	1.68484100	6.05922600
H	4.08688800	2.56647400	6.27803100
B	4.76494300	1.14259700	1.91234700
O	4.78731500	-0.21949600	1.78705900
O	5.83185400	1.77937200	1.34198100
C	5.91175400	-0.55980000	0.92359000
C	6.79095600	0.75442300	0.95946900
C	7.40069500	1.15098800	-0.37831400
H	7.97998600	2.07176500	-0.25698500
H	8.07502600	0.37010500	-0.74680600
H	6.62470600	1.33505000	-1.11925100
C	7.86711800	0.74544600	2.04899900
H	8.66582200	0.03387100	1.81625100
H	8.30657700	1.74553100	2.11558800
H	7.44606100	0.49352800	3.02567900
C	5.32400500	-0.86044900	-0.45352100
H	6.10121600	-1.15255500	-1.16744400
H	4.61431800	-1.68915600	-0.36216600
H	4.79074800	0.01178900	-0.83115300
C	6.59123200	-1.79935000	1.49407000
H	5.88845300	-2.63793600	1.47487600
H	7.46286600	-2.07141000	0.88847800
H	6.91113900	-1.64953400	2.52597000
C	4.26100600	4.18330900	2.03498400
C	5.41681700	4.97138000	1.84201600
C	5.38137400	6.02100800	0.96417000
C	3.02670600	5.48384100	0.55930800
C	4.15657100	6.33690000	0.33262600
C	1.78719900	5.87358100	-0.00041700
C	4.02064100	7.48929000	-0.48316300
C	1.67473300	7.02587700	-0.74751600
H	0.91565600	5.27105000	0.17533300
C	2.80047100	7.83573500	-1.01352100
H	0.70332500	7.30499800	-1.14470600

H	6.31713600	4.71189900	2.38656300
H	6.25834700	6.63391500	0.77478900
H	4.89873000	8.10691500	-0.65247200
H	2.69800100	8.72984000	-1.62109700
N	3.12775800	4.34801000	1.35026400
O	1.77252400	3.11963700	-1.54090200
O	3.69875900	1.98310100	-1.09217500
B	2.48624600	2.43607000	-0.55713200
C	3.60674900	2.05890100	-2.54393100
C	3.21459300	4.59147500	-2.80910000
H	3.77667500	4.72293900	-3.73964800
H	2.43852600	5.35695300	-2.76366000
H	3.89174400	4.75036500	-1.96729000
C	1.62671400	3.03004800	-3.94115300
H	0.92799900	3.87149700	-3.97979900
H	2.18704000	3.00931000	-4.88315800
H	1.04147800	2.11180900	-3.85960600
C	2.56408900	3.20784900	-2.74956700
C	3.10223400	0.70382900	-3.05610400
H	3.03481500	0.69700900	-4.14858600
H	3.79448700	-0.08615900	-2.75456600
H	2.11554500	0.46162800	-2.65231700
C	4.98914100	2.34253100	-3.12119300
H	5.63383100	1.46640000	-3.00391700
H	4.92075500	2.56145400	-4.19276300
H	5.46386900	3.18842700	-2.62006000
C	0.78313600	0.78656800	1.45496100
C	1.63514800	0.87485300	0.29176800
H	2.51603300	0.23898900	0.30129700
H	1.11824500	0.83821600	-0.66940700
H	-0.26817800	1.01586600	1.28981100
C	0.94187000	-0.26987700	2.48182000
C	0.21195400	-0.18468700	3.68223200
C	1.77679600	-1.38705000	2.30717600
C	0.35868700	-1.13580000	4.68723400
H	-0.44855700	0.66398500	3.83459300
C	1.92938700	-2.33974700	3.31594500
H	2.33787400	-1.50017600	1.38721900
C	1.23150200	-2.21516100	4.51713200
H	-0.20267500	-1.03101200	5.61208100
H	2.59976600	-3.18099300	3.15964100
H	1.35547700	-2.95209700	5.30542900

TS-IV

0 1

Mn	1.87585600	1.54212600	1.09744600
S	3.91059900	1.44071300	6.59390000
O	-0.30591900	1.82745400	3.06366200
O	-0.00357300	2.27224400	-1.03630300
C	3.14872700	2.86671800	3.50355300
H	3.89155600	3.17130900	4.25107700
H	2.17430000	2.83628400	4.00733900
C	3.18984400	0.47056500	4.00677900
H	2.15823200	0.56203000	4.35504200
H	3.27512500	-0.49238800	3.51490000
C	6.09548200	0.09509600	6.41833400
H	7.06042500	-0.34217400	6.65056200
C	0.56684000	1.77015700	2.29043000
C	4.17076200	0.49893000	5.14534800
C	0.74820800	1.95961700	-0.20093700
C	5.43113100	0.94218200	7.26352600
H	5.73726000	1.29321900	8.23955300
N	3.43077400	1.51879600	2.98415900
C	5.37433200	-0.15867900	5.21224400
H	5.71667700	-0.80618500	4.41373000
B	4.67894200	1.36911400	2.25393000
O	5.23199400	0.14627100	1.95819100
O	5.46078100	2.43520000	1.88941500
C	6.40516400	0.40536200	1.12966900
C	6.75020000	1.89974100	1.49098200
C	7.27243600	2.73750800	0.33007200
H	7.46029500	3.75952200	0.67353900
H	8.21299600	2.32826700	-0.05497300
H	6.54606900	2.78190600	-0.48390100
C	7.66714200	2.03406800	2.71084100
H	8.68603200	1.70059200	2.48947300
H	7.70491900	3.08649400	3.00774100
H	7.28317400	1.45877700	3.55905100
C	5.99234800	0.22081100	-0.33196100
H	6.84219100	0.37820000	-1.00362000
H	5.62945300	-0.79967700	-0.48178400
H	5.18756100	0.90247600	-0.61636200
C	7.47875300	-0.60833500	1.50780600
H	7.13353300	-1.61587100	1.25585900
H	8.40375300	-0.41751400	0.95258900
H	7.70113100	-0.58131400	2.57663500
C	3.12423100	3.89340900	2.40621800
C	3.47953100	5.23004300	2.69770200
C	3.49847700	6.15734700	1.68884100
C	2.94719600	4.35339700	0.13882200
C	3.26425600	5.73048200	0.35955200
C	2.85784400	3.88634400	-1.19356700
C	3.37974000	6.60661600	-0.74944400
C	3.00222400	4.75644400	-2.25188400
H	2.71984700	2.82701400	-1.35067800
C	3.23980200	6.13312800	-2.03367900
H	2.93978000	4.37669200	-3.26694100
H	3.72391800	5.49783000	3.72048300
H	3.73347100	7.20015600	1.88416300
H	3.60103500	7.65418800	-0.56265200
H	3.33565200	6.80709800	-2.87972100
N	2.78045100	3.47984300	1.19257000
O	3.24108200	-0.13754400	-2.39480200
O	1.03432000	-0.63900800	-2.03939300
B	2.25849900	-0.40777100	-1.47170500
C	1.21787300	-0.71474400	-3.47638100
C	3.49053200	-0.55434200	-4.76225500
H	3.00461200	-0.50716500	-5.74314200
H	4.42046700	0.02074800	-4.81501300
H	3.74704400	-1.59395800	-4.54849500
C	2.41841000	1.53979600	-3.90159000
H	3.39752900	2.01958700	-3.80773700
H	2.01934900	1.75639400	-4.89780800
H	1.74565900	1.97534000	-3.15894400
C	2.58774200	0.03371900	-3.68390900
C	0.01647400	-0.05989400	-4.14951100
H	0.15749900	-0.00861900	-5.23510900
H	-0.88120300	-0.65321100	-3.95036600
H	-0.15464900	0.94610200	-3.76233000
C	1.28360600	-2.20385900	-3.82861500
H	0.37143100	-2.69109100	-3.47231400
H	1.36181400	-2.35983500	-4.90944800
H	2.13698300	-2.68724800	-3.34290500
C	1.39621100	-0.71207900	0.93766600
C	2.49027100	-0.47175000	0.06701100
H	3.10741200	1.06055900	0.07072900
H	3.46645700	-0.81483400	0.40201700
C	1.48580400	-1.53320400	2.16105000
C	2.57488300	-2.38706700	2.41702200
C	0.44313500	-1.50697600	3.10577100
C	2.64554400	-3.13625700	3.59176500
H	3.38385300	-2.45501400	1.69684400
C	0.51149300	-2.25562800	4.27708800
H	-0.40893300	-0.85839300	2.92794600
C	1.62015300	-3.06755100	4.53536000
H	3.50576000	-3.77711300	3.76783400
H	-0.30032000	-2.19907000	4.99756800
H	1.67686700	-3.64575400	5.45308900
H	0.40300000	-0.66852300	0.50017900

TS-IVA

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Mn	1.87355700	1.70066800	1.21173200
S	3.86703900	1.32502400	6.59929400
O	-0.08438600	2.35623400	3.31097300
O	-0.09625500	2.69341300	-0.72705600
C	3.51513000	2.82062700	3.45317400
H	4.31871300	3.01326700	4.17410800
H	2.56209800	3.00196400	3.96389000
C	3.06523200	0.44980400	4.01298200

H	2.06231500	0.74471100	4.33323400
H	2.98305900	-0.52108200	3.52364100
C	5.79821800	-0.37247800	6.51790700
H	6.66941400	-0.95885500	6.78838000
C	0.71274800	2.16303700	2.48007500
C	4.00179000	0.31311500	5.18224100
C	0.69351500	2.26149700	0.00850400
C	5.26418900	0.59668600	7.32335900
H	5.59890500	0.91699600	8.30054500
N	3.52721100	1.41930100	2.99064100
C	5.07678800	-0.53365100	5.29629300
H	5.33273400	-1.24554700	4.52040300
B	4.73271900	1.01942100	2.28871200
O	5.05870500	-0.29213500	2.04621500
O	5.69160400	1.91448700	1.88986800
C	6.25547000	-0.27092700	1.20743600
C	6.87041900	1.13688000	1.54373100
C	7.57210600	1.82852700	0.38174600
H	7.94680100	2.80316500	0.70935300
H	8.42409600	1.23485000	0.03244500
H	6.88873200	1.99200000	-0.45379400
C	7.76430200	1.12679100	2.78746100
H	8.70937700	0.60740300	2.59954600
H	7.98809300	2.16002800	3.06928600
H	7.26077500	0.64793700	3.63305100
C	5.79341400	-0.38099100	-0.24409400
H	6.64726400	-0.40133200	-0.92910600
H	5.21671600	-1.29705100	-0.38658600
H	5.14780000	0.45896100	-0.51278900
C	7.12354400	-1.46208900	1.58995500
H	6.59705500	-2.39039100	1.34813900
H	8.06443700	-1.44876000	1.02881700
H	7.35444400	-1.46712900	2.65752700
C	3.66449700	3.76809200	2.28959000
C	4.38547800	4.97091400	2.45617900
C	4.57285600	5.79934800	1.38040100
C	3.40279000	4.15063200	0.00839900
C	4.11012100	5.39009700	0.10656900
C	3.03147100	3.68528300	-1.27821600
C	4.35933100	6.14877200	-1.06568000
C	3.30711400	4.43685800	-2.39978900
H	2.55343800	2.72008900	-1.36378300
C	3.96033300	5.68673900	-2.29837600
H	3.01859100	4.05990400	-3.37686700
H	4.78168900	5.21534400	3.43622600
H	5.10374300	6.74221800	1.47994200
H	4.88544900	7.09486900	-0.96883100
H	4.15842400	6.26959300	-3.19294000
N	3.12132900	3.39970100	1.13224500
O	1.38422300	0.23216900	-2.08430800
O	3.08614900	-1.28290100	-1.90995000
B	2.16313000	-0.51686700	-1.23374900
C	3.07600700	-0.85054000	-3.29885000
C	1.55581500	0.99004800	-4.36440400
H	1.80178400	0.70949900	-5.39467500
H	0.53610400	1.38581900	-4.34865600
H	2.23062600	1.78804600	-4.04738500
C	0.56087200	-1.23983900	-3.78675200
H	-0.42024600	-0.76981800	-3.67217000
H	0.65725400	-1.59271300	-4.81846700
H	0.60191200	-2.10309300	-3.11564100
C	1.64593700	-0.21657700	-3.43771100
C	3.33578000	-2.06139400	-4.18624700
H	3.26482400	-1.78775200	-5.24490500
H	4.34414200	-2.44441900	-4.00051400
H	2.62533400	-2.86538100	-3.98381500
C	4.20259300	0.17654600	-3.45343900
H	5.14952200	-0.28684500	-3.16263000
H	4.29031300	0.52079300	-4.48885000
H	4.03895800	1.04667900	-2.80997200
C	1.08853100	-0.41557400	1.27330200
C	2.15623800	-0.46705000	0.32458600
H	1.37353900	-0.75864800	2.26483900
H	2.93201900	0.94157700	0.07184800
H	3.06843500	-0.89180200	0.73914600
C	-0.37057700	-0.53648600	1.06856900
C	-1.16185400	-0.78383300	2.20685000
C	-1.03048200	-0.42891100	-0.16807000
C	-2.54445800	-0.91684800	2.12058800
H	-0.67551200	-0.86194600	3.17658800
C	-2.41480200	-0.56334400	-0.25392100
H	-0.46465200	-0.20988800	-1.06207500
C	-3.18433700	-0.80888700	0.88437400
H	-3.12314900	-1.10328600	3.02174200
H	-2.89645800	-0.46949500	-1.22440900
H	-4.26347400	-0.91099400	0.81060300

TS-IVB

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Mn	1.88488900	1.47508100	1.04588800
S	4.56726100	0.65855800	6.15592000
O	-0.24931200	1.88717200	3.03485500
O	0.06819900	2.58535500	-0.96374400
C	3.24151300	2.56043600	3.50232100
H	3.96927900	2.80110100	4.28779800
H	2.25309500	2.48853800	3.96840900
C	3.29241000	0.07191800	3.66440200
H	2.31146700	0.18698400	4.13619900
H	3.23689600	-0.77687900	2.98520000
C	6.32575800	-1.13267000	5.58812200
H	7.18862200	-1.78701600	5.64579900
C	0.62737800	1.79621000	2.26888500
C	4.37708700	-0.22622200	4.66092600
C	0.79332800	2.10017800	-0.18477400
C	6.01429400	-0.21269900	6.55247000
H	6.53969900	-0.00151800	7.47384200
N	3.54686300	1.27509900	2.84030200
C	5.39229400	-1.13692500	4.50696000
H	5.46872200	-1.76792000	3.62852200
B	4.86427300	1.29319000	2.20539700
O	5.46023400	0.23140100	1.59107000
O	5.65730000	2.41381200	2.27388800
C	6.68445600	0.74620900	0.98227500
C	6.98990500	2.00874200	1.86402500
C	7.63585500	3.17577400	1.12722700
H	7.79183700	4.00581500	1.82348200
H	8.61004700	2.88667400	0.71766600
H	7.00148800	3.53168400	0.31299400
C	7.76178000	1.68383300	3.14625100
H	8.80426000	1.42720700	2.93167900
H	7.74959900	2.56292700	3.79774900
H	7.29952900	0.85432600	3.68911500
C	6.35572800	1.11732500	-0.46556000
H	7.23831500	1.50836800	-0.98164500
H	6.01144700	0.22737900	-0.99110000
H	5.55754600	1.86419800	-0.51079300
C	7.73808400	-0.35073400	1.03864800
H	7.40802900	-1.20036100	0.43580100
H	8.69315700	0.01075900	0.64098400
H	7.89307100	-0.70068800	2.06159400
C	3.27095700	3.66130500	2.46569400
C	3.68361700	4.96638700	2.81026800
C	3.81262500	5.91274500	1.82510200
C	3.20762400	4.19613200	0.19888300
C	3.61373000	5.53943200	0.47320900
C	3.11155000	3.76903200	-1.14969500
C	3.83640700	6.43157500	-0.60667300
C	3.35846700	4.65621500	-2.17464500
H	2.87632000	2.73117800	-1.35034100
C	3.70392800	6.00197300	-1.90741700
H	3.29123700	4.31283700	-3.20297200
H	3.90278600	5.19418300	3.84829600
H	4.10869400	6.93165500	2.05997900
H	4.12898300	7.45460400	-0.38488900
H	3.88166700	6.68827700	-2.73014500
N	2.95747400	3.31021000	1.22221000
O	2.16877400	0.35058800	-2.41683100
O	0.47079300	-1.11510400	-1.96785400
B	1.56202000	-0.45189600	-1.48330800
C	0.19314700	-0.62938500	-3.31095600

C	2.50987000	-0.75755400	-4.50307900
H	2.13195400	-0.96799500	-5.50850500
H	3.46256100	-0.22686800	-4.59658000
H	2.70159200	-1.70751000	-3.99517200
C	1.34703500	1.46566000	-4.37984400
H	2.32756000	1.90593800	-4.59028100
H	0.81129900	1.35941700	-5.32940100
H	0.79661100	2.15324200	-3.73488000
C	1.53688800	0.11200700	-3.70169600
C	-1.02225400	0.29452800	-3.20455100
H	-1.32408700	0.66787400	-4.18875600
H	-1.85695300	-0.27407800	-2.78307900
H	-0.82609100	1.14379400	-2.54852800
C	-0.14744200	-1.83431900	-4.18400100
H	-1.06338900	-2.30276700	-3.81161700
H	-0.32002500	-1.52622000	-5.22117600
H	0.64577300	-2.58466100	-4.16800600
C	1.09529000	-0.57287900	1.01706900
C	2.07439600	-0.65635400	-0.00872400
H	1.26048600	-1.05081400	1.97845600
H	3.00631500	0.81460600	-0.07379900
H	0.05085900	-0.50555000	0.73254500
C	3.26089500	-1.57381000	0.11390100
C	4.23801800	-1.59595600	-0.89406700
C	3.37049900	-2.51277300	1.14872200
C	5.29782000	-2.49747100	-0.85324400
H	4.16086000	-0.88500400	-1.70950100
C	4.44659900	-3.39999800	1.20896700
H	2.59229600	-2.57941300	1.90037700
C	5.41895700	-3.39593600	0.20977100
H	6.03559800	-2.49591600	-1.65175100
H	4.50638000	-4.11392200	2.02638500
H	6.24852900	-4.09649600	0.24631000
H	-0.60770200	-5.23987000	0.95614400
H	0.61943600	-5.25413600	2.23483300
H	-0.93776400	-4.43869300	2.49820000
C	-0.62919500	1.55285600	2.00455500
C	-0.07620000	2.17376600	3.14607500
C	0.88359100	3.13711500	2.98951300
C	0.73063100	2.78496500	0.57320100
C	1.32138200	3.46674300	1.68586200
C	1.21388500	3.08677900	-0.72211200
C	2.33682700	4.43177900	1.46439200
C	2.20759000	4.02320500	-0.90556000
H	0.81208000	2.55592300	-1.56720000
C	2.77429200	4.71070800	0.19130000
H	2.56296700	4.22779100	-1.91093200
H	-0.42176400	1.86983200	4.12834600
H	1.32548500	3.63928700	3.84585300
H	2.76443400	4.93849300	2.32551500
H	3.55495200	5.44719900	0.02676700
N	-0.26397600	1.84117200	0.75715000
C	0.34715200	-0.54826700	-0.93795600
H	0.19863400	-1.30046600	-1.72048200
C	1.63522000	-0.20479600	-0.71066400
H	1.85200400	0.48102500	0.10610400
C	2.84442100	-0.68570300	-1.38827400
C	2.81607500	-1.50095300	-2.53659600
C	4.10363300	-0.32509500	-0.87204900
C	3.99386800	-1.94561400	-3.12832300
H	1.85821800	-1.77945600	-2.96512100
C	5.28430900	-0.76895500	-1.46385800
H	4.14271500	0.31190300	0.00868700
C	5.23563800	-1.58501500	-2.59529000
H	3.94607100	-2.57368300	-4.01412500
H	6.24297900	-0.47787600	-1.04238800
H	6.15342000	-1.93274300	-3.06116500

TS-V

0 1

Mn	-1.34257300	0.70677700	-0.64553200
S	-2.66981800	-1.06560400	-1.70068200
O	-3.61833700	2.58860800	-0.38916500
O	-0.66084700	1.72856900	-3.31794900
C	-1.72827400	0.54312300	2.18908600
H	-1.60677100	0.04813500	3.16225000
H	-2.68625700	1.08054600	2.19832800
C	-3.02794100	-1.20472800	1.05158800
H	-2.80382500	-2.25336600	1.26414900
H	-3.70285200	-0.83601500	1.82968800
C	-5.14353800	-0.40407200	-1.99746300
H	-6.08902200	-0.10306200	-2.43520500
C	-2.74128500	1.83136600	-0.48850100
C	-3.70083000	-1.05014500	-0.27542100
C	-0.90005300	1.38845800	-2.22996200
C	-3.99119300	-0.51774900	-2.71033600
H	-3.83242800	-0.36909000	-3.76947100
N	-1.75549000	-0.42161700	1.08689600
C	-4.97162000	-0.68558800	-0.59605900
H	-5.75527200	-0.55600800	0.14279900
B	-0.50348500	-1.26218000	0.95421100
O	-0.67475800	-2.60631600	0.62118800
O	0.50674000	-1.08065100	1.90054900
C	0.42666800	-3.36395900	1.17029300
C	1.05278200	-2.37200900	2.24680800
C	2.57737300	-2.28115900	2.20946400
H	2.91132600	-1.54005100	2.94315500
H	3.03420800	-3.24364000	2.46619300
H	2.93988900	-1.97218200	1.22818400
C	0.58749300	-2.65216300	3.68119400
H	0.97341900	-3.60318700	4.06255700
H	0.94990300	-1.84818700	4.32949400
H	-0.50500800	-2.66884400	3.74496900
C	1.37614700	-3.73496200	0.02786000
H	2.19033500	-4.37609800	0.38194300
H	0.81010100	-4.28664800	-0.72940300
H	1.80673000	-2.85694100	-0.44772100
C	-0.15989300	-4.64774600	1.76031200

TS-VA

0 1

Mn	1.56500800	0.94540700	1.06614300
S	1.32475400	-1.69376500	1.22132100
O	-0.16866400	1.25475100	3.45146700
O	-0.71521500	1.10423400	-0.78206400
C	3.61460100	1.63067000	2.98957500
H	4.64912400	1.70842800	3.35227900
H	2.96627300	1.45566100	3.85878100
C	3.47508400	-0.81803600	2.77489100
H	4.22272200	-1.44753700	2.28801000
H	3.79111000	-0.67125000	3.81314600
C	0.01423000	-2.26631100	3.36418600
H	-0.77030700	-2.58116400	4.04313500
C	0.52139600	1.10678900	2.52715000
C	2.13366800	-1.47865300	2.76867900
C	0.17778700	1.10871900	-0.03530100
C	-0.14105400	-2.21734800	2.01259000
H	-1.00505900	-2.48614200	1.42082500
N	3.44615600	0.49984700	2.06943200
C	1.31189300	-1.82697000	3.79788500
H	1.59775800	-1.72964100	4.83974500
B	4.31106700	0.56093600	0.84037900
O	4.95129400	-0.60220900	0.42353800
O	5.09428800	1.69250900	0.61696400
C	6.14659700	-0.22907100	-0.30536000
C	6.40417700	1.24965400	0.18944400
C	6.91778600	2.20154200	-0.88582100
H	7.04446000	3.20205200	-0.45960600
H	7.88961100	1.86811400	-1.26663600
H	6.21783200	2.27913800	-1.71898100
C	7.30200000	1.32481800	1.43073700
H	8.33986100	1.06008400	1.20462300
H	7.28226100	2.34941800	1.81486900
H	6.93849300	0.65892600	2.22023000
C	5.86116800	-0.33653900	-1.80521100
H	6.76770900	-0.15365200	-2.39165200
H	5.50832800	-1.34956600	-2.02219800
H	5.08605400	0.36294600	-2.11538100
C	7.24396400	-1.22225800	0.07305000

H	6.97052600	-2.21888200	-0.28713100
H	8.19742500	-0.94420300	-0.38977600
H	7.38318400	-1.28034700	1.15486000
C	3.20470400	2.94233200	2.37029900
C	3.80975900	4.12796500	2.83888300
C	3.36677500	5.33928400	2.37472500
C	1.78141000	4.13202100	0.96058000
C	2.32734700	5.37387900	1.41894400
C	0.77622300	4.17250900	-0.03385000
C	1.84047400	6.59587400	0.88777900
C	0.33050500	5.37267000	-0.53724000
H	0.38851300	3.24754500	-0.42223400
C	0.85821600	6.59911800	-0.07261100
H	-0.42554800	5.37224000	-1.31573600
H	4.61384800	4.05751300	3.56369500
H	3.80616900	6.27065900	2.72191500
H	2.26909400	7.52566700	1.25256900
H	0.49438900	7.53620000	-0.48316700
N	2.23429900	2.92617500	1.45706300
C	2.66896400	0.54890600	-0.74963900
H	2.66404500	-0.53173100	-0.93480500
C	2.74482600	1.21842800	-1.92716800
H	2.73712100	0.63416700	-2.85558900
C	2.81017500	2.66565800	-2.19316200
C	2.13877200	3.18377500	-3.31623100
C	3.57332900	3.55219400	-1.41417200
C	2.19215300	4.54025900	-3.62658100
H	1.55698100	2.50827400	-3.93923600
C	3.65214700	4.90423200	-1.74369800
H	4.11139100	3.16260500	-0.56121400
C	2.95400900	5.40917700	-2.84048000
H	1.64777400	4.91955200	-4.48772500
H	4.24965100	5.57013900	-1.12681900
H	3.00591300	6.46660800	-3.08523800

TS-VB

0 1

Mn	1.53501200	1.13293100	0.89717000
S	0.93543700	-1.37798200	0.70405700
O	-0.22809000	1.35731200	3.26035300
O	-0.67508000	1.96073000	-0.86556100
C	3.45288000	1.27379300	3.03698400
H	4.44807900	1.18264900	3.49623500
H	2.70952100	0.97341400	3.78742000
C	3.23180800	-1.04837800	2.24366900
H	3.85373600	-1.61005800	1.54511400
H	3.65421200	-1.19850600	3.24415000
C	-0.37605100	-2.08404200	2.81074400
H	-1.17485500	-2.39329700	3.47566600
C	0.46285900	1.23263700	2.33363100
C	1.81800400	-1.53375300	2.22055100
C	0.20369400	1.67303800	-0.15885200
C	-0.56776600	-1.78790100	1.49619600
H	-1.48128500	-1.83493100	0.91956100
N	3.30985400	0.39451300	1.86947600
C	0.98911100	-1.91663300	3.23118100
H	1.32295600	-2.03604800	4.25659300
B	4.28057900	0.69889500	0.74701900
O	5.06680600	-0.34889800	0.26057600
O	5.01162700	1.88633100	0.81488900
C	6.29708000	0.19976300	-0.26855100
C	6.37791000	1.60902600	0.44761800
C	6.87847400	2.74562900	-0.43923300
H	6.85911000	3.68279400	0.12647400
H	7.90850800	2.56496500	-0.76670900
H	6.24483000	2.86799400	-1.31910300
C	7.17439600	1.57962300	1.75844900
H	8.24550900	1.42934600	1.58866100
H	7.03554900	2.53621600	2.27197000
H	6.81314400	0.78498400	2.41920700
C	6.18692900	0.27775700	-1.79437400
H	7.12343000	0.63343000	-2.23671800
H	5.97879700	-0.72177300	-2.18645900
H	5.37317000	0.93212500	-2.10426500
C	7.42253000	-0.76496400	0.10276900

H	7.26522000	-1.71892400	-0.41017500
H	8.39491600	-0.36861500	-0.21027500
H	7.45254100	-0.95995300	1.17697700
C	3.21611500	2.71442100	2.65630100
C	3.81432300	3.73947300	3.42106800
C	3.58700500	5.04839500	3.08556000
C	2.22231200	4.25522400	1.22079500
C	2.78539200	5.34522900	1.95851500
C	1.45802200	4.54850000	0.06593600
C	2.53859300	6.67759900	1.54014100
C	1.24153500	5.85349100	-0.31874400
H	1.07240500	3.73278600	-0.52341200
C	1.77606600	6.93136800	0.42421800
H	0.65547100	6.05424600	-1.21059800
H	4.44789000	3.47028600	4.25971800
H	4.02387000	5.86101800	3.65981100
H	2.96941200	7.49077800	2.11831900
H	1.59061100	7.95306800	0.10691300
N	2.42767100	2.95022000	1.61078100
C	2.82653800	1.03763700	-0.96885500
C	3.24566900	2.18428600	-1.53773600
H	3.53665500	3.04451700	-0.94323200
C	2.43079400	-0.06550100	-1.88617800
C	2.99027500	-1.35492400	-1.81469300
C	1.42186800	0.15152600	-2.84380600
C	2.56391000	-2.37436300	-2.66524400
H	3.77343600	-1.54631000	-1.09201400
C	0.98516100	-0.87173900	-3.68453400
H	0.96112700	1.13226200	-2.90359100
C	1.55444000	-2.14382100	-3.60139800
H	3.02095900	-3.35838400	-2.59086700
H	0.19734500	-0.67295100	-4.40713200
H	1.21623000	-2.94262300	-4.25586900
H	3.36088300	2.29589800	-2.62084200

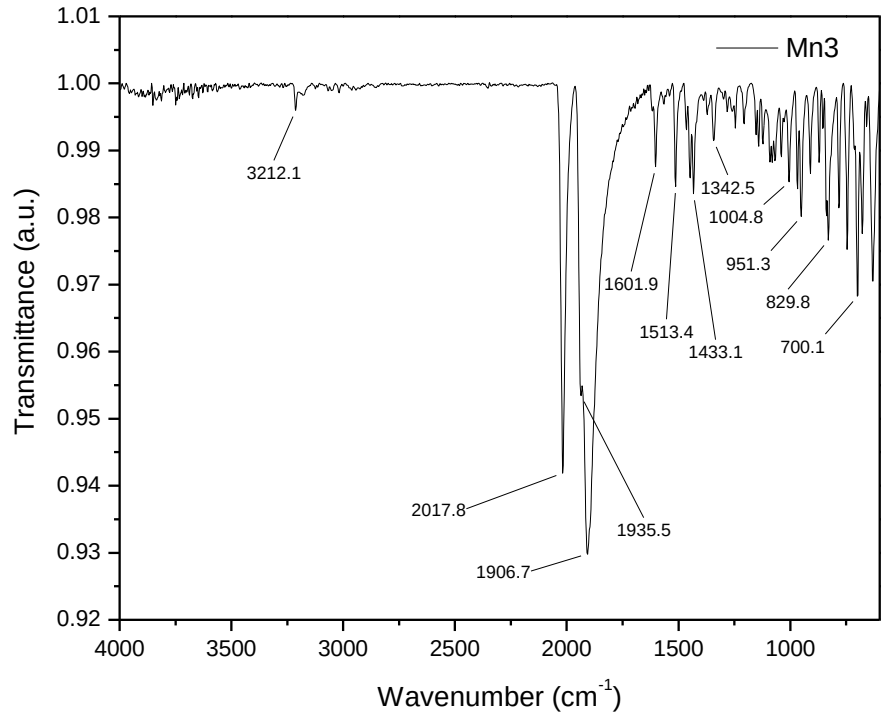
TS-VI

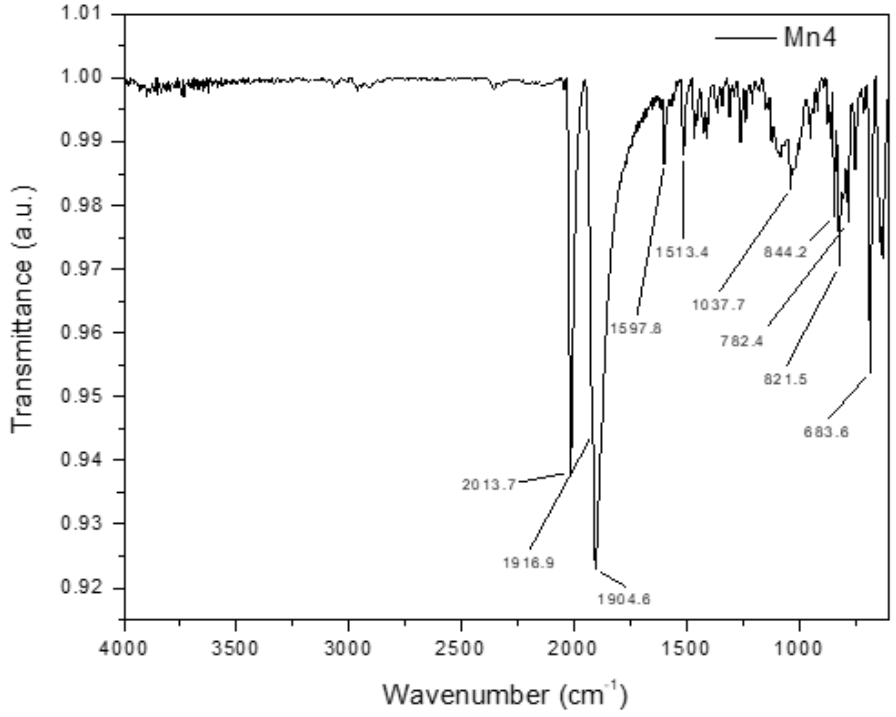
0 1

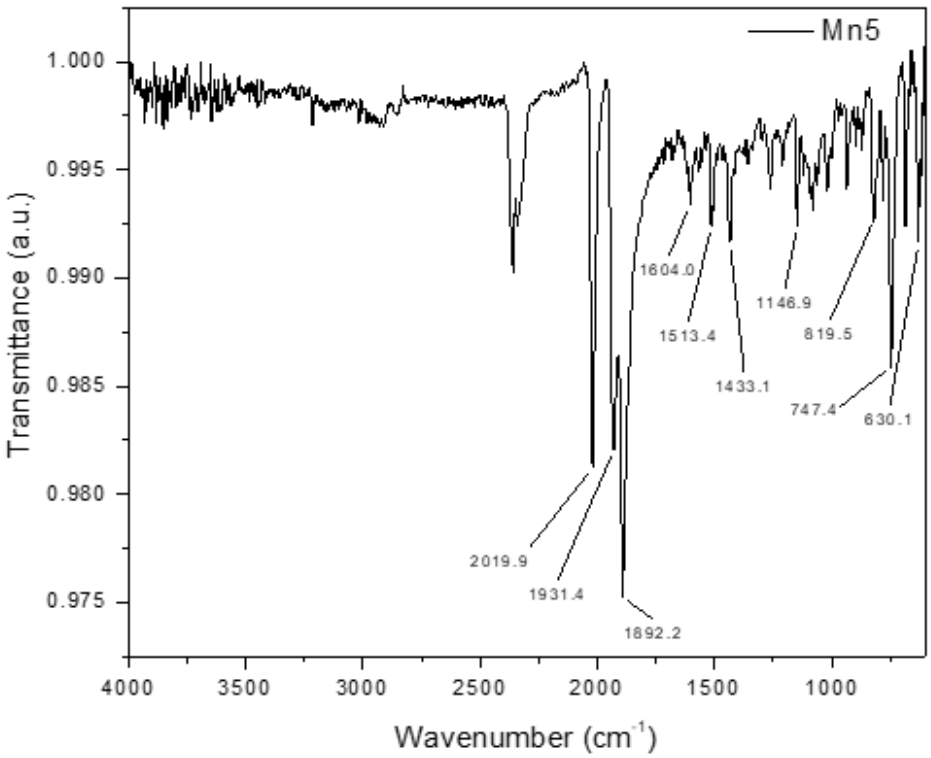
Mn	1.59166500	1.29090000	1.13195200
S	6.33958100	-1.22686100	3.53887100
O	0.32069500	0.99722800	3.80193000
O	-1.07858500	1.84902700	0.05585000
C	3.74238600	1.86555000	3.15207500
H	4.69355100	1.96077200	3.68858100
H	2.98329300	1.61153300	3.89905900
C	3.66208100	-0.57830600	2.76825600
H	2.66351200	-0.65933200	3.20461900
H	3.72593200	-1.29512700	1.94969100
C	5.57256400	-1.13803300	5.99791600
H	5.56983900	-1.17692900	7.08154000
C	0.87057400	1.13110900	2.78544700
C	4.65697200	-0.86292900	3.85627900
C	-0.02522900	1.64537900	0.50015200
C	6.68552400	-1.35761500	5.23497000
H	7.68793300	-1.59304200	5.56673900
N	3.79268200	0.77461200	2.15787200
C	4.41742200	-0.85452300	5.20671800
H	3.43316600	-0.65539400	5.61879300
B	4.91890800	0.89231800	1.24285800
O	5.55553500	-0.17897600	0.68503900
O	5.52150400	2.09821800	0.98738000
C	6.59470800	0.34474600	-0.19217600
C	6.80195700	1.80919700	0.35556600
C	7.06533400	2.86009400	-0.71514700
H	7.13234300	3.84768000	-0.24730400
H	8.01576300	2.65951000	-1.22201600
H	6.27175400	2.89027900	-1.46236000
C	7.85186000	1.90653100	1.46635900
H	8.86354800	1.75278300	1.07804900
H	7.80104500	2.90544900	1.91055400
H	7.66361500	1.17274500	2.25553000
C	6.04635900	0.29889200	-1.61845700
H	6.78073100	0.67306600	-2.33855300
H	5.81642600	-0.73876500	-1.86772100
H	5.12641200	0.87959900	-1.71116100
C	7.81623600	-0.55924200	-0.06792200

H	7.56387600	-1.56069700	-0.42943800
H	8.64208300	-0.17544500	-0.67710400
H	8.15249000	-0.64748300	0.96661200
C	3.39611900	3.19394500	2.52426900
C	4.11363000	4.33742100	2.94414700
C	3.83156100	5.55639200	2.38848500
C	2.14171900	4.45069400	1.01380300
C	2.83757400	5.64502700	1.38757200
C	1.16605600	4.54181700	-0.00892600
C	2.53440600	6.87158900	0.74222900
C	0.89931800	5.74497700	-0.62296200
H	0.65757900	3.64874000	-0.32730900
C	1.58392500	6.92398500	-0.24896000
H	0.15699400	5.78274400	-1.41420400
H	4.89468900	4.22097000	3.68721300
H	4.37186500	6.45087700	2.68700300
H	3.07568200	7.76371700	1.04602500
H	1.36027400	7.86233500	-0.74734400
N	2.42974500	3.23804800	1.60840500
C	2.18386400	1.51900100	-0.87864600
H	1.49849000	1.25879800	-1.68886700
C	3.16286100	2.37950000	-1.23688400
H	3.85063600	2.75452700	-0.48398400
C	3.36294300	3.00536700	-2.55371600
C	2.80712500	2.51042100	-3.74782400
C	4.13599300	4.17952500	-2.62969600
C	3.02061400	3.15893400	-4.96063300
H	2.20474200	1.60898700	-3.71969900
C	4.34827600	4.83205300	-3.84271500
H	4.55286000	4.58934500	-1.71289400
C	3.79404100	4.32260900	-5.01800500
H	2.58408500	2.75323200	-5.86988100
H	4.94416000	5.74088700	-3.86980700
H	3.95979100	4.82486100	-5.96700700
O	0.81846500	-1.08087200	-1.07157500
B	1.75752000	-0.68459500	-0.14491800
O	2.92839600	-1.41610600	-0.22100000
C	2.65532100	-2.54541900	-1.09335100
C	1.48039000	-2.00058900	-1.98060900
C	2.23421100	-3.70718100	-0.18588600
H	2.06120200	-4.62466200	-0.75739200
H	3.03172300	-3.89721500	0.53904300
H	1.32134000	-3.46322200	0.36600100
C	3.92543400	-2.90803500	-1.85074400
H	4.71062800	-3.17610500	-1.13691300
H	3.74892000	-3.76699700	-2.50794200
H	4.28498300	-2.07542400	-2.45564700
C	1.97227900	-1.19671600	-3.18721600
H	2.39355000	-1.85097200	-3.95748300
H	1.12462100	-0.65645300	-3.61989800
H	2.72930300	-0.46599200	-2.89309500
C	0.46497300	-3.04884000	-2.42002400
H	-0.31933700	-2.57243900	-3.01634700
H	0.94392700	-3.81741700	-3.03730100
H	-0.00875700	-3.53091600	-1.56236900
H	1.30658700	-0.43227600	1.00924000

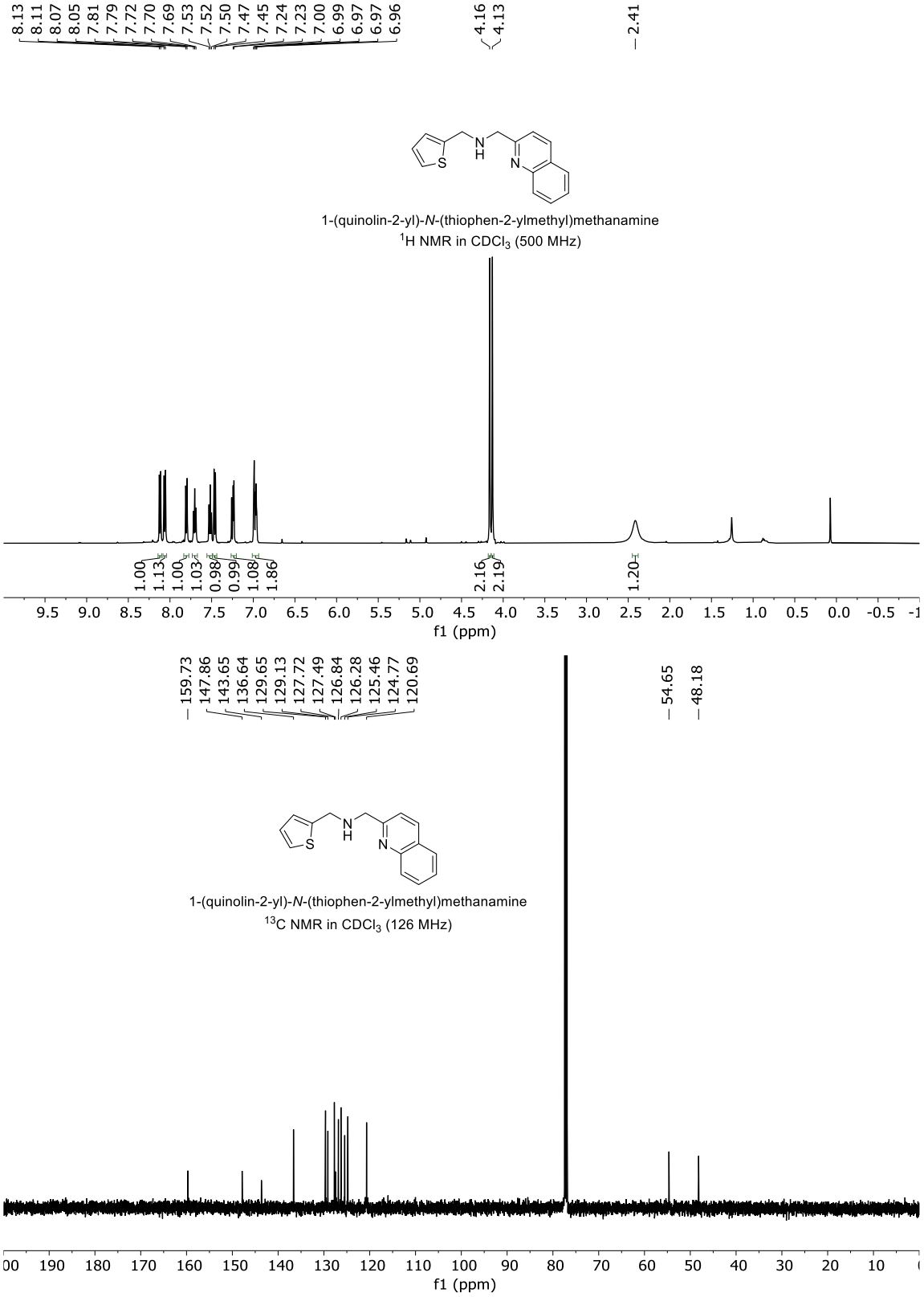
11. IR spectra of manganese complexes:

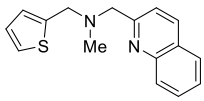





Mn5
Transmittance (a.u.)
1.000
0.995
0.990
0.985
0.980
0.975
4000
3500
3000
2500
2000
1500
1000
Wavenumber (cm-1)
2019.9
1931.4
1892.2
1604.0
1513.4
1433.1
1146.9
819.5
747.4
630.1

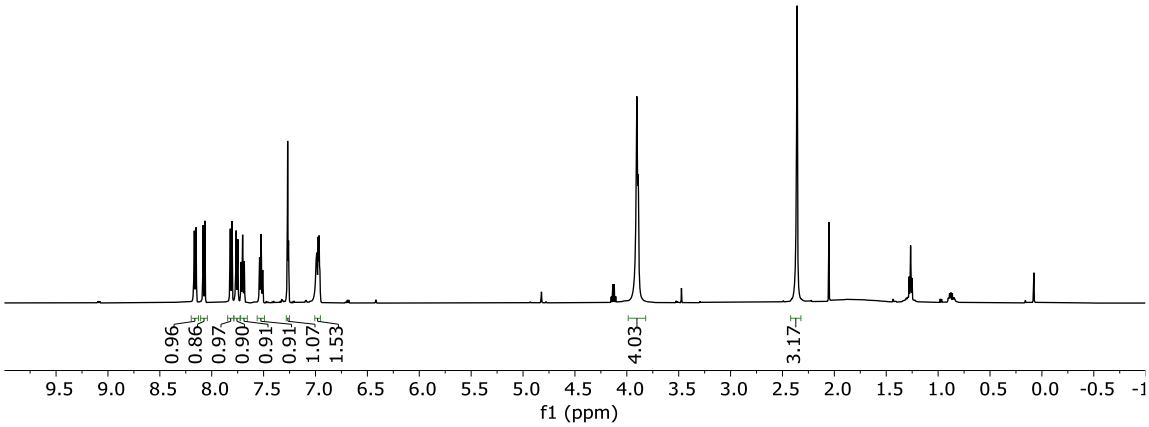
12. ^{1}H, ^{13}C, and ^{11}B spectra of synthesized compounds.

