

Purine-substituted imidazolium mesomeric betaines and their tautomeric N-heterocyclic carbenes. Formation of a cyclic borane adduct.

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DFT Calculations

11aA

Energy: -675.499793 H

Number of imaginary frequencies: 0

N	-6.705400	-1.688537	-1.233935
C	-6.561842	-3.026088	-1.227653
N	-5.883218	-3.777827	-0.367356
C	-5.273966	-3.096487	0.609844
C	-5.345154	-1.666525	0.723478
C	-6.091143	-1.043152	-0.255142
N	-4.514364	-3.562392	1.629474
C	-4.184155	-2.436121	2.274046
N	-4.637521	-1.249466	1.802343
N	-6.233360	0.378582	-0.246376
C	-5.679081	1.175988	0.669519
N	-6.015152	2.436426	0.376248
C	-6.802874	2.433850	-0.756968
C	-6.940048	1.138790	-1.148285
C	-5.606696	3.608404	1.127998
H	-7.070057	-3.549430	-2.034679
H	-3.561645	-2.466614	3.163907
H	-5.070041	0.787674	1.487108
H	-7.193684	3.345650	-1.181316
H	-7.460610	0.667044	-1.966390
H	-6.486586	4.132744	1.508567
H	-4.988296	3.289539	1.967420
H	-5.027286	4.278438	0.488264

11aB

Energy: -675.479567 H

Number of imaginary frequencies: 0

N	-6.668394	-1.621883	-1.157301
C	-6.573705	-2.951682	-1.231553
N	-5.907268	-3.768852	-0.424138

C	-5.292517	-3.094863	0.542305
C	-5.289388	-1.700786	0.763148
C	-6.041186	-0.972591	-0.176604
N	-4.519322	-3.609627	1.544414
C	-4.099965	-2.542851	2.298796
N	-4.531681	-1.389724	1.872770
N	-6.193732	0.412989	-0.175008
C	-5.629322	1.256907	0.767307
N	-6.066778	2.460267	0.330135
C	-6.857410	2.390887	-0.813977
C	-6.943044	1.087426	-1.141395
C	-5.728879	3.693988	1.001215
H	-7.109763	-3.417241	-2.055716
H	-3.464933	-2.681414	3.165036
H	-7.287698	3.262166	-1.286169
H	-7.446438	0.569053	-1.940407
H	-6.632240	4.213117	1.338913
H	-5.114262	3.434241	1.863158
H	-5.164916	4.357047	0.336381
H	-4.317356	-4.587716	1.684626

12

Energy: -674.926579 H

Number of imaginary frequencies: 0

N	-6.767810	-1.598196	-1.067480
C	-6.707248	-2.937295	-1.116560
N	-6.021767	-3.765348	-0.344832
C	-5.291976	-3.135546	0.595211
C	-5.257423	-1.701147	0.763649
C	-6.051178	-0.980120	-0.125077
N	-4.468875	-3.704038	1.503164
C	-3.991110	-2.616682	2.144930
N	-4.397983	-1.395435	1.777048
N	-6.154150	0.440450	-0.152302
C	-5.860603	1.285306	0.890514
N	-6.148381	2.499424	0.334677
C	-6.603756	2.420165	-0.975232
C	-6.612414	1.104655	-1.282327
C	-5.996791	3.726364	1.069346
H	-7.311555	-3.395248	-1.902302
H	-3.274618	-2.731794	2.957826
H	-6.872809	3.285359	-1.565138
H	-6.900672	0.563259	-2.168657
H	-6.953691	4.255290	1.167563
H	-5.627792	3.457146	2.060104
H	-5.276263	4.396711	0.583344

14

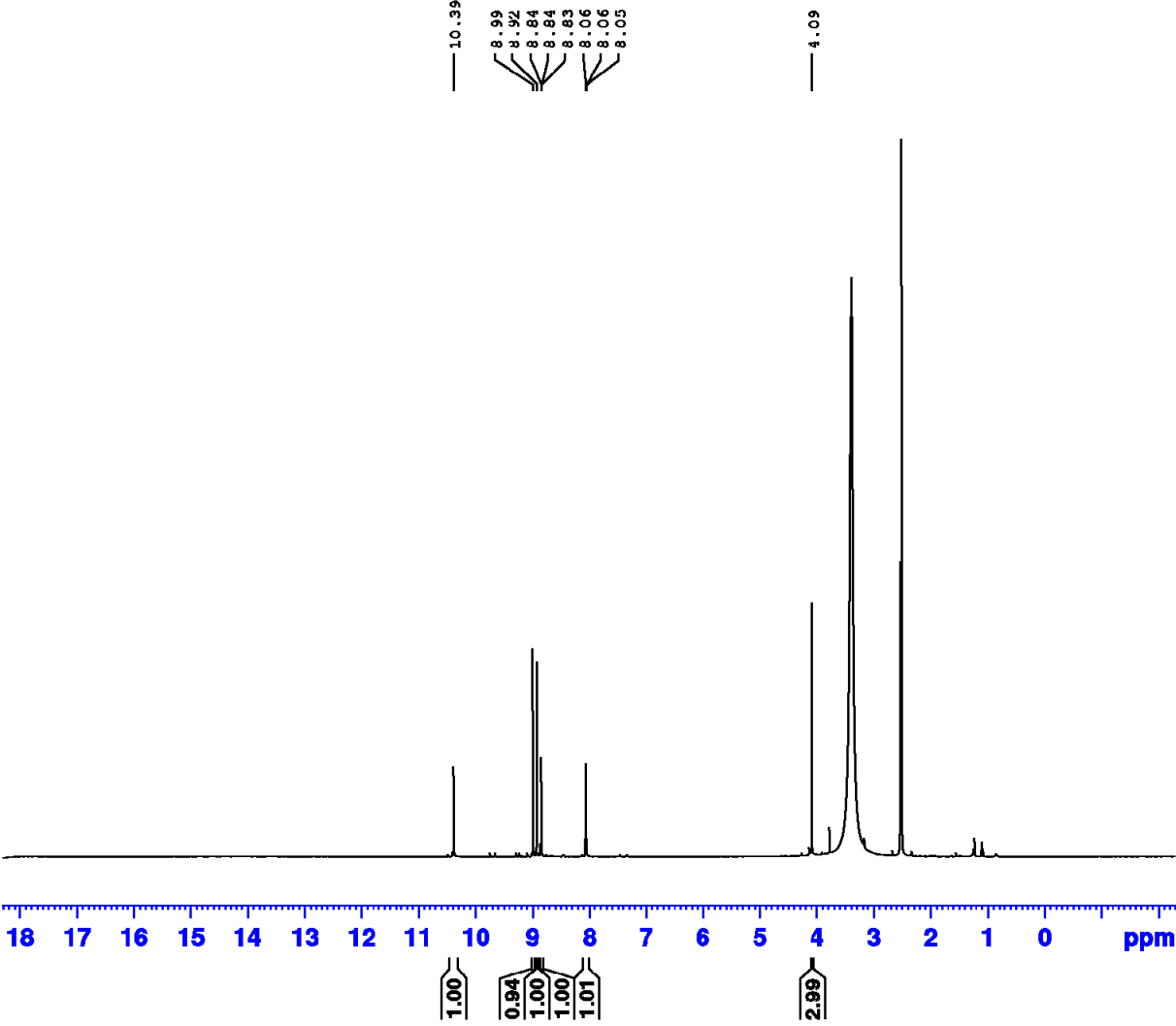
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Number of imaginary frequencies: 0

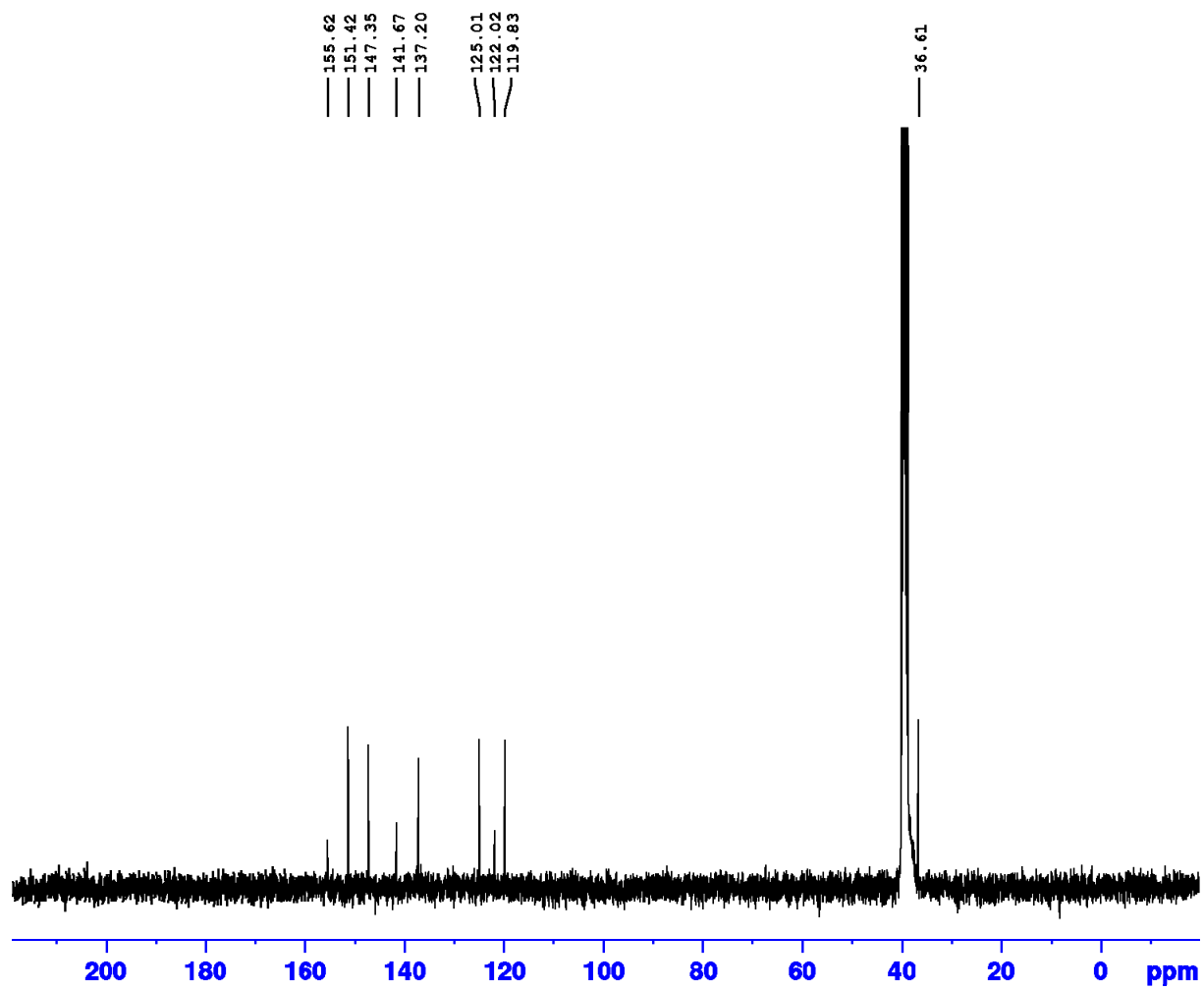
N	-4.541703	-0.693990	-7.600000
C	-4.315378	-1.992613	-7.922901
N	-3.776835	-2.958216	-7.188412
C	-3.426114	-2.578843	-5.948355
C	-3.639429	-1.263742	-5.512393
C	-4.187456	-0.356224	-6.377430
N	-2.836597	-3.277033	-4.932198
C	-2.728202	-2.379363	-3.960326
N	-3.189919	-1.127644	-4.245091
B	-3.447213	0.212279	-3.435633
C	-3.905319	1.286646	-4.627736
N	-4.297340	0.965921	-5.893193
N	-4.056927	2.624177	-4.566108
C	-4.532130	3.124568	-5.766948
C	-4.686364	2.075855	-6.606870
C	-4.716658	-0.092230	-2.443249
C	-2.081767	0.654853	-2.671915
C	-3.672330	3.483119	-3.458716
C	-5.265184	1.029220	-1.564159
C	-0.891014	0.984487	-3.572458
H	-4.615670	-2.266816	-8.931259
H	-2.300857	-2.608115	-2.991426
H	-4.717525	4.178063	-5.908244
H	-5.020571	1.994039	-7.628748
H	-4.384744	-0.913948	-1.789071
H	-5.546311	-0.515715	-3.029321
H	-2.256154	1.488461	-1.976625
H	-1.805953	-0.185128	-2.015048
H	-2.626857	3.786016	-3.563796
H	-4.311945	4.367814	-3.464063
H	-3.805125	2.954276	-2.519041
H	-6.047522	0.668177	-0.885302
H	-5.718719	1.833007	-2.159747
H	-4.484088	1.476373	-0.935149
H	0.019810	1.204948	-3.002417
H	-0.661081	0.149686	-4.245320
H	-1.091163	1.856580	-4.210925

NMR Spectroscopy

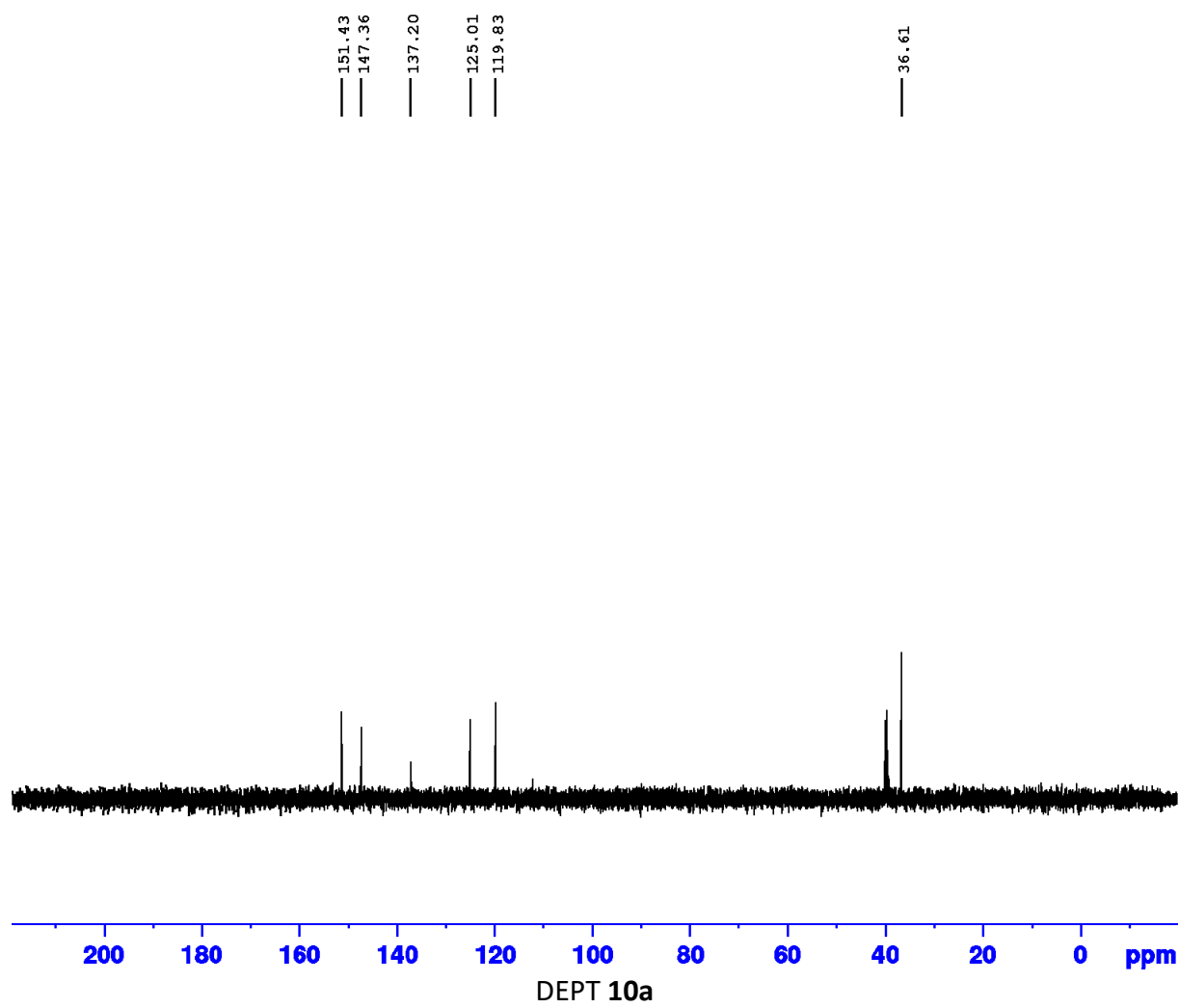
1-Methyl-3-(9H-purin-6-yl)-1H-imidazolium chloride 10a



