SUPPORTING INFORMATION

Snapshot of Inorganic Janovsky Complex Analogues featuring a Nucleophilic Boron Center

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CONTENTS

1. Synthesis, physical and spectroscopic data for all new compounds

General considerations: All reactions were performed under an atmosphere of dry argon using standard Schlenk or dry box techniques; solvents were dried over Na metal, K metal or CaH_2., and distilled under nitrogen. Reagents were of analytical grade, obtained from commercial suppliers and used without further purification. ^{1}H, ^{13}C, ^{11}B and ^{31}P NMR spectra were recorded on a Bruker AVIII 400 MHz or Bruker AV 400 MHz, spectrometers at 298 K. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, m = multiplet. Coupling constants *J* are given in Hz. In the ^{13}C NMR spectra of compounds **2**, **3**, **4**, **5**, **6, 7** signals for the carbon atoms directly bonding to the boron atom could not be observed, presumable due to the coupling with the boron atom. Electrospray ionization (ESI) mass spectra were obtained at the Mass Spectrometry Laboratory at the Division of Chemistry and Biological Chemistry, Nanyang Technological University. Melting points were measured with OptiMelt (Stanford Research System).

Compound 2/2’: Phenyl lithium (0.007 g, 0.081 mmol) was added into a THF-d_8 (0.45 mL) solution of 1,3,2,5-diazadiborinine **1** (0.025 g, 0.067 mmol) in a J-Young NMR tube at room temperature. The tube was sealed, shaken and the reaction was monitored by NMR spectroscopy, which indicated the formation of **2** (Figure S1).* Subsequently, 12-crown-4 ether (22 μL, 0.134 mmol) was added into the solution. After 2 hours, the red crystal generated was filtered off, washed with THF (5 ml), and then dried under vacuum to afford **2’** as a red powder (0.038 g, 70% yield).
(*Single crystals of **2** suitable for X-ray diffraction analysis were obtained from a concentrated solution of THF at –10 °C without addition of 12-crown-4.)
M.p.: 125 °C (dec.); ^{1}H NMR (400 MHz, C_5D_5N): δ = 0.87 (s, 12 H, CH_3), 3.67 (s, 32 H, OCH_2CH_2O), 3.94 (s, 4 H, CH_2), 6.85-8.92 (m, 15 H, ArH); ^{13}C NMR (100 MHz, C_5D_5N): δ = 26.1 (CH_3), 62.1 ($\underline{C}(CH_3)_2$), 70.6 (OCH_2CH_2O), 81.9 (CH_2), 125.3 (CH x2), 126.9 (CH x4), 127.2 (CH x3), 133.2 (CH x2); ^{13}C NMR (DEPT-135, 100 MHz, C_5D_5N): δ = 26.1 (CH3), 125.3 (CH x2), 126.9 (CH x4), 127.2 (CH x3), 133.2 (CH x2); 136.3 (CH x4); ^{11}B NMR (76.8 MHz, C_5D_5N): δ = –0.9 (s), 1.4 (s); HRMS (ESI): *m/z* calcd for $C_{28}H_{31}B_2N_2O_2$: 449.2572 [(*M*)]$^-$; found: 449.2589.

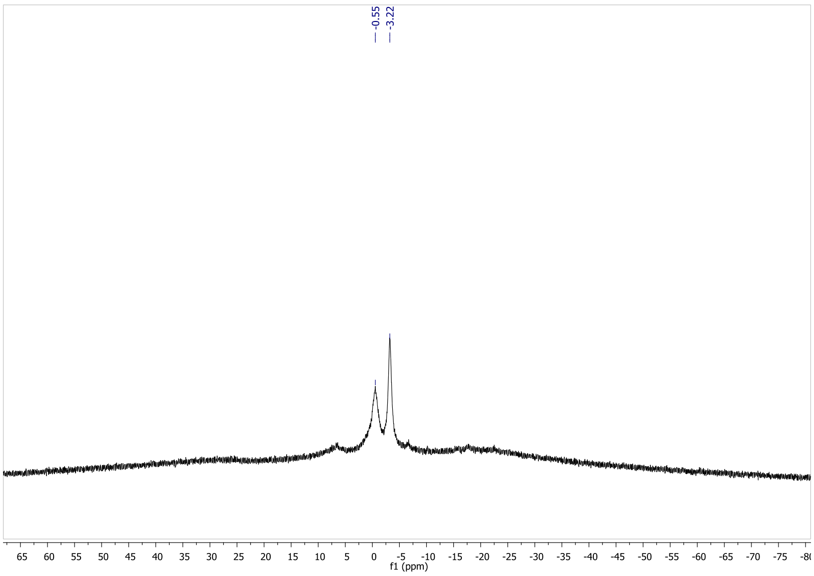


Figure S1. ^{11}B NMR (THF-d_8) spectrum of a mixture of **1** and **Phenyl lithium** after 2 hours at ambient temperature.

Compound 3: Methyl iodide (5 μL, 0.081 mmol) was added into a THF-d_8 (0.45 mL) solution of **2** (0.031 g, 0.067 mmol) in a J-Young NMR tube at room temperature. The reaction occurred immediately as confirmed by NMR spectroscopy. After removal of all volatiles, the solid residue was recrystallized from a THF/hexane mixed solution to afford colorless crystals of **3** (0.024 g, 76% yield).
Mp: 173 °C. ^{1}H NMR (400 MHz, THF-d_8): δ = 0.35 (s, 3 H, BCH_3), 0.61 (s, 12 H, CH_3), 3.92-3.97 (m, 4 H, CH_2), 7.00-7.91 (m, 15 H, ArH); ^{13}C NMR (100 MHz, THF-d_8): δ = 25.6 (CH_3), 25.7 (CH_3), 68.0 ($\underline{C}(CH_3)_2$), 81.8 (CH_2), 125.4 (CH x1), 127.3 (CH x1), 127.4 (CH x1), 127.5 (CH x2), 127.9 (CH x2), 128.0 (CH x2), 133.4 (CH x2), 135.2 (CH x2), 135.4 (CH x2); ^{13}C NMR (DEPT-135, 100 MHz, THF-d_8): δ = 25.6 (CH_3), 25.7 (CH_3), 125.4 (CH x1), 127.3

(CH x1), 127.4 (CH x1), 127.5 (CH x2), 127.9 (CH x2), 128.0 (CH x2), 133.4 (CH x2), 135.2 (CH x2), 135.4 (CH x2); ^{11}B NMR (76.8 MHz, THF-d_8): = –19.3 (s), –0.8 (s). HRMS (ESI): m/z calcd for $C_{29}H_{35}B_2N_2O_2$: 465.2885 [(M+H)]$^+$; found: 465.2896.

Compound 4: Cy$_3$PAuCl (0.034 g, 0.067 mmol) was added into a THF-d_8 (0.45 mL) solution of **2** (0.031 g, 0.067 mmol) in a J-Young NMR tube at room temperature. The reaction occurred immediately as confirmed by NMR spectroscopy. After removal of all volatiles, the solid residue was recrystallized from a THF/hexane mixed solution to afford colorless crystals of **4** (0.040 g, 65% yield).

M.p.: 175 °C (dec.); ^{1}H NMR (400 MHz, THF-d_8): δ = 0.64 (s, 6 H, CH_3), 0.66 (s, 6 H, CH_3), 1.26-2.11 (m, 33 H), 4.01-4.07 (m, 4 H, CH_2), 7.12-7.95 (m, 15 H, ArH); ^{13}C NMR (100 MHz, THF-d_8): δ = 25.2 (CH_3), 25.5 (CH_3), 26.7 (CH_2), 27.7 (CH_2), 27.8 (CH_2), 31.4 (CH_2), 33.4 (CH), 33.7 (CH), 69.0 ($\underline{C}(CH_3)_2$), 82.1 (CH_2), 126.9 (CH x1), 127.6 (CH x2), 127.67 (CH x1), 127.70 (CH x1), 128.18 (CH x2), 128.20 (CH x2), 133.3 (CH x2), 135.1 (CH x2), 135.3 (CH x2); ^{13}C NMR (DEPT-135, 100 MHz, THF-d_8): δ = 25.2 (CH_3), 25.5 (CH_3), 33.4 (CH), 33.7 (CH), 126.9 (CH x1), 127.6 (CH x2), 127.68 (CH x1), 127.70 (CH x1), 128.19 (CH x2), 128.21 (CH x2), 133.3 (CH x2), 135.1 (CH x2), 135.3 (CH x2); ^{11}B NMR (76.8 MHz, THF-d_8): δ = –11.6 (s), –0.4 (s); ^{31}P NMR (162 MHz, $CDCl_3$): δ = 53.3 (s); HRMS (ESI): *m/z* calcd for $C_{46}H_{65}AuB_2N_2O_2P$: 927.4635 [(M+H)]$^+$; found: 927.4644.

Compound 5: By following the procedure for the synthesis of **2’**, the reaction of **1** with the **methyl lithium** solution afforded **5** as a red powder (0.039 g, 77 % yield).

M.p.: 110 °C (dec.); ^{1}H NMR (400 MHz, C_5D_5N) δ = 0.96 (s, 3 H, BCH_3), 1.17 (s, 6 H, CH_3), 1.47 (s, 6 H, CH_3), 3.67 (s, 32 H, OCH_2CH_2O), 3.87 (d, J = 7.2 Hz, 2 H, CH_2), 3.97 (d, J = 7.2 Hz, 2 H, CH_2), 6.80-8.84 (m, 10 H, ArH); ^{13}C NMR (100 MHz, C_5D_5N): δ = 26.6 (CH_3), 29.0 (CH_3), 61.3 ($\underline{C}(CH_3)_2$), 70.8 (OCH_2CH_2O), 82.0 (CH_2), 117.5 (CH x1), 124.8 (CH x1), 126.8 (CH x2), 127.2 (CH x2), 133.0 (CH x2), 133.8 (CH x2); ^{13}C NMR (DEPT-135, 100 MHz, C_5D_5N): δ = 26.6 (CH_3), 29.0 (CH_3), 117.5 (CH x1), 124.8 (CH x1), 126.9 (CH x2), 127.2 (CH x2), 133.1 (CH x2), 133.8 (CH x2); ^{11}B NMR (76.8 MHz, C_5D_5N): δ = –1.3 (s), 0.5 (s); HRMS (ESI): *m/z* calcd for $C_{23}H_{29}B_2N_2O_2$: 387.2415 [(M)]$^-$; found: 387.2431.

Compound 6: By following the procedure for the synthesis of **2’**, the reaction of **1** with **(phenylethynyl)lithium** afforded **6** as a red powder (0.045 g, 80 % yield).

M.p.: 166 °C (dec.); ^{1}H NMR (400 MHz, C_5D_5N): δ = 1.51 (s, 6 H, CH_3), 1.86 (s, 6 H, CH_3), 3.67 (s, 32 H, OCH_2CH_2O), 3.93 (d, J = 7.2 Hz, 2 H, CH_2), 4.06 (d, J = 7.2 Hz, 2 H, CH_2), 6.85-8.84 (m, 15 H, ArH); ^{13}C NMR (100 MHz, C_5D_5N): δ = 26.3 (CH_3), 27.5 (CH_3), 61.3 ($\underline{C}(CH_3)_2$), 70.8 (OCH_2CH_2O), 81.9 (CH_2), 118.2 (CH x1), 125.3 (CH x1), 127.0 (CH x1), 127.1 (CH x2), 127.3 (CH x2), 128.7 (C_q), 129.2 (CH x2), 131.7 (CH x2), 132.0 (C_q), 133.1 (CH x2), 133.8 (CH x2); ^{13}C NMR (DEPT-135, 100 MHz, C_5D_5N): δ = 26.3 (CH_3), 27.5 (CH_3), 118.2 (CH x1), 125.3 (CH x1), 127.0 (CH x1), 127.1 (CH x2), 127.3 (CH x2), 129.2 (CH x2), 131.7 (CH x2), 133.1 (CH x2), 133.8 (CH x2); B NMR (76.8 MHz, C_5D_5N): δ = –3.9 (s), –0.4 (s); HRMS (ESI): *m/z* calcd for $C_{30}H_{31}B_2N_2O_2$: 473.2572 [(M)]$^-$; found: 473.2580.

Compound 7: By following the procedure for the synthesis of **2’**, the reaction of **2** and **1 -lithio-1-methylimidazolide** afforded **7** as a red powder (0.045 g, 82 % yield).

M.p.: 98 °C (dec.); ^{1}H NMR (400 MHz, C_5D_5N): δ = 0.85 (s, 6 H, CH_3), 0.93 (s, 6 H, CH_3), 3.68 (s, 32 H, OCH_2CH_2O), 3.92-3.96 (m, 4 H, CH_2), 4.01 (s, 3 H, NCH_3), 6.88-8.93 (m, 12 H); ^{13}C NMR (100 MHz, C_5D_5N): δ = 24.4 (CH_3), 27.1 (CH_3), 36.6 (NCH_3), 62.1 ($\underline{C}(CH_3)_2$), 70.6 (OCH_2CH_2O), 81.7 (CH_2), 118.3 (CH x1), 121.0 (CH x1), 125.2 (CH x1), 126.6 (CH x1), 126.7 (CH x1), 127.2 (CH x3), 128.3 (CH x1), 133.3 (CH x3); ^{13}C NMR (DEPT-135, 100 MHz, C_5D_5N): δ = 24.4 (CH_3), 27.1 (CH_3), 36.6 (NCH_3), 118.3 (CH x1), 121.0 (CH x1), 125.2 (CH x1), 126.6 (CH x1), 126.7 (CH x1), 127.3 (CH x3), 128.3 (CH x1), 133.3 (CH x3); ^{11}B NMR (76.8 MHz, C_5D_5N): δ = –1.8 (s), –1.1 (s); HRMS (ESI): *m/z* calcd for $C_{26}H_{31}B_2N_4O_2$: 453.2633 [(M)]$^-$; found: 453.2639.