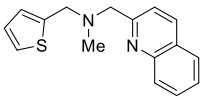




N-methyl-1-(quinolin-2-yl)-*N*-(thiophen-2-ylmethyl)methanamine

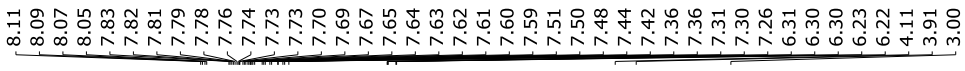
^{1}H NMR in $CDCl_3$ (500 MHz)

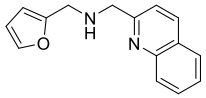




N-methyl-1-(quinolin-2-yl)-*N*-(thiophen-2-ylmethyl)methanamine

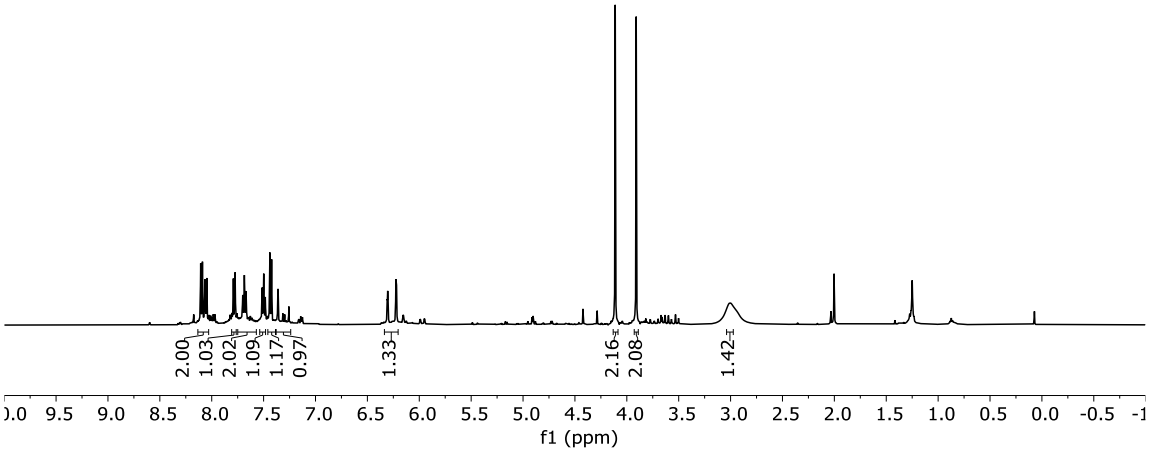
^{13}C NMR in $CDCl_3$ (126 MHz)

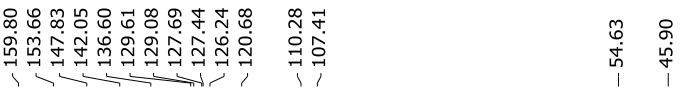


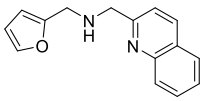


1-(furan-2-yl)-*N*-(quinolin-2-ylmethyl)methanamine

^{1}H NMR in $CDCl_3$ (500 MHz)

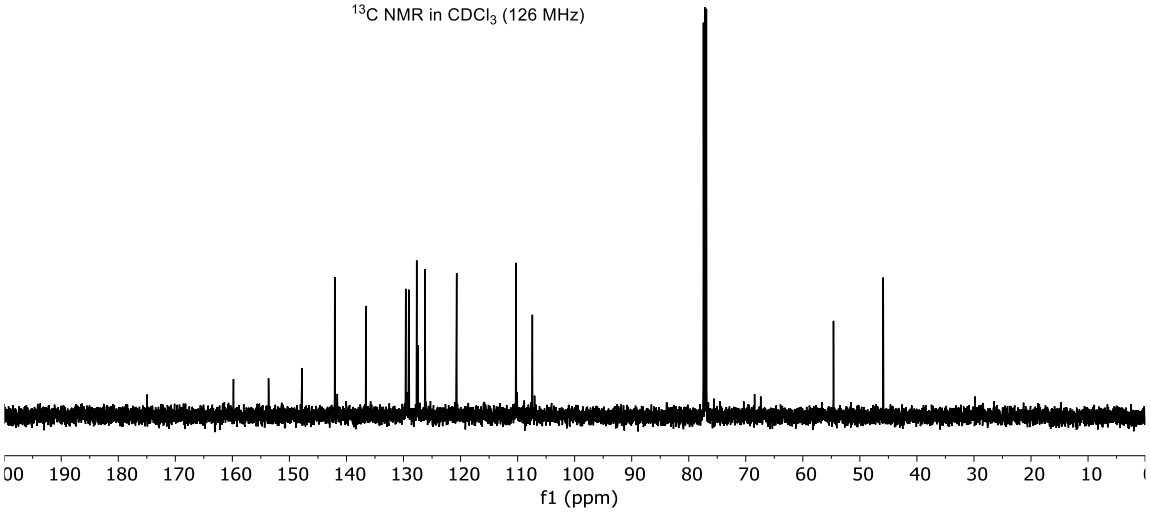


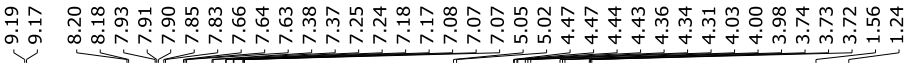


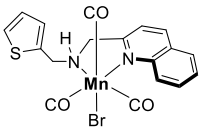


1-(furan-2-yl)-*N*-(quinolin-2-ylmethyl)methanamine

^{13}C NMR in $CDCl_3$ (126 MHz)

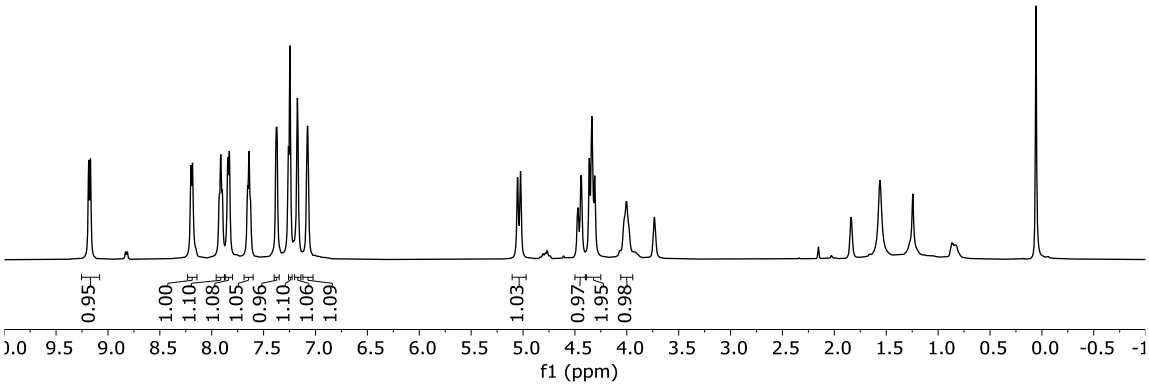


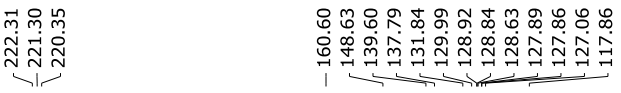


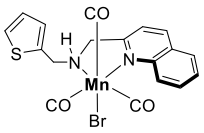


Mn3

^{1}H NMR in $CDCl_3$ (500 MHz)

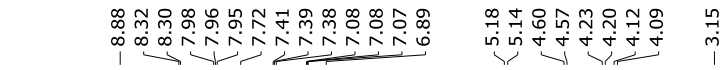


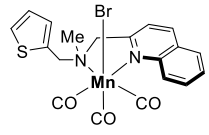




Mn3

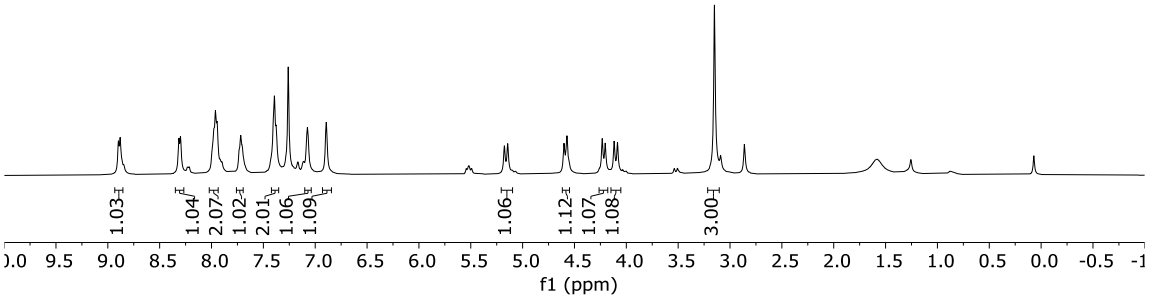
^{13}C NMR in $CDCl_3$ (126 MHz)

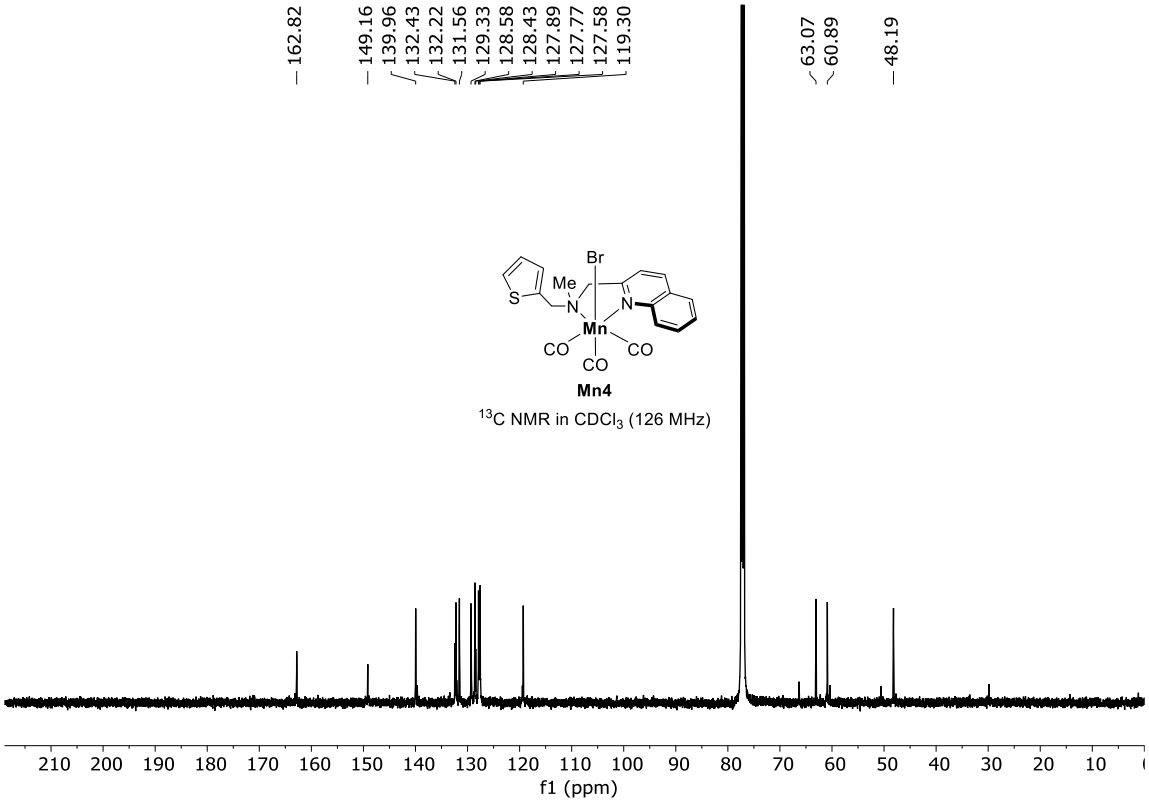




Mn4

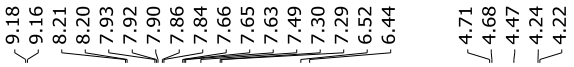
^{1}H NMR in $CDCl_3$ (500 MHz)

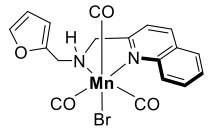




Mn4

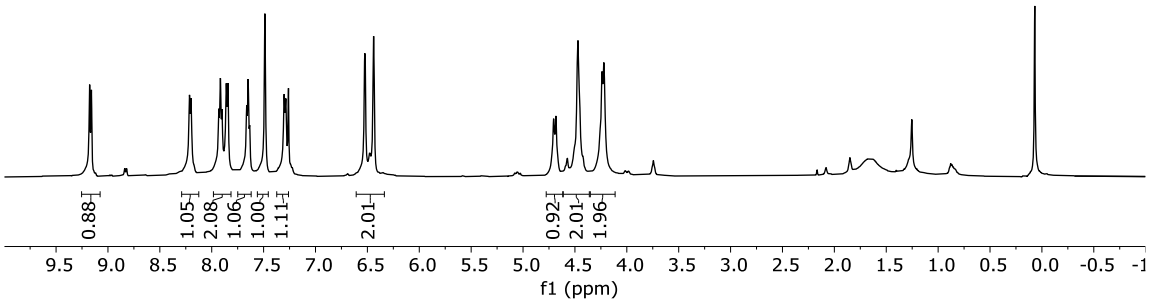
^{13}C NMR in $CDCl_3$ (126 MHz)

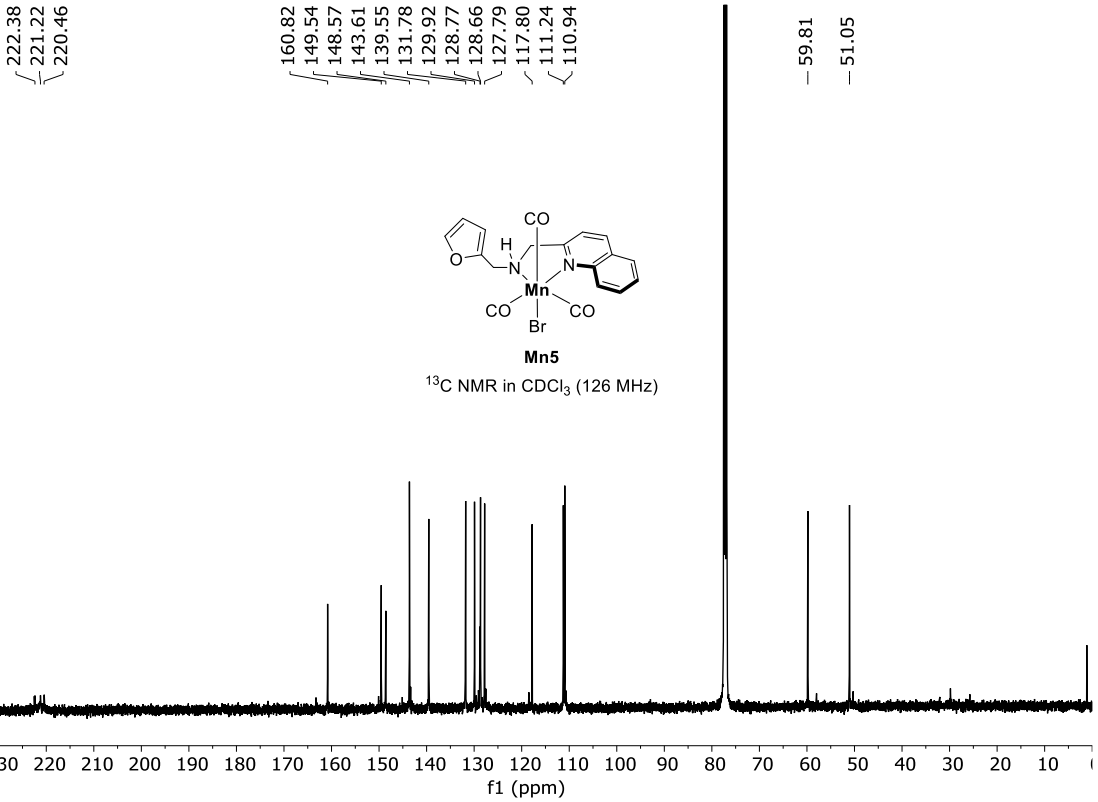




Mn5

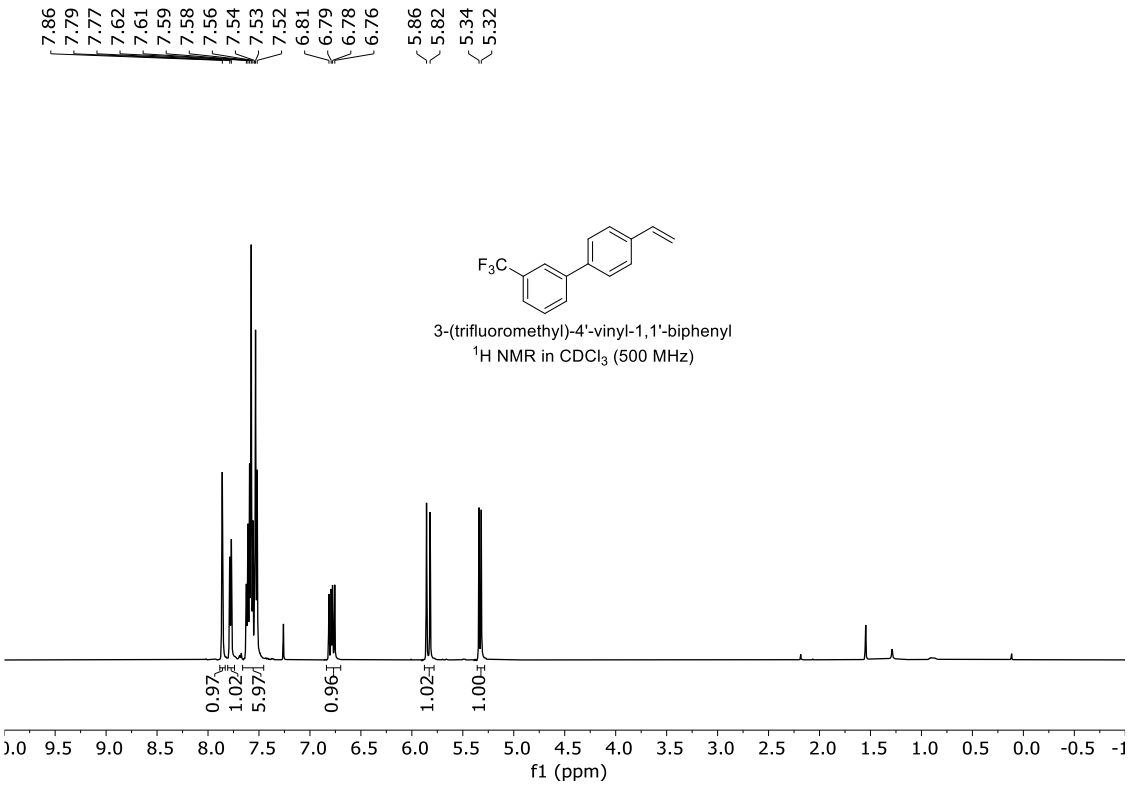
^{1}H NMR in $CDCl_3$ (500 MHz)

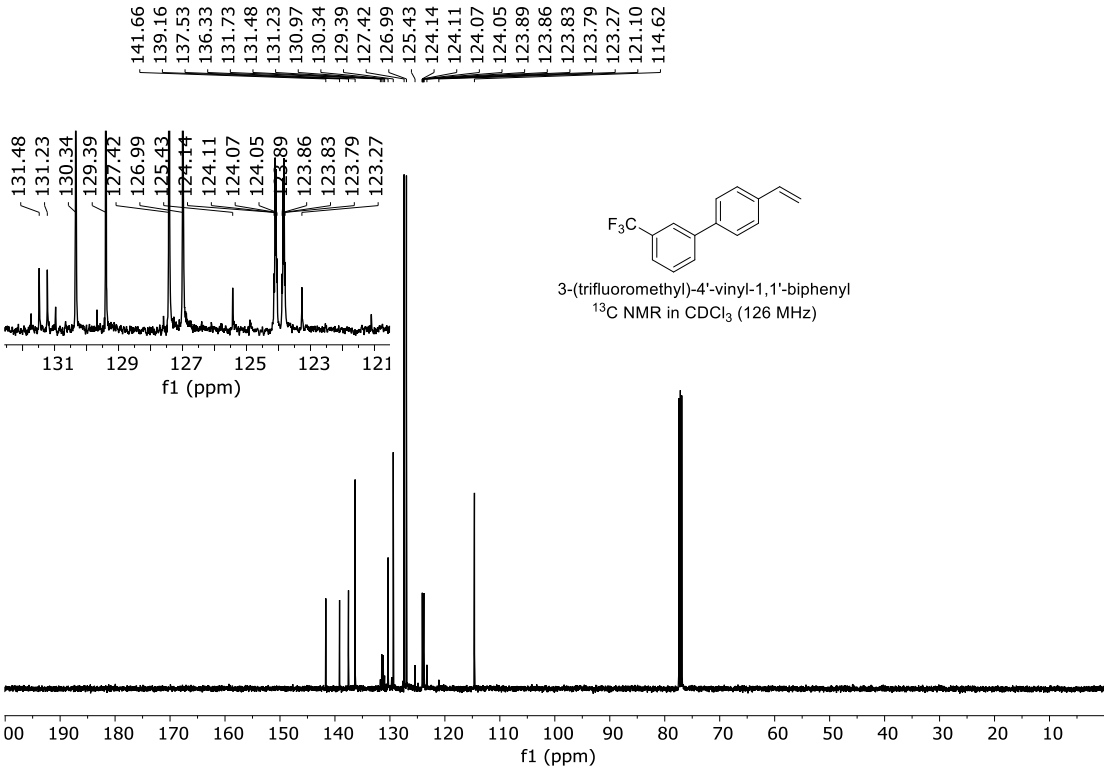


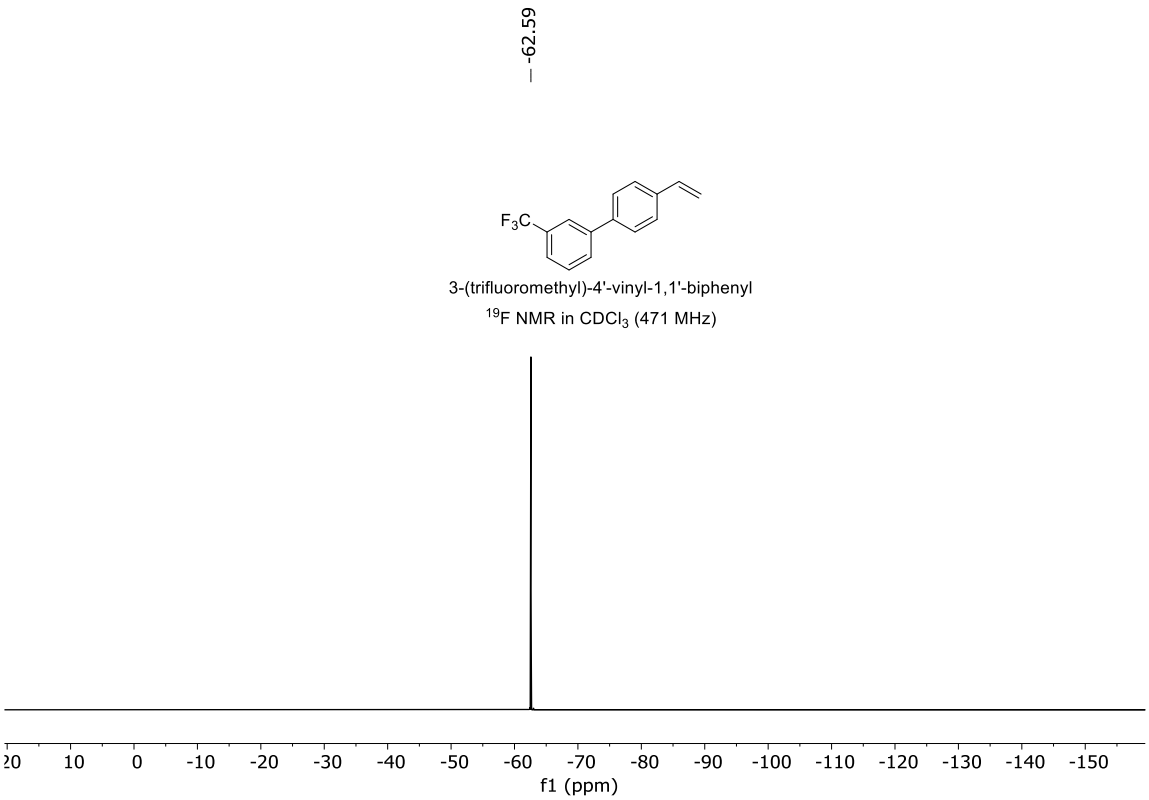


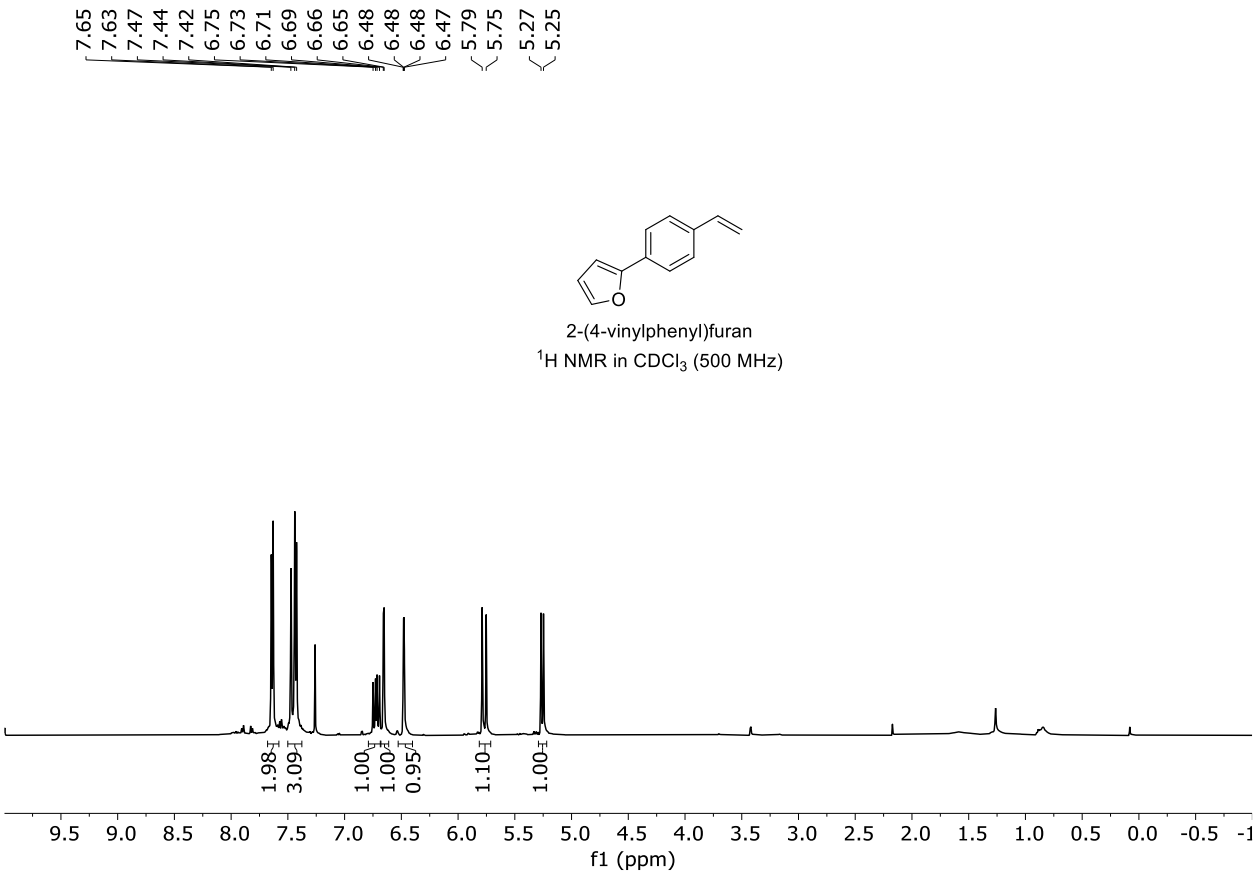
Mn5

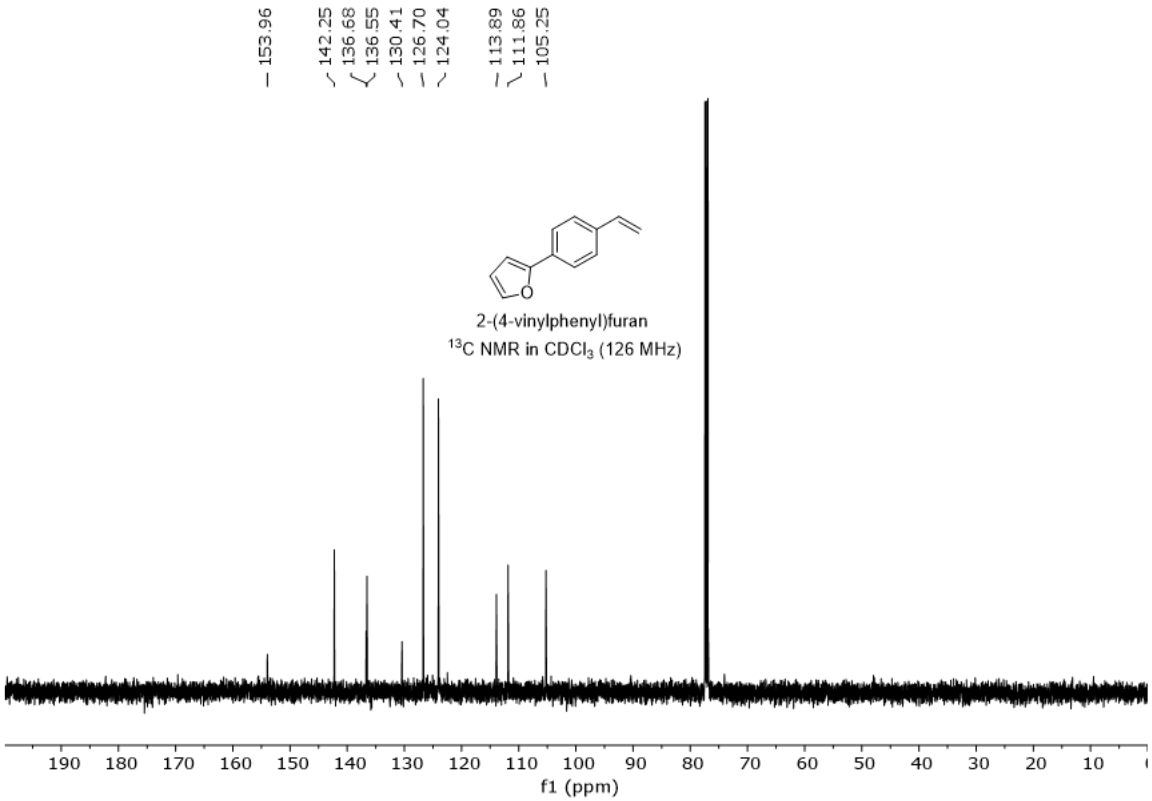
^{13}C NMR in $CDCl_3$ (126 MHz)

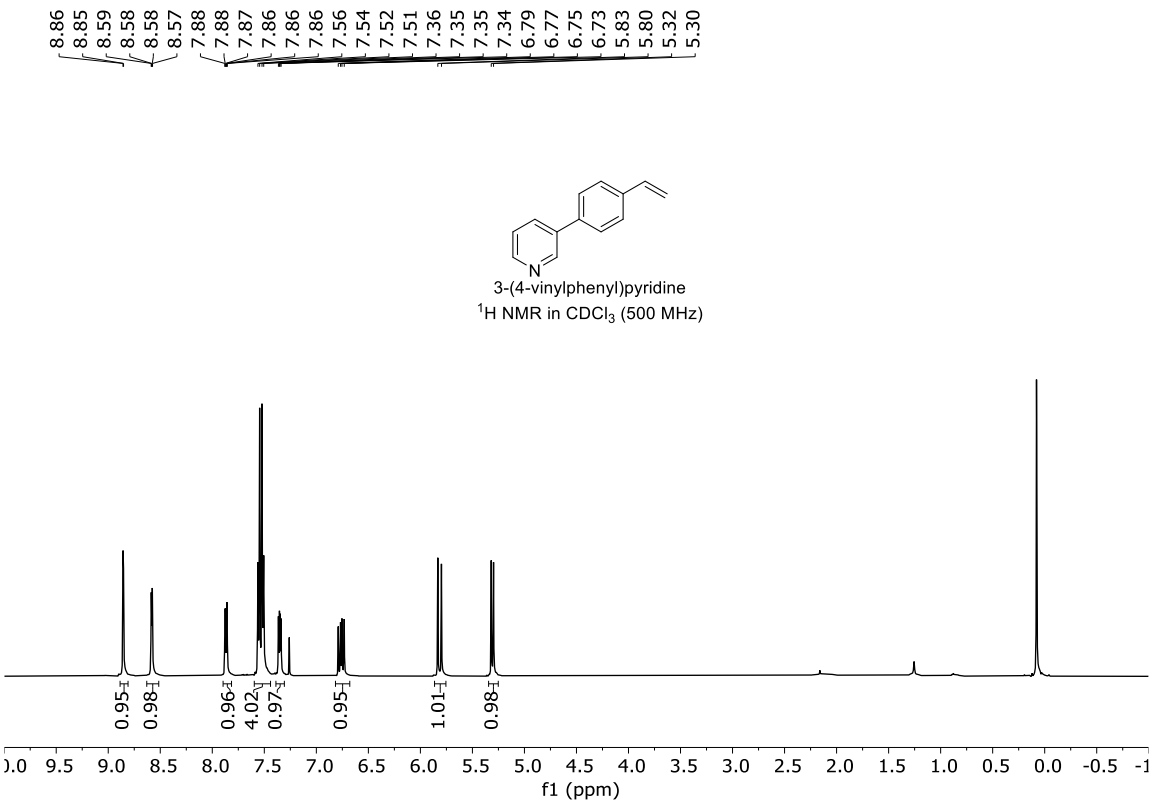

7.86
7.79
7.77
7.62
7.61
7.59
7.58
7.56
7.54
7.53
7.52
6.81
6.79
6.78
6.76
5.86
5.82
5.34
5.32
F3C
3-(trifluoromethyl)-4'-vinyl-1,1'-biphenyl
1H NMR in CDCl3 (500 MHz)
0.97
1.02
5.97
0.96
1.02
1.00
f1 (ppm)

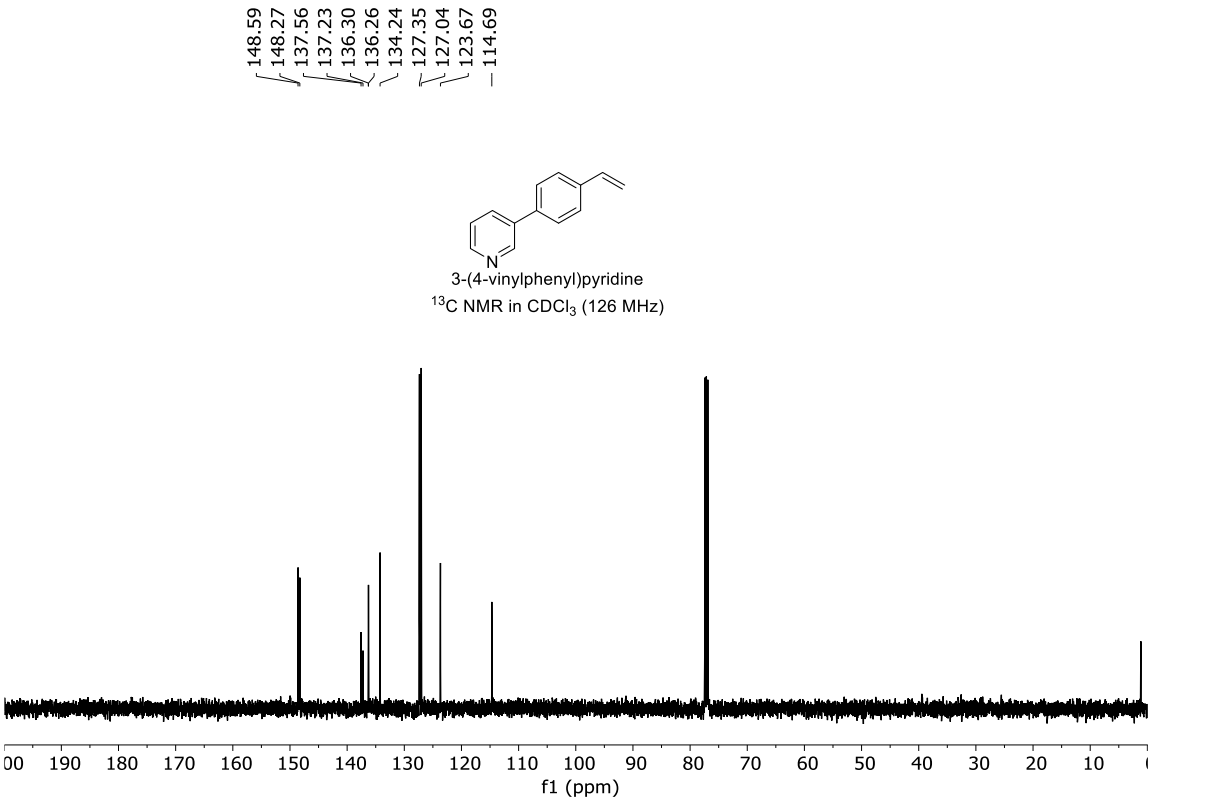

141.66
139.16
137.53
136.33
131.73
131.48
131.23
130.97
130.34
129.39
127.42
126.99
125.43
124.14
124.11
124.07
124.05
123.89
123.86
123.83
123.79
123.27
121.10
114.62
131.48
131.23
130.34
129.39
127.42
126.99
125.43
124.14
124.11
124.07
124.05
123.89
123.86
123.83
123.79
123.27
131
129
127
125
123
f1 (ppm)
F3C
3-(trifluoromethyl)-4'-vinyl-1,1'-biphenyl
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

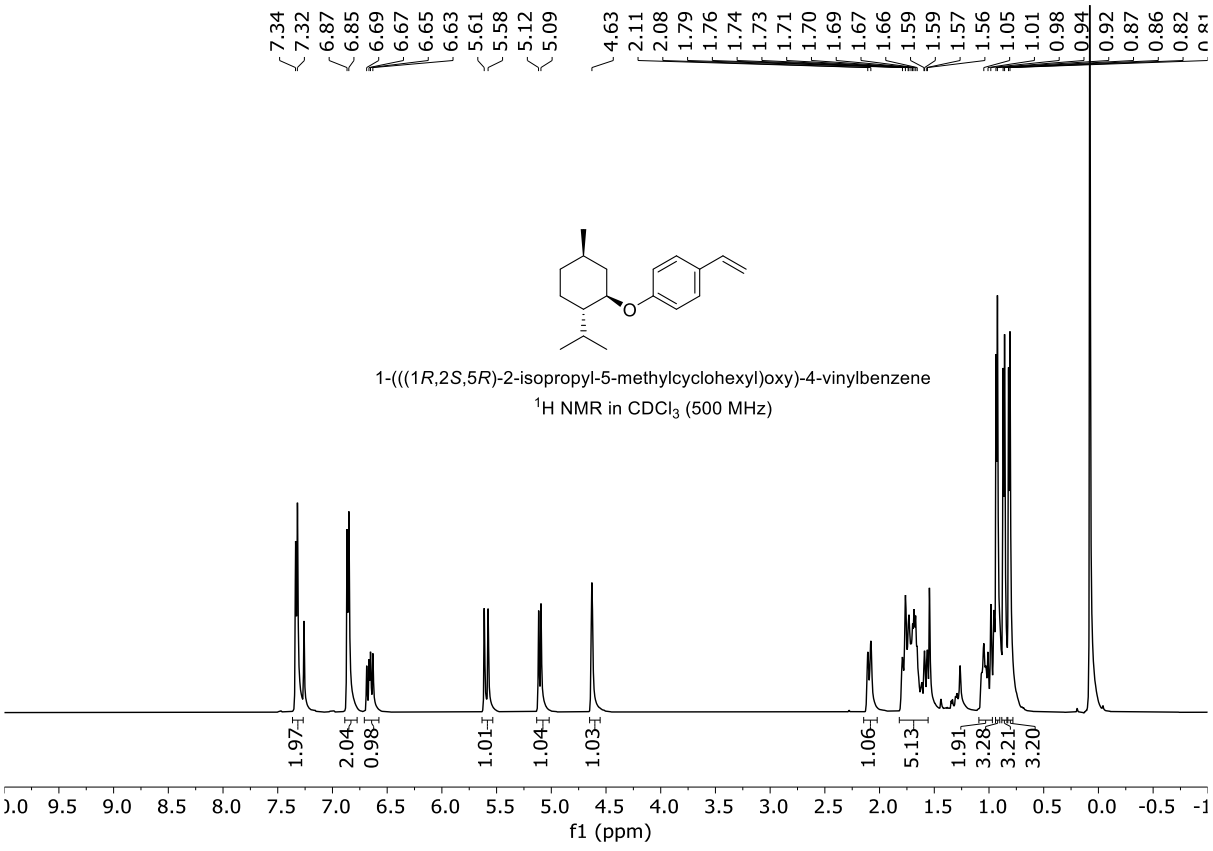

-62.59
F3C
3-(trifluoromethyl)-4'-vinyl-1,1'-biphenyl
19F NMR in CDCl3 (471 MHz)
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)

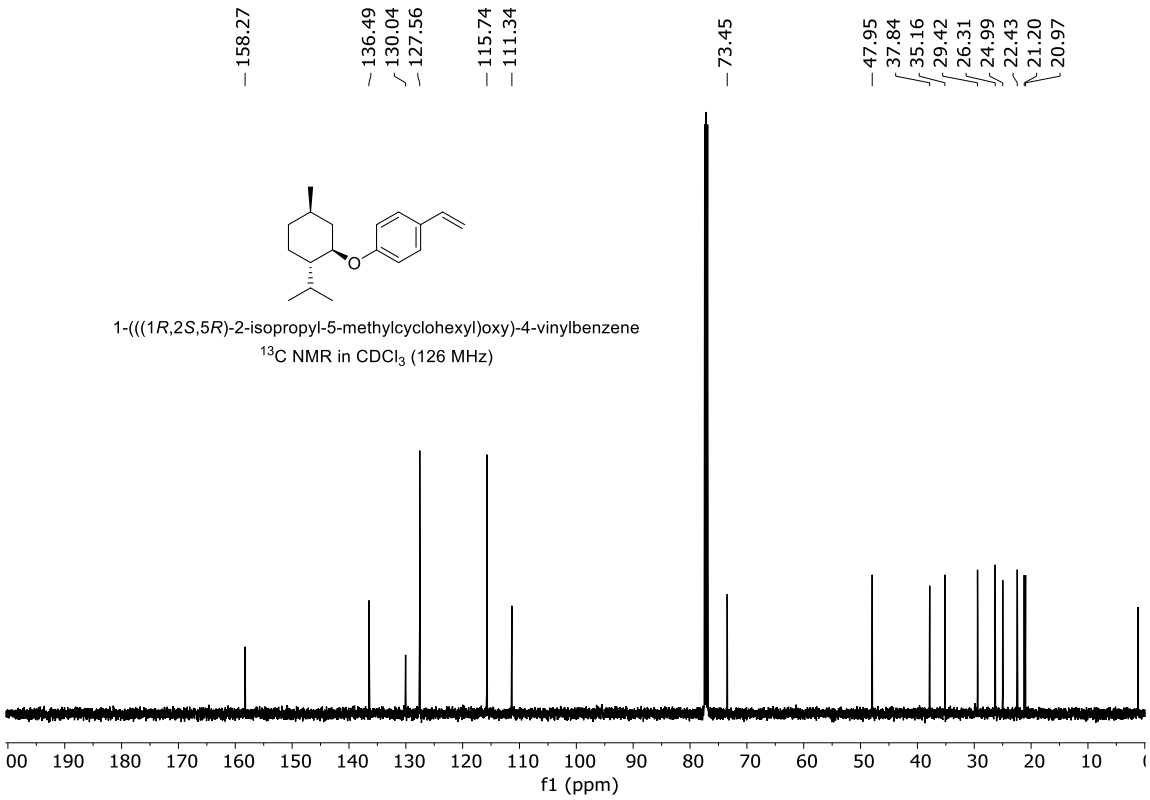

7.65
7.63
7.47
7.44
7.42
6.75
6.73
6.71
6.69
6.66
6.65
6.48
6.48
6.48
6.47
5.79
5.75
5.27
5.25
O
2-(4-vinylphenyl)furan
1H NMR in CDCl3 (500 MHz)
1.98
3.09
1.00
1.00
0.95
1.10
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


153.96
142.25
136.68
136.55
130.41
126.70
124.04
113.89
111.86
105.25
2-(4-vinylphenyl)furan
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


8.86
8.85
8.59
8.58
8.58
8.57
7.88
7.88
7.87
7.86
7.86
7.86
7.56
7.54
7.52
7.51
7.36
7.35
7.35
7.34
6.79
6.77
6.75
6.73
5.83
5.80
5.32
5.30
3-(4-vinylphenyl)pyridine
1H NMR in CDCl3 (500 MHz)
0.95
0.98
0.96
4.02
0.97
0.95
1.01
0.98
f1 (ppm)

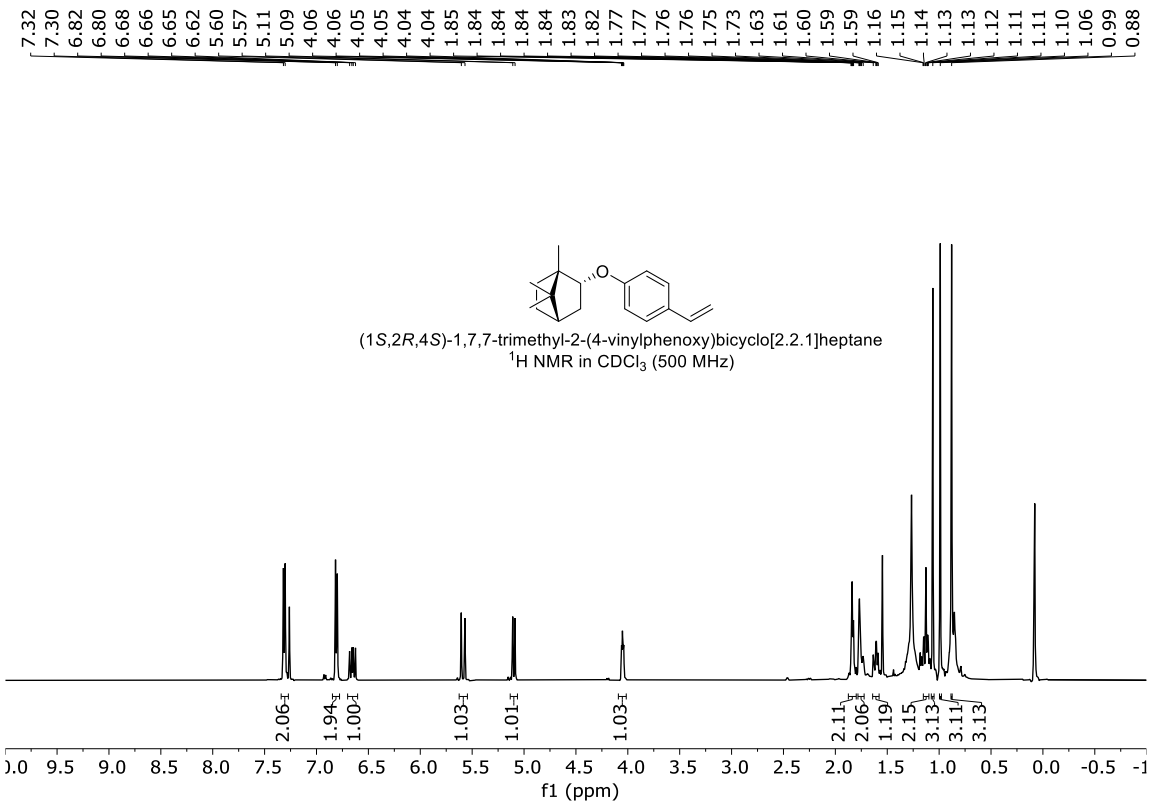

148.59
148.27
137.56
137.23
136.30
136.26
134.24
127.35
127.04
123.67
114.69
N
3-(4-vinylphenyl)pyridine
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


7.34
7.32
6.87
6.85
6.69
6.67
6.65
6.63
5.61
5.58
5.12
5.09
4.63
2.11
2.08
1.79
1.76
1.74
1.73
1.71
1.70
1.69
1.67
1.66
1.59
1.59
1.57
1.56
1.05
1.01
0.98
0.94
0.92
0.87
0.86
0.82
O
1-(((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)-4-vinylbenzene
1H NMR in CDCl3 (500 MHz)
1.97
2.04
0.98
1.01
1.04
1.03
1.06
5.13
1.91
3.28
3.21
3.20
f1 (ppm)



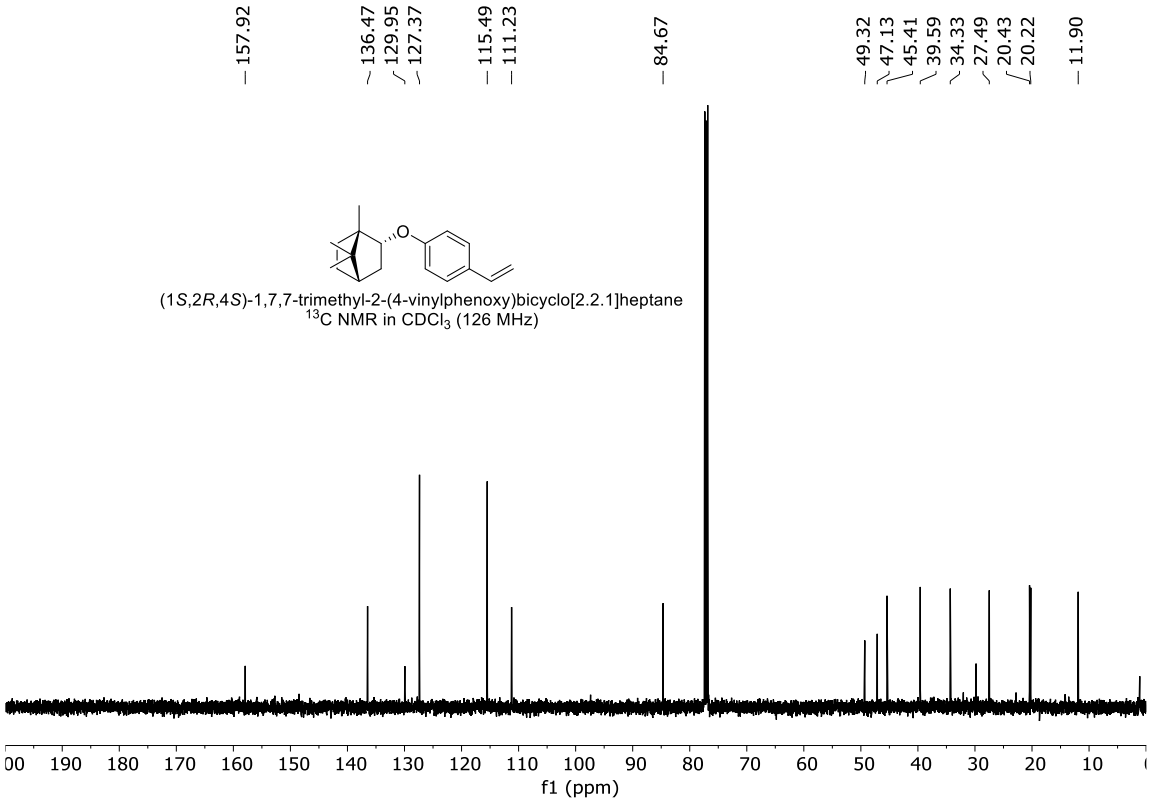
1-(((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl)oxy)-4-vinylbenzene

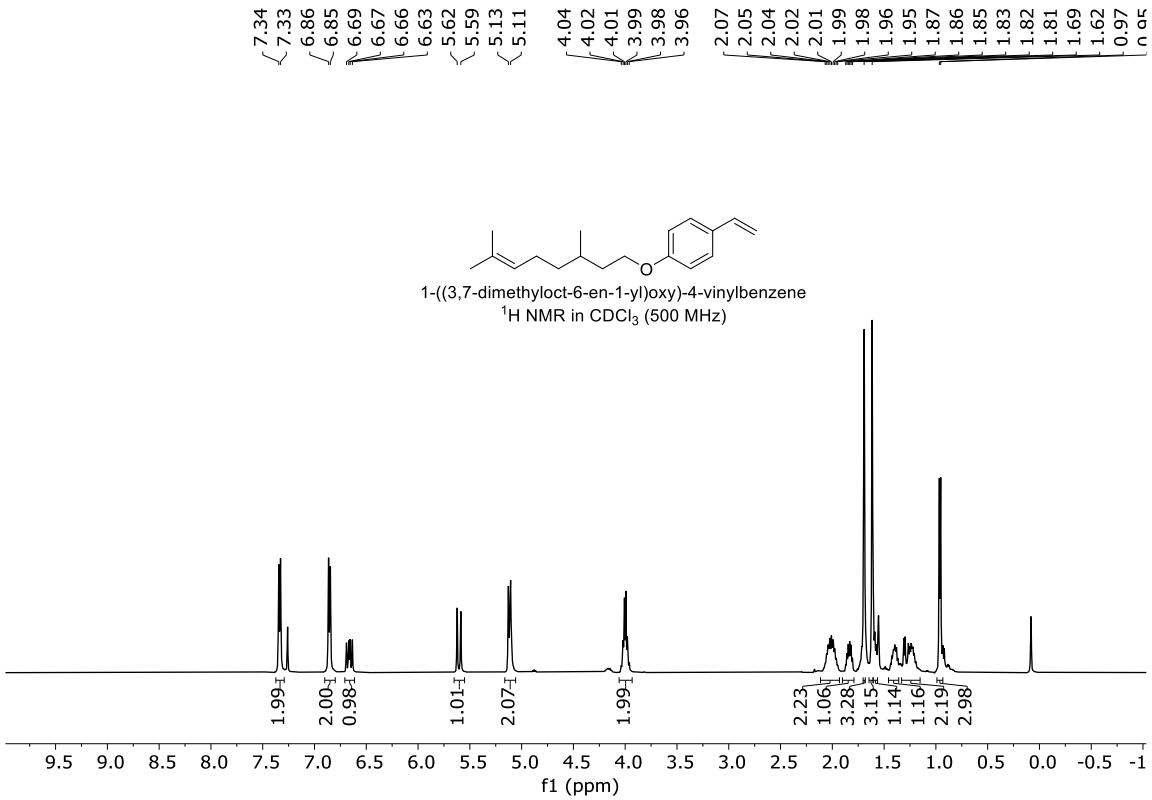
^{13}C NMR in $CDCl_3$ (126 MHz)