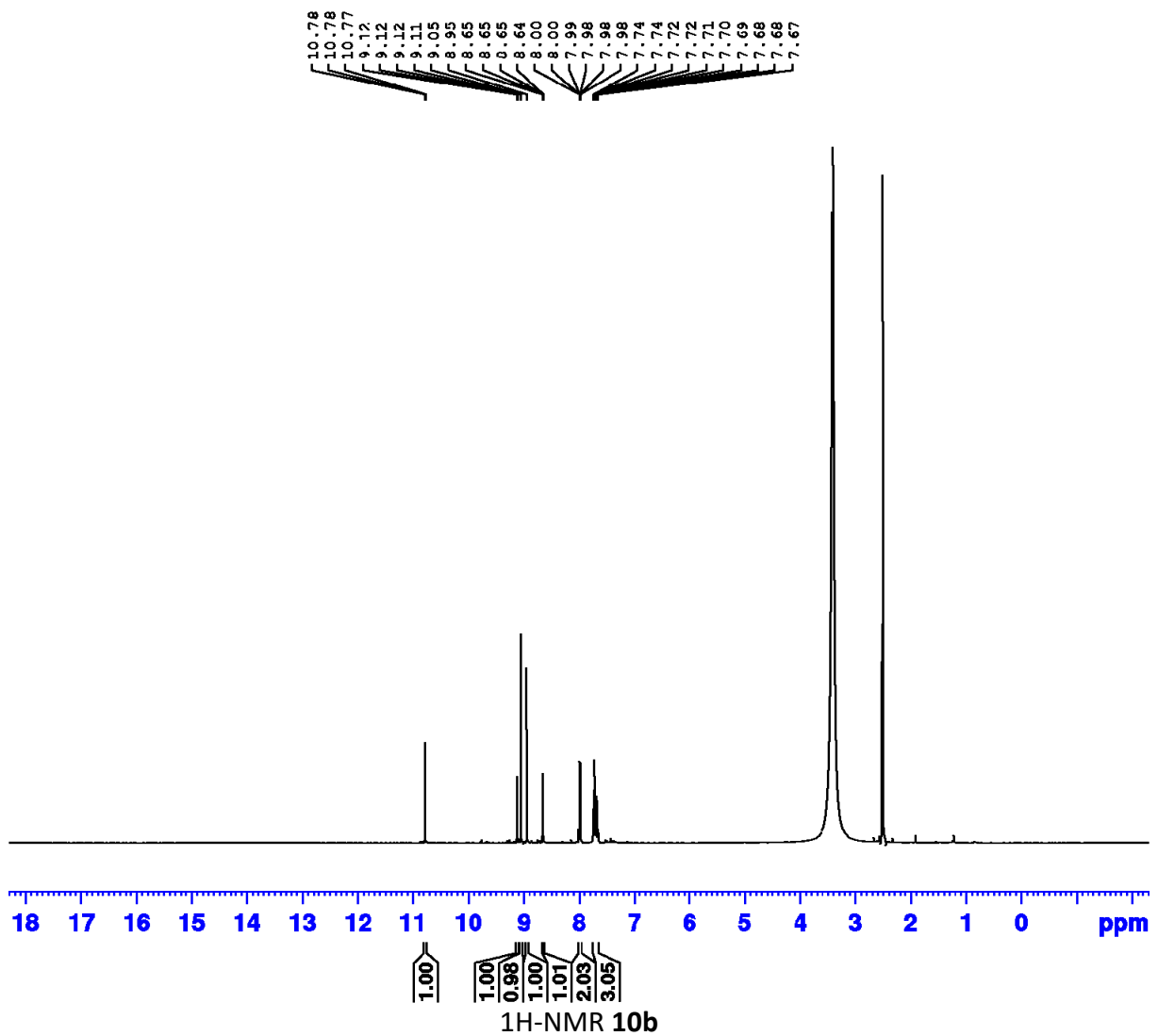
1H-NMR 10a

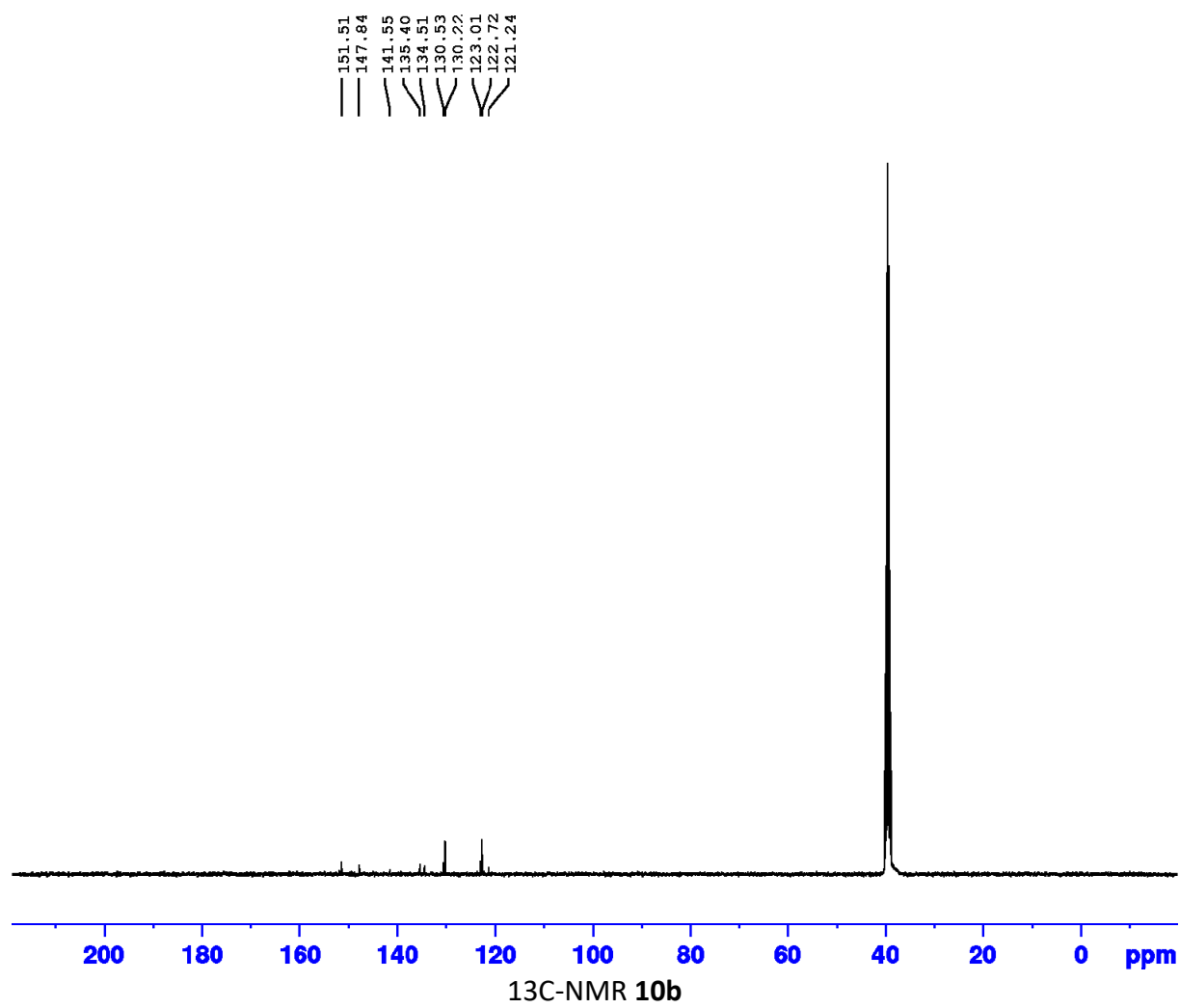


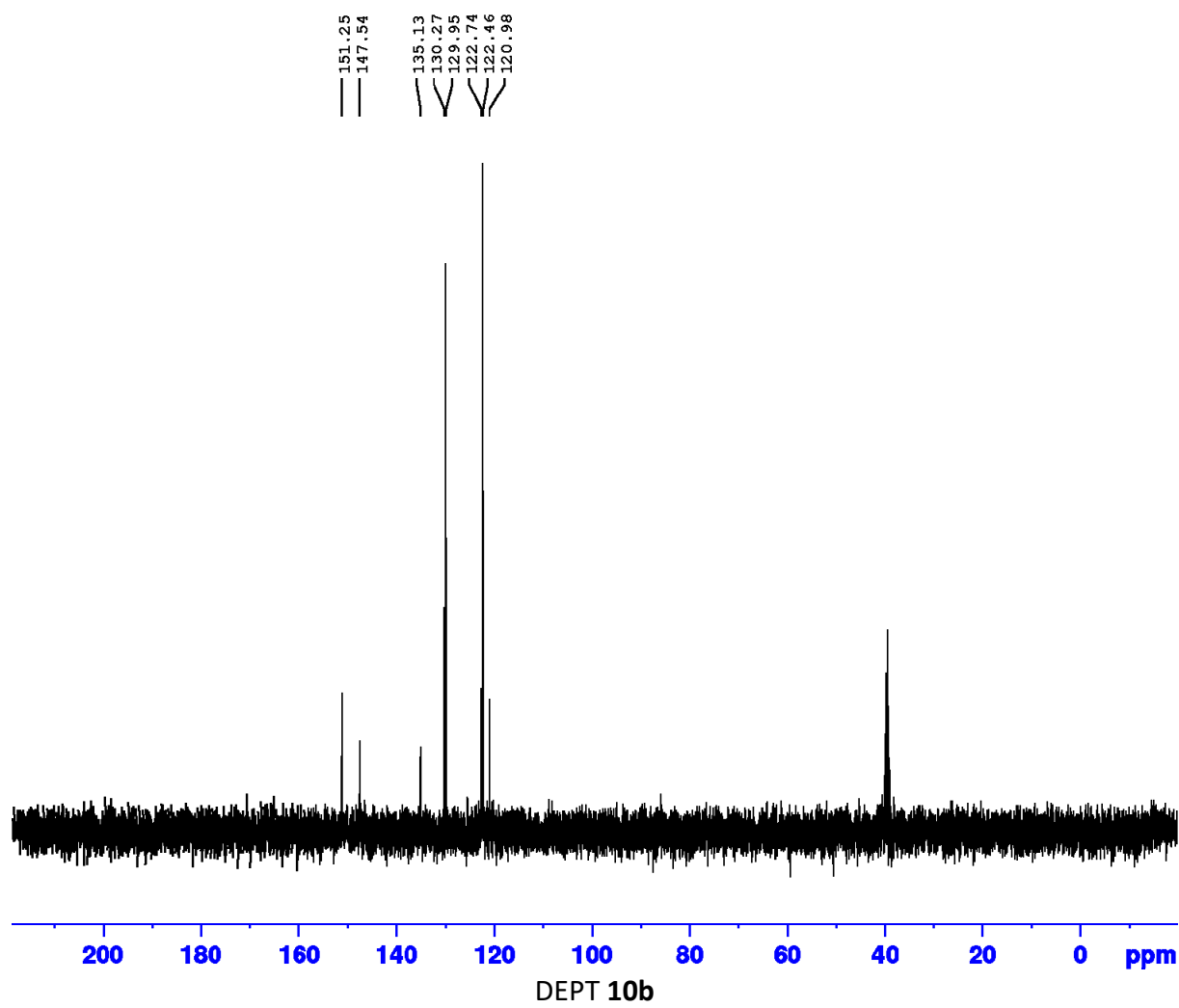
13C-NMR 10a



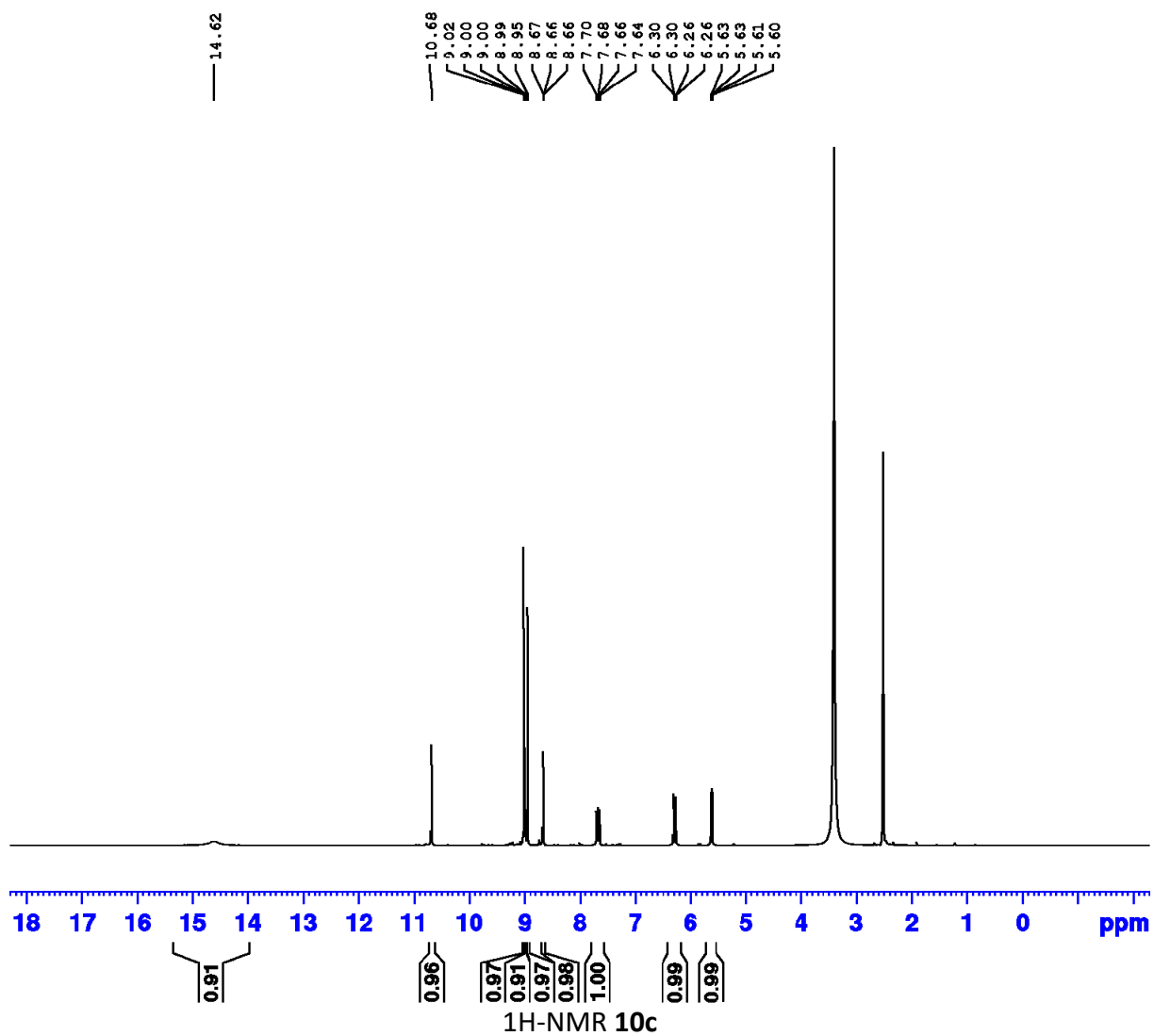
1-Phenyl-3-(9H-purin-6-yl)-1H-imidazolium chloride 10b

