Electronic Supplementary Material (ESI) for ChemComm.

Supporting Material

1,2,4,3-Triazaborole-based Neutral Oxoborane Stabilized by a Lewis Acid

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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 argon by using standard Schlenk or dry box techniques; solvents were dried over Na metal, K metal or CaH_2. Reagents were of analytical grade, obtained from commercial suppliers and used without further purification. ^{1}H, ^{13}C, ^{11}B, and $^{27}Al\{^{1}H\}$ NMR spectra were obtained with a Bruker AV 300, Bruker AV 400 or Bruker AVIII 400MHz BBFO1, spectrometers at 298 K unless otherwise stated. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, sept = septet, m = multiplet, br = broad signal. Coupling constants *J* are given in Hz. 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. IR spectrum was measured using Shimadzu IR Prestige-21 FITR spectrometer. N-(2,6-diisopropylphenyl)pivalimidoyl chloride **[(DippN=C(^{t}Bu)Cl)]** was synthesized according to literature report.[1]

Synthesis of compound 1: **1** was generated *in situ* using a modified literature procedure.[2] Phenyl hydrazine (0.99 mL, 10.0 mmol) and NEt_3 (2.09 mL, 15.0 mmol) were added dropwise to a THF solution of **[(DippN=C(^{t}Bu)Cl)]** (2.80 g, 10.0 mmol). After 4 h at room temperature, all volatiles were evaporated in *vacuo*. Toluene (40 mL) was then added and filtered to give a toluene solution of **1**, which was used subsequently for the next reaction.

Synthesis of compound 2: 1.0 M BCl_3 in *n*-hexane (11.0 mL, 11.0 mmol) was added dropwise to a toluene solution of **1** at room temperature. The solution was refluxed for 3 h, and then cooled to room temperature and filtered. All volatiles were evaporated to afford **2** as pale yellow solid in 66 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.15 (d, ^{3}J = 6.0 Hz, 6H, CH_3), 1.19 (s, 9H, C(CH)$_3$), 1.26 (d, ^{3}J = 6.0 Hz, 6H, CH_3), 2.78 (sept, J = 6.0 Hz, CHMe$_2$), 7.14 (t, ^{3}J = 8.0 Hz, 1H, ArH), 7.23 (d, ^{3}J = 8.0 Hz, 2H, ArH), 7.38 (t, ^{3}J = 8.0 Hz, 3H, ArH) 7.81 (d, ^{3}J = 8.0 Hz, 2H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz): 22.8 (CH$_3$), 25.8 (CH$_3$), 28.7(CH), 30.0 (CH$_3$), 35.5 (CMe$_3$), 119.7 (CH), 124.1 (CH), 124.3 (CH), 129.0 (CH), 134.1 (Ar-C), 142.7 (CN), 146.6 (CN), 156.8 (C=N); ^{11}B NMR ($CDCl_3$, 128 MHz): 24.4; M.p.: 159 ^{o}C; HRMS (ESI): *m/z* calcd for $C_{23}H_{32}BClN_3$: 396.2378 [(M+H)]$^{+}$; found: 396.2352.

Synthesis of compound 3: H_2O (14 µL, 0.778 mmol) was added to a dichloromethane solution of **2** (0.30 g, 0.758 mmol) at room temperature. The reaction mixture was stirred for few minutes, and then NEt_3 (0.11 mL, 0.789 mmol) was added to the mixture. The solvent was then removed under vacuum and the residue was extracted with benzene. Evaporation of benzene under vacuum followed by washing with minimum amount of pentane afforded borinic acid **3** as a colourless solid in 73 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.10 (d, ^{3}J = 6.0 Hz, 6H,

$CH(CH_3)_2$), 1.17 (s, 9H, CH_3), 1.25 (d, ^3J = 6.0 Hz, 6H, $CH(CH_3)_2$) 2.96 (sept, ^3J = 6.0 Hz, 2H, $CHMe_2$), 3.25 (s, 1H, O*H*), 7.00 (t, 1H, ^3J = 8.0 Hz, Ar*H*), 7.24 (d, 2H, ^3J = 8.0 Hz, Ar*H*), 7.32 – 7.40 (m, 3H, Ar*H*), 7.69 (d, ^3J = 8.0 Hz, 2H, Ar*H*); ^{13}C NMR ($CDCl_3$, 100 MHz): 22.3 (*C*H), 26.3 (*C*H), 28.6 (*C*H), 29.6 (CH_3), 35.3 (CMe_3), 117.2 (*C*H), 122.1 (*C*H), 124.3 (*C*H), 129.1 (2 x *C*H), 133.6 (Ar-*C*), 143.8 (*C*-N), 147.5 (*C*-N), 154.3(*C*=N); ^{11}B NMR ($CDCl_3$, 128 MHz): 23.4; M.p.: 116 ^oC; HRMS (ESI): *m/z* calcd for $C_{23}H_{33}BN_3O$: 378.2717 $[(M+H)]^+$; found: 378.2702.

Synthesis of compound 5: Borinic acid **3** (0.283 g, 0.769 mmol) and $AlCl_3$ (0.100 g, 0.750 mmol) were dissolved in DCM in glove box. The solution was then stirred at room temperature for 1 h. The solvent was removed under vacuum to afford oxoborane **5** as a light pale yellow solid in 95 % yield. ^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.26 (d, ^3J = 6.0 Hz, 6H, C*H*), 1.29 – 1.31 (m, 15H), 2.66 (sept, ^3J = 6.0Hz, 2H, $CHMe_2$), 7.30-7.37 (m, 3H, Ar-C*H*), 7.47-7.57 (m, 5H, Ar-C*H*), 10.22 (br, 1H, N*H*); ^{13}C NMR (CD_2Cl_2, 100 MHz): 22.6 (CH_3), 26.0 (CH_3), 28.6(CH_3), 29.7 (*C*H), 36.3 (CMe_3), 121.5 (*C*H), 124.9 (*C*H), 127.4 (*C*H), 130.3 (*C*H), 130.6 (*C*H), 130.8 (Ar-*C*), 136.8 (*C*-N), 145.6 (*C*-N), 160.7 (*C*=N); ^{11}B NMR (CD_2Cl_2, 128 MHz): 18.9; ^{27}Al{^{1}H} (CD_2Cl_2, 104 MHz): 87.3; M.p.: 250 ^oC (Decomposed); HRMS (ESI): *m/z* calcd for $C_{23}H_{33}AlBCl_3N_3O$: 510.1598 $[(M+H)]^+$; found: 510.1617.

2. Crystal Structure Determination of Compounds 2, 3 and 5

X-ray data collection and structural refinement. Intensity data for compounds **2**, **3** and **5** were collected using a Bruker APEX II diffractometer. The crystals of **2**, **3** and **5** were measured at 103(2) K. The structure was solved by direct phase determination (SHELXS-97) and refined for all data by full-matrix least squares methods on F^2.[3] 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: 1000877-1000879 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**	**5**
Formula	$C_{23}H_{31}BClN_3$	$C_{23}H_{32}BN_3O$	$C_{23}H_{32}AlBCl_3N_3O$
Fw	395.77	377.33	510.65
cryst syst	Orthorhombic	Monoclinic	Monoclinic
space group	*P* b c a	*C* 1 c 1	*P* 1 21/n 1
Size (mm^3)	0.12 x 0.12 x 0.38	0.24 x 0.30 x 0.34	0.30 x 0.34 x 0.42
T, K	103(2)	103(2)	103(2)
a, Å	9.7748(16)	18.898(4)	9.7657(12)
b, Å	18.042(4)	13.4431(19)	17.953(2)
c, Å	24.277(5)	17.569(3)	16.2032(18)
α, deg	90	90	90
β, deg	90	100.681(5)	106.333(3)
γ, deg	90	90	90
V, A^3	4281.4(14)	4386.0(14)	2671.5(6)
Z	8	8	4
d_{calcd} $g\cdot cm^{-3}$	1.228	1.143	1.270
μ, mm^{-1}	0.192	0.070	0.396
Refl collected	54744	15879	8582
T_{min}/ T_{max}	0.9522	0.9931	0.9562
N_{measd}	3769	6195	8020
$[R_{int}]$	0.1427	0.0960	0.1253
R [I>2sigma(I)]	0.0671	0.0816	0.0631
R_w[I>2sigma(I)]	0.2030	0.2270	0.1666
GOF	1.098	1.029	1.044
Largest diff peak/hole[$e\cdot Å^{-3}$]	0.417/-0.695	0.609/-0.673	0.954/-0.818

