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Supplementary.Material

Luminescent P-Benzyl Dithienophospholes – A Joint Experimental and Theoretical Investigation

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Figure S1. Fluroescence spectra of the P-benzyl dithienophospholes.

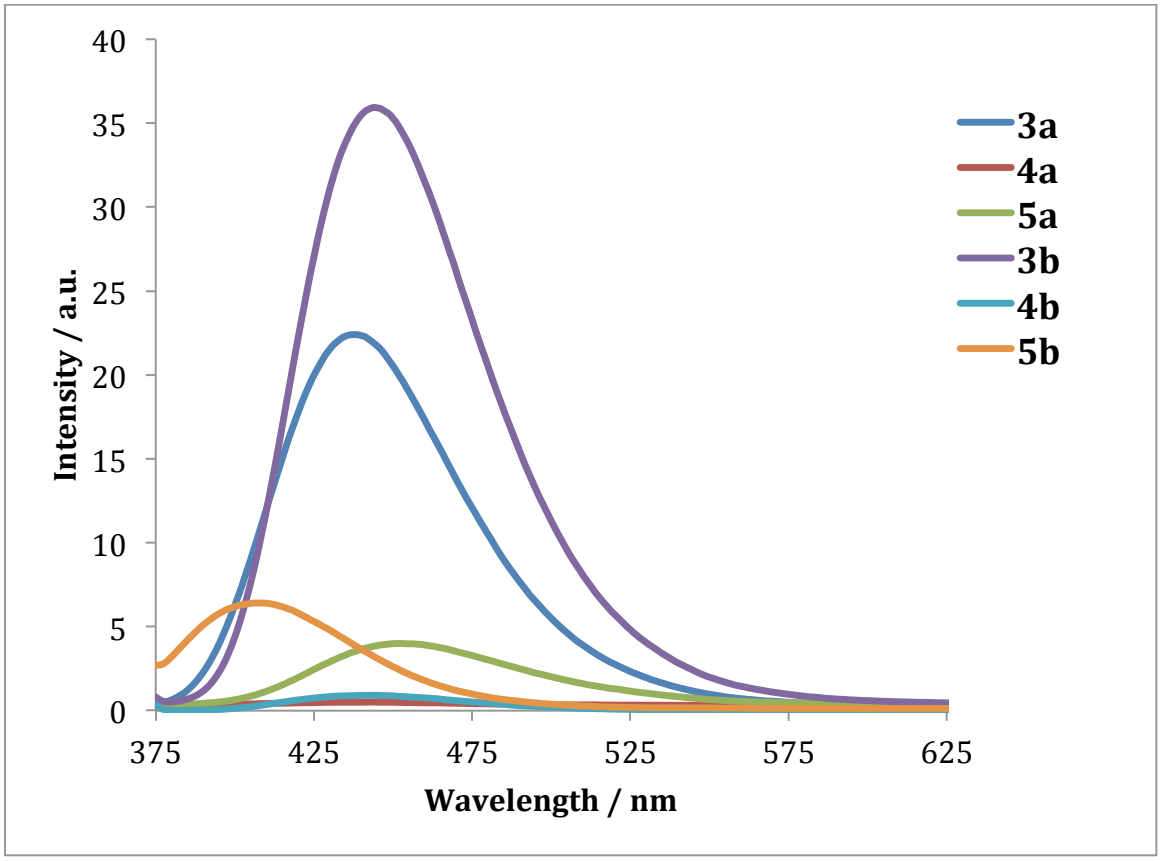


Table S1. Cartesian coordinates of minimized **2a**.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.459123	3.201114	-0.387305
2	6	0	-0.348825	2.140911	-0.713795
3	6	0	0.311412	0.886856	-0.554498
4	6	0	1.625407	1.029763	-0.123413
5	16	0	2.058745	2.695815	0.101453
6	1	0	0.217709	4.256134	-0.405489
7	1	0	-1.373614	2.258491	-1.049166
8	6	0	2.336317	-0.215610	0.025482
9	16	0	3.950723	-0.630049	0.511943
10	6	0	2.323554	-2.549709	-0.144504
11	6	0	3.606230	-2.328319	0.290932
12	1	0	1.934797	-3.541759	-0.351007
13	1	0	4.379838	-3.058357	0.491307
14	15	0	-0.078770	-0.871423	-0.925389
15	6	0	-2.588812	-0.840213	0.414096
16	6	0	-3.006462	0.285983	1.139383
17	6	0	-3.511071	-1.460126	-0.444960
18	6	0	-4.309478	0.776723	1.015390
19	1	0	-2.306181	0.779040	1.809822
20	6	0	-4.812878	-0.971766	-0.572369
21	1	0	-3.205392	-2.333444	-1.017797
22	6	0	-5.217594	0.150067	0.158149
23	1	0	-4.614219	1.646793	1.591917
24	1	0	-5.512172	-1.468935	-1.240128
25	1	0	-6.231863	0.529044	0.062257
26	6	0	1.583459	-1.339874	-0.292151
27	6	0	-1.179209	-1.362010	0.546416
28	1	0	-0.711691	-1.011921	1.471836
29	1	0	-1.174160	-2.458746	0.561814

SCF Energy: -1715.88822414 a.u.

Table S2. Cartesian coordinates of minimized **2a-rot**.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.870117	-3.018870	-0.269429
2	6	0	1.224336	-2.614877	0.872225
3	6	0	1.002645	-1.206899	0.901668
4	6	0	1.508117	-0.566900	-0.223333
5	16	0	2.246740	-1.682276	-1.329150
6	1	0	2.156873	-4.022512	-0.555944
7	1	0	0.925925	-3.304573	1.655482
8	6	0	1.333522	0.864097	-0.215059
9	16	0	1.778287	2.136034	-1.308885
10	6	0	0.568134	2.771537	0.902862
11	6	0	1.094260	3.331064	-0.234560
12	1	0	0.114474	3.360985	1.693341
13	1	0	1.128876	4.377048	-0.510799
14	15	0	0.366171	0.006256	2.123114
15	6	0	-2.193896	-0.251985	0.699792
16	6	0	-2.698220	0.925631	0.125821
17	6	0	-2.339355	-1.453241	-0.012100
18	6	0	-3.326221	0.905996	-1.121550
19	1	0	-2.599643	1.867112	0.661530
20	6	0	-2.966757	-1.477144	-1.259718
21	1	0	-1.958101	-2.378174	0.414187
22	6	0	-3.461953	-0.296605	-1.820657
23	1	0	-3.710870	1.830352	-1.545562
24	1	0	-3.069939	-2.419455	-1.792275
25	1	0	-3.951960	-0.314395	-2.790818
26	6	0	0.692233	1.351543	0.917237
27	6	0	-1.522598	-0.225954	2.047771
28	1	0	-1.927043	0.582343	2.669229
29	1	0	-1.707766	-1.157044	2.597672

SCF Energy: -1715.94582876 a.u.

Table S3. Cartesian coordinates of minimized **3a**.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.350420	3.206375	0.569106
2	6	0	0.408328	2.097133	0.851895
3	6	0	-0.297799	0.889543	0.595577
4	6	0	-1.581968	1.104388	0.121446
5	16	0	-1.941617	2.791537	-0.016876
6	1	0	-0.077838	4.248674	0.672849
7	1	0	1.422293	2.148102	1.232353
8	6	0	-2.348684	-0.104429	-0.133786
9	16	0	-3.963268	-0.394986	-0.685761
10	6	0	-2.472035	-2.441032	-0.099174
11	6	0	-3.729689	-2.119071	-0.548081
12	1	0	-2.143321	-3.461510	0.065794
13	1	0	-4.542986	-2.787477	-0.799459
14	15	0	0.021852	-0.910198	0.713551
15	6	0	2.526695	-0.782958	-0.585139
16	6	0	2.961218	0.243365	-1.437021
17	6	0	3.414301	-1.274501	0.386017
18	6	0	4.253514	0.764560	-1.328963
19	1	0	2.284831	0.634652	-2.194109
20	6	0	4.705119	-0.752937	0.495429
21	1	0	3.084022	-2.054664	1.066226
22	6	0	5.130405	0.267103	-0.361612
23	1	0	4.573608	1.555832	-2.002431
24	1	0	5.379245	-1.144362	1.253171
25	1	0	6.136962	0.668840	-0.277067
26	6	0	-1.677519	-1.285512	0.137695
27	6	0	1.127118	-1.341466	-0.711899
28	1	0	0.643356	-0.991200	-1.630711
29	1	0	1.140622	-2.438922	-0.742709
30	8	0	0.479759	-1.486647	2.023259

SCF Energy: -1791.16321614 a.u.

Table S4. Cartesian coordinates of minimized **3a-rot**.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.695629	-3.083688	-0.572392
2	6	0	1.216152	-2.649301	0.639360
3	6	0	1.039263	-1.238815	0.668830
4	6	0	1.393357	-0.625995	-0.521324
5	16	0	1.941690	-1.771324	-1.696015
6	1	0	1.931564	-4.095390	-0.876130
7	1	0	1.017352	-3.314602	1.472872
8	6	0	1.267812	0.822664	-0.520949
9	16	0	1.612603	2.045749	-1.694677
10	6	0	0.746290	2.785046	0.640668
11	6	0	1.144942	3.295687	-0.570576
12	1	0	0.435166	3.406055	1.473946
13	1	0	1.203104	4.332979	-0.874035
14	15	0	0.472312	0.023291	1.868591
15	6	0	-2.181529	-0.173997	0.738802
16	6	0	-2.705267	1.005408	0.187579
17	6	0	-2.433965	-1.387382	0.080350
18	6	0	-3.455500	0.975427	-0.990203
19	1	0	-2.527156	1.955422	0.686442
20	6	0	-3.182973	-1.421328	-1.097994
21	1	0	-2.043364	-2.313931	0.494785
22	6	0	-3.695652	-0.238948	-1.638871
23	1	0	-3.855161	1.900588	-1.397974
24	1	0	-3.369202	-2.372509	-1.590450
25	1	0	-4.282004	-0.264488	-2.553754
26	6	0	0.813939	1.365202	0.669602
27	6	0	-1.375168	-0.138643	2.014201
28	1	0	-1.673385	0.702178	2.652528
29	1	0	-1.525316	-1.048573	2.608434
30	8	0	1.126380	0.078011	3.220384

SCF Energy: -1791.19105562 a.u.