2. Crystal Structure Determination of Compounds 2, 3, 4, 5, 6 and 7

X-ray data collection and structural refinement. Intensity data for compounds **2**, **3**, **4**, **5**, **6** and **7** were collected using a Bruker APEX II diffractometer. The crystals of **3**, **4**, **5**, **6** and **7** were measured at 100(2) K and the crystal of **2** was measured at 103(2). The structure was solved by direct phase determination (SHELXS-97)[1] and refined for all data by full-matrix least squares methods on F^2.[2] All non-hydrogen atoms were subjected to anisotropic refinement. The hydrogen atoms were generated geometrically and allowed to ride in their respective parent atoms; they were assigned appropriate isotropic thermal parameters and included in the structure-factor calculations. CCDC: 1569030-1569035 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallography Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Summary of Data Collection and Structure Refinement.

	2	**3·(toluene)$_{0.5}$**	**4**
Formula	$C_{44}H_{63}B_2LiN_2O_6$	$C_{32.50}H_{38}B_2N_2O_2$	$C_{46}H_{64}AuB_2N_2O_2P$
Fw	744.52	510.27	926.54
cryst syst	triclinic	triclinic	monoclinic
space group	*P-1*	*P-1*	*P 1 21/c 1*
Size (mm^3)	0. 100 x 0.240 x 0.320	0.140 x 0.220 x 0.320	0.100 x 0.220 x 0.320
T, K	103(2)	100(2)	100(2)
a, Å	17.0101(4)	13.8934(5)	21.6138(7)
b, Å	17.8543(5)	14.2385(4)	11.4783(3)
c, Å	28.3178(7)	16.4845(5)	18.9214(5)
α, deg	79.6457(17) °	107.9003(9)°	90°
β, deg	87.6737(15)°	98.7434(11)°	114.5269(10)°
γ, deg	88.4679(17) °	106.7165(9)°	90°
V, A^3	8451.5(4)	2866.72(16)	4270.6(2)
Z	8	4	4
d_{calcd}g·cm^{-3}	1.170	1.182	1.441
μ, mm^{-1}	0.592	0.072	3.521
Refl collected	29269	130017	71330
T_{min}/T_{max}	0.8330/0.9430	0.9770/0.9900	0.3990/0.7200
N_{measd}	29269	13661	8075
[R_{int}]	0.1677	0.1284	0.0613
R [I>2sigma(I)]	0.0956	0.0724	0.0379
R_w[I>2sigma(I)]	0.2796	0.1369	0.0819
GOF	1.022	1.115	1.182
Largest diff peak/hole[e·Å^{-3}]	0.557/-0.500	0.409/-0.267	2.166/-1.183

	5·(THF)	**6·(THF)$_{1.5}$**	**7·(THF)$_2$**
Formula	$C_{43}H_{69}B_2LiN_2O_{11}$	$C_{52}H_{75}B_2LiN_2O_{11.50}$	$C_{50}H_{79}B_2LiN_4O_{12}$
Fw	818.56	940.70	956.73
cryst syst	triclinic	monoclinic	monoclinic
space group	*P-1*	*P 1 21/n 1*	*P 1 21/c 1*
Size (mm^3)	0.142 x 0.206 x 0.217	0.060 x 0.300 x 0.320	0.179 x 0.186 x 0.236
T, K	100(2)	100(2)	100(2)
a, Å	11.8344(4)	12.1544(3)	11.7547(3)
b, Å	12.2694(4)	23.3935(6)	28.7561(8)
c, Å	15.7797(5)	17.8383(5)	15.7165(4)
α, deg	92.1118(10)°	90°	90^o
β, deg	103.9532(11)°	96.1514(10)°	108.0772(12)^o
γ, deg	93.1230(10)°	90°	90^o
V, A^3	2217.36(13)	5042.8(2)	5050.3(2)
Z	2	4	4
d_{calcd}g·cm^{-3}	1.226	1.239	1.258
μ, mm^{-1}	0.086	0.085	0.088
Refl collected	44237	62962	48424
T_{min}/ T_{max}	0.9820/0.9880	0.9730/0.9950	0.9800/0.9840
N $_{measd}$	9013	11104	8908
[R_{int}]	0.0828	0.1118	0.0562
R [I>2sigma(I)]	0.0635	0.0596	0.0725
R_w[I>2sigma(I)]	0.1598	0.1644	0.1614
GOF	1.032	1.018	1.191
Largest diff peak/hole[e·Å^{-3}]	0.532/-0.430	0.430/-0.519	0.503 /-0.344

3. Theoretical calculation

Gaussian 09E was used for all density functional theory (DFT) calculations.[3] Geometry optimization, frequency calculations, and Natural bond order (NBO) analysis on compound **2** was performed at the B3LYP/6-311G(d,p) level of theory.

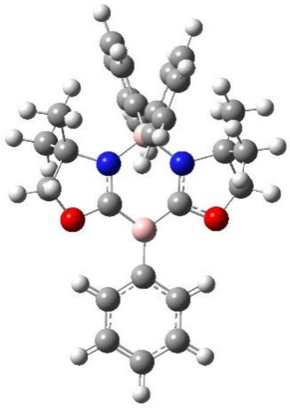
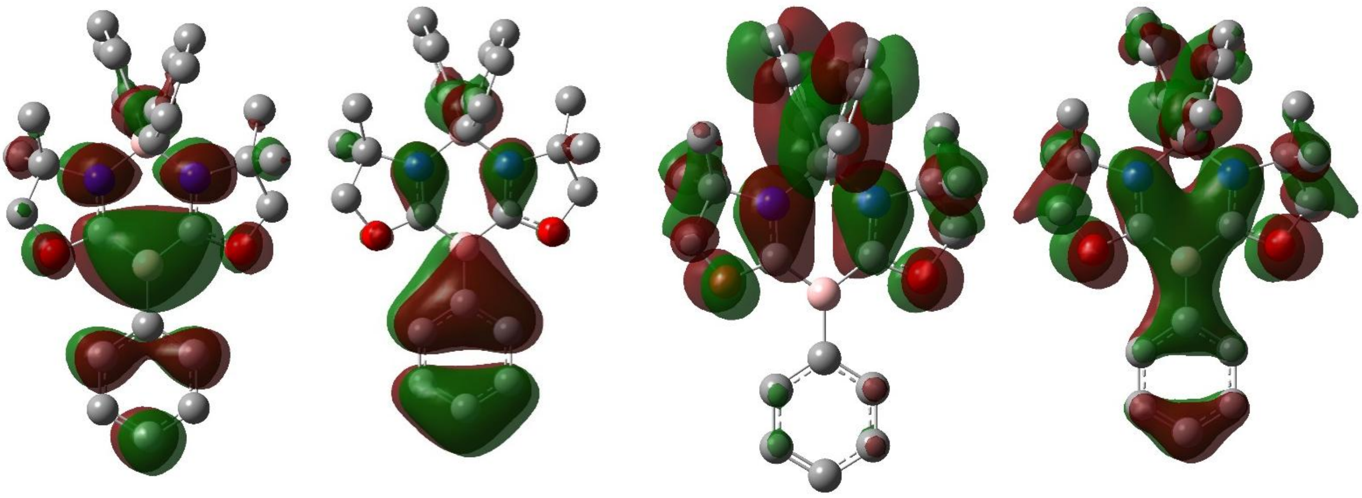


Figure S2. Calculated optimized structures for **2** at B3LYP/6-311G(d,p) level of theory.

Table S2. Optimized structures of **2** (atom, x-, y-, z- positions in Å)

B	-1.078108	-0.000019	0.000024
B	2.114265	0.000110	0.000175
C	-1.966595	0.725964	1.201600
C	-1.329901	0.982785	2.431831
H	-0.303074	0.655959	2.559984
C	-1.959383	1.653009	3.478787
H	-1.422472	1.834758	4.405617
C	-3.275445	2.097099	3.337373
H	-3.773953	2.616668	4.149940
C	-3.934903	1.867833	2.132255
H	-4.957138	2.211221	1.998504
C	-3.284266	1.200000	1.089923
H	-3.828053	1.061202	0.162203
C	-1.966207	-0.726118	-1.201754
C	-3.283840	-1.200327	-1.090448
H	-3.827920	-1.061613	-0.162883
C	-3.934102	-1.868237	-2.132979
H	-4.956322	-2.211772	-1.999500
C	-3.274298	-2.097362	-3.337926
H	-3.772503	-2.616983	-4.150647
C	-1.958264	-1.653061	-3.478983
H	-1.421093	-1.834693	-4.405685
C	-1.329157	-0.982790	-2.431842
H	-0.302351	-0.655799	-2.559712
C	-1.817653	2.416768	-2.032801
H	-1.751330	1.690764	-2.843556
H	-1.962521	3.413513	-2.465032
H	-2.701095	2.183482	-1.439202
C	-0.547844	2.423268	-1.177247
C	-0.669502	3.471901	-0.046377
H	-1.492292	3.240652	0.627211
H	-0.844843	4.464852	-0.477617
H	0.253107	3.507349	0.537872

C	0.681746	2.747432	-2.029744
H	0.593671	2.321822	-3.038762
H	0.900739	3.814785	-2.100420
C	1.235310	1.029861	-0.651223
C	1.235337	-1.029703	0.651546
C	-0.547745	-2.423264	1.177392
C	-1.817577	-2.416934	2.032902
H	-1.751357	-1.690966	2.843699
H	-1.962350	-3.413716	2.465075
H	-2.701022	-2.183713	1.439286
C	-0.669287	-3.471819	0.046436
H	-1.492086	-3.240582	-0.627148
H	-0.844549	-4.464821	0.477587
H	0.253338	-3.507128	-0.537794
C	0.681826	-2.747408	2.029918
H	0.593685	-2.321883	3.038966
H	0.900894	-3.814752	2.100520
C	3.688534	0.000130	0.000156
C	4.455799	1.062701	-0.546965
H	3.939735	1.908283	-0.981610
C	5.848588	1.063681	-0.549356
H	6.379202	1.907805	-0.983922
C	6.567869	0.000156	0.000094
H	7.653757	0.000158	0.000053
C	5.848630	-1.063385	0.549568
H	6.379277	-1.907498	0.984116
C	4.455841	-1.062430	0.547241
H	3.939817	-1.908032	0.981896
N	-0.126639	1.090299	-0.655690
N	-0.126602	-1.090239	0.655899
O	1.754463	2.108012	-1.340097
O	1.754530	-2.107851	1.340376



HOMO HOMO-2 HOMO-3 HOMO-4

Figure S3. Plots of the frontier orbitals of compounds **2**.

Table S3. The NPA charges of **2** calculated at B3LYP/6-311G(d,p) level of theory.

Atom	No	Charge Natural	Core	Valence	Rydberg	Total
B	1	0.82974	1.99886	2.13951	0.03188	4.17026
B	2	0.05230	1.99861	2.93257	0.01653	4.94770
C	3	-0.27999	1.99891	4.25105	0.03003	6.27999
C	4	-0.19214	1.99907	4.17623	0.01684	6.19214
H	5	0.21139	0.00000	0.78625	0.00237	0.78861
C	6	-0.21792	1.99914	4.20069	0.01809	6.21792
H	7	0.19268	0.00000	0.80571	0.00161	0.80732
C	8	-0.23263	1.99914	4.21466	0.01883	6.23263
H	9	0.19053	0.00000	0.80780	0.00167	0.80947
C	10	-0.22112	1.99914	4.20367	0.01831	6.22112
H	11	0.18973	0.00000	0.80859	0.00167	0.81027
C	12	-0.22019	1.99907	4.20461	0.01652	6.22019
H	13	0.19538	0.00000	0.80184	0.00278	0.80462
C	14	-0.27999	1.99891	4.25106	0.03003	6.27999
C	15	-0.22020	1.99907	4.20461	0.01652	6.22020
H	16	0.19538	0.00000	0.80185	0.00278	0.80462
C	17	-0.22112	1.99914	4.20367	0.01831	6.22112
H	18	0.18973	0.00000	0.80859	0.00167	0.81027
C	19	-0.23263	1.99914	4.21466	0.01883	6.23263
H	20	0.19053	0.00000	0.80780	0.00167	0.80947
C	21	-0.21792	1.99914	4.20069	0.01809	6.21792
H	22	0.19268	0.00000	0.80571	0.00161	0.80732
C	23	-0.19214	1.99907	4.17623	0.01684	6.19214
H	24	0.21139	0.00000	0.78624	0.00237	0.78861
C	25	-0.57936	1.99925	4.56918	0.01092	6.57936
H	26	0.21532	0.00000	0.78312	0.00156	0.78468
H	27	0.19072	0.00000	0.80790	0.00138	0.80928
H	28	0.21410	0.00000	0.78442	0.00148	0.78590
C	29	0.11407	1.99914	3.86273	0.02406	5.88593
C	30	-0.58572	1.99927	4.57488	0.01157	6.58572