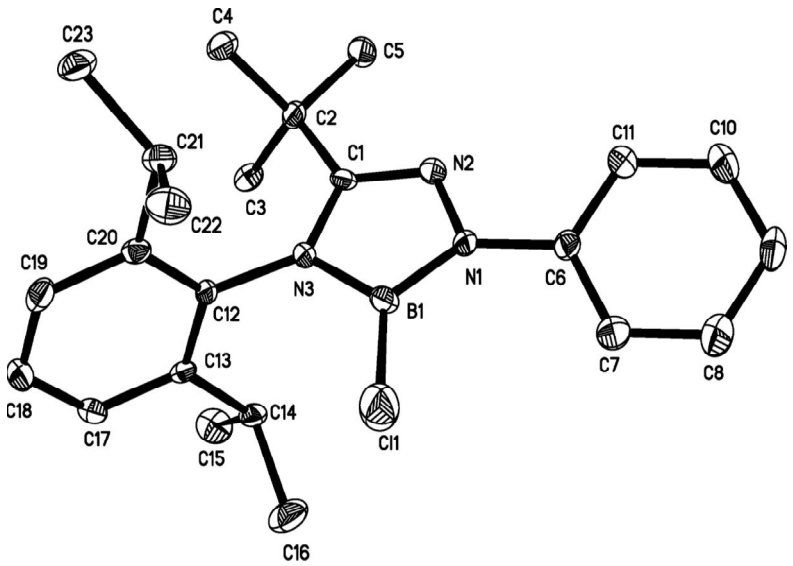

Figure S1. ORTEP drawing of **2** with 30% probability ellipsoid. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [^{o}]: B1–Cl1 1.733(4), B1–N1 1.410(5), B1–N3 1.428(5), C1–N2 1.291(5), C1–N3 1.407(4), N1–B1–N3 105.3(3), N1–B1–Cl1 128.9(3), N3–B1–Cl1 125.8(3), N1–B1–N3 105.3(3).

3. DFT calculation results

Method

Gaussian 09 was used for all density functional theory (DFT) calculations.[4] Geometry optimization and frequency calculations on compounds **5** and **6** were performed at the B3LYP/6-31G(d,p) level of theory. Natural bond order (NBO) analysis of **5** and **6** was performed at M052X/6-311G(d,p) level of theory.

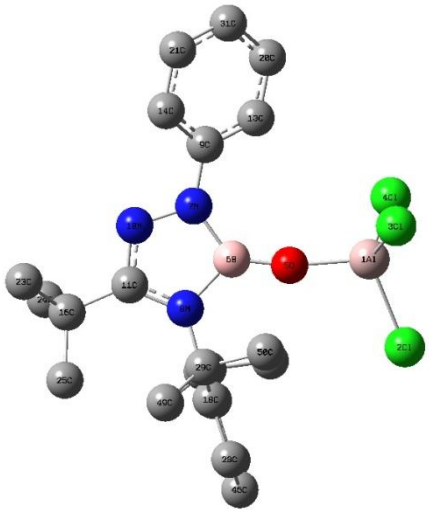

Figure S2. Optimized geometry of **5** obtained at B3LYP/6-31G(d,p) level of theory . Selected computed bond lengths [Å] and angles [º]: B6–O5 1.297, O5–Al1 1.780, B6–N7 1.459, B6–N6 1.511, C11–N10 1.336, C11–N8 1.345, Al1–O5–B6 169.5, O5–B6–N7 131.6, O5–B6–N8 126.9, N7–B6–N8 101.5.

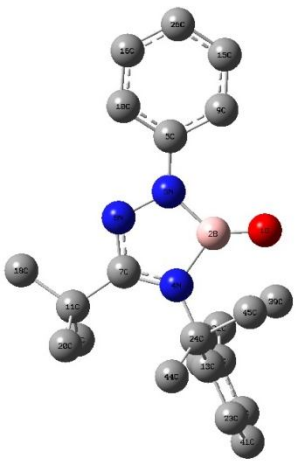

Figure S3. Optimized geometry of **6** obtained at B3LYP/6-31G(d,p) level of theory. Selected computed bond lengths [Å] and angles [º]: B2–O1 1.264, B2–N3 1.503, B2–N4 1.570, C7–N6 1.344, C7–N4 1.333, O1–B2–N3 133.2, O1–B2–N4 128.8, N3–B2–N4 98.0.

(a) Mode #150 (1627 cm^{-1}); B–O **(b) Mode #186 (3627 cm^{-1}); N–H**

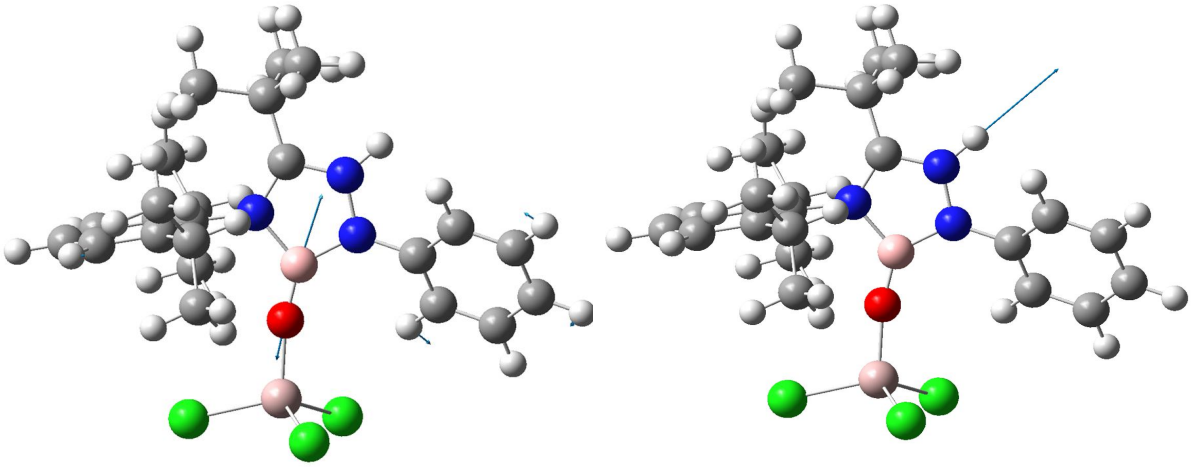

Figure S4. DFT-calculated vibrational modes of **5** and their assignments.