Table S5. Cartesian coordinates of minimized **4a**.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.471272	3.208644	0.867232
2	6	0	0.314363	2.092438	1.013781
3	6	0	-0.356570	0.914007	0.586760
4	6	0	-1.643243	1.153597	0.129992
5	16	0	-2.046320	2.835177	0.212140
6	1	0	-0.227267	4.234935	1.109408
7	1	0	1.320802	2.116035	1.415742
8	6	0	-2.375736	-0.032592	-0.271740
9	16	0	-3.978550	-0.304041	-0.867963
10	6	0	-2.433703	-2.363698	-0.501288
11	6	0	-3.695610	-2.025772	-0.924476
12	1	0	-2.077038	-3.386385	-0.444837
13	1	0	-4.487782	-2.683228	-1.258587
14	15	0	0.005623	-0.878974	0.514487
15	6	0	2.502617	-0.554312	-0.827874
16	6	0	2.815670	0.696718	-1.381455
17	6	0	3.505164	-1.257905	-0.142181
18	6	0	4.099247	1.233454	-1.254795
19	1	0	2.050498	1.251736	-1.919947
20	6	0	4.788157	-0.721396	-0.013216
21	1	0	3.274382	-2.223456	0.299000
22	6	0	5.089965	0.525433	-0.568716
23	1	0	4.325139	2.201043	-1.696152
24	1	0	5.552319	-1.279479	0.521777
25	1	0	6.090176	0.939910	-0.471555
26	6	0	-1.675569	-1.219893	-0.130339
27	6	0	1.114661	-1.126775	-0.972940
28	1	0	0.589460	-0.683323	-1.826662
29	1	0	1.144062	-2.212353	-1.123001
30	16	0	0.580623	-1.795043	2.157388

SCF Energy: -2114.15866674 a.u.

Table S6. Cartesian coordinates of minimized **5a**.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.952843	1.783353	2.670267
2	6	0	0.078725	1.163818	1.812697
3	6	0	0.771738	0.373494	0.853869
4	6	0	2.157293	0.416463	0.995047
5	16	0	2.619758	1.420094	2.315622
6	1	0	0.719919	2.443996	3.495405
7	1	0	-0.996976	1.281241	1.863435
8	6	0	2.899784	-0.355443	0.013177
9	16	0	4.575932	-0.643294	-0.261969
10	6	0	2.866279	-1.773926	-1.865259
11	6	0	4.214268	-1.658762	-1.630094
12	1	0	2.454554	-2.364775	-2.676011
13	1	0	5.027258	-2.110538	-2.183816
14	15	0	0.379605	-0.693939	-0.541265
15	6	0	-1.909575	-2.159707	0.327043
16	6	0	-2.284537	-1.755250	1.617491
17	6	0	-2.908384	-2.489956	-0.601172
18	6	0	-3.633553	-1.670719	1.967464
19	1	0	-1.521283	-1.526876	2.357975
20	6	0	-4.258376	-2.407104	-0.250139
21	1	0	-2.634410	-2.839180	-1.594932
22	6	0	-4.623373	-1.992437	1.033393
23	1	0	-3.911169	-1.368121	2.973281
24	1	0	-5.021157	-2.678804	-0.974393
25	1	0	-5.672336	-1.936137	1.309872
26	6	0	2.112376	-1.021502	-0.921562
27	6	0	-0.449898	-2.277220	-0.050503
28	1	0	0.158536	-2.670792	0.772061
29	1	0	-0.314779	-2.953659	-0.903830
30	6	0	-0.541265	0.148879	-1.924451
31	1	0	-1.232555	-0.598195	-2.330136
32	1	0	0.213847	0.352243	-2.691282
33	6	0	-1.268358	1.419379	-1.533187
34	6	0	-0.629065	2.659941	-1.669374
35	6	0	-2.586580	1.375806	-1.056682
36	6	0	-1.296303	3.839996	-1.333909
37	1	0	0.387922	2.708521	-2.052998
38	6	0	-3.251995	2.557173	-0.719435
39	1	0	-3.100212	0.422484	-0.959293
40	6	0	-2.608703	3.790600	-0.855760
41	1	0	-0.794500	4.795865	-1.455262
42	1	0	-4.276950	2.513110	-0.361659
43	1	0	-3.130882	4.708649	-0.601442

SCF Energy: -1986.76994080 a.u.

Table S7. Cartesian coordinates of minimized **5a-rot**.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.039098	-1.215320	3.198403
2	6	0	0.694533	-0.592948	2.219281
3	6	0	0.064463	-0.711837	0.949130
4	6	0	-1.136029	-1.416637	0.989050
5	16	0	-1.498415	-1.944897	2.587345
6	1	0	0.189145	-1.292867	4.253643
7	1	0	1.633607	-0.086141	2.407664
8	6	0	-1.811802	-1.551265	-0.290208
9	16	0	-3.263646	-2.327135	-0.796663
10	6	0	-1.837149	-1.113542	-2.602817
11	6	0	-2.991473	-1.840232	-2.446992
12	1	0	-1.505134	-0.726566	-3.559878
13	1	0	-3.707970	-2.122441	-3.207670
14	15	0	0.348835	-0.184066	-0.746854
15	6	0	-0.763907	2.380351	-0.309995
16	6	0	-1.961516	2.586800	-1.010033
17	6	0	-0.640235	2.881072	0.994118
18	6	0	-3.018525	3.277913	-0.414143
19	1	0	-2.066830	2.221105	-2.029082
20	6	0	-1.697478	3.571473	1.590087
21	1	0	0.289338	2.745710	1.542782
22	6	0	-2.889632	3.768868	0.888017
23	1	0	-3.937466	3.440524	-0.970290
24	1	0	-1.585894	3.962167	2.597600
25	1	0	-3.709738	4.311911	1.349009
26	6	0	-1.161666	-0.946146	-1.361705
27	6	0	0.391717	1.651143	-0.959013
28	1	0	0.424737	1.824945	-2.042501
29	1	0	1.357067	1.975629	-0.553065
30	6	0	1.856407	-0.938554	-1.511509
31	1	0	1.808362	-0.699439	-2.581281
32	1	0	1.724539	-2.021821	-1.413358
33	6	0	3.158031	-0.468842	-0.895958
34	6	0	3.714361	-1.154974	0.194447
35	6	0	3.836949	0.640824	-1.422515
36	6	0	4.923186	-0.732526	0.752724
37	1	0	3.212947	-2.032703	0.596027
38	6	0	5.045051	1.063347	-0.863015
39	1	0	3.436644	1.163559	-2.289069
40	6	0	5.588386	0.379502	0.228110
41	1	0	5.351222	-1.280122	1.587733
42	1	0	5.566334	1.916745	-1.287268
43	1	0	6.532087	0.702463	0.658107

SCF-Energy: -1986.77424553 a.u.

Table S8. Cartesian coordinates of minimized **5b**.

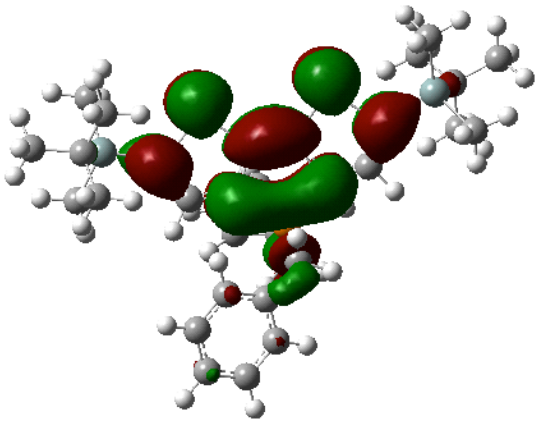
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.784027	-1.386316	0.231311
2	6	0	-2.455946	-0.041692	0.213283
3	6	0	-1.084547	0.198283	-0.070827
4	6	0	-0.347690	-0.969278	-0.262352
5	16	0	-1.351997	-2.354475	-0.098772
6	1	0	-3.183769	0.740801	0.399032
7	6	0	1.065699	-0.769355	-0.528645
8	16	0	2.384064	-1.816260	-0.878089
9	6	0	2.857269	0.721008	-0.841580
10	6	0	3.515202	-0.479035	-1.050369
11	1	0	3.361857	1.679730	-0.908116
12	15	0	0.041868	1.592736	-0.212197
13	6	0	-1.596409	3.515363	-1.496673
14	6	0	-2.819925	2.990764	-1.940216
15	6	0	-1.570173	4.802416	-0.937664
16	6	0	-3.994942	3.736567	-1.819882
17	1	0	-2.852467	2.004408	-2.397216
18	6	0	-2.745477	5.547403	-0.816329
19	1	0	-0.625484	5.237419	-0.616952
20	6	0	-3.960966	5.014393	-1.254352
21	1	0	-4.933376	3.324071	-2.179920
22	1	0	-2.708638	6.547029	-0.392497
23	1	0	-4.873758	5.596899	-1.168148
24	6	0	1.477806	0.560823	-0.541254
25	6	0	-0.321292	2.712683	-1.641304
26	1	0	-0.345343	2.061656	-2.522338
27	1	0	0.554588	3.365524	-1.744152
28	6	0	0.179107	2.601165	1.330284
29	1	0	-0.746902	3.184618	1.390289
30	1	0	0.995671	3.312365	1.150450
31	6	0	0.410668	1.791702	2.587292
32	6	0	1.708689	1.430396	2.976193
33	6	0	-0.673141	1.412299	3.392014
34	6	0	1.918537	0.698975	4.146976
35	1	0	2.560968	1.730202	2.370642
36	6	0	-0.463355	0.681360	4.563106
37	1	0	-1.683928	1.699784	3.111153
38	6	0	0.832723	0.321048	4.941635
39	1	0	2.929622	0.432879	4.442292
40	1	0	-1.310614	0.402281	5.183303
41	1	0	0.996634	-0.242419	5.855836
42	6	0	6.388421	-0.825352	0.156890
43	6	0	5.468698	-2.383846	-2.432978
44	6	0	5.876837	0.689780	-2.566201
45	1	0	4.858573	-2.340633	-3.343346
46	1	0	6.502036	-2.580933	-2.742966
47	1	0	5.135535	-3.250541	-1.849353
48	1	0	6.932242	0.602416	-2.851471