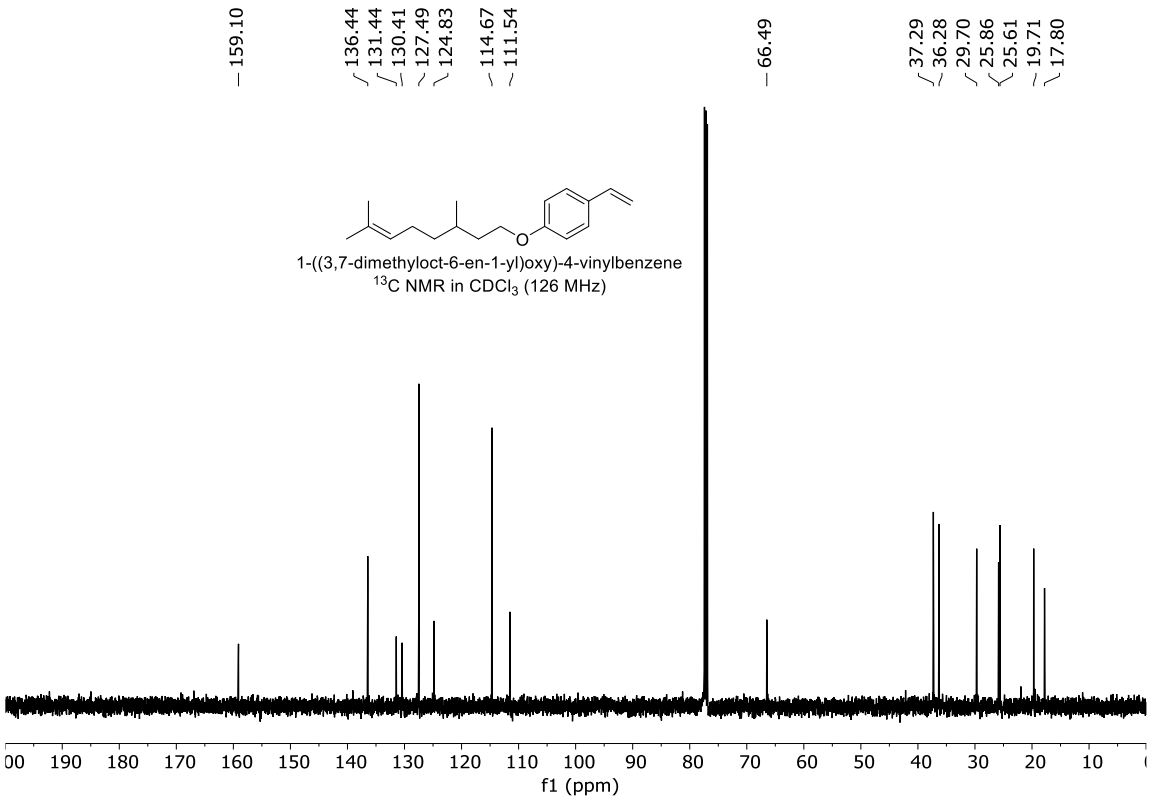


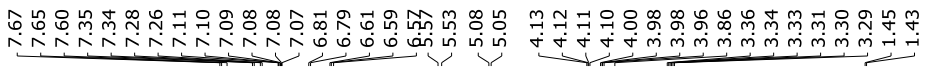
(1*S*,2*R*,4*S*)-1,7,7-trimethyl-2-(4-vinylphenoxy)bicyclo[2.2.1]heptane

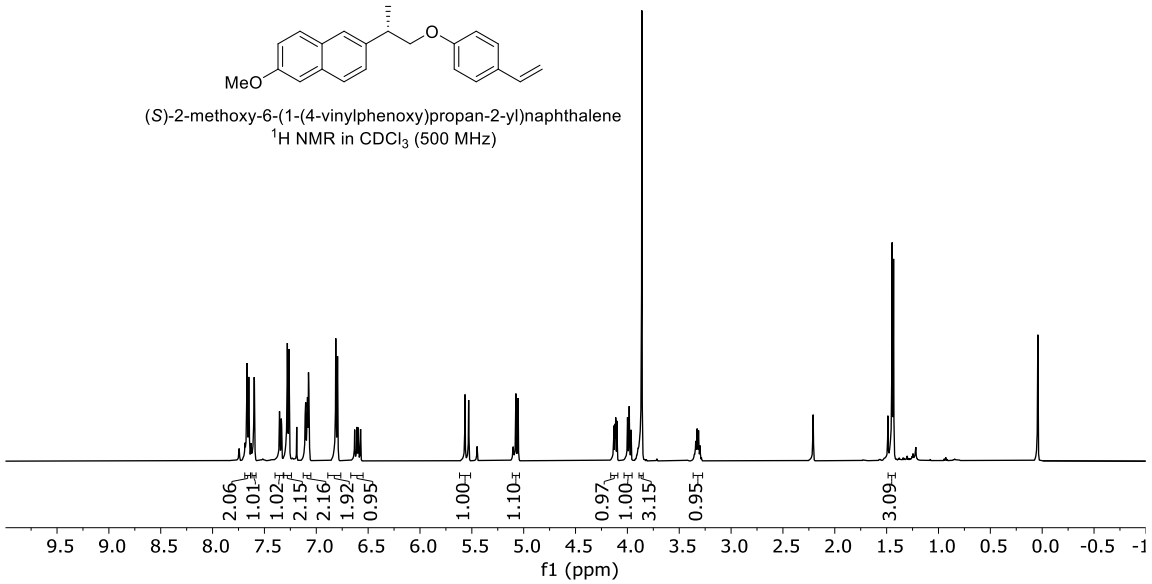
^{1}H NMR in $CDCl_3$ (500 MHz)

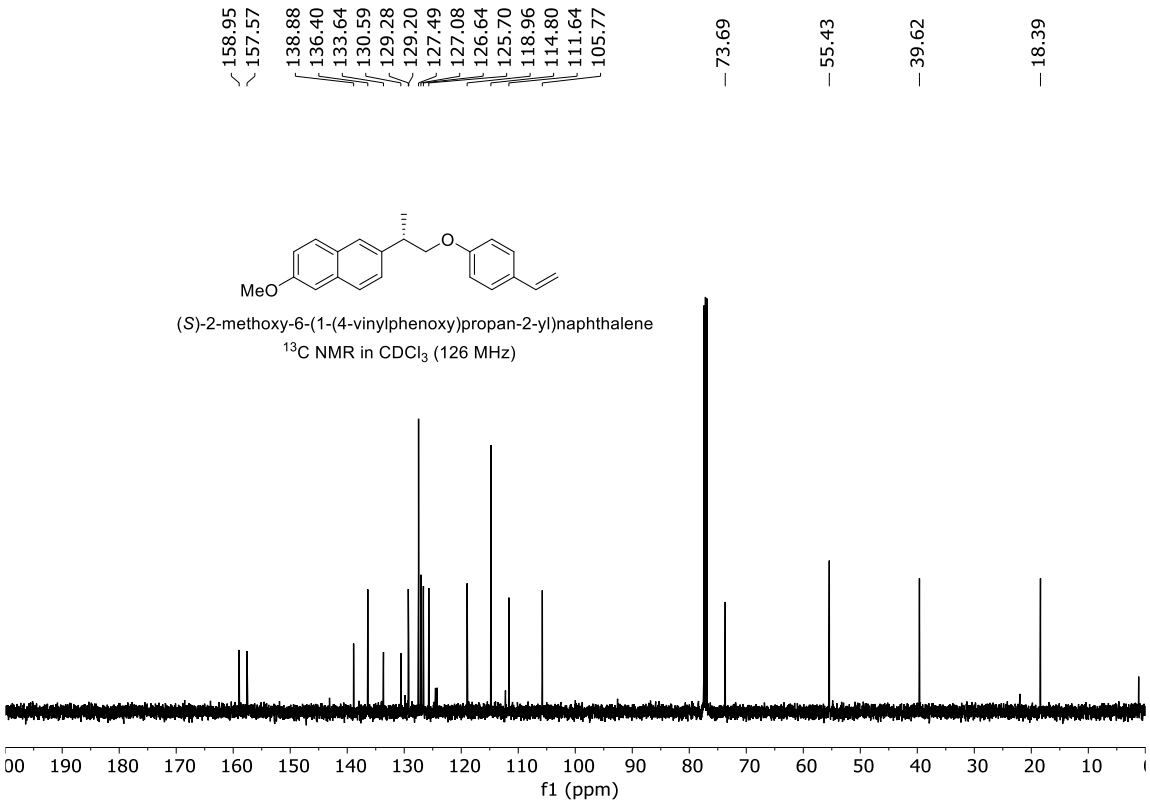

157.92
136.47
129.95
127.37
115.49
111.23
84.67
49.32
47.13
45.41
39.59
34.33
27.49
20.43
20.22
11.90
O
(1S,2R,4S)-1,7,7-trimethyl-2-(4-vinylphenoxy)bicyclo[2.2.1]heptane
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

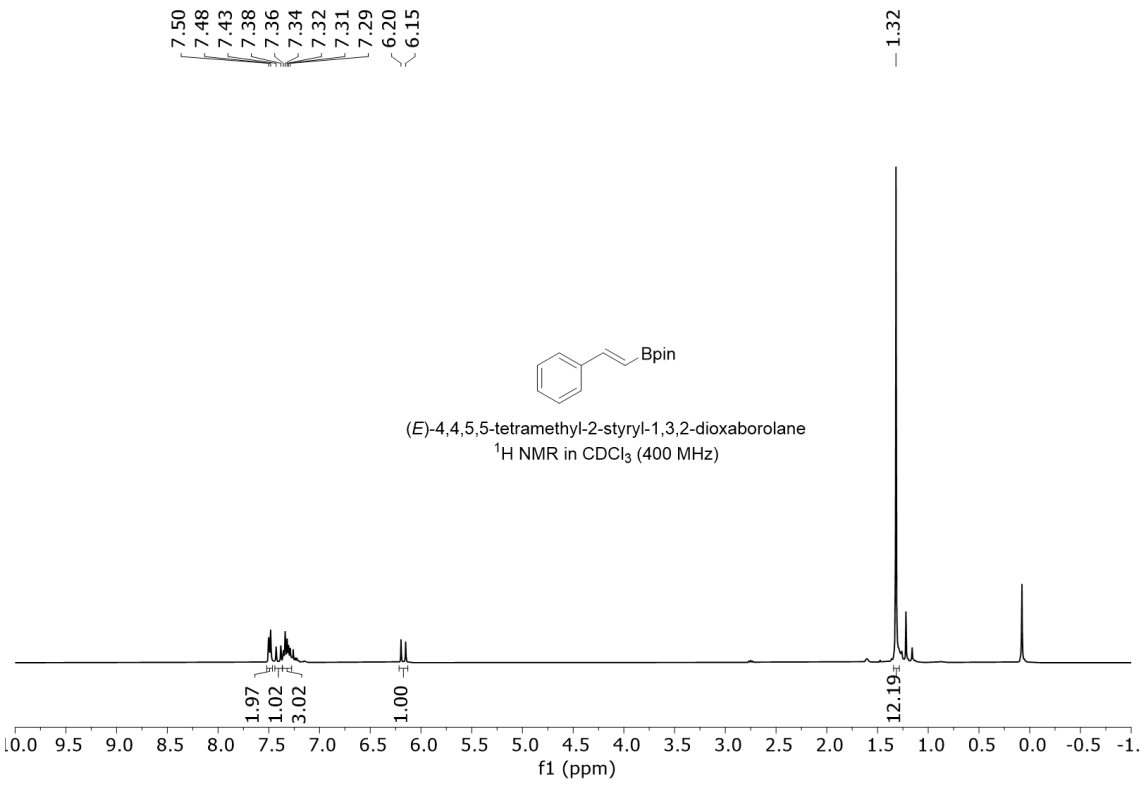

7.34
7.33
6.86
6.85
6.69
6.67
6.66
6.63
5.62
5.59
5.13
5.11
4.04
4.02
4.01
3.99
3.98
3.96
2.07
2.05
2.04
2.02
2.01
1.99
1.98
1.96
1.95
1.87
1.86
1.85
1.83
1.82
1.81
1.69
1.62
0.97
O
1-((3,7-dimethyloct-6-en-1-yl)oxy)-4-vinylbenzene
1H NMR in CDCl3 (500 MHz)
1.99
2.00
0.98
1.01
2.07
1.99
2.23
1.06
3.28
3.15
1.14
1.16
2.19
2.98
f1 (ppm)

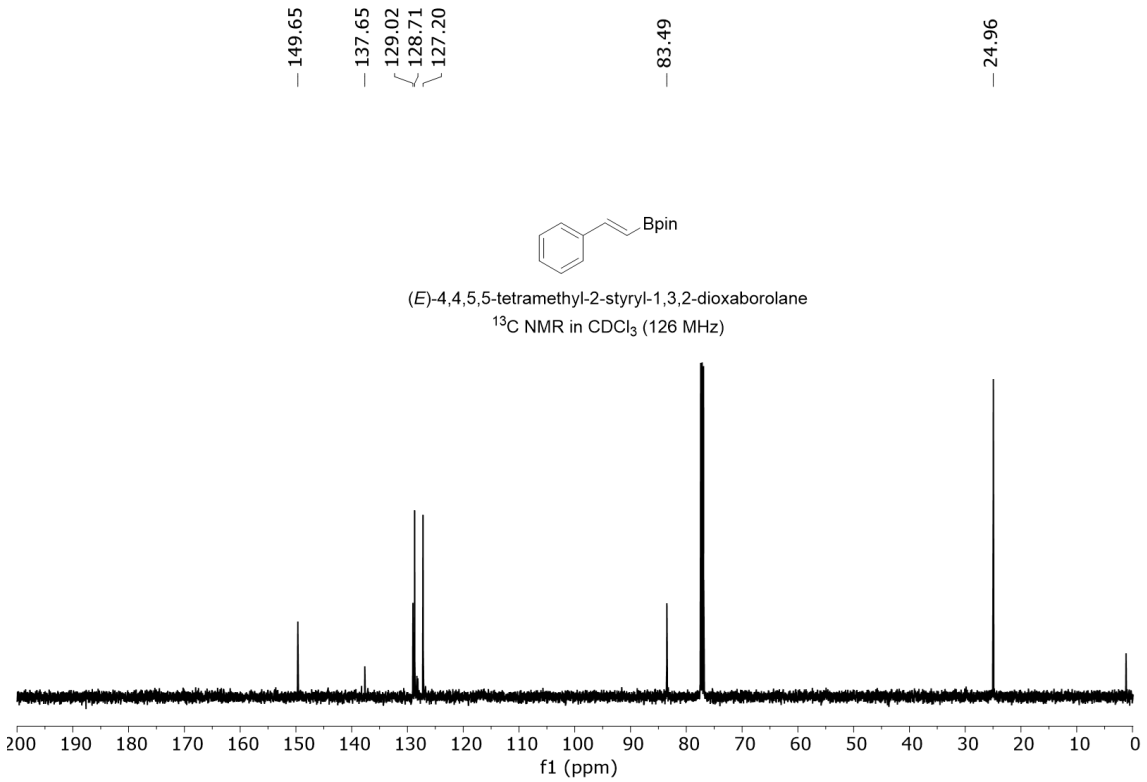

159.10
136.44
131.44
130.41
127.49
124.83
114.67
111.54
66.49
37.29
36.28
29.70
25.86
25.61
19.71
17.80
O
1-((3,7-dimethyloct-6-en-1-yl)oxy)-4-vinylbenzene
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

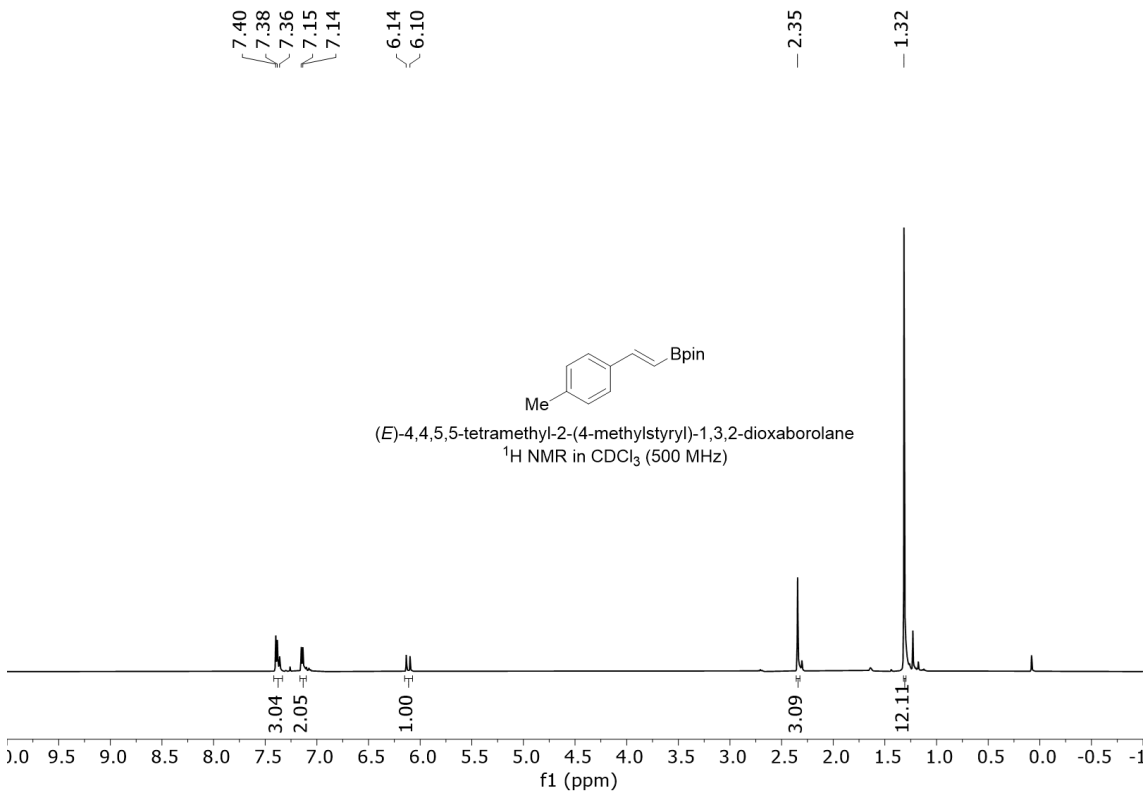

7.67
7.65
7.60
7.35
7.34
7.28
7.26
7.11
7.10
7.09
7.08
7.08
7.07
6.81
6.79
6.61
6.59
6.57
5.57
5.53
5.08
5.05
4.13
4.12
4.11
4.10
4.00
3.98
3.98
3.96
3.86
3.36
3.34
3.33
3.31
3.30
3.29
1.45
1.43

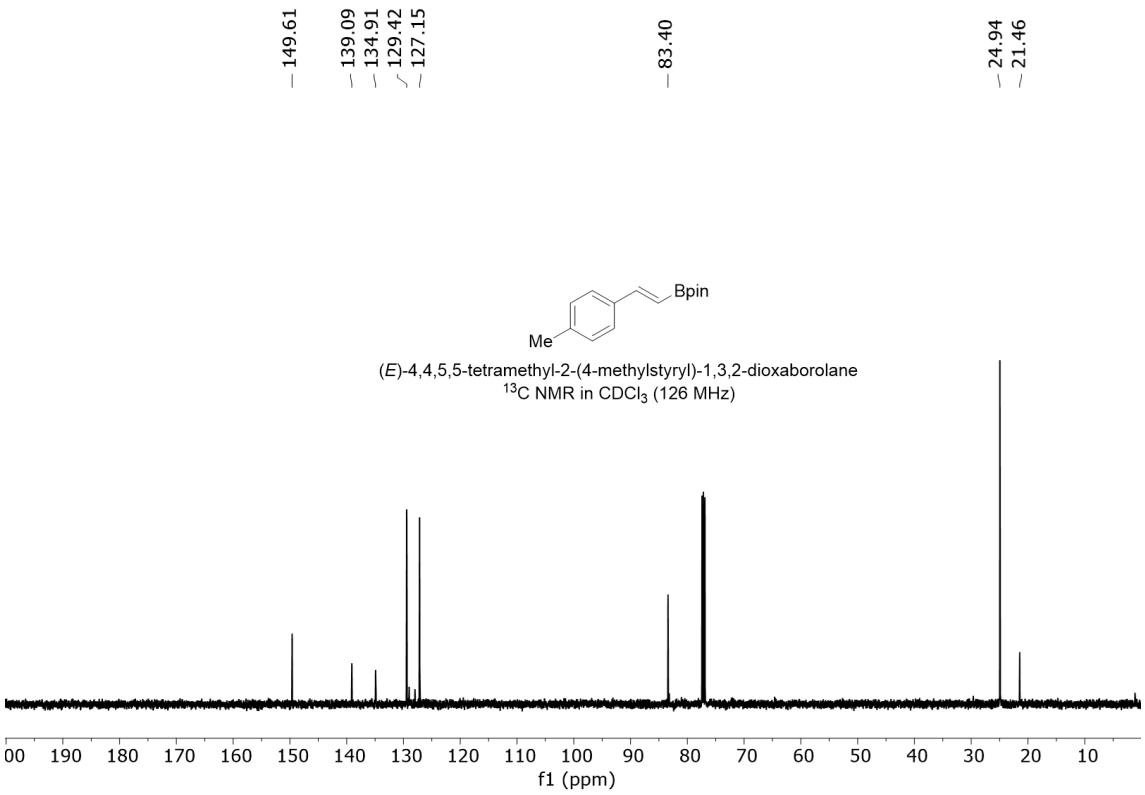

MeO
O
(S)-2-methoxy-6-(1-(4-vinylphenoxy)propan-2-yl)naphthalene
1H NMR in CDCl3 (500 MHz)
2.06
1.01
1.02
2.15
2.16
1.92
0.95
1.00
1.10
0.97
1.00
3.15
0.95
3.09
f1 (ppm)

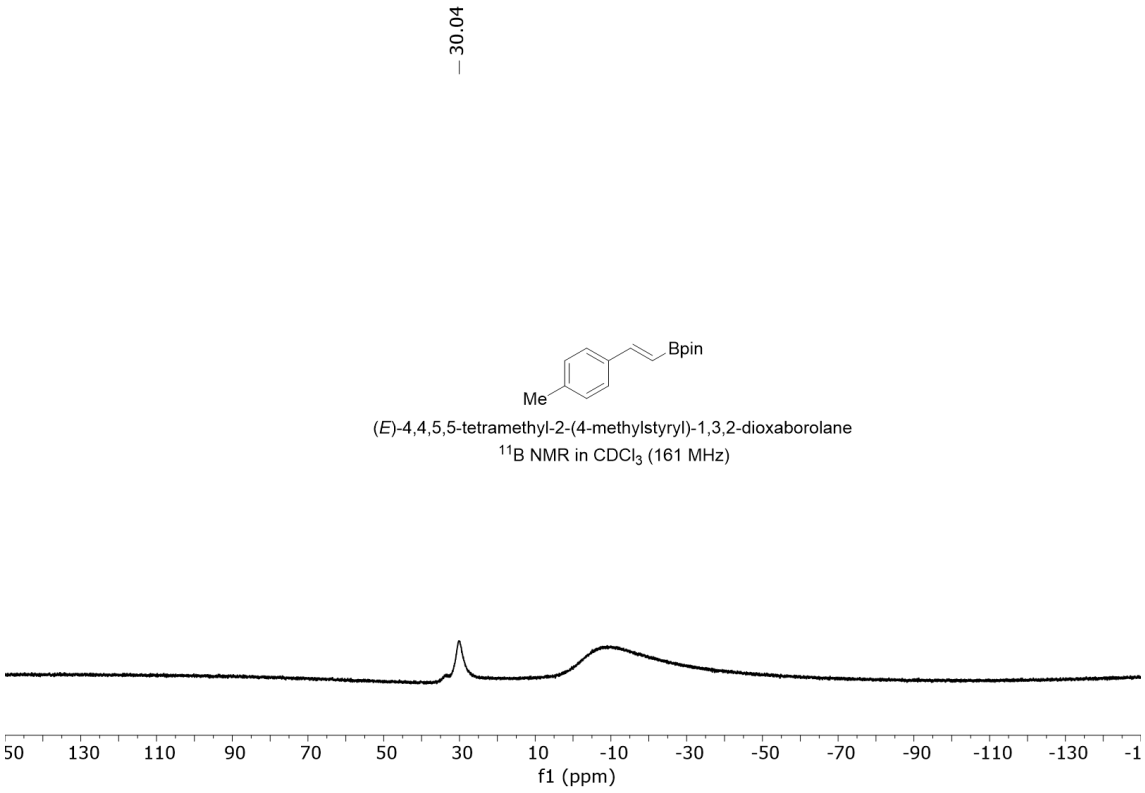

158.95
157.57
138.88
136.40
133.64
130.59
129.28
129.20
127.49
127.08
126.64
125.70
118.96
114.80
111.64
105.77
73.69
55.43
39.62
18.39
MeO
O
(S)-2-methoxy-6-(1-(4-vinylphenoxy)propan-2-yl)naphthalene
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

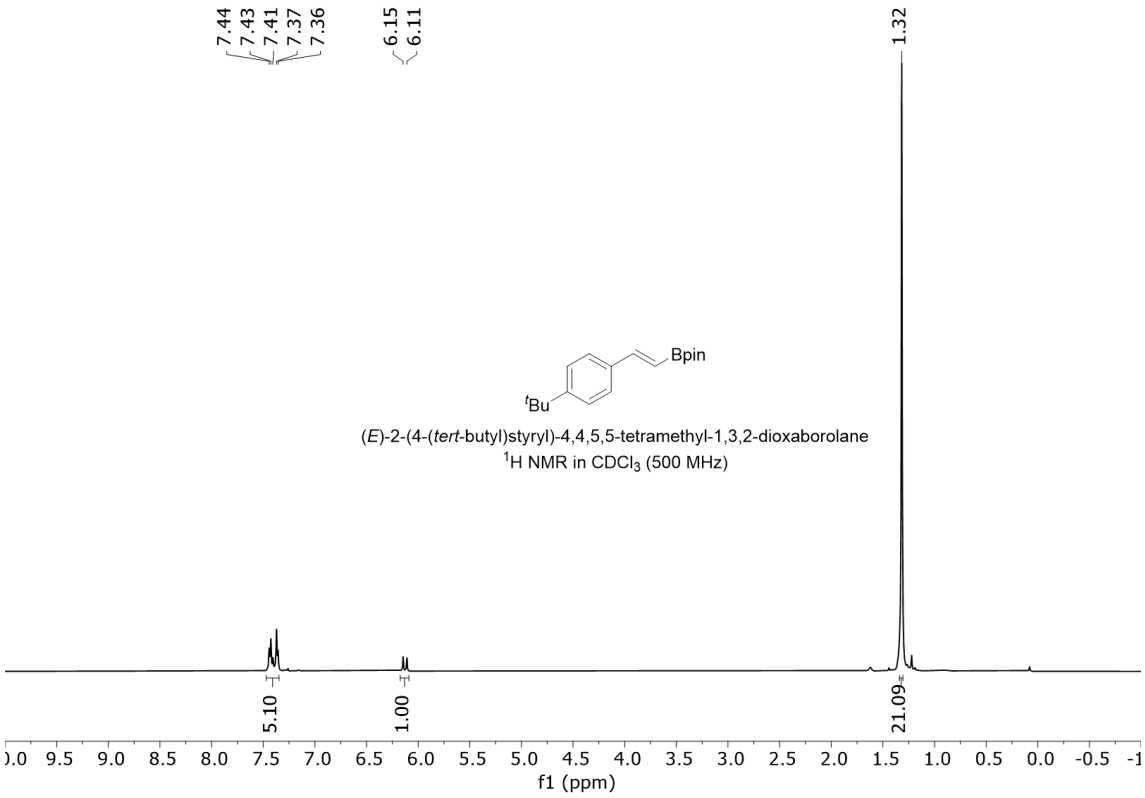

7.50
7.48
7.43
7.38
7.36
7.34
7.32
7.31
7.29
6.20
6.15
1.32
Bpin
(E)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane
1H NMR in CDCl3 (400 MHz)
1.97
1.02
3.02
1.00
12.19
f1 (ppm)


149.65
137.65
129.02
128.71
127.20
83.49
24.96
Bpin
(E)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

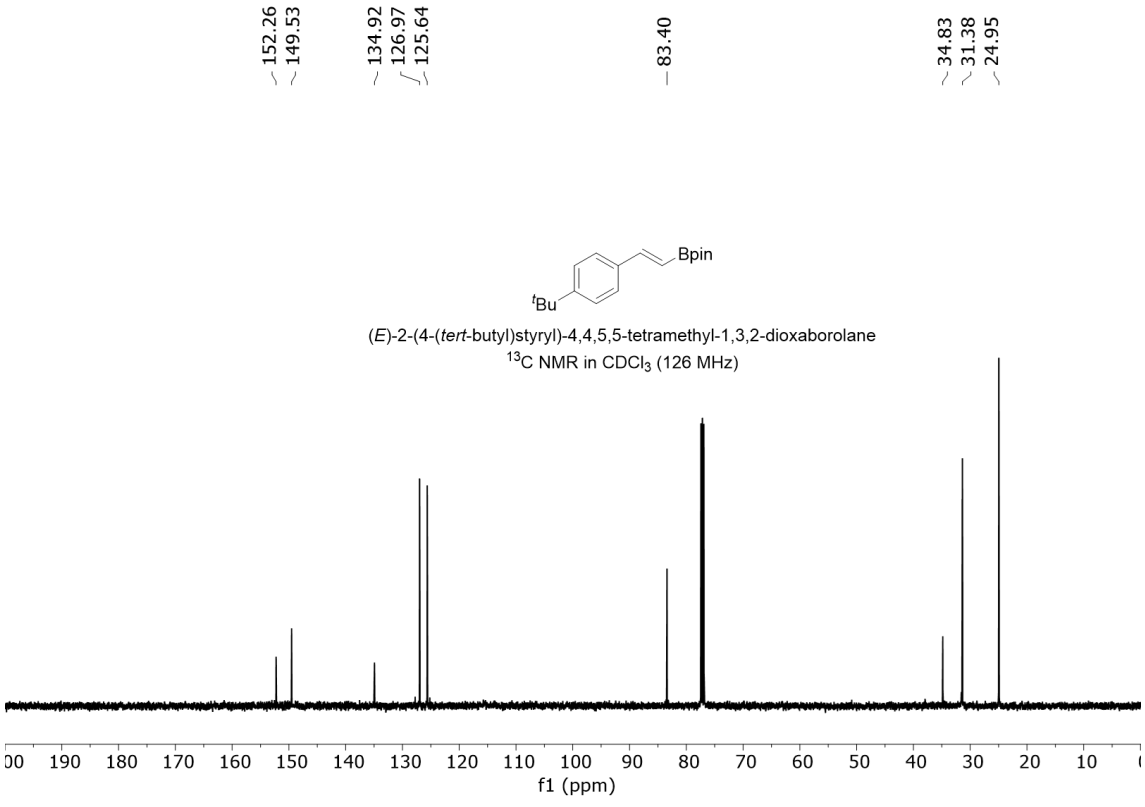

7.40
7.38
7.36
7.15
7.14
6.14
6.10
2.35
1.32
Bpin
Me
(E)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
3.04
2.05
1.00
3.09
12.11
f1 (ppm)


149.61
139.09
134.91
129.42
127.15
83.40
24.94
21.46
Bpin
Me
(E)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


30.04
Bpin
Me
(E)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane
11B NMR in CDCl3 (161 MHz)
50 130 110 90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -1
f1 (ppm)

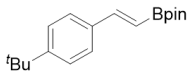


(*E*)-2-(4-(*tert*-butyl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (500 MHz)



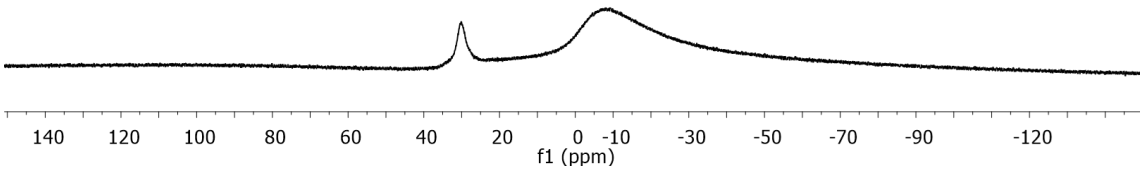
(*E*)-2-(4-(*tert*-butyl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)

30.07

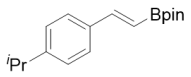


(*E*)-2-(4-(*tert*-butyl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

^{11}B NMR in $CDCl_3$ (161 MHz)

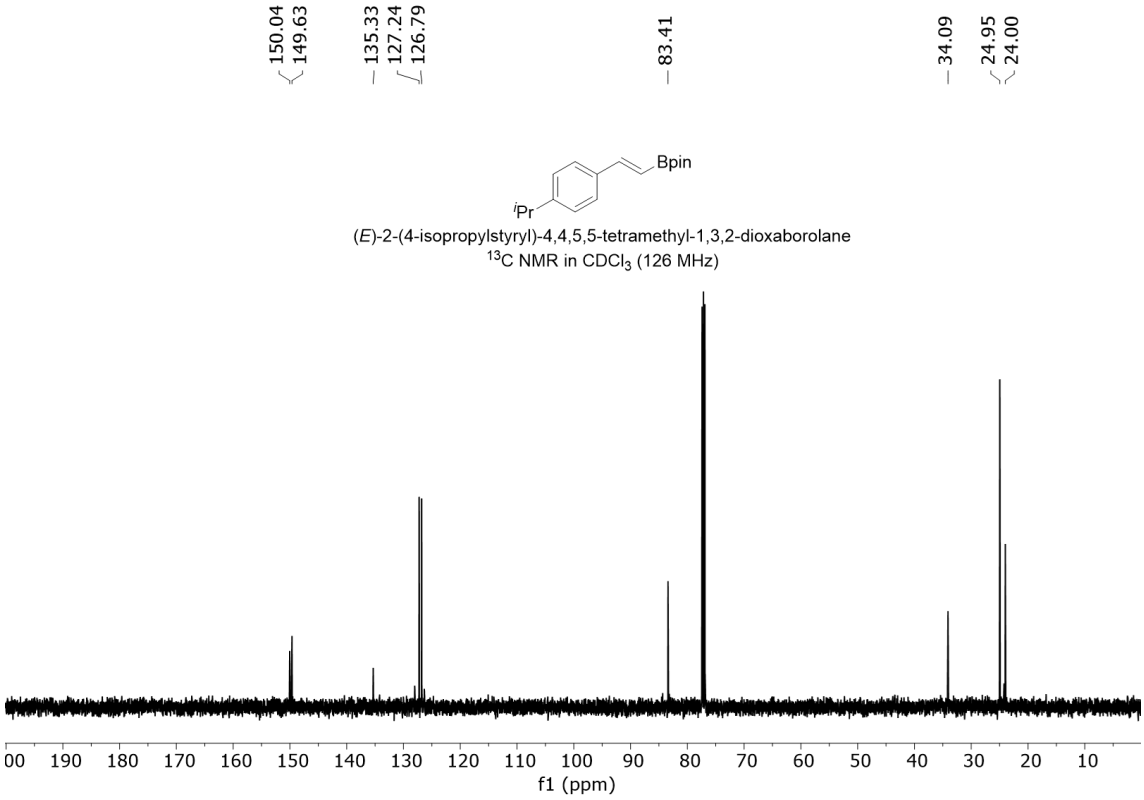


7.43 7.42 7.40 7.36 7.21 7.19 6.14 6.10 2.94 2.93 2.91 2.90 2.89 2.87 2.86 1.31 1.25 1.24



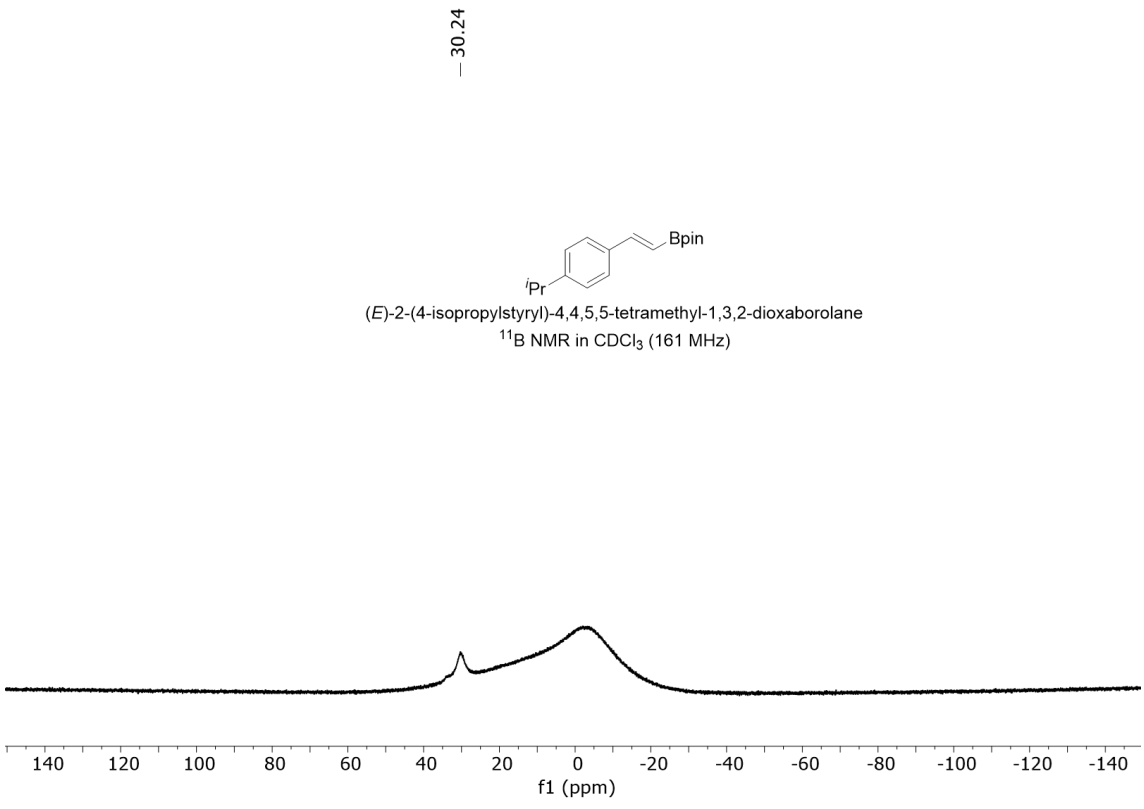
(*E*)-2-(4-isopropylstyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

^{1}H NMR in $CDCl_3$ (500 MHz)



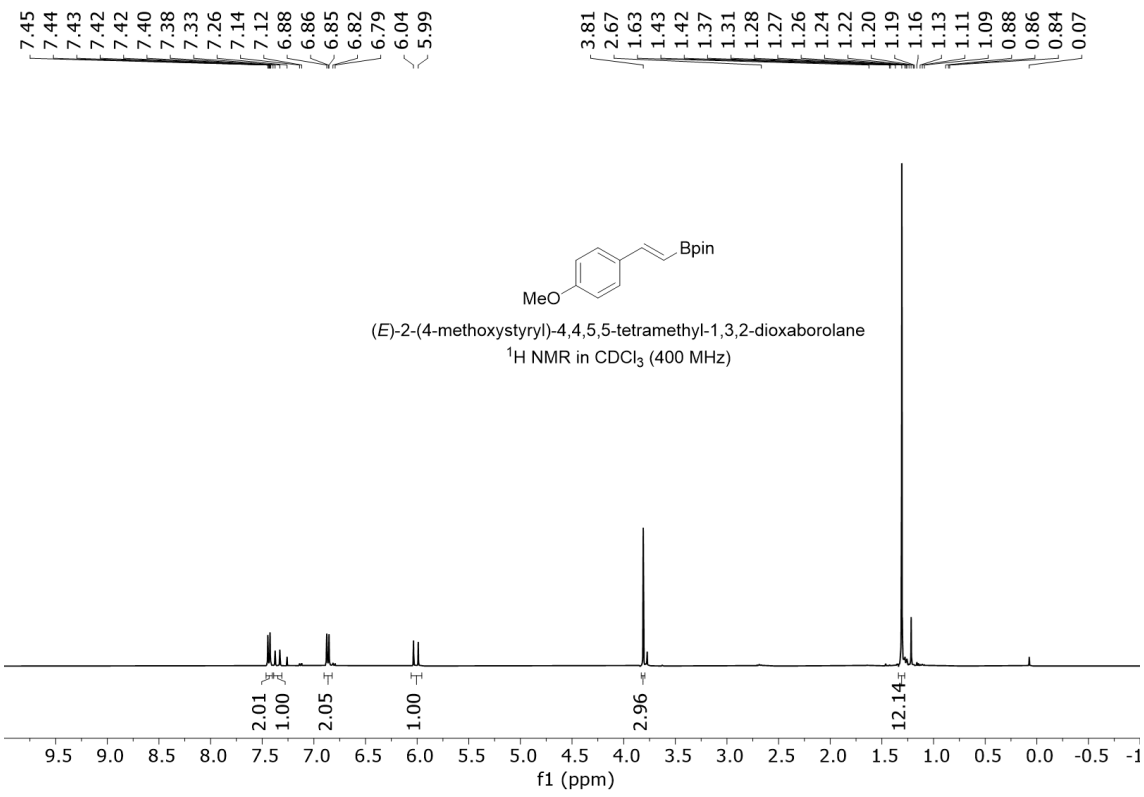
(*E*)-2-(4-isopropylstyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

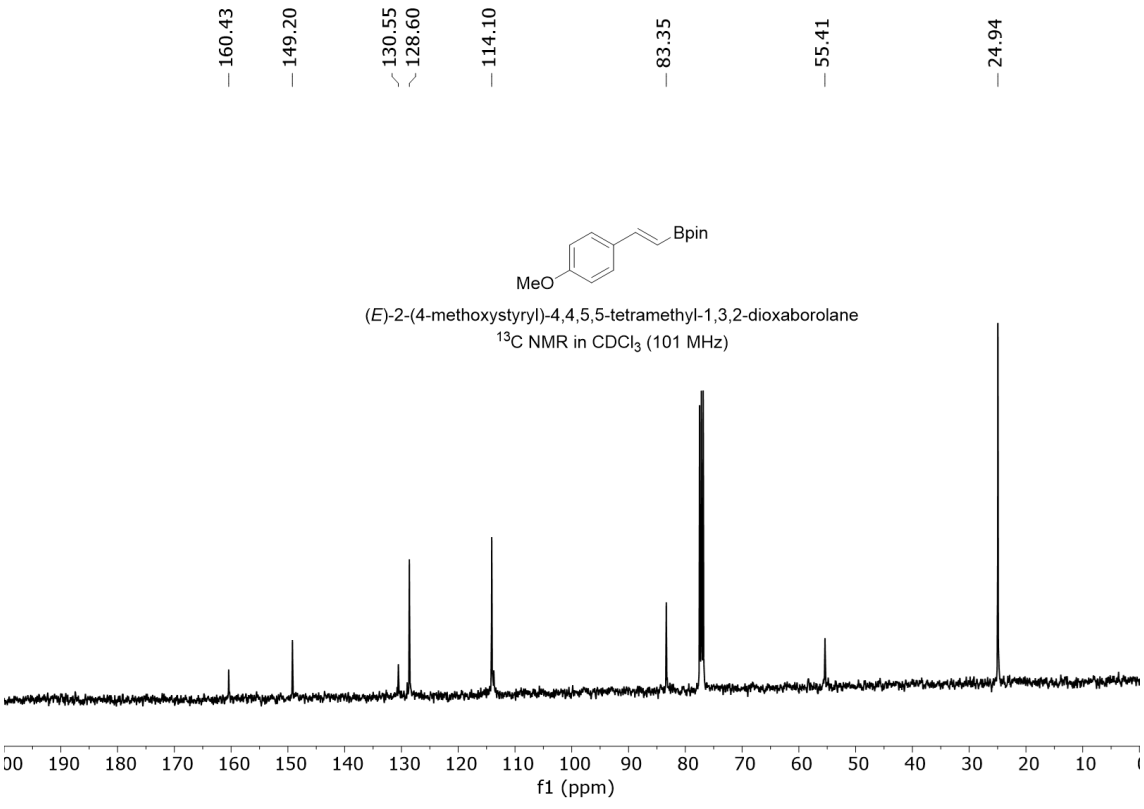
^{13}C NMR in $CDCl_3$ (126 MHz)

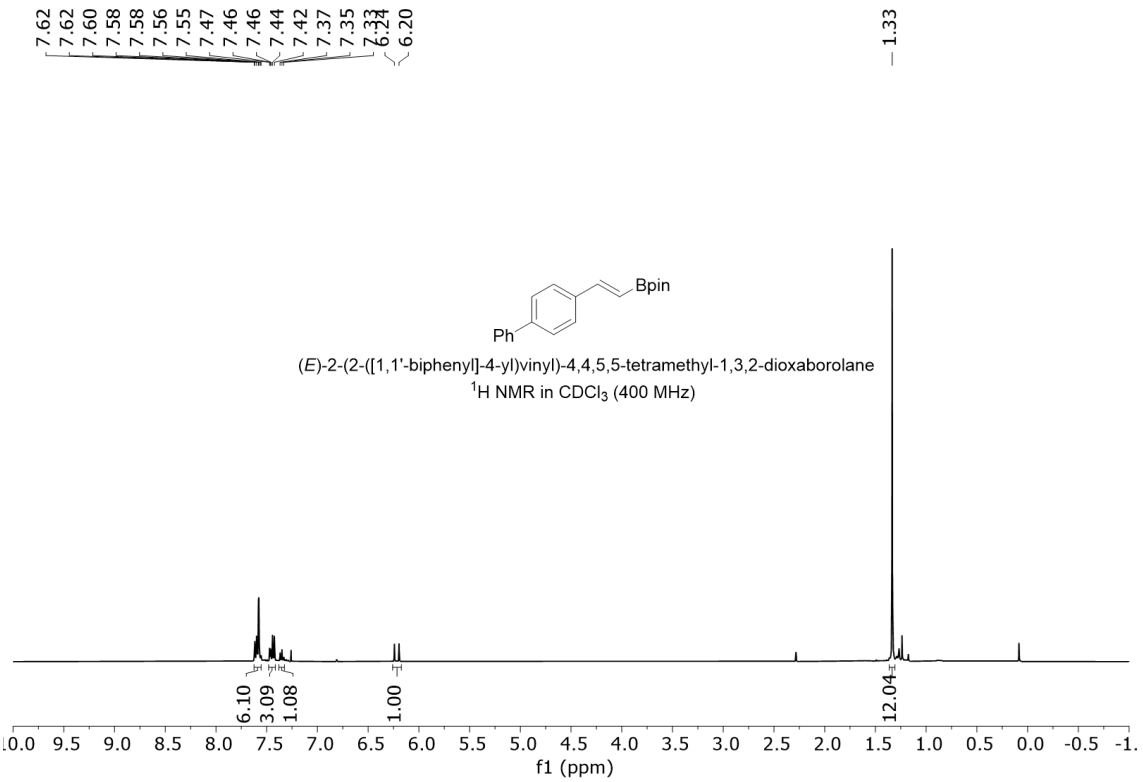


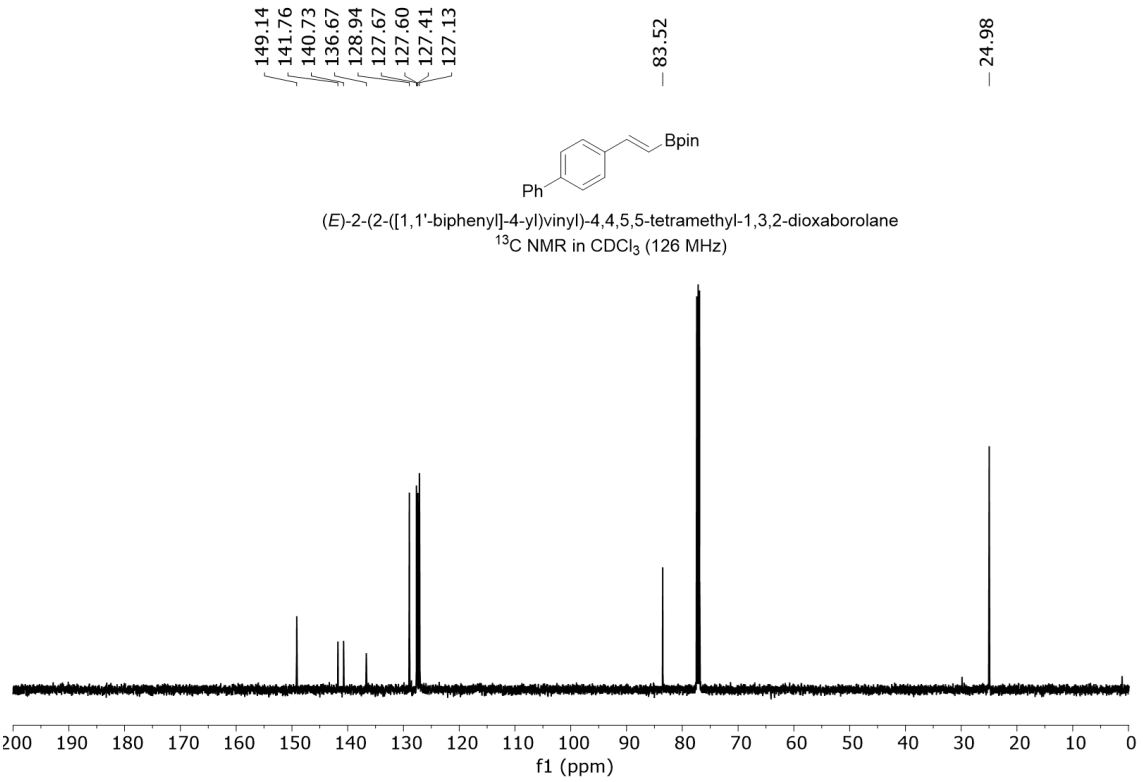
(*E*)-2-(4-isopropylstyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

^{11}B NMR in $CDCl_3$ (161 MHz)

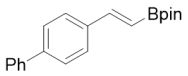

7.45
7.44
7.43
7.42
7.42
7.40
7.38
7.33
7.26
7.14
7.12
6.88
6.86
6.85
6.82
6.79
6.04
5.99
3.81
2.67
1.63
1.43
1.42
1.37
1.31
1.28
1.27
1.26
1.24
1.22
1.20
1.19
1.16
1.13
1.11
1.09
0.88
0.86
0.84
0.07
Bpin
MeO
(E)-2-(4-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
1H NMR in CDCl3 (400 MHz)
2.01
1.00
2.05
1.00
2.96
12.14
f1 (ppm)


160.43
149.20
130.55
128.60
114.10
83.35
55.41
24.94
Bpin
MeO
(E)-2-(4-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
13C NMR in CDCl3 (101 MHz)
f1 (ppm)


7.62
7.62
7.60
7.58
7.58
7.56
7.55
7.47
7.46
7.46
7.44
7.42
7.37
7.35
6.24
6.20
1.33
Bpin
Ph
(E)-2-(2-([1,1'-biphenyl]-4-yl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
1H NMR in CDCl3 (400 MHz)
6.10
3.09
1.08
1.00
12.04
f1 (ppm)

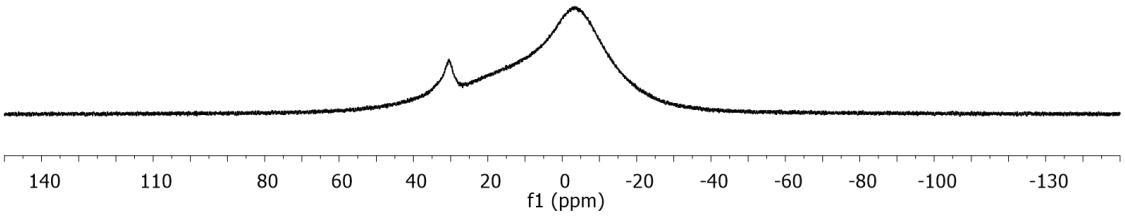

149.14
141.76
140.73
136.67
128.94
127.67
127.60
127.41
127.13
83.52
24.98
Bpin
Ph
(E)-2-(2-([1,1'-biphenyl]-4-yl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

30.42



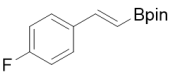
(*E*)-2-(2-([1,1'-biphenyl]-4-yl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