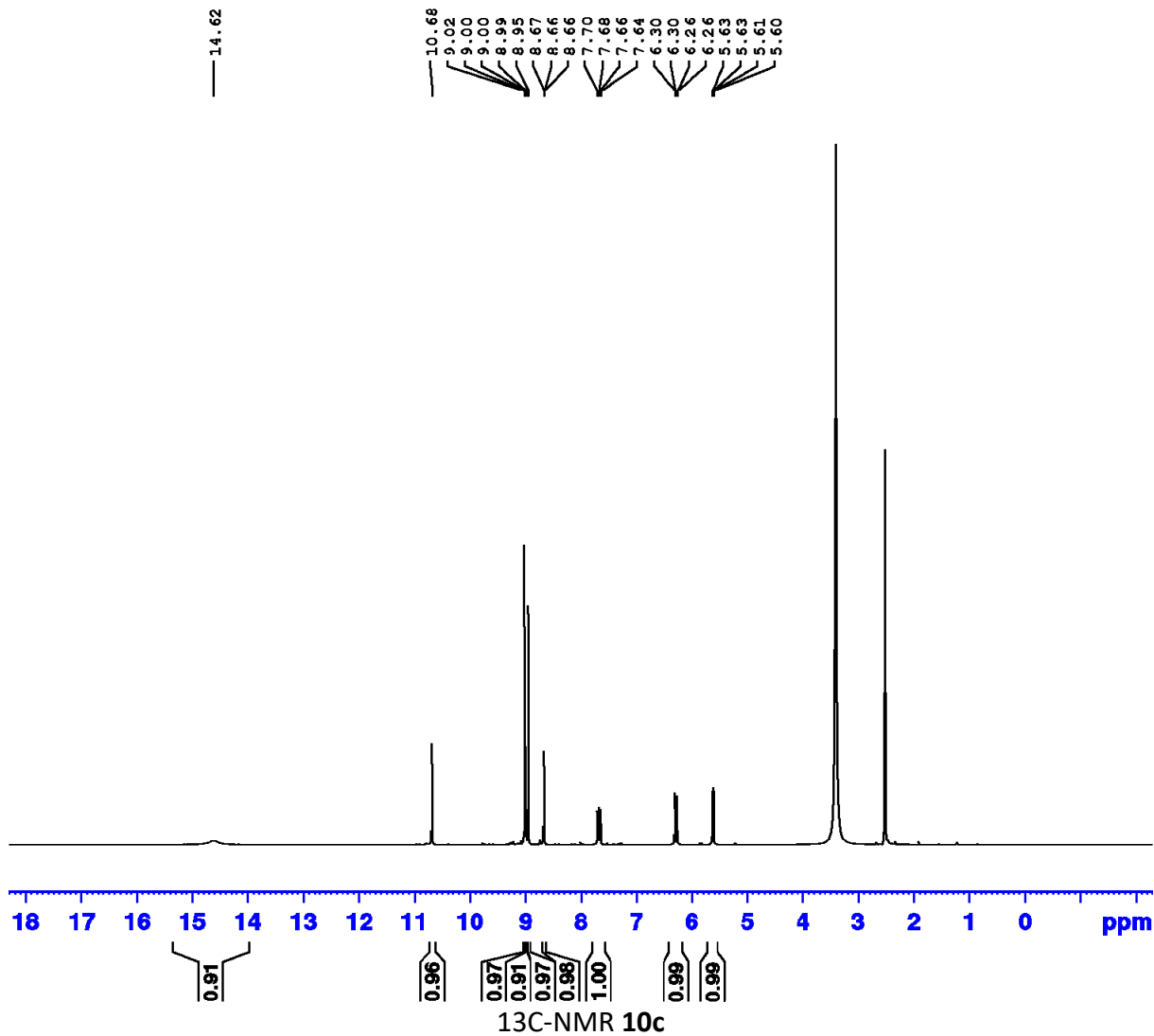




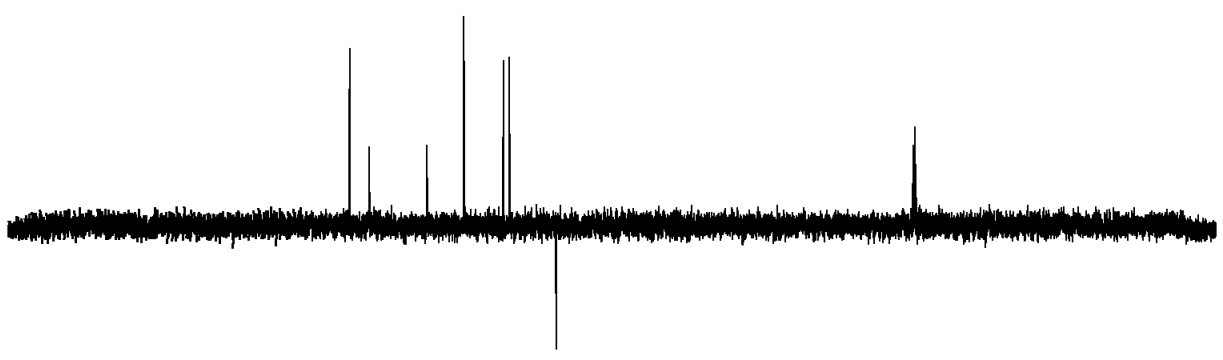


1-Vinyl-3-(9H-purin-6-yl)-1H-imidazolium chloride 10c



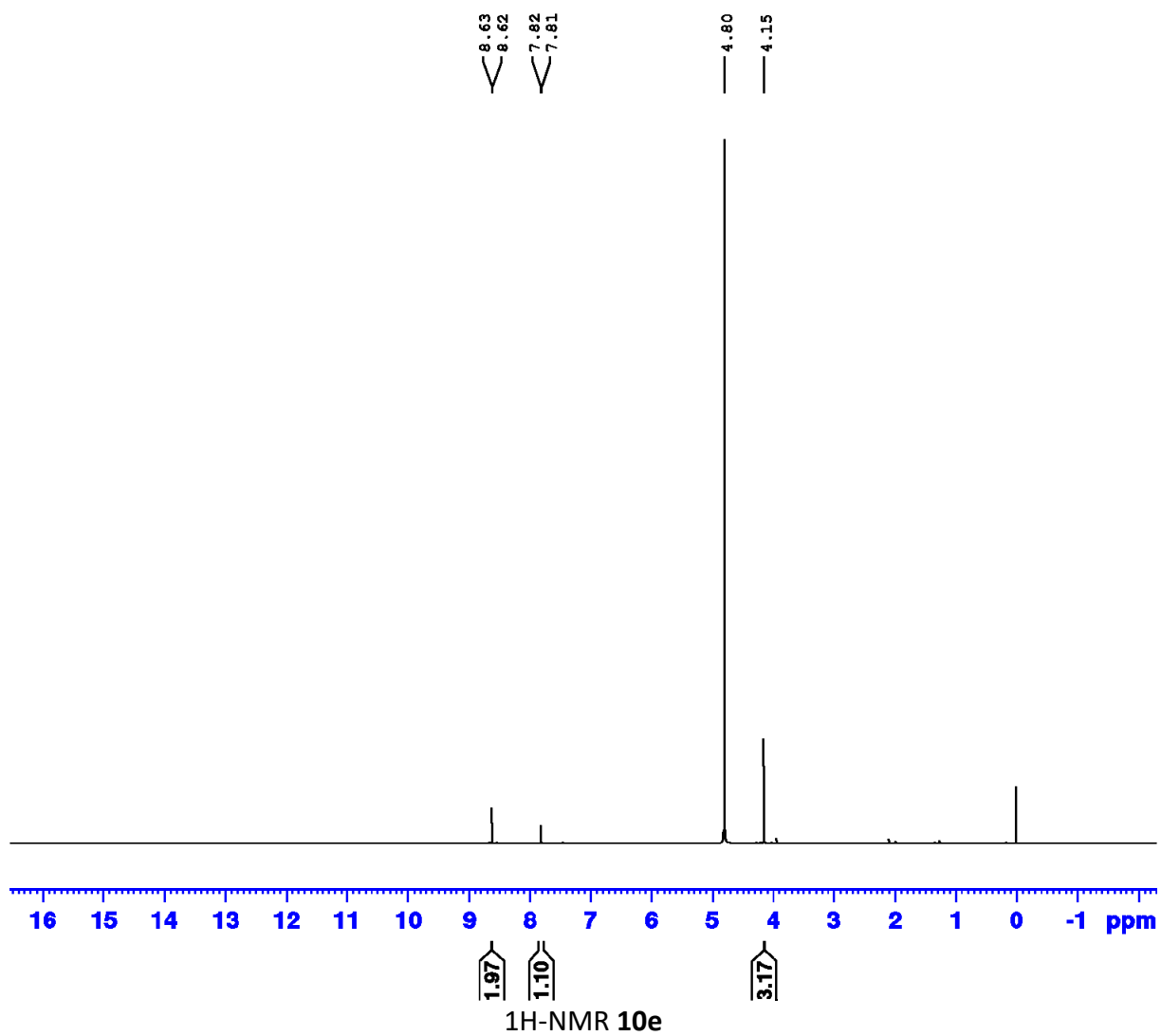


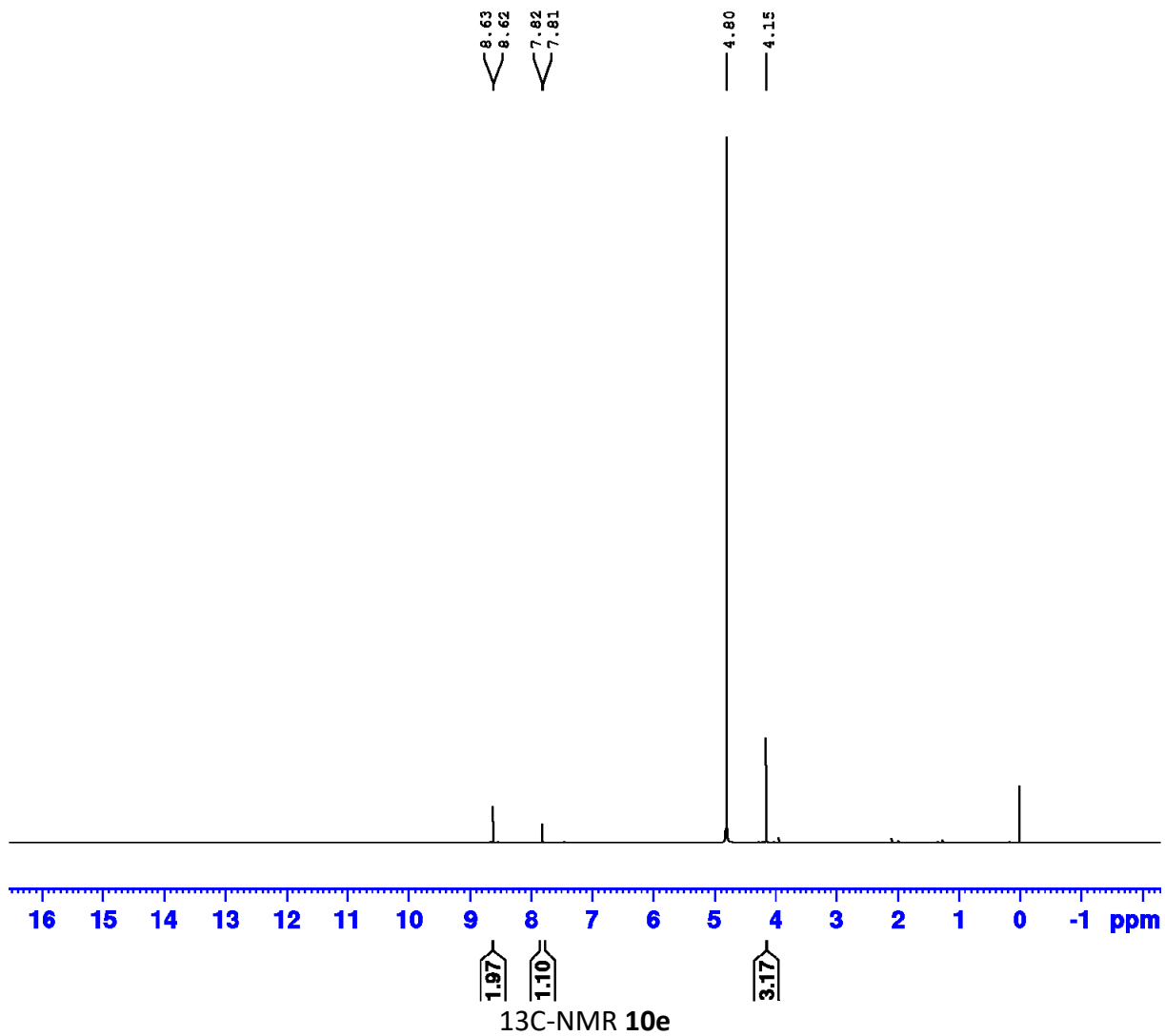
151.41
147.49
136.06
128.82
120.92
119.78
110.76

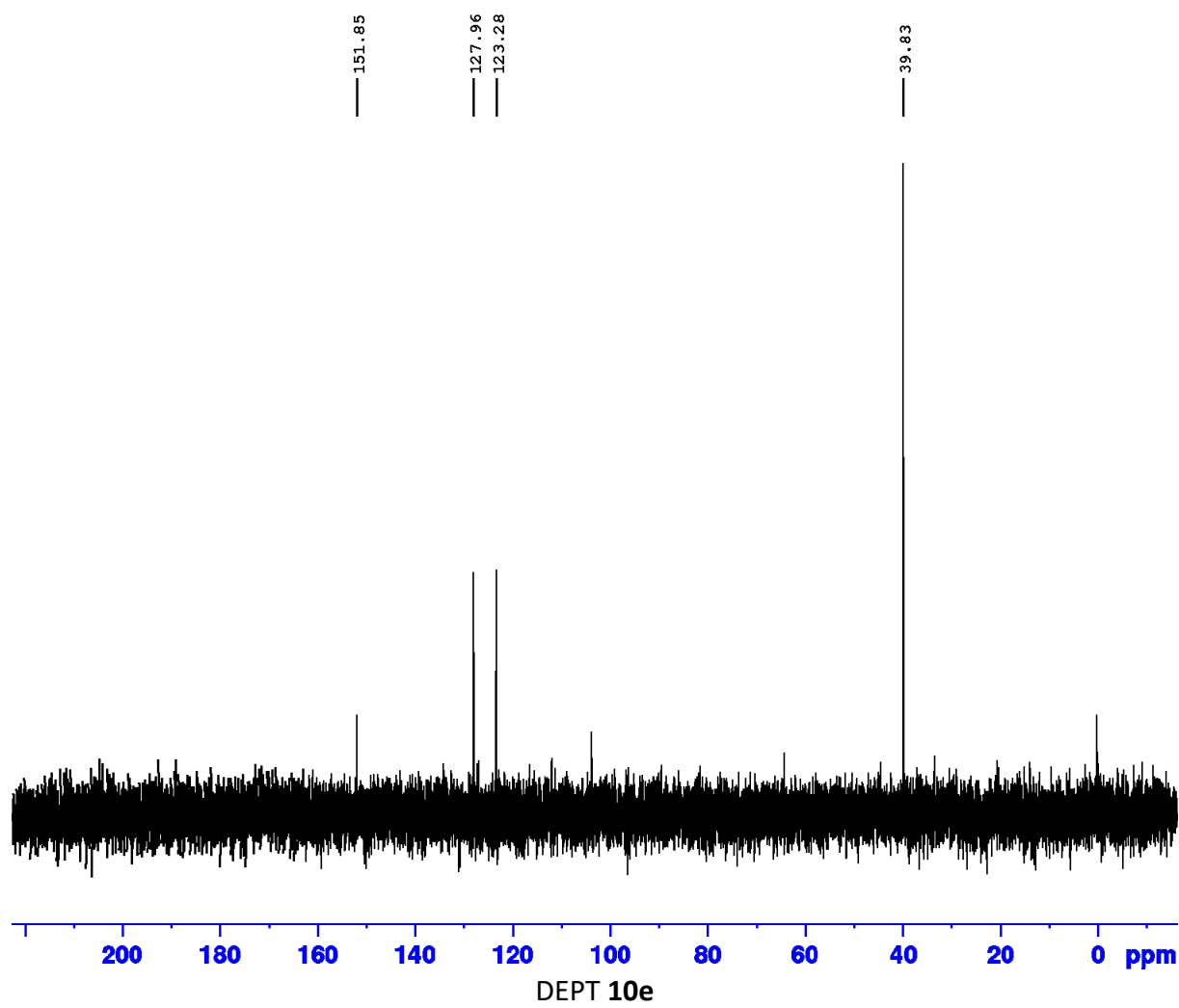


200 180 160 140 120 100 80 60 40 20 0 ppm
DEPT 10c

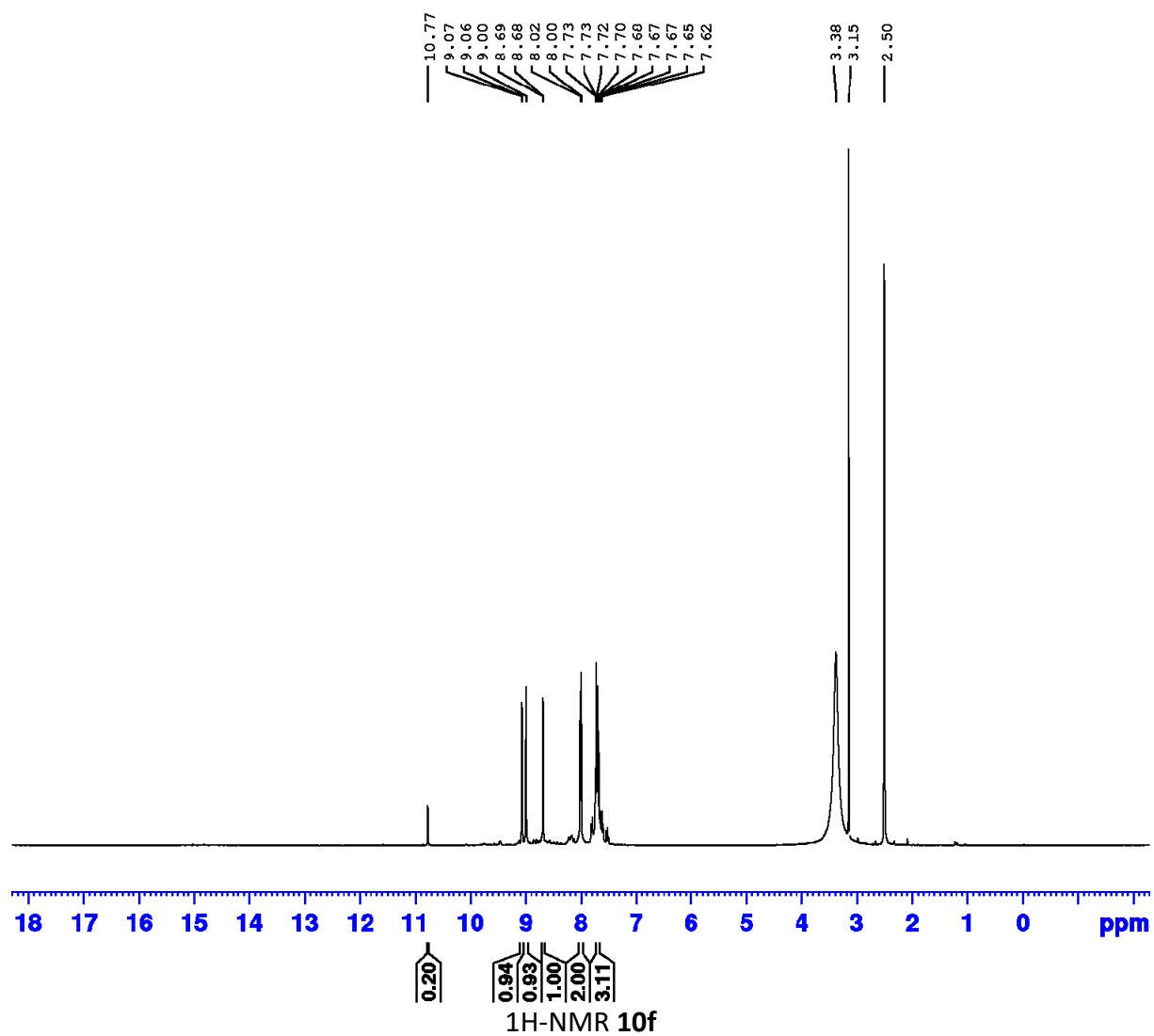
(2-Chloro-9H-purin-6-yl)-1-methyl-1H-imidazolium chloride 10e

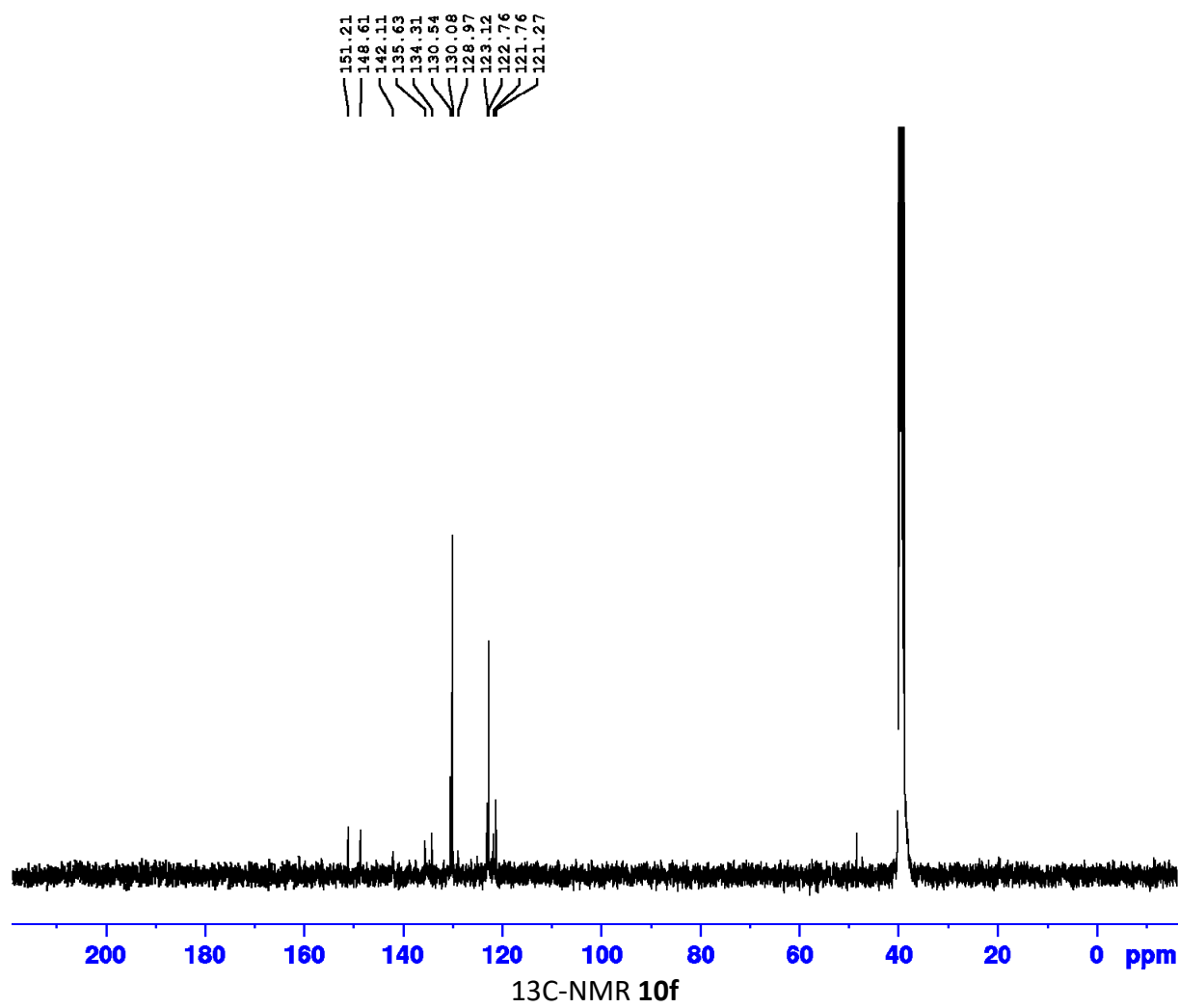


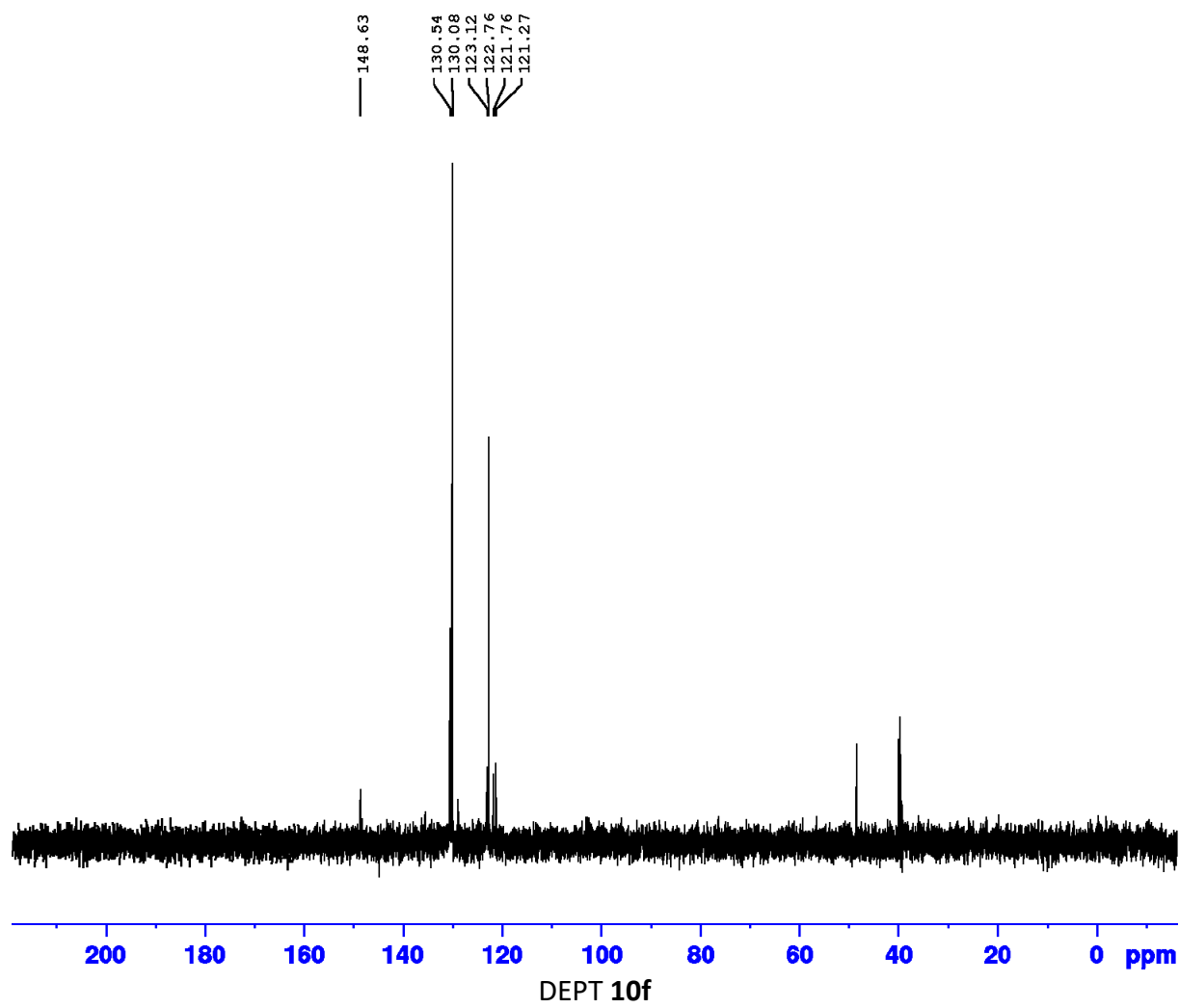




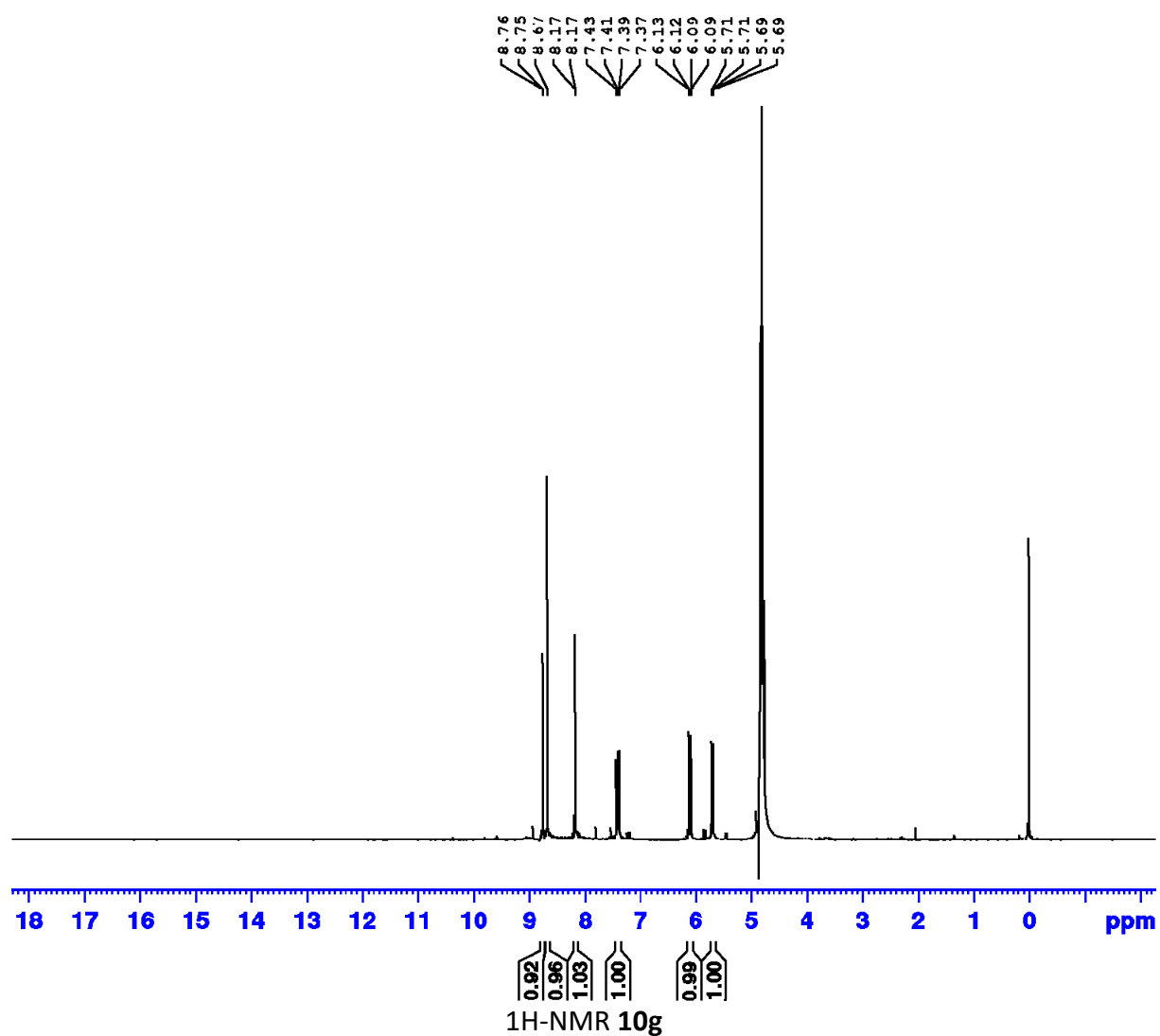
1-Phenyl-3-(2-chloro-9H-purin-6-yl)-1H-imidazolium chloride 10f