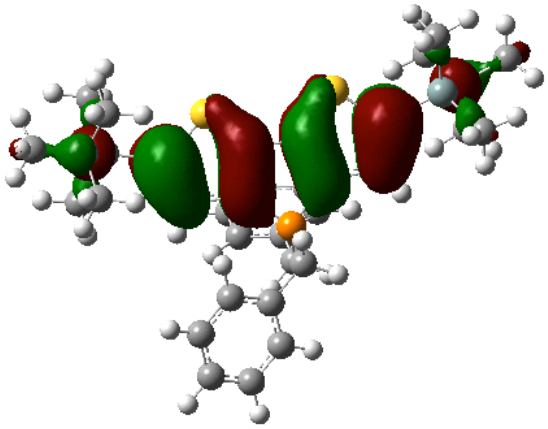
49	1	0	5.288347	0.705879	-3.491406
50	1	0	5.753846	1.661789	-2.073736
51	6	0	-4.164341	-3.855528	1.390229
52	6	0	-5.383026	-1.026646	1.765044
53	6	0	-5.452894	-2.376415	-1.087721
54	1	0	-3.630938	-4.555610	0.736183
55	1	0	-3.569121	-3.733448	2.303305
56	1	0	-5.107327	-4.335373	1.678340
57	1	0	-5.554371	-0.029163	1.343171
58	1	0	-6.362844	-1.436034	2.038925
59	1	0	-4.808752	-0.905813	2.691386
60	6	0	-4.695632	-3.312266	-2.055218
61	1	0	-3.702156	-2.925304	-2.314908
62	1	0	-4.568557	-4.320864	-1.643264
63	1	0	-5.257477	-3.417217	-2.994400
64	6	0	-6.844240	-2.982817	-0.789034
65	1	0	-7.407776	-3.107724	-1.724698
66	1	0	-6.774436	-3.972494	-0.321287
67	1	0	-7.445323	-2.340349	-0.134035
68	6	0	-5.640127	-1.000652	-1.763226
69	1	0	-6.207668	-0.303543	-1.133785
70	1	0	-4.678392	-0.532477	-2.009261
71	1	0	-6.198267	-1.114325	-2.703578
72	6	0	6.288311	0.517821	0.911486
73	1	0	5.254761	0.750098	1.199374
74	1	0	6.881752	0.477601	1.836260
75	1	0	6.673551	1.356596	0.318621
76	6	0	7.869411	-1.091649	-0.201311
77	1	0	8.292664	-0.303555	-0.836200
78	1	0	8.476219	-1.129678	0.714490
79	1	0	8.003689	-2.049851	-0.717070
80	6	0	5.883121	-1.958319	1.076589
81	1	0	4.841388	-1.806036	1.385612
82	1	0	5.953394	-2.943440	0.599220
83	1	0	6.491697	-2.000638	1.991334
84	14	0	5.360356	-0.761688	-1.469037
85	14	0	-4.488680	-2.185908	0.567354

SCF-Energy: -3040.01529667 a.u.

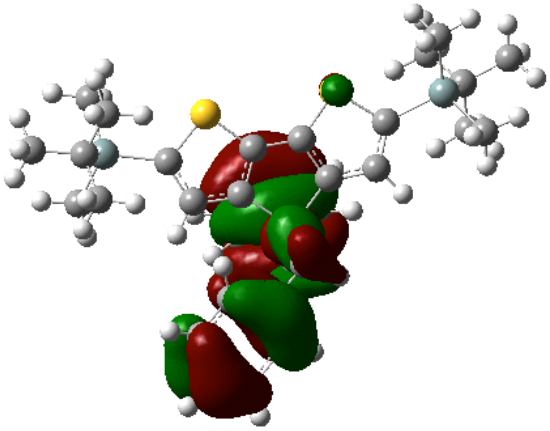
Figure S2. Frontier orbitals of **5b'**.