H	31	0.22068	0.00000	0.77767	0.00165	0.77932
H	32	0.18248	0.00000	0.81590	0.00162	0.81752
H	33	0.21143	0.00000	0.78723	0.00135	0.78857
C	34	-0.01779	1.99903	3.99742	0.02135	6.01779
H	35	0.16570	0.00000	0.83228	0.00203	0.83430
H	36	0.17784	0.00000	0.82050	0.00166	0.82216
C	37	0.41623	1.99873	3.54899	0.03605	5.58377
C	38	0.41625	1.99873	3.54897	0.03605	5.58375
C	39	0.11407	1.99914	3.86273	0.02406	5.88593
C	40	-0.57935	1.99925	4.56918	0.01092	6.57935
H	41	0.21531	0.00000	0.78312	0.00156	0.78469
H	42	0.19072	0.00000	0.80790	0.00138	0.80928
H	43	0.21409	0.00000	0.78443	0.00148	0.78591
C	44	-0.58572	1.99927	4.57488	0.01157	6.58572
H	45	0.22068	0.00000	0.77767	0.00165	0.77932
H	46	0.18248	0.00000	0.81590	0.00162	0.81752
H	47	0.21143	0.00000	0.78722	0.00135	0.78857
C	48	-0.01780	1.99903	3.99742	0.02135	6.01780
H	49	0.16570	0.00000	0.83228	0.00203	0.83430
H	50	0.17784	0.00000	0.82050	0.00166	0.82216
C	51	-0.22954	1.99900	4.21140	0.01915	6.22954
C	52	-0.21082	1.99911	4.19426	0.01744	6.21082
H	53	0.20727	0.00000	0.78980	0.00294	0.79273
C	54	-0.22516	1.99914	4.20704	0.01897	6.22516
H	55	0.18152	0.00000	0.81671	0.00177	0.81848
C	56	-0.27018	1.99914	4.24875	0.02228	6.27018
H	57	0.18239	0.00000	0.81581	0.00179	0.81761
C	58	-0.22516	1.99914	4.20704	0.01897	6.22516
H	59	0.18152	0.00000	0.81671	0.00177	0.81848
C	60	-0.21082	1.99911	4.19427	0.01744	6.21082
H	61	0.20726	0.00000	0.78980	0.00294	0.79274
N	62	-0.71120	1.99924	5.68635	0.02561	7.71120
N	63	-0.71119	1.99924	5.68634	0.02560	7.71119
O	64	-0.56541	1.99974	6.54811	0.01756	8.56541
O	65	-0.56540	1.99974	6.54810	0.01756	8.56540

===

* Total *	-1.00000	67.96984	171.27921	0.75095	240.00000

4. References

[1] G. M. Sheldrick, SHELXL-97, Program for Crystal Structure Refinement; University of Göttingen: Göttingen, Germany, **1997**.

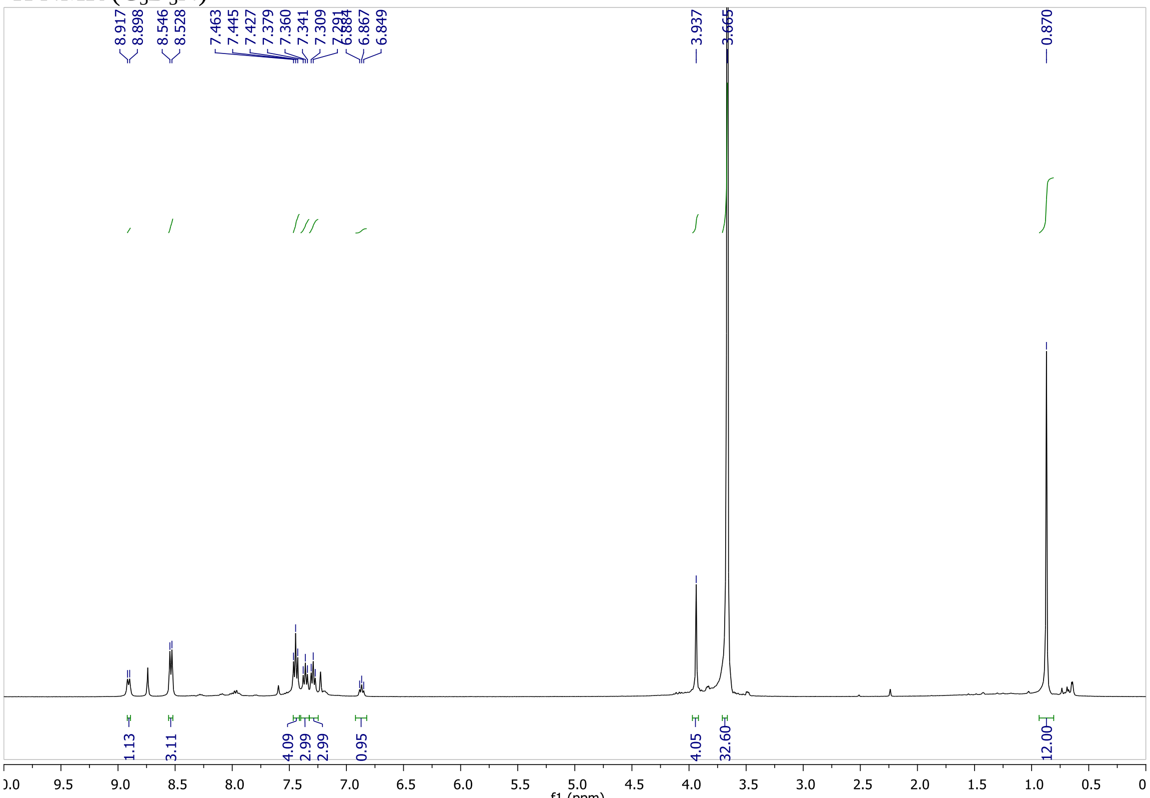
[2] Bruker AXS SHELXTL, Madison, WI; SHELX-97G. M. Sheldrick, *Acta Crystallogr. A*, **2008**, *64*, 112–122, SHELX-2013, http://shelx.uni-ac.gwdg.de/SHELX/index.php.

[3] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

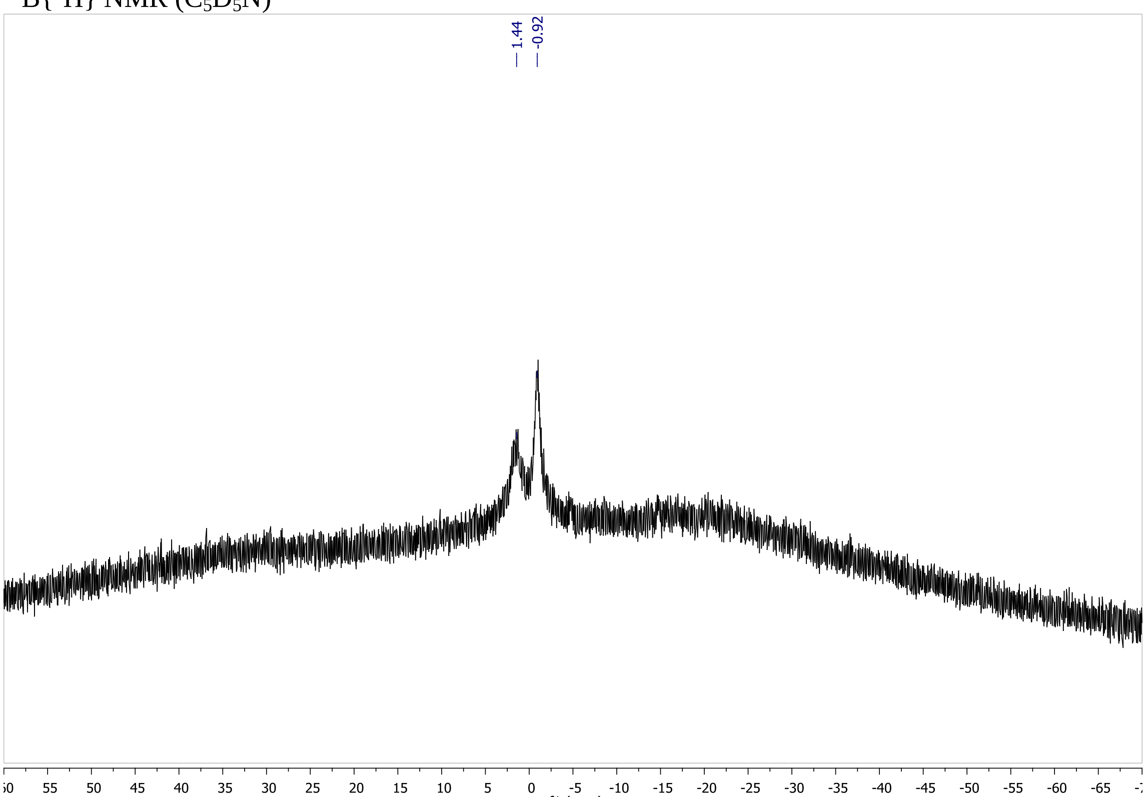
5. NMR spectra

Compound 2

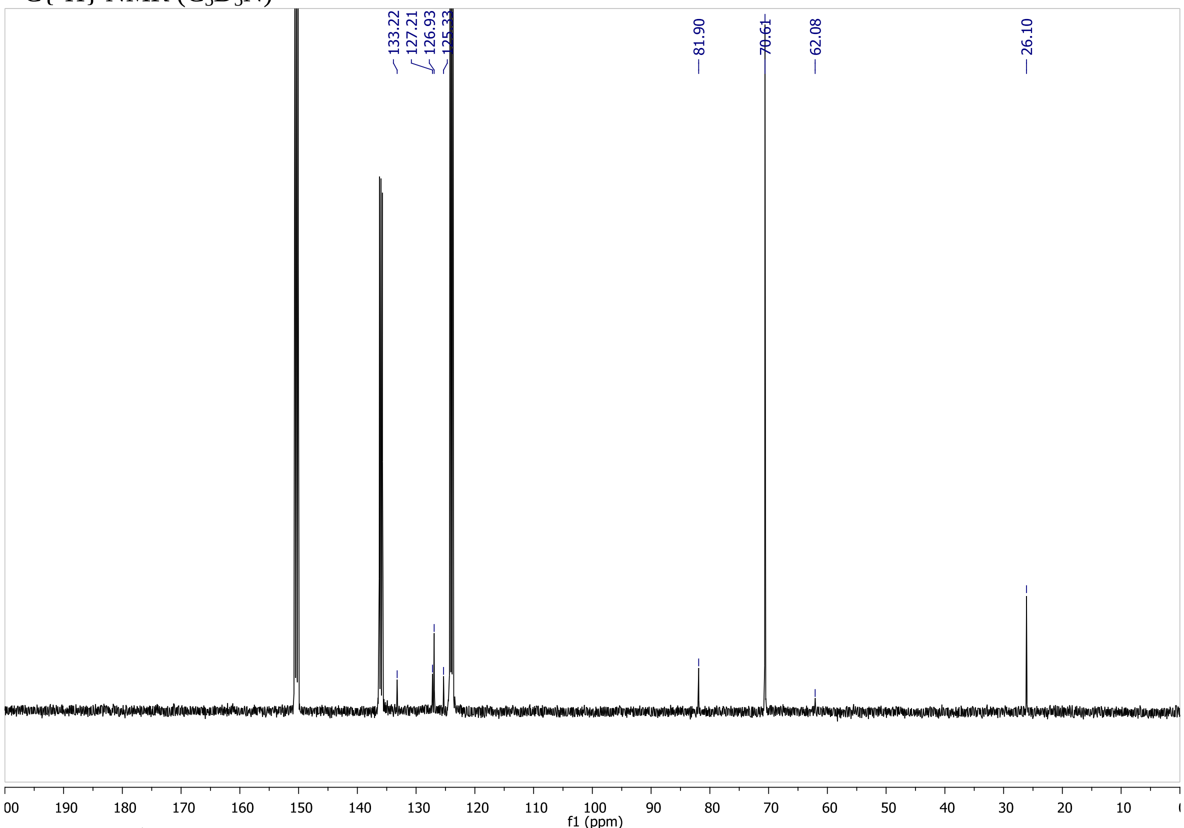
^{1}H NMR (C_5D_5N)