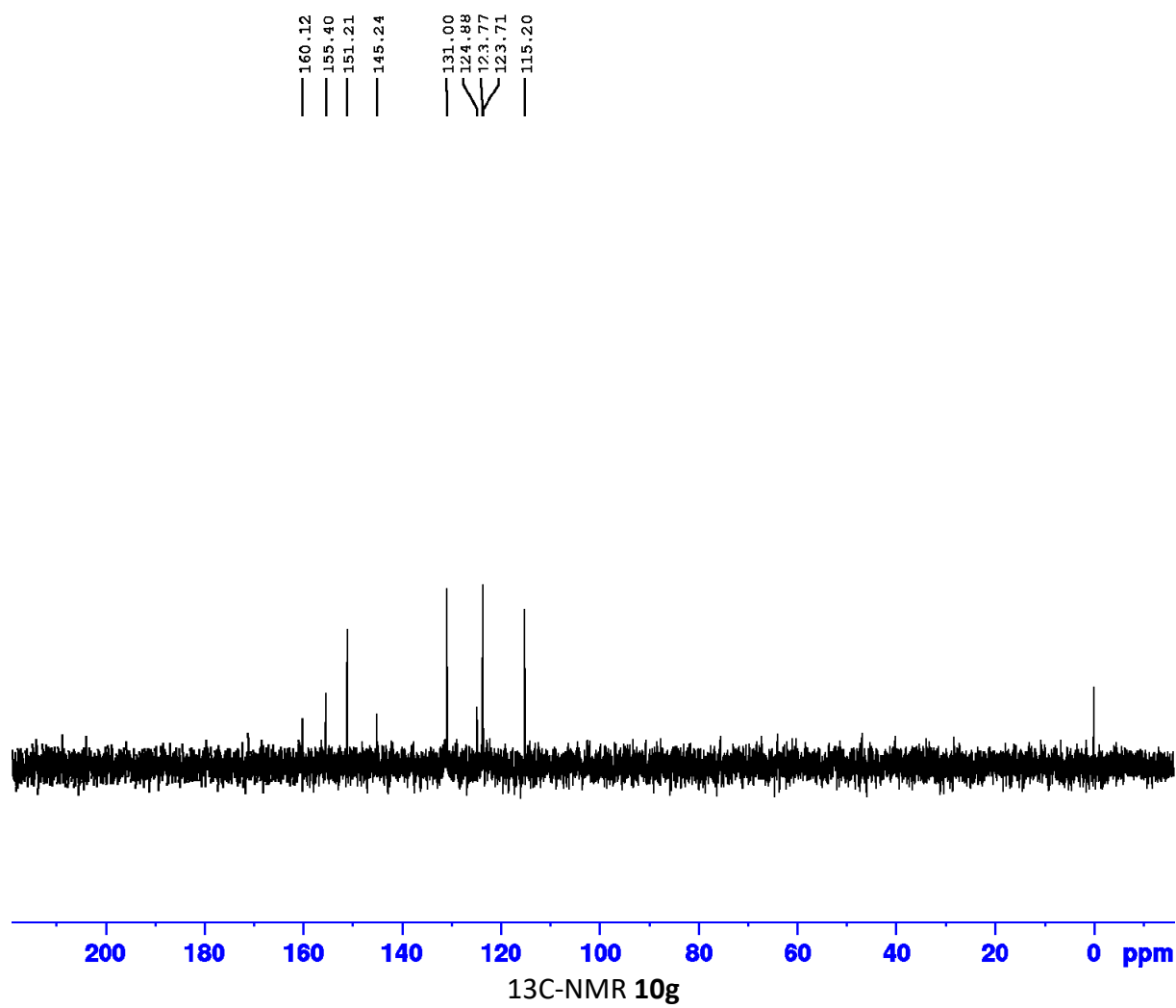


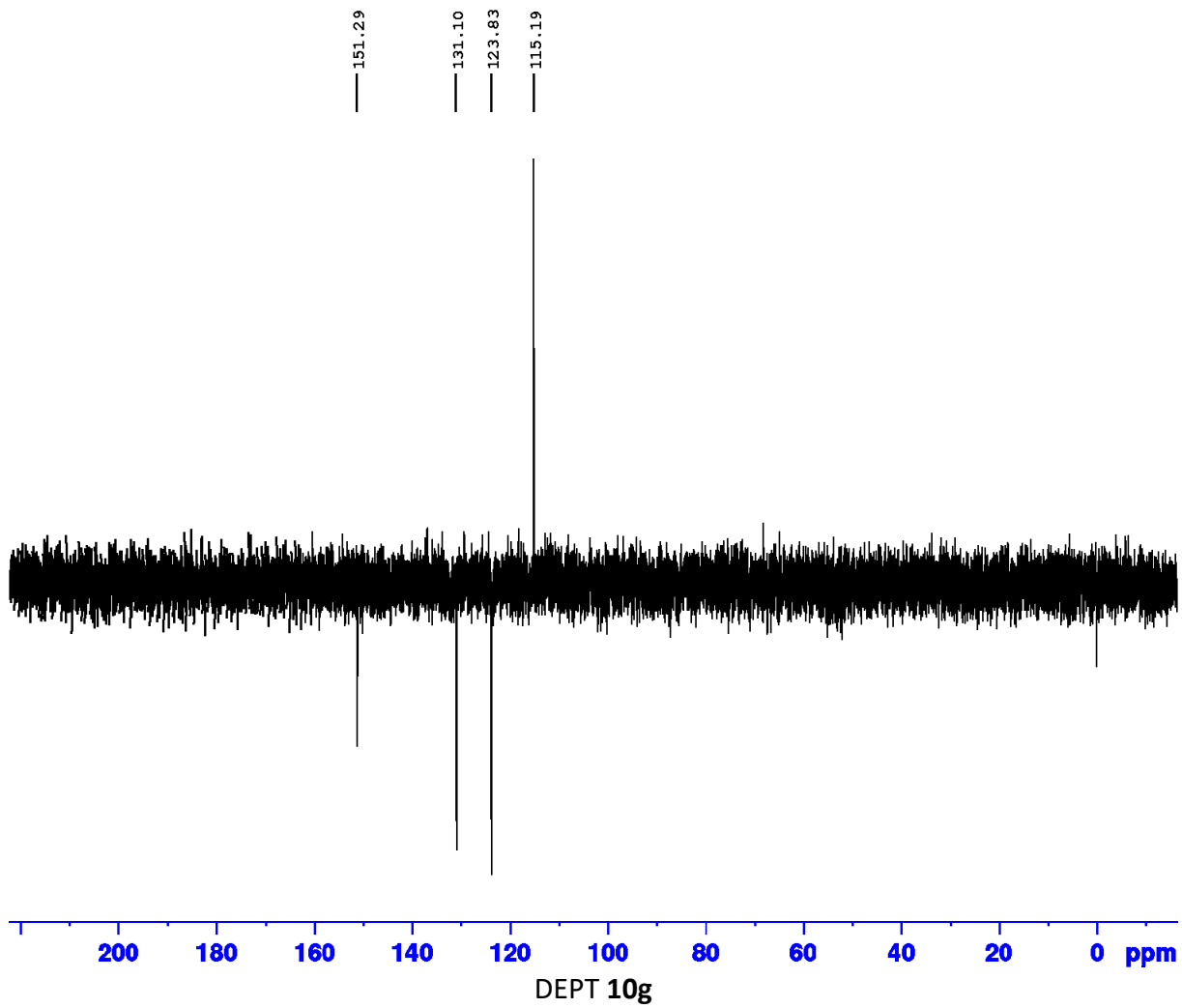




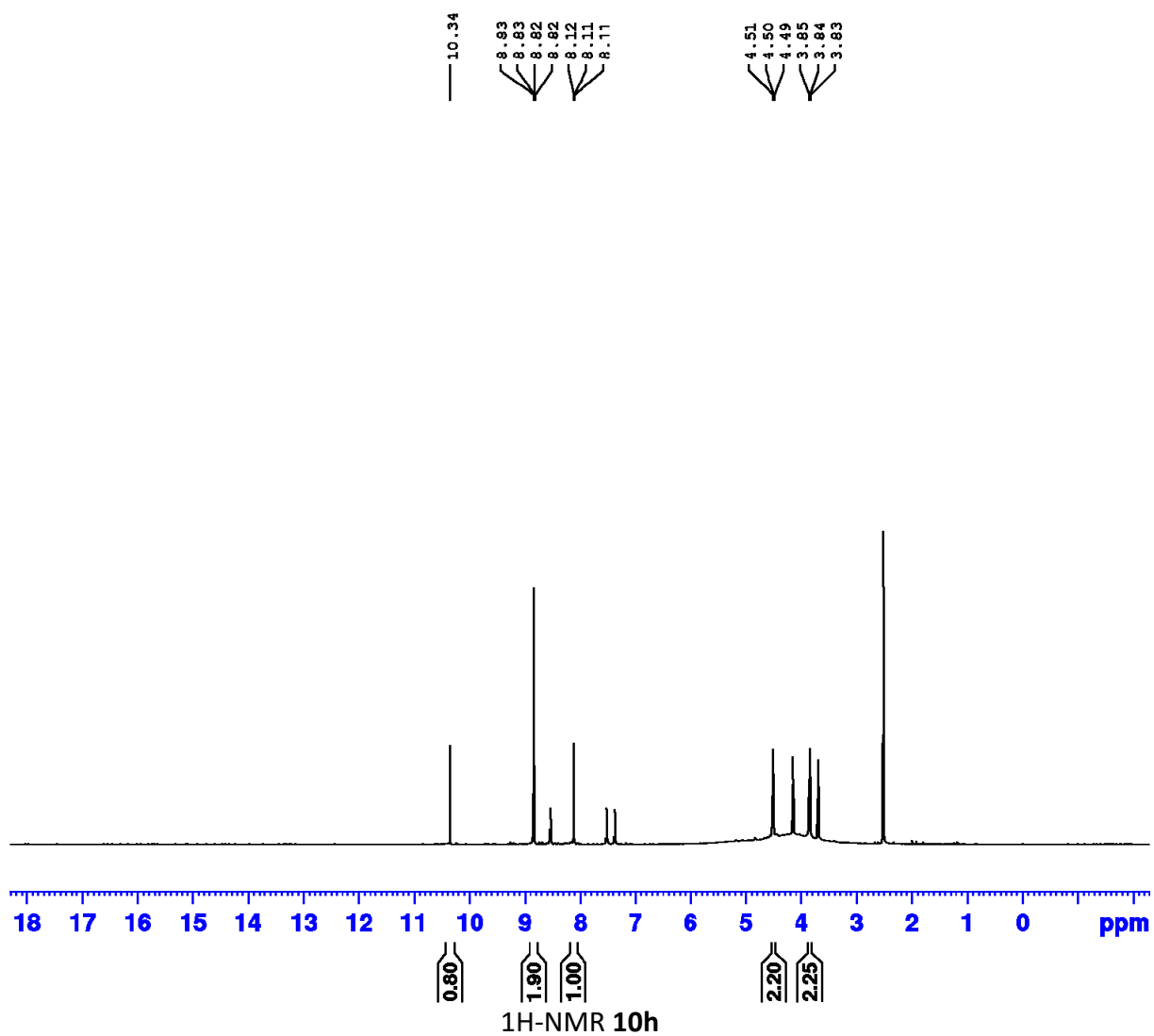
3-(2-Chloro-9H-purin-6-yl)-1-vinyl-1H-imidazolium chloride 10g