LUMO; *E* = -2.94 eV

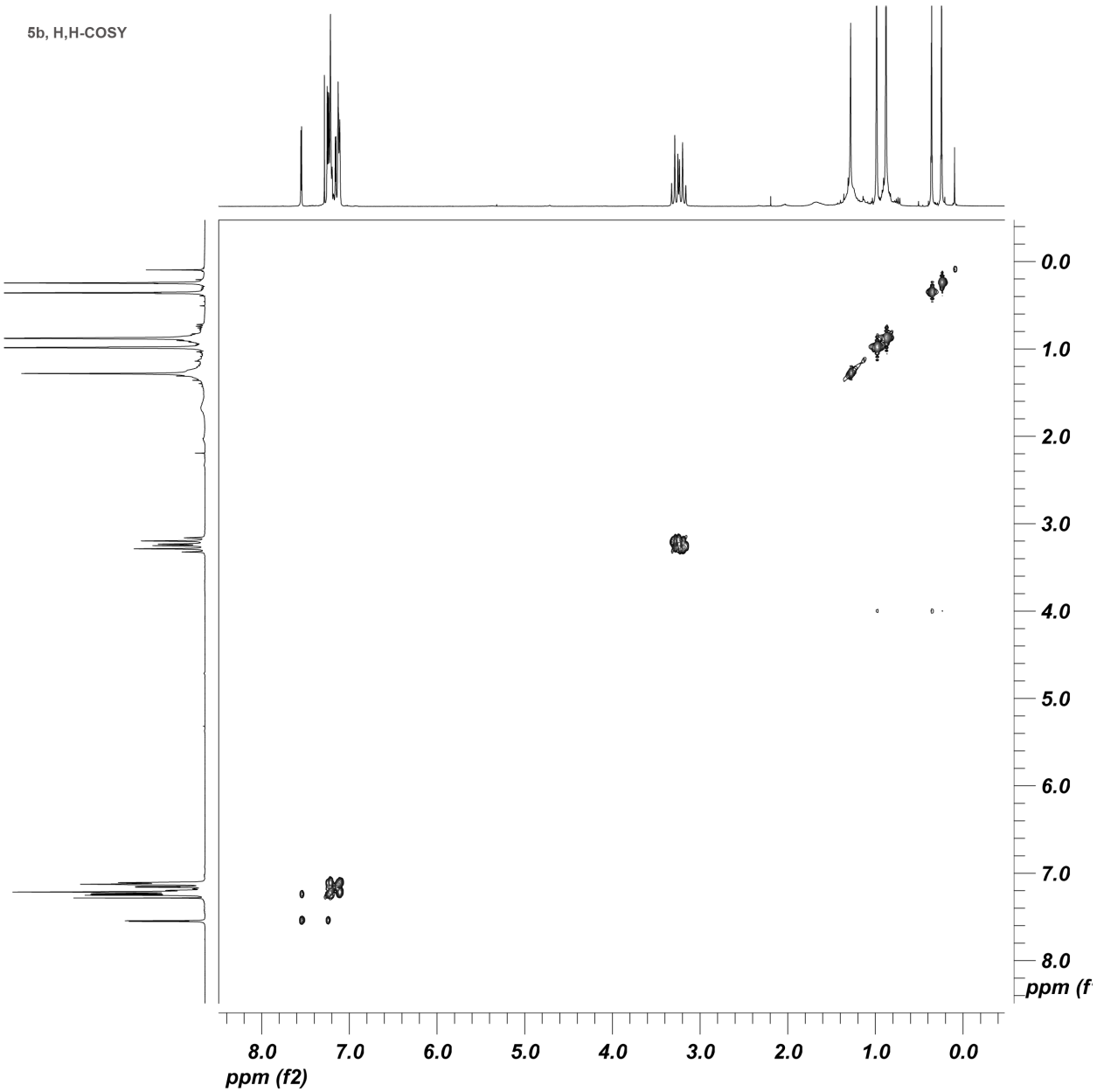


HOMO; *E* = -6.58 eV

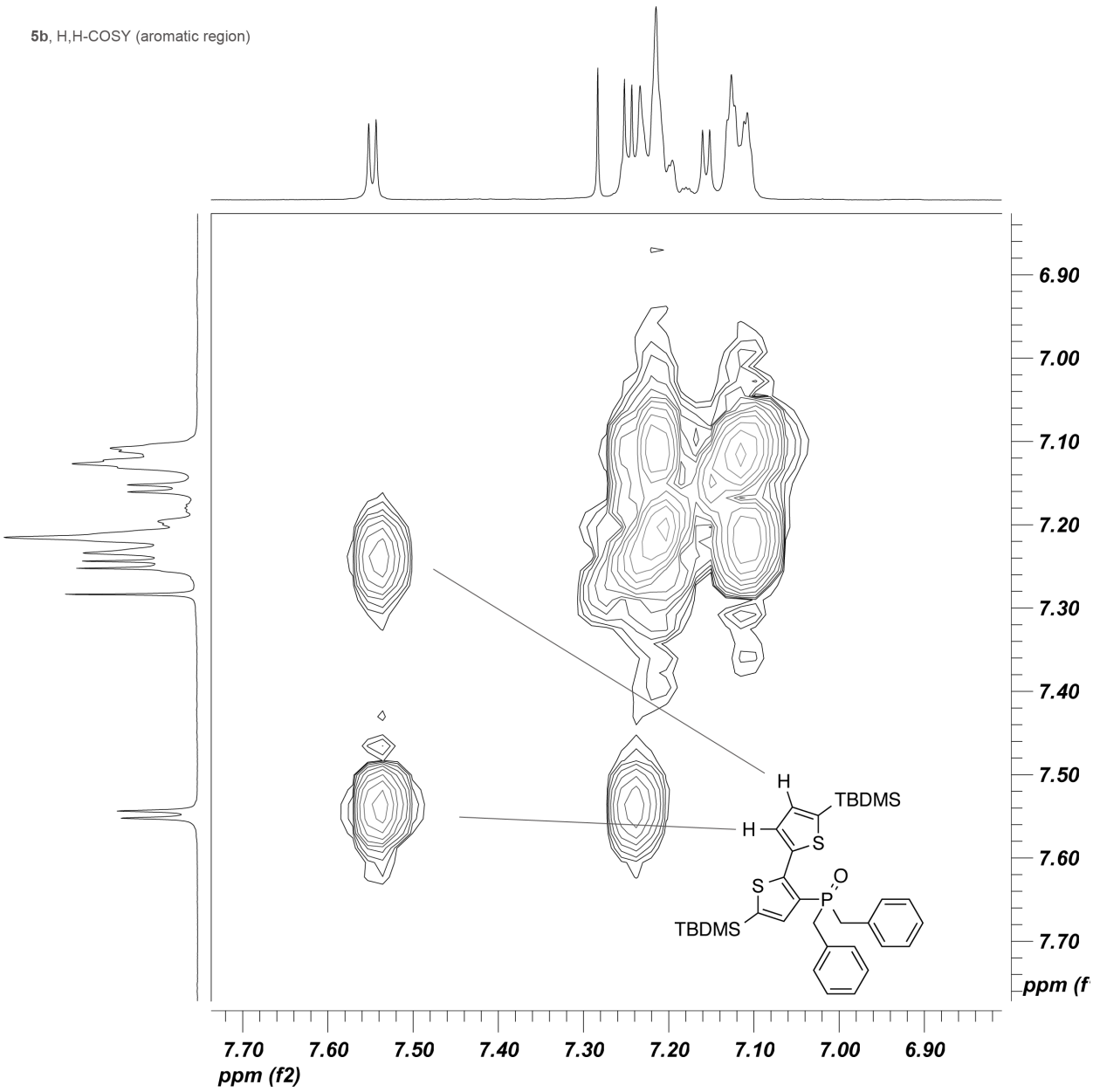


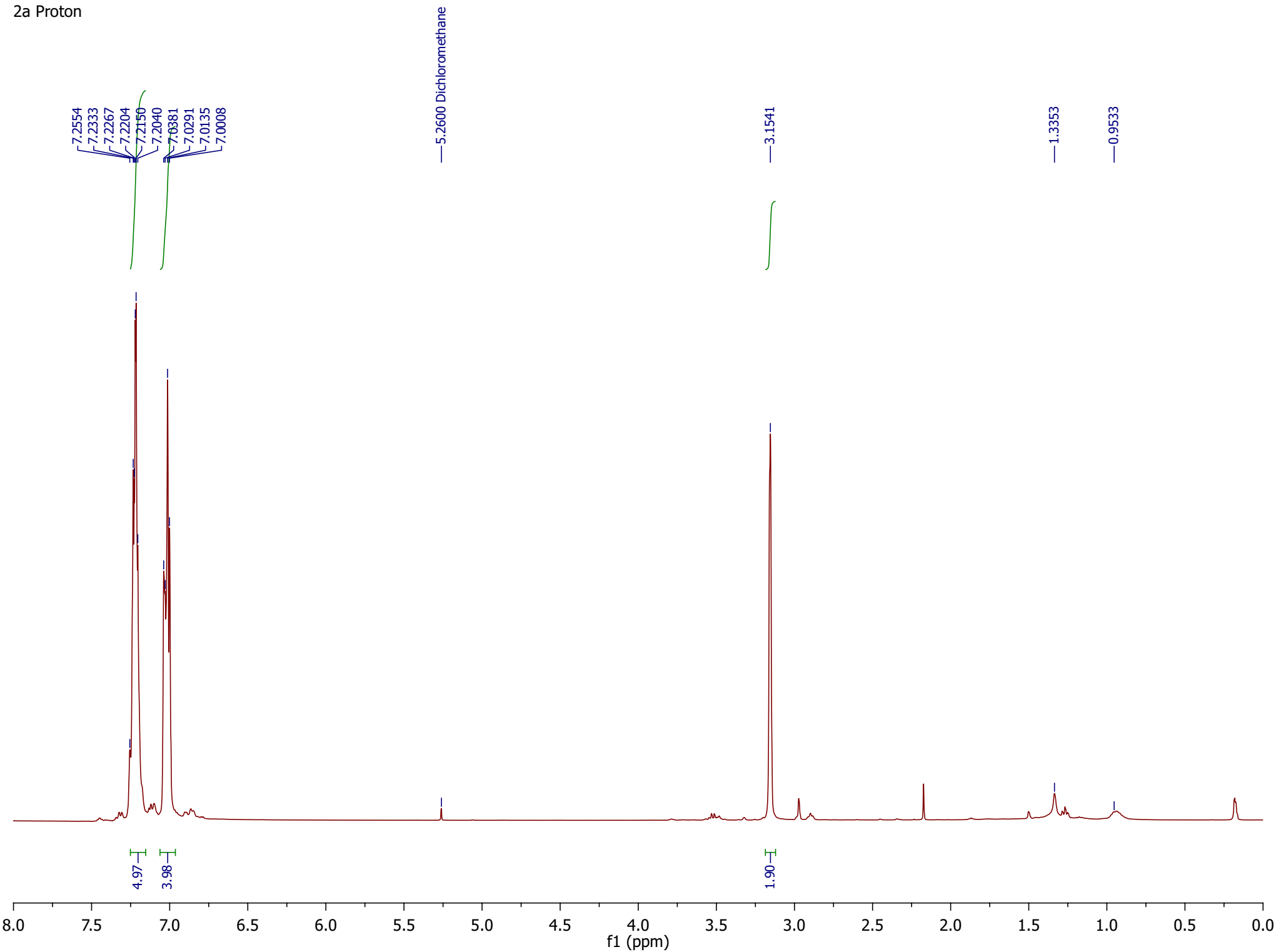
HOMO-1; *E* = -7.34 eV

Figure S3. ^{1}H, $^{13}C\{^{1}H\}$, and $^{31}P\{^{1}H\}$ NMR spectra of **2a,b – 5a,b** and $^{1}H,^{1}H$-COSY of **5b**.

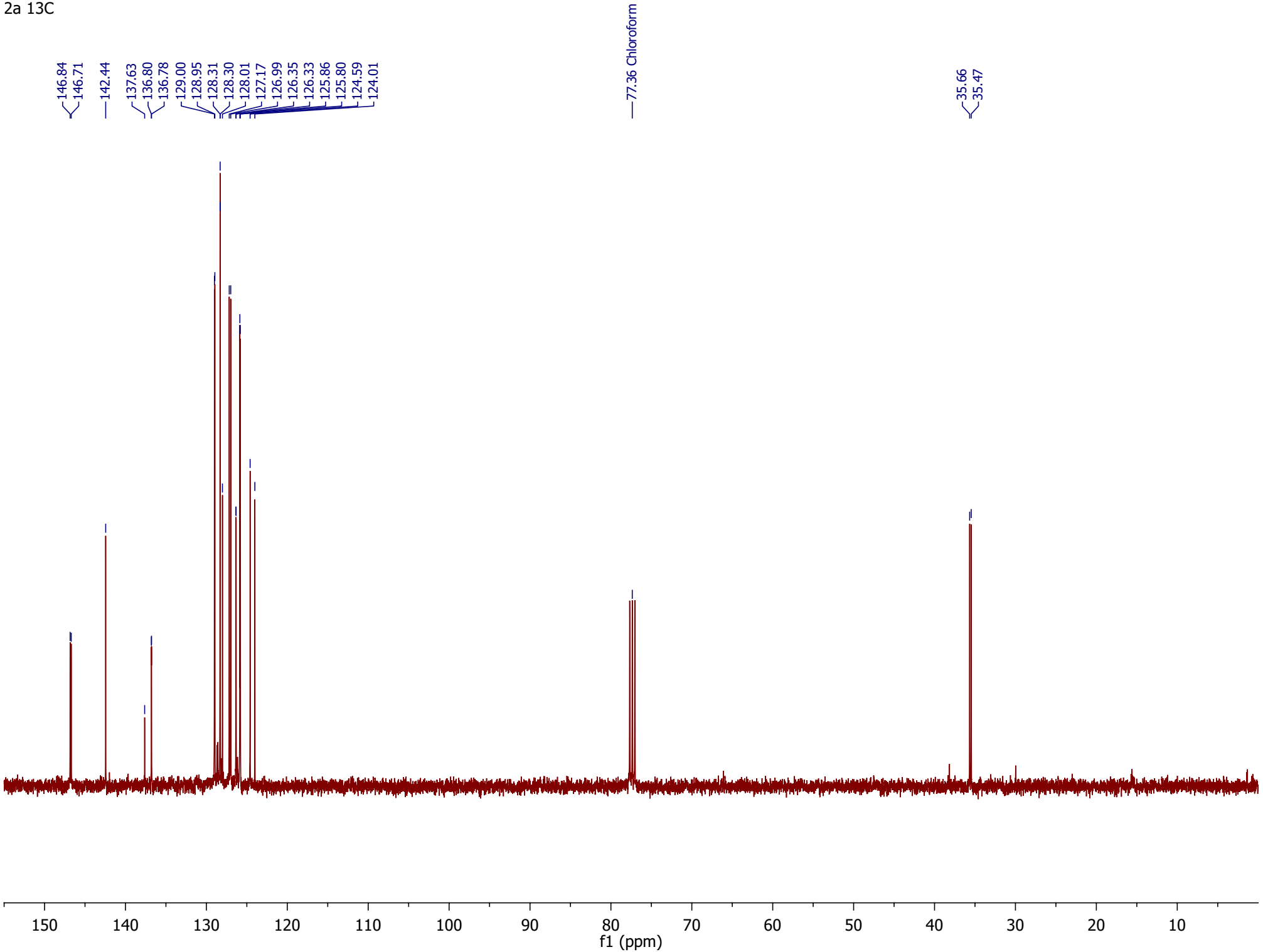


5b, H,H-COSY (aromatic region)