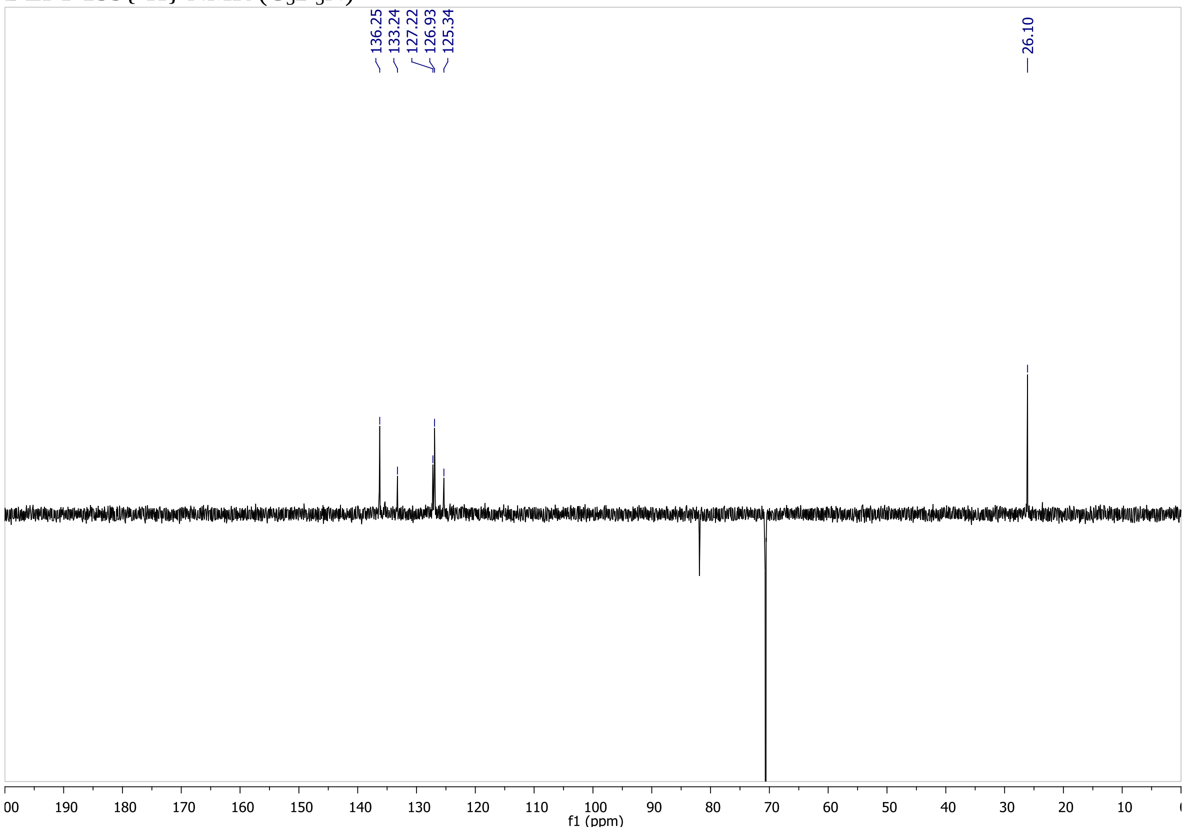
$^{11}B\{^1H\}$ NMR (C_5D_5N)



$^{13}C\{^{1}H\}$ NMR (C_5D_5N)

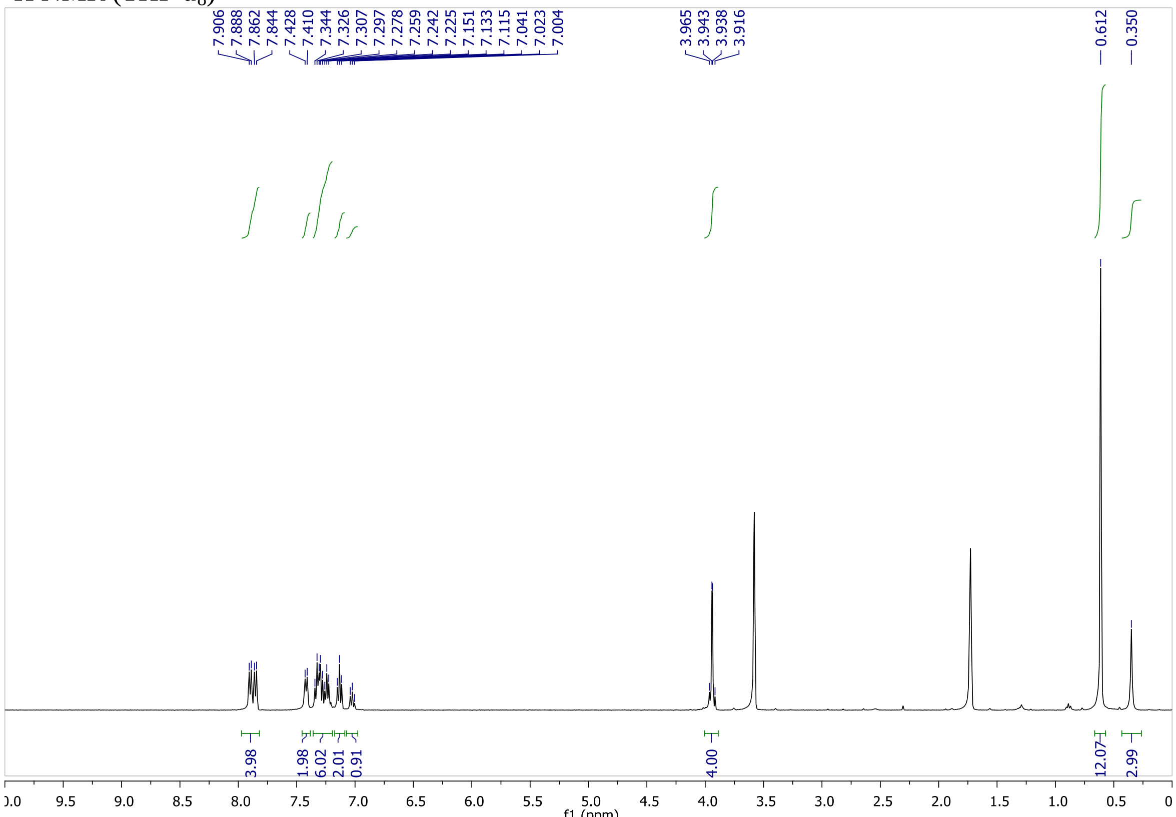


DEPT-135$\{^{1}H\}$ NMR (C_5D_5N)

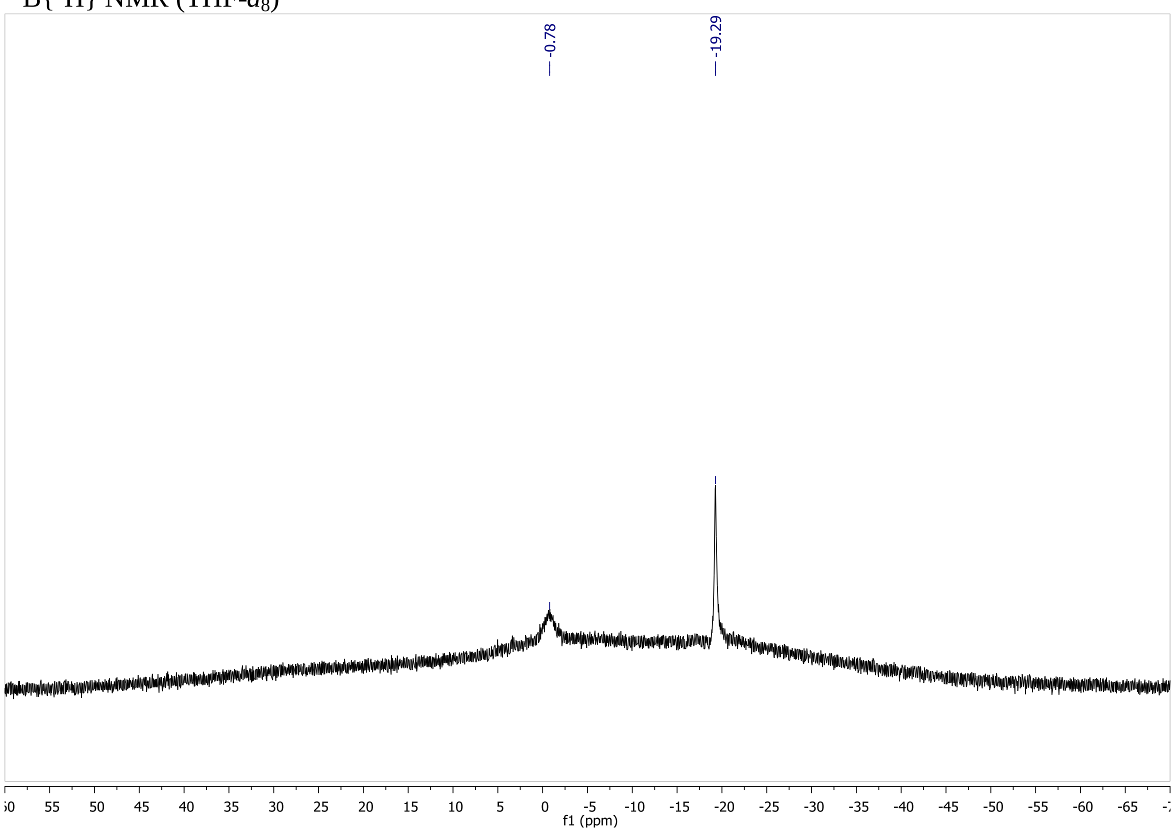


Compound 3

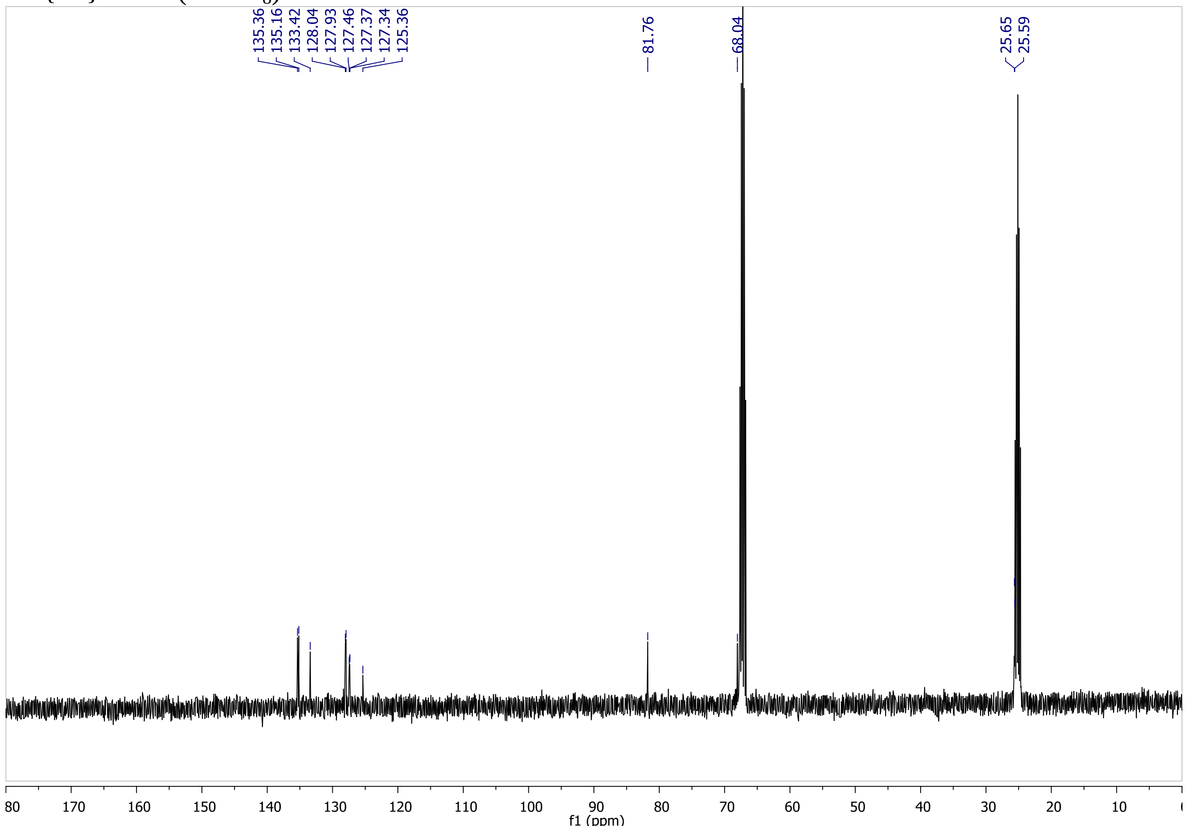
^{1}H NMR (THF-d_8)