^{11}B NMR in $CDCl_3$ (161 MHz)



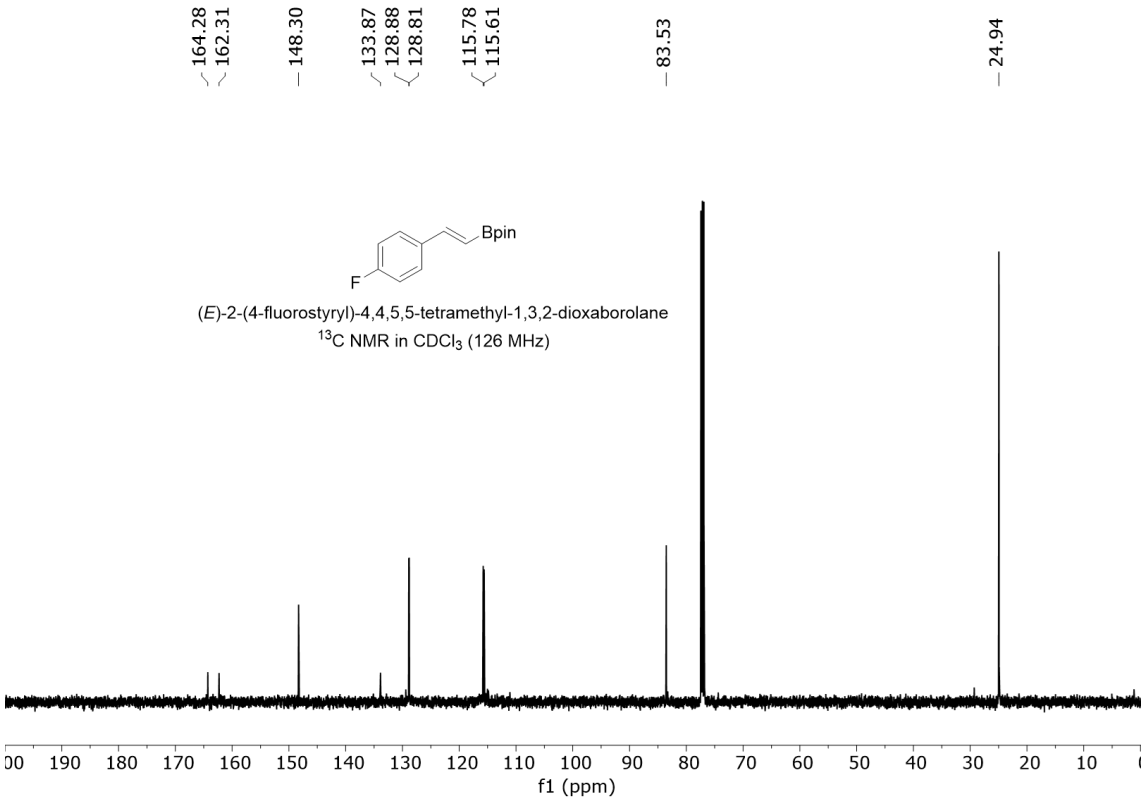
7.47
7.45
7.44
7.37
7.33
7.04
7.02
7.00
6.09
6.05

1.31



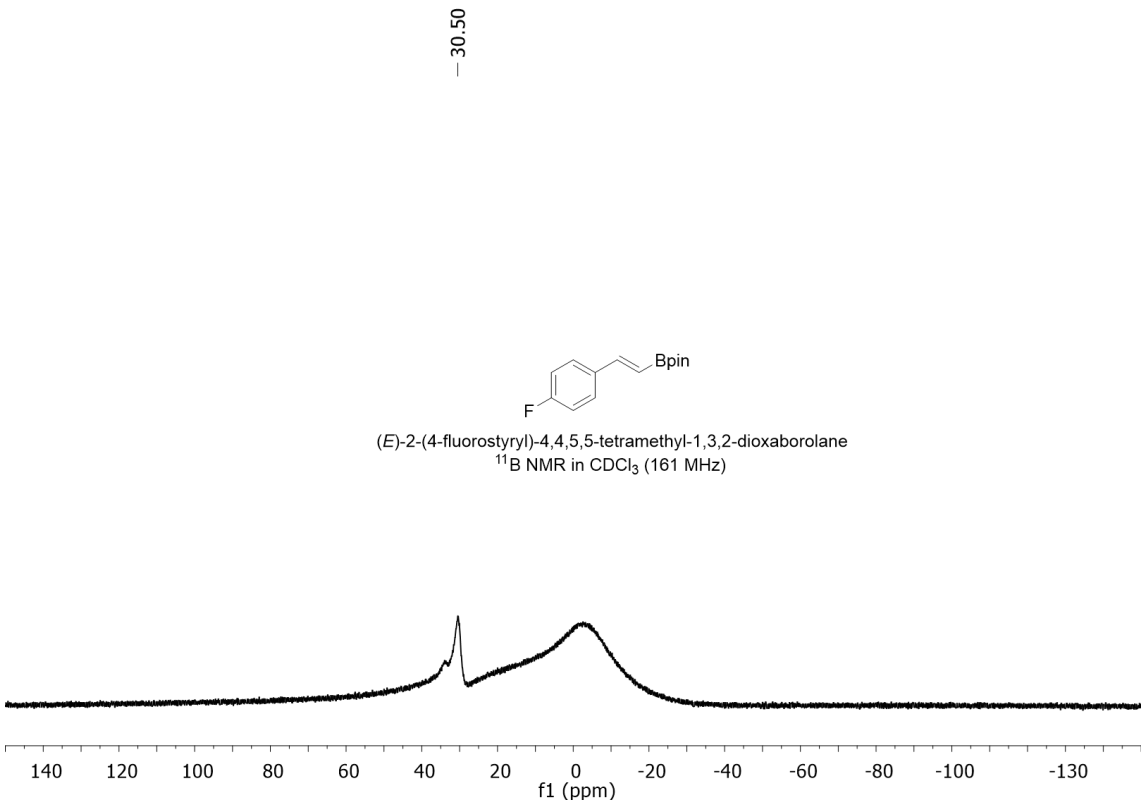
(*E*)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

^{1}H NMR in $CDCl_3$ (500 MHz)



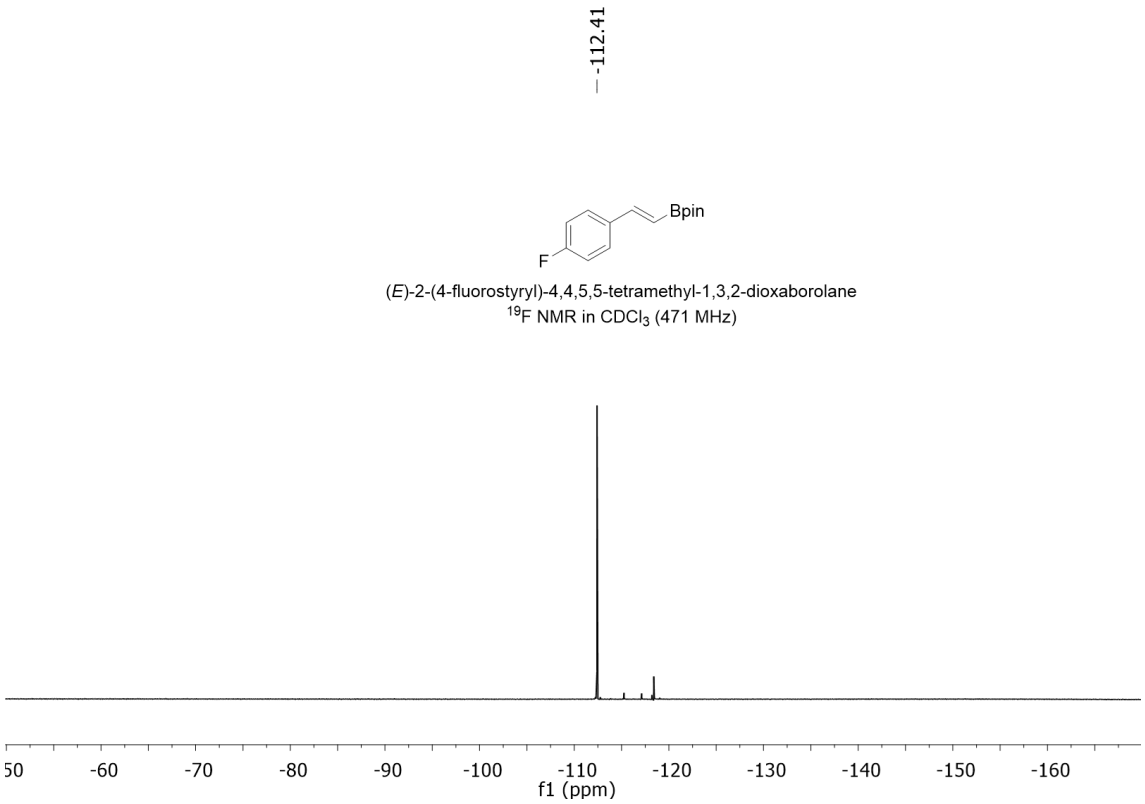
(*E*)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

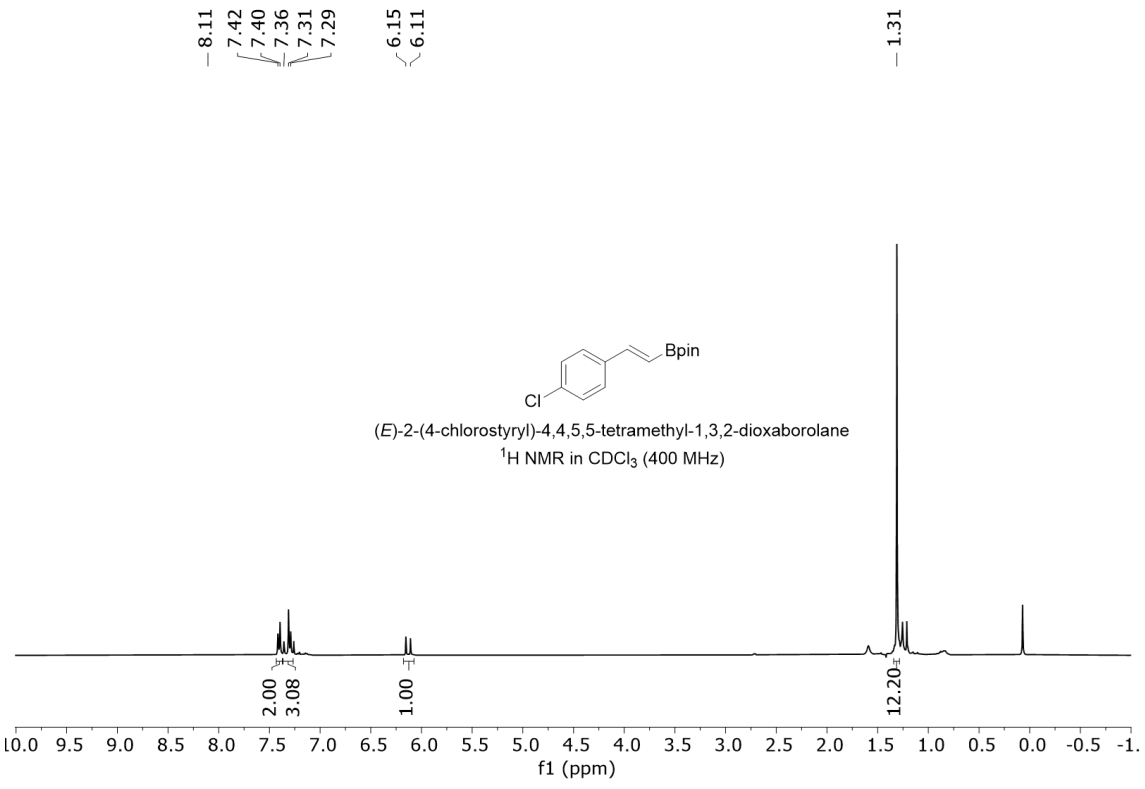
^{13}C NMR in $CDCl_3$ (126 MHz)

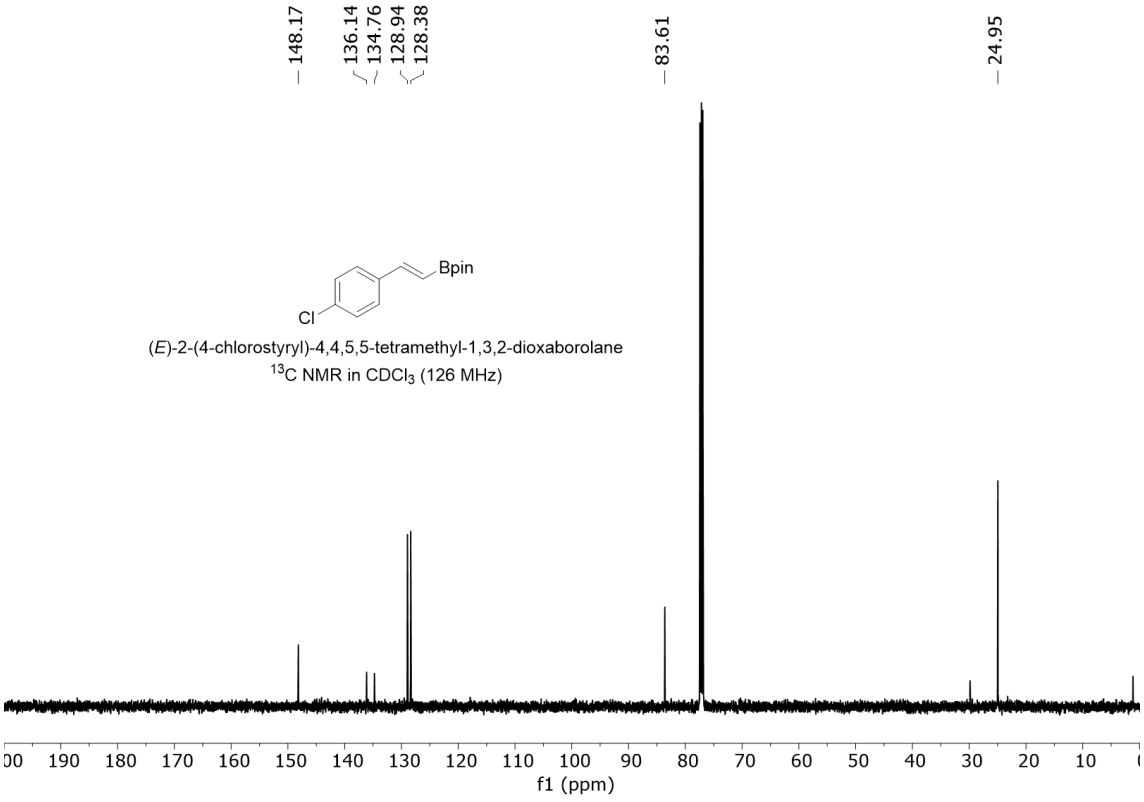


(*E*)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

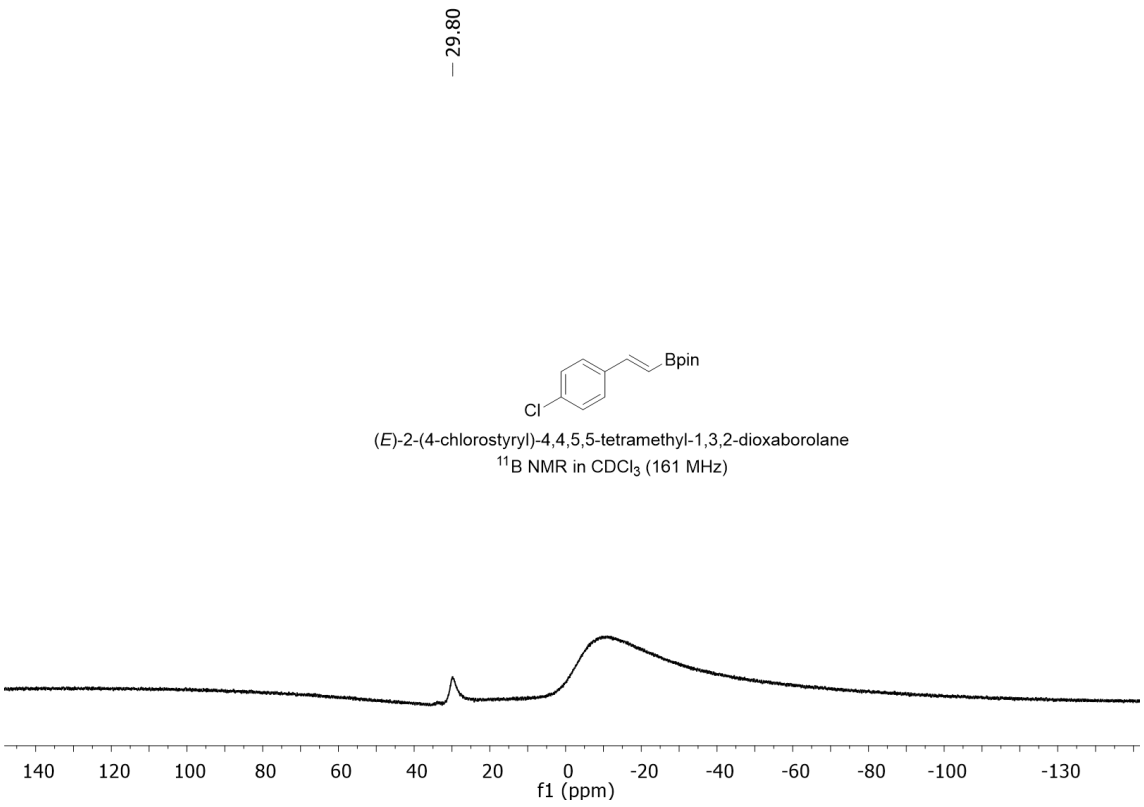
^{11}B NMR in $CDCl_3$ (161 MHz)


-112.41
Bpin
F
(E)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
19F NMR in CDCl3 (471 MHz)
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

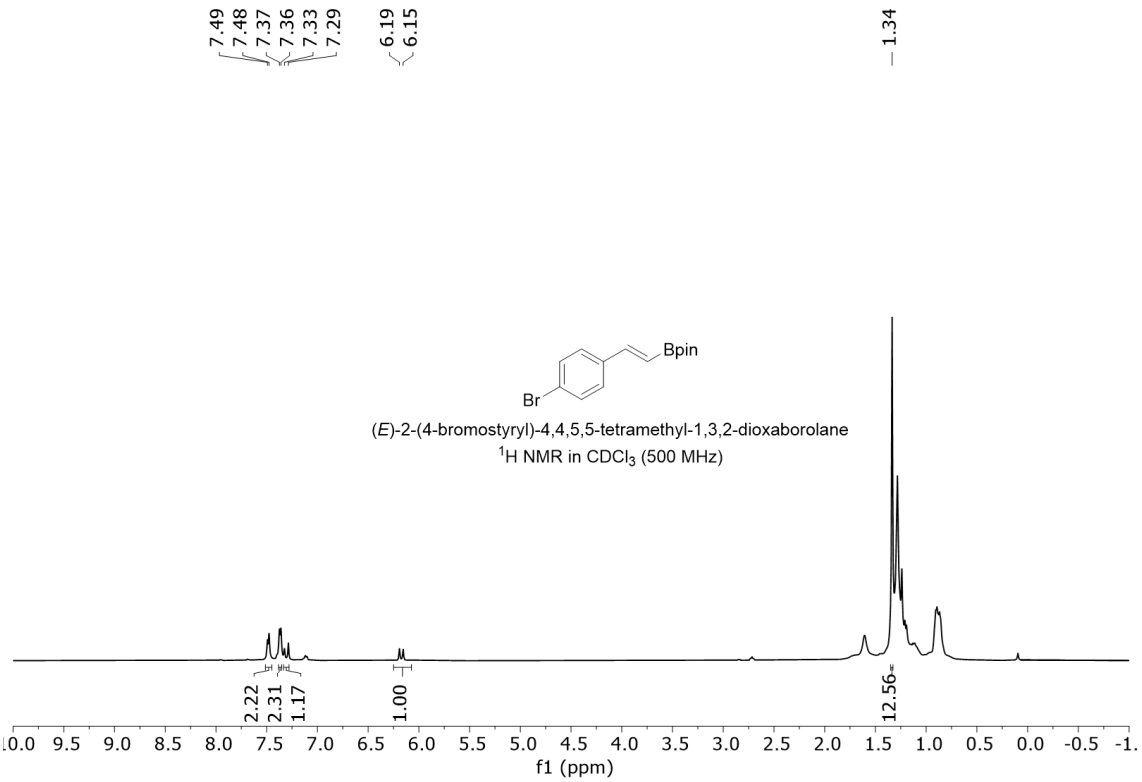

8.11
7.42
7.40
7.36
7.31
7.29
6.15
6.11
1.31
Bpin
Cl
(E)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
1H NMR in CDCl3 (400 MHz)
2.00
3.08
1.00
12.20
f1 (ppm)

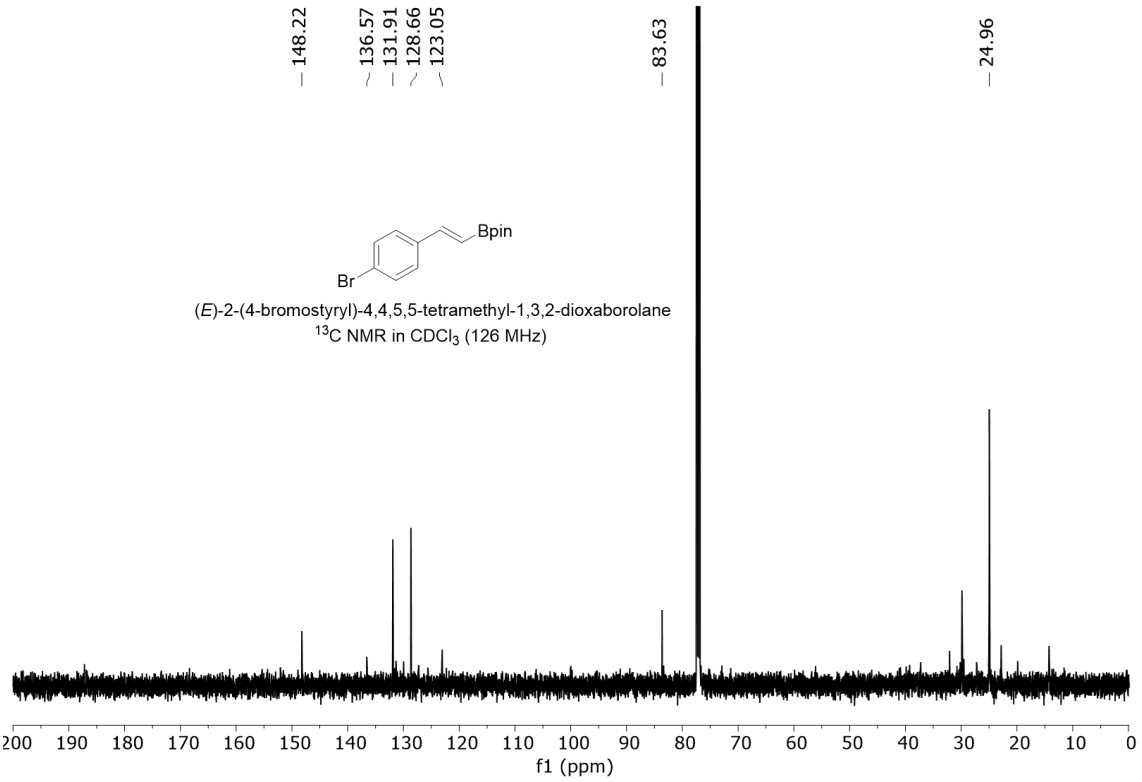


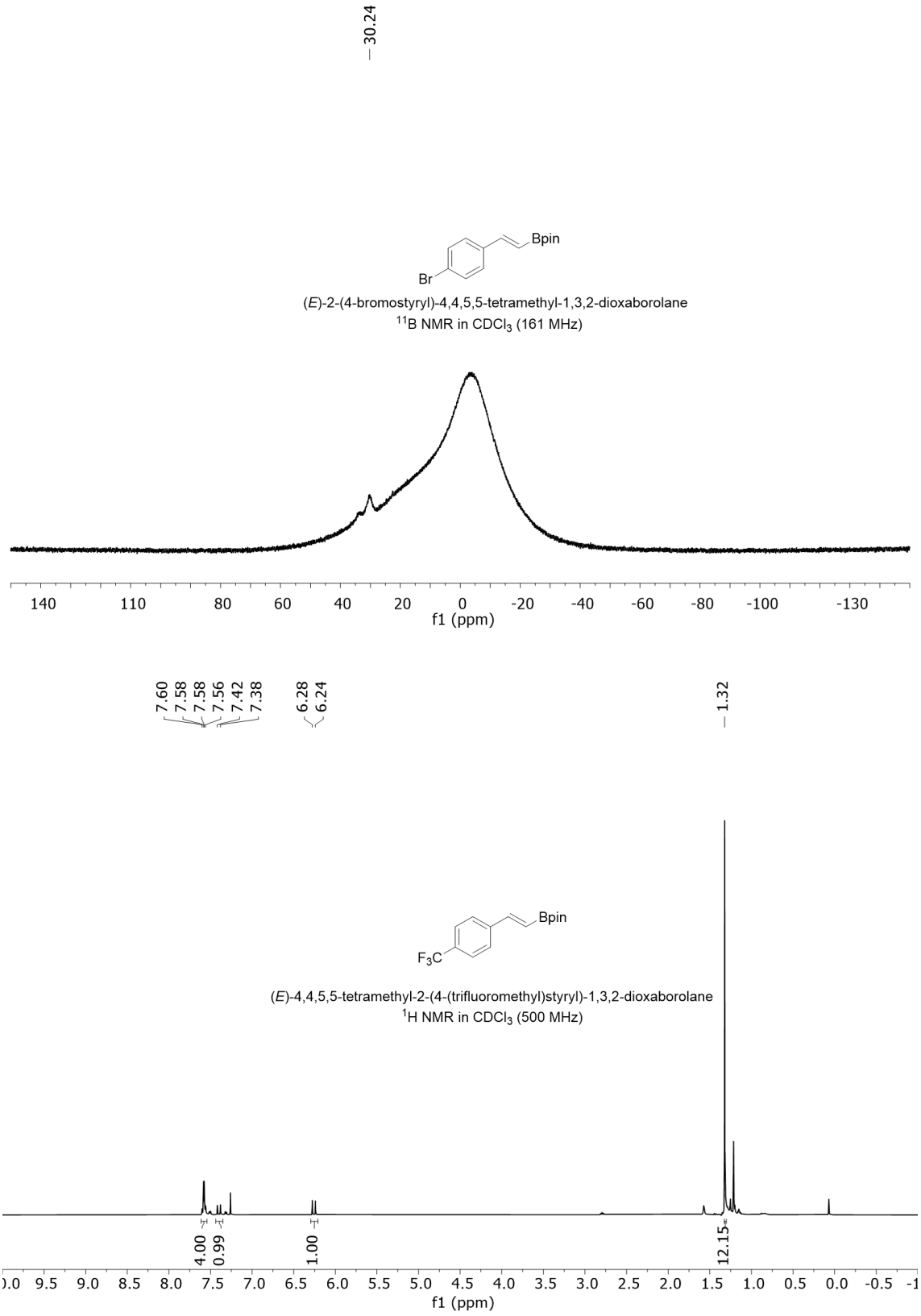
(*E*)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)

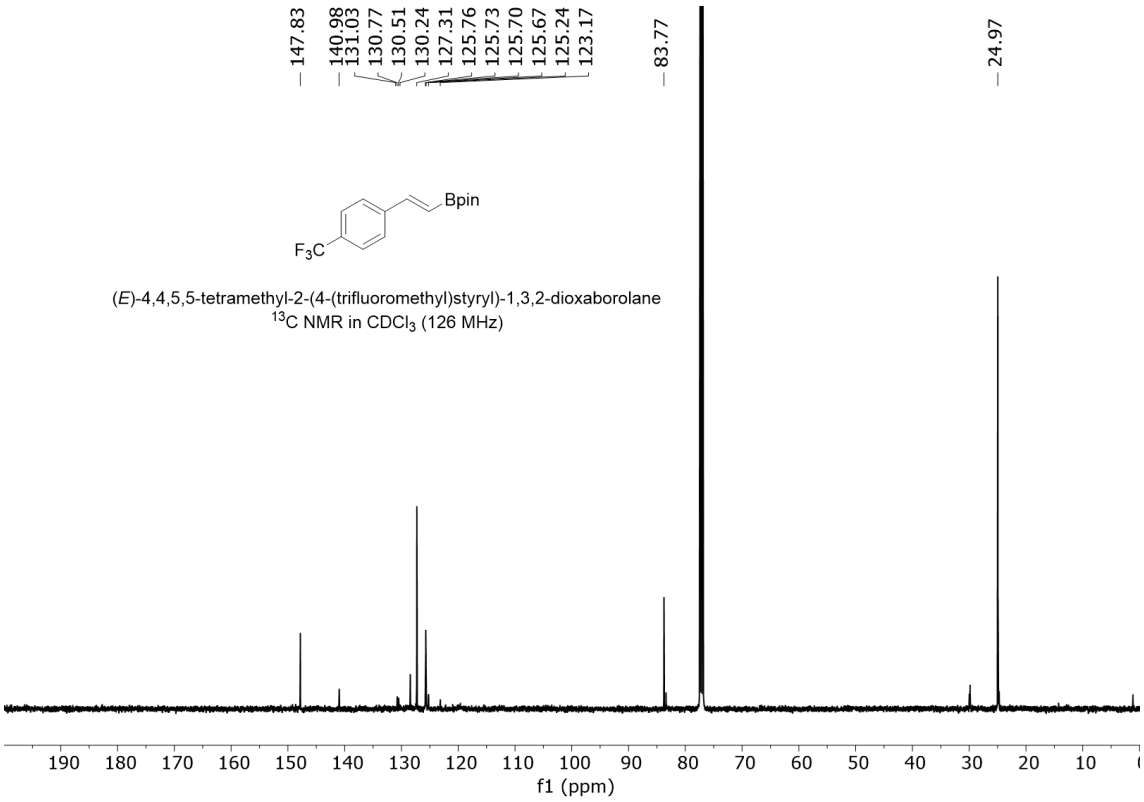


(*E*)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (161 MHz)

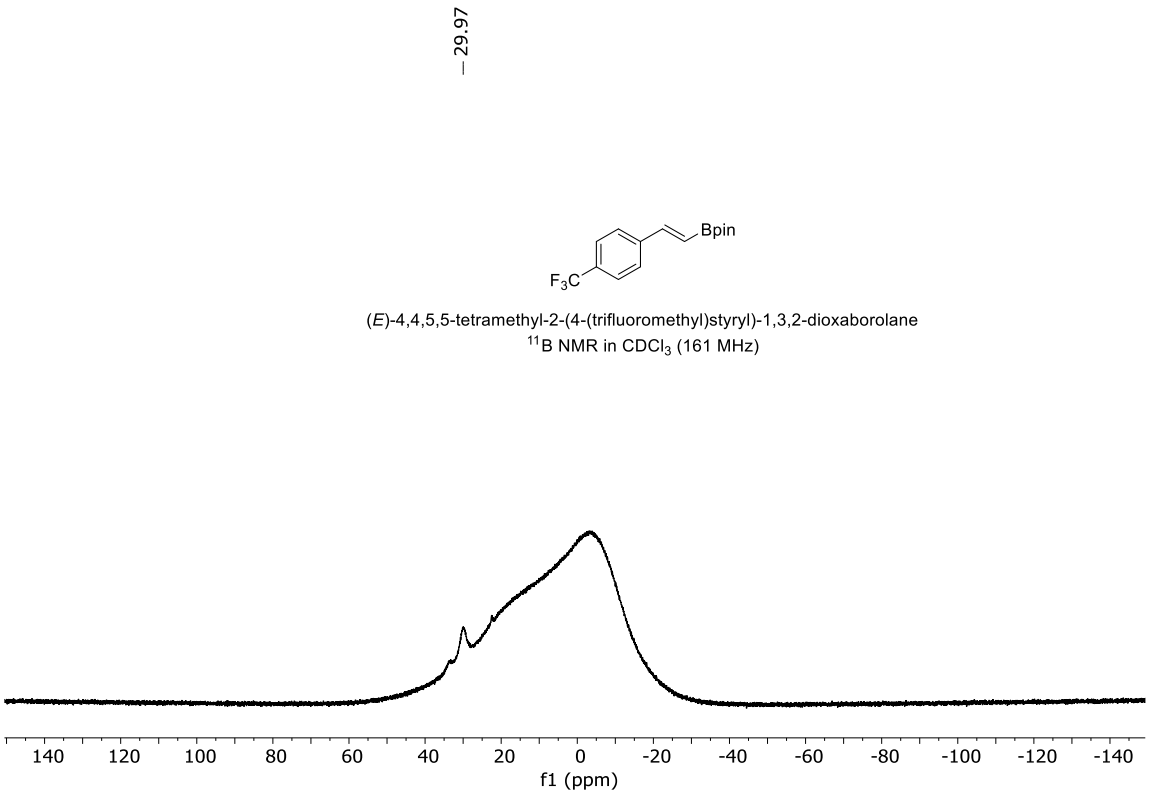

7.49
7.48
7.37
7.36
7.33
7.29
6.19
6.15
1.34
Bpin
Br
(E)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
2.22
2.31
1.17
1.00
12.56
f1 (ppm)


148.22
136.57
131.91
128.66
123.05
83.63
24.96
Bpin
Br
(E)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

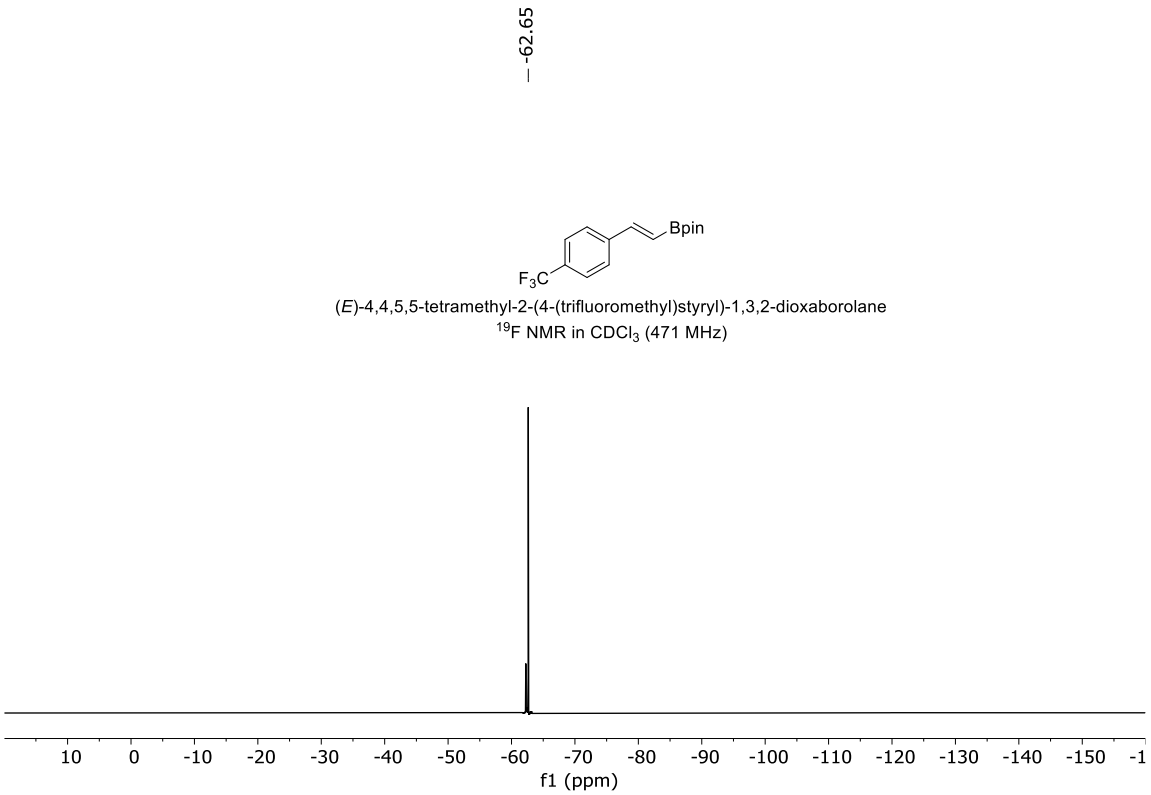

30.24
Bpin
Br
(E)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
11B NMR in CDCl3 (161 MHz)
140 110 80 60 40 20 0 -20 -40 -60 -80 -100 -130
f1 (ppm)
7.60
7.58
7.58
7.56
7.42
7.38
6.28
6.24
1.32
Bpin
F3C
(E)-4,4,5,5-tetramethyl-2-(4-(trifluoromethyl)styryl)-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
4.00
0.99
1.00
12.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



(*E*)-4,4,5,5-tetramethyl-2-(4-(trifluoromethyl)styryl)-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)

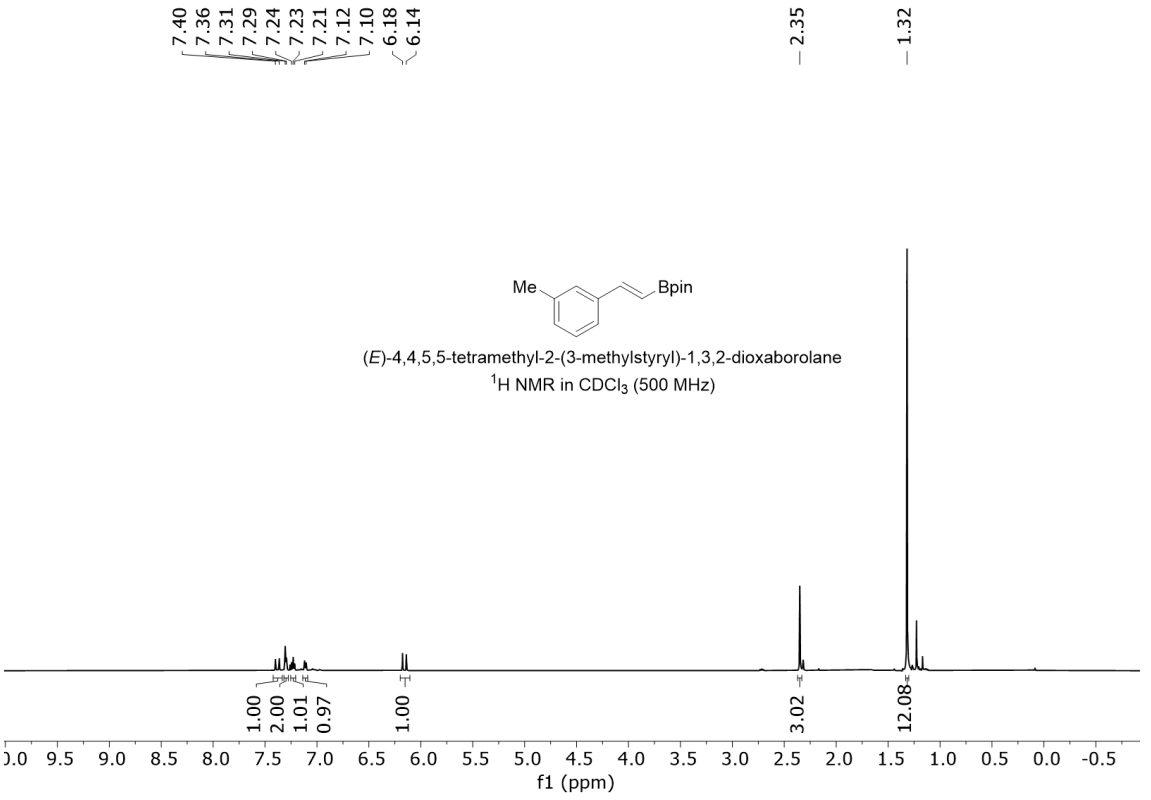


(*E*)-4,4,5,5-tetramethyl-2-(4-(trifluoromethyl)styryl)-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (161 MHz)



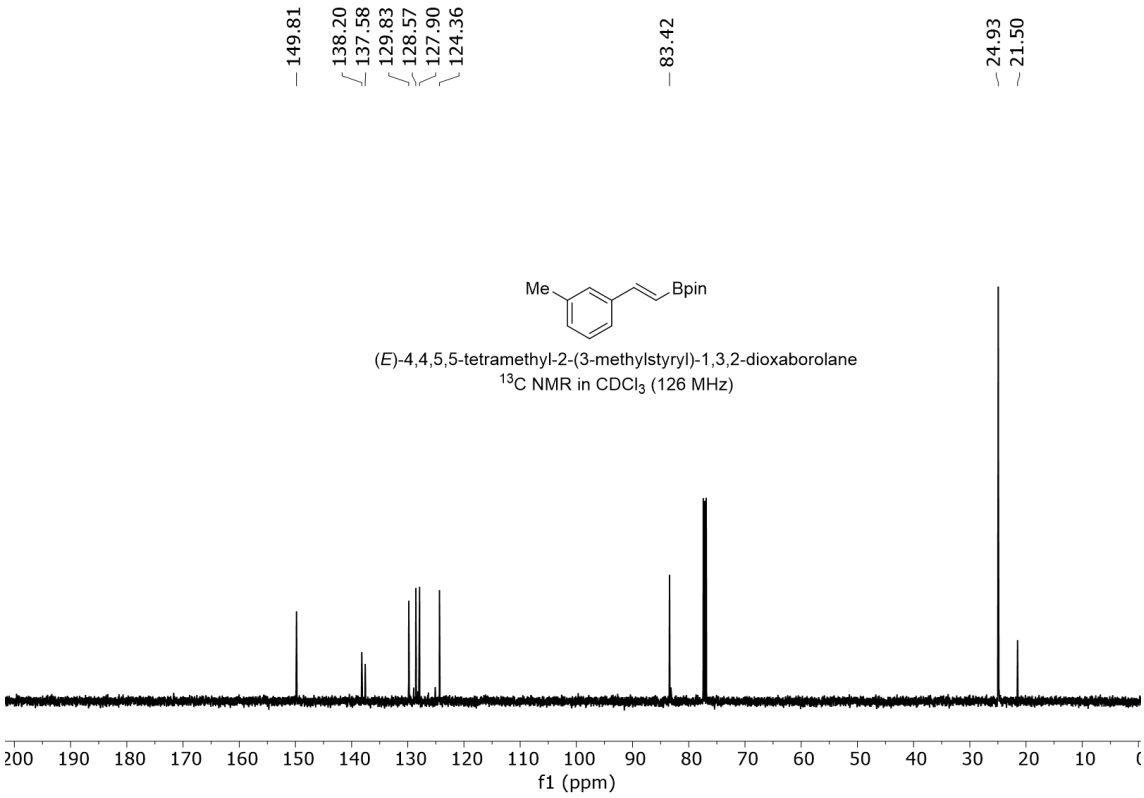
(*E*)-4,4,5,5-tetramethyl-2-(4-(trifluoromethyl)styryl)-1,3,2-dioxaborolane

^{19}F NMR in $CDCl_3$ (471 MHz)

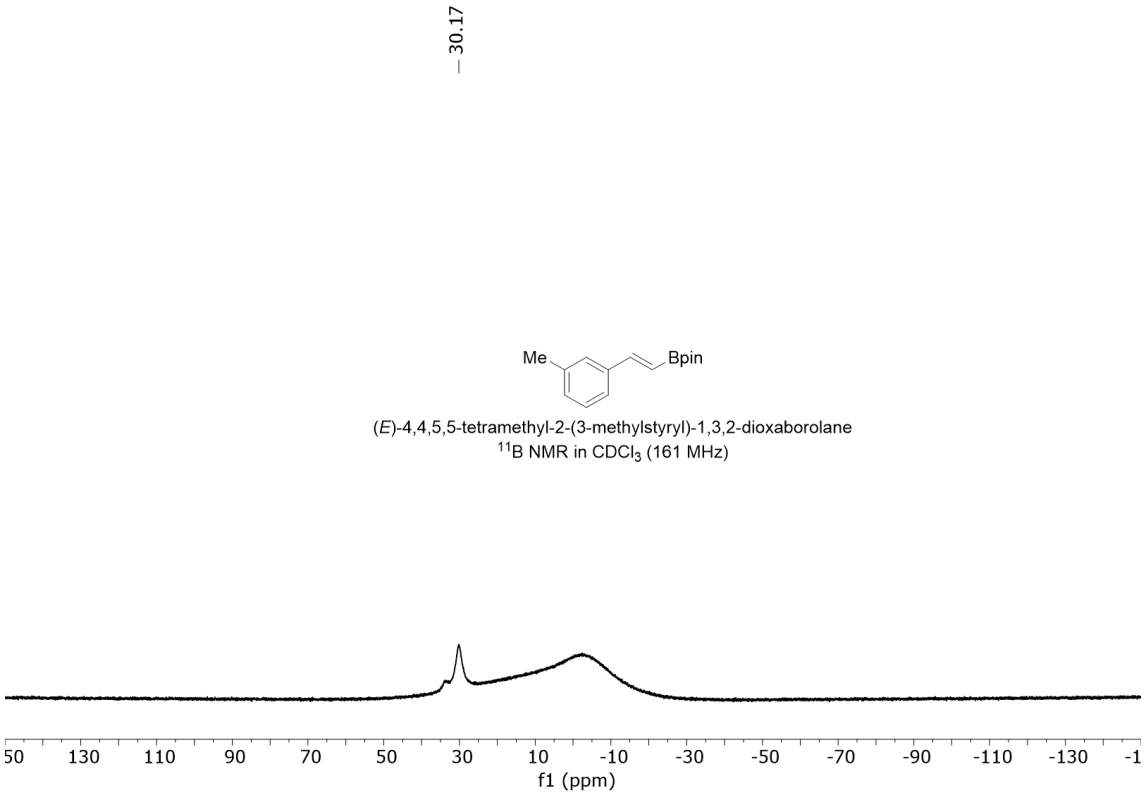


(*E*)-4,4,5,5-tetramethyl-2-(3-methylstyryl)-1,3,2-dioxaborolane

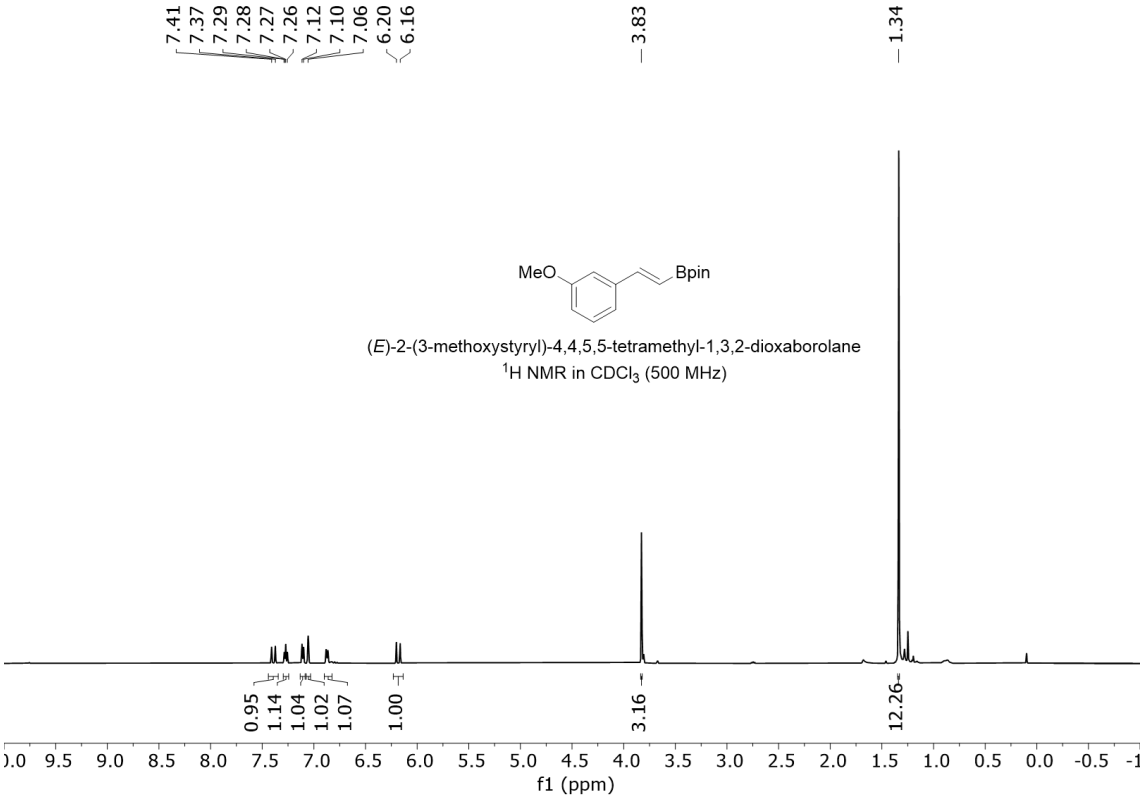
^{1}H NMR in $CDCl_3$ (500 MHz)



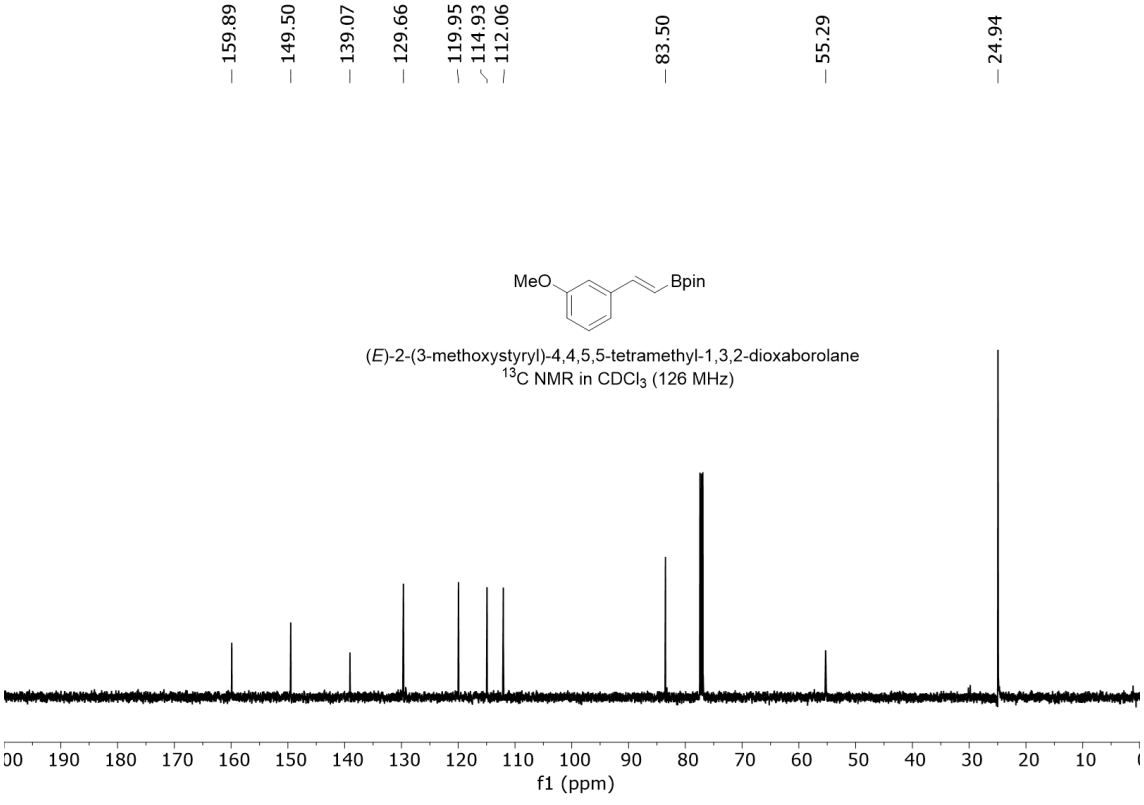
(*E*)-4,4,5,5-tetramethyl-2-(3-methylstyryl)-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)