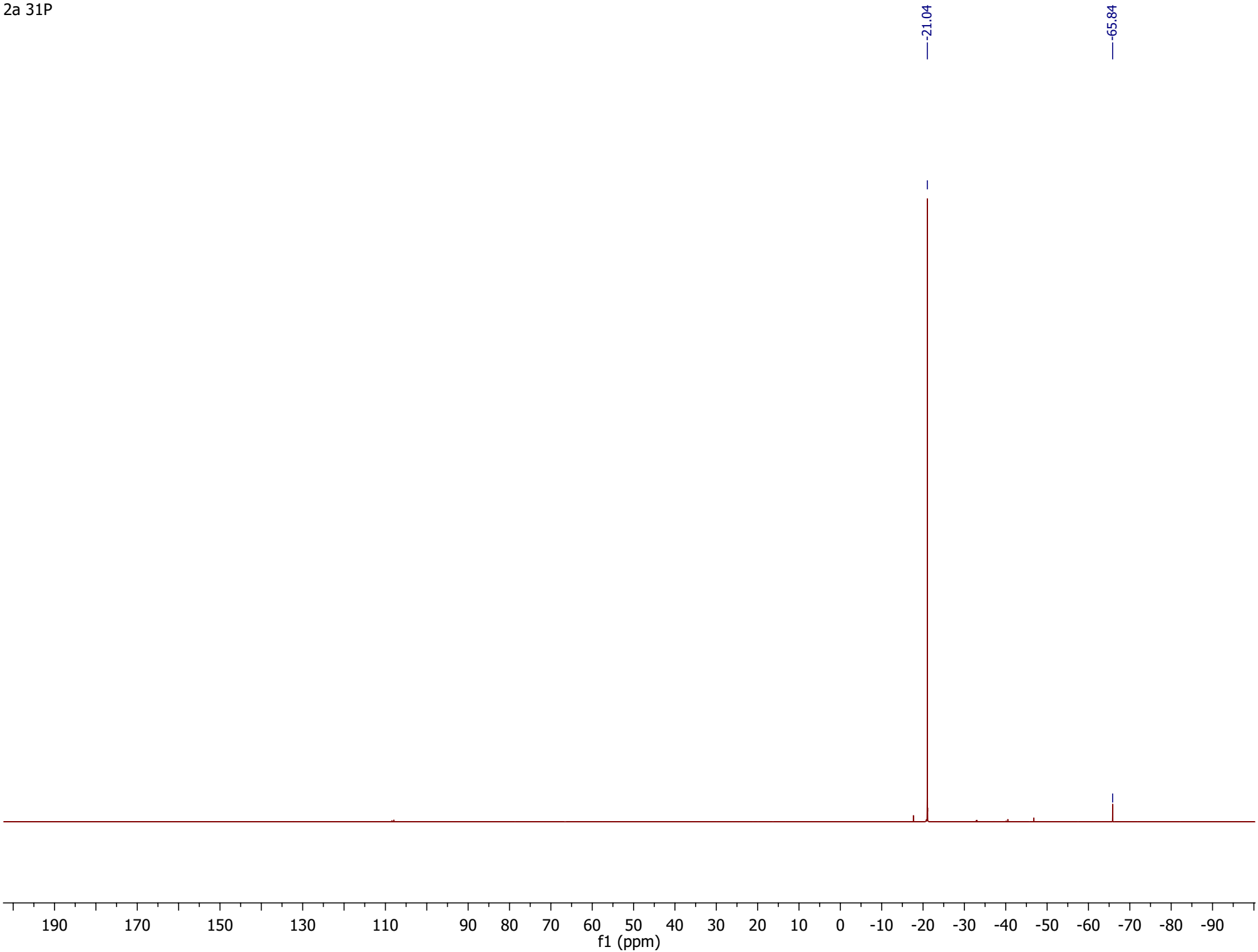


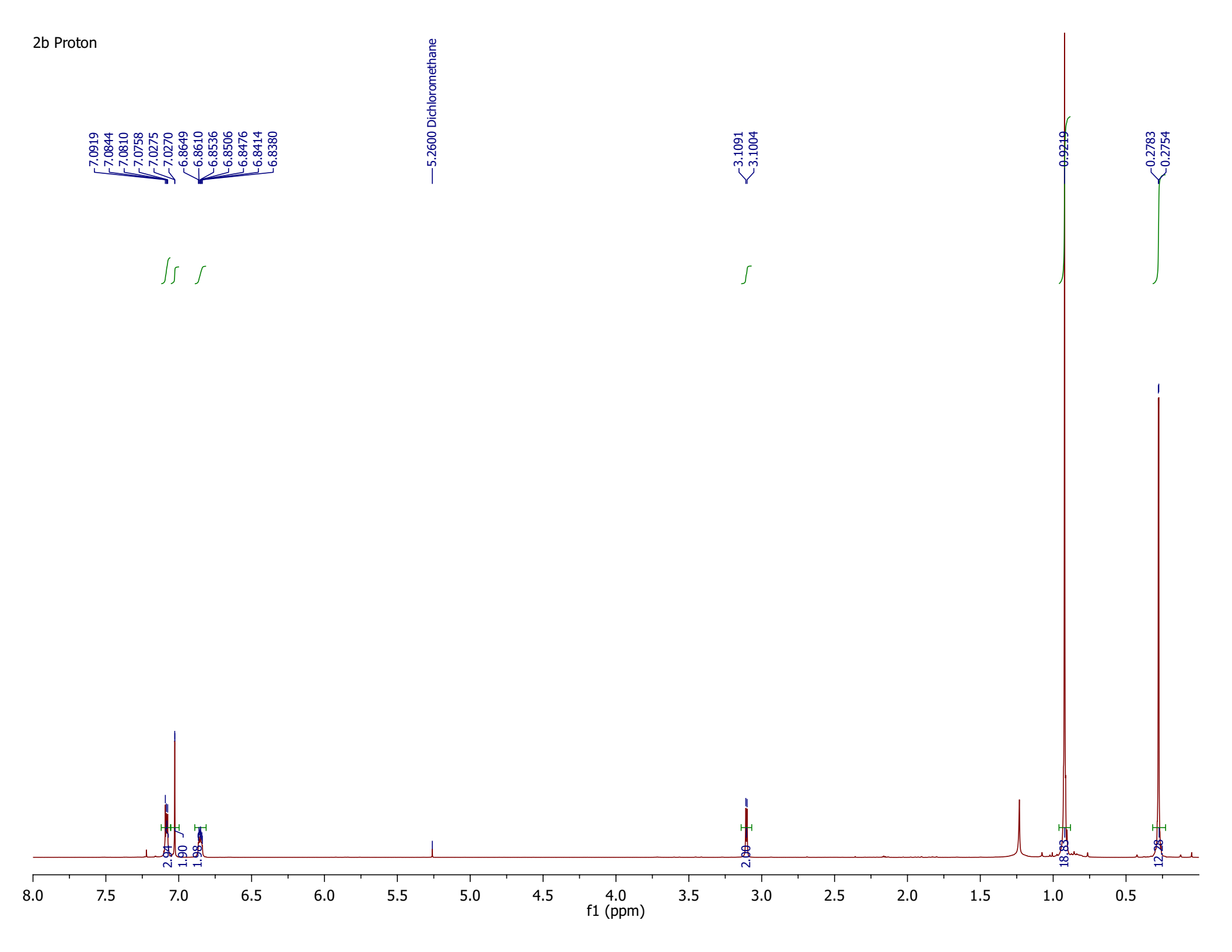

2a Proton
7.2554
7.2333
7.2267
7.2204
7.2150
7.2040
7.0381
7.0291
7.0135
7.0008
5.2600 Dichloromethane
3.1541
1.3353
0.9533
4.97
3.98
1.90
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

2a 13C

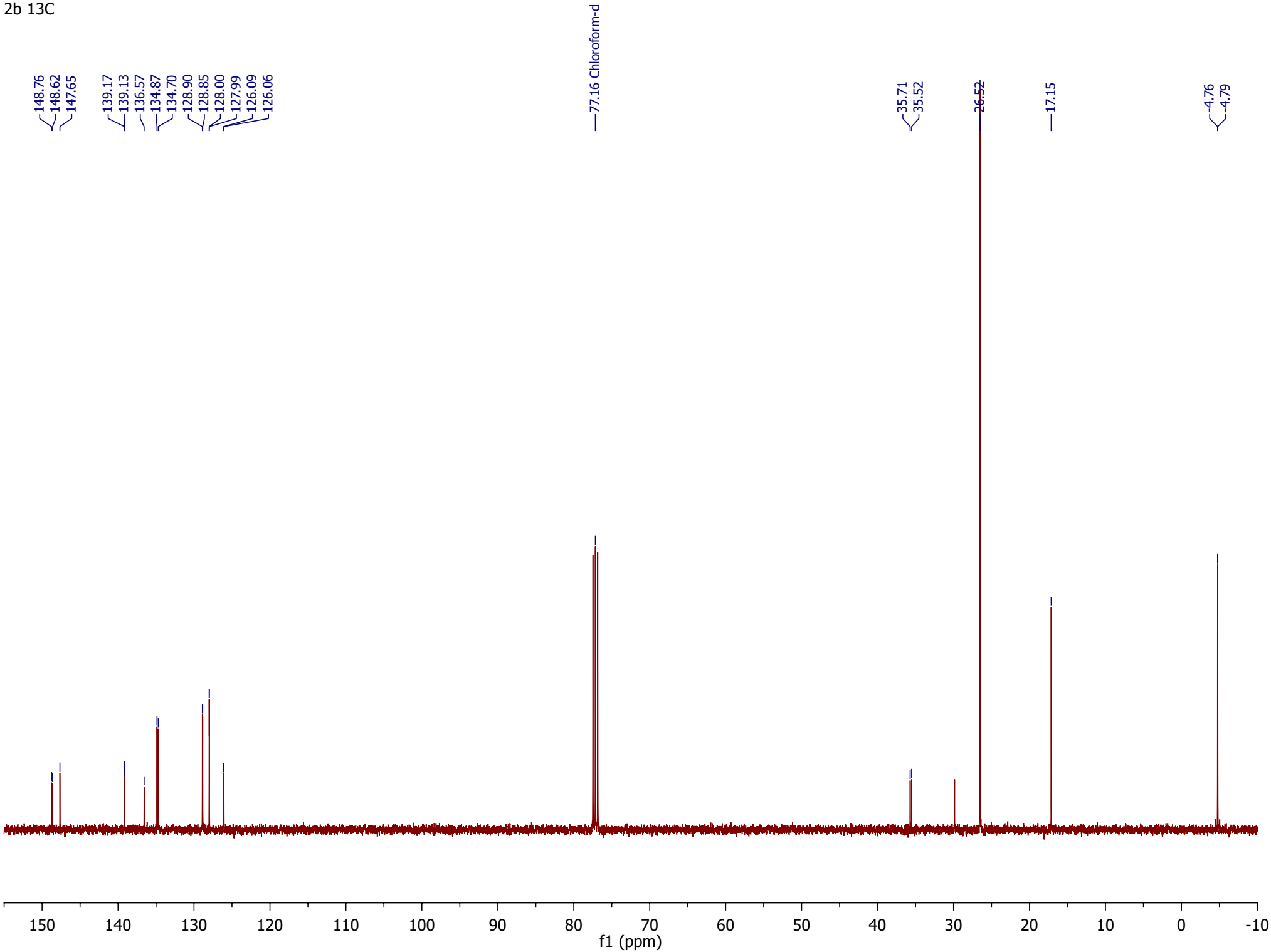

146.84
146.71
142.44
137.63
136.80
136.78
129.00
128.95
128.31
128.30
128.01
127.17
126.99
126.35
126.33
125.86
125.80
124.59
124.01
77.36 Chloroform
35.66
35.47
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