Solid-state IR Spectrum of compound 5

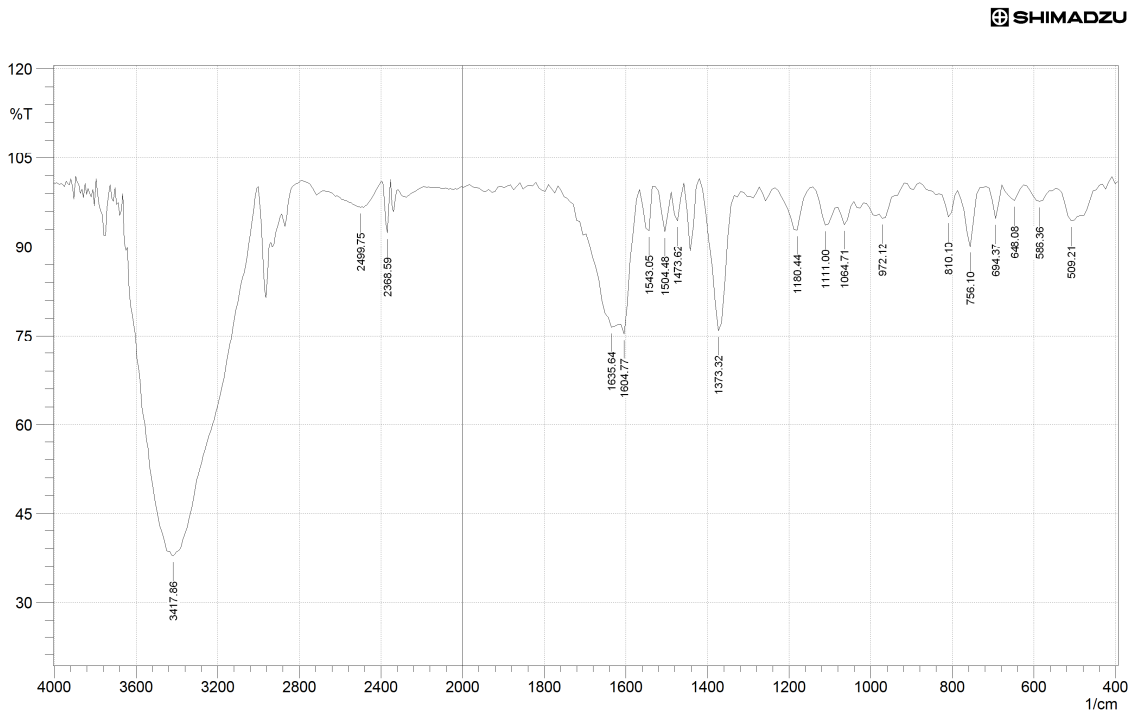

Table S2. Second-Order Perturbation Theory Analysis of Fock Matrix in NBO Basis. Important donor-acceptor interactions in **5**.

Donor NBO	Acceptor NBO	$E^{(2)}$ (kcal/mol)	E(*j*)-E(*i*) (au)	F(*l*, *j*) (au)
BD(2) C9-C14	BD*(2) C13-C18	24.68	0.39	0.088
BD(2) C9-C14	BD*(2) C19-C27	28.57	0.39	0.095
BD(2) C12-C16	BD*(2) C17-C25	31.61	0.38	0.098
BD(2) C12-C16	BD*(2) C24-C30	23.30	0.39	0.085
BD(2) C13-C18	BD*(2) C9-C14	35.09	0.34	0.099
BD(2) C13-C18	BD(2) C19-C27	28.76	0.36	0.092
BD(2) C17-C25	BD*(2) C12-C16	29.12	0.36	0.092
BD(2) C17-C25	BD*(2) C24-C30	30.95	0.37	0.097
BD(2) C19-C27	BD*(2) C9-C14	29.54	0.35	0.092
BD(2) C19-C27	BD*(2) C13-C18	29.93	0.37	0.095
BD(2) C24-C30	BD*(2) C12-C16	33.96	0.36	0.099
BD(2) C24-C30	BD*(2) C17-C25	28.14	0.36	0.091
BD(1) O5-B6	LP*(4) Al1	49.71	1.35	0.245
CR(1) O5	LP*(4) Al1	15.28	19.55	0.521
LP(2) O5	LP*(1) Al1	25.77	0.72	0.133
LP(2) O5	LP*(4) Al1	115.06	0.86	0.289
LP(1) O5	BD*(1) B6-N7	17.98	0.93	0.117
LP(1) O5	BD*(1) B6-N8	18.88	0.87	0.116
LP(3) O5	LP*(1) B6	80.15	0.40	0.169
BD(2) N8-C11	LP*(1) B6	24.30	0.48	0.106
LP(1) N7	LP*(1) B6	62.59	0.38	0.143
LP(1) N7	BD*(2) C9-C14	18.07	0.40	0.078
LP(1) N10	BD*(2) N8-C11	110.75	0.34	0.176

Table S3. Second-Order Perturbation Theory Analysis of Fock Matrix in NBO Basis. Important donor-acceptor interactions in **6**

Donor NBO	Acceptor NBO	$E^{(2)}$ (kcal/mol)	E(*j*)-E(*i*) (au)	F(*l*, *j*) (au)
BD(2) C5-C10	BD*(2) C9-C15	22.23	0.38	0.083
BD(2) C5-C10	BD*(2) C16-C26	32.18	0.37	0.098
BD(2) C8-C12	BD*(2) C13-C23	31.69	0.37	0.097
BD(2) C8-C12	BD*(2) C22-C41	26.00	0.38	0.087
BD(2) C9-C15	BD*(2) C5-C10	31.75	0.34	0.095
BD(2) C9-C15	BD*(2) C16-C26	26.31	0.36	0.087
BD(2) C13-C23	BD*(2) C8-C12	27.58	0.36	0.089
BD(2) C13-C23	BD*(2) C22-C41	31.87	0.36	0.096
BD(2) C16-C26	BD*(2) C9-C15	30.05	0.37	0.095
BD(2) C22-C41	BD*(2) C8-C12	32.42	0.36	0.097
BD(2) C22-C41	BD*(2) C13-C23	27.60	0.37	0.090
CR(1) N4	LP*(1) B2	10.55	14.84	0.403
LP(1) N3	BD*(1) B2-N4	34.71	0.42	0.112
LP(1) N4	BD*(2) C5-C10	44.66	0.37	0.118
LP(1) N4	LP*(1) B2	340.37	0.61	0.413
LP(1) N4	BD*(1) B2-N4	27.01	0.53	0.107
LP(1) N4	BD*(1) C7-C11	10.84	0.83	0.093
LP(1) N4	BD*(1) C8-C12	12.91	0.48	0.071
LP(1) N6	LP*(1) C7	122.82	0.23	0.172
BD(1) N4-C7	LP*(1) B2	19.03	1.18	0.152
BD(1) N4-C8	LP*(1) B2	21.65	1.07	0.154
LP(1) O1	RY*(1) B2	20.97	1.86	0.177
LP(2) O1	LP*(1) B2	58.04	0.44	0.153
LP(2) O1	BD*(1) B2-N3	25.37	0.77	0.128
LP(3) O1	BD*(1) B2-N4	127.94	0.34	0.189
BD(1) B2-N4	LP*(1) C7	183.59	0.18	0.185

XYZ Coordinates of Optimized Geometries

=== Compound **5** ===

Al	2.017355	-2.301979	0.037230
Cl	0.698128	-4.002116	-0.053818
Cl	3.107195	-2.201771	1.893523
Cl	3.321974	-2.232508	-1.693281
O	1.007543	-0.838238	-0.045576
B	0.477330	0.342535	-0.131017
N	1.077495	1.666343	-0.258282
N	-0.995183	0.681202	-0.095947
C	2.405623	2.159078	-0.171421
N	0.042691	2.586963	-0.247436
C	-1.162062	2.011060	-0.206208
C	-2.009625	-0.332365	0.130509
C	3.441565	1.406140	-0.736248
C	2.679639	3.380705	0.458688
H	0.229244	3.531050	-0.557719
C	-2.402026	2.891554	-0.373641
C	-2.539160	-1.024414	-0.977347
C	-2.351230	-0.654737	1.461265
H	3.231380	0.460891	-1.224765
C	4.748796	1.881040	-0.659065
C	3.991458	3.854311	0.503450
H	1.888073	3.940118	0.950495
C	-2.218022	4.182830	0.461822
C	-2.514244	3.263199	-1.876340
C	-3.711132	2.215729	0.075818
C	-2.110665	-0.752097	-2.417112
C	-3.476495	-2.032337	-0.720040
C	-3.289734	-1.674636	1.655205
C	-1.708611	0.016264	2.674270
H	5.548442	1.284943	-1.088204
C	5.029865	3.107559	-0.052312
H	4.198825	4.801247	0.994016
H	-2.086561	3.956702	1.524790
H	-3.111645	4.805264	0.354506
H	-1.367714	4.791993	0.133677
H	-1.633076	3.809415	-2.231306
H	-3.388441	3.906226	-2.024150
H	-2.638004	2.374279	-2.501371
H	-3.949007	1.327421	-0.510579
H	-4.525678	2.936284	-0.054513
H	-3.682314	1.928928	1.129774
H	-1.453307	0.124609	-2.419690
C	-3.308143	-0.432229	-3.333781
C	-1.296059	-1.933489	-2.982673
H	-3.901994	-2.585906	-1.551517
C	-3.853581	-2.353014	0.579424
H	-3.571567	-1.951998	2.666174
H	-1.166119	0.904642	2.331465
C	-2.742187	0.495132	3.712391
C	-0.676130	-0.923145	3.331998
H	6.051112	3.473811	-0.005953
H	-3.976583	-1.294023	-3.435776
H	-2.955437	-0.172801	-4.338634
H	-3.907126	0.404973	-2.955751
H	-0.436782	-2.169875	-2.350221
H	-0.932804	-1.695830	-3.989357
H	-1.911759	-2.837498	-3.051946
H	-4.574864	-3.146050	0.755703
H	-3.497030	1.157030	3.271605
H	-2.237338	1.044497	4.515006
H	-3.270391	-0.344279	4.177322
H	-1.159246	-1.834984	3.700896
H	-0.196578	-0.426102	4.183363
H	0.105590	-1.221671	2.628876