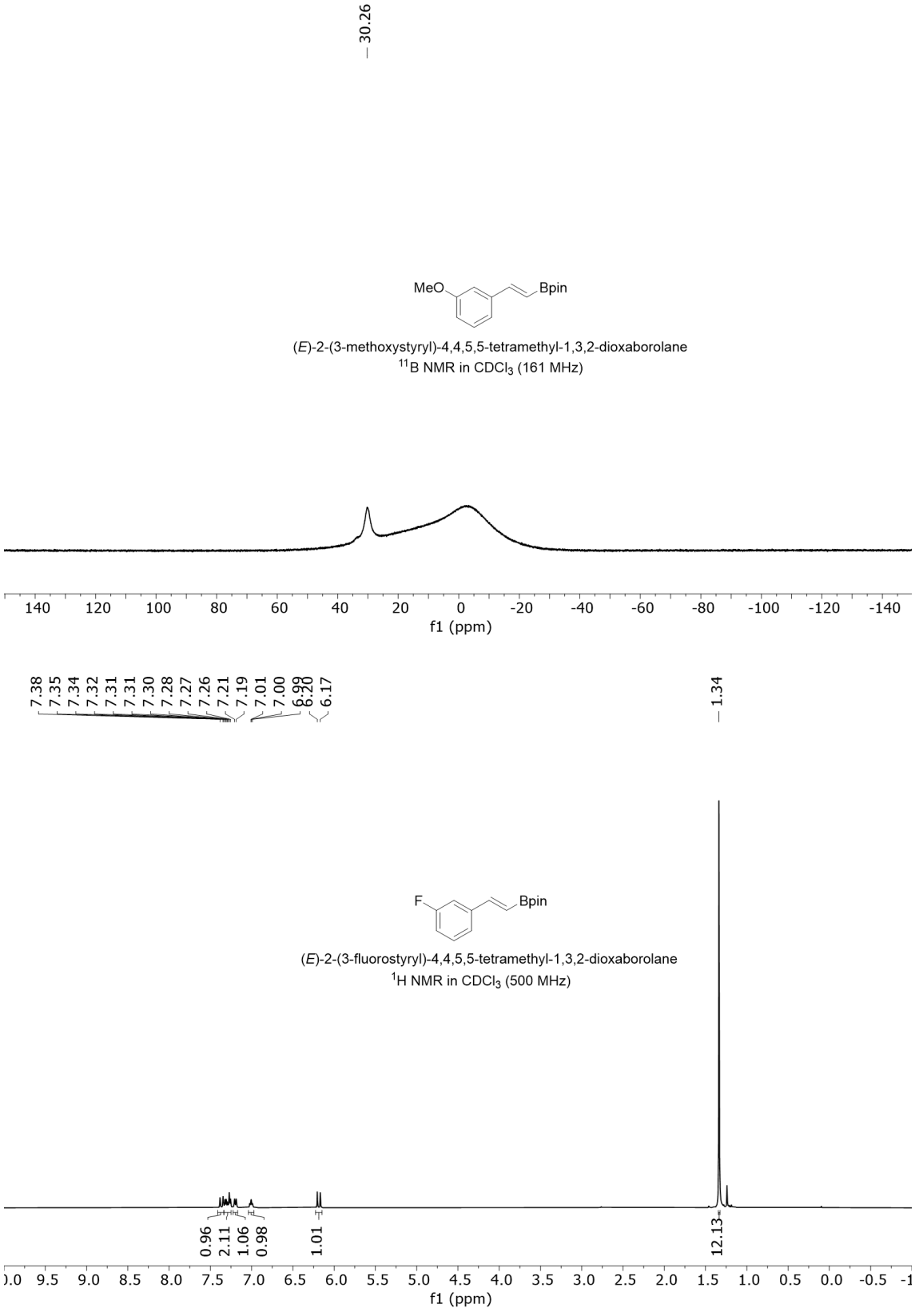
(*E*)-4,4,5,5-tetramethyl-2-(3-methylstyryl)-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (161 MHz)

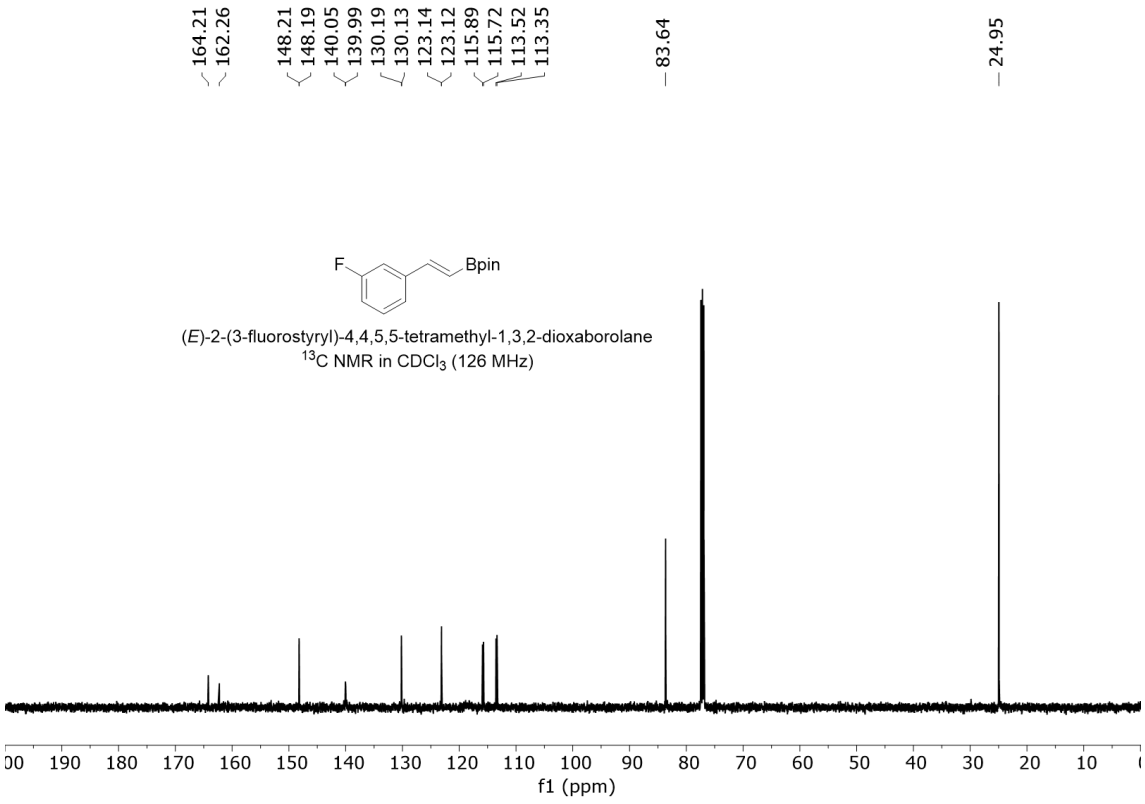


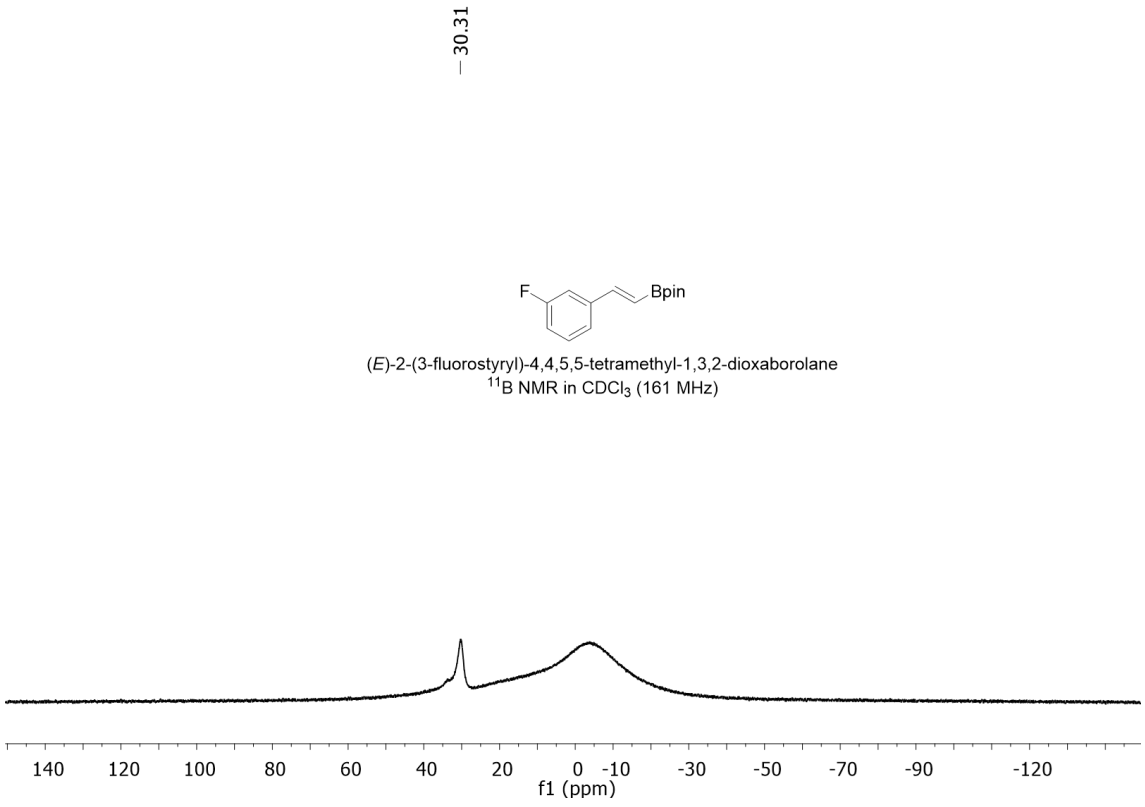
(*E*)-2-(3-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (500 MHz)

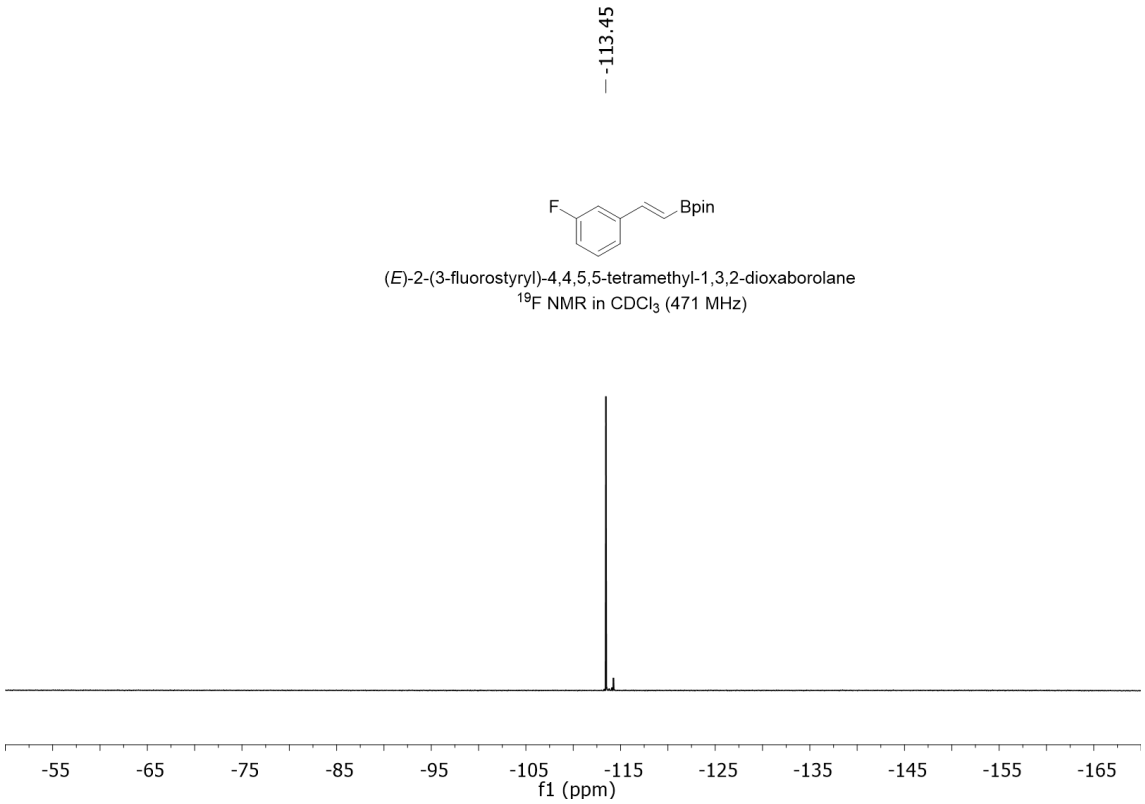


(*E*)-2-(3-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)

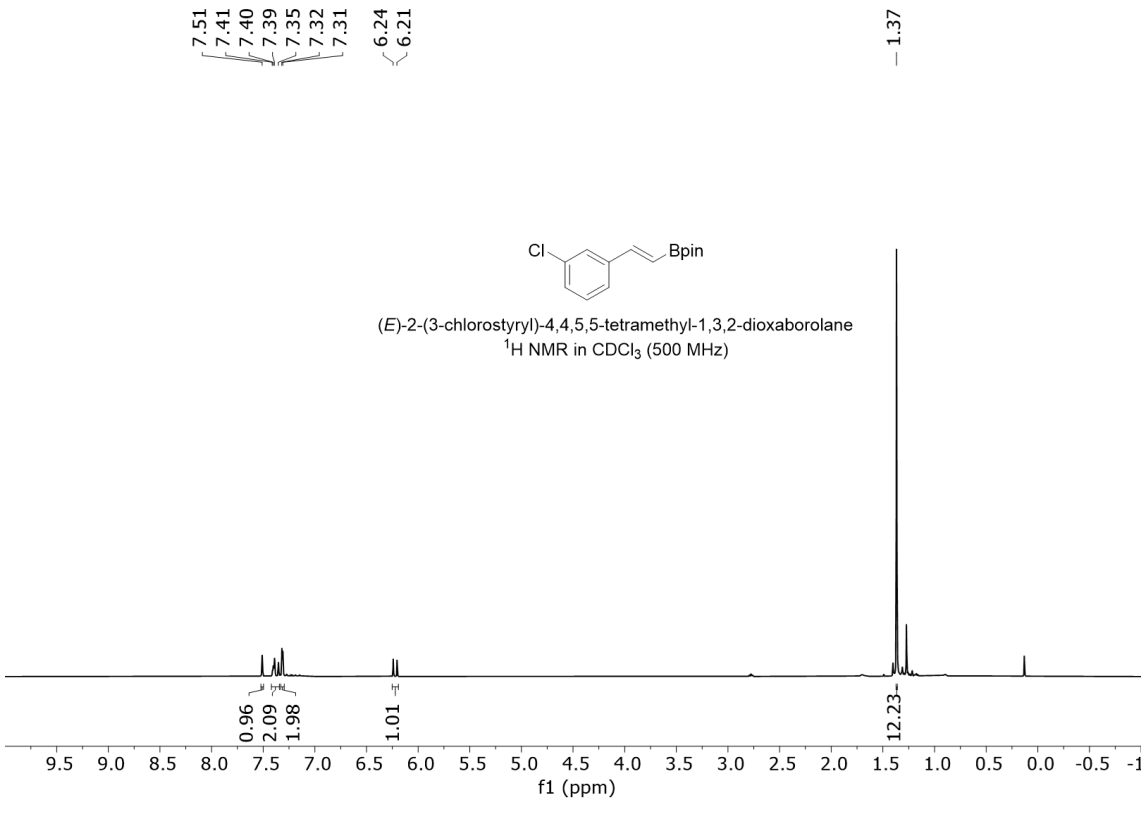

30.26
MeO
Bpin
(E)-2-(3-methoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
11B NMR in CDCl3 (161 MHz)
140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140
f1 (ppm)
7.38
7.35
7.34
7.32
7.31
7.31
7.30
7.28
7.27
7.26
7.21
7.19
7.01
7.00
6.99
6.20
6.17
1.34
F
Bpin
(E)-2-(3-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
0.96
2.11
1.06
0.98
1.01
12.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


164.21
162.26
148.21
148.19
140.05
139.99
130.19
130.13
123.14
123.12
115.89
115.72
113.52
113.35
83.64
24.95
F
Bpin
(E)-2-(3-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

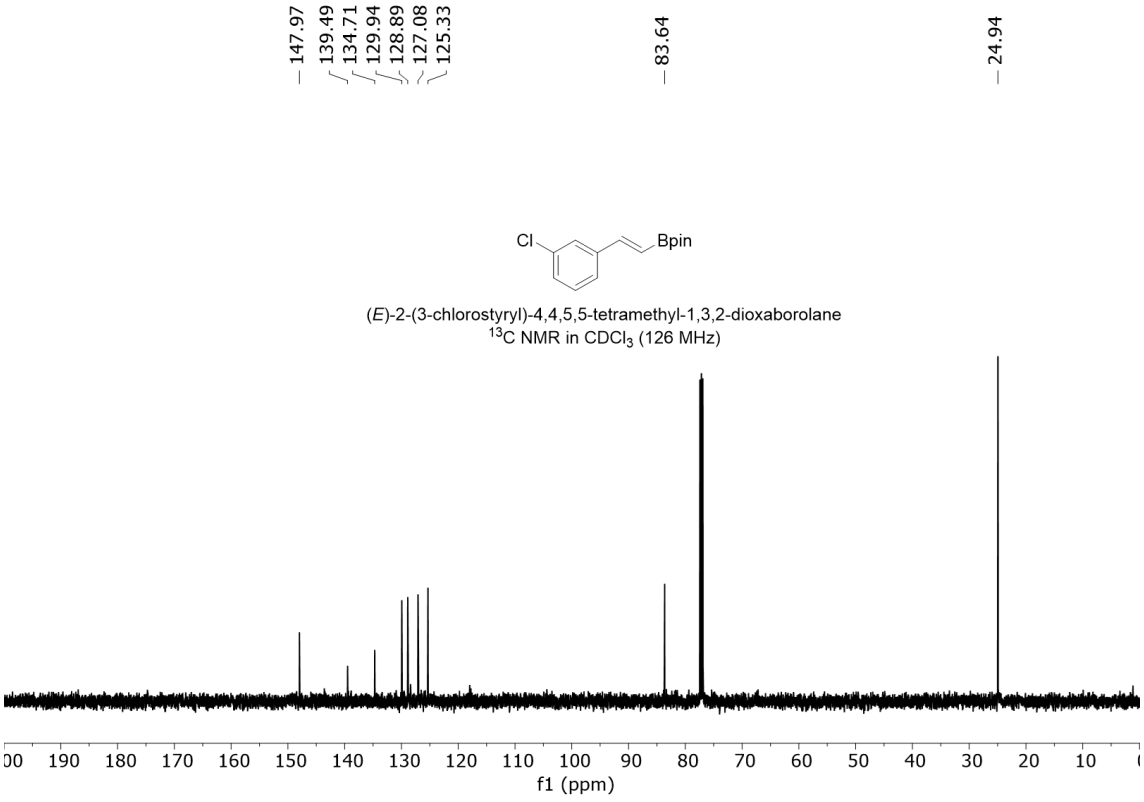

30.31
F
Bpin
(E)-2-(3-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
11B NMR in CDCl3 (161 MHz)
f1 (ppm)



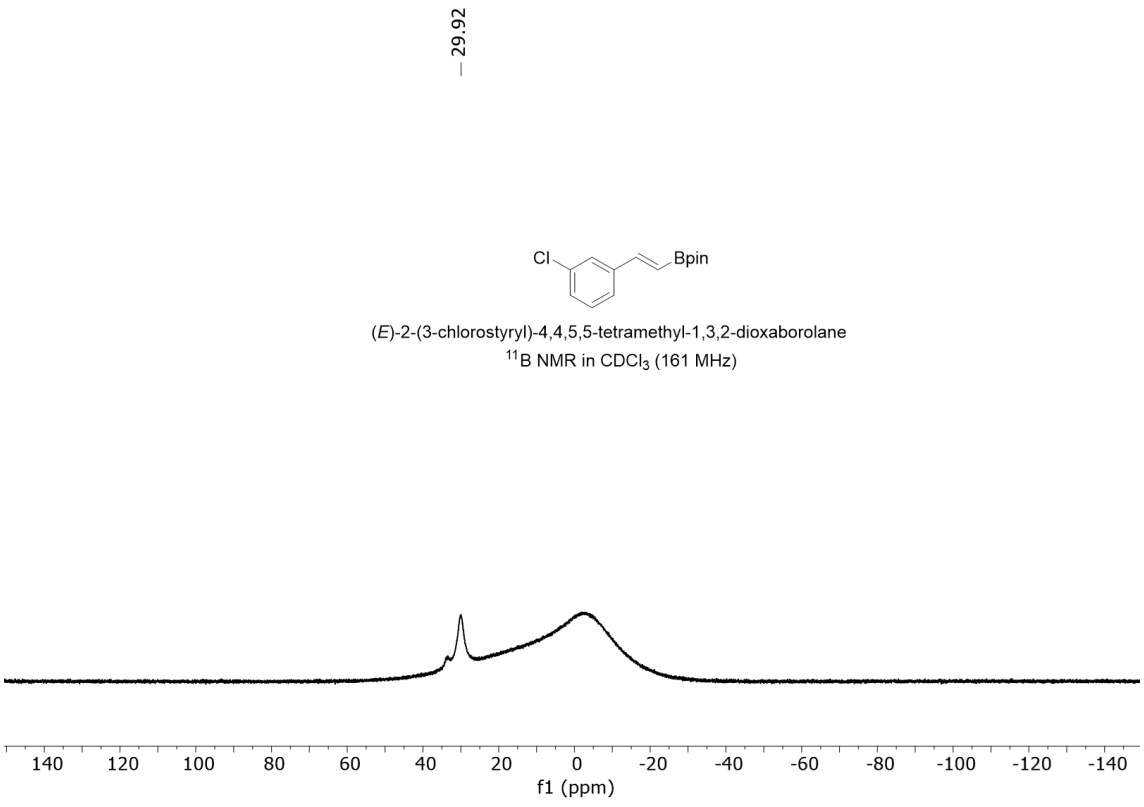
(*E*)-2-(3-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{19}F NMR in $CDCl_3$ (471 MHz)



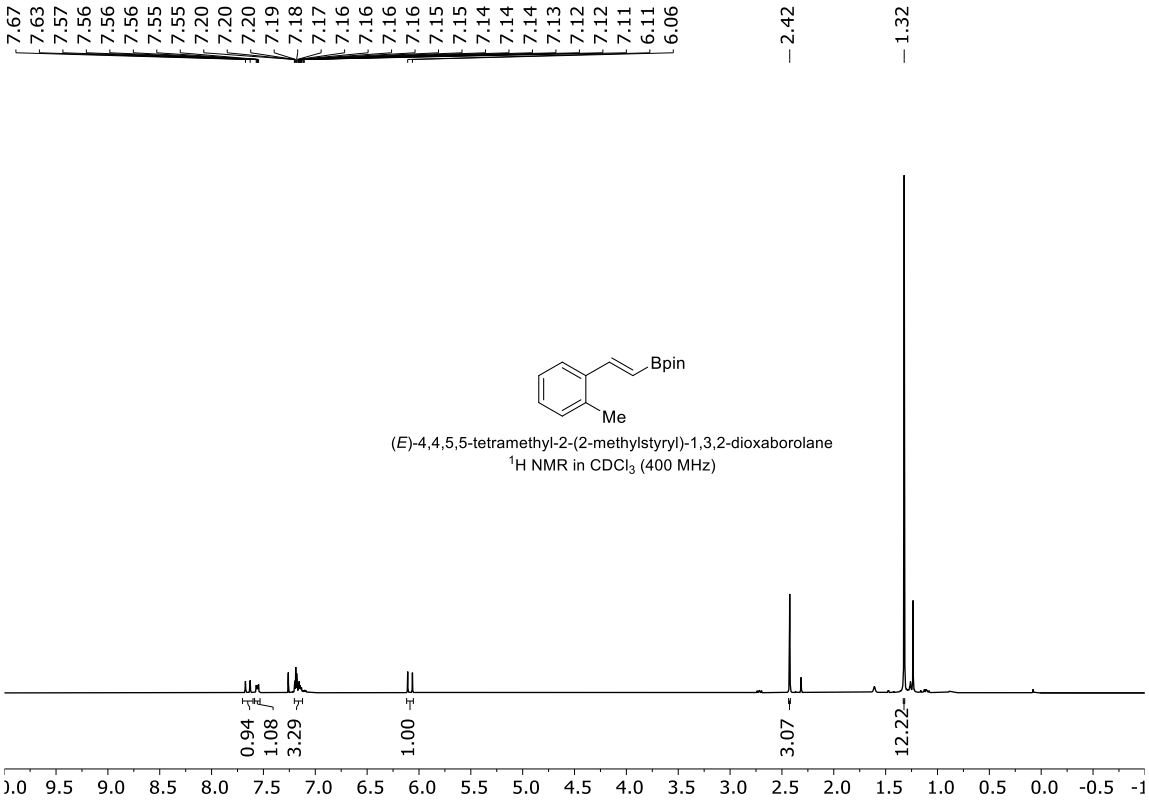
(*E*)-2-(3-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (500 MHz)

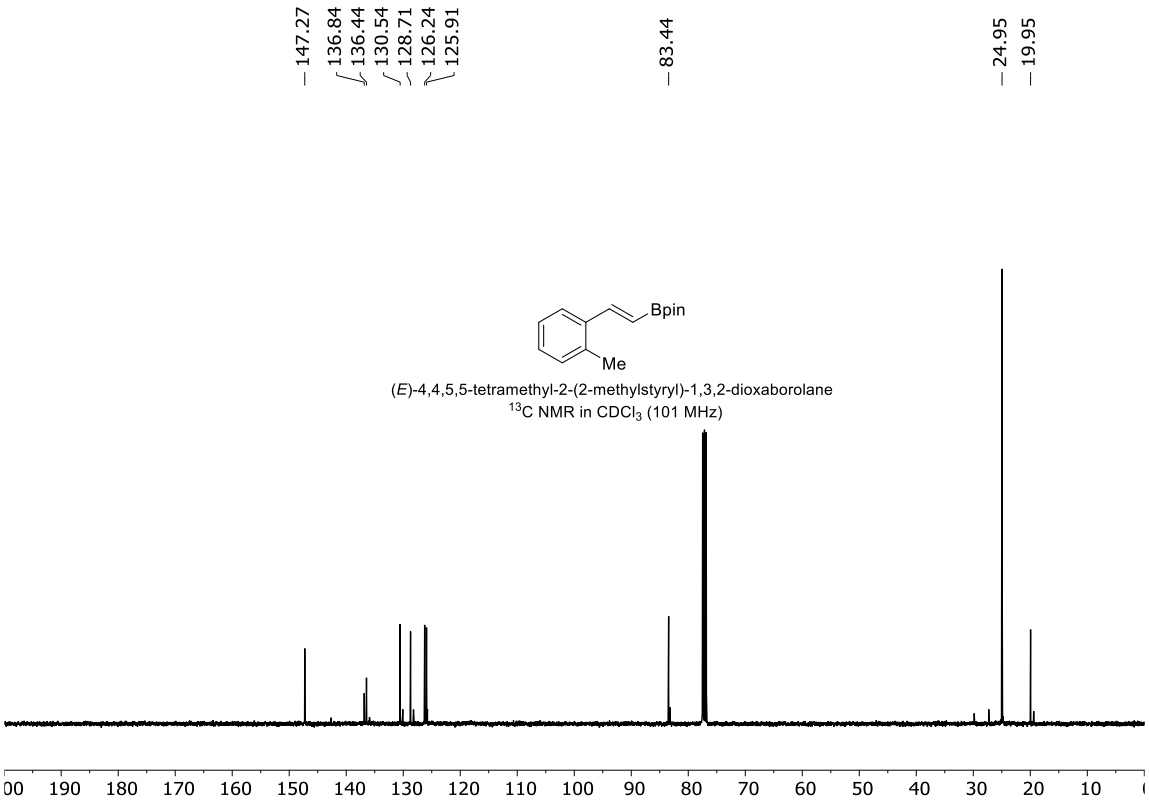


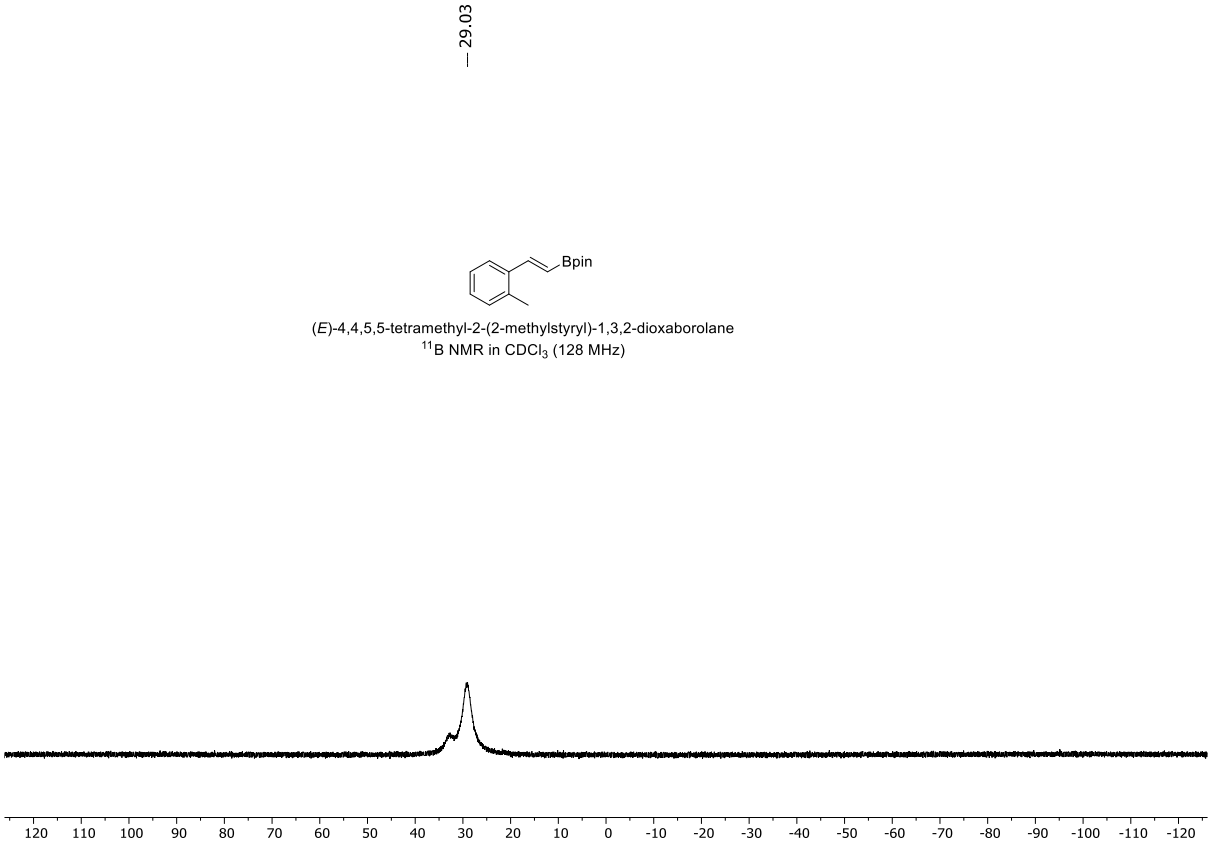
(*E*)-2-(3-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)



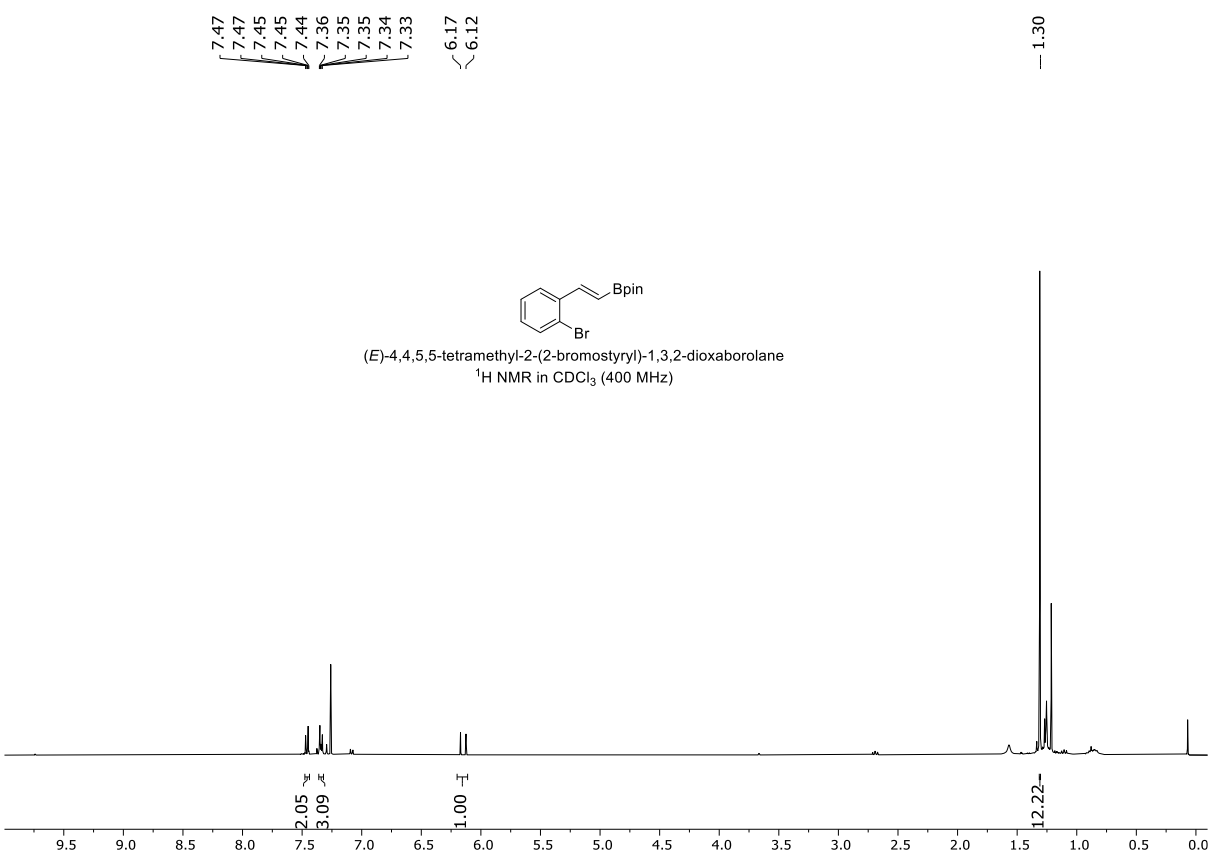
(*E*)-2-(3-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (161 MHz)


7.67
7.63
7.57
7.56
7.56
7.56
7.55
7.55
7.20
7.20
7.20
7.19
7.18
7.17
7.16
7.16
7.16
7.16
7.15
7.15
7.14
7.14
7.14
7.13
7.12
7.12
7.11
6.11
6.06
2.42
1.32
Bpin
Me
(E)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane
1H NMR in CDCl3 (400 MHz)
0.94
1.08
3.29
1.00
3.07
12.22
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1

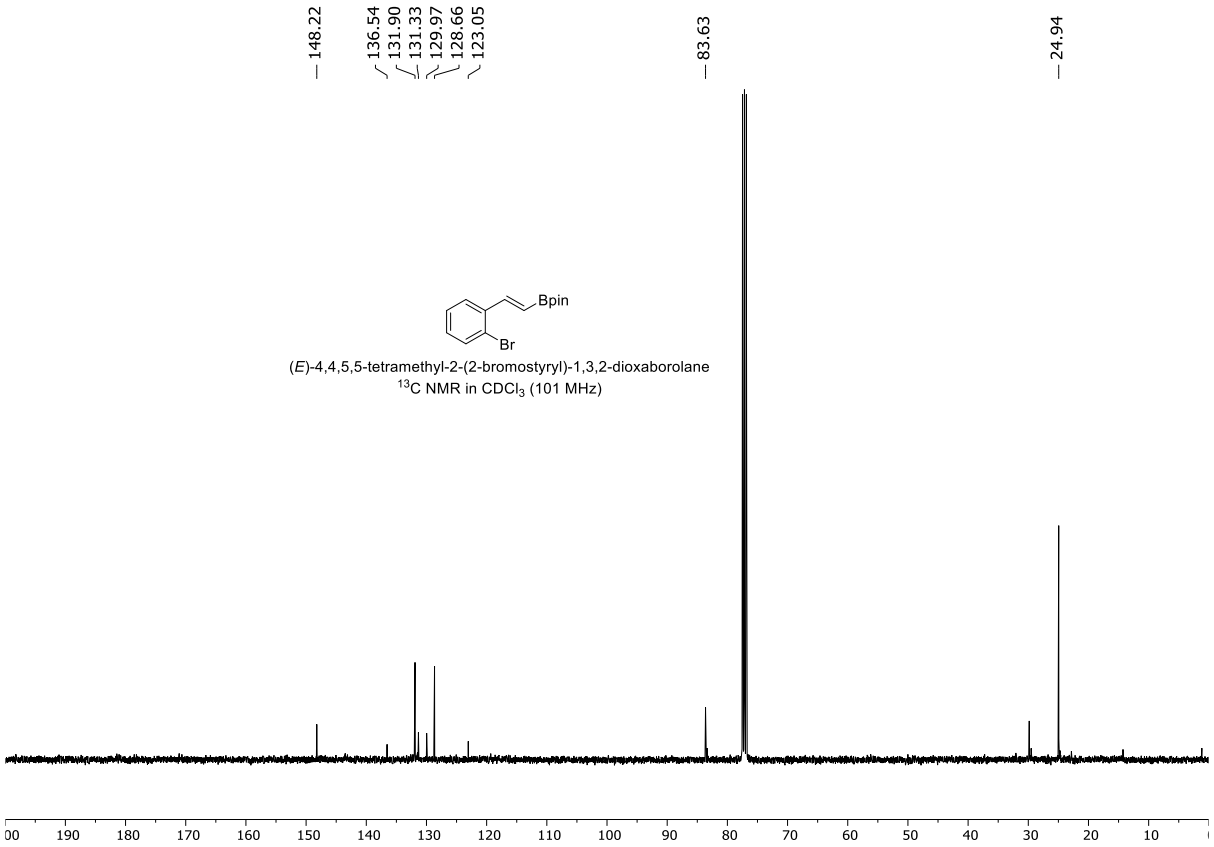

147.27
136.84
136.44
130.54
128.71
126.24
125.91
83.44
24.95
19.95
Bpin
Me
(E)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane
13C NMR in CDCl3 (101 MHz)
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10



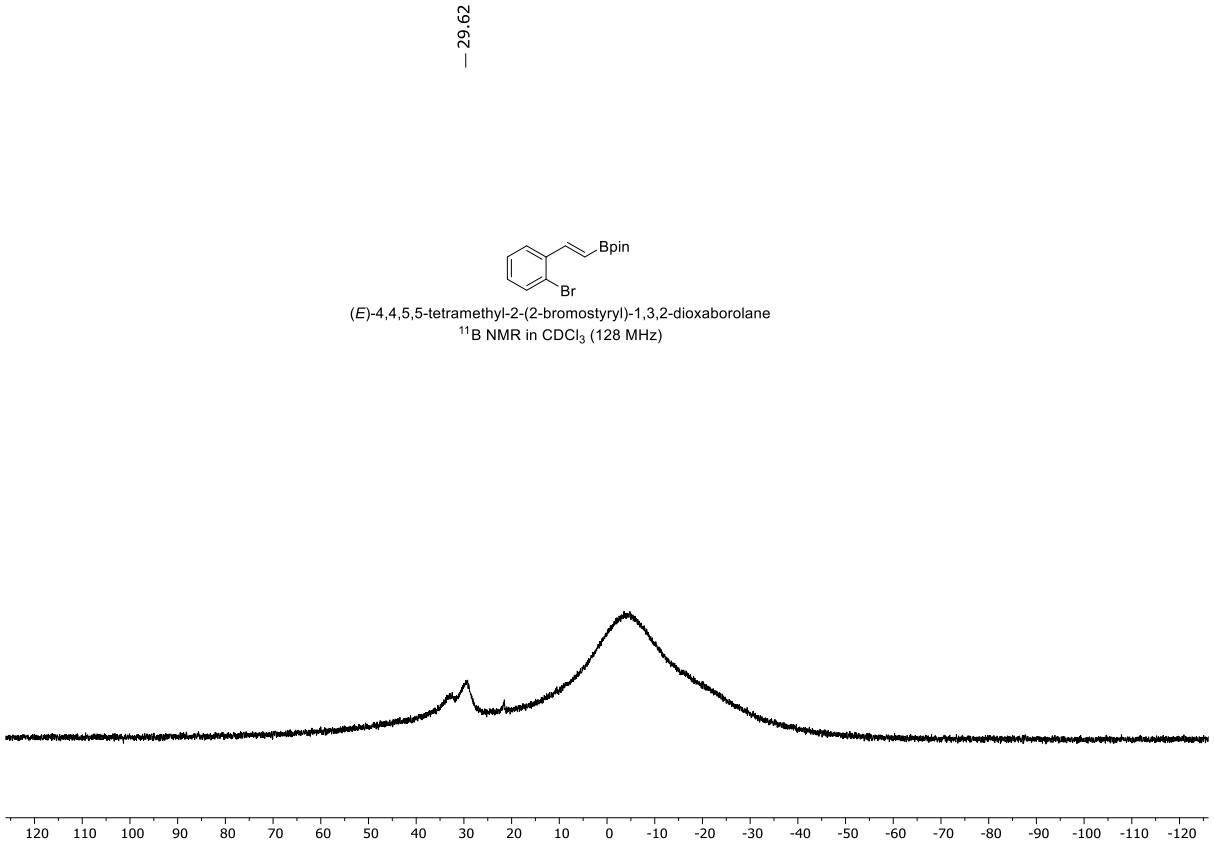
(*E*)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (128 MHz)



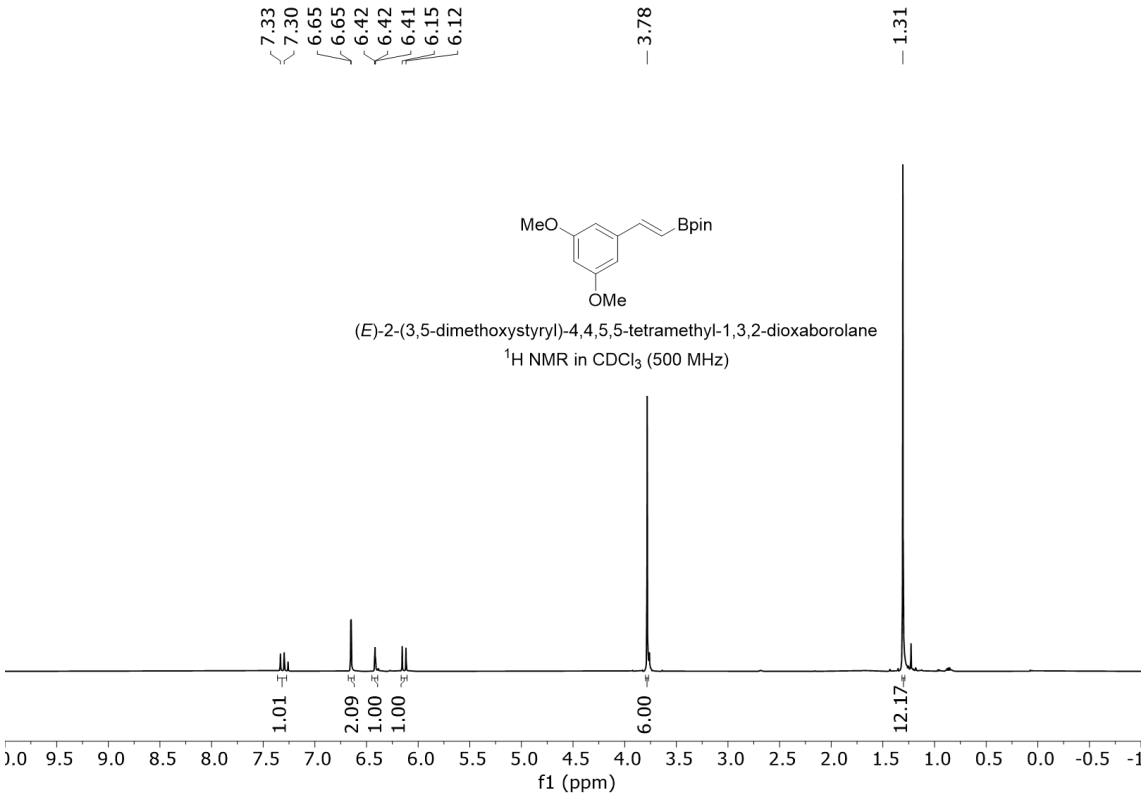
(*E*)-4,4,5,5-tetramethyl-2-(2-bromostyryl)-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (400 MHz)

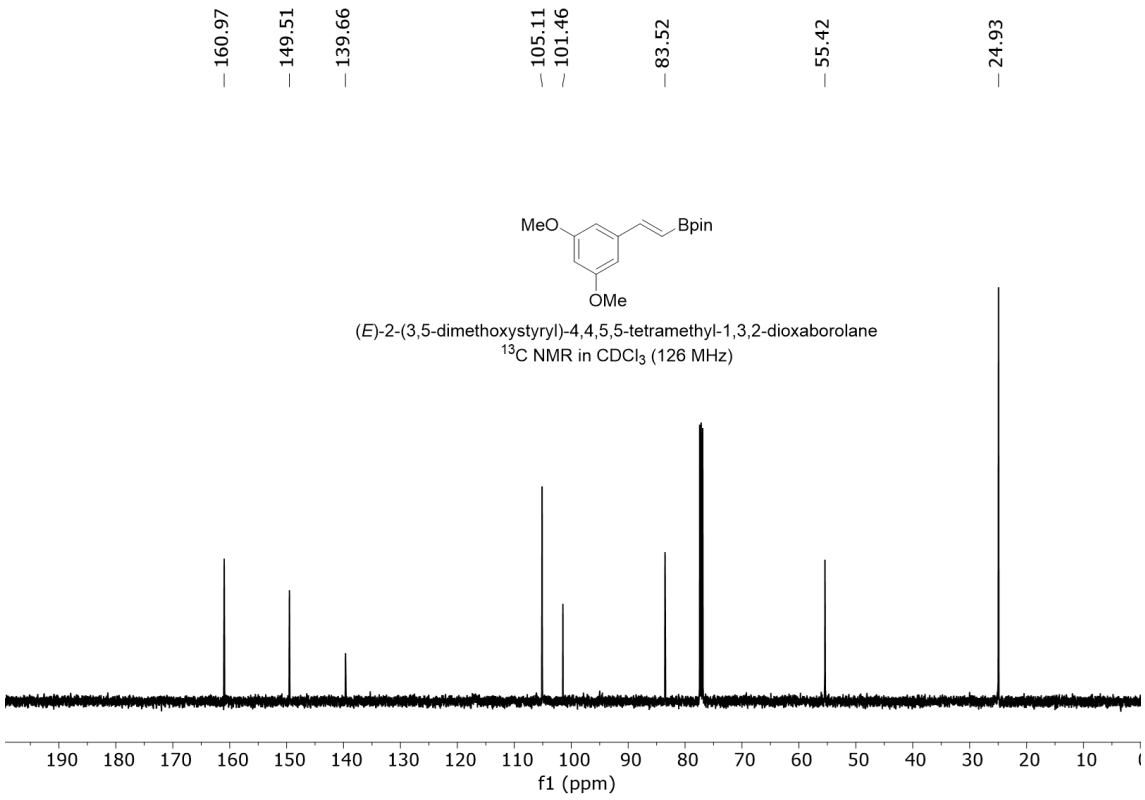


(*E*)-4,4,5,5-tetramethyl-2-(2-bromostyryl)-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (101 MHz)

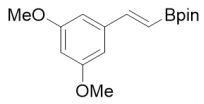


(*E*)-4,4,5,5-tetramethyl-2-(2-bromostyryl)-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (128 MHz)

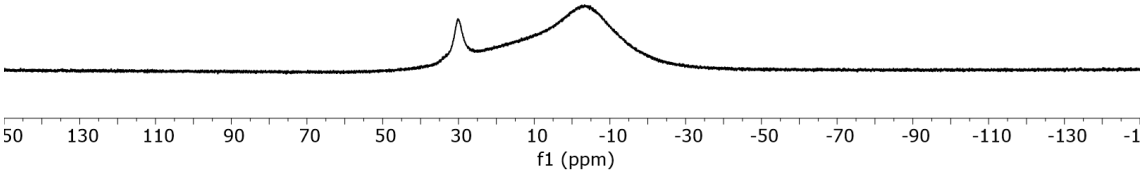

7.33
7.30
6.65
6.65
6.42
6.42
6.41
6.15
6.12
3.78
1.31
MeO
Bpin
OMe
(E)-2-(3,5-dimethoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
1.01
2.09
1.00
1.00
6.00
12.17
f1 (ppm)


160.97
149.51
139.66
105.11
101.46
83.52
55.42
24.93
MeO
Bpin
OMe
(E)-2-(3,5-dimethoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

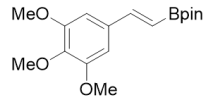
30.21



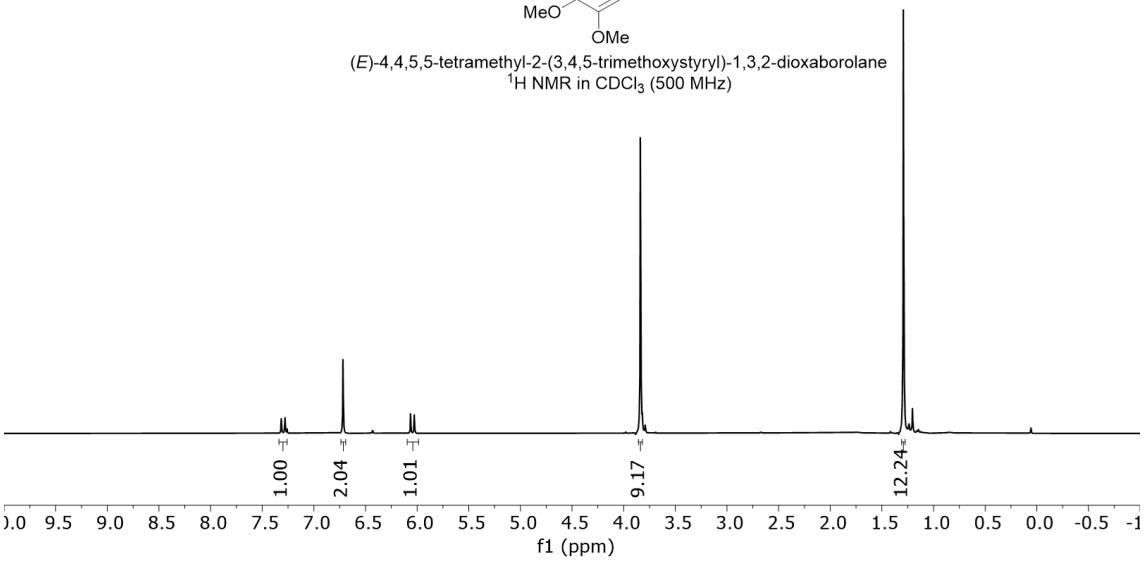
(*E*)-2-(3,5-dimethoxystyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (161 MHz)