2a 31P

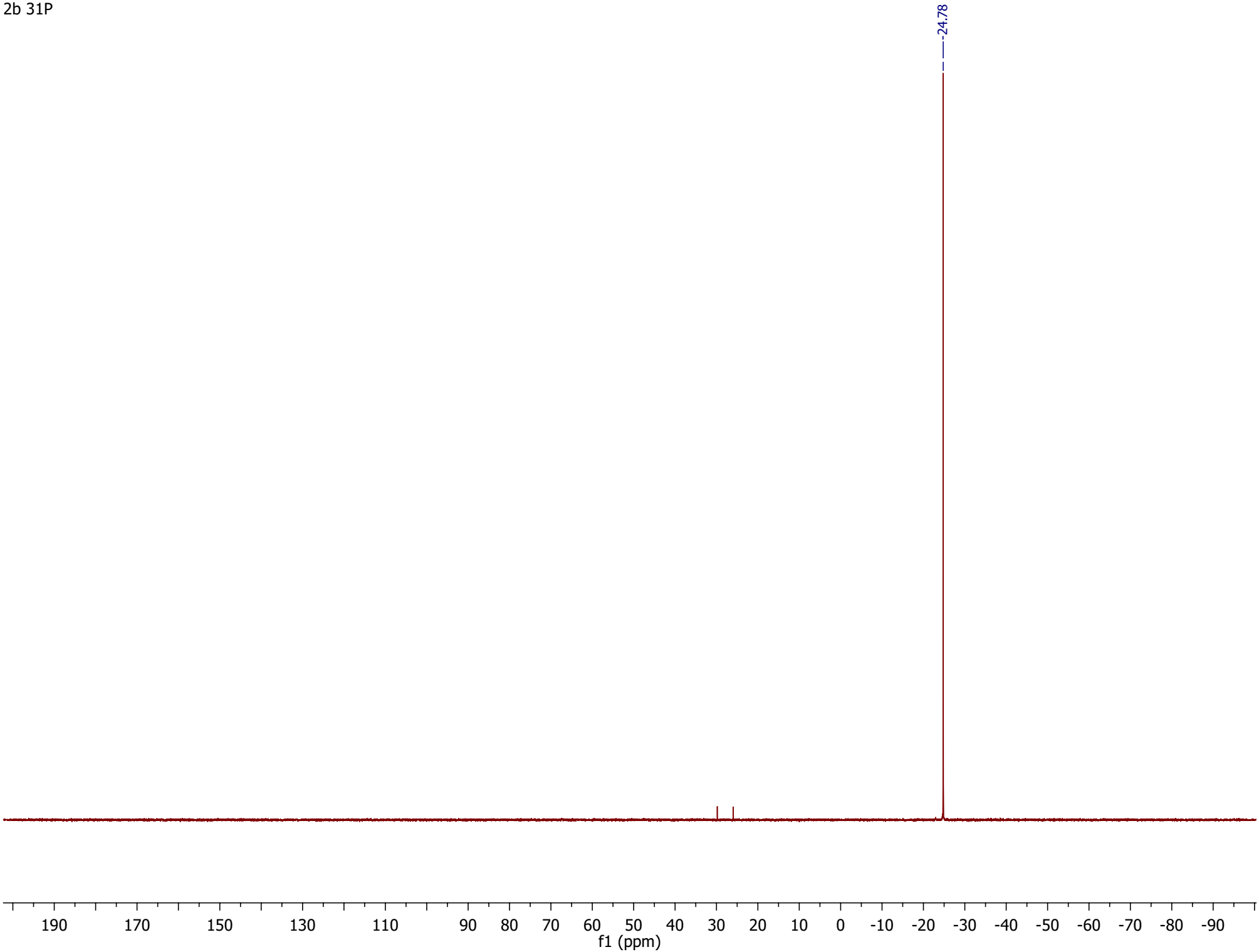

-21.04
-65.84
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

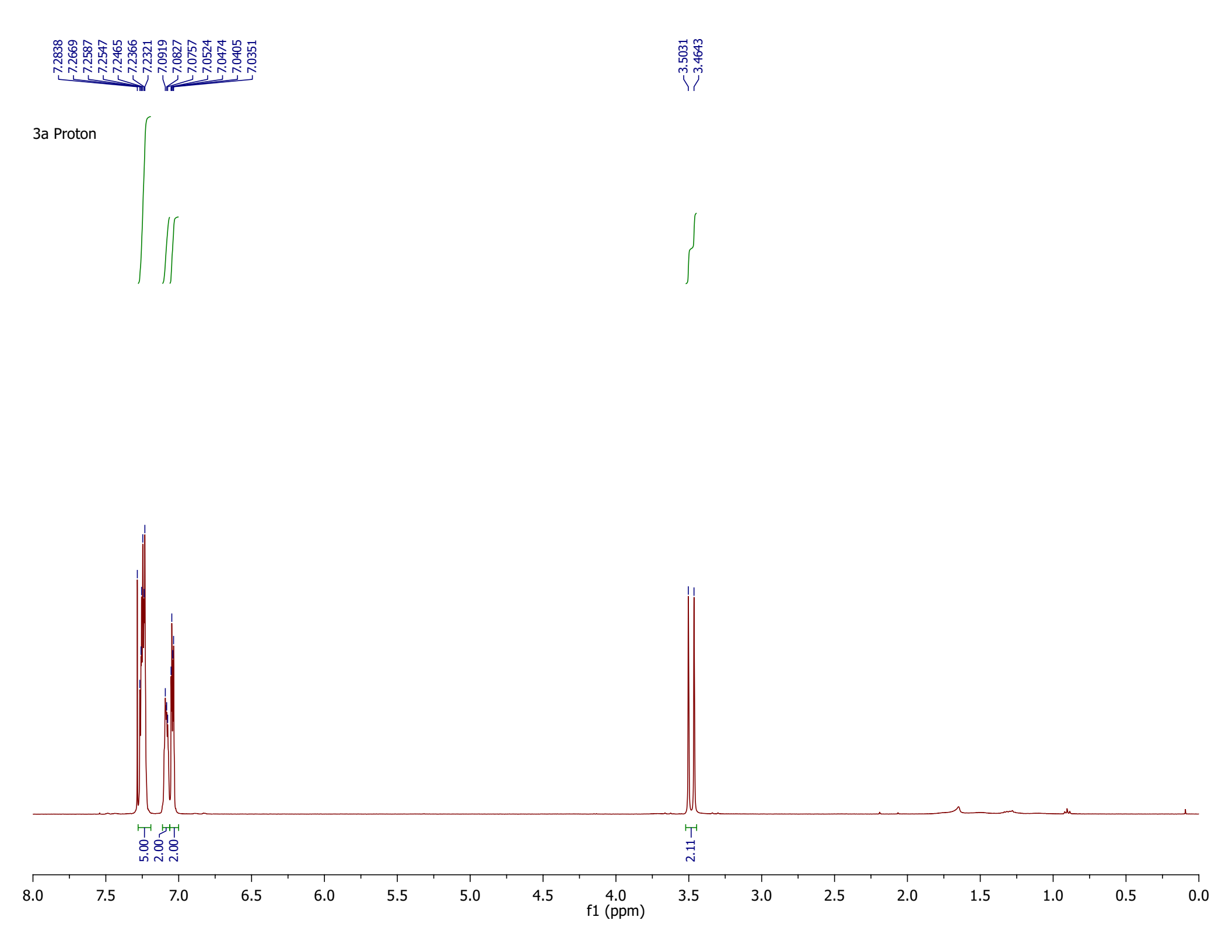

2b Proton
7.0919
7.0844
7.0810
7.0758
7.0275
7.0270
6.8649
6.8610
6.8536
6.8506
6.8476
6.8414
6.8380
5.2600 Dichloromethane
3.1091
3.1004
0.9219
0.2783
0.2754
2.94
1.90
1.98
2.00
18.83
12.28
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

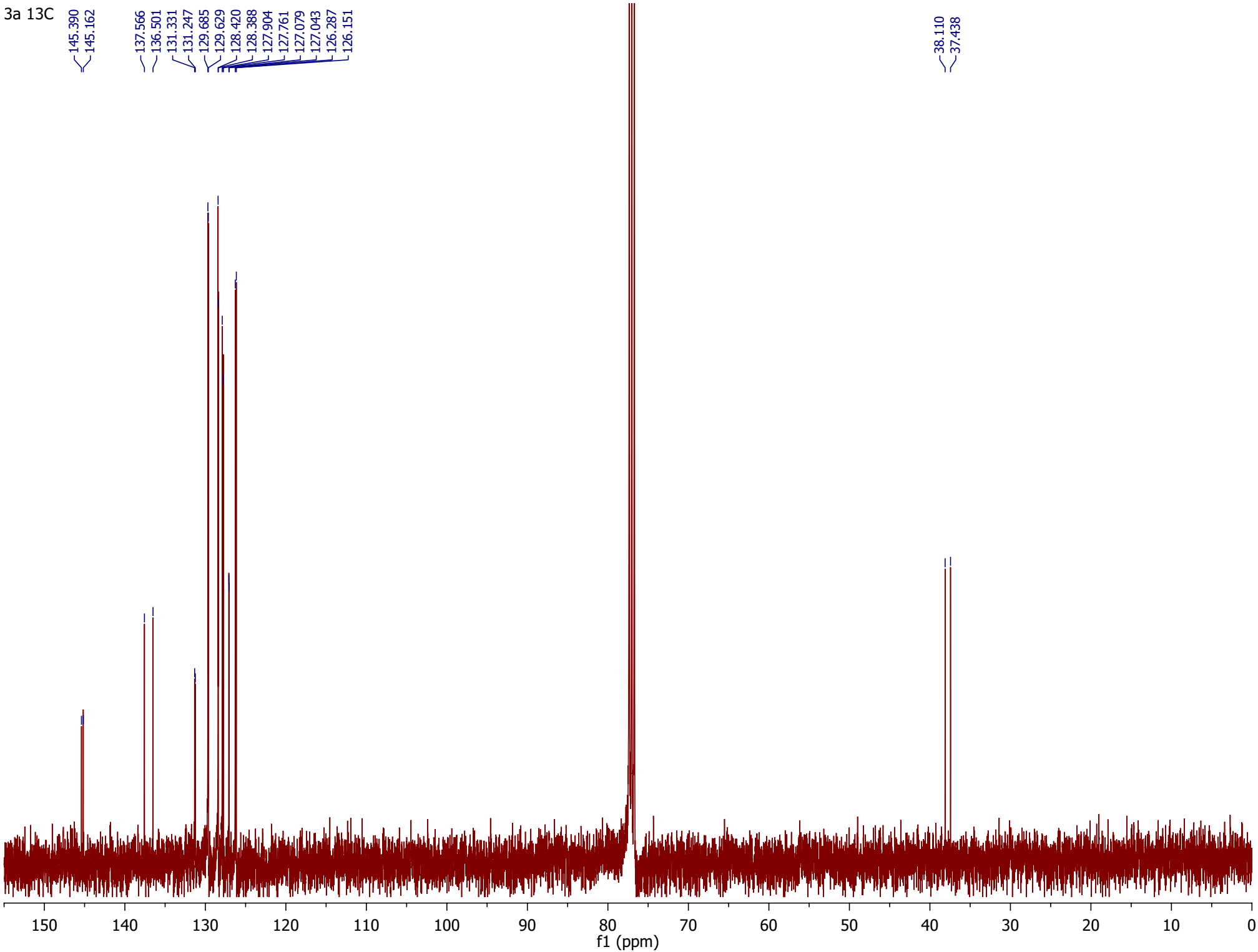
2b 13C


148.76
148.62
147.65
139.17
139.13
136.57
134.87
134.70
128.90
128.85
128.00
127.99
126.09
126.06
77.16 Chloroform-d
35.71
35.52
26.52
17.15
-4.76
-4.79
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