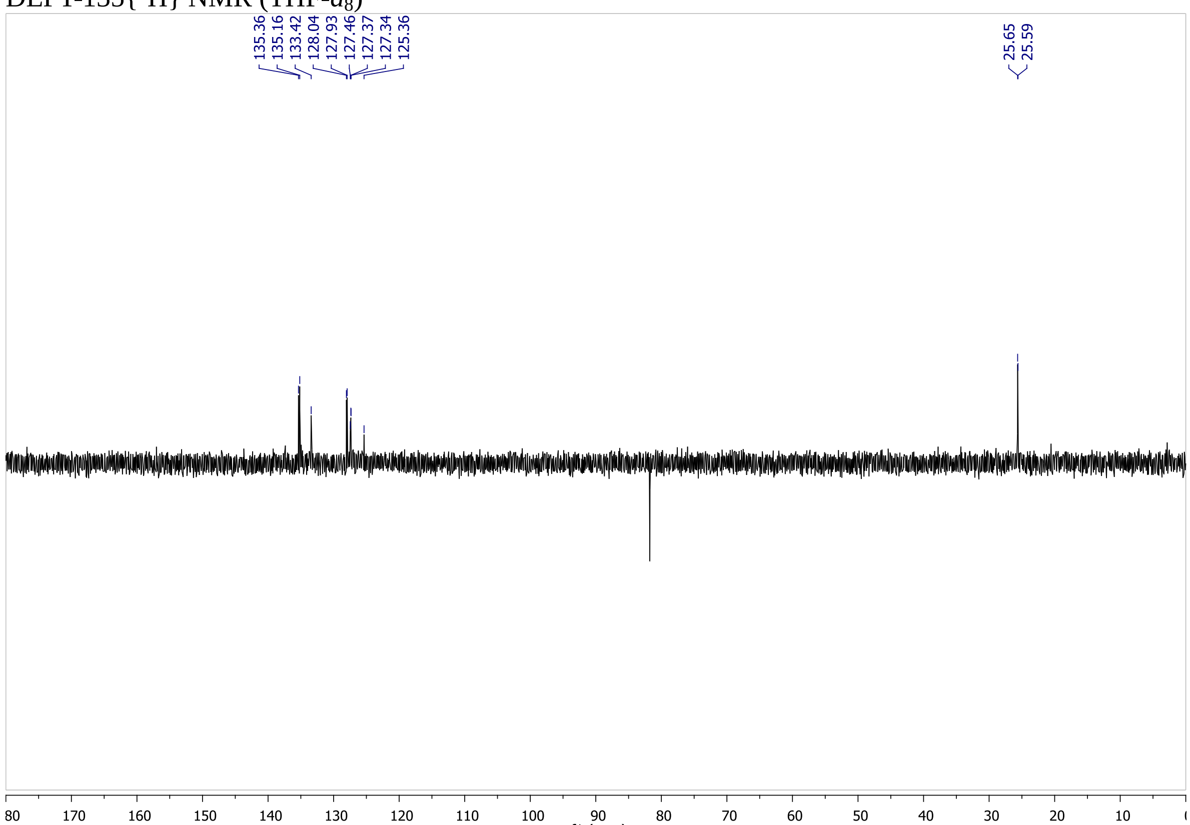
$^{11}B\{^{1}H\}$ NMR (THF-d_8)



$^{13}C\{^{1}H\}$ NMR (THF-d_8)

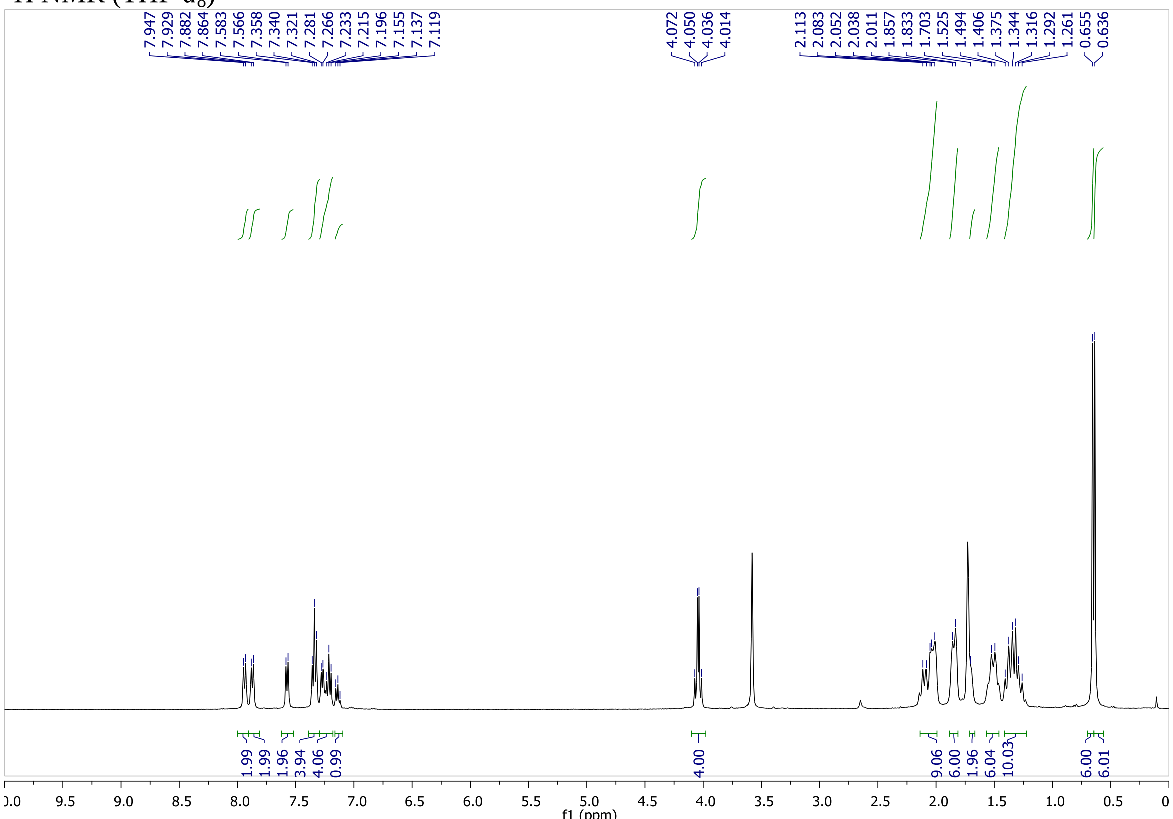


DEPT-135$\{^{1}H\}$ NMR (THF-d_8)

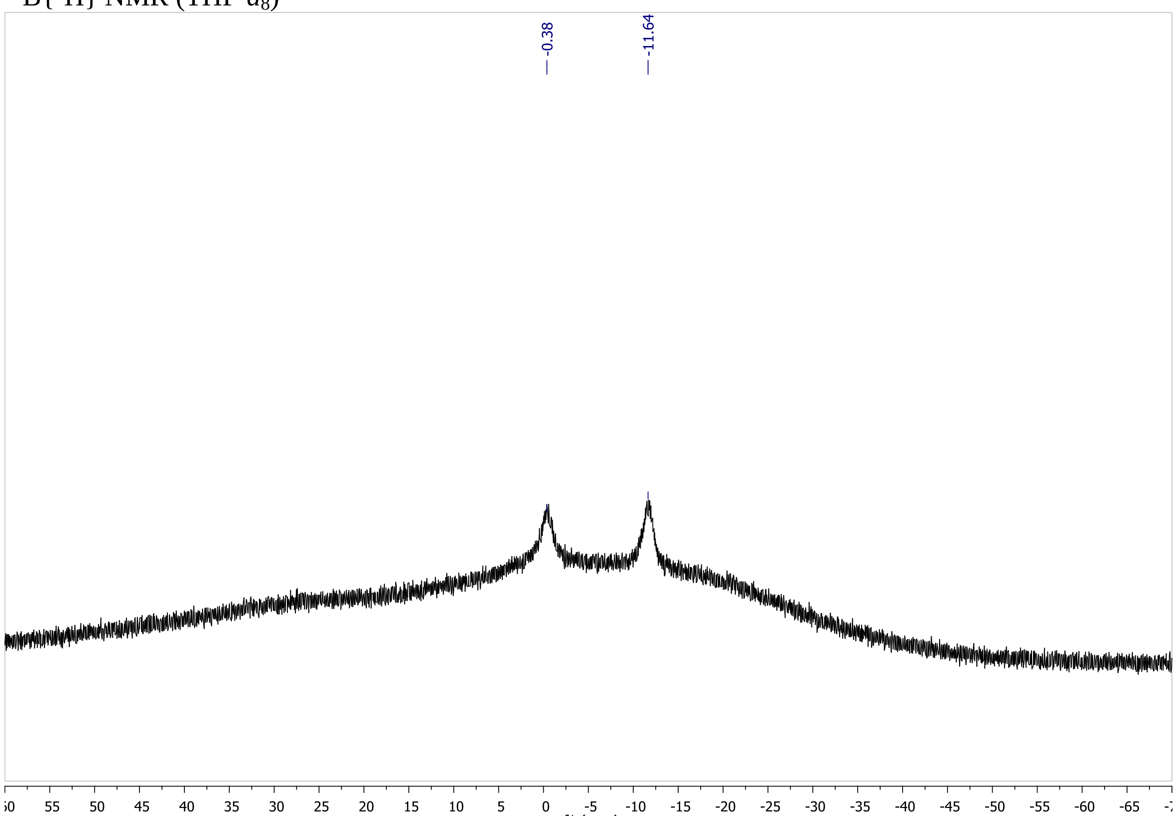


Compound 4

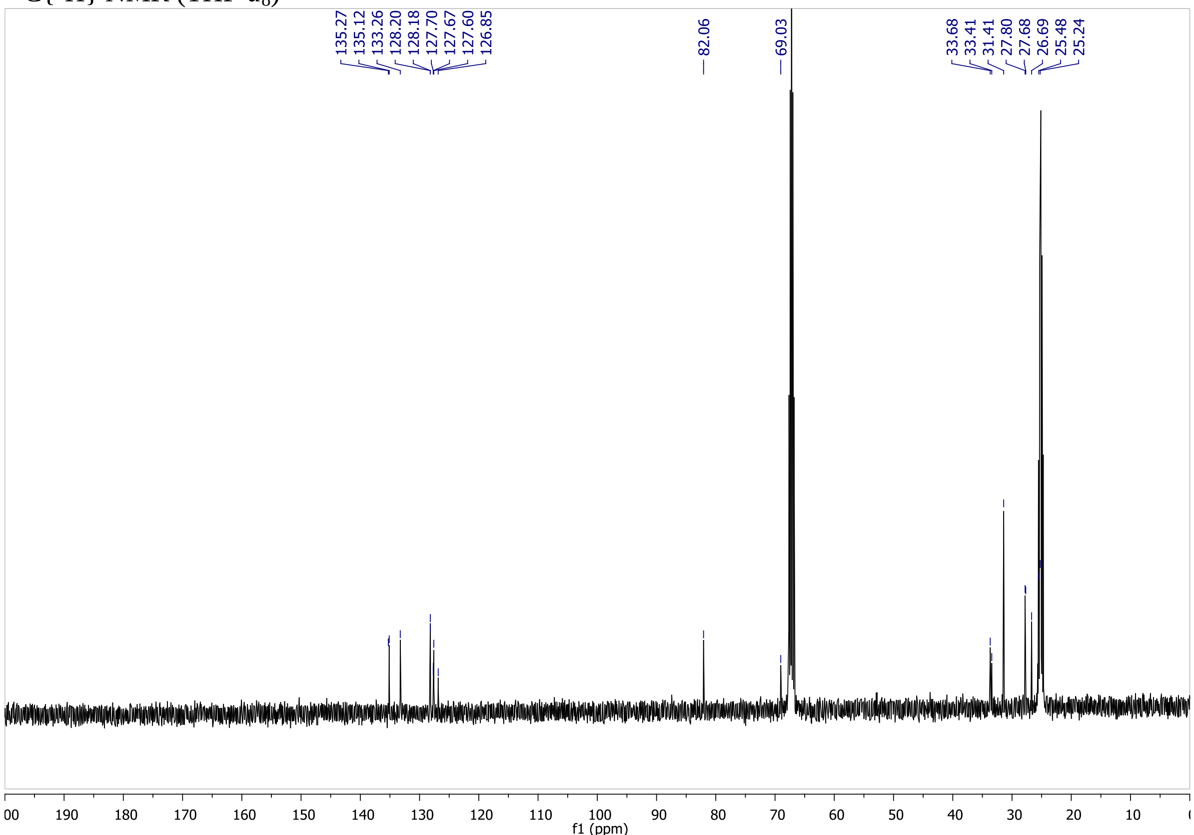
^{1}H NMR (THF-d_8)



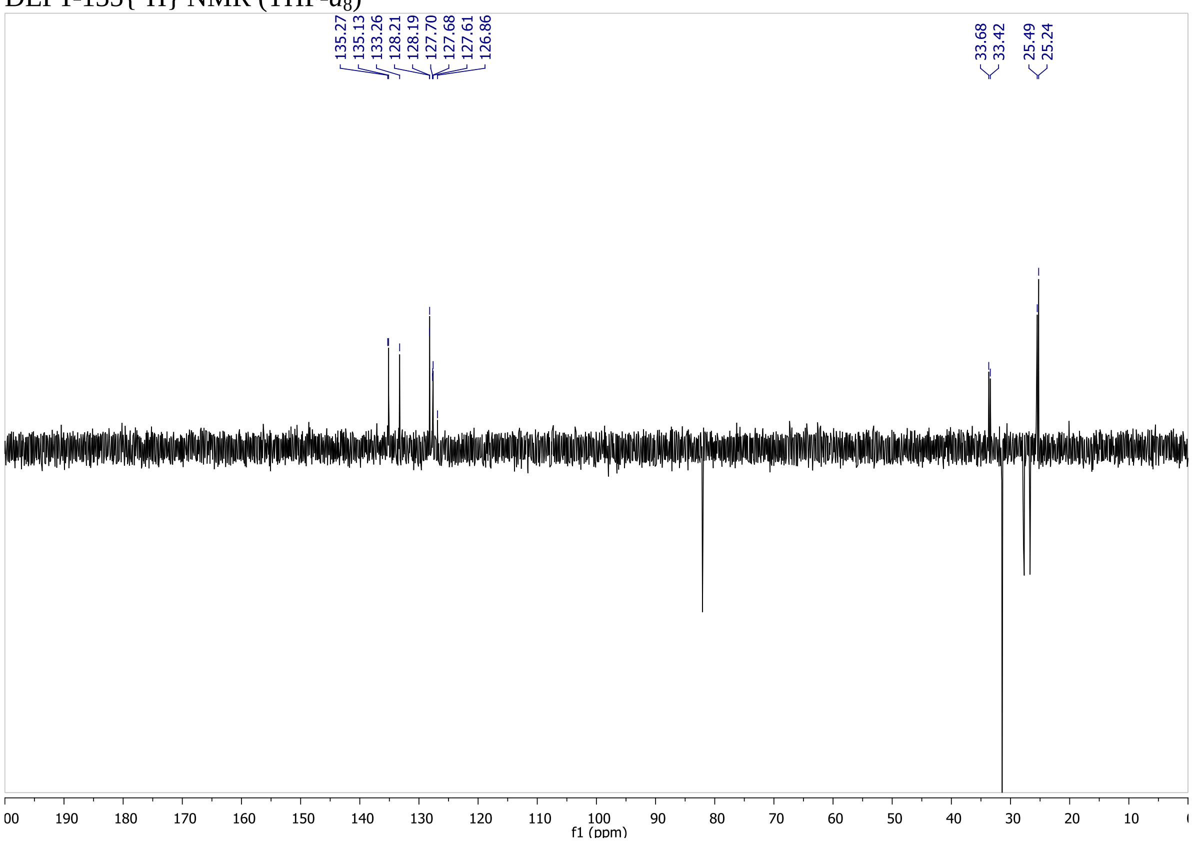
^{11}B{^{1}H} NMR (THF-d_8)