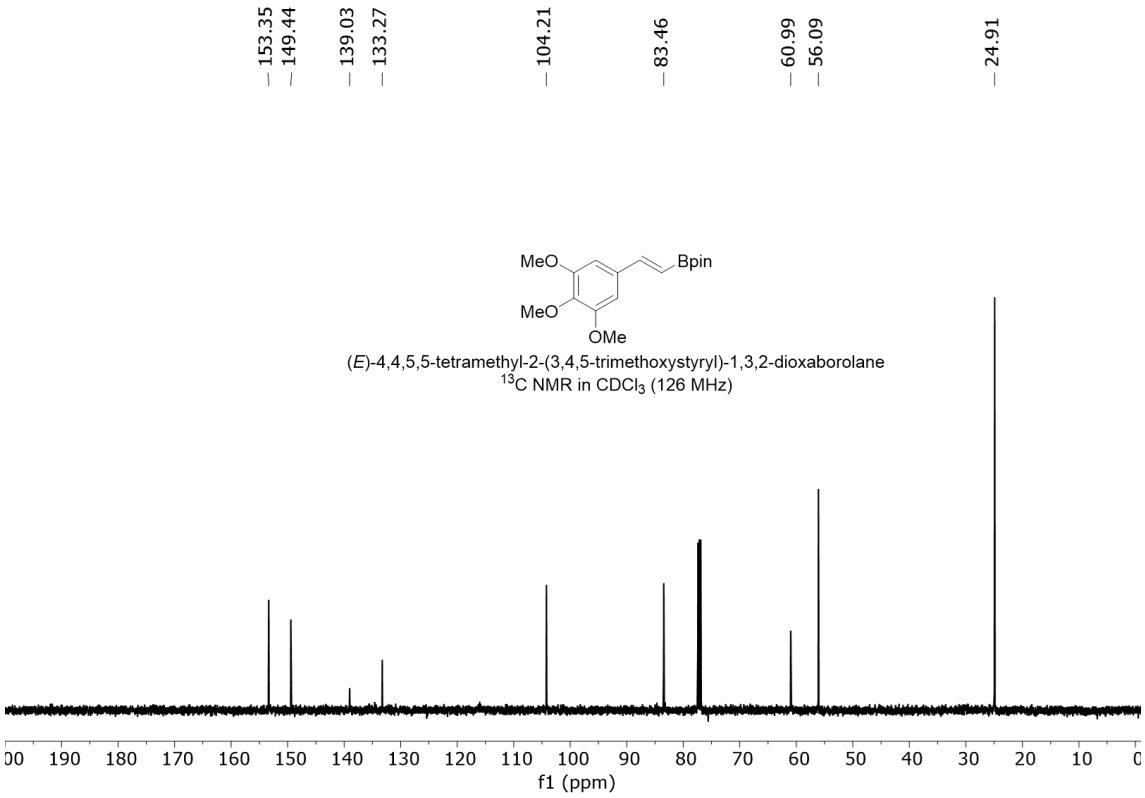


7.32
7.28
6.72
6.06
6.03
3.84
1.29

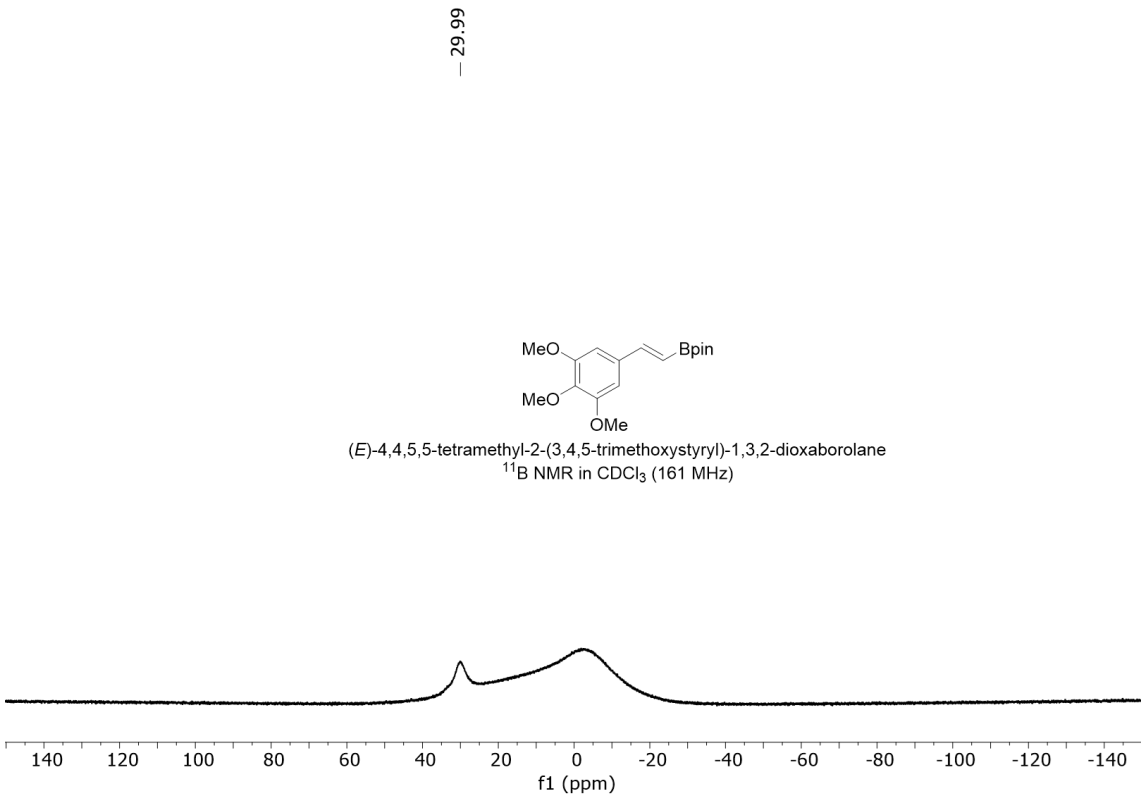


(*E*)-4,4,5,5-tetramethyl-2-(3,4,5-trimethoxystyryl)-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (500 MHz)

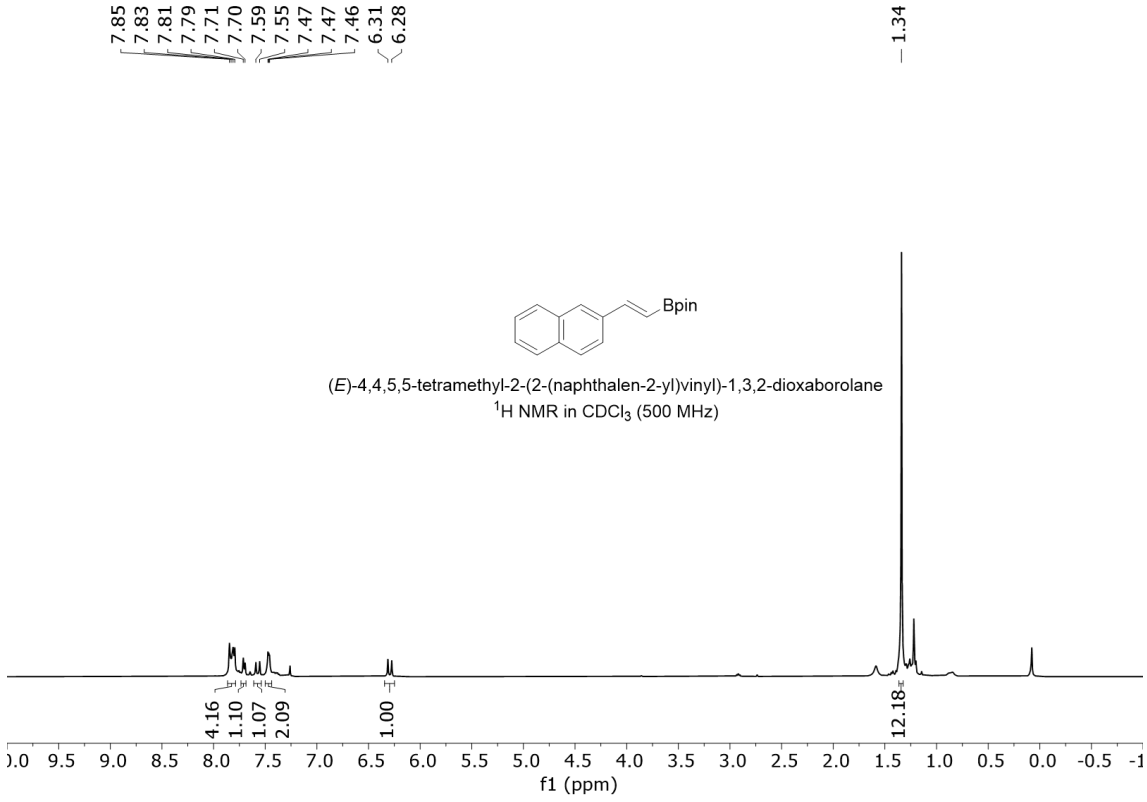


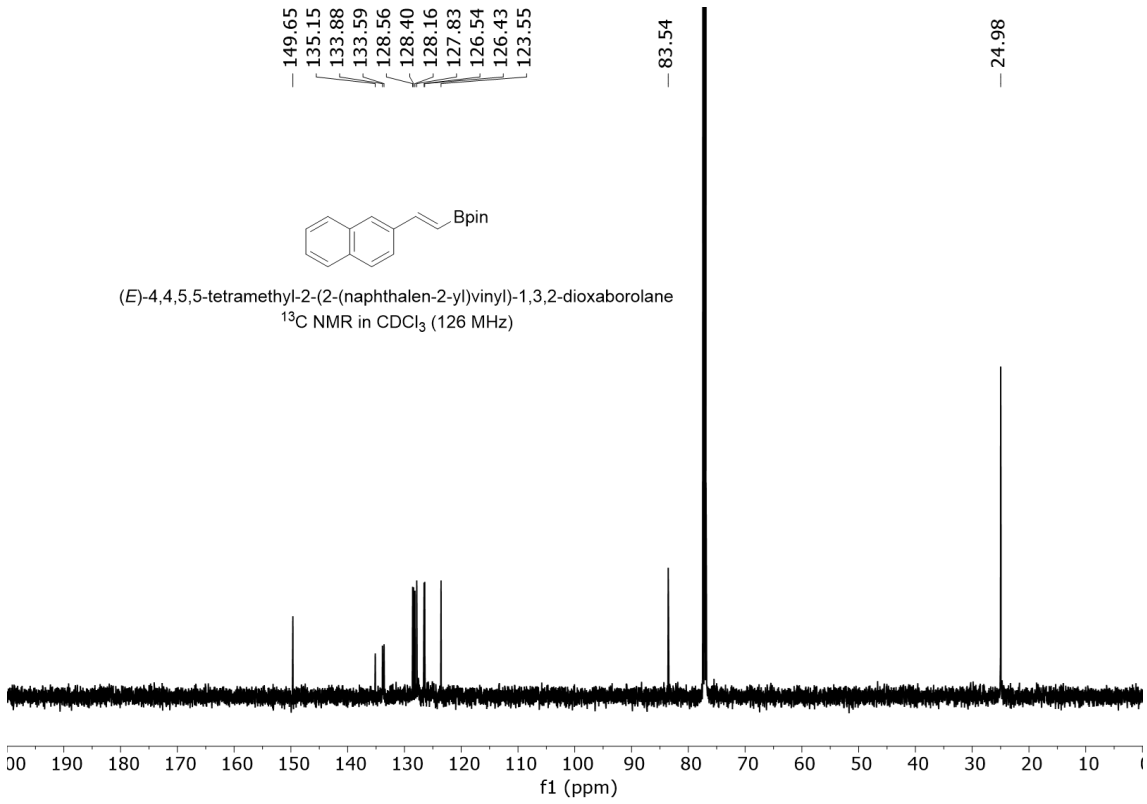


(*E*)-4,4,5,5-tetramethyl-2-(3,4,5-trimethoxystyryl)-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)

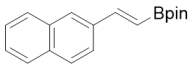


(*E*)-4,4,5,5-tetramethyl-2-(3,4,5-trimethoxystyryl)-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (161 MHz)


7.85
7.83
7.81
7.79
7.71
7.70
7.59
7.55
7.47
7.47
7.46
6.31
6.28
1.34
Bpin
(E)-4,4,5,5-tetramethyl-2-(2-(naphthalen-2-yl)vinyl)-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
4.16
1.10
1.07
2.09
1.00
12.18
f1 (ppm)

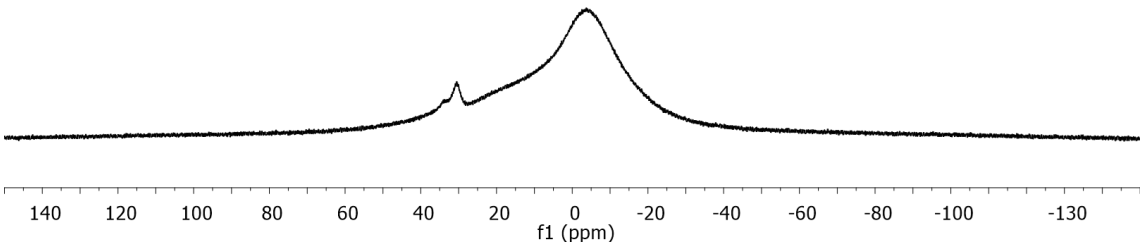

149.65
135.15
133.88
133.59
128.56
128.40
128.16
127.83
126.54
126.43
123.55
83.54
24.98
Bpin
(E)-4,4,5,5-tetramethyl-2-(2-(naphthalen-2-yl)vinyl)-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

30.57



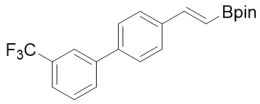
(*E*)-4,4,5,5-tetramethyl-2-(2-(naphthalen-2-yl)vinyl)-1,3,2-dioxaborolane

^{11}B NMR in $CDCl_3$ (161 MHz)



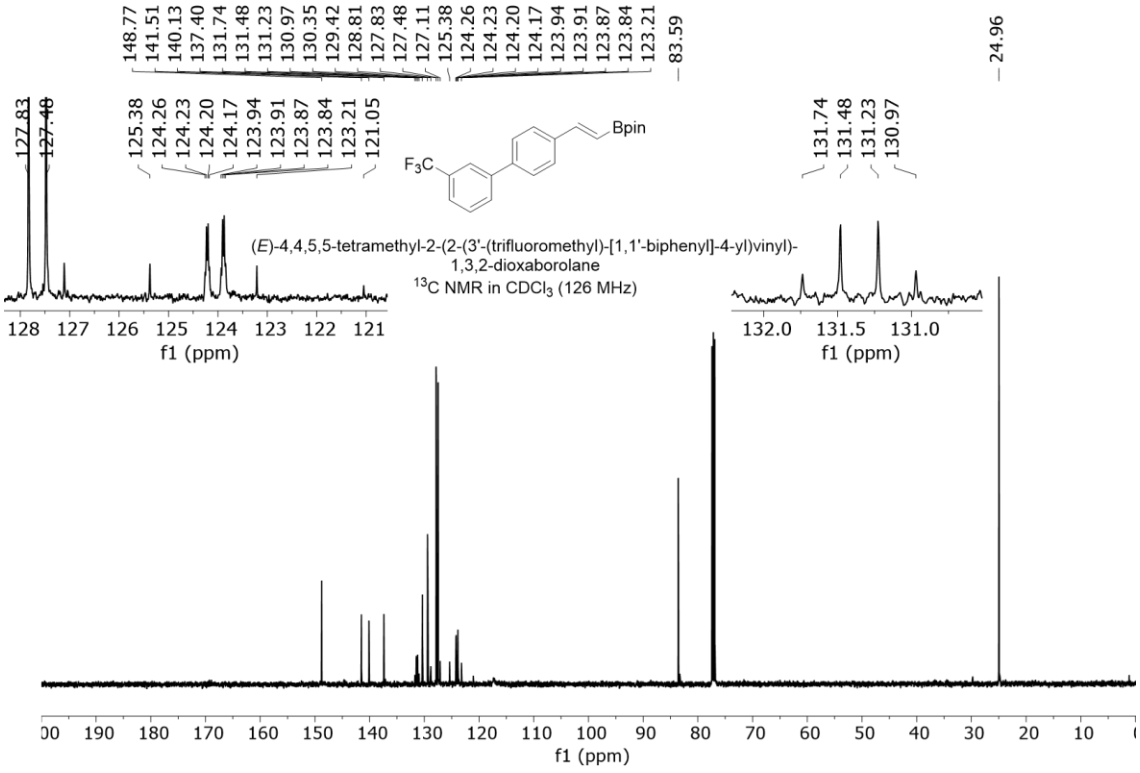
7.84
7.78
7.76
7.61
7.59
7.56
7.55
7.53
7.47
7.43
6.26
6.22

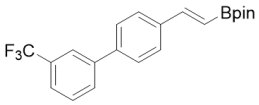
1.33



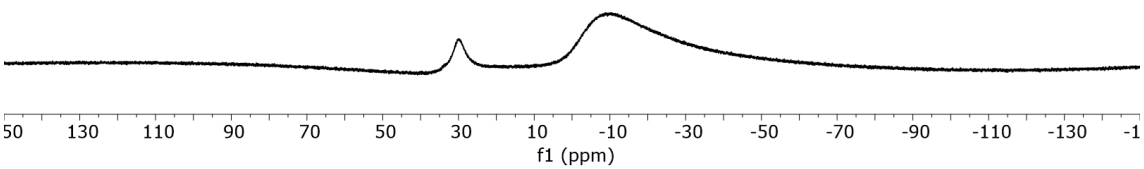
(*E*)-4,4,5,5-tetramethyl-2-(2-(3'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)vinyl)-1,3,2-dioxaborolane

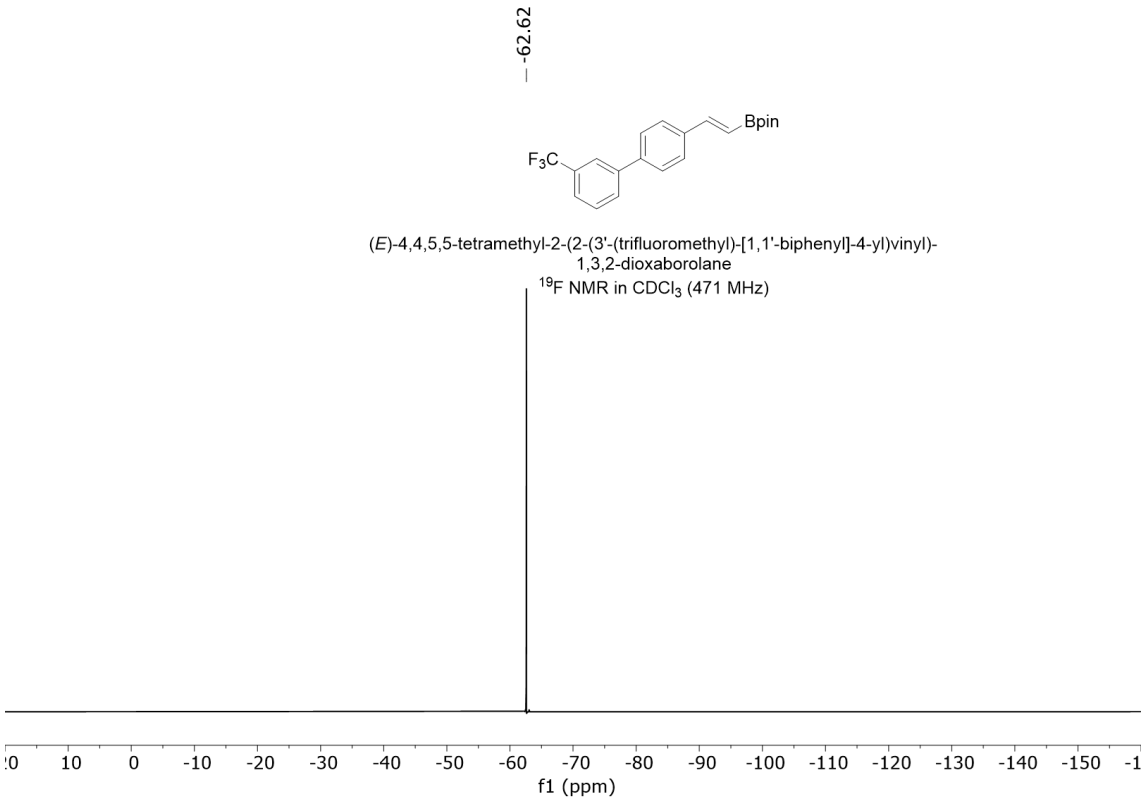
^{1}H NMR in $CDCl_3$ (500 MHz)

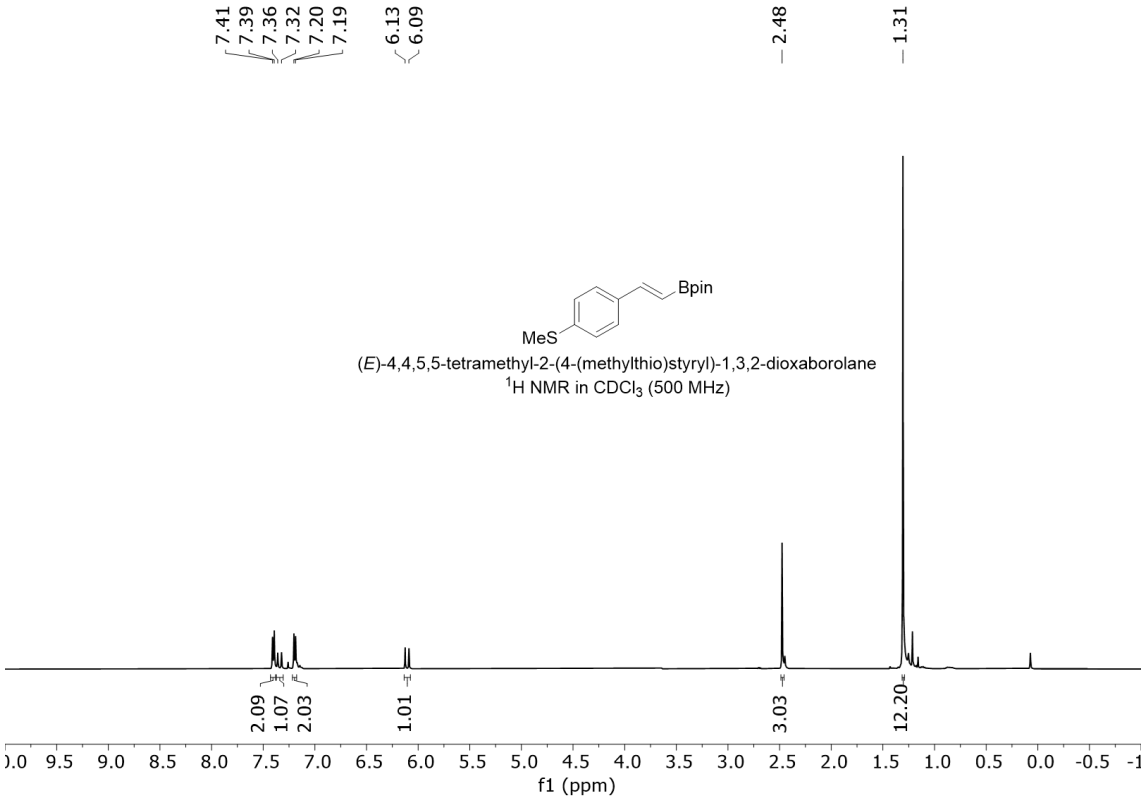


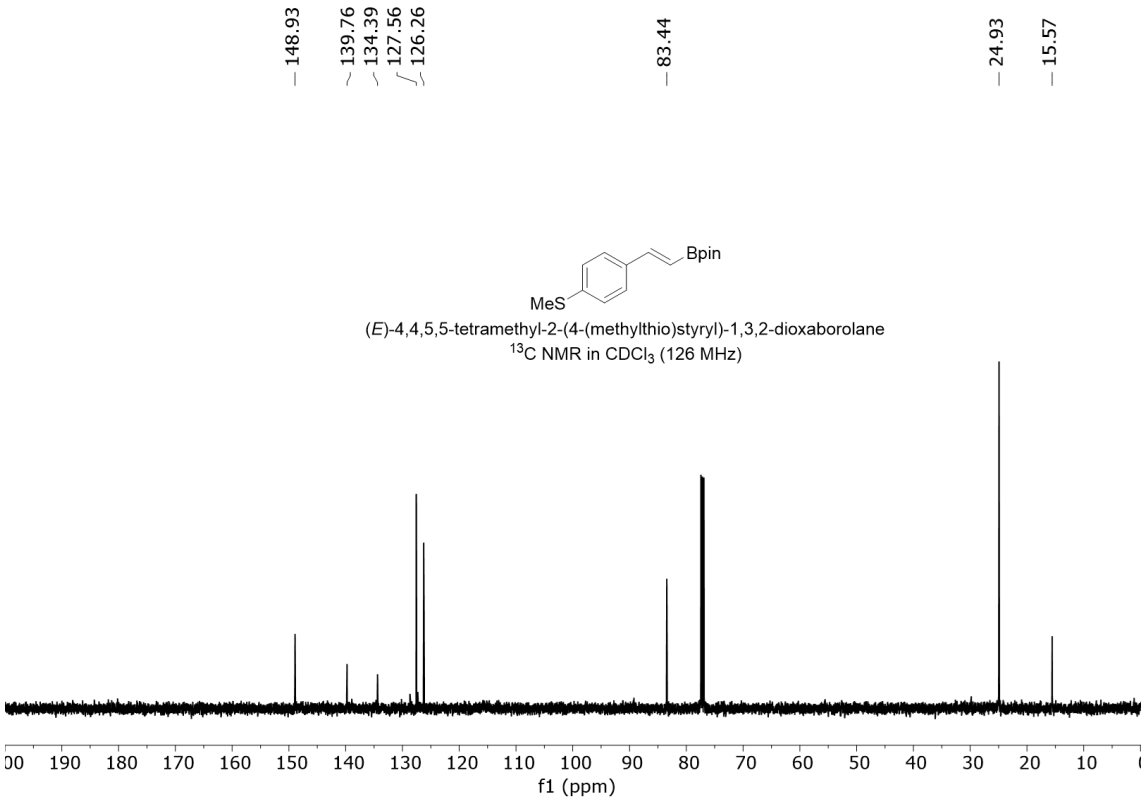


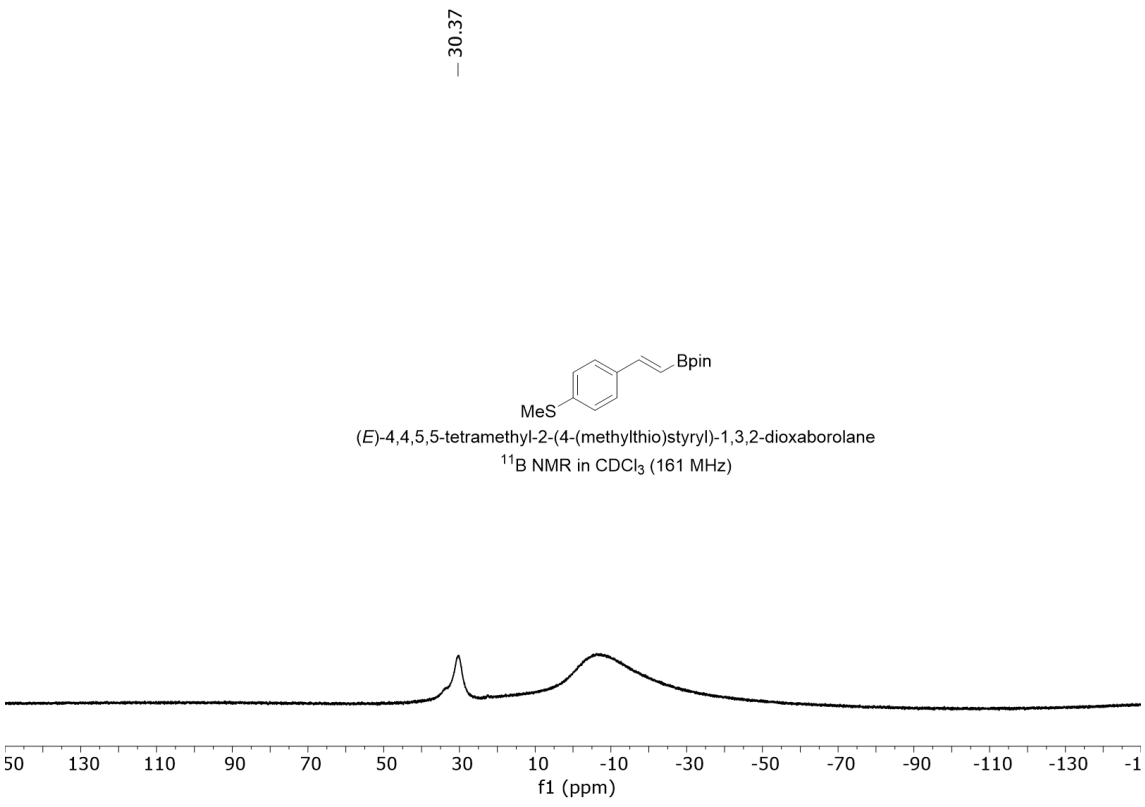
(*E*)-4,4,5,5-tetramethyl-2-(2-(3'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)vinyl)-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (500 MHz)

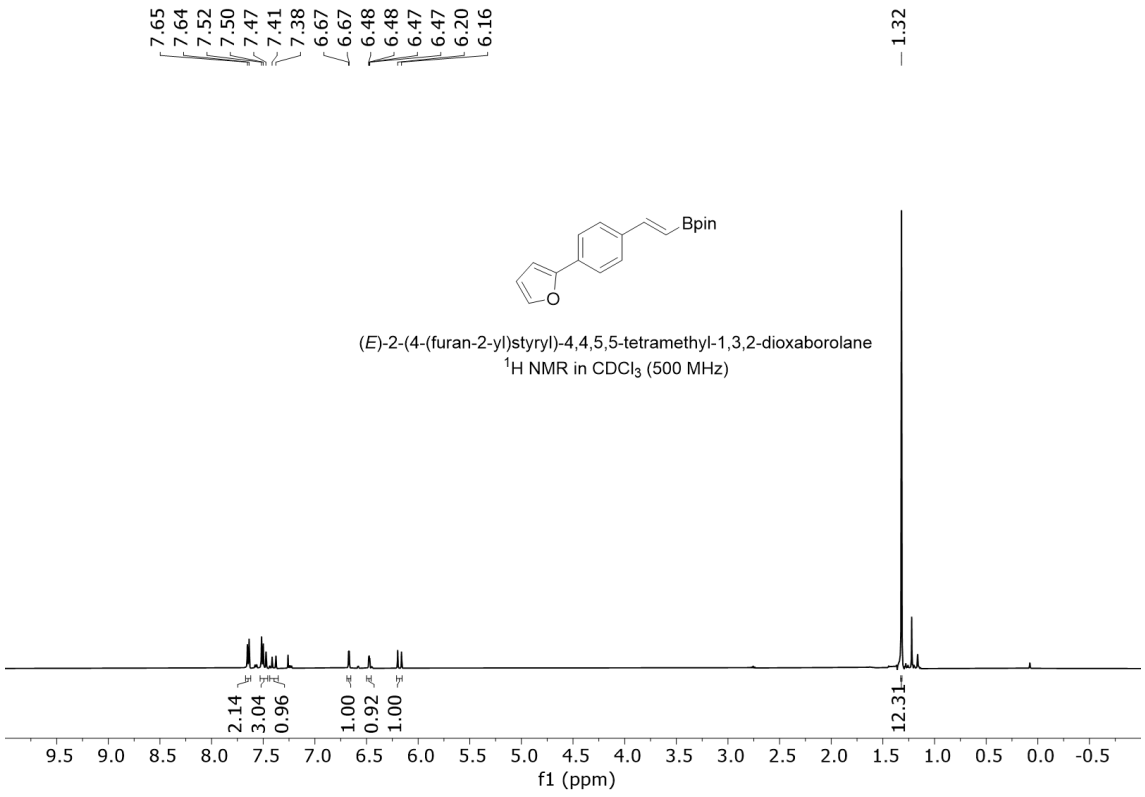


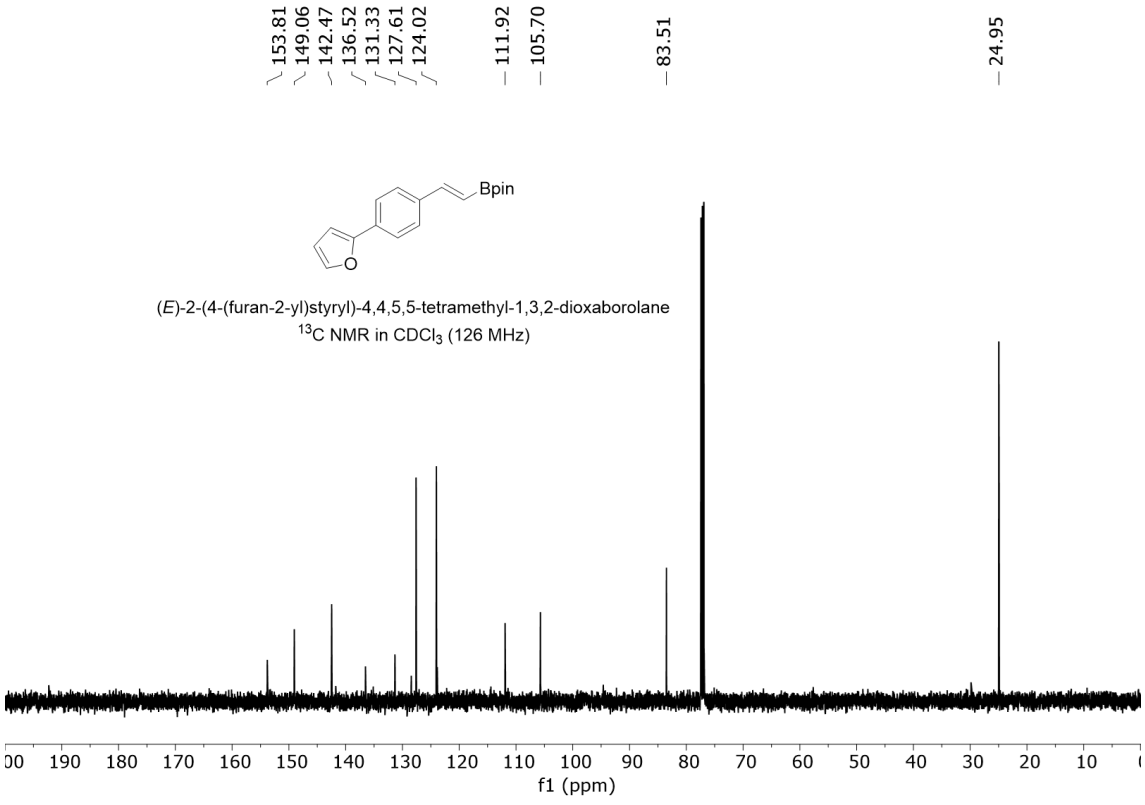

-62.62
Bpin
F3C
(E)-4,4,5,5-tetramethyl-2-(2-(3'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)vinyl)-1,3,2-dioxaborolane
19F NMR in CDCl3 (471 MHz)
f1 (ppm)

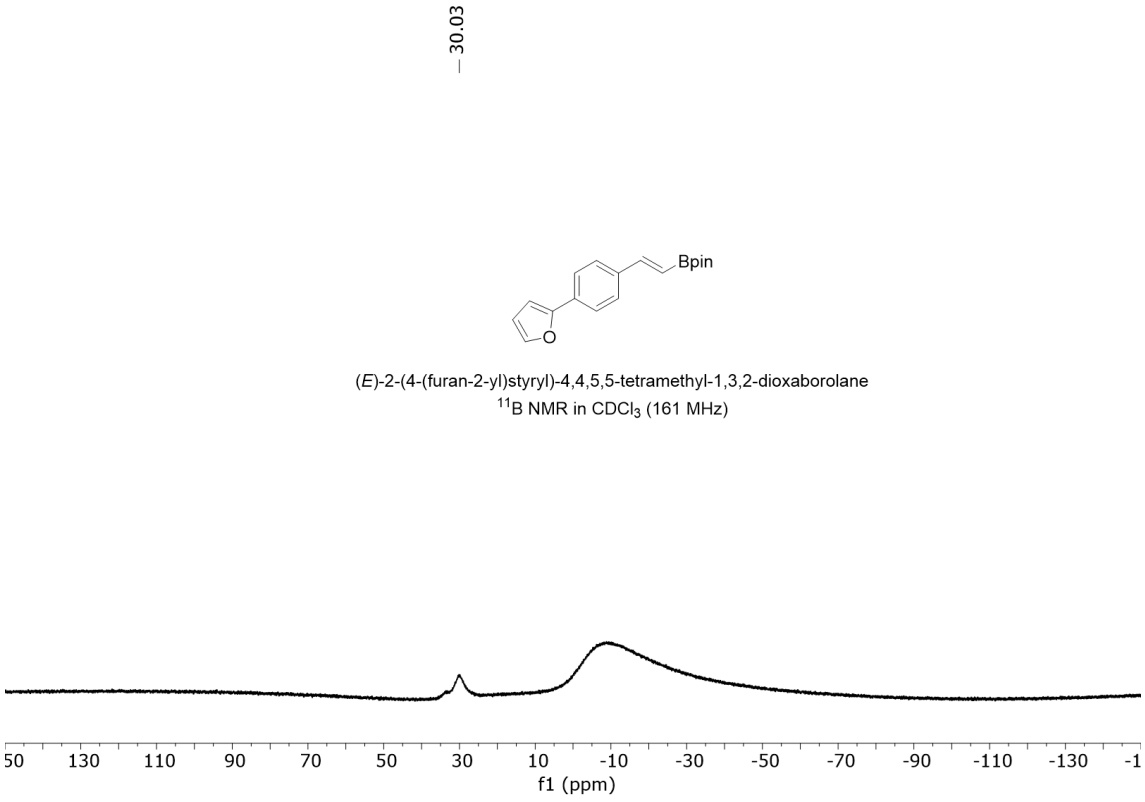

7.41
7.39
7.36
7.32
7.20
7.19
6.13
6.09
2.48
1.31
Bpin
MeS
(E)-4,4,5,5-tetramethyl-2-(4-(methylthio)styryl)-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
2.09
1.07
2.03
1.01
3.03
12.20
f1 (ppm)


148.93
139.76
134.39
127.56
126.26
83.44
24.93
15.57
Bpin
MeS
(E)-4,4,5,5-tetramethyl-2-(4-(methylthio)styryl)-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


30.37
Bpin
MeS
(E)-4,4,5,5-tetramethyl-2-(4-(methylthio)styryl)-1,3,2-dioxaborolane
11B NMR in CDCl3 (161 MHz)
f1 (ppm)

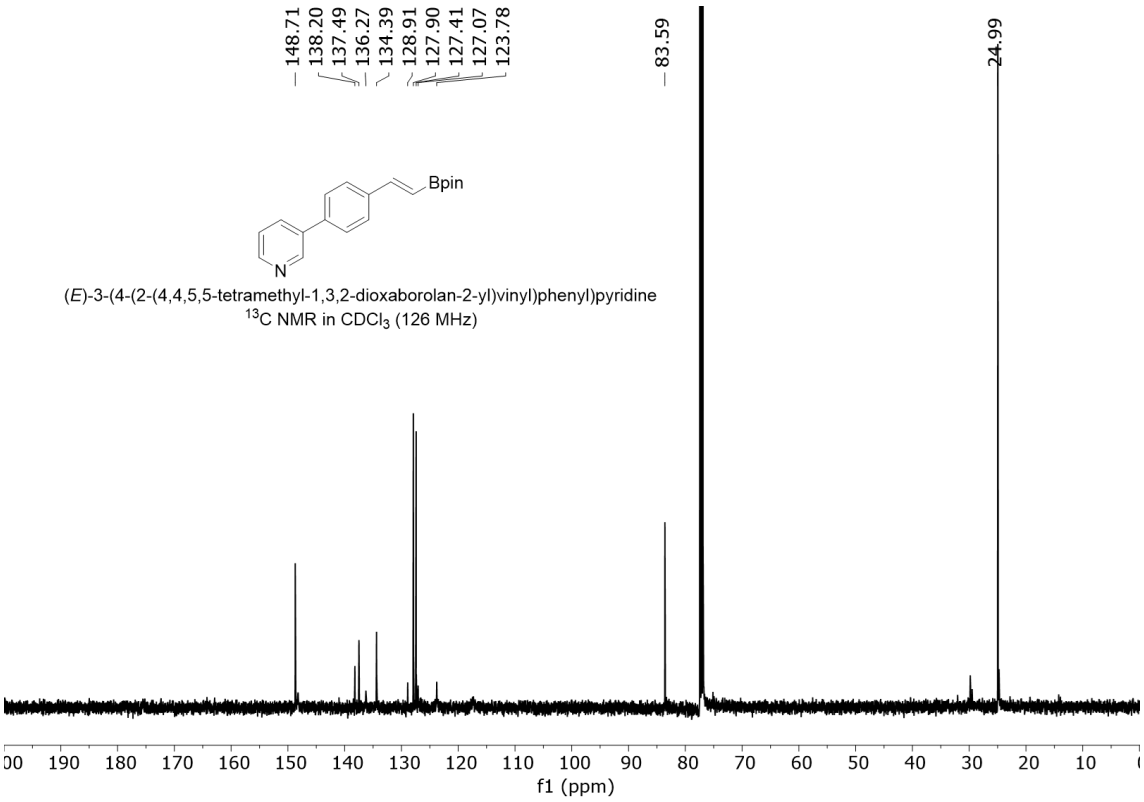

7.65
7.64
7.52
7.50
7.47
7.41
7.38
6.67
6.67
6.48
6.48
6.47
6.47
6.20
6.16
1.32
Bpin
O
(E)-2-(4-(furan-2-yl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
2.14
3.04
0.96
1.00
0.92
1.00
12.31
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


153.81
149.06
142.47
136.52
131.33
127.61
124.02
111.92
105.70
83.51
24.95
Bpin
O
(E)-2-(4-(furan-2-yl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
13C NMR in CDCl3 (126 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)



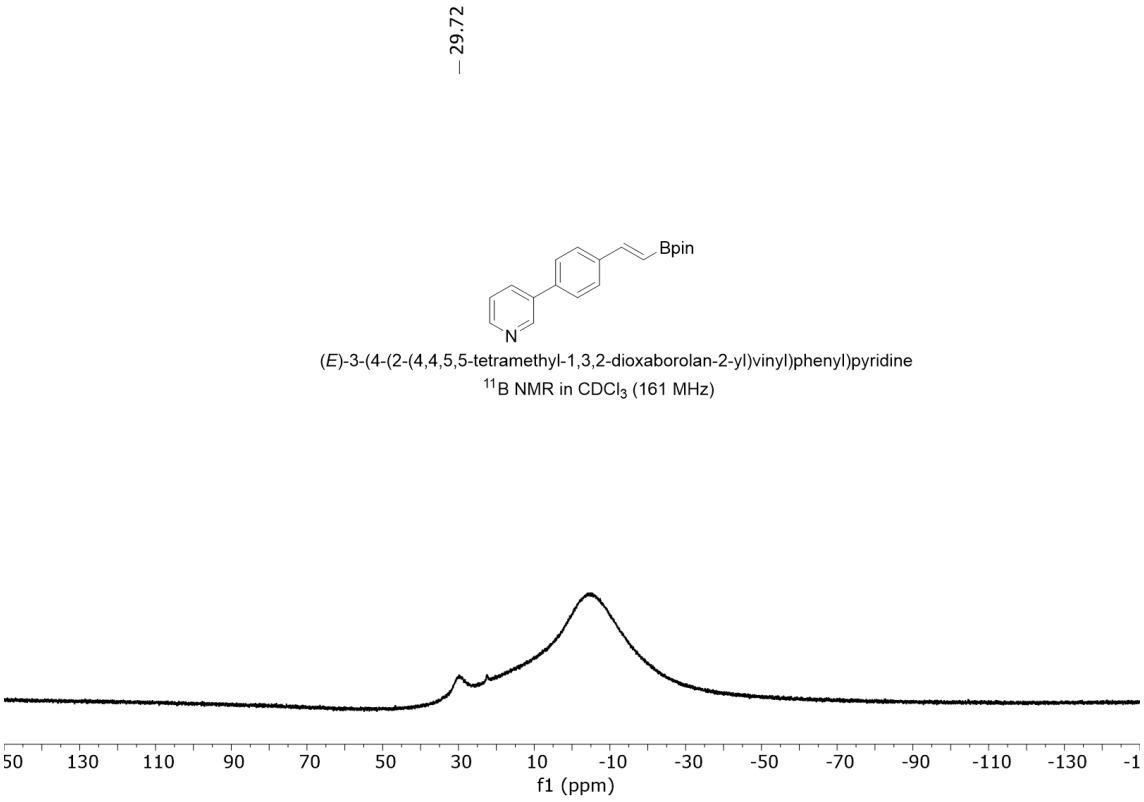
(*E*)-2-(4-(furan-2-yl)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (161 MHz)

(*E*)-3-(4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)phenyl)pyridine
^{1}H NMR in $CDCl_3$ (500 MHz)



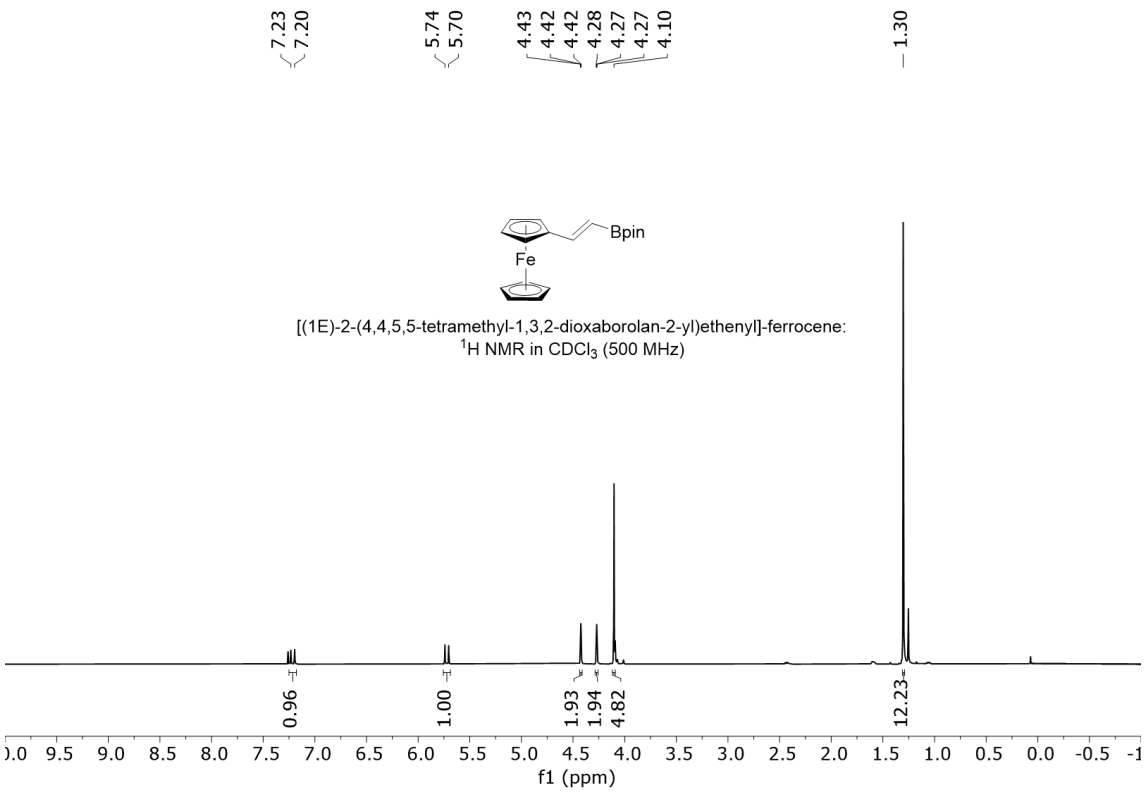
(*E*)-3-(4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)phenyl)pyridine

^{13}C NMR in $CDCl_3$ (126 MHz)

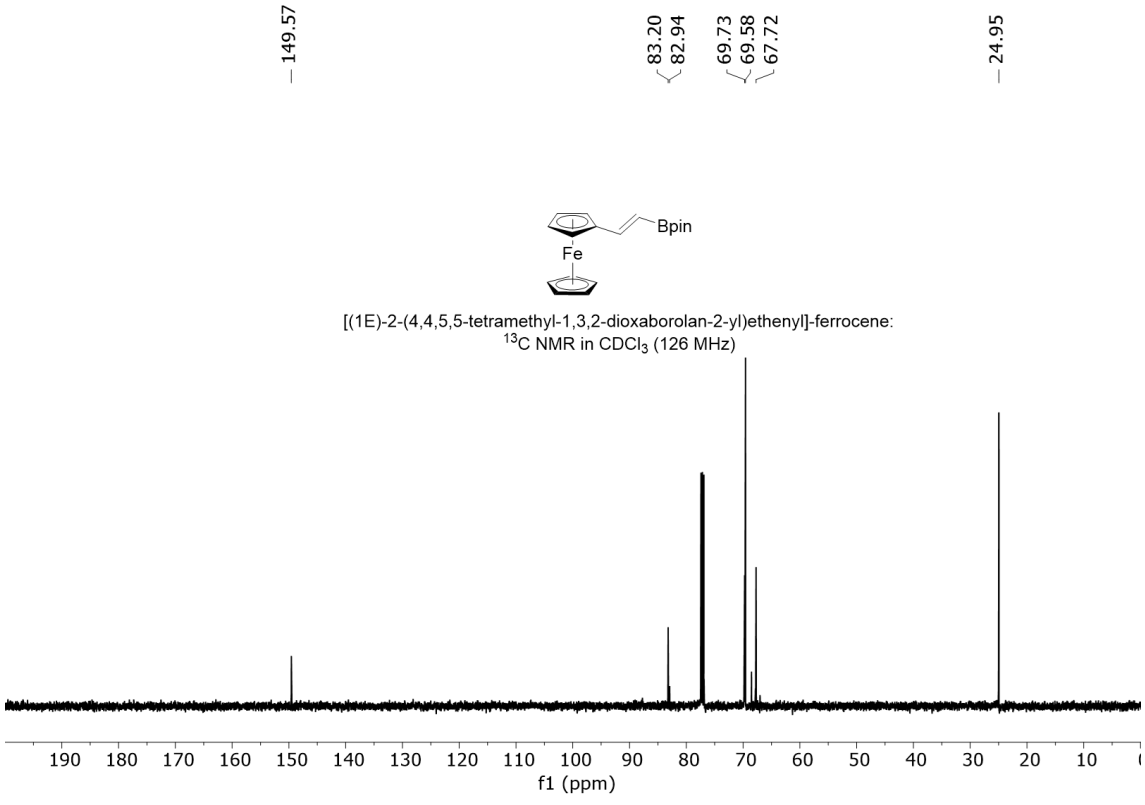


(*E*)-3-(4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)phenyl)pyridine

^{11}B NMR in $CDCl_3$ (161 MHz)