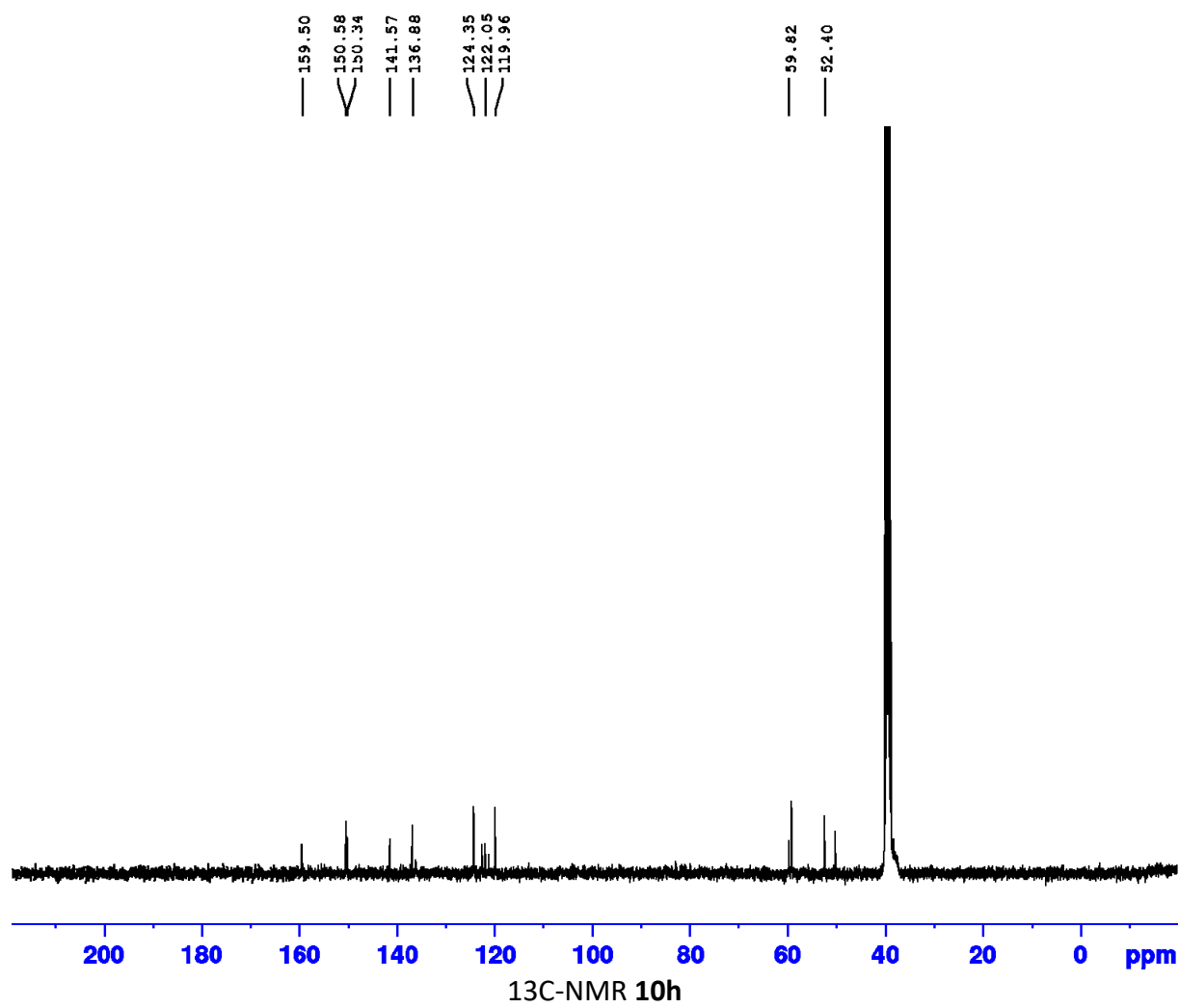


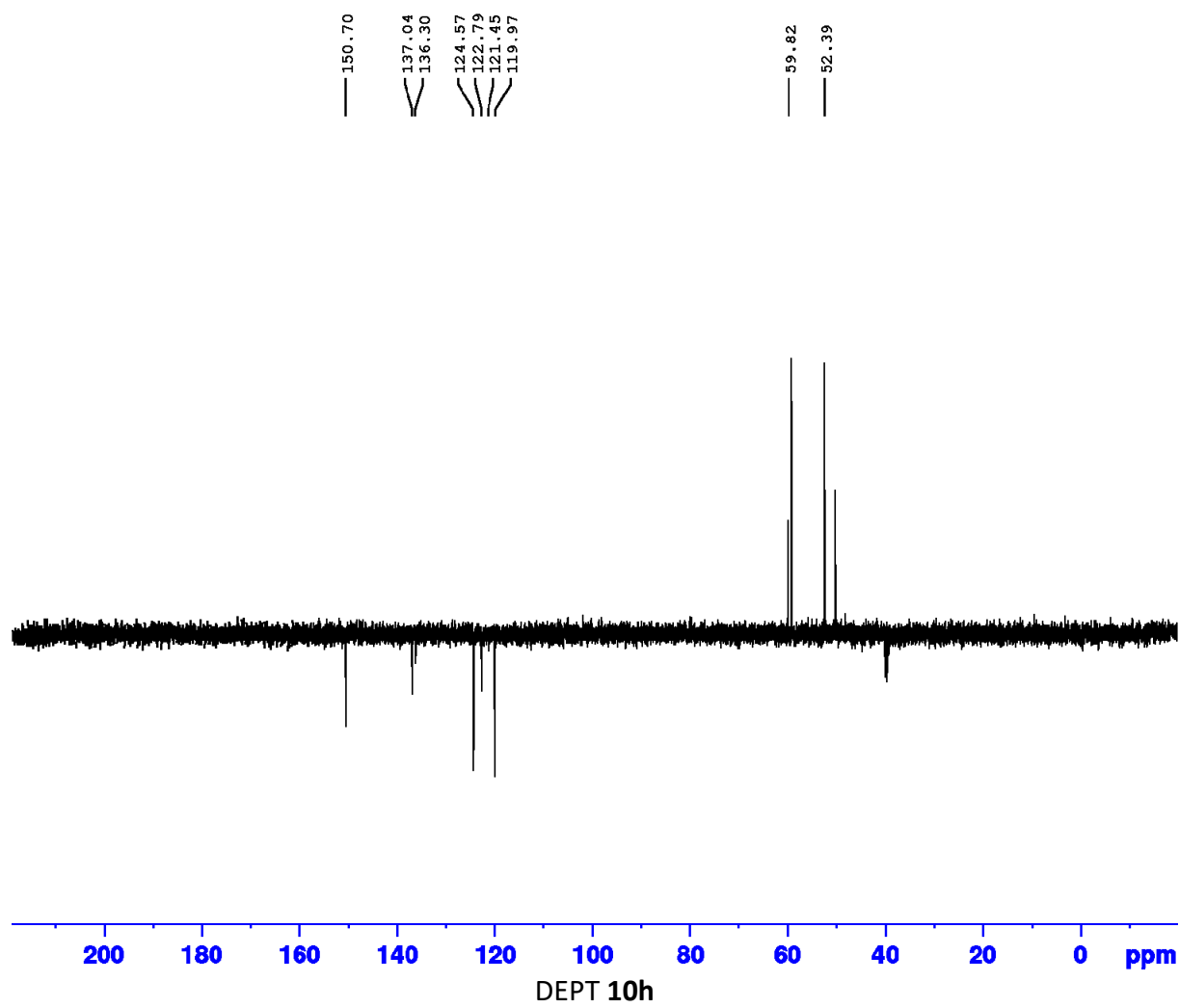




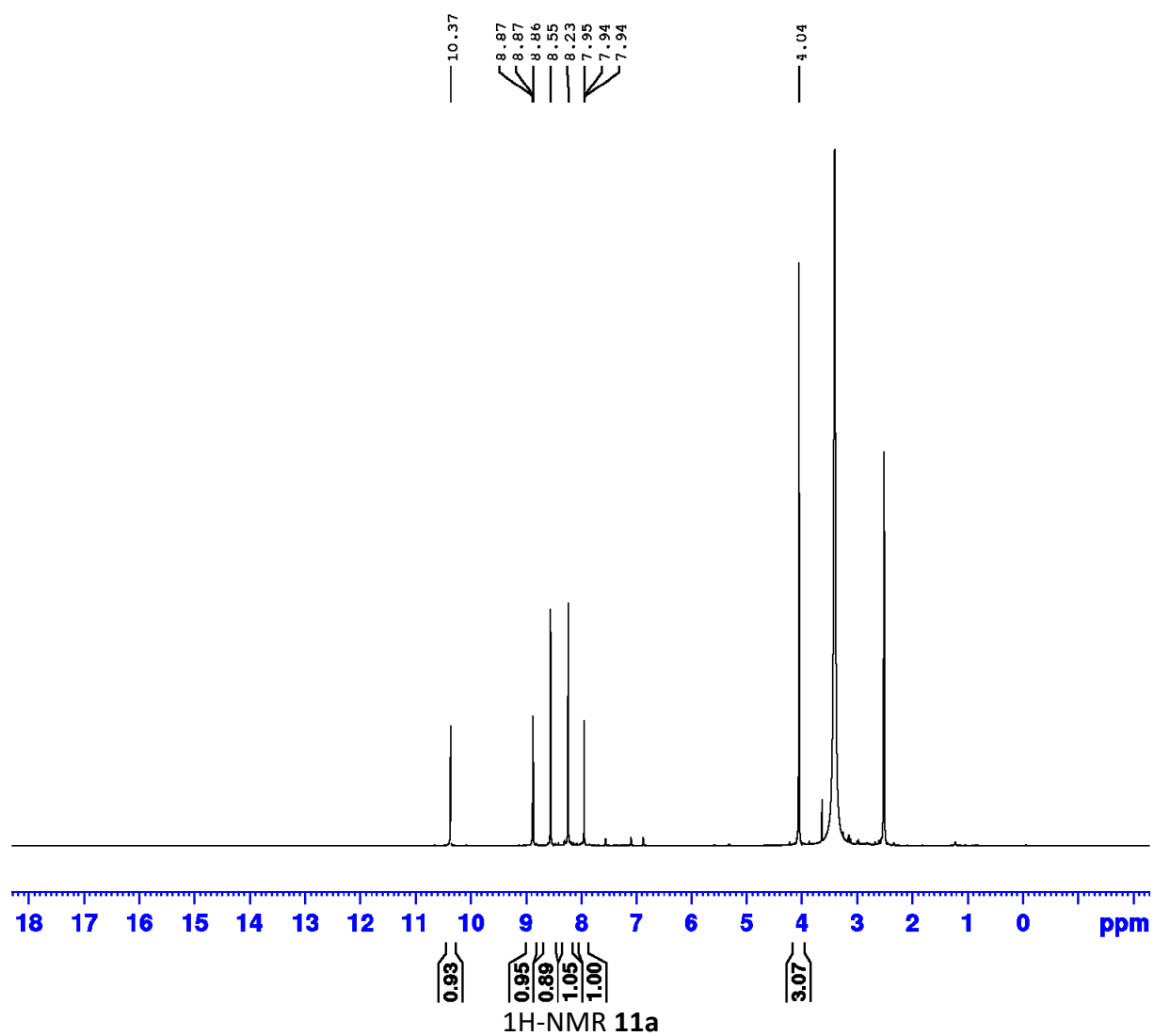
3-(2-Chloro-9H-purin-6-yl)-1-(2-hydroxyethyl)-1H-imidazolium chloride 10h

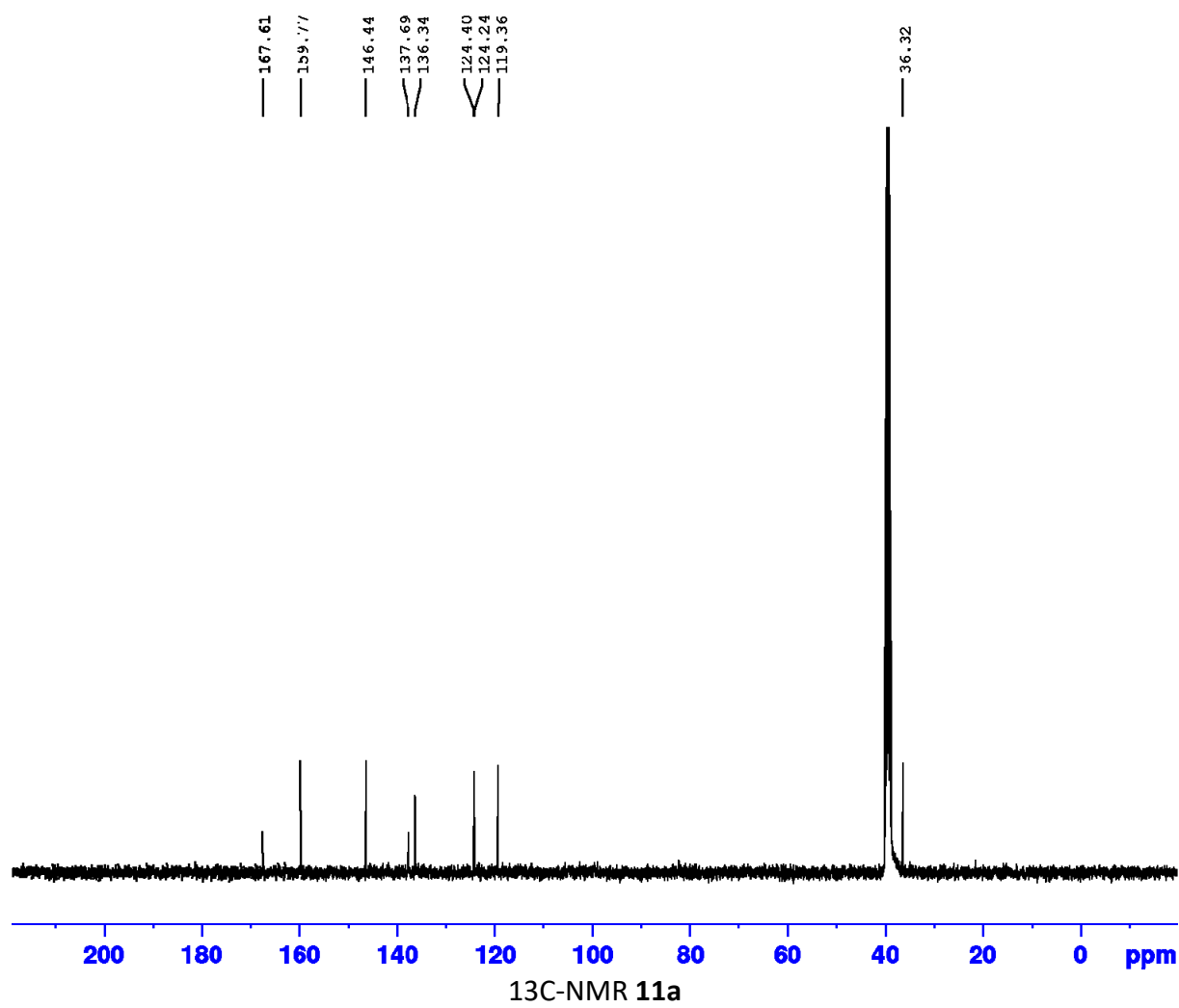


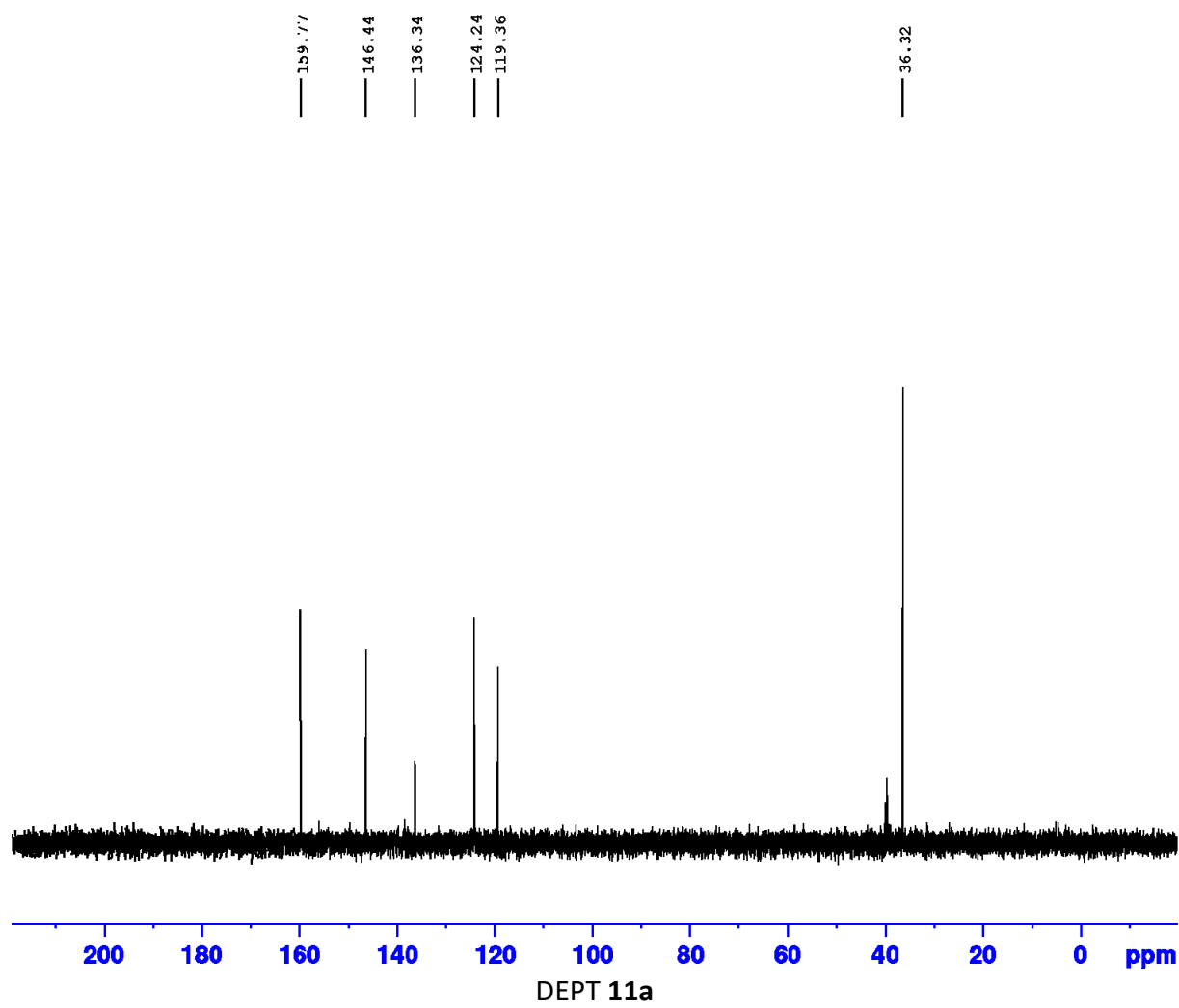




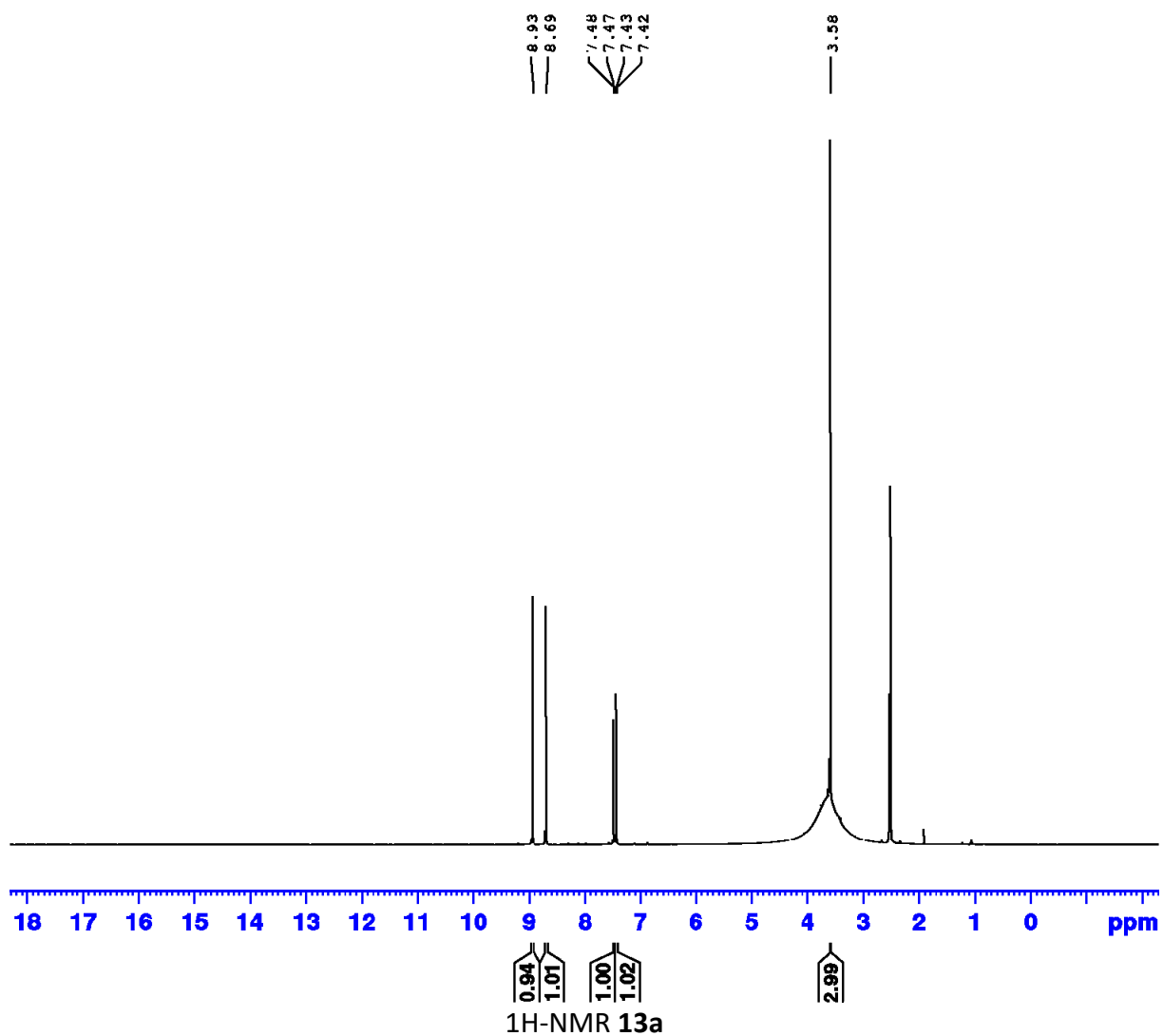
6-(1-Methyl-1H-imidazolium-3-yl)purin-7-ide 11a