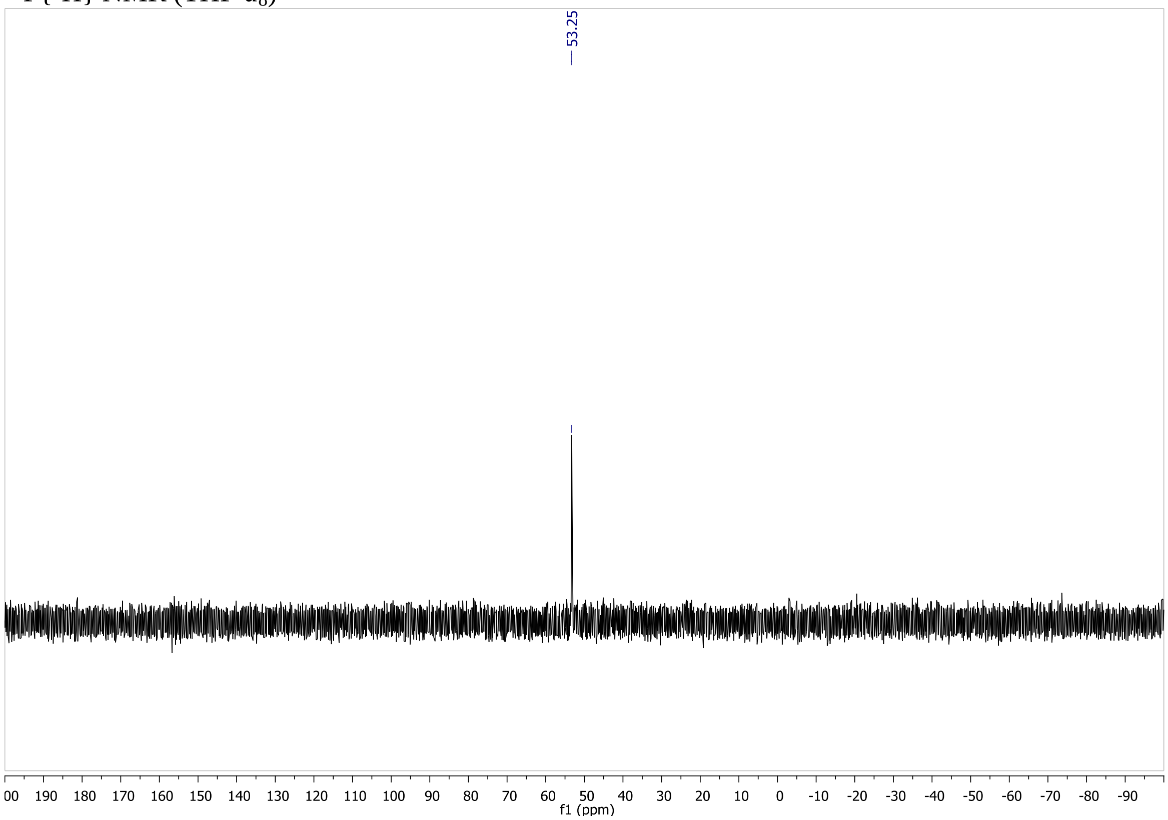
$^{13}C\{^1H\}$ NMR (THF-d_8)



DEPT-135$\{^1H\}$ NMR (THF-d_8)

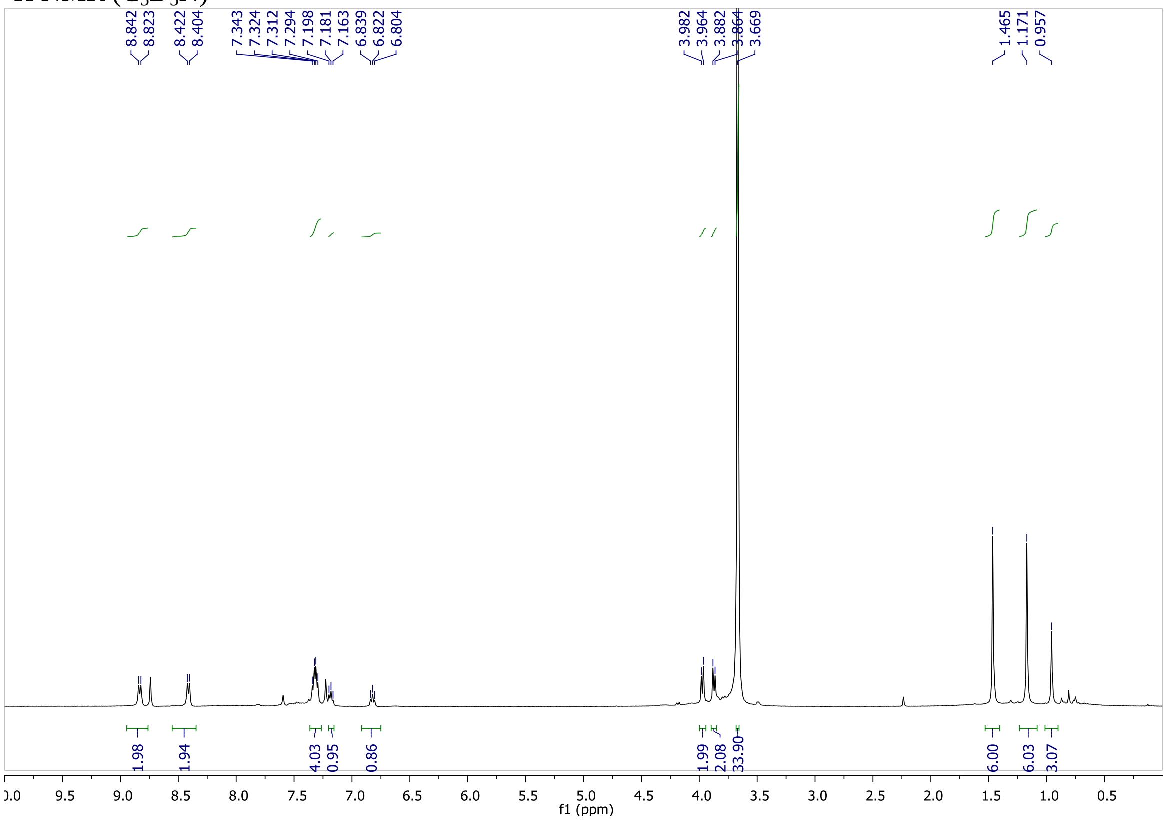


$^{31}P\{^{1}H\}$ NMR (THF-d_8)

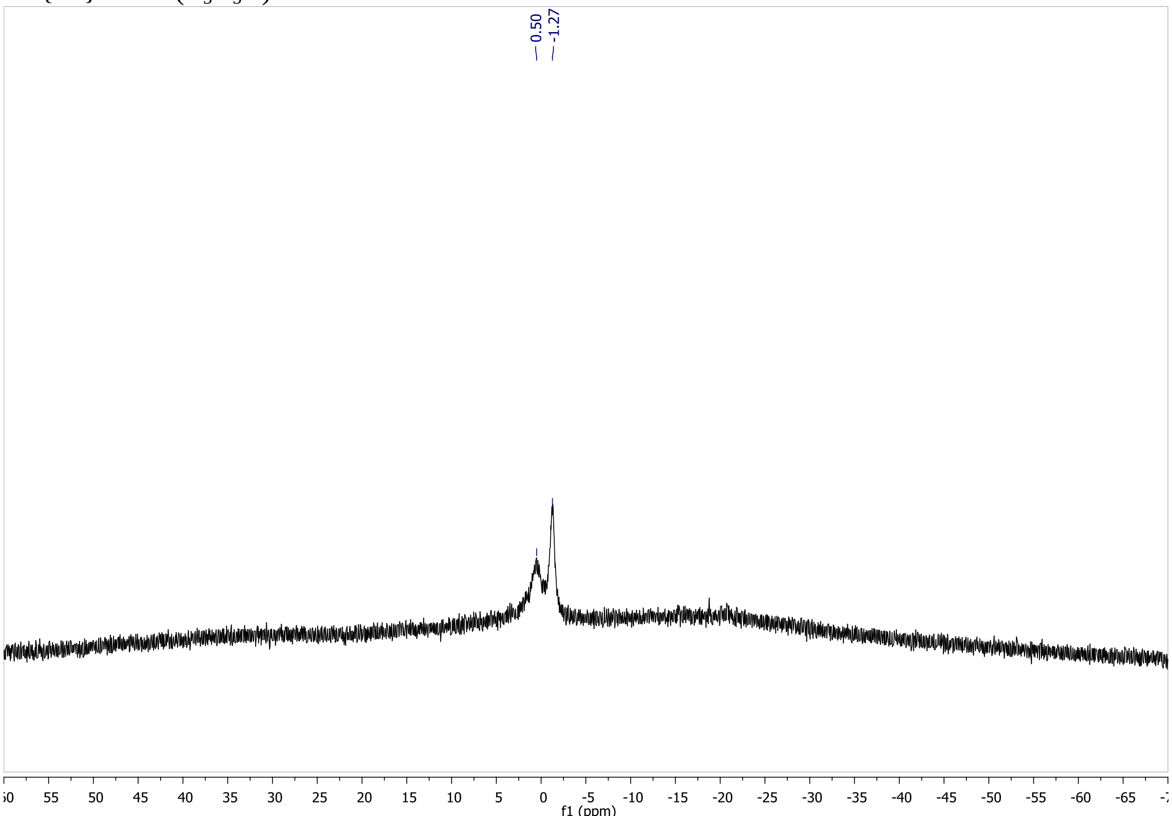


Compound 5

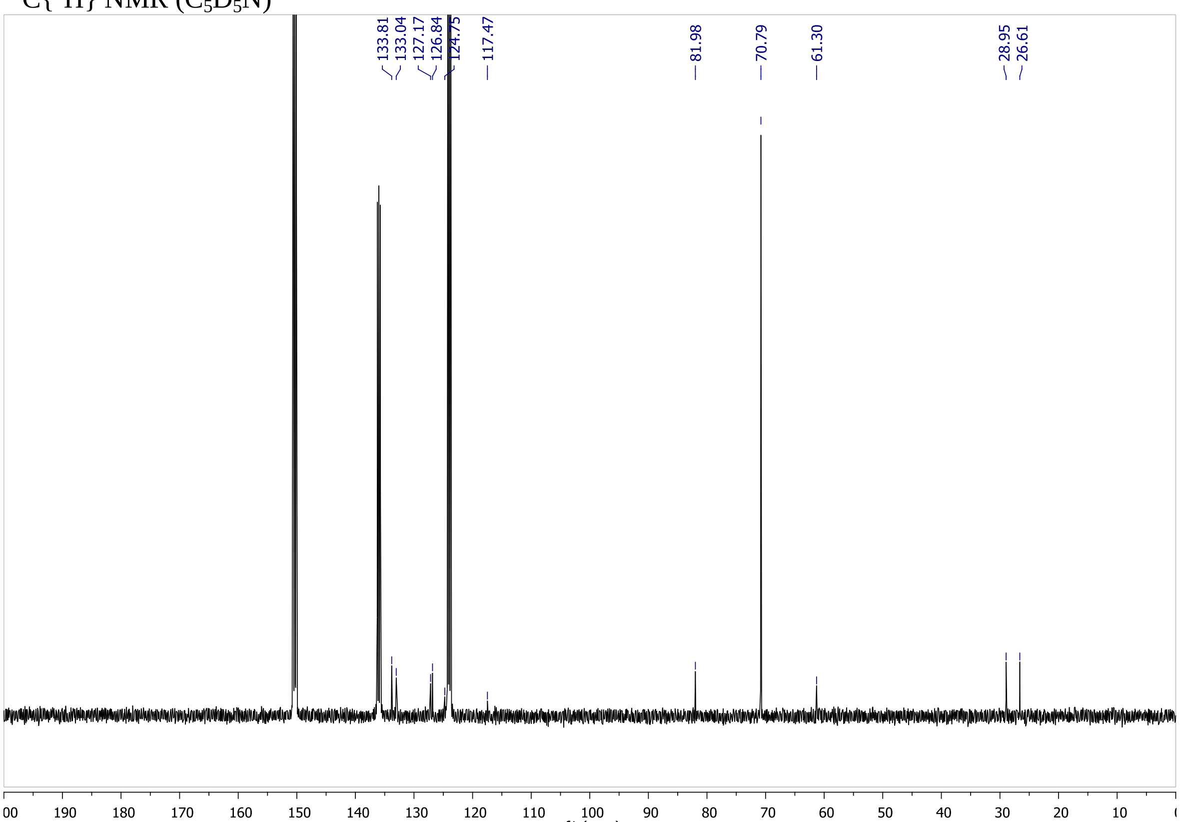
^{1}H NMR (C_5D_5N)