=== Compound **6** ===

O	0.764668	0.888855	-2.073219
B	0.832463	0.481989	-0.878640
N	1.978797	0.236232	0.061208
N	-0.332410	0.057693	0.084053
C	3.357926	0.204985	-0.173695
N	1.485506	-0.262125	1.257181
C	0.141858	-0.293419	1.279168
C	-1.702335	0.038761	-0.366642
C	3.835197	0.813548	-1.350898
C	4.268479	-0.387474	0.716312
C	-0.582126	-0.711737	2.560350
C	-2.460703	1.228580	-0.303335
C	-2.202346	-1.130736	-0.981752
H	3.111821	1.238331	-2.039290
C	5.201053	0.835384	-1.606692
C	5.637856	-0.346847	0.443755
H	3.925376	-0.917317	1.601082
C	0.430107	-0.925351	3.707895
C	-1.588427	0.376835	2.995451

C	-1.331380	-2.044545	2.323271	C	-4.323325	0.018260	-1.296598
C	-1.854958	2.557405	0.142949	H	-3.945958	-2.007130	-1.888895
C	-3.783483	1.183402	-0.761714	H	-0.450924	-2.298581	-0.601084
C	-3.531598	-1.118942	-1.422199	C	-2.001763	-3.692084	-1.065184
C	-1.310358	-2.334262	-1.278816	C	-0.758347	-2.219150	-2.718074
H	5.557601	1.306397	-2.519196	H	7.180714	0.293991	-0.920373
C	6.115027	0.266280	-0.712212	H	-3.666476	3.754005	0.482631
H	6.329371	-0.811415	1.142216	H	-2.255335	4.285634	1.392858
H	1.166231	-1.701660	3.470856	H	-3.143864	2.838663	1.905366
H	-0.111318	-1.252133	4.600457	H	-0.704406	2.782425	-1.704776
H	0.956184	-0.000202	3.975685	H	-0.918109	4.295226	-0.785398
H	-1.091870	1.339376	3.159241	H	-2.271472	3.626823	-1.717088
H	-2.056932	0.073621	3.938455	H	-5.353229	0.005079	-1.643705
H	-2.377610	0.516686	2.254813	H	-2.433538	-3.783936	-0.061957
H	-2.110266	-1.937858	1.565978	H	-1.275341	-4.502154	-1.196789
H	-1.806687	-2.359591	3.259054	H	-2.804289	-3.861856	-1.791757
H	-0.644037	-2.836726	2.007782	H	-1.576461	-2.276905	-3.446696
H	-0.955245	2.340133	0.728315	H	-0.063261	-3.042545	-2.924542
C	-2.787993	3.398036	1.032600	H	-0.233975	-1.269352	-2.862922
C	-1.405574	3.362830	-1.097122	H	2.036971	-0.139165	2.095271
H	-4.393283	2.080192	-0.714630				