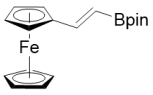


[(1E)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]-ferrocene:
^{1}H NMR in $CDCl_3$ (500 MHz)

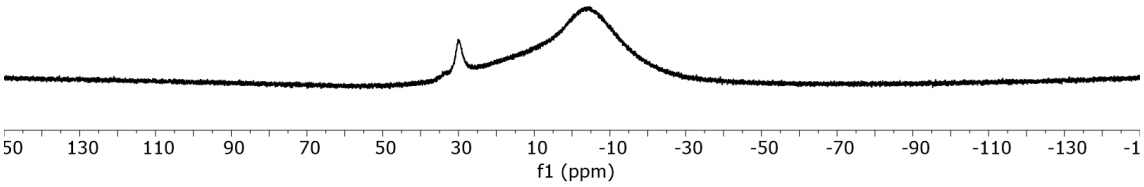


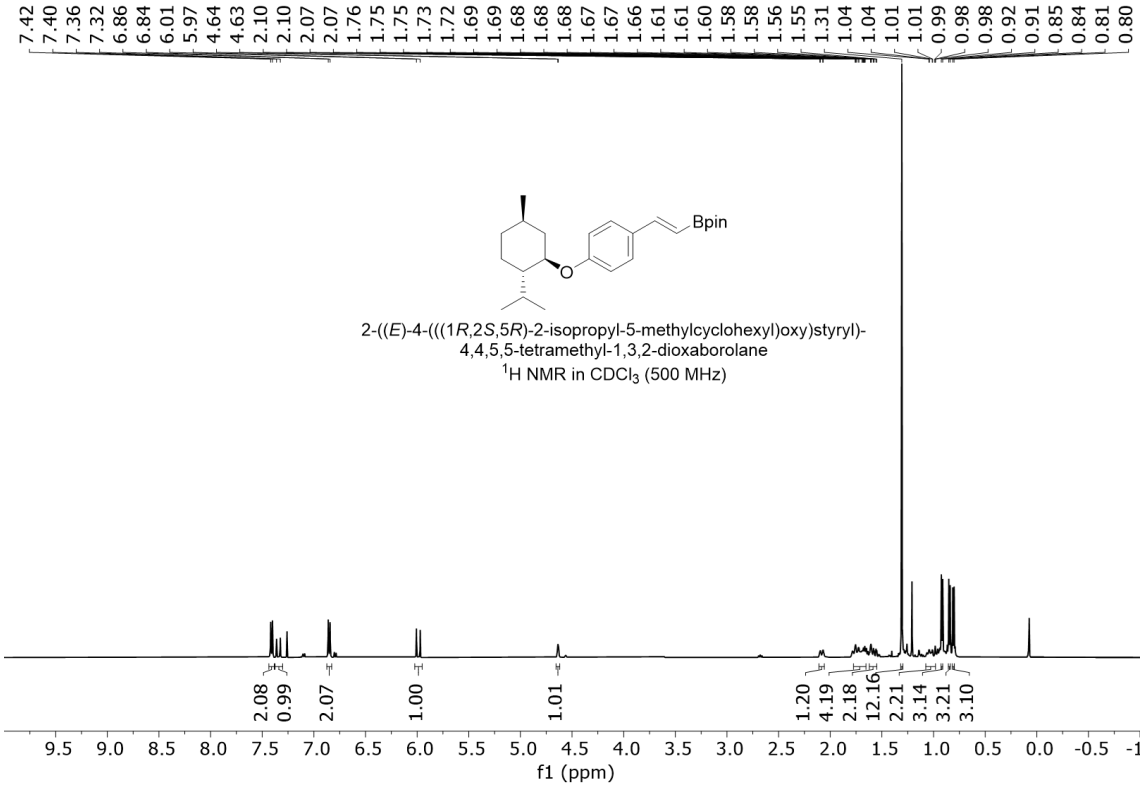
[(1E)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]-ferrocene:
^{13}C NMR in $CDCl_3$ (126 MHz)

29.89

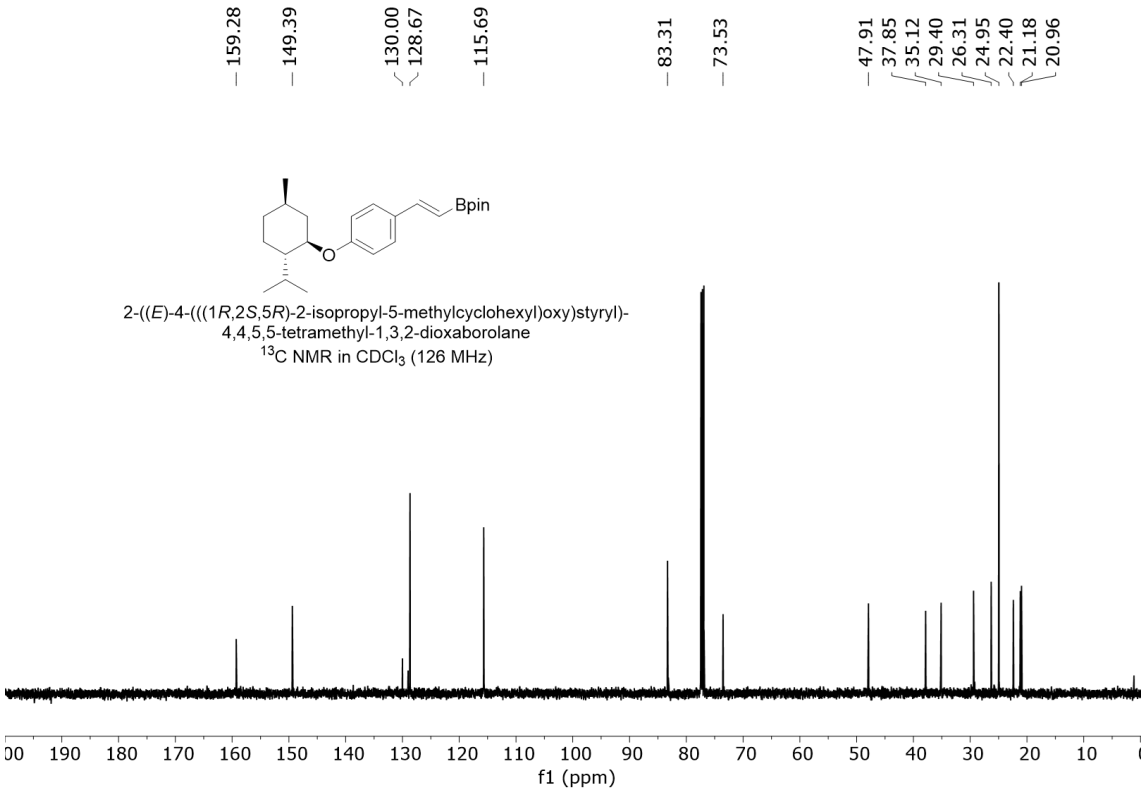


[(1E)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]-ferrocene:
^{11}B NMR in $CDCl_3$ (161 MHz)

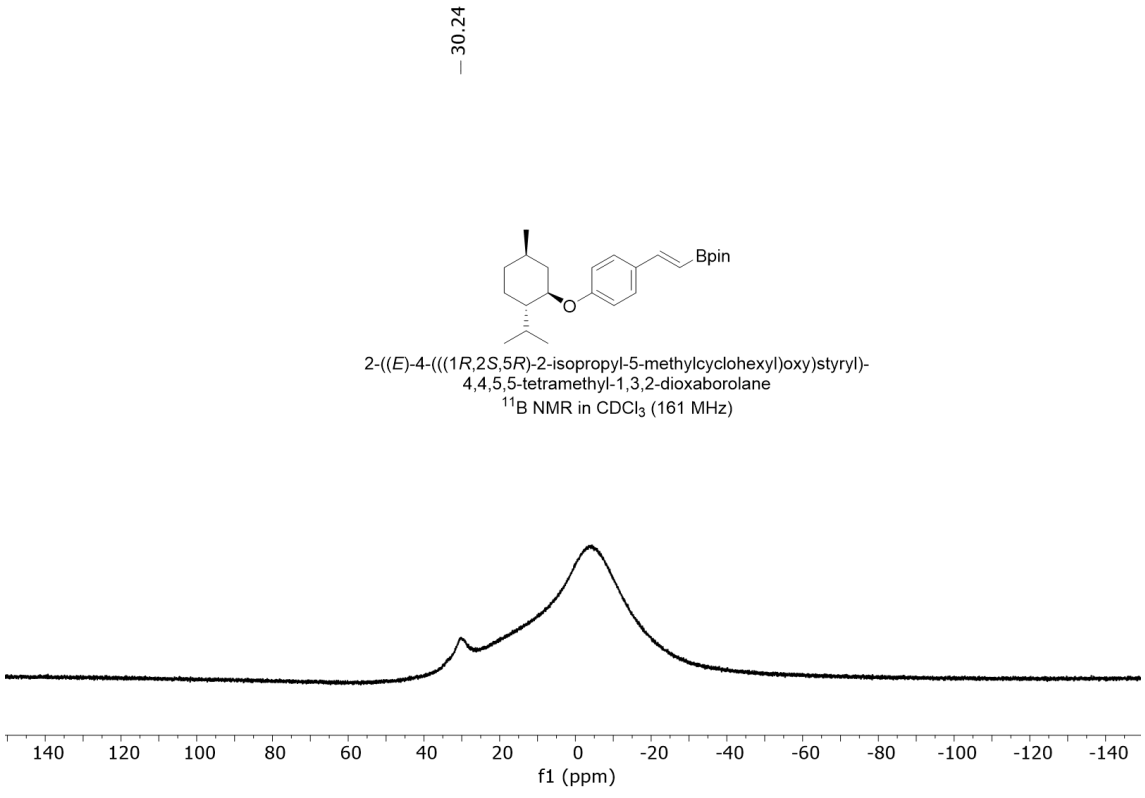




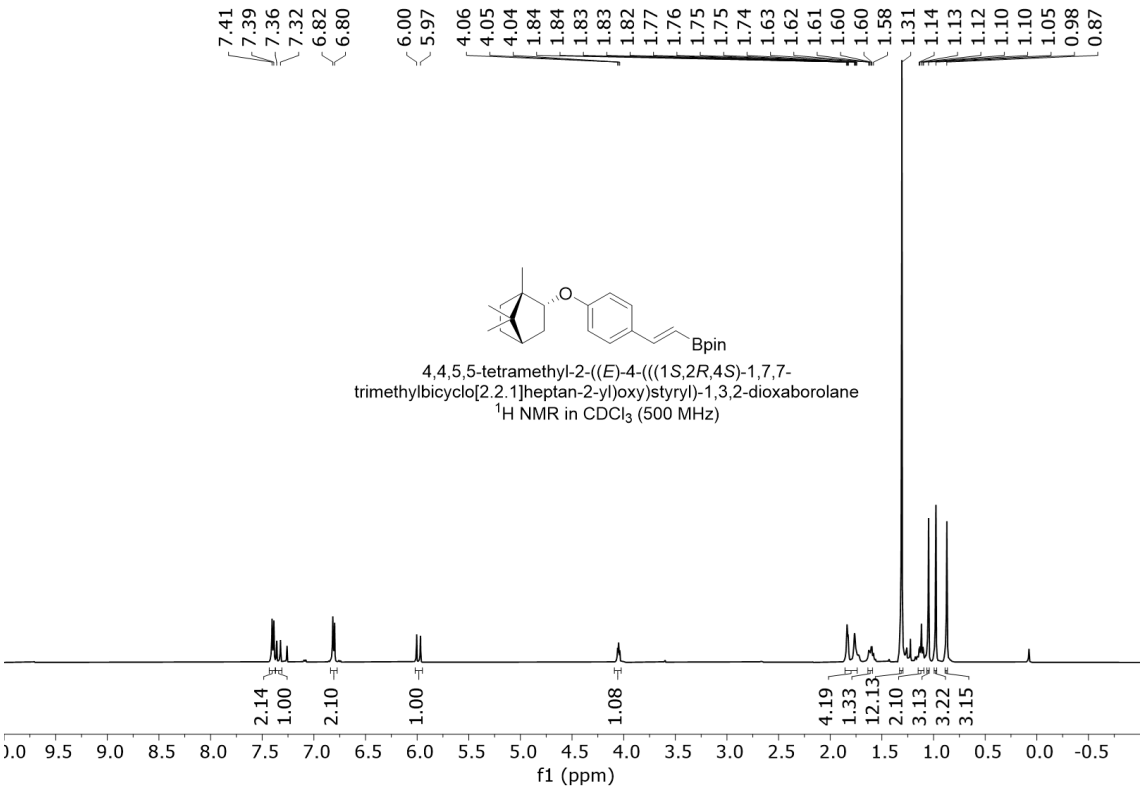
2-((*E*)-4-(((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl)oxy)styryl)-
4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (500 MHz)



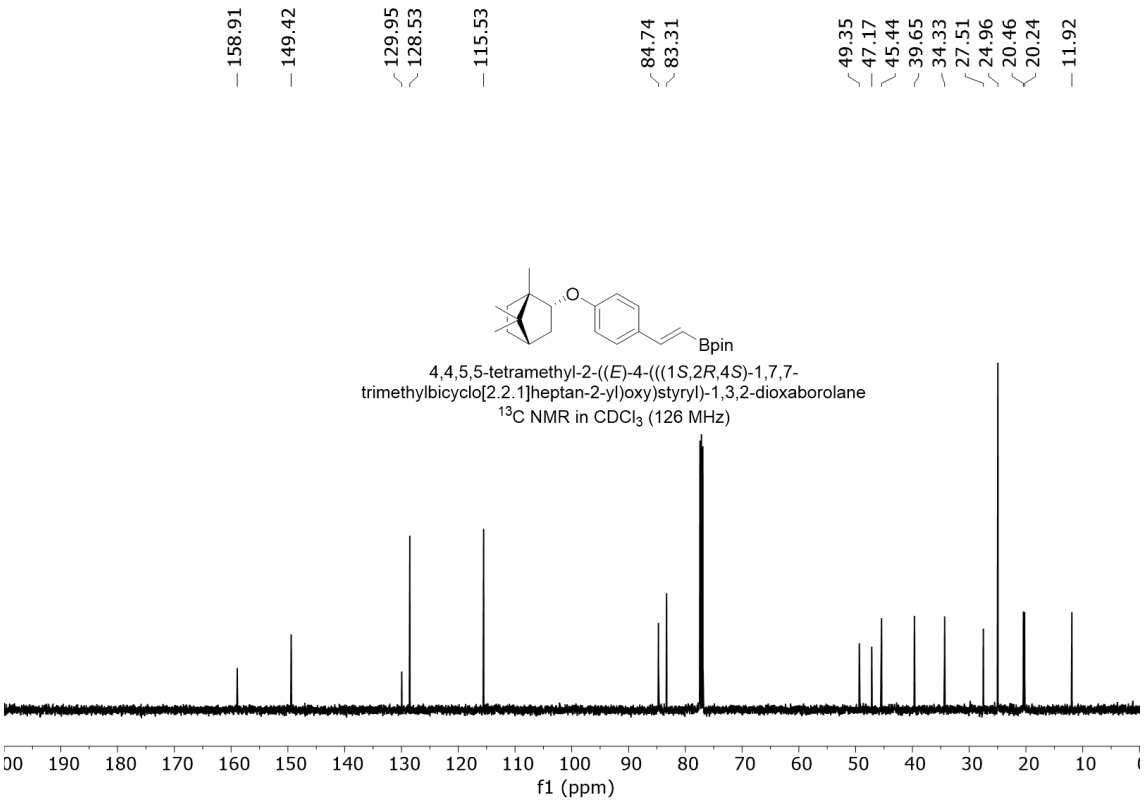
2-((*E*)-4-(((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl)oxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)



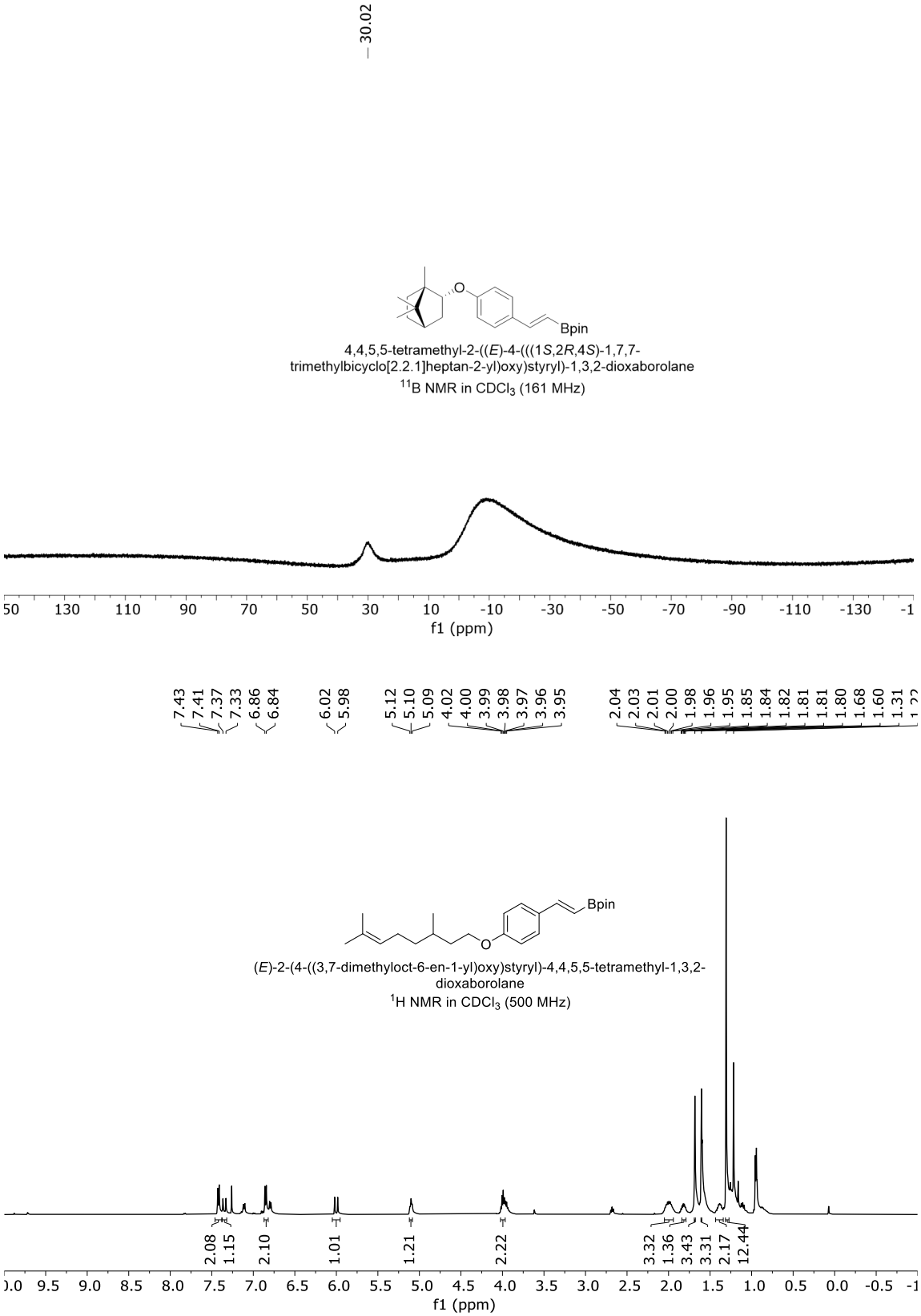
2-((*E*)-4-(((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl)oxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{11}B NMR in $CDCl_3$ (161 MHz)

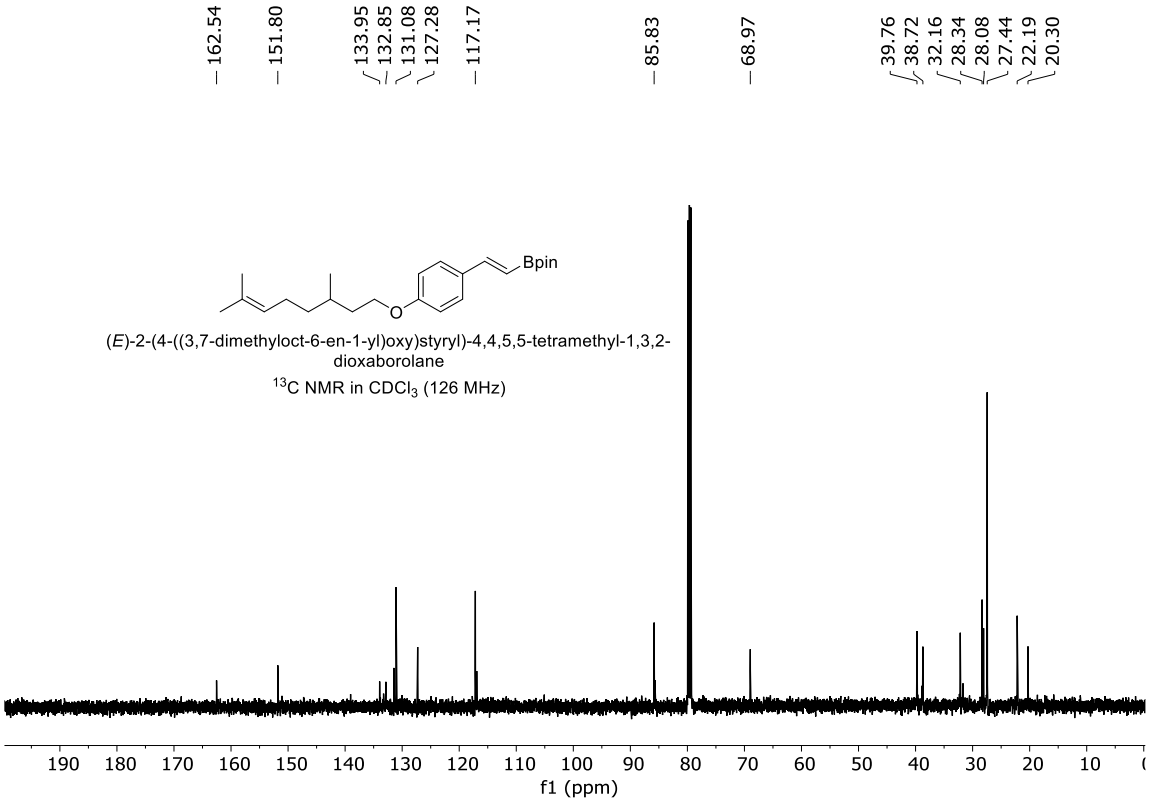


4,4,5,5-tetramethyl-2-((*E*)-4-(((1*S*,2*R*,4*S*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)styryl)-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (500 MHz)



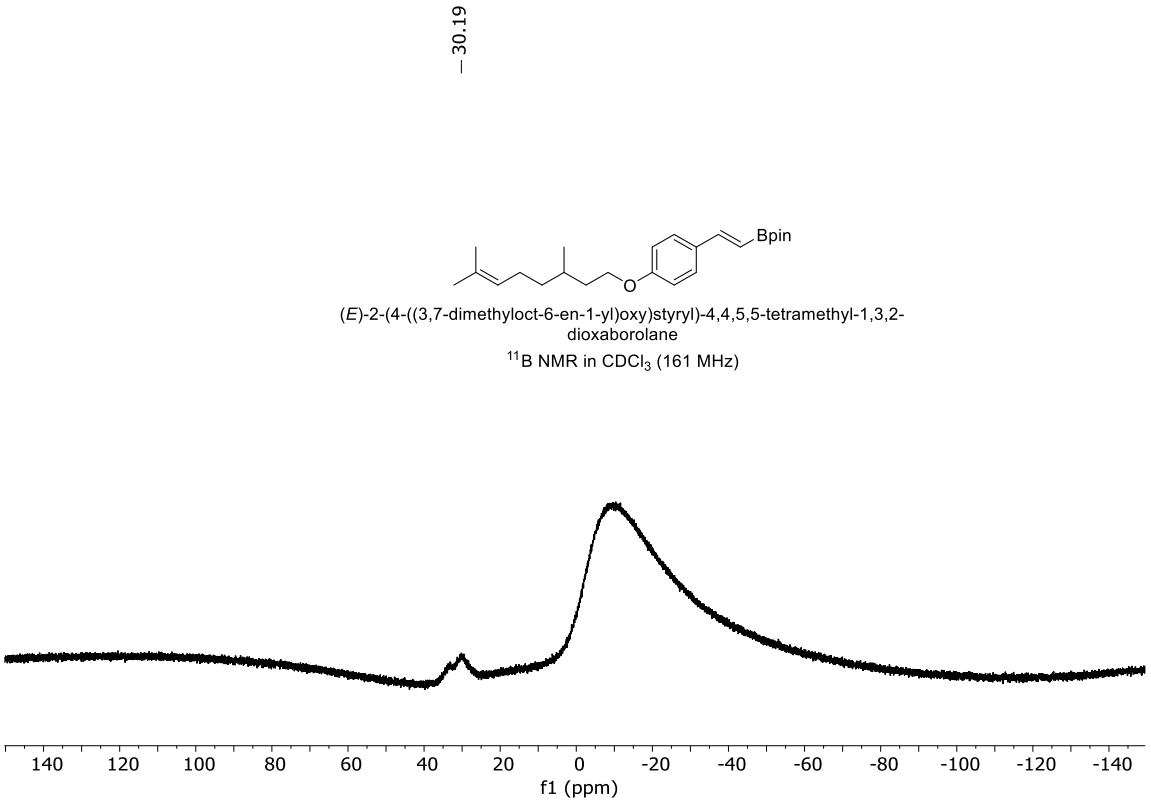
4,4,5,5-tetramethyl-2-((*E*)-4-(((1*S*,2*R*,4*S*)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)styryl)-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)


30.02
Bpin
4,4,5,5-tetramethyl-2-((E)-4-(((1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)styryl)-1,3,2-dioxaborolane
11B NMR in CDCl3 (161 MHz)
50 130 110 90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -1
f1 (ppm)
7.43 7.41 7.37 7.33 6.86 6.84 6.02 5.98 5.12 5.10 5.09 4.02 4.00 3.99 3.98 3.97 3.96 3.95 2.04 2.03 2.01 2.00 1.98 1.96 1.95 1.85 1.84 1.82 1.81 1.81 1.80 1.68 1.60 1.31
Bpin
(E)-2-(4-((3,7-dimethyloct-6-en-1-yl)oxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
1H NMR in CDCl3 (500 MHz)
2.08 1.15 2.10 1.01 1.21 2.22 3.32 1.36 3.43 3.31 2.17 12.44
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)



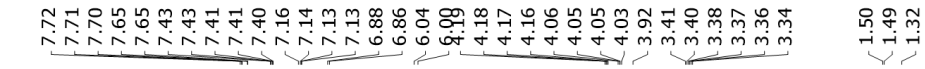
(*E*)-2-(4-((3,7-dimethyloct-6-en-1-yl)oxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

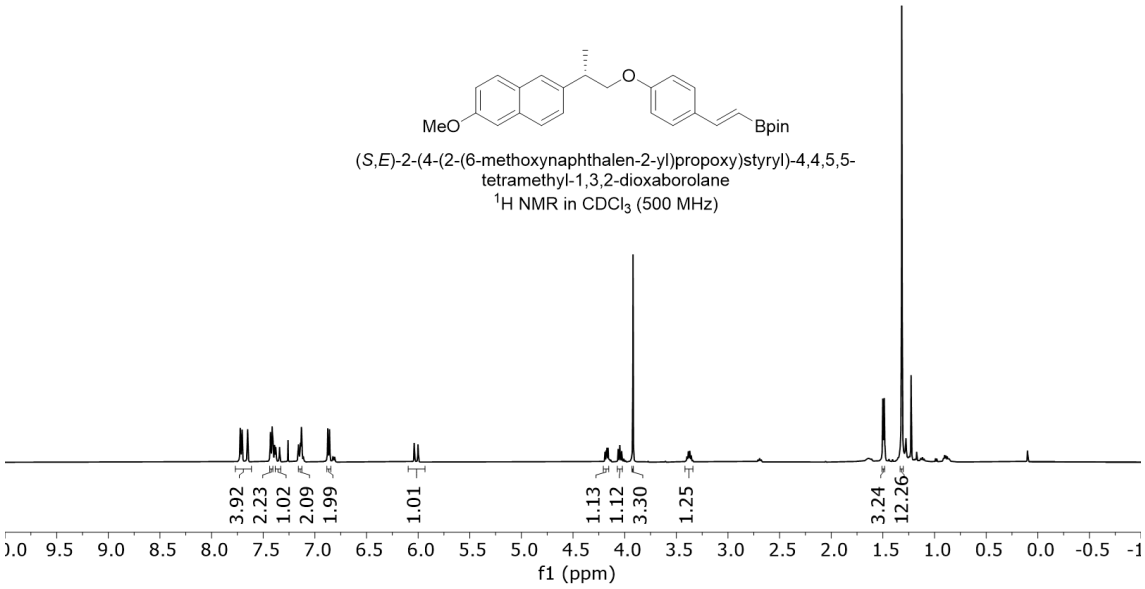
^{13}C NMR in $CDCl_3$ (126 MHz)



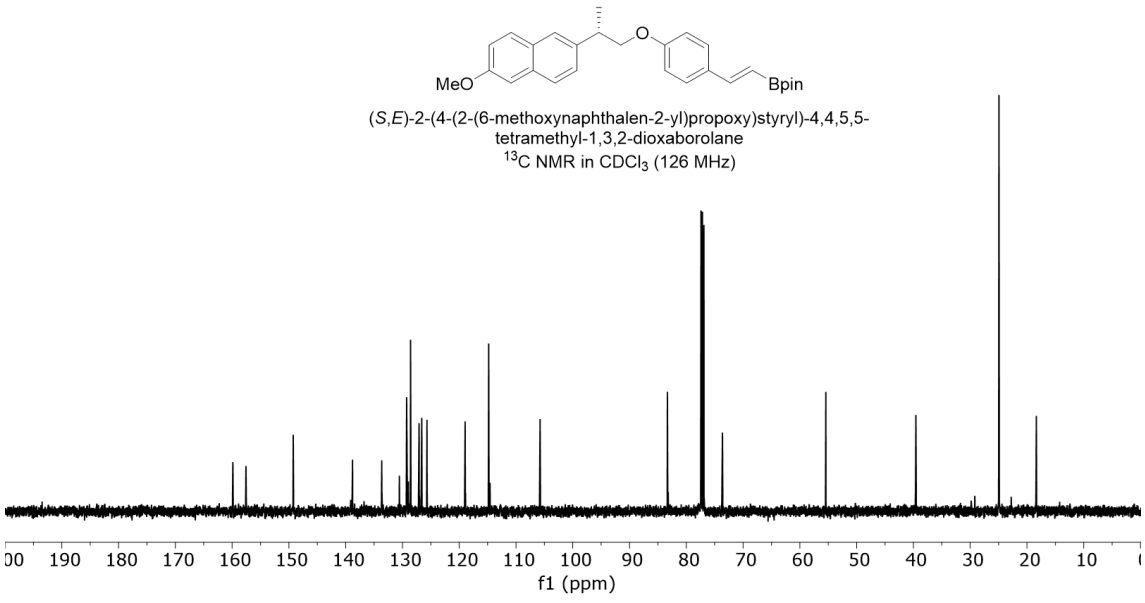
(*E*)-2-(4-((3,7-dimethyloct-6-en-1-yl)oxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

^{11}B NMR in $CDCl_3$ (161 MHz)



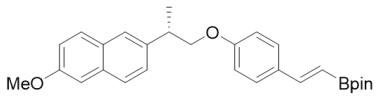


(*S*,*E*)-2-(4-(2-(6-methoxynaphthalen-2-yl)propoxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{1}H NMR in $CDCl_3$ (500 MHz)



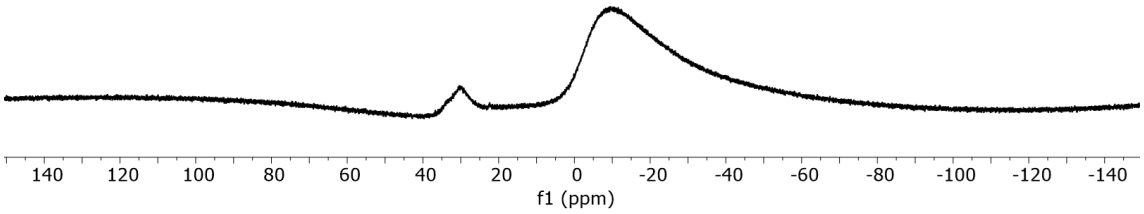
(*S*,*E*)-2-(4-(2-(6-methoxynaphthalen-2-yl)propoxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane
^{13}C NMR in $CDCl_3$ (126 MHz)

30.15

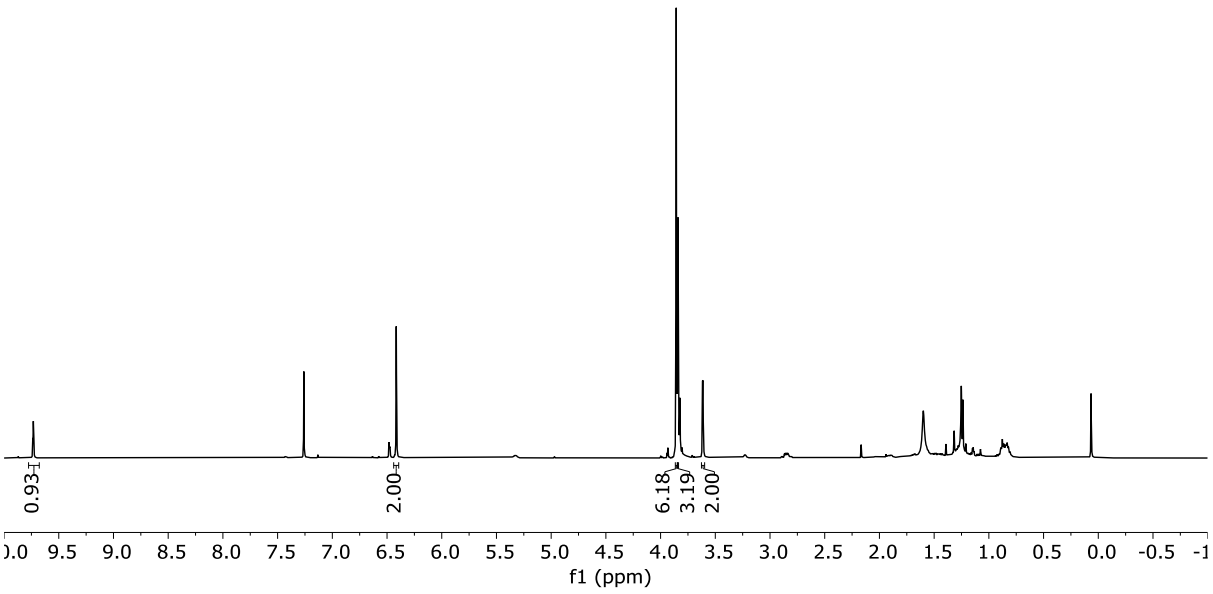


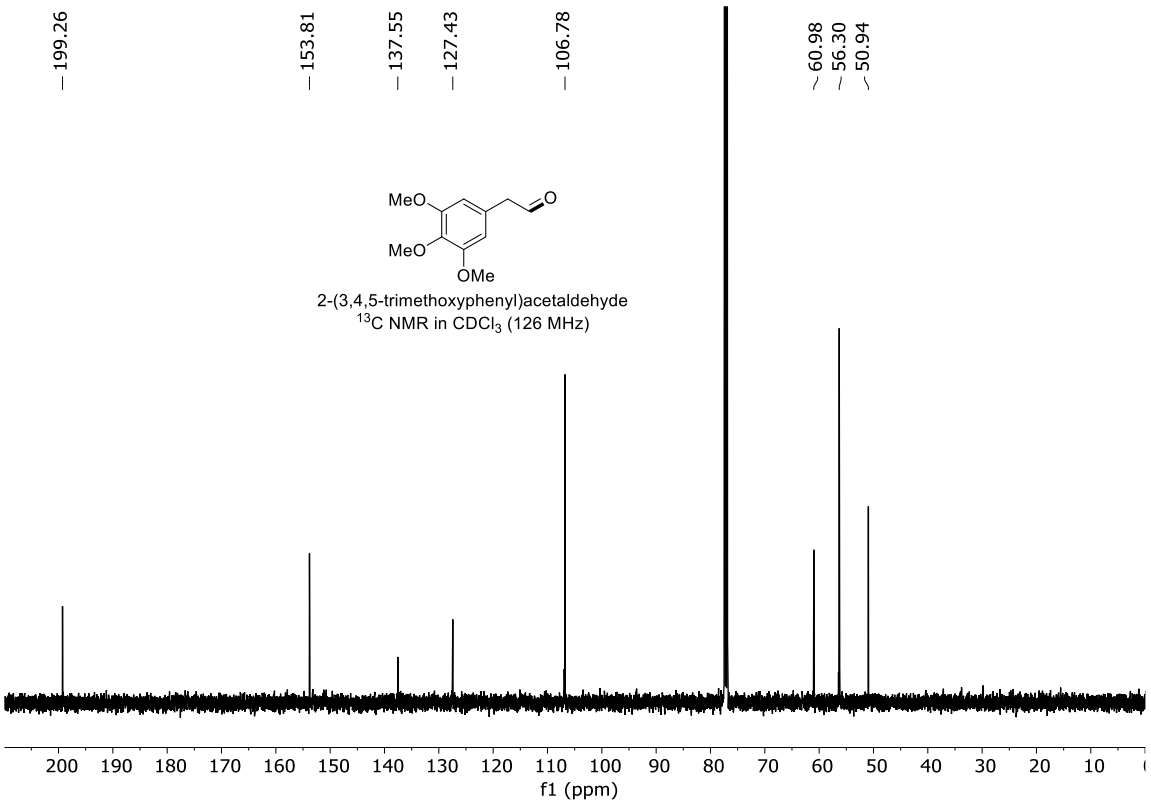
(*S*,*E*)-2-(4-(2-(6-methoxynaphthalen-2-yl)propoxy)styryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

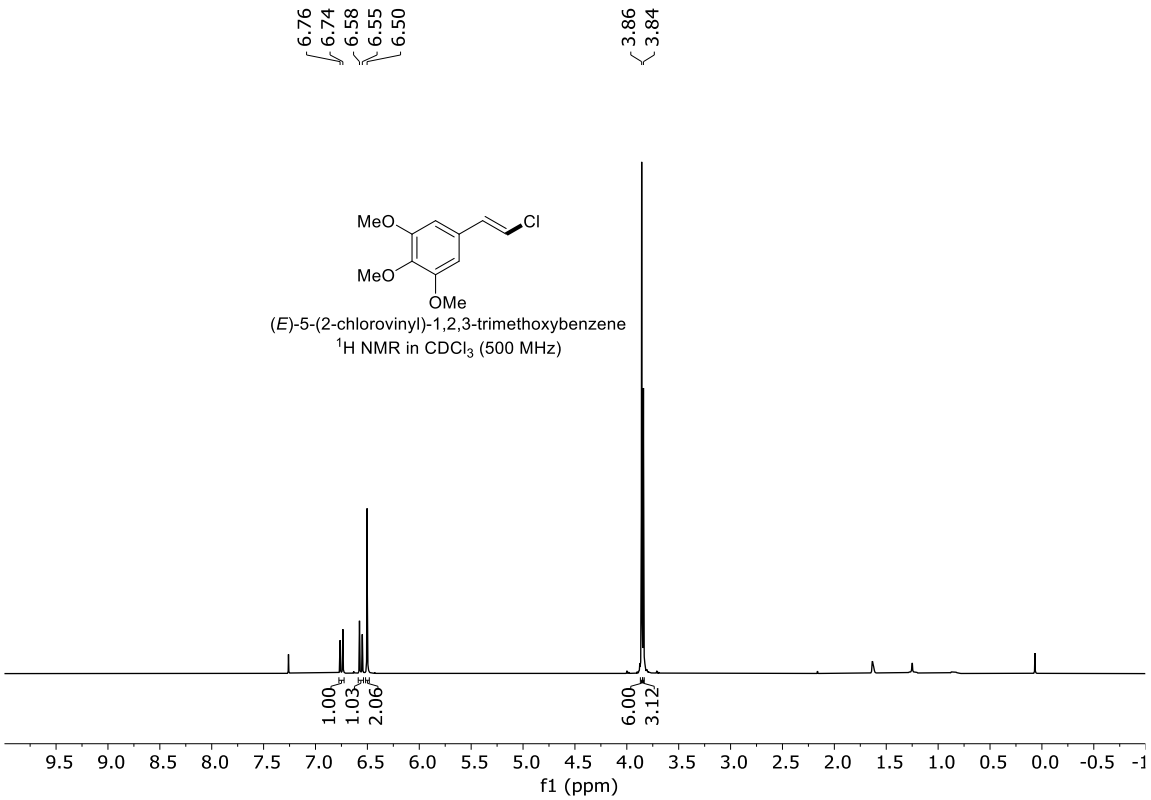
^{11}B NMR in $CDCl_3$ (161 MHz)

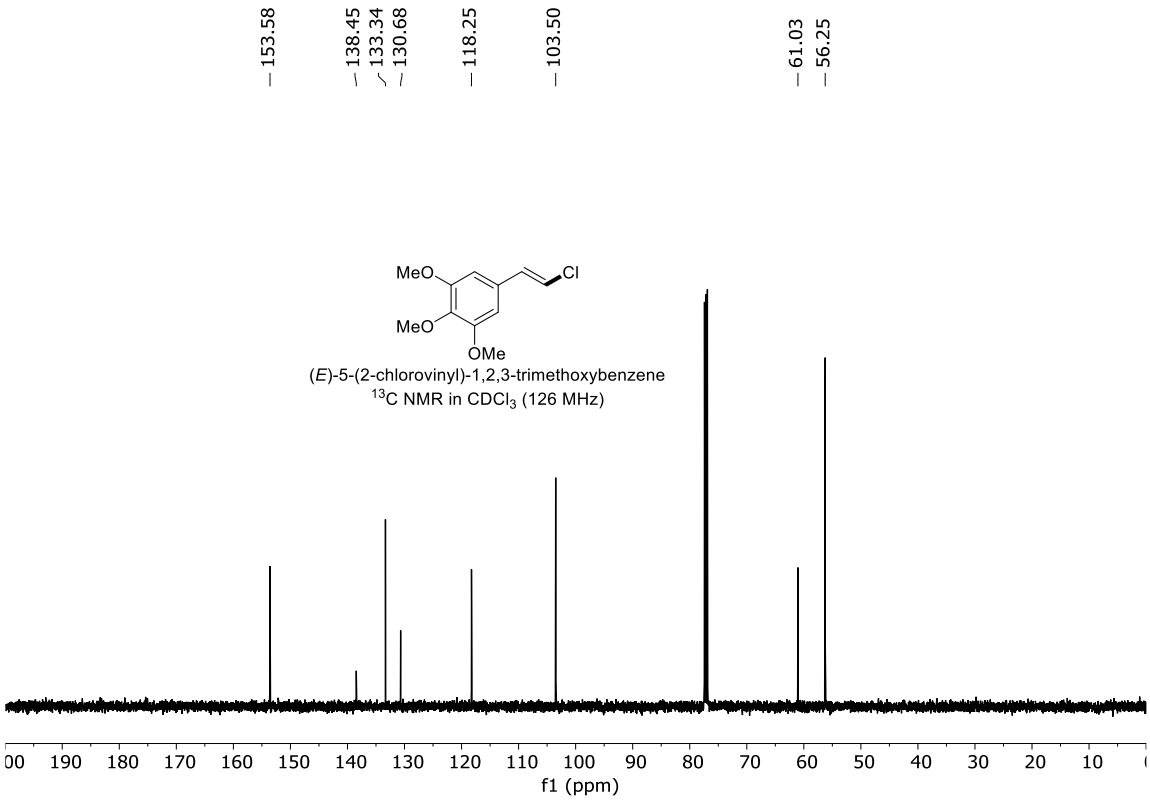


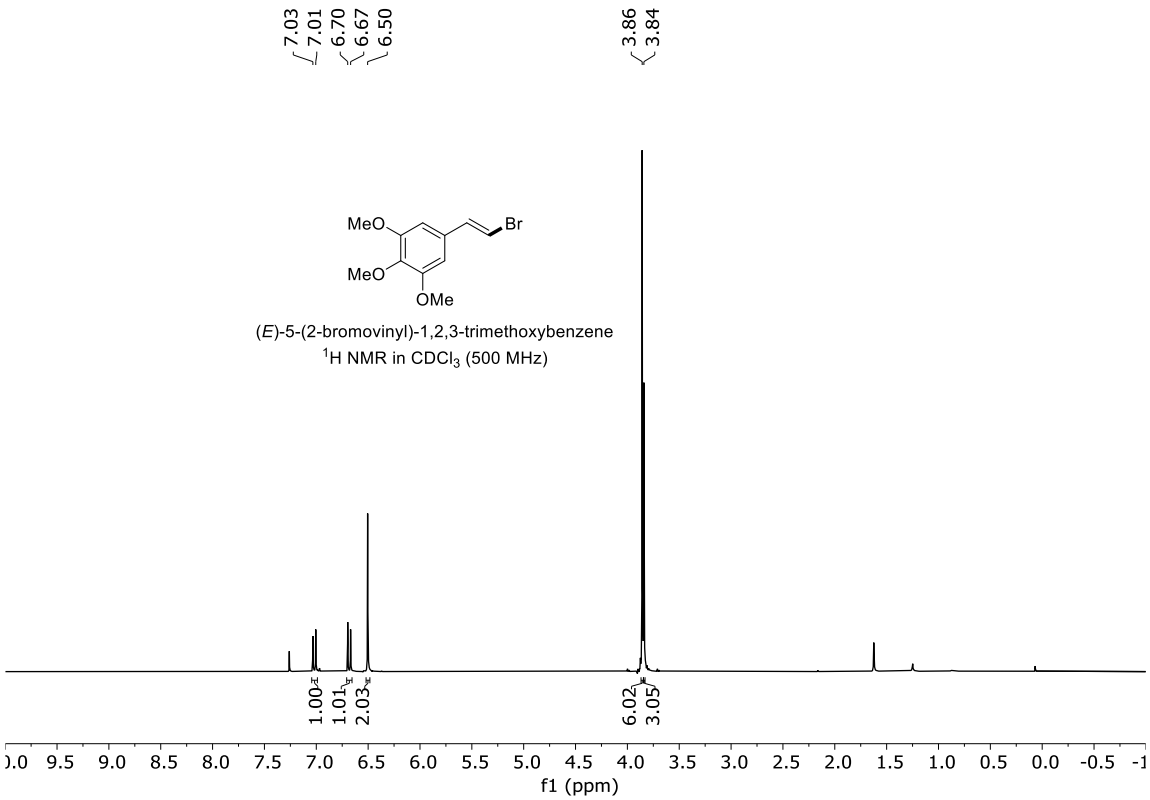
9.74
9.73
9.73
6.42
3.86
3.84
3.62
3.61

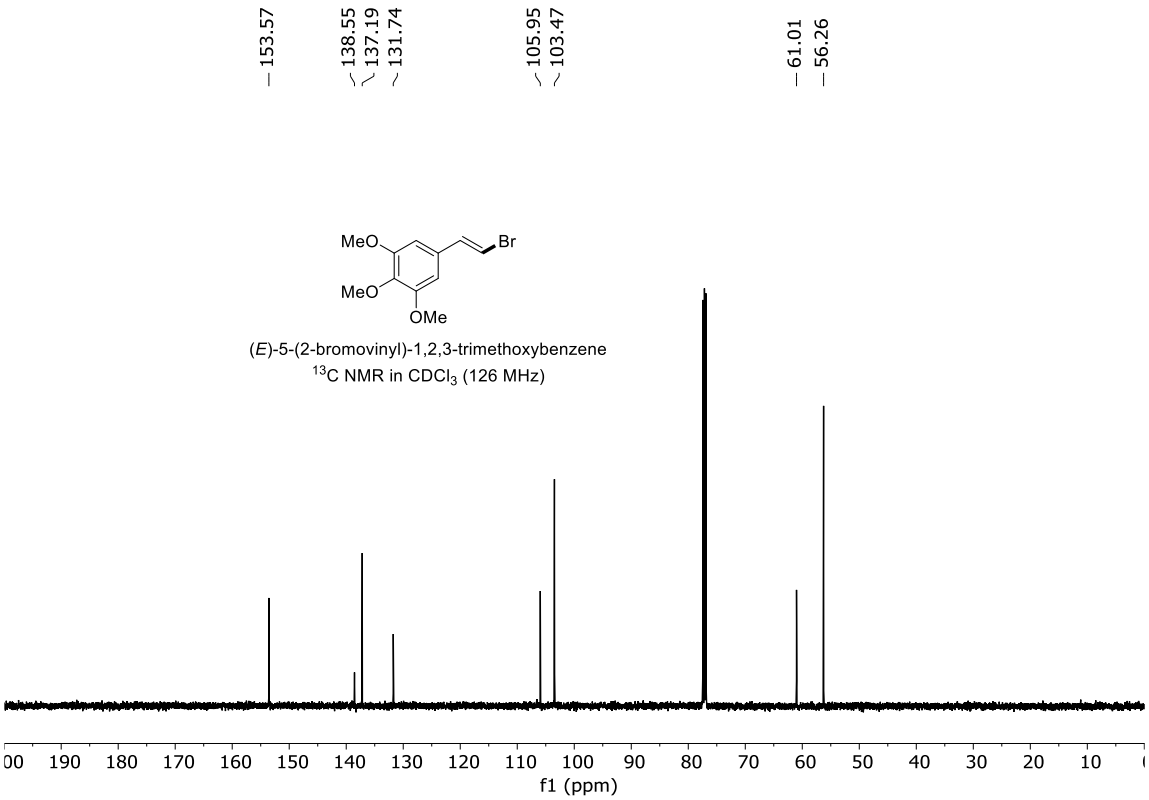


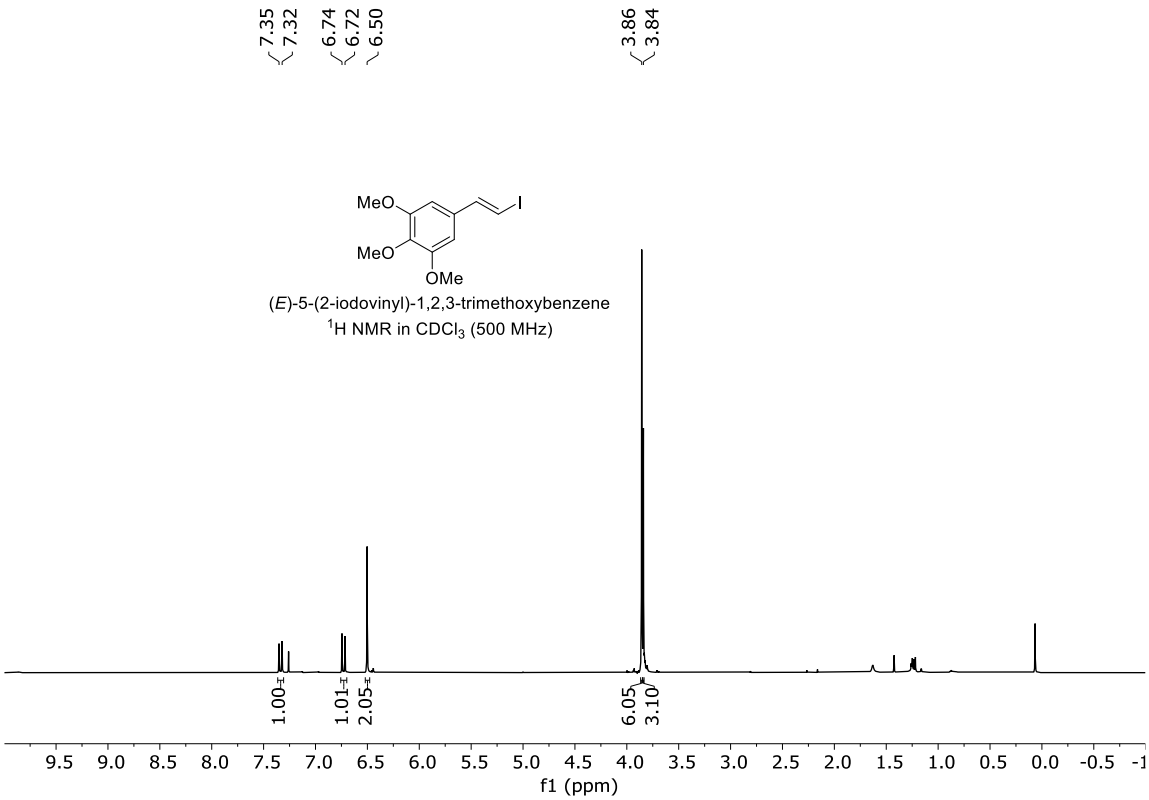

199.26
153.81
137.55
127.43
106.78
60.98
56.30
50.94
MeO
MeO
OMe
O
2-(3,4,5-trimethoxyphenyl)acetaldehyde
13C NMR in CDCl3 (126 MHz)
f1 (ppm)