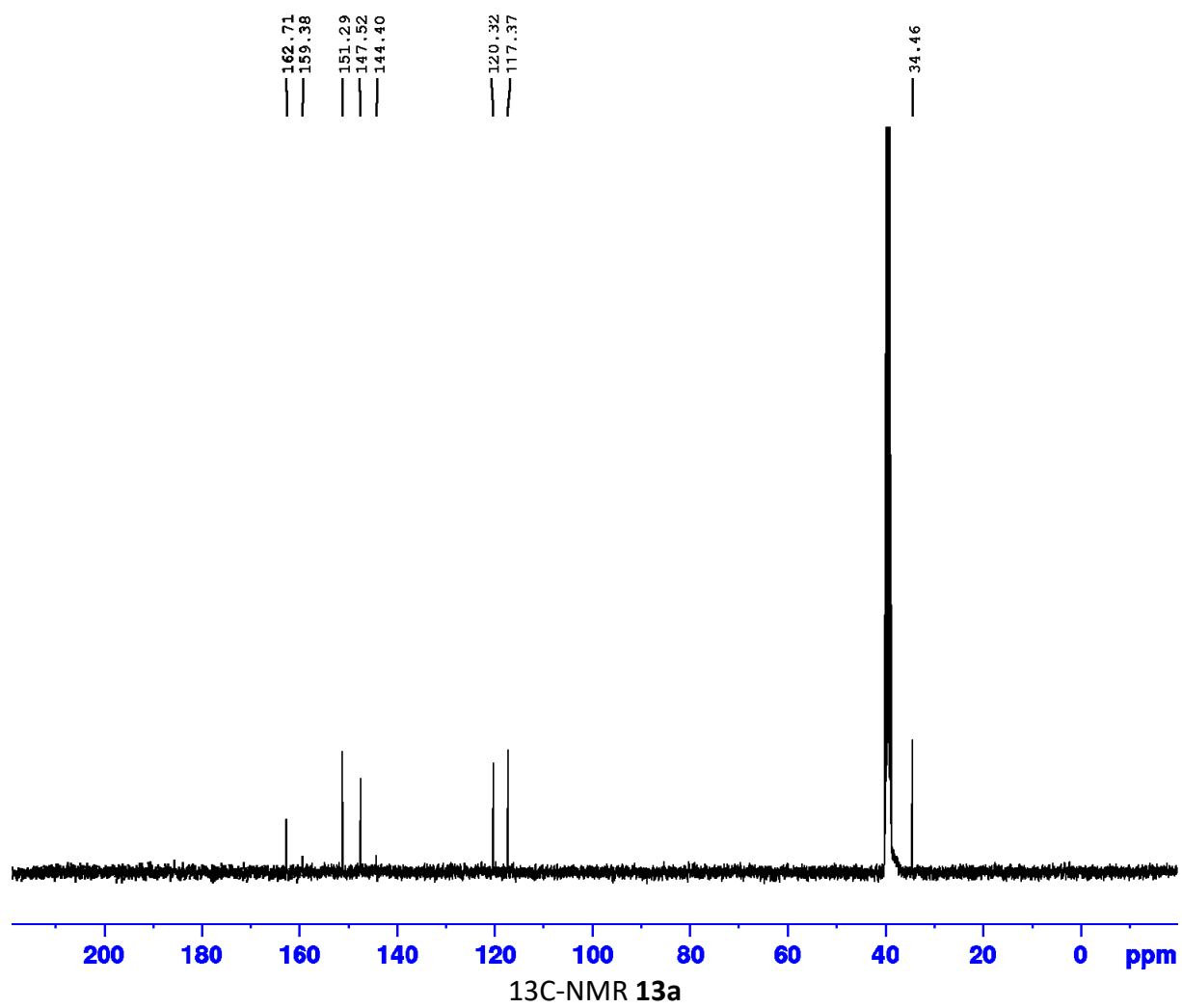


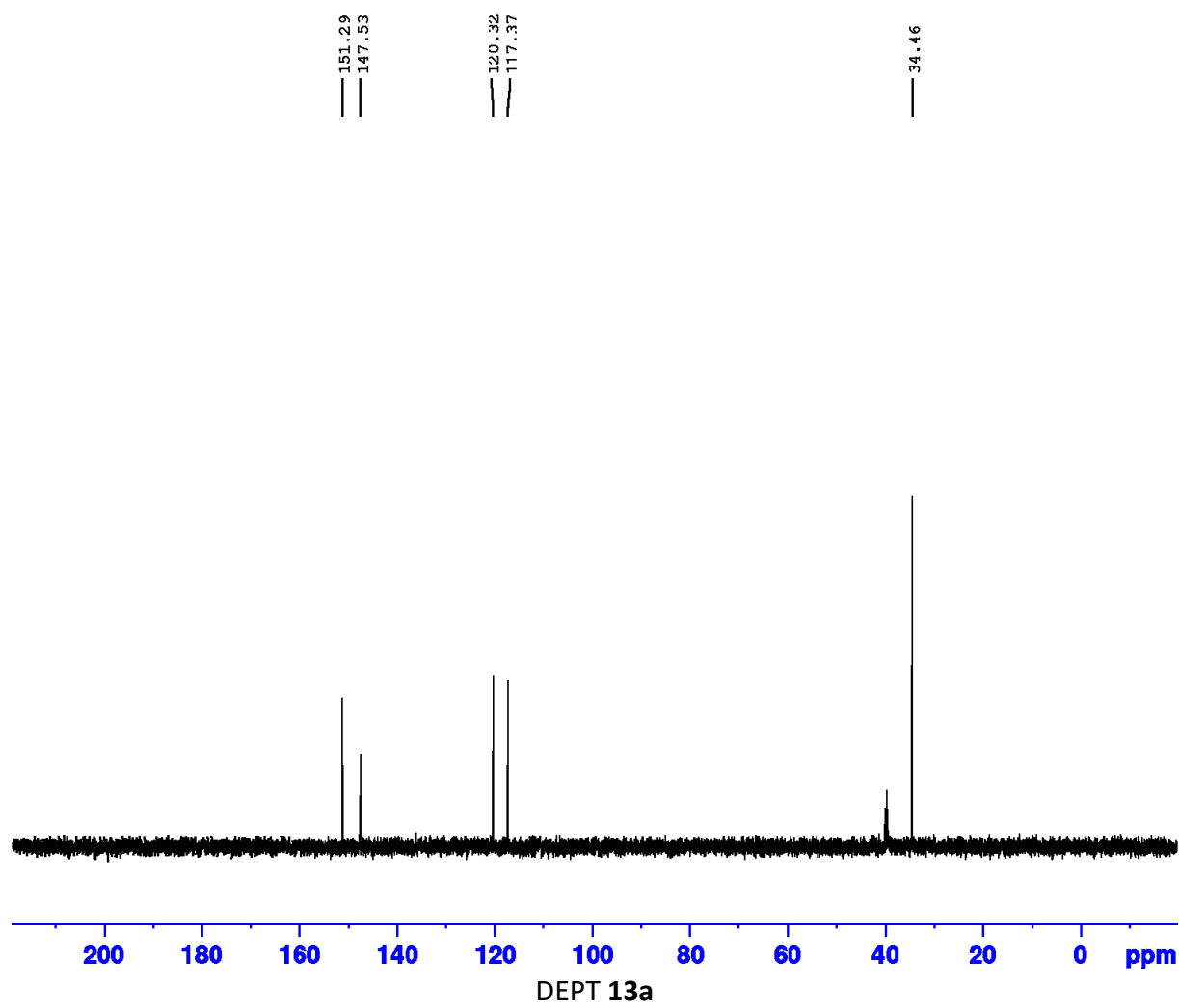




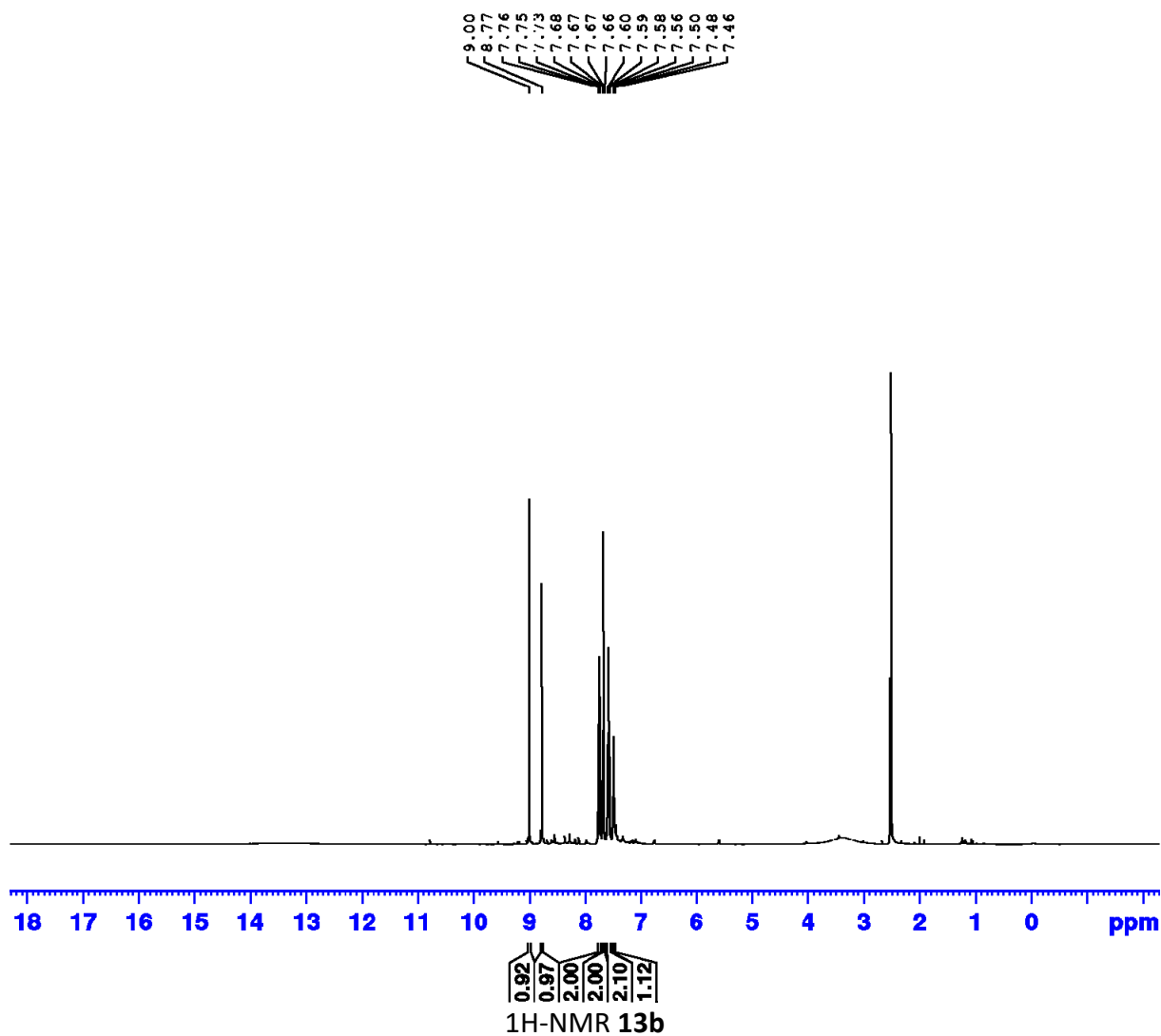
1-Methyl-3-(9H-purin-6-yl)-1,3-dihydro-2H-imidazole-2-thione 13a

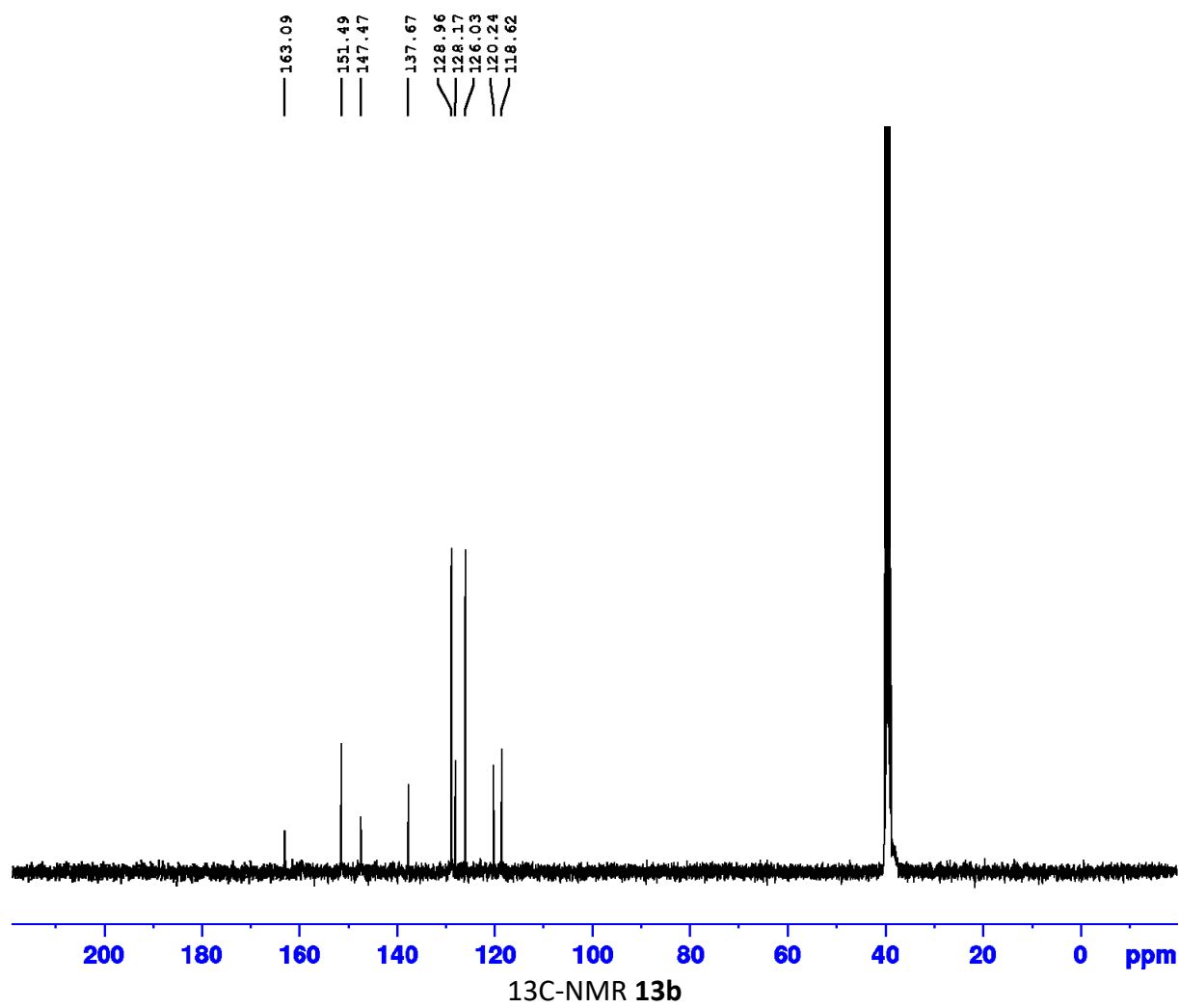


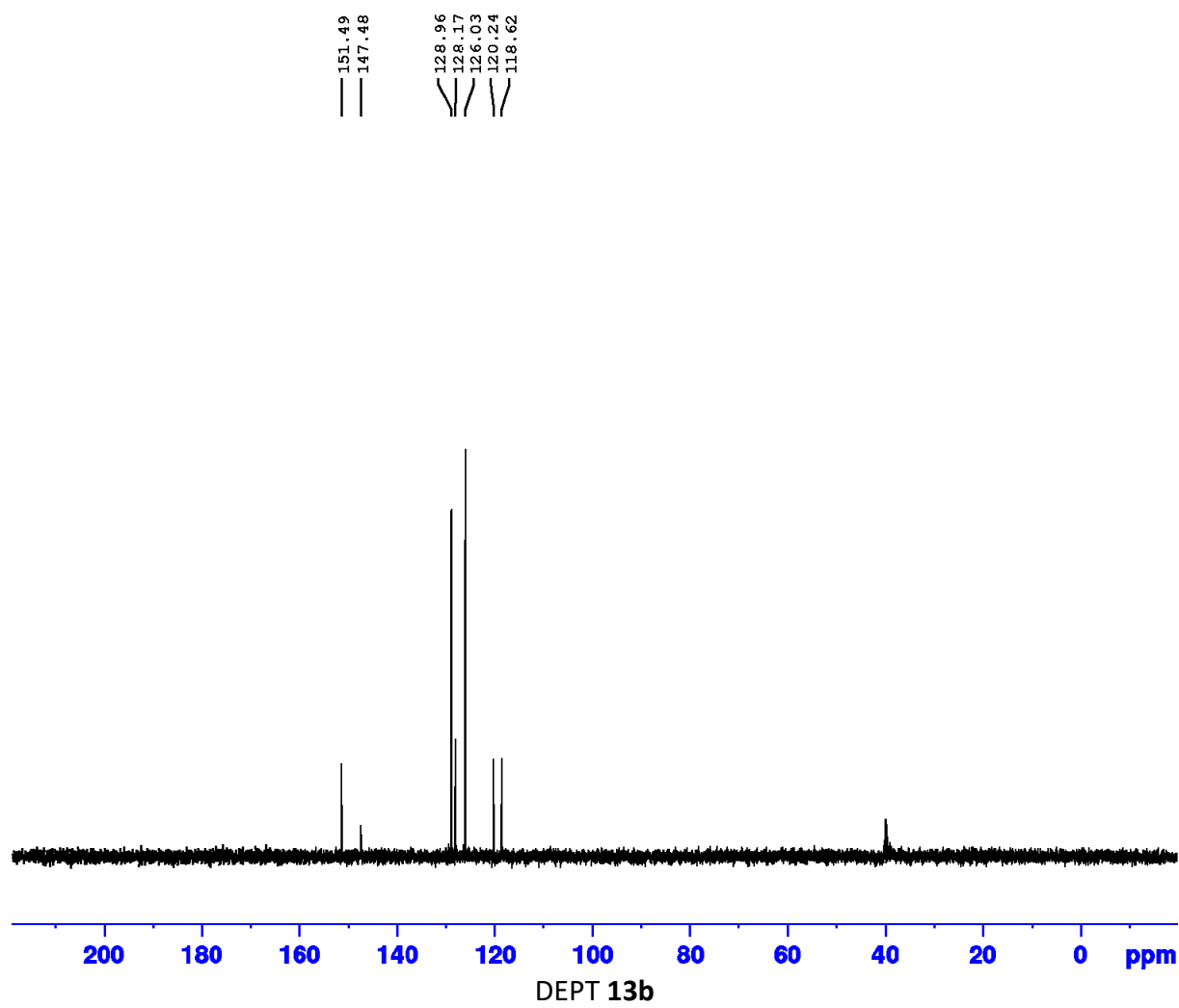




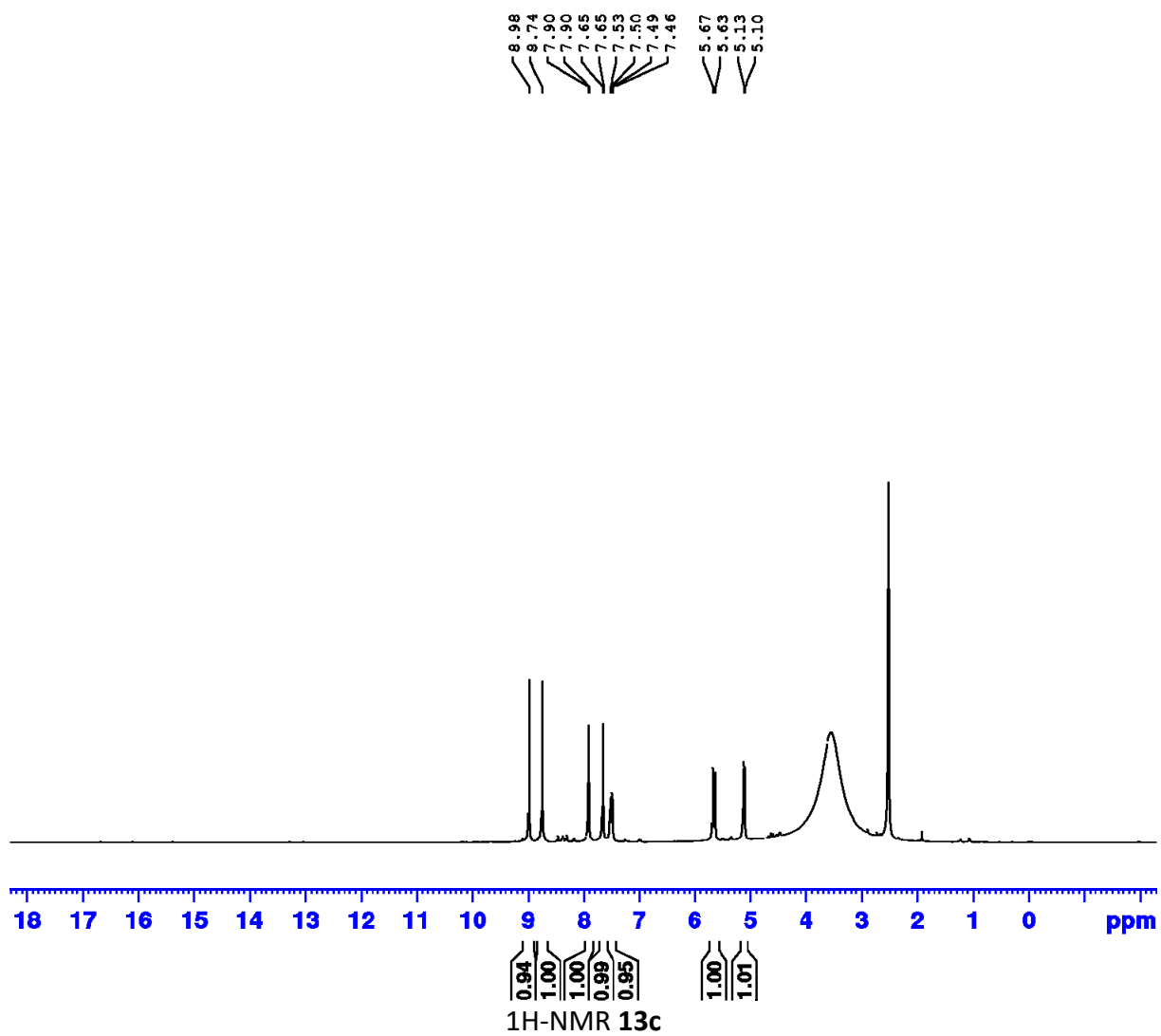
1-Phenyl-3-(9H-purin-6-yl)-1,3-dihydro-2H-imidazole-2-thione 13b