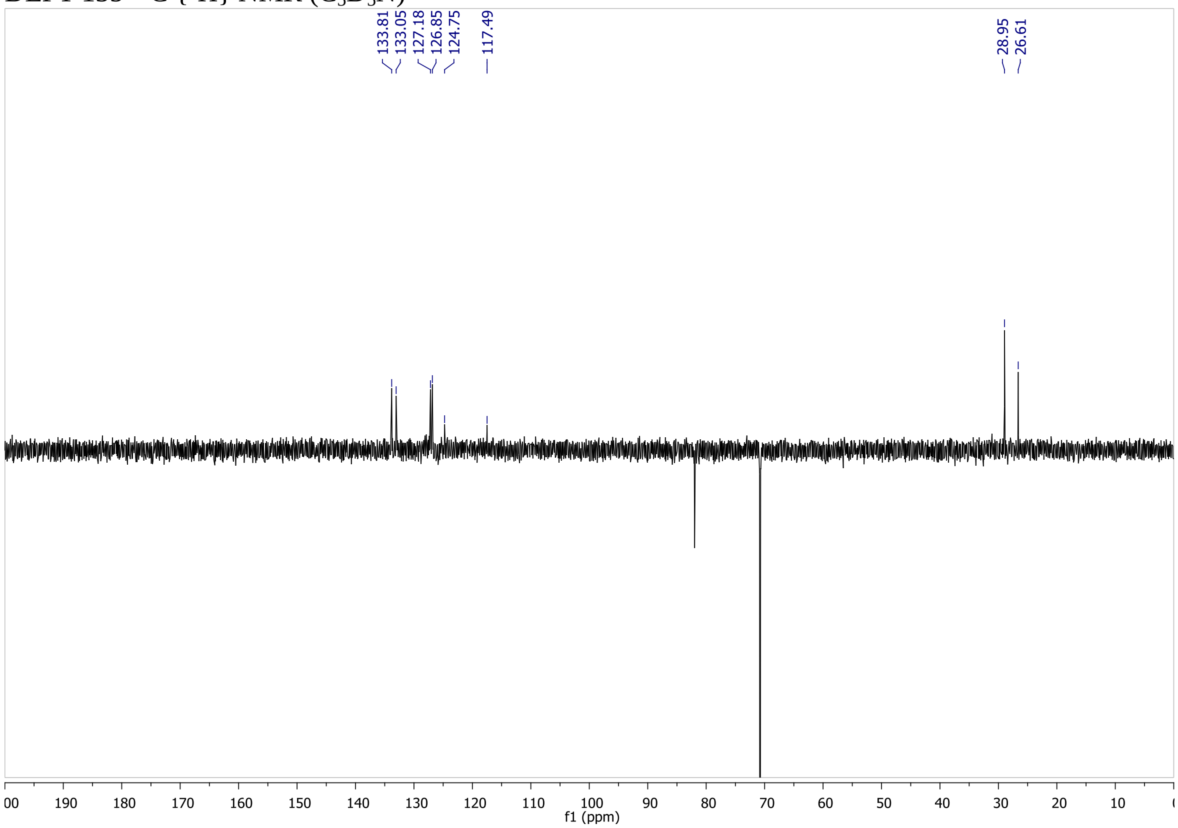
$^{11}B\{^{1}H\}$ NMR (C_5D_5N)



$^{13}C\{^{1}H\}$ NMR (C_5D_5N)

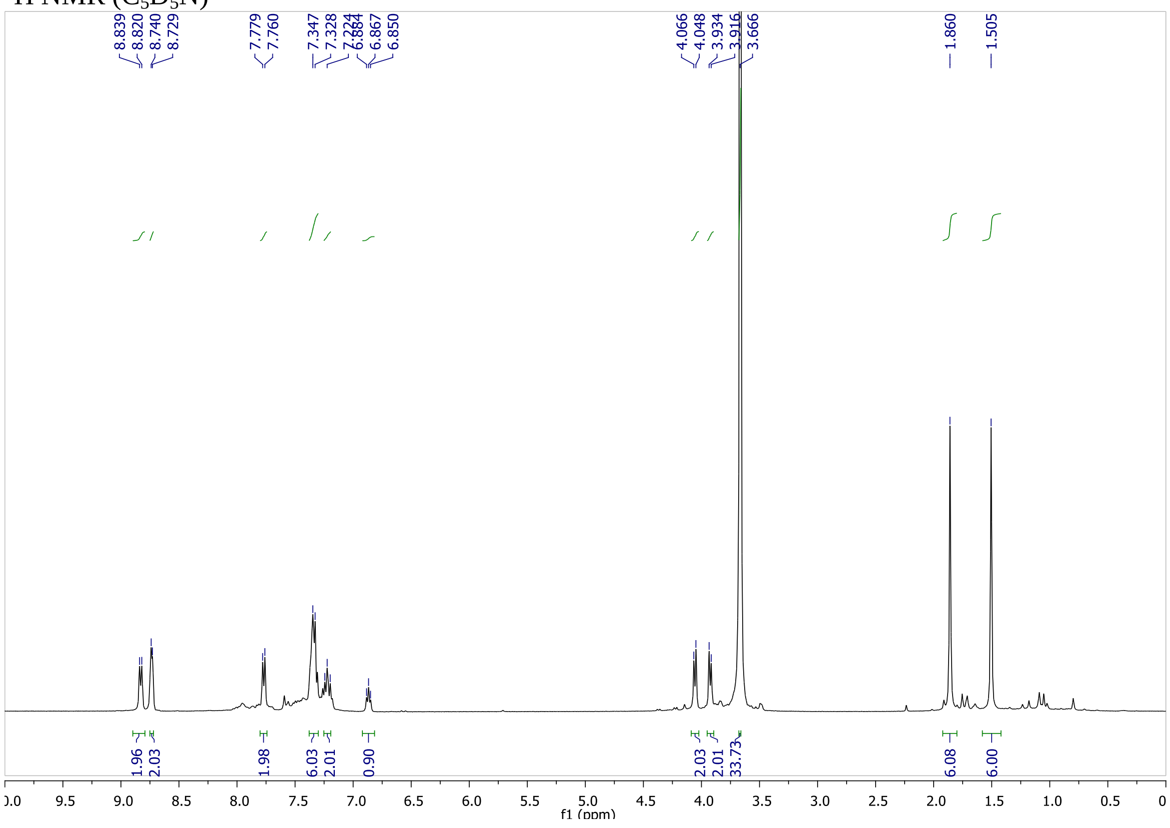


DEPT-135 $^{13}C\{^{1}H\}$ NMR (C_5D_5N)

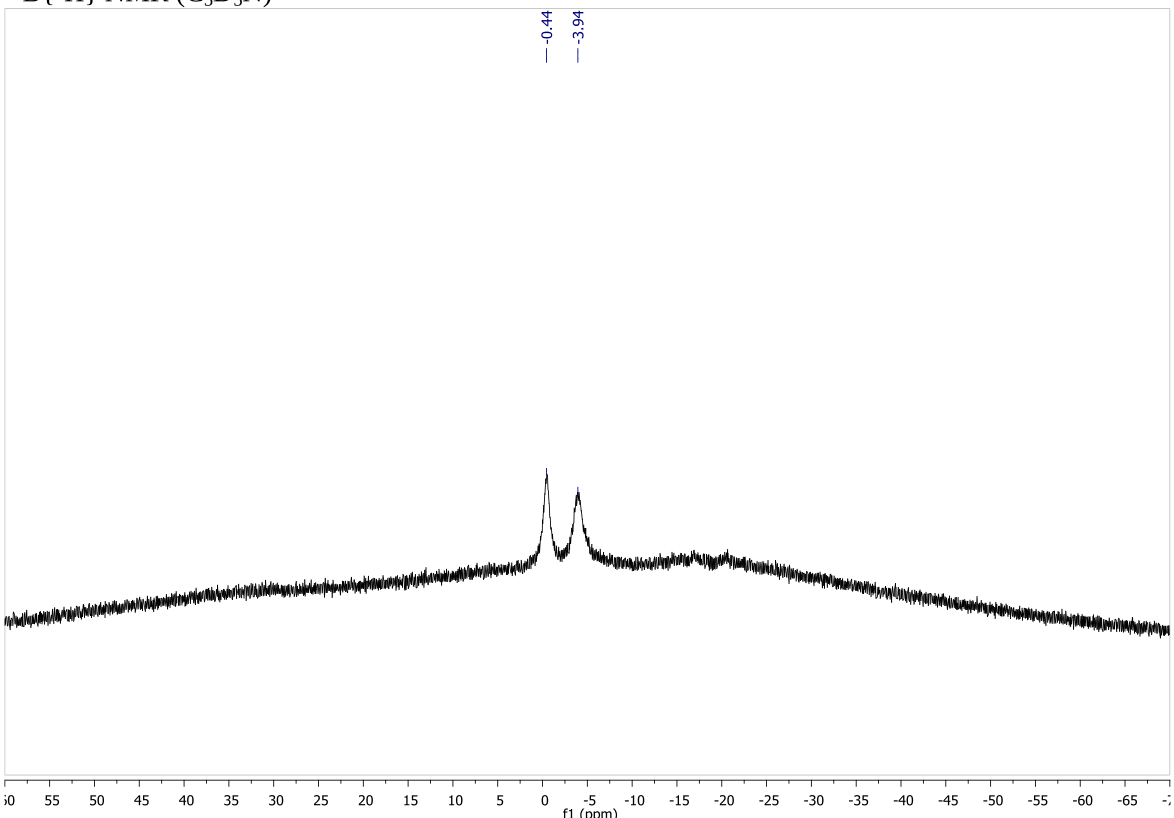


Compound 6

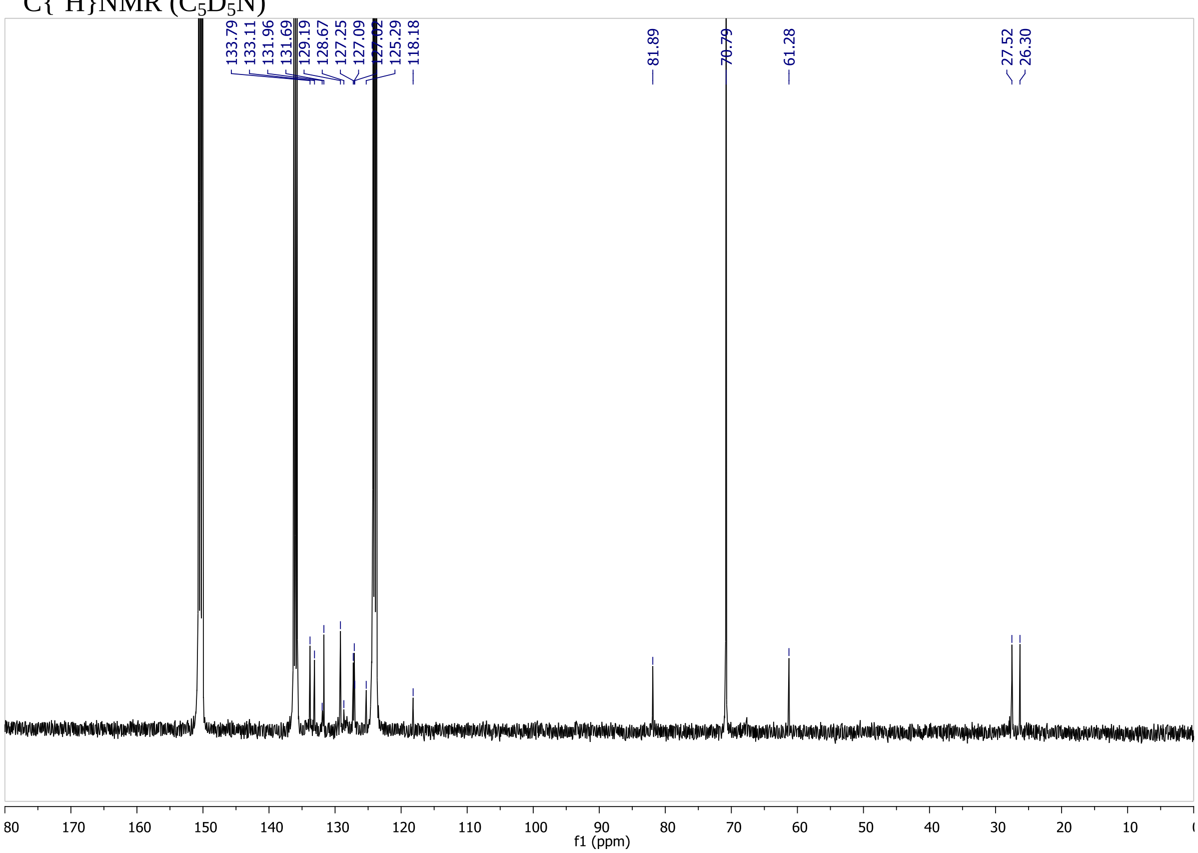
^{1}H NMR (C_5D_5N)