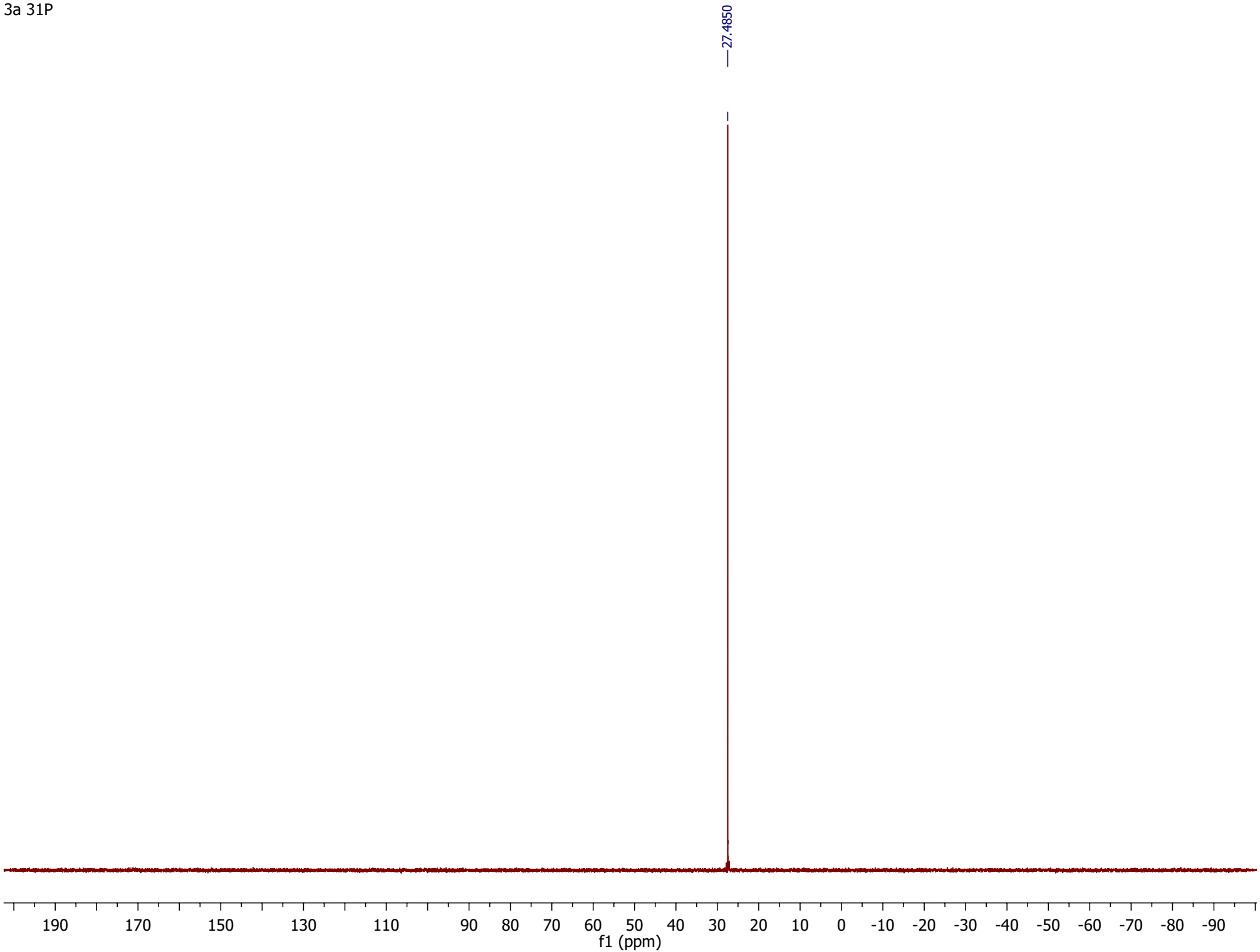
2b 31P

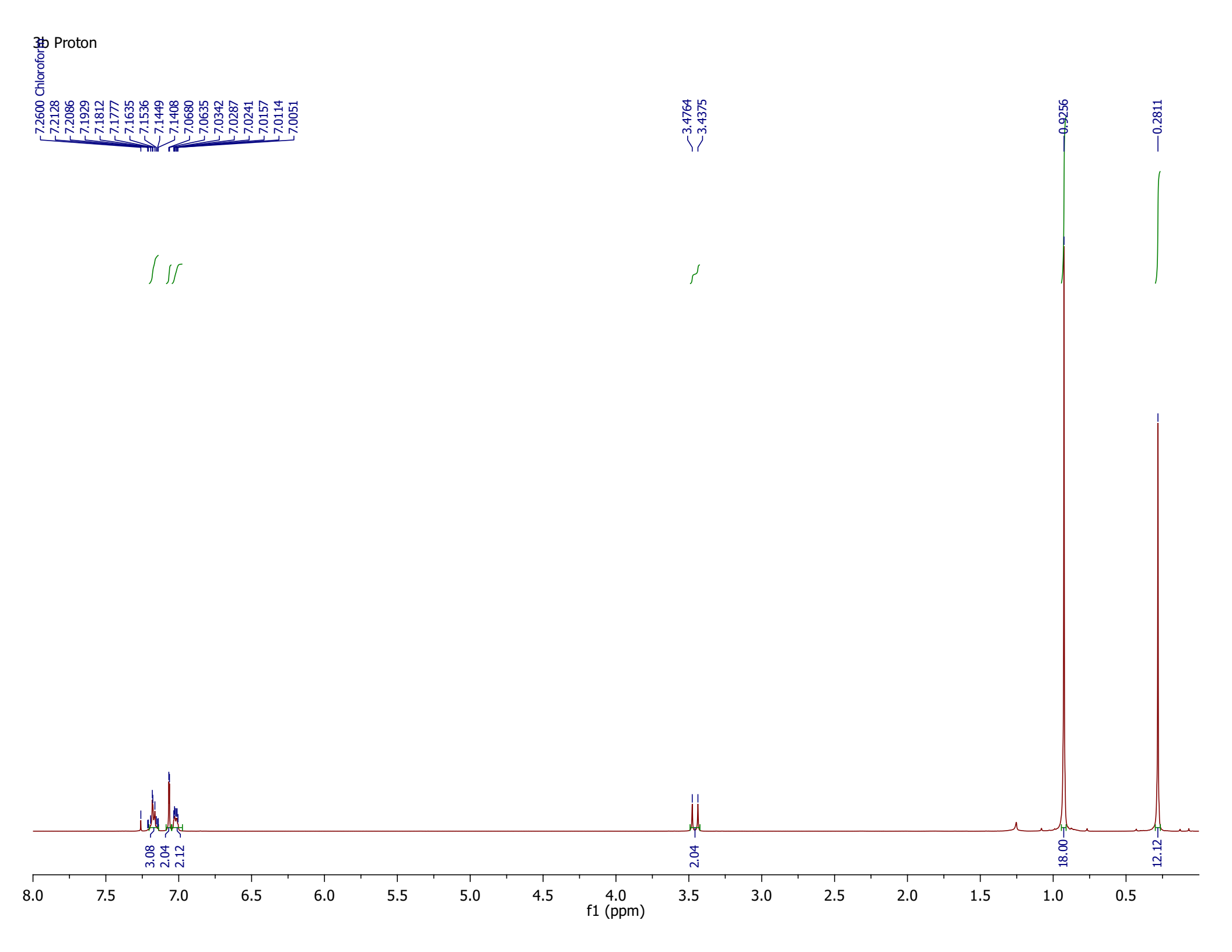

-24.78
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

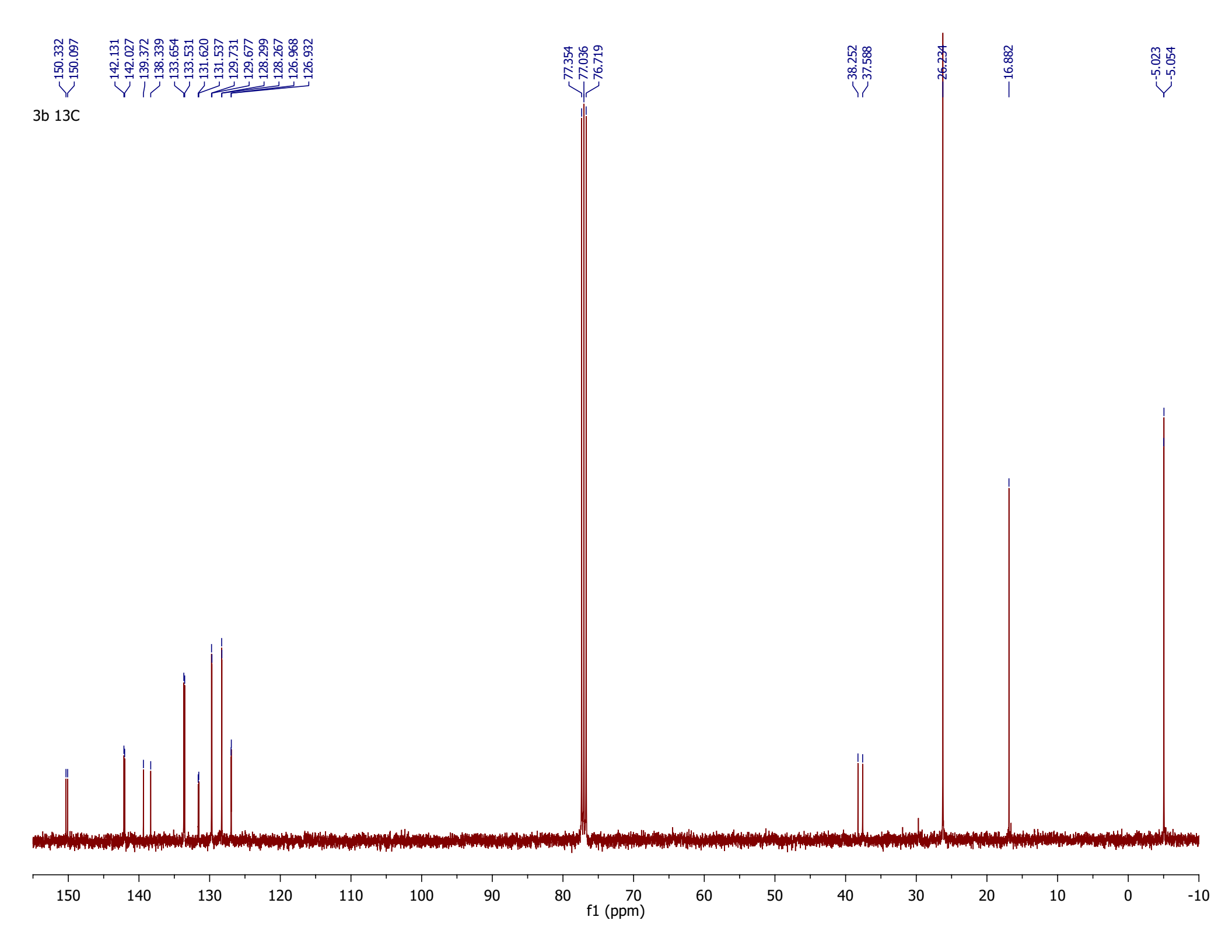

7.2838
7.2669
7.2587
7.2547
7.2465
7.2366
7.2321
7.0919
7.0827
7.0757
7.0524
7.0474
7.0405
7.0351
3.5031
3.4643
3a Proton
5.00
2.00
2.00
2.11
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