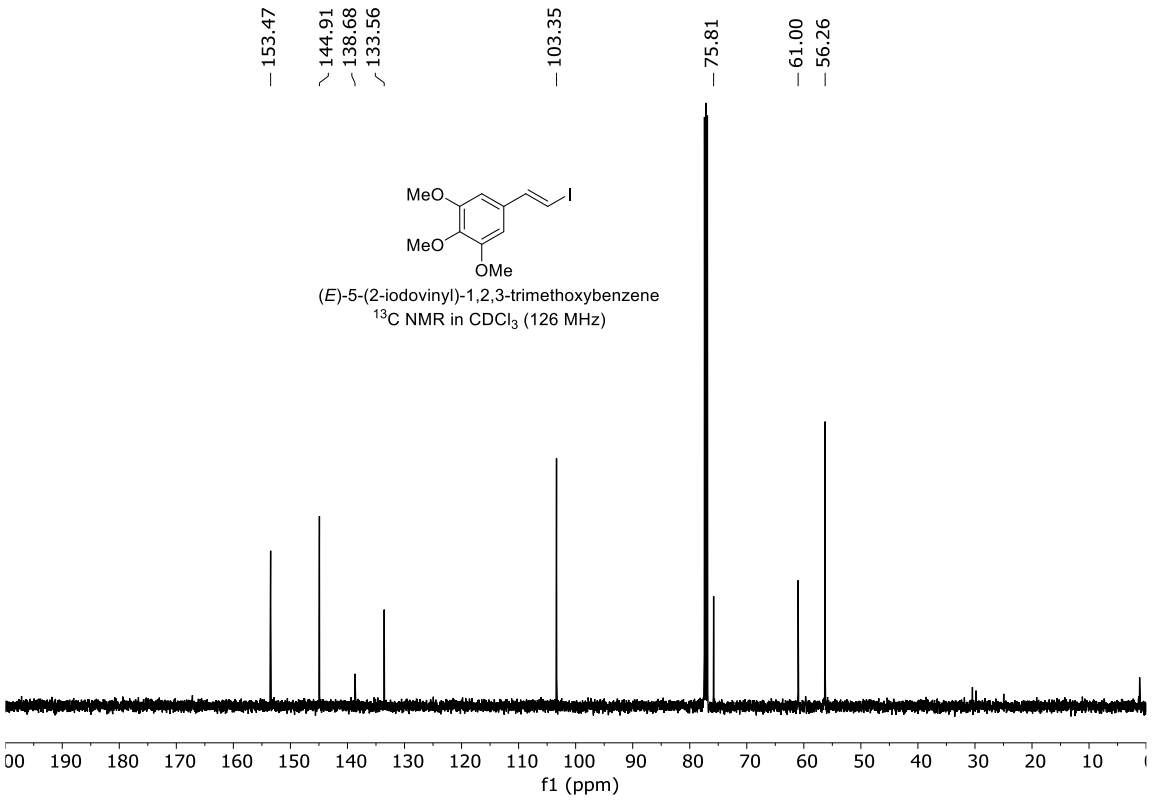

6.76
6.74
6.58
6.55
6.50
3.86
3.84
MeO
MeO
OMe
Cl
(E)-5-(2-chlorovinyl)-1,2,3-trimethoxybenzene
1H NMR in CDCl3 (500 MHz)
1.00
1.03
2.06
6.00
3.12
f1 (ppm)


153.58
138.45
133.34
130.68
118.25
103.50
61.03
56.25
MeO
MeO
OMe
Cl
(E)-5-(2-chlorovinyl)-1,2,3-trimethoxybenzene
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


7.03
7.01
6.70
6.67
6.50
3.86
3.84
MeO
MeO
OMe
Br
(E)-5-(2-bromovinyl)-1,2,3-trimethoxybenzene
1H NMR in CDCl3 (500 MHz)
1.00
1.01
2.03
6.02
3.05
f1 (ppm)

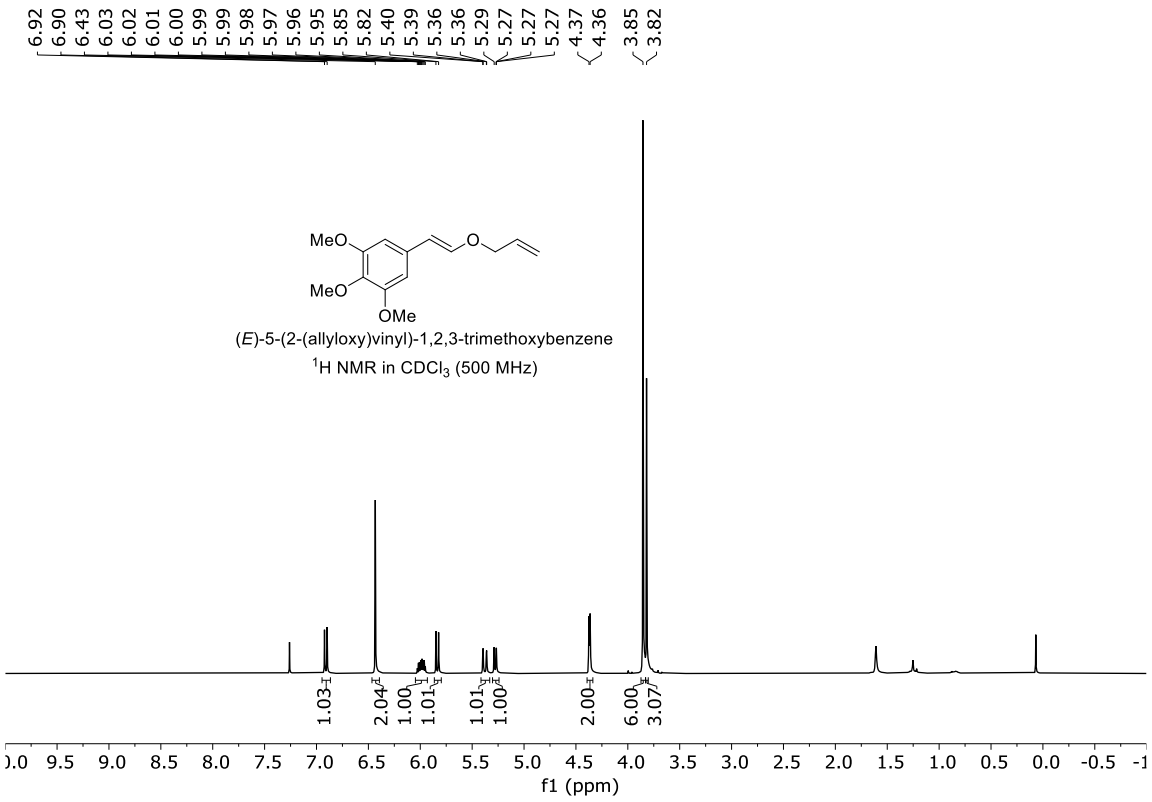

153.57
138.55
137.19
131.74
105.95
103.47
61.01
56.26
MeO
MeO
OMe
Br
(E)-5-(2-bromovinyl)-1,2,3-trimethoxybenzene
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


7.35
7.32
6.74
6.72
6.50
3.86
3.84
MeO
MeO
OMe
I
(E)-5-(2-iodovinyl)-1,2,3-trimethoxybenzene
1H NMR in CDCl3 (500 MHz)
1.00
1.01
2.05
6.05
3.10
f1 (ppm)



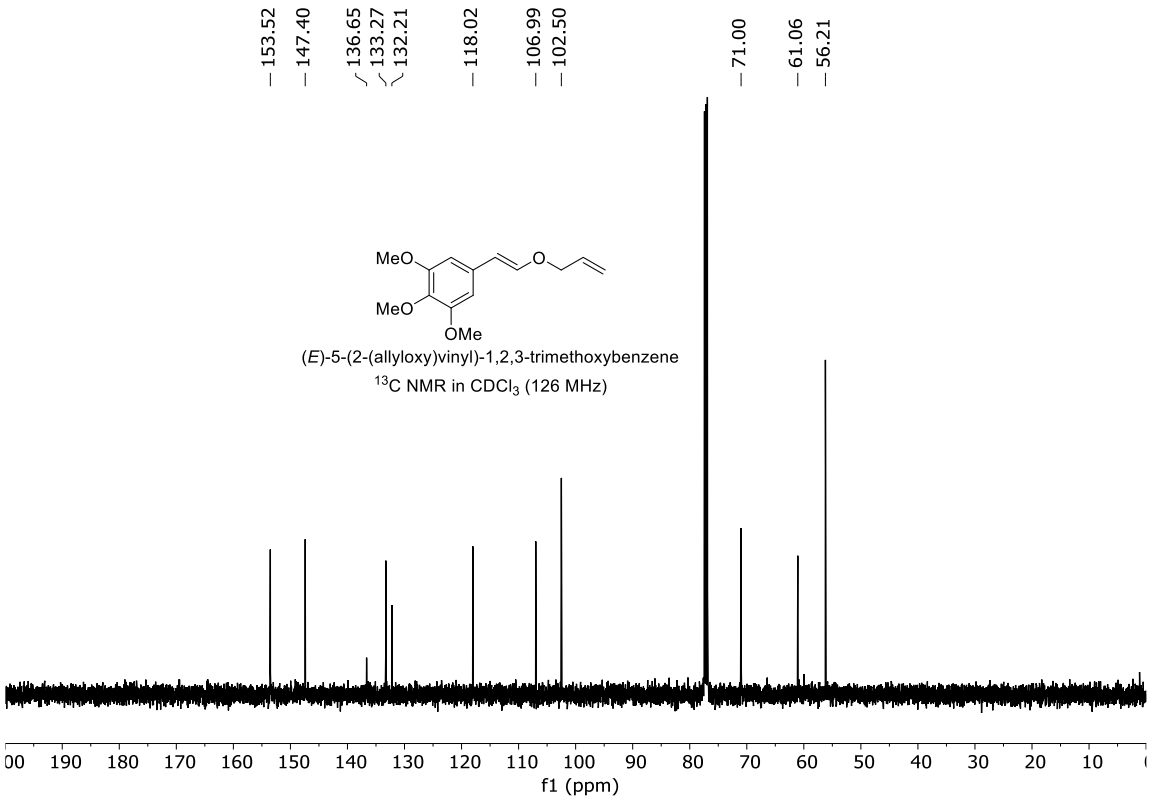
(*E*)-5-(2-iodovinyl)-1,2,3-trimethoxybenzene

^{13}C NMR in $CDCl_3$ (126 MHz)



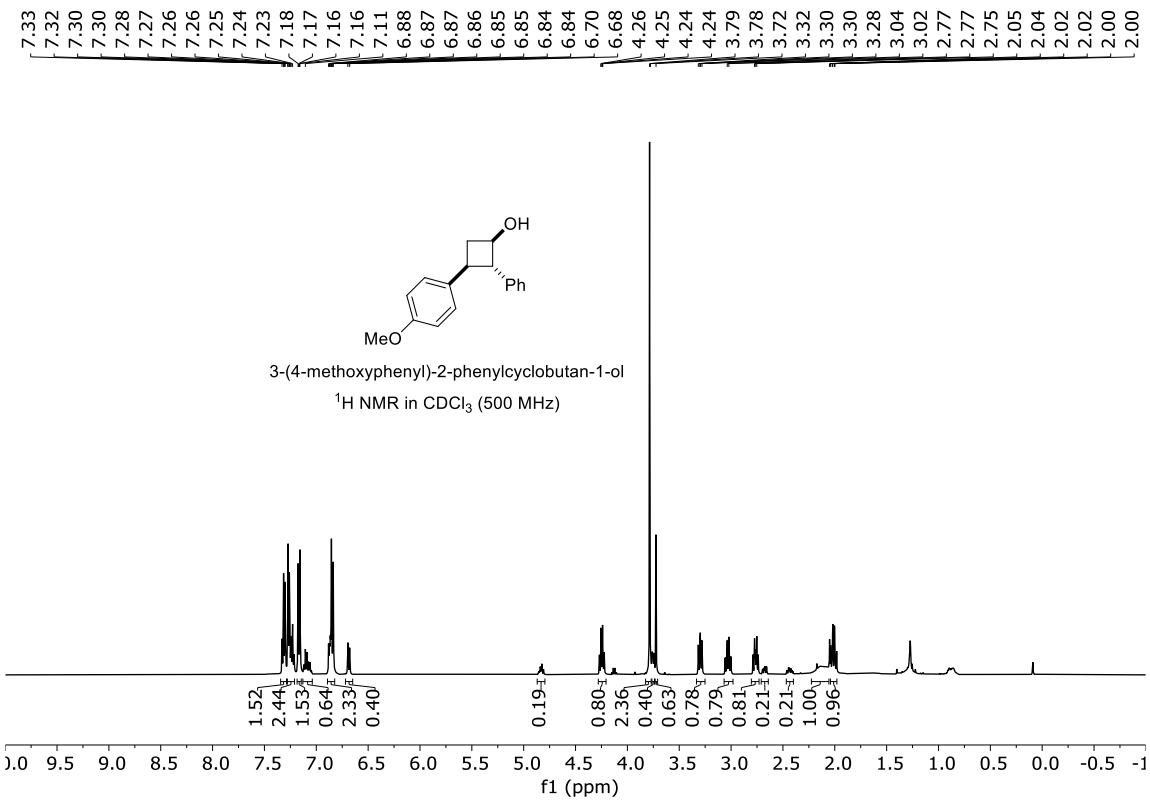
(*E*)-5-(2-(allyloxy)vinyl)-1,2,3-trimethoxybenzene

^{1}H NMR in $CDCl_3$ (500 MHz)



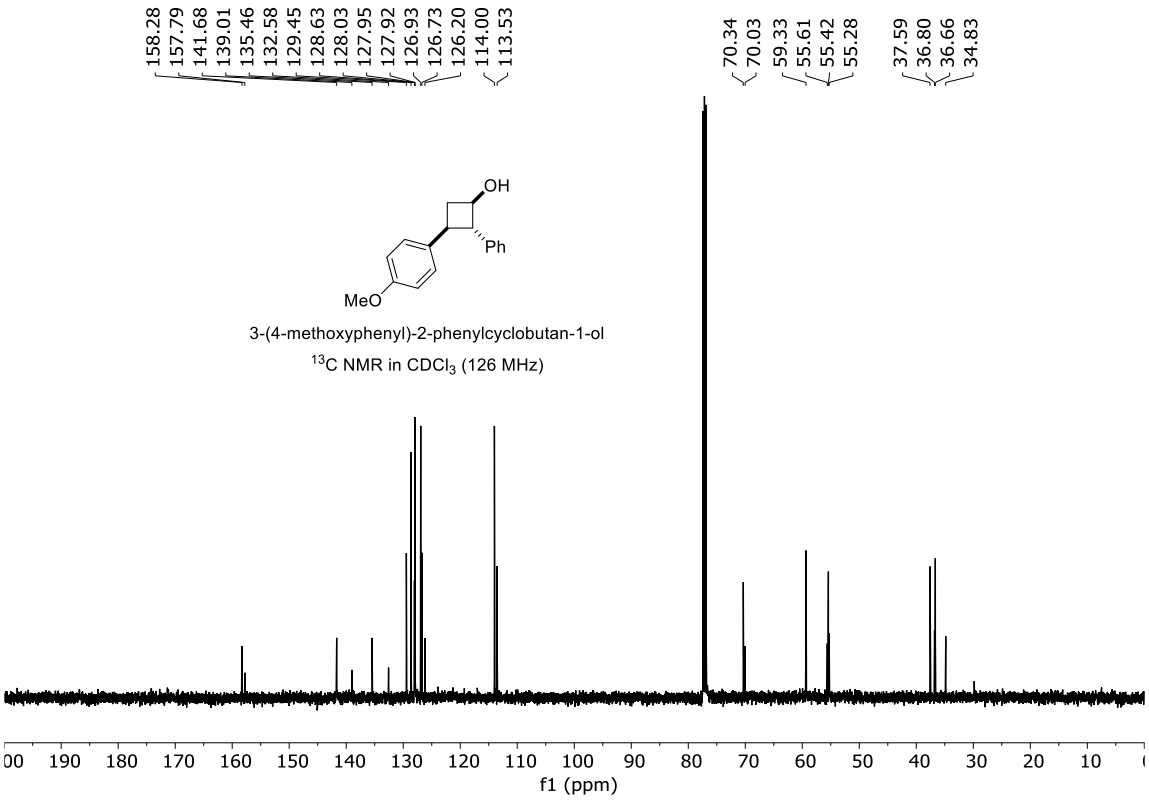
(*E*)-5-(2-(allyloxy)vinyl)-1,2,3-trimethoxybenzene

^{13}C NMR in $CDCl_3$ (126 MHz)



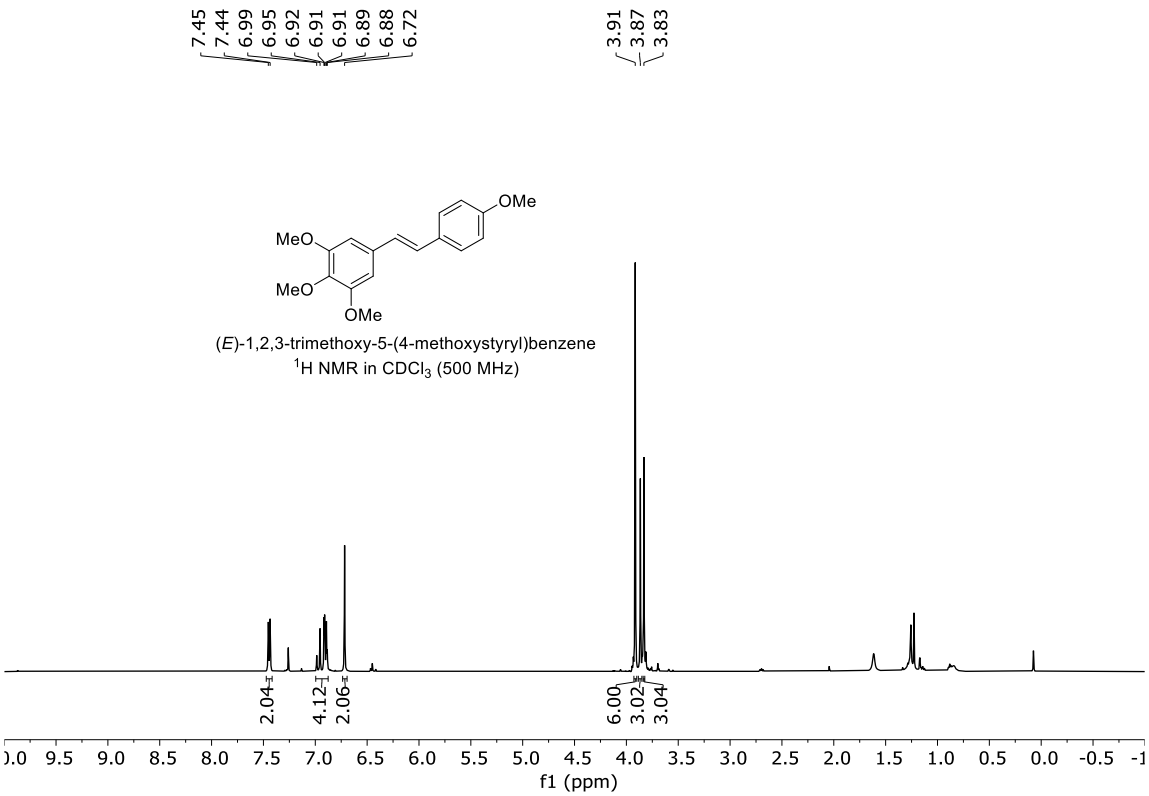
3-(4-methoxyphenyl)-2-phenylcyclobutan-1-ol

^{1}H NMR in $CDCl_3$ (500 MHz)



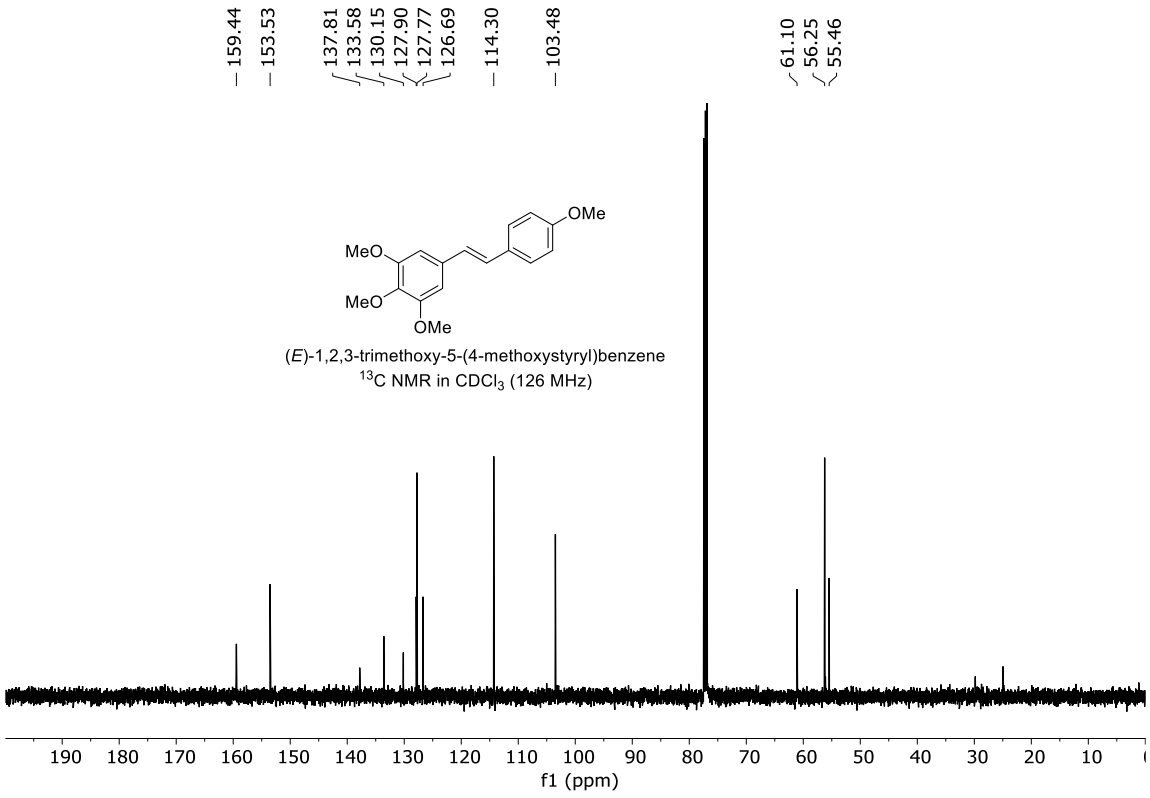
3-(4-methoxyphenyl)-2-phenylcyclobutan-1-ol

^{13}C NMR in $CDCl_3$ (126 MHz)

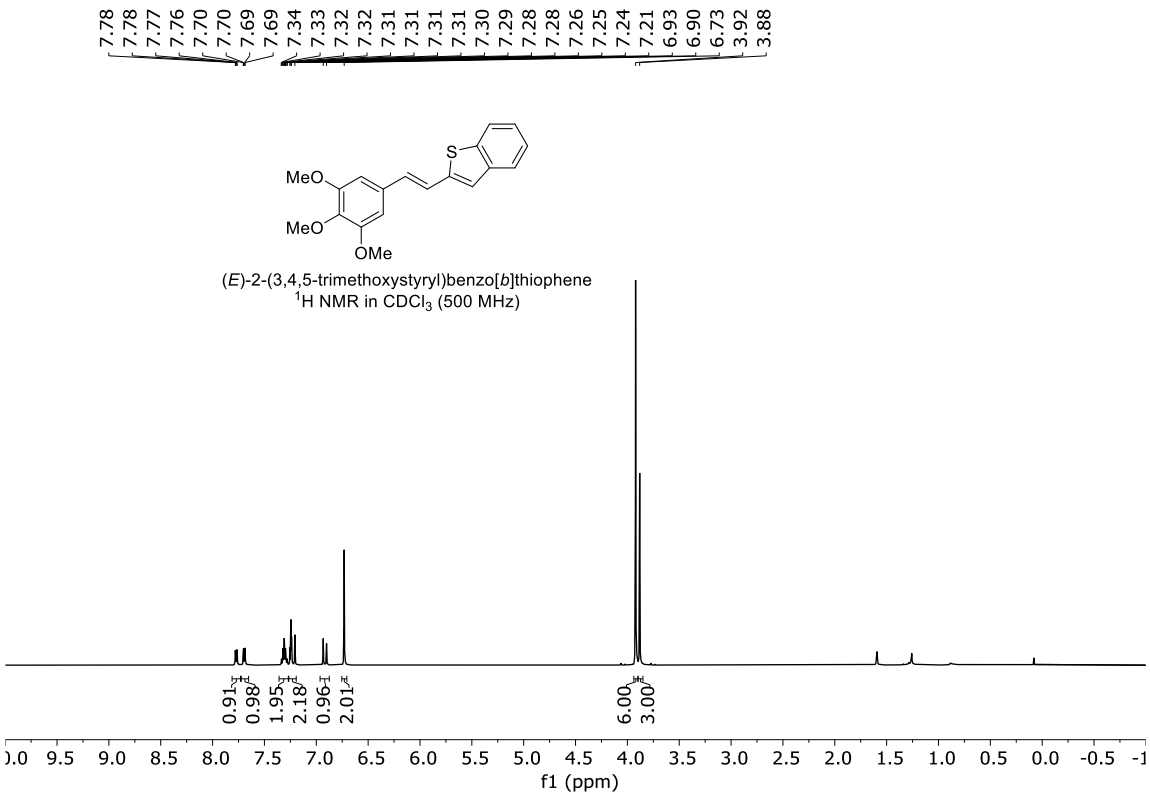


(*E*)-1,2,3-trimethoxy-5-(4-methoxystyryl)benzene

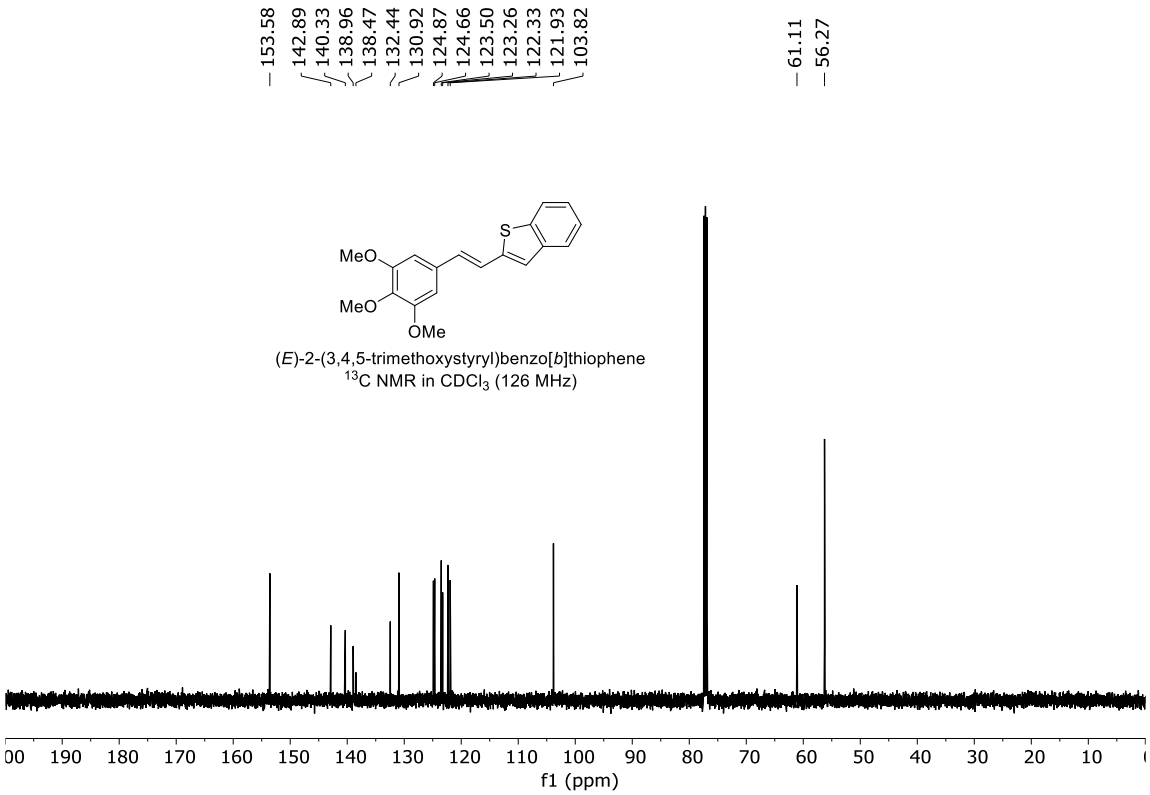
^{1}H NMR in $CDCl_3$ (500 MHz)



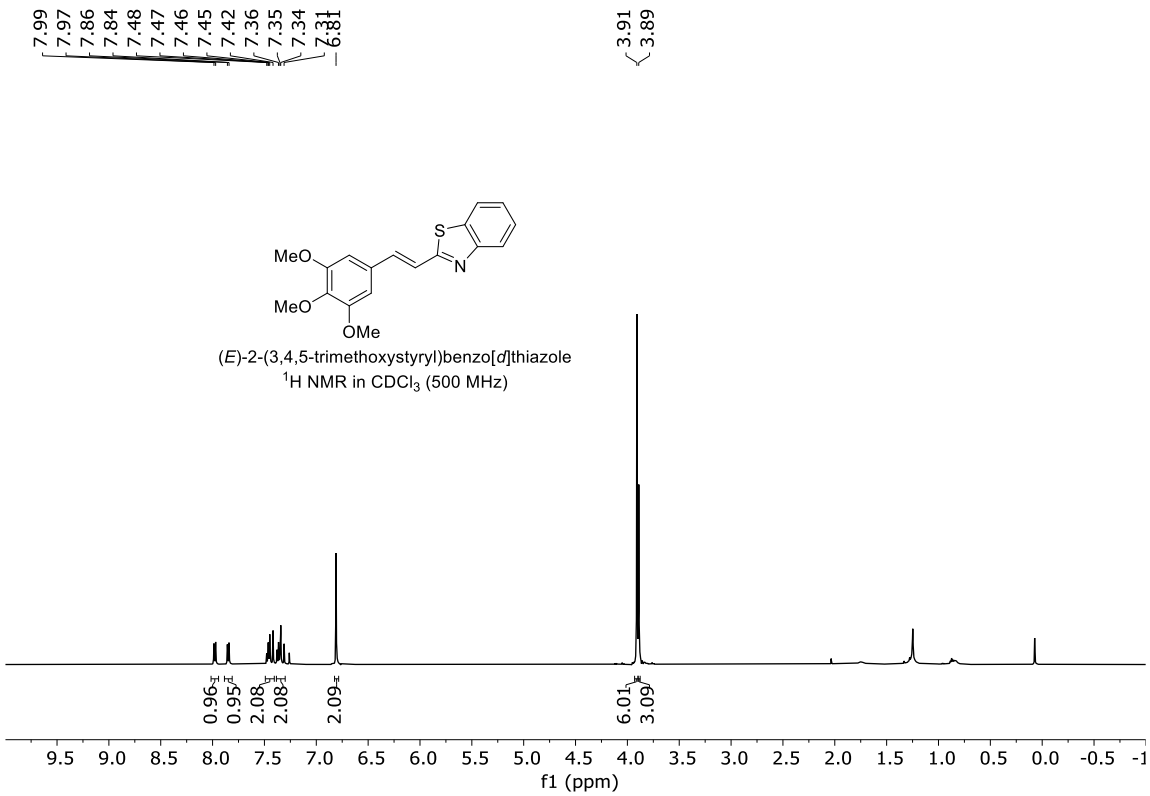
(*E*)-1,2,3-trimethoxy-5-(4-methoxystyryl)benzene
^{13}C NMR in $CDCl_3$ (126 MHz)



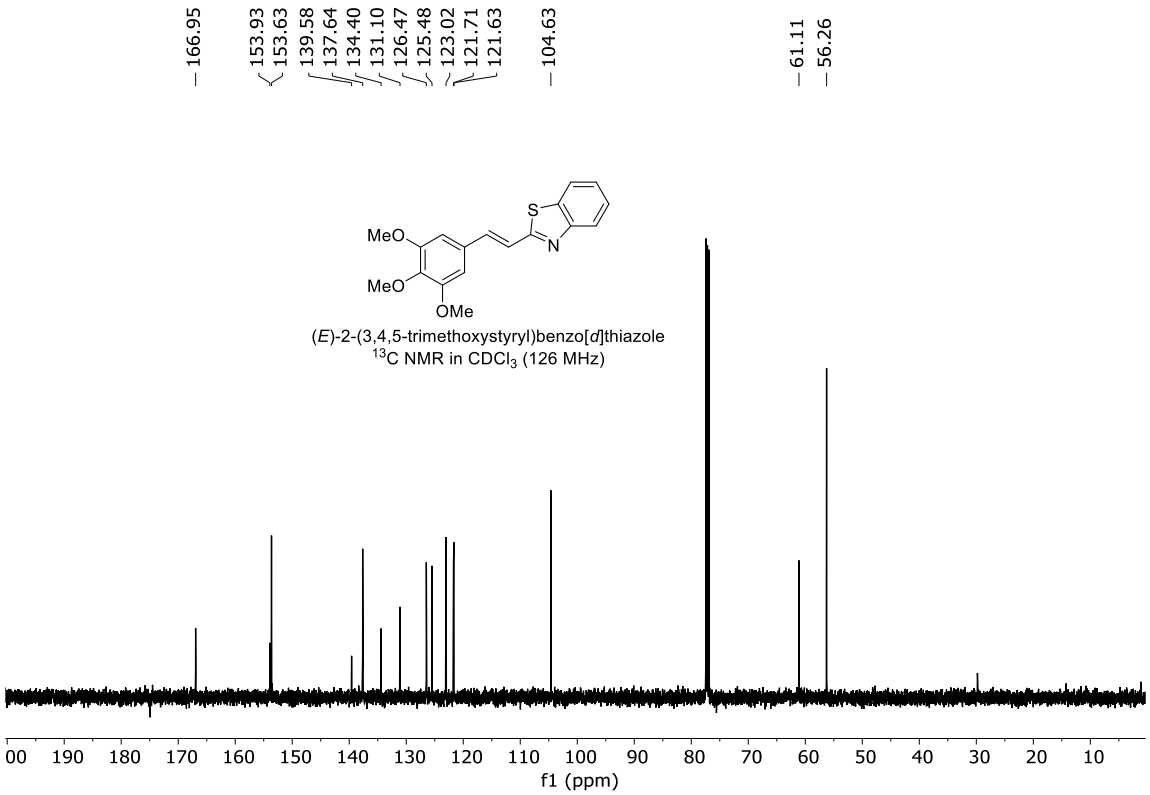
(*E*)-2-(3,4,5-trimethoxystyryl)benzo[*b*]thiophene
^{1}H NMR in $CDCl_3$ (500 MHz)

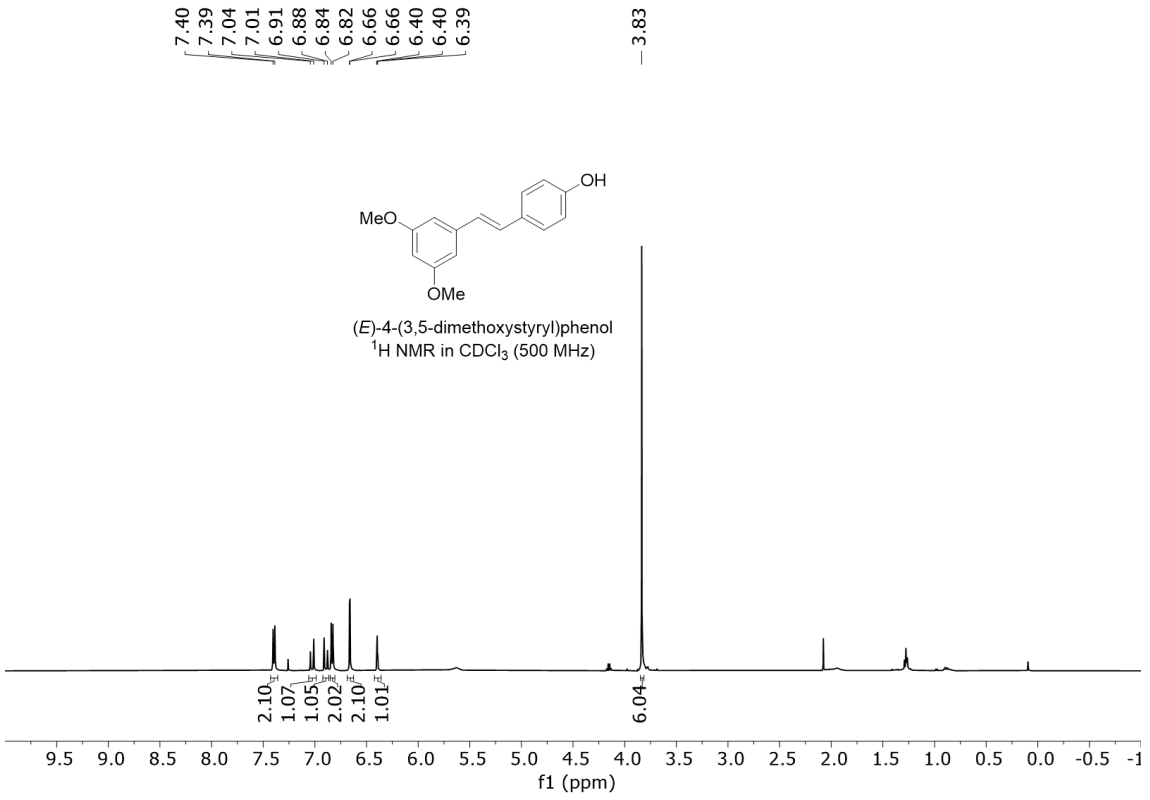


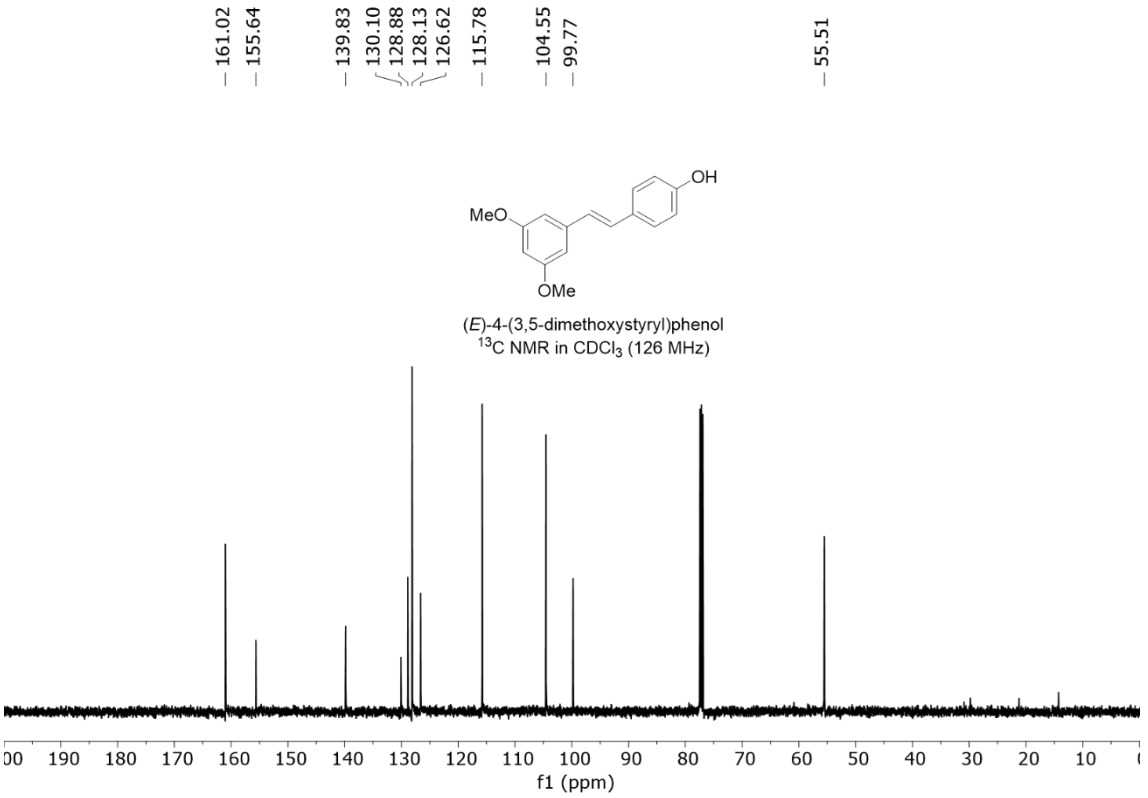
(*E*)-2-(3,4,5-trimethoxystyryl)benzo[*b*]thiophene
^{13}C NMR in $CDCl_3$ (126 MHz)

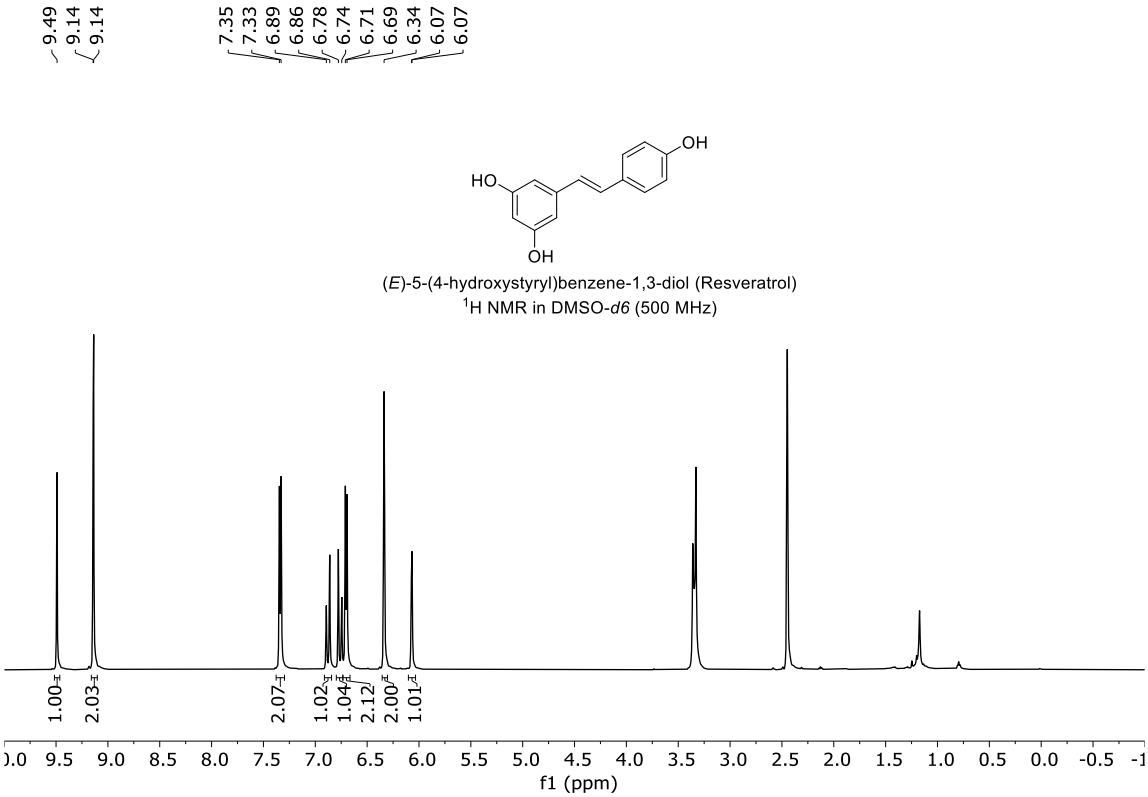


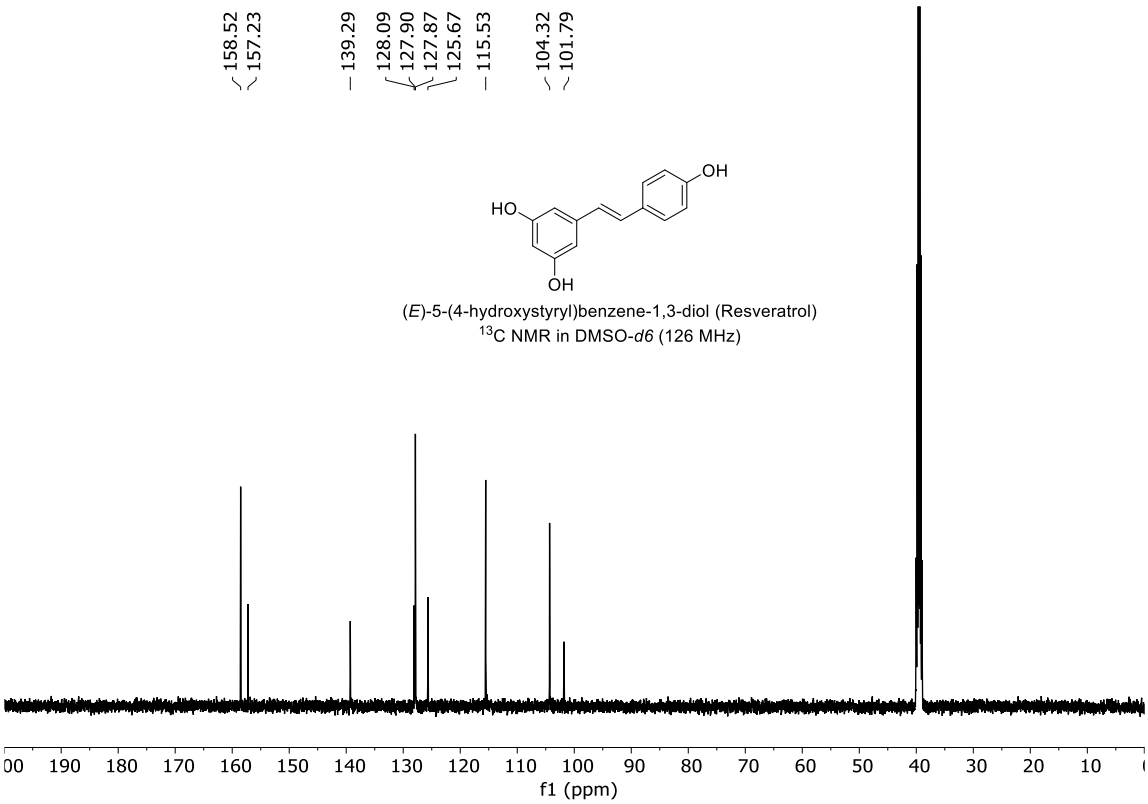
(*E*)-2-(3,4,5-trimethoxystyryl)benzo[*d*]thiazole
^{1}H NMR in $CDCl_3$ (500 MHz)


166.95
153.93
153.63
139.58
137.64
134.40
131.10
126.47
125.48
123.02
121.71
121.63
104.63
61.11
56.26
MeO
MeO
OMe
S
N
(E)-2-(3,4,5-trimethoxystyryl)benzo[d]thiazole
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


7.40
7.39
7.04
7.01
6.91
6.88
6.84
6.82
6.66
6.66
6.40
6.40
6.39
3.83
OH
MeO
OMe
(E)-4-(3,5-dimethoxystyryl)phenol
1H NMR in CDCl3 (500 MHz)
2.10
1.07
1.05
2.02
2.10
1.01
6.04
f1 (ppm)


161.02
155.64
139.83
130.10
128.88
128.13
126.62
115.78
104.55
99.77
55.51
OH
MeO
OMe
(E)-4-(3,5-dimethoxystyryl)phenol
13C NMR in CDCl3 (126 MHz)
f1 (ppm)


9.49
9.14
9.14
7.35
7.33
6.89
6.86
6.78
6.74
6.71
6.69
6.34
6.07
6.07
OH
HO
OH
(E)-5-(4-hydroxystyryl)benzene-1,3-diol (Resveratrol)
1H NMR in DMSO-d6 (500 MHz)
1.00
2.03
2.07
1.02
1.04
2.12
2.00
1.01
f1 (ppm)


158.52
157.23
139.29
128.09
127.90
127.87
125.67
115.53
104.32
101.79
HO
OH
OH
(E)-5-(4-hydroxystyryl)benzene-1,3-diol (Resveratrol)
13C NMR in DMSO-d6 (126 MHz)
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

13. References:

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