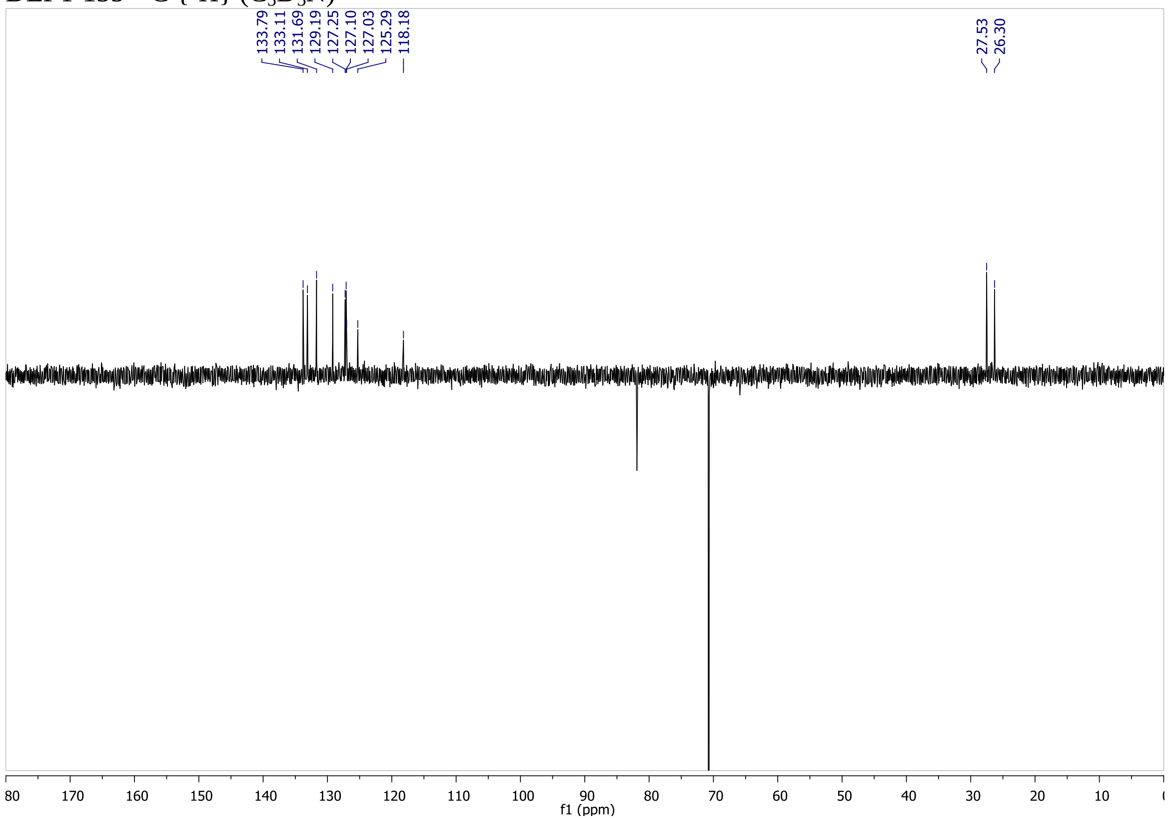
$^{11}B\{^{1}H\}$ NMR (C_5D_5N)



$^{13}C\{^{1}H\}$NMR (C_5D_5N)

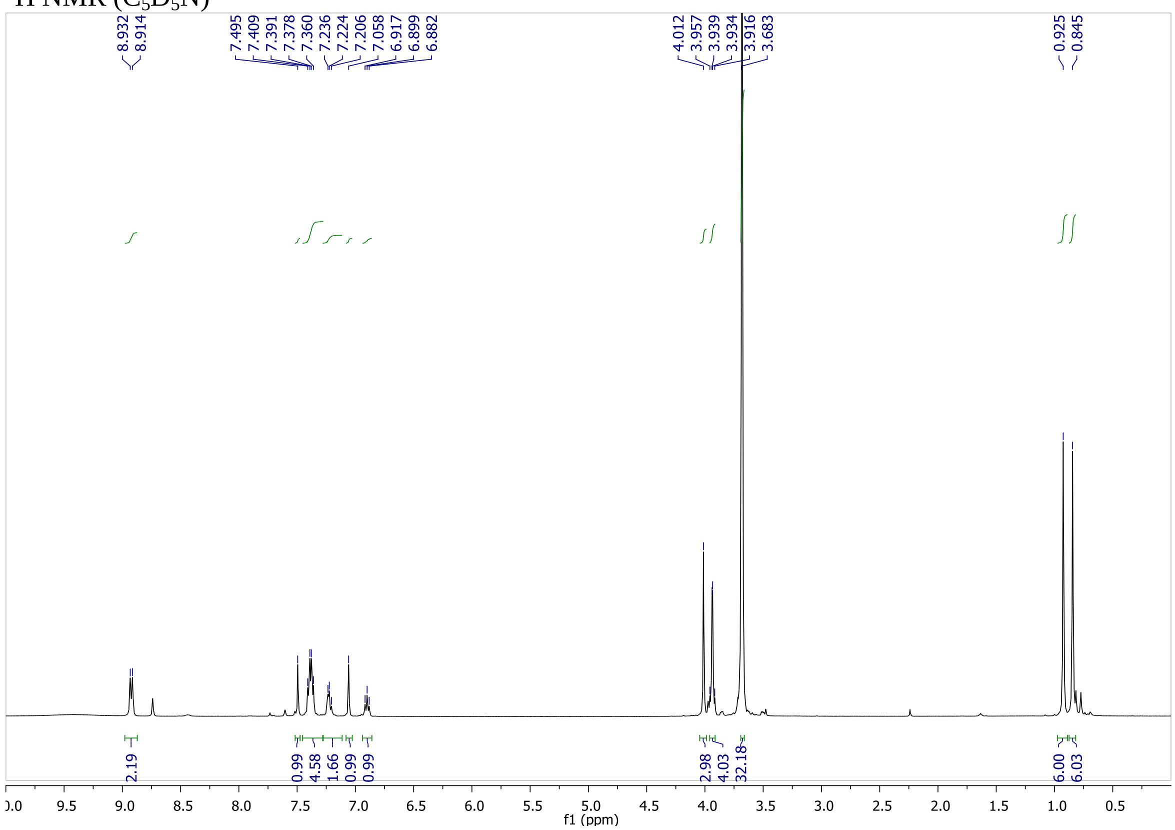


DEPT-135 $^{13}C\{^{1}H\}$ (C_5D_5N)

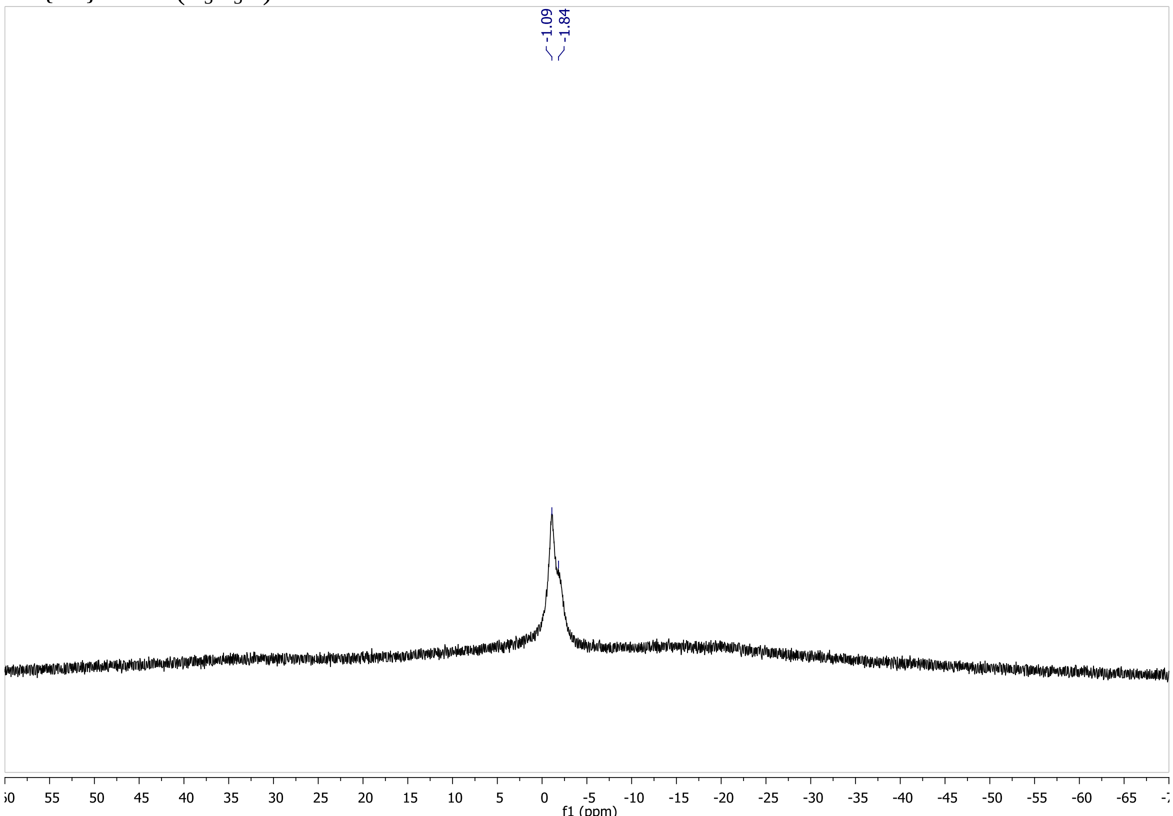


Compound 7

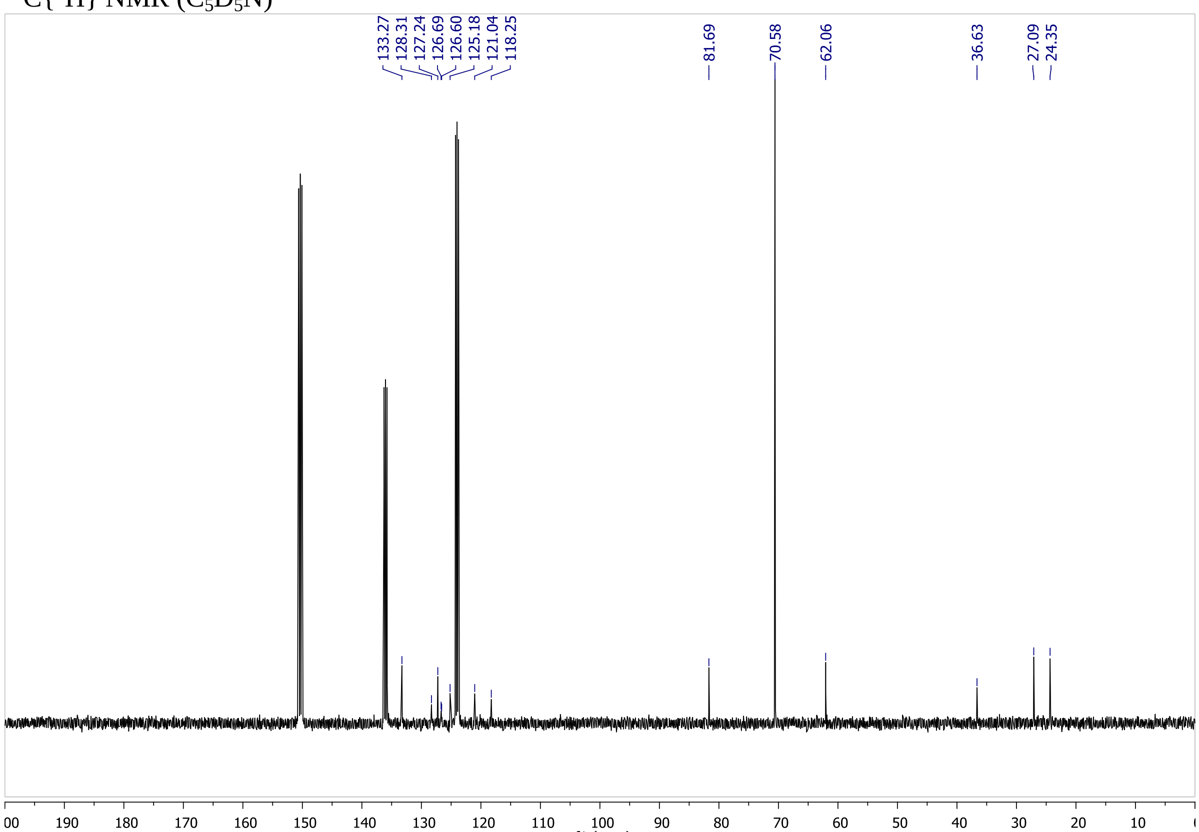
^{1}H NMR (C_5D_5N)



$^{11}B\{^{1}H\}$ NMR (C_5D_5N)



$^{13}C\{^{1}H\}$ NMR (C_5D_5N)



DEPT-135 $^{13}C\{^{1}H\}$ NMR (C_5D_5N)