4. References

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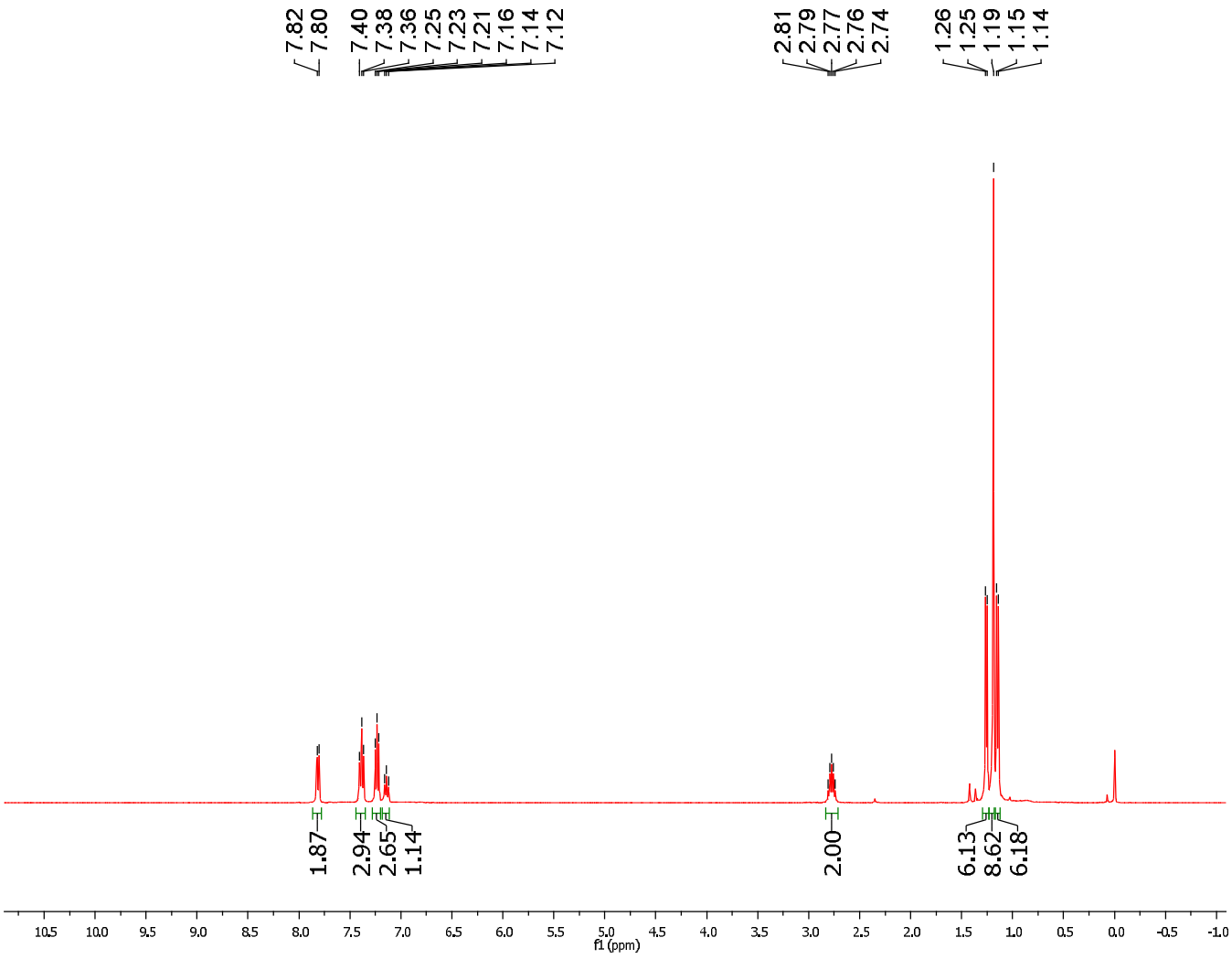
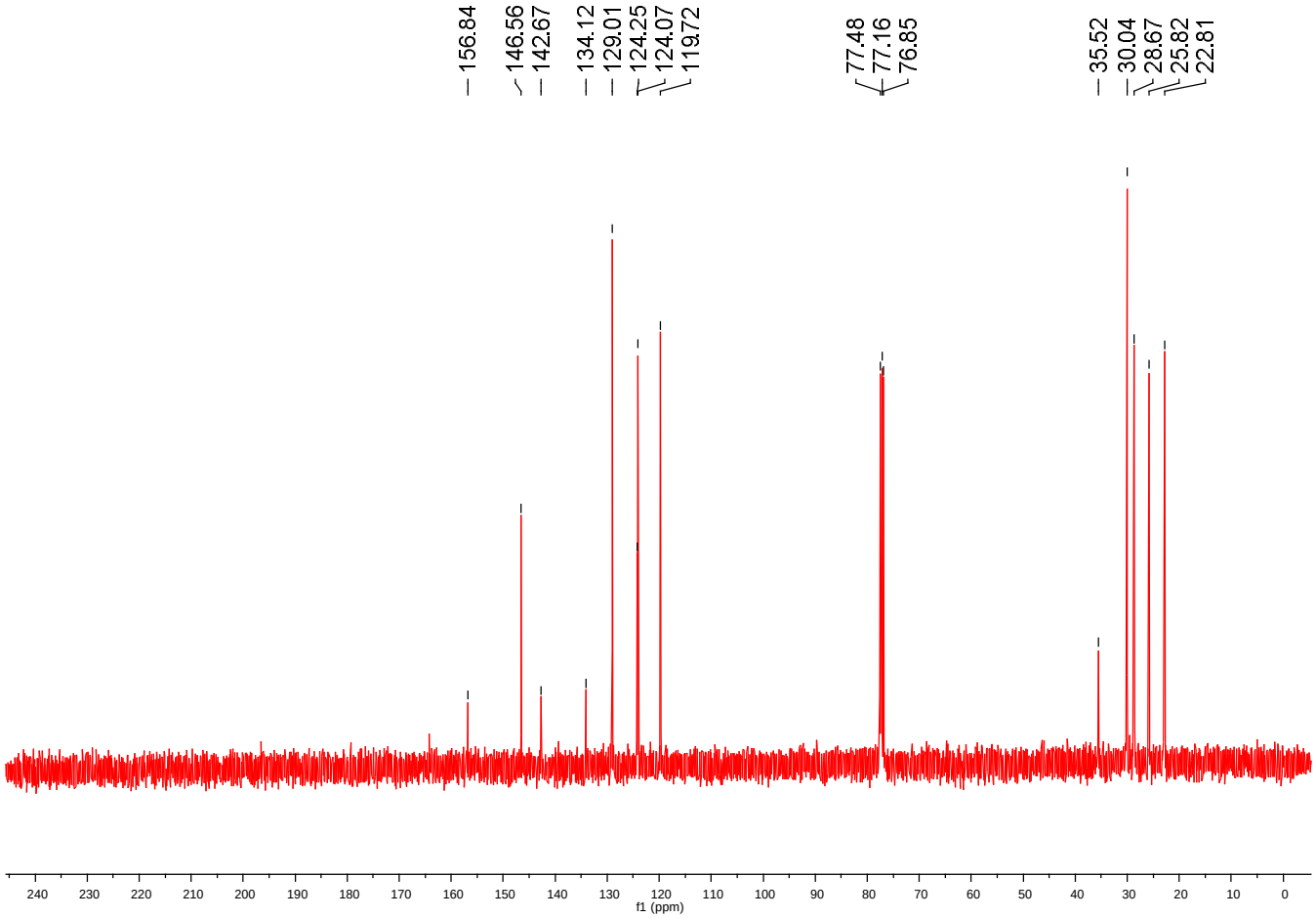
5. NMR spectra

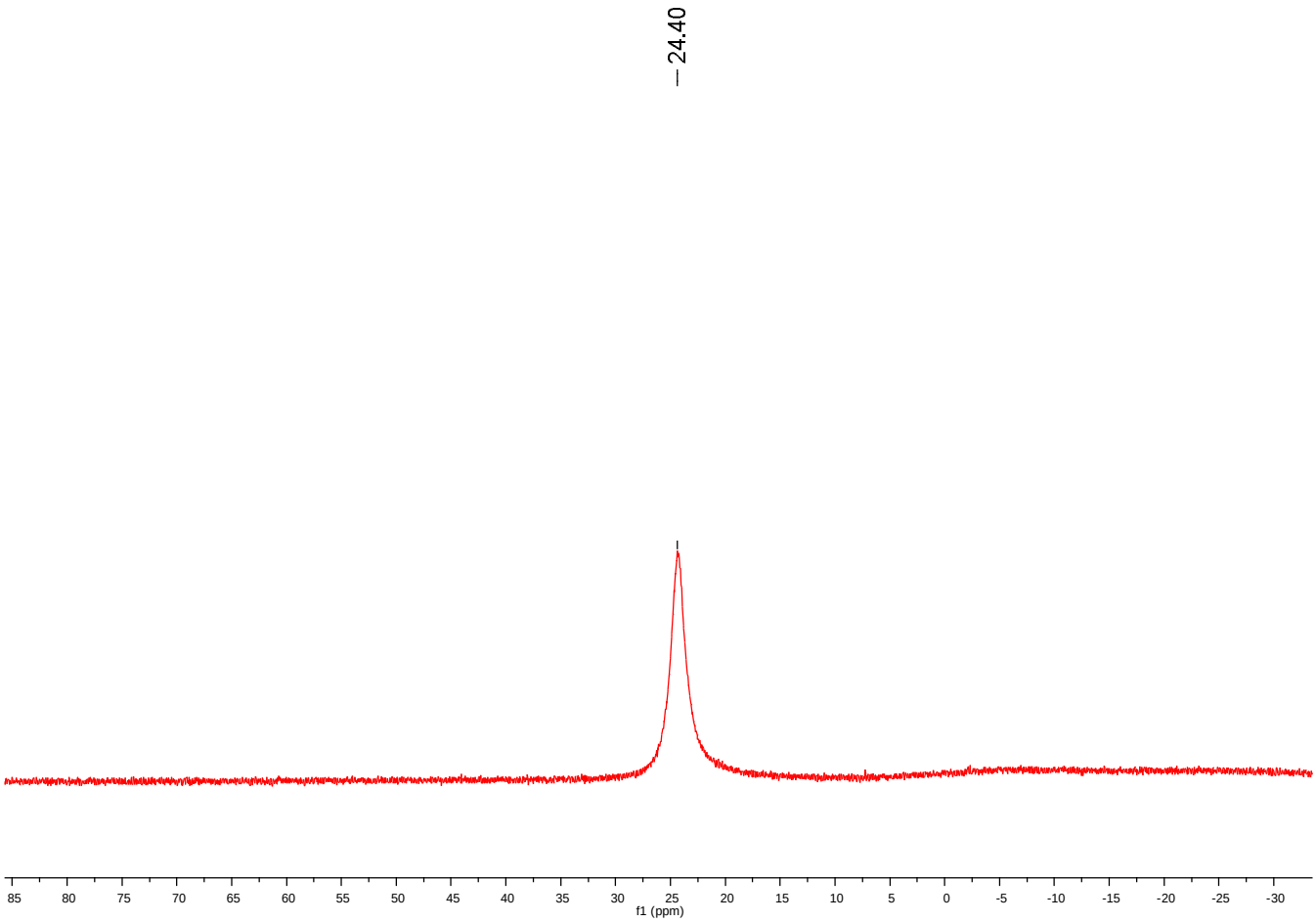
Compound 2; ^{1}H NMR ($CDCl_3$)