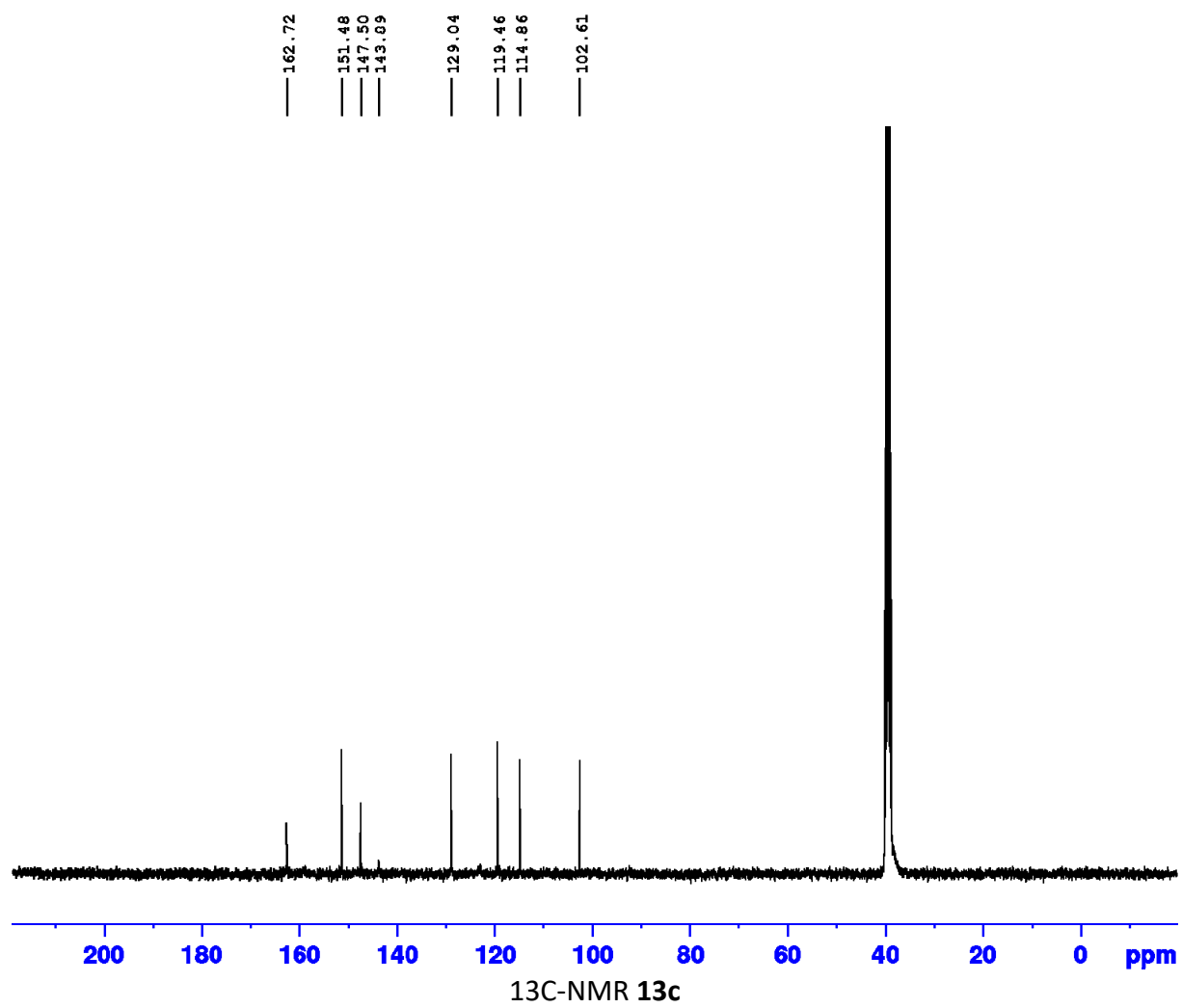


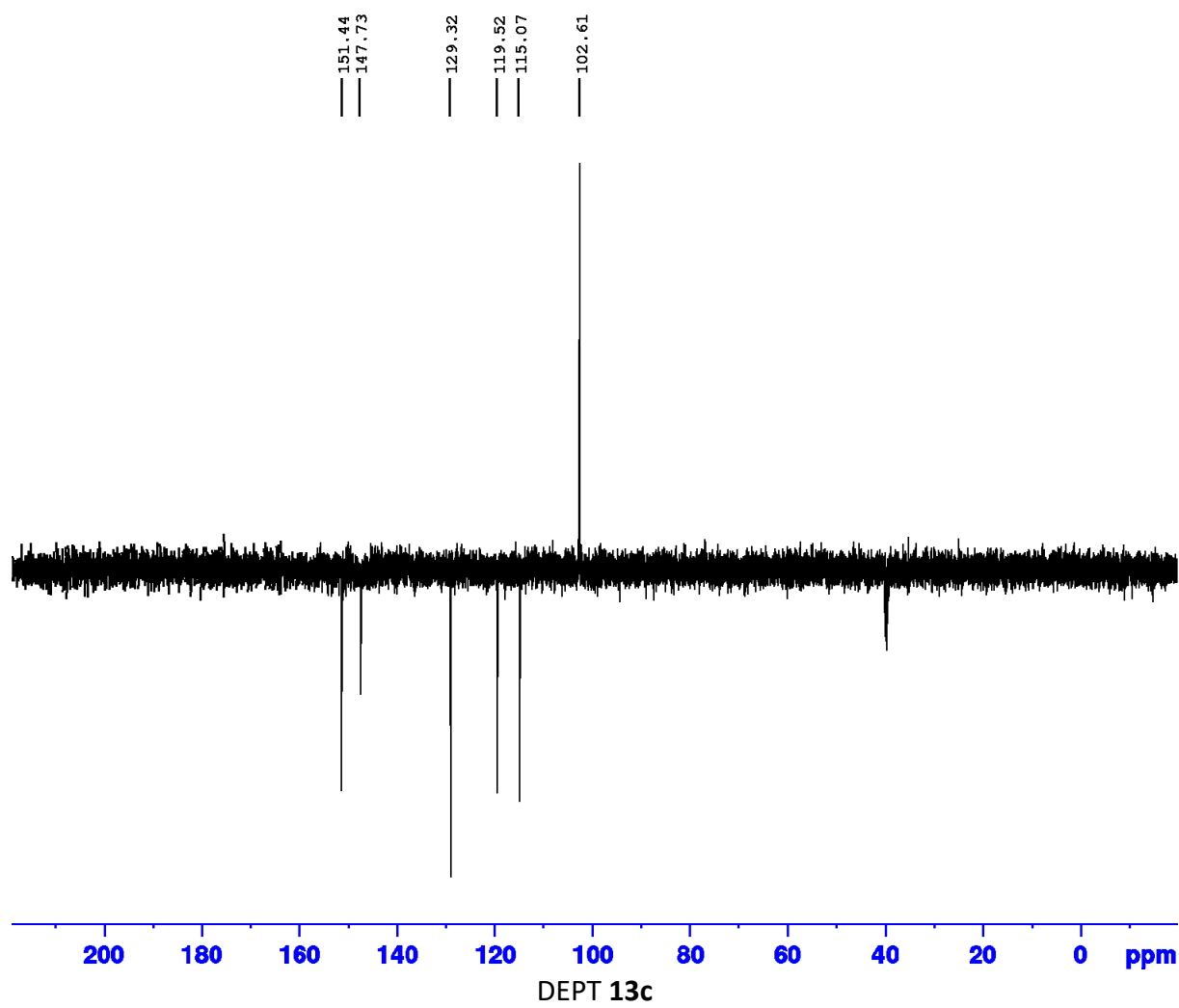




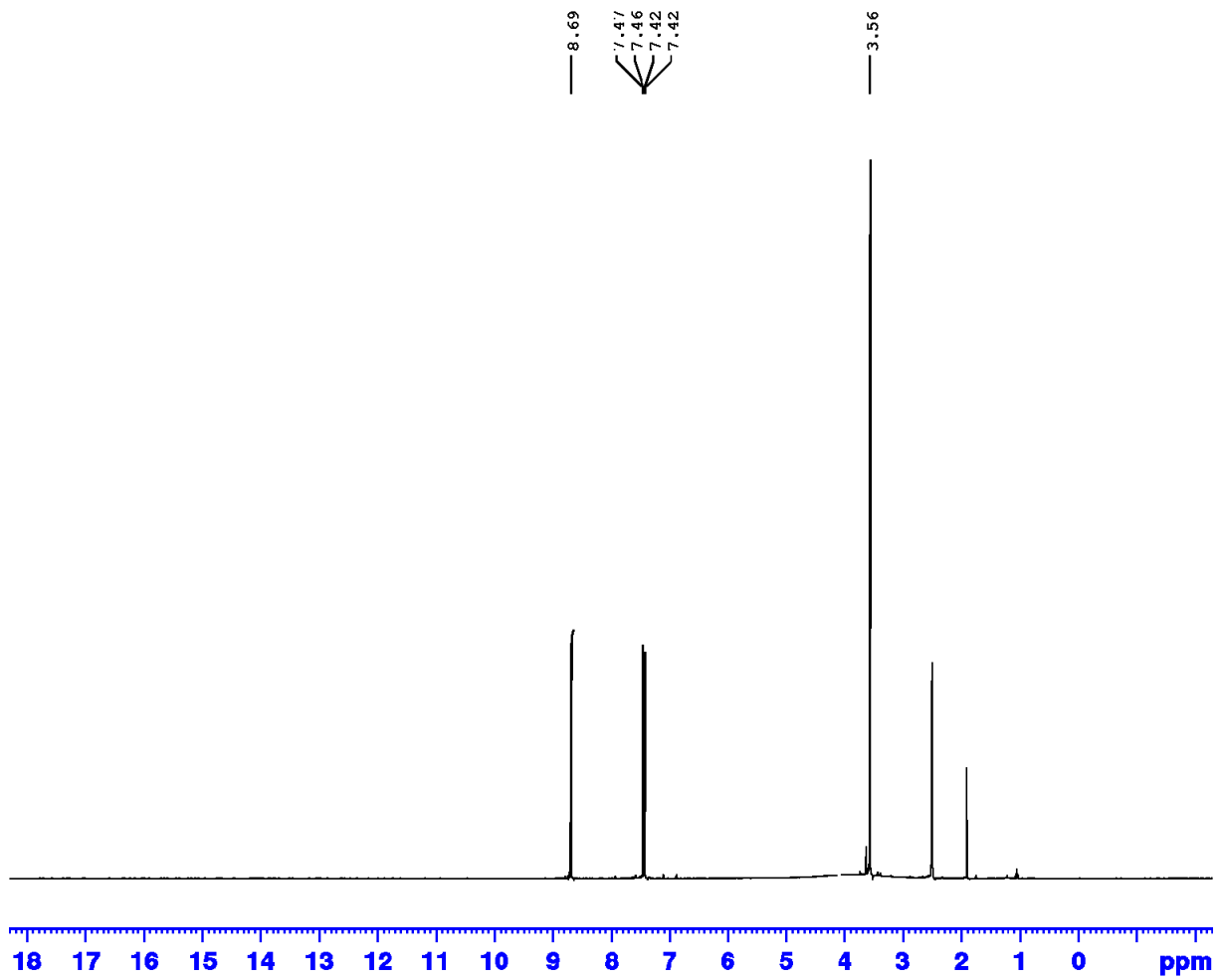
1-(9H-Purin-6-yl)-3-vinyl-1,3-dihydro-2H-imidazole-2-thione 13c





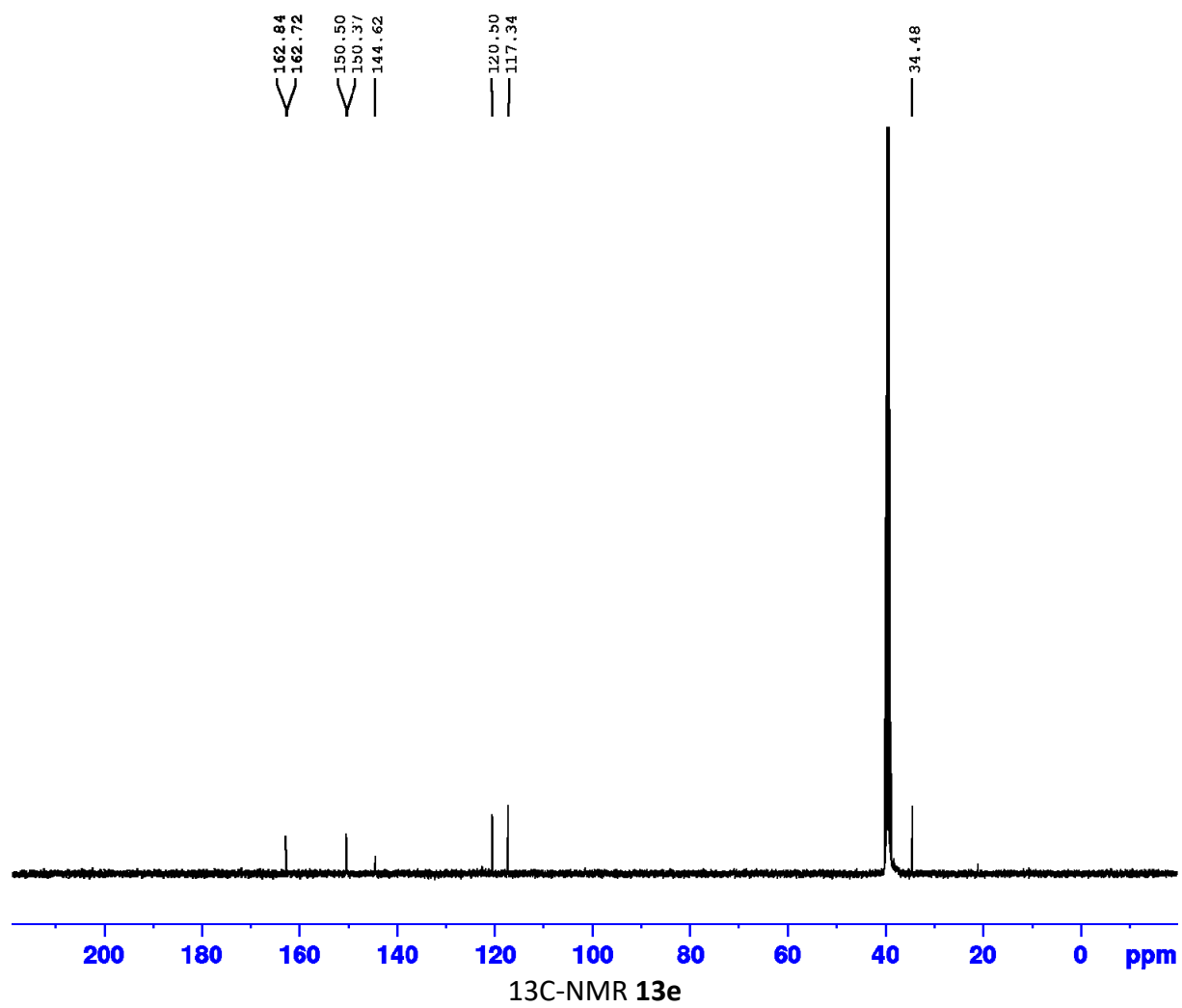


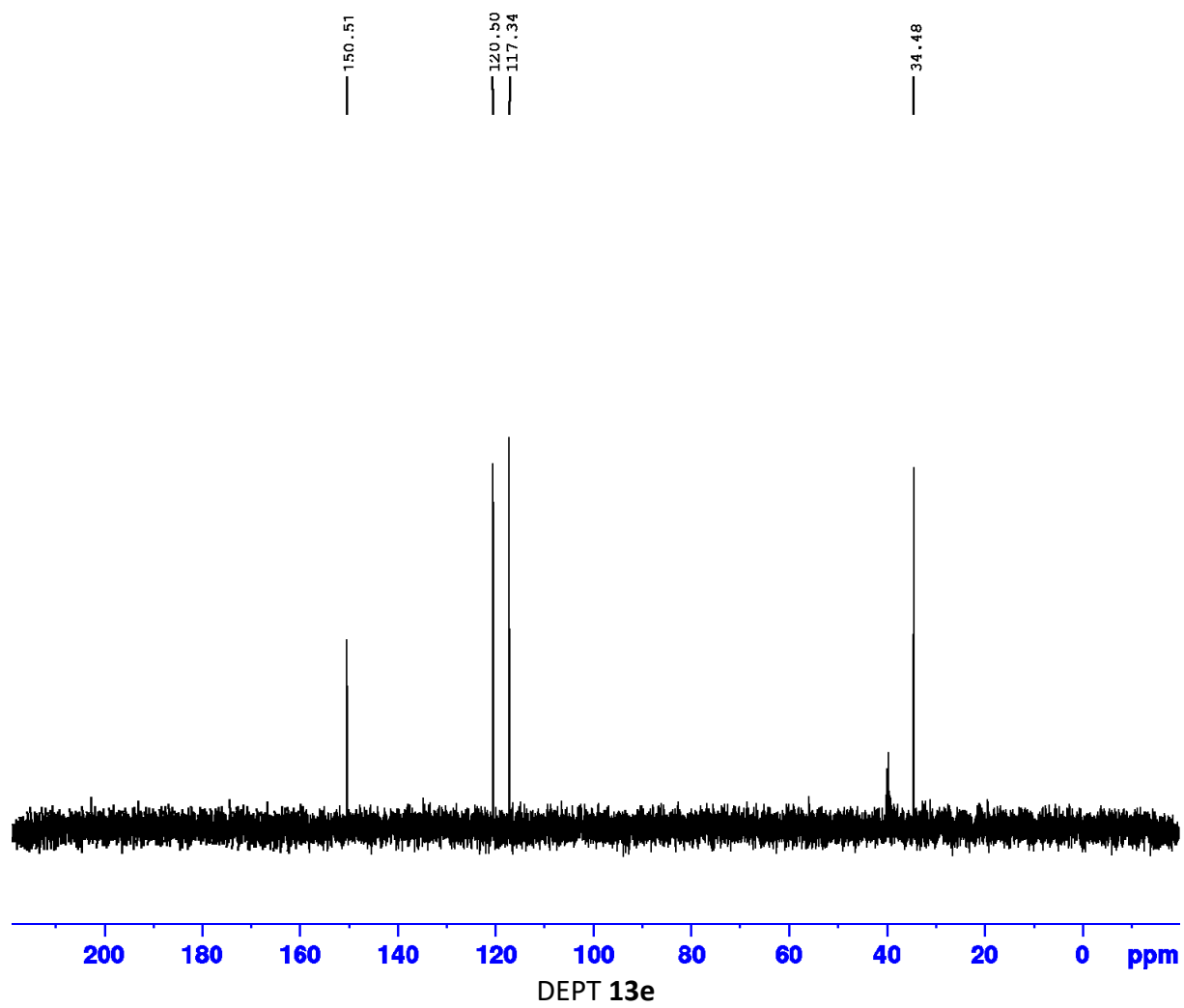
1-(2-Chloro-9H-purin-6-yl)-3-methyl-1,3-dihydro-2H-imidazole-2-thione 13e