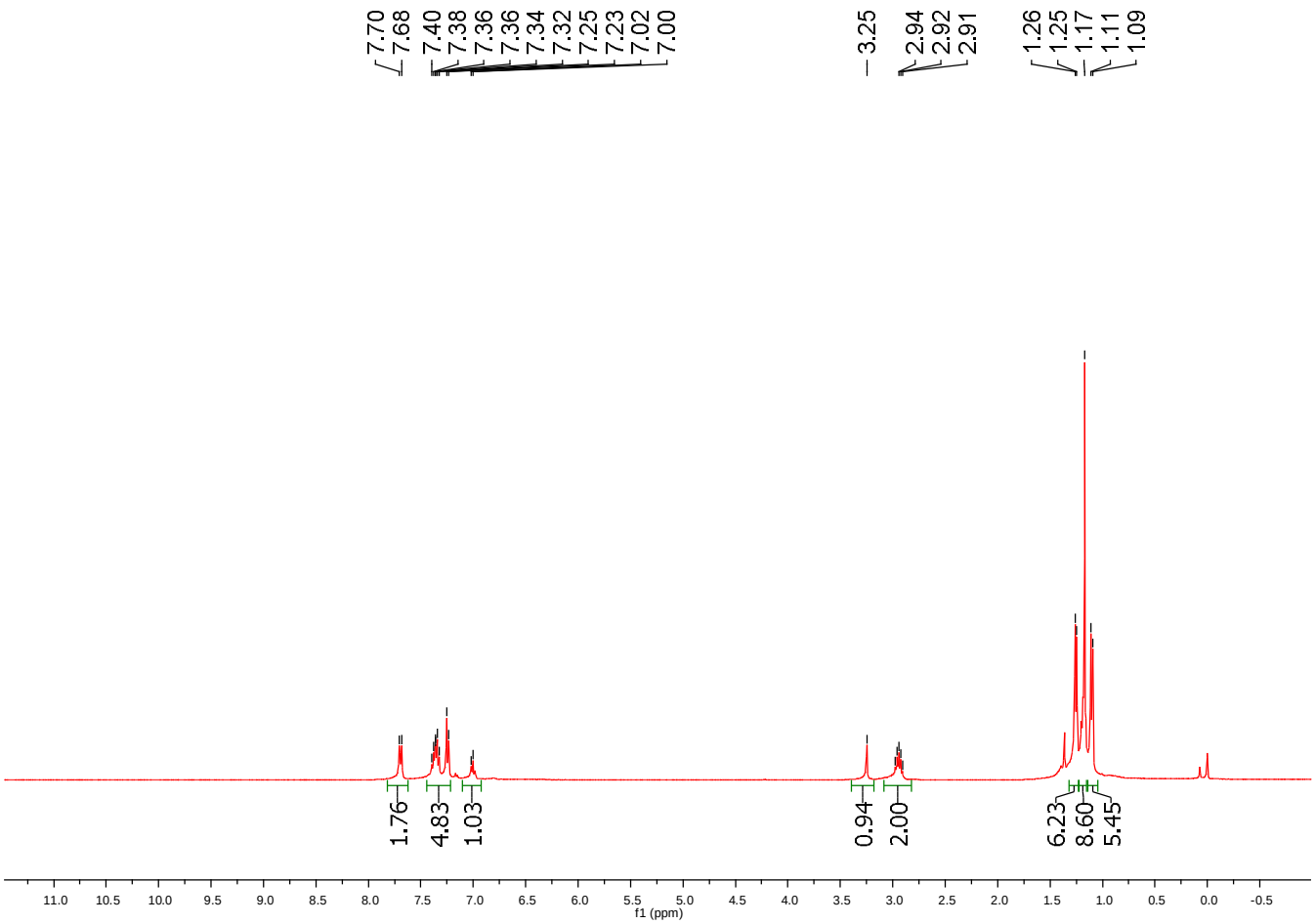
Compound 2; ^{13}C NMR ($CDCl_3$)



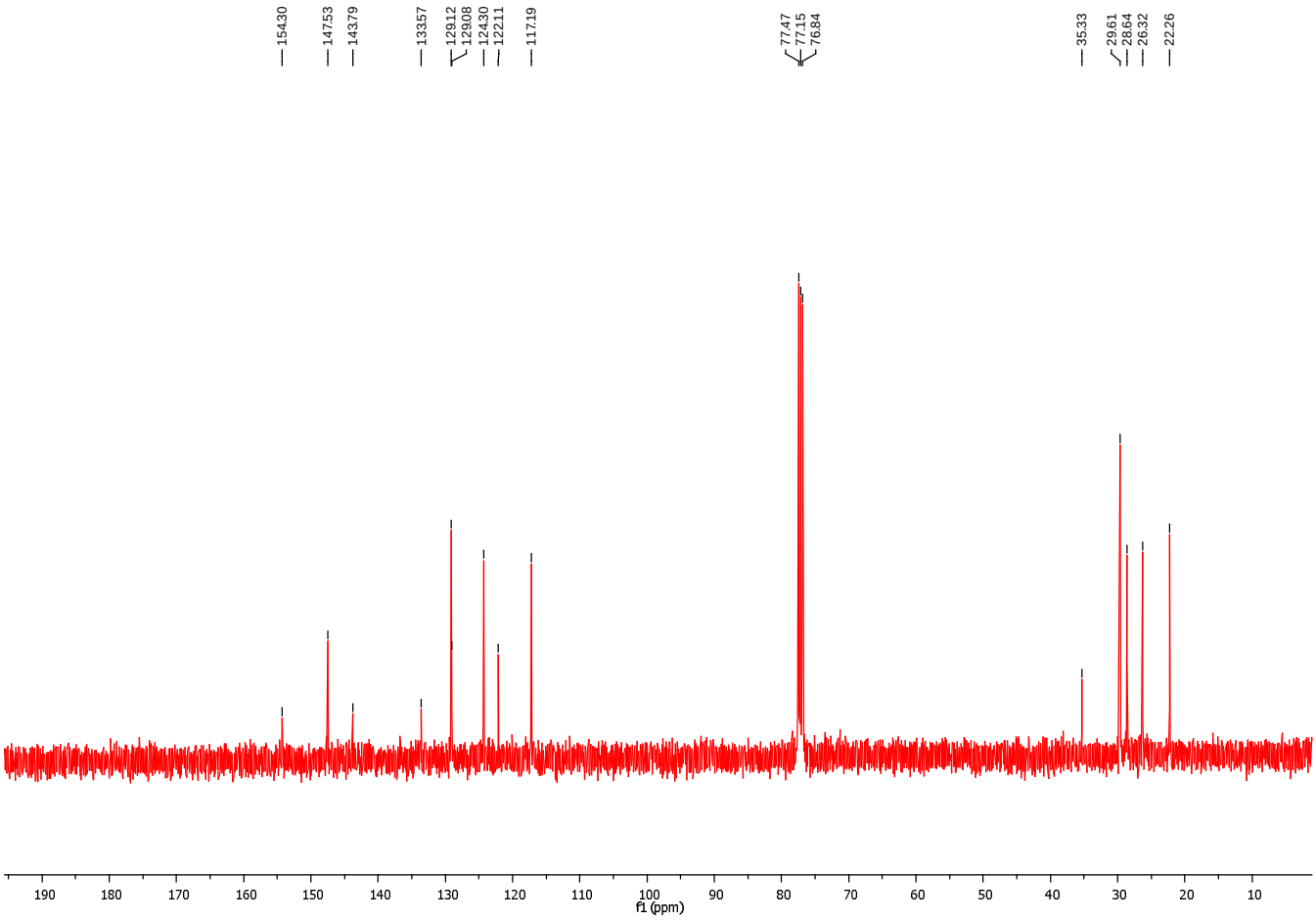
Compound 2; ^{11}B NMR ($CDCl_3$)



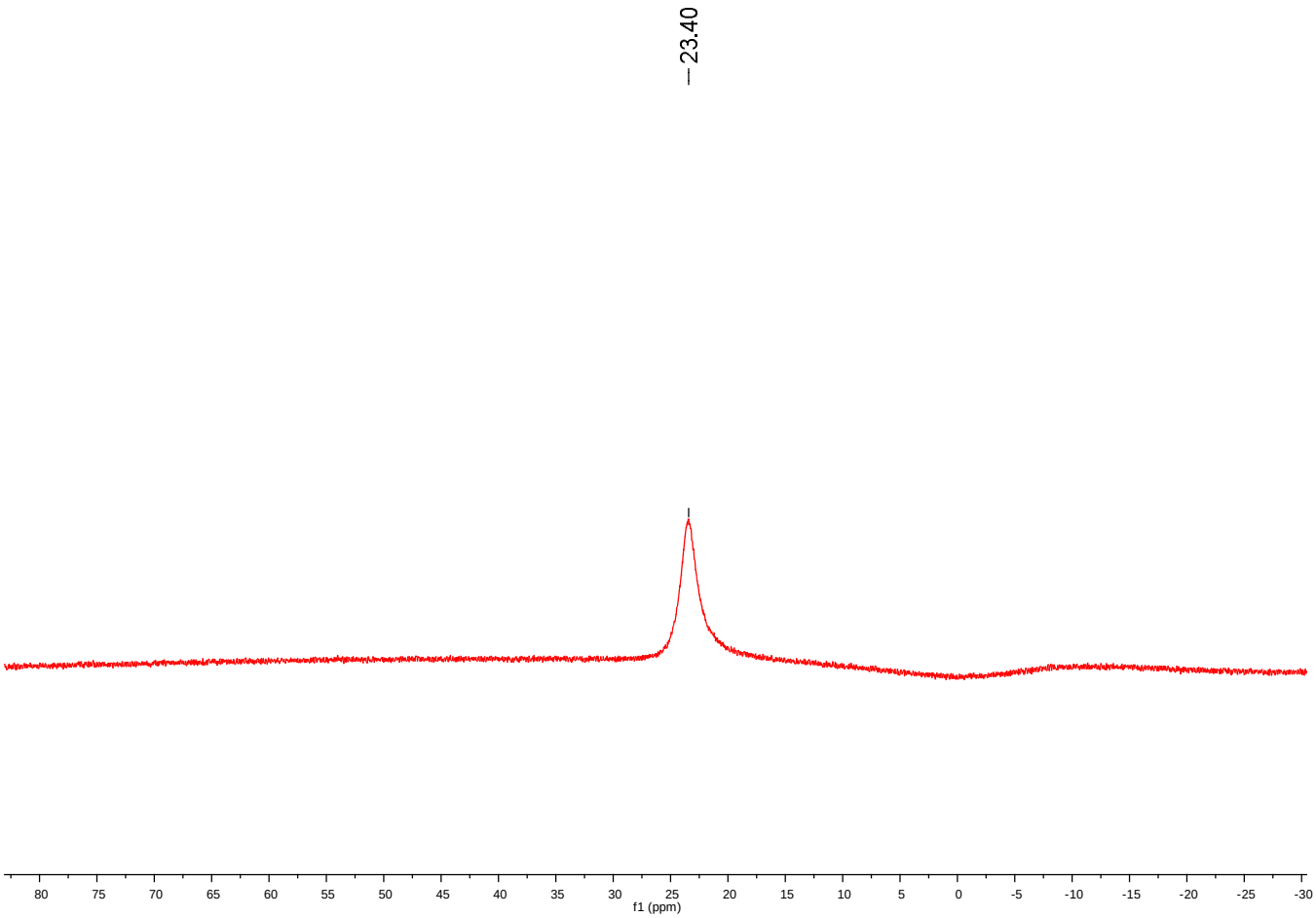
Compound 3; ^{1}H NMR ($CDCl_3$)



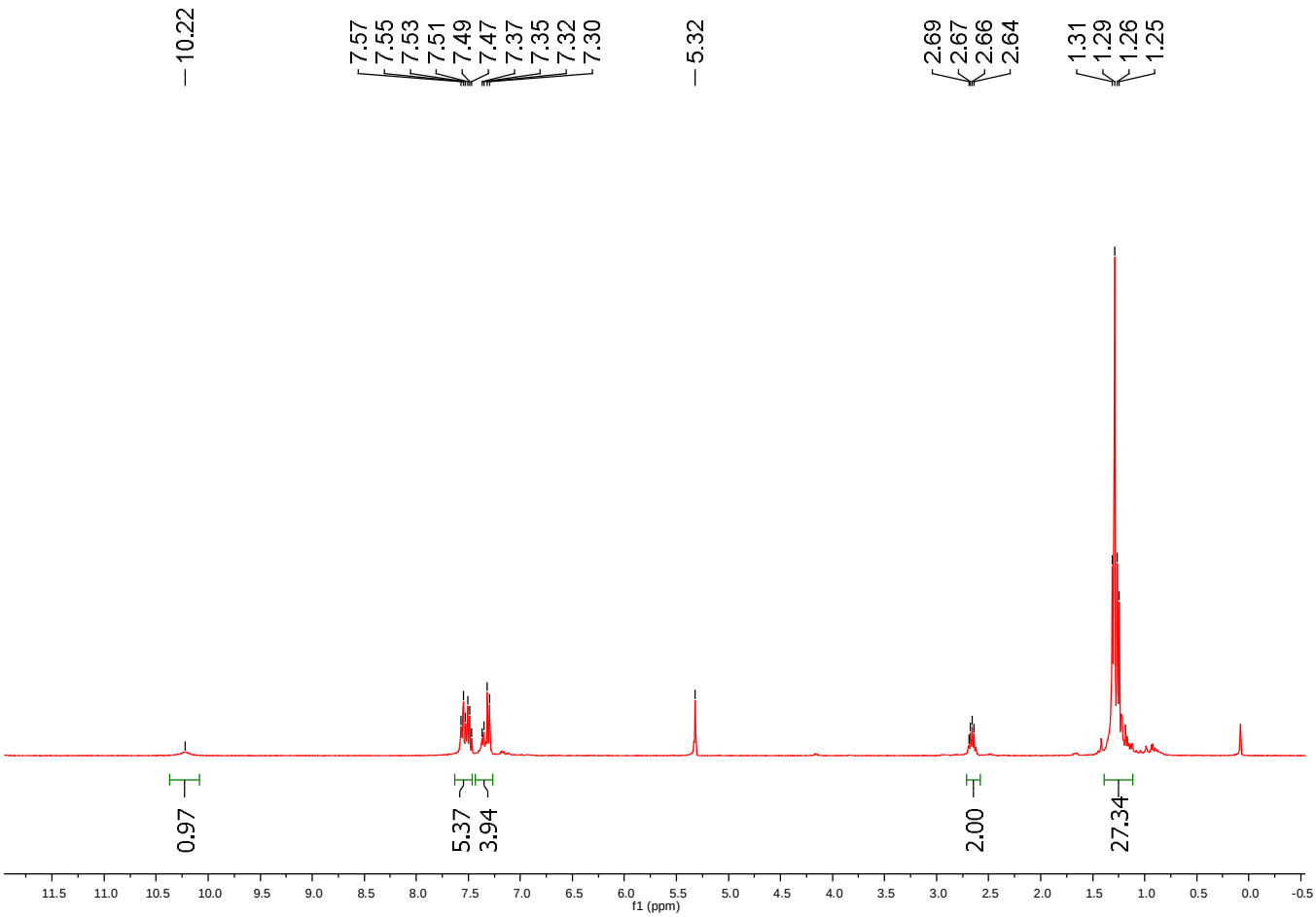
Compound 3; ^{13}C NMR ($CDCl_3$)