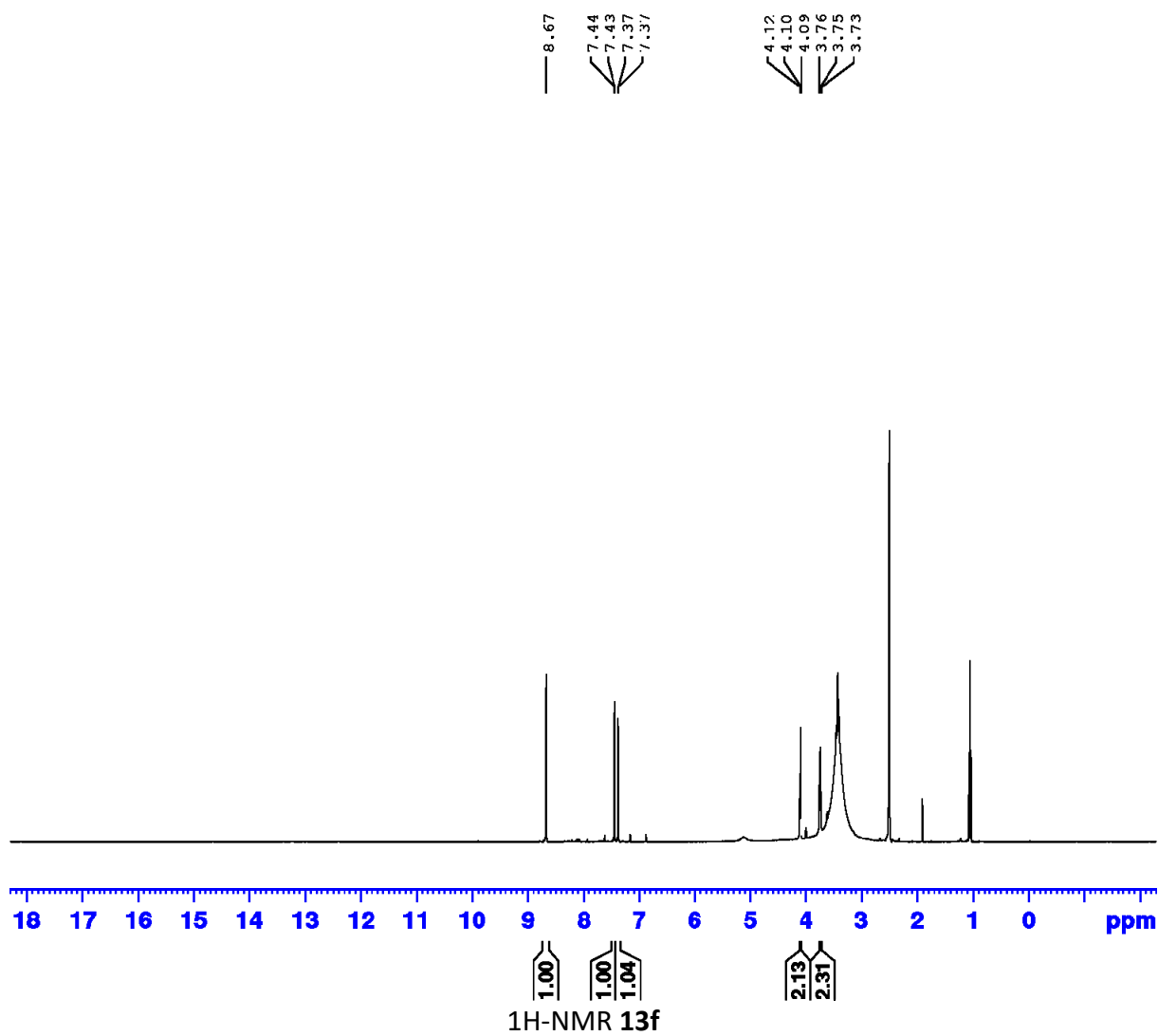
1.06
1.00
0.97
3.08

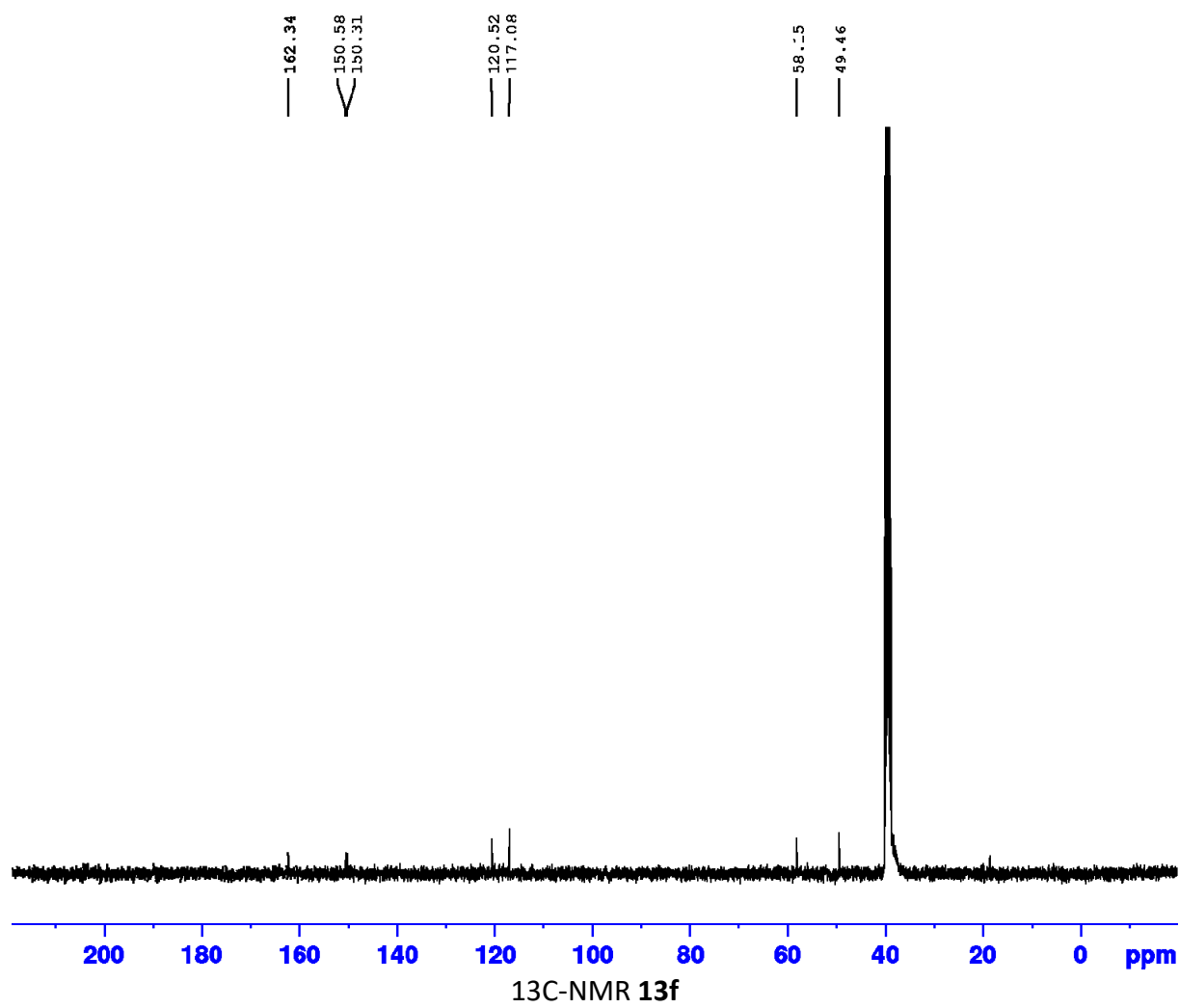
1H-NMR 13e

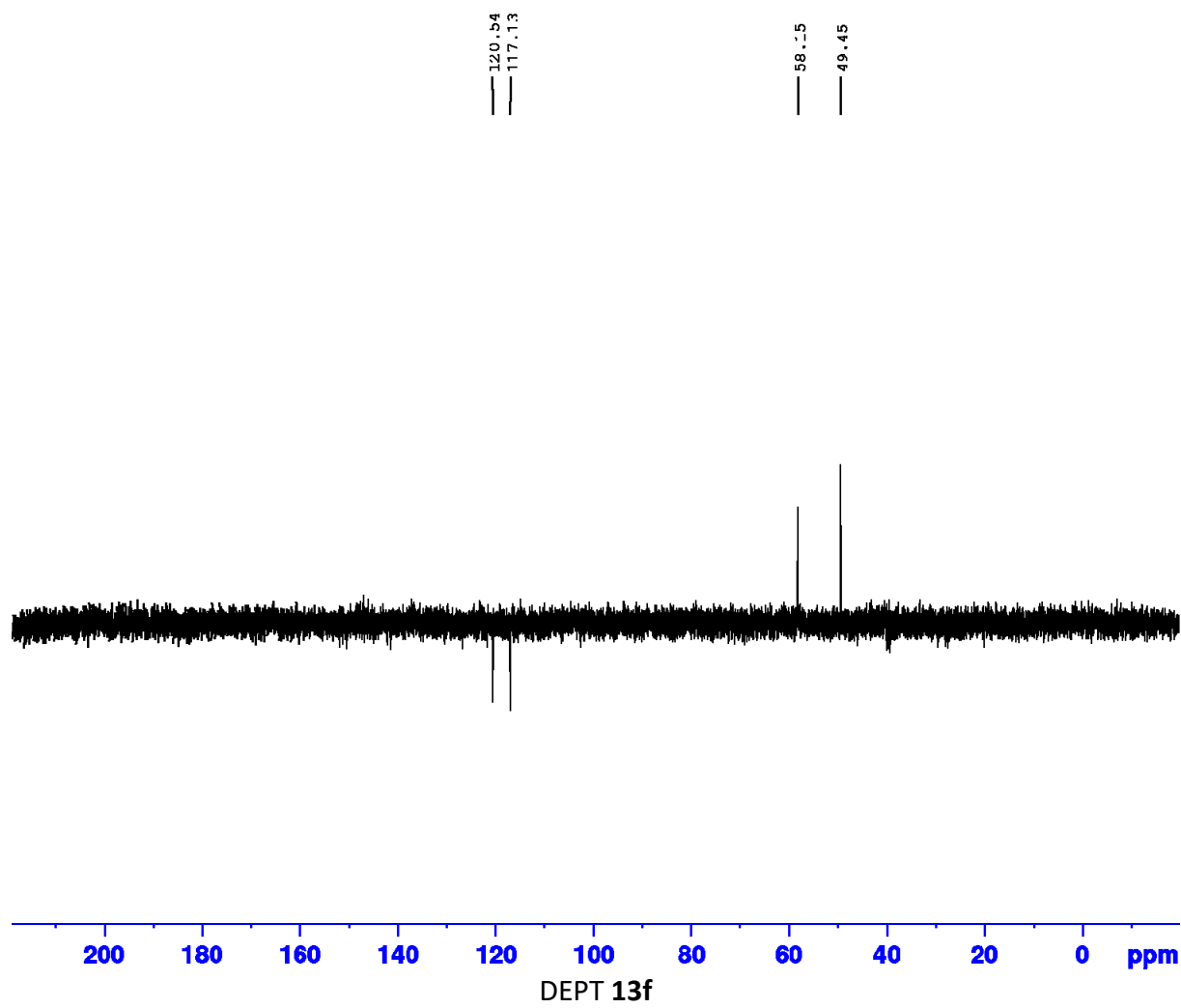




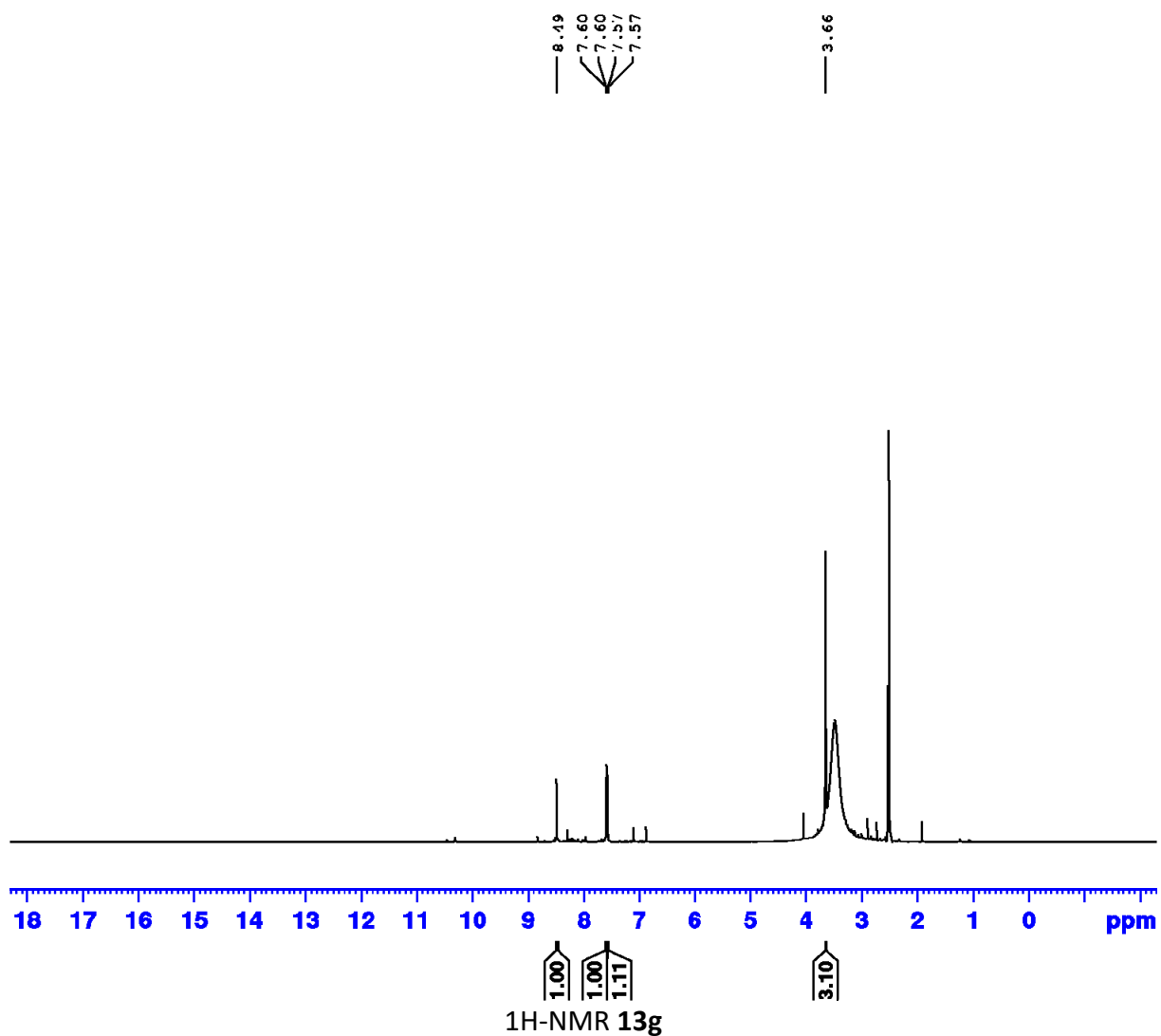
1-(2-Chloro-9H-purin-6-yl)-3-(2-hydroxyethyl)-1,3-dihydro-2H-imidazole-2-thione 13f

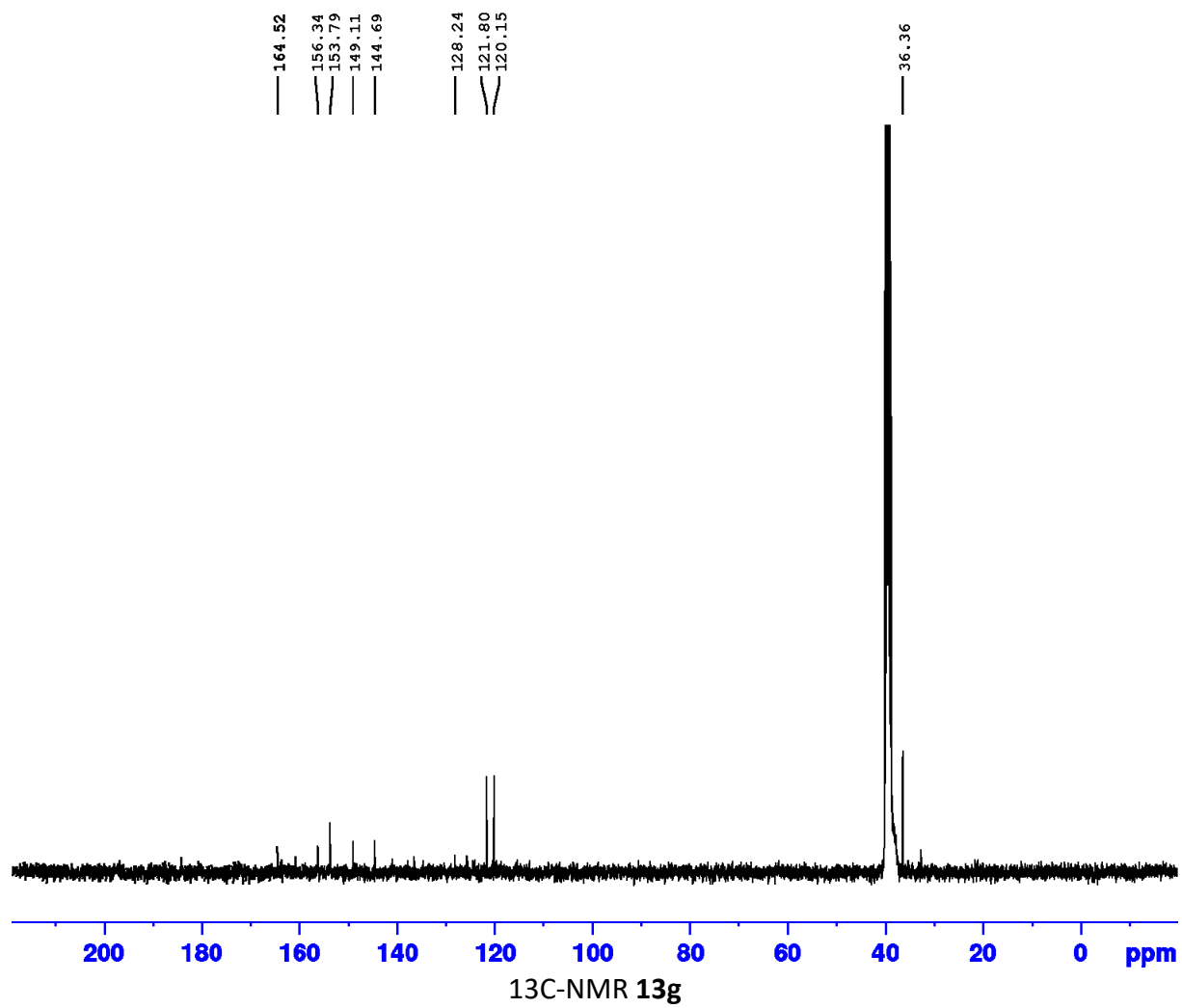


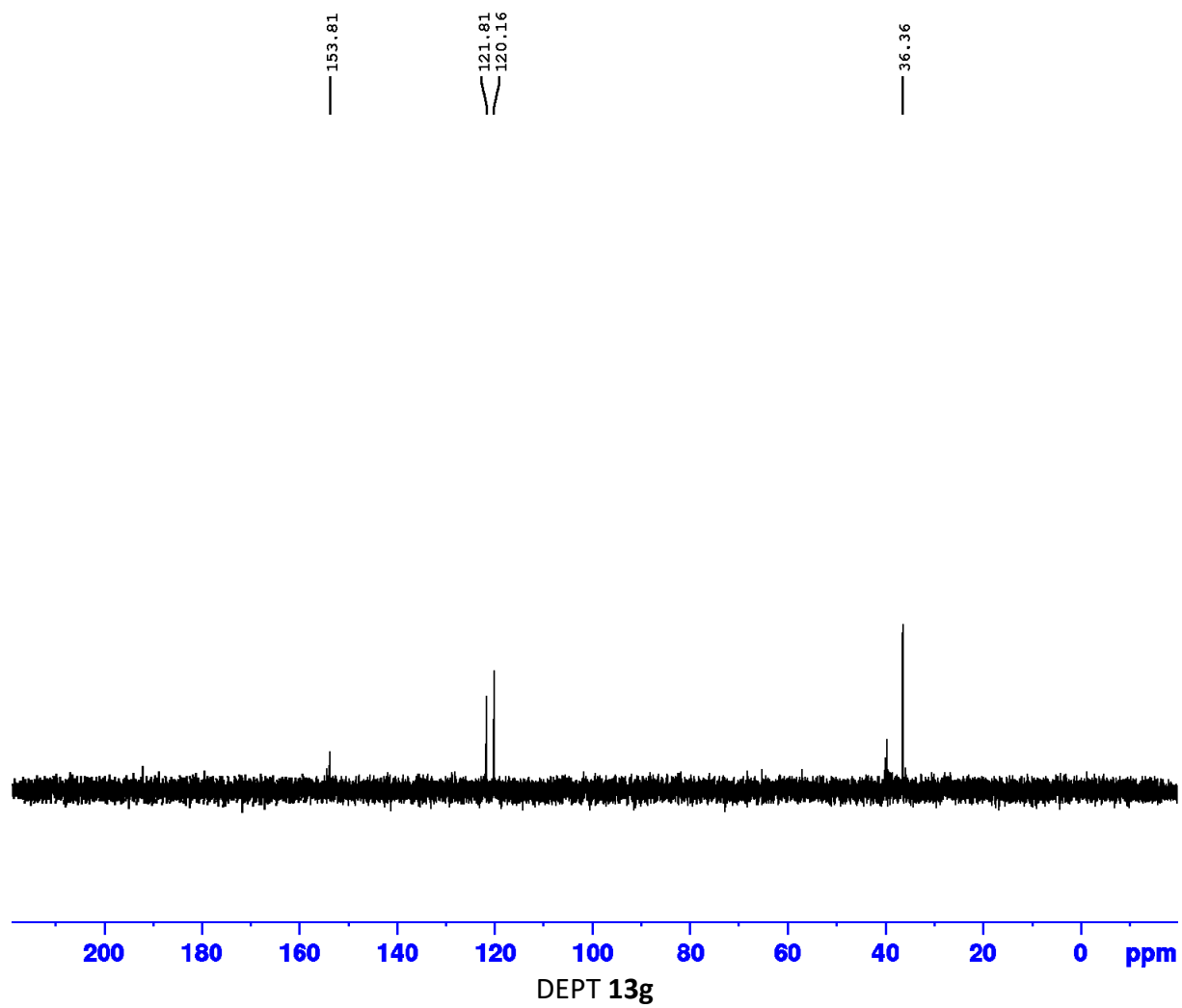




1-(2-Chloro-9H-purin-6-yl)-3-methyl-1,3-dihydro-2H-imidazole-2-selenone 13g







7,7-Diethyl-8-methyl-7,8-dihydroimidazo[2',1':3,4][1,4,2] diazaborinino[1,6,5-gh]purinium-7-ide 14