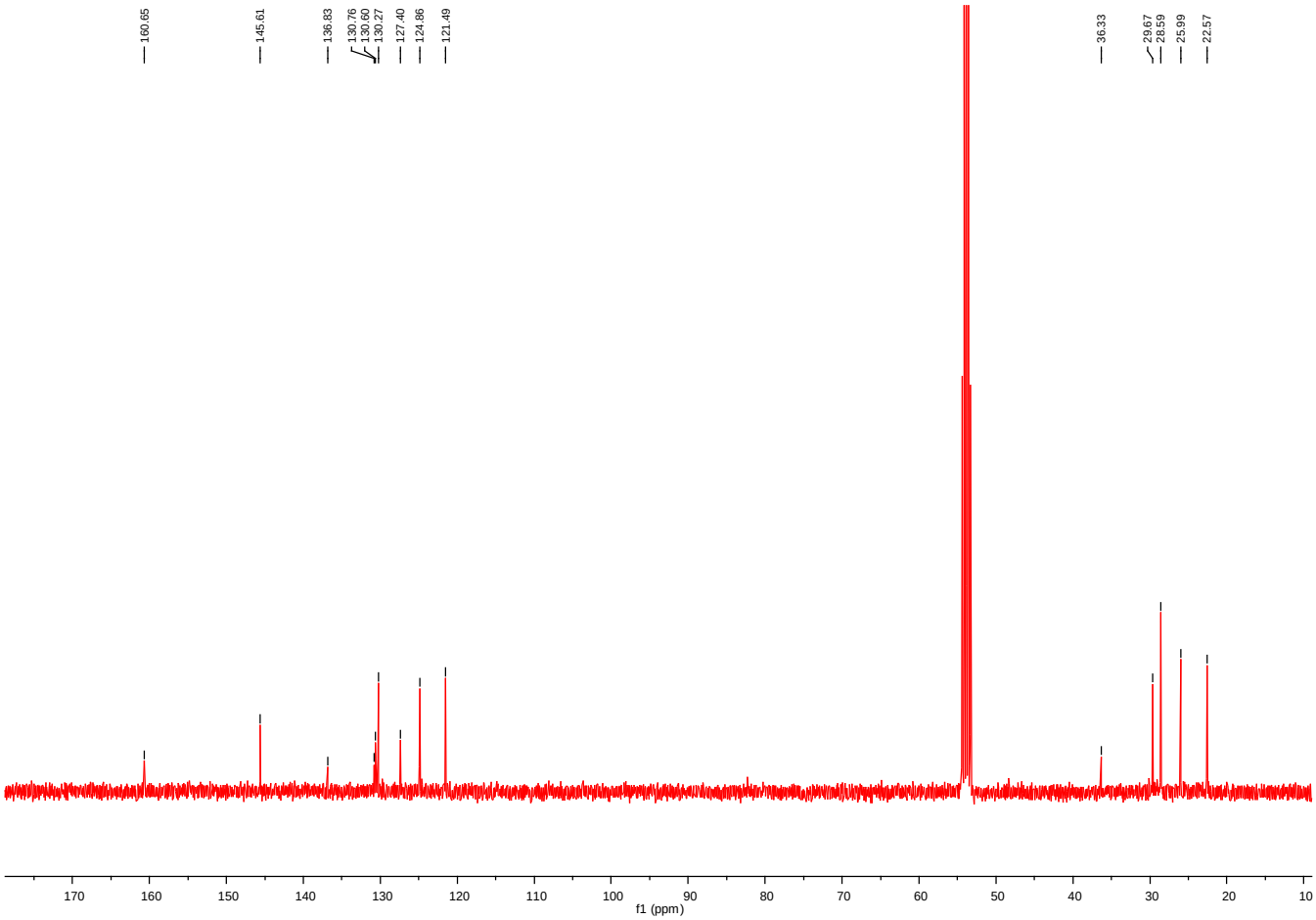
Compound 3; ^{11}B NMR ($CDCl_3$)



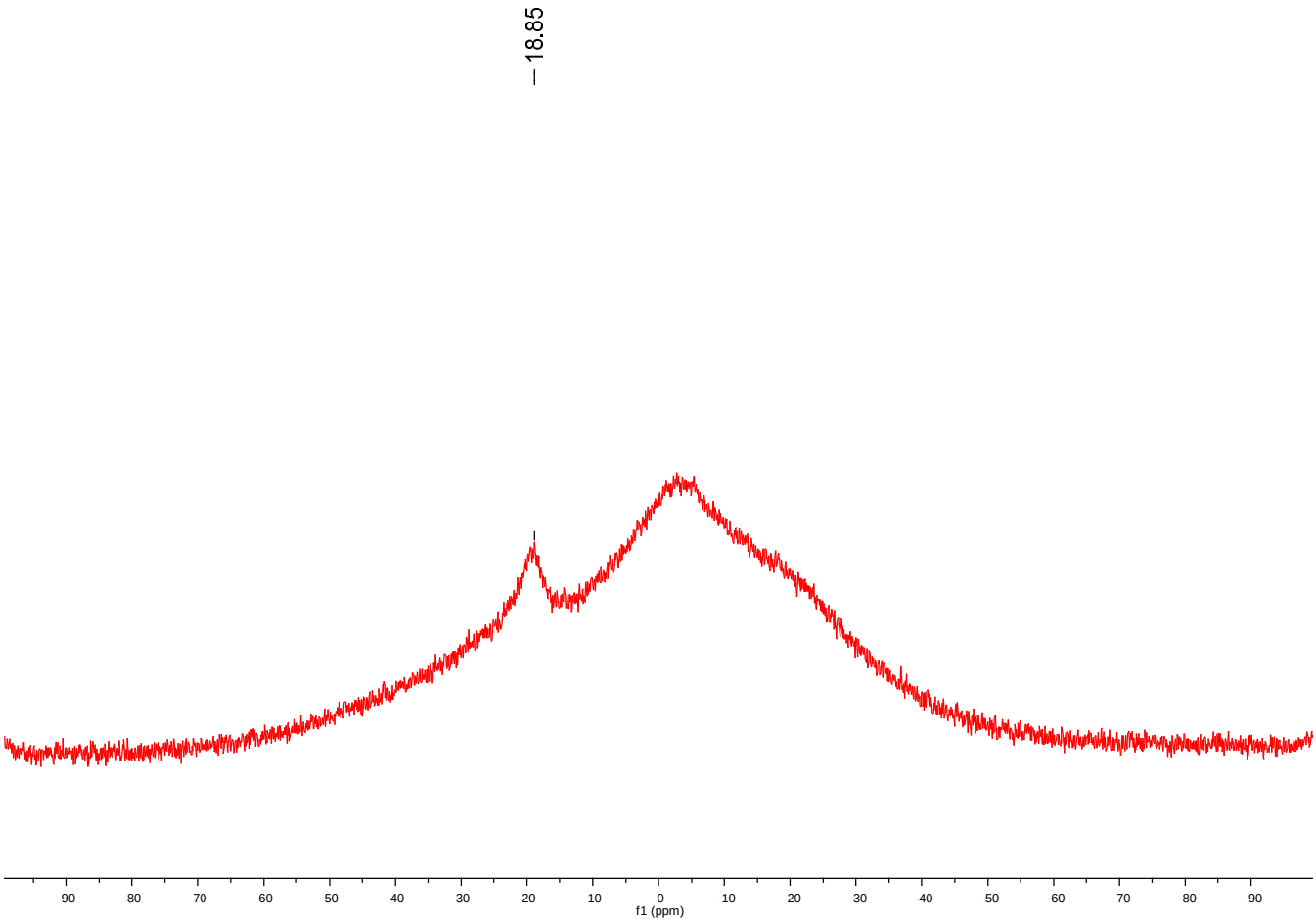
Compound 5; ^{1}H NMR (CD_2Cl_2)



Compound 5; ^{13}C NMR (CD_2Cl_2)



Compound 5; ^{11}B NMR (CD_2Cl_2)



Compound 5; $^{27}Al\{^{1}H\}$ NMR (CD_2Cl_2)