3a 13C
145.390
145.162
137.566
136.501
131.331
131.247
129.685
129.629
128.420
128.388
127.904
127.761
127.079
127.043
126.287
126.151
38.110
37.438
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

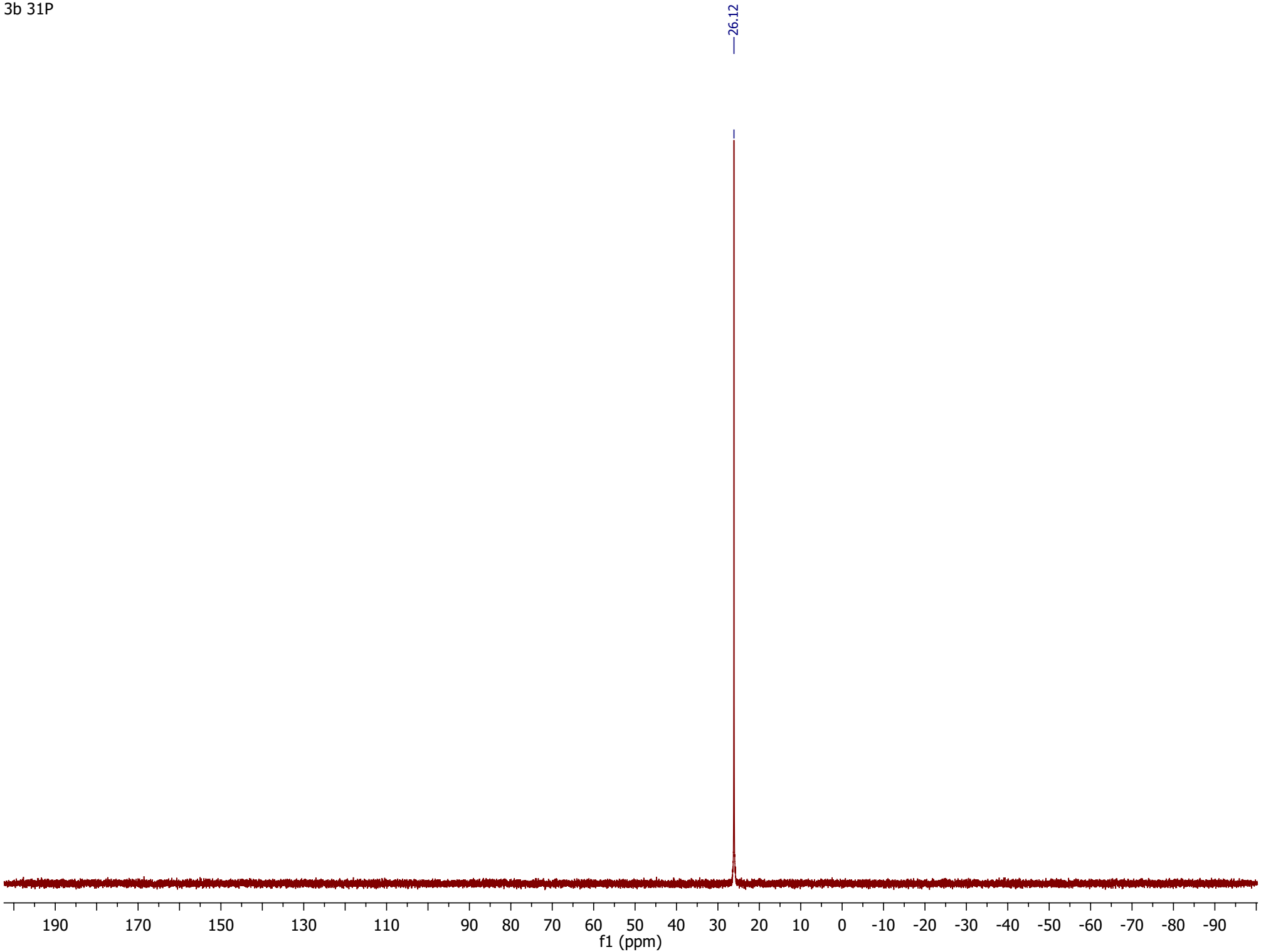
3a 31P

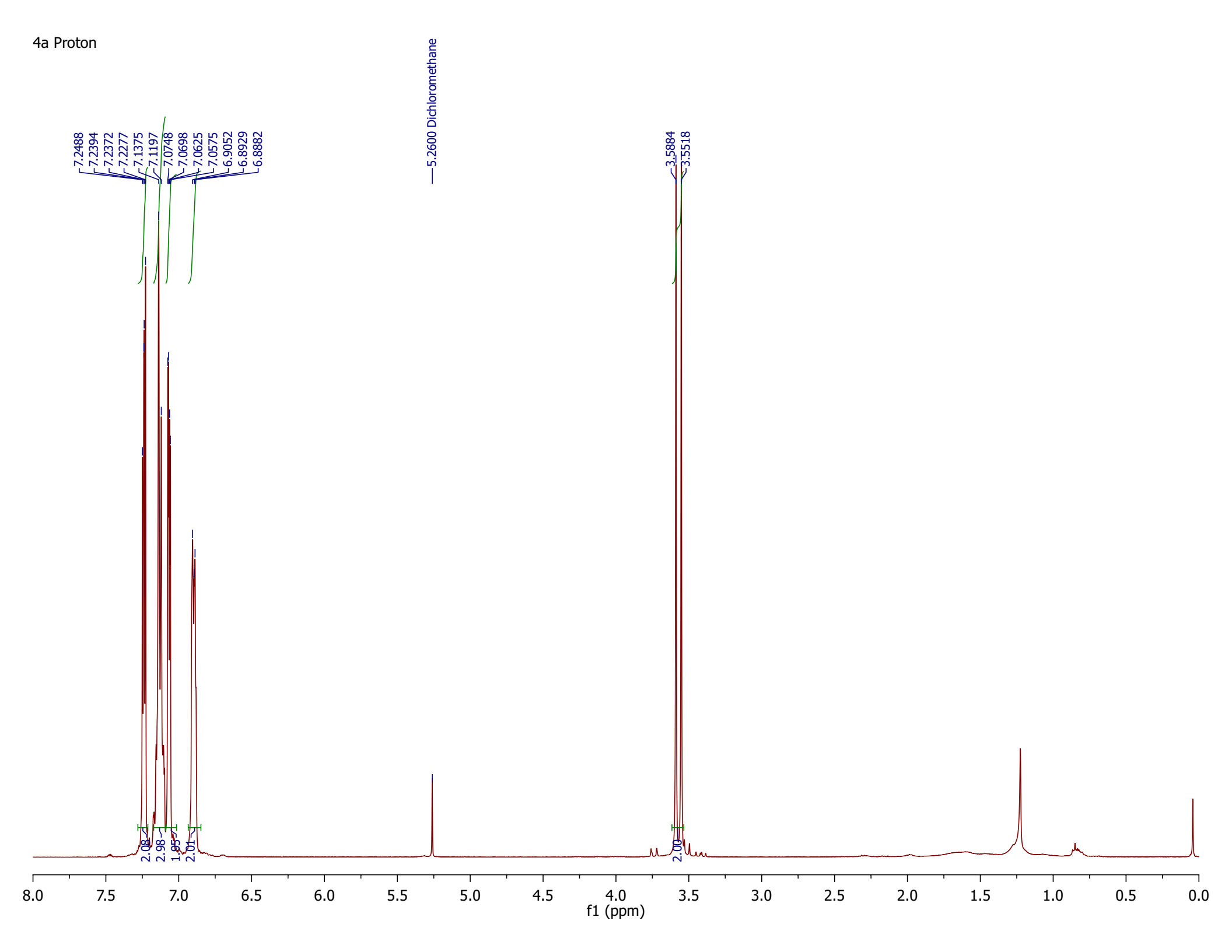

27.4850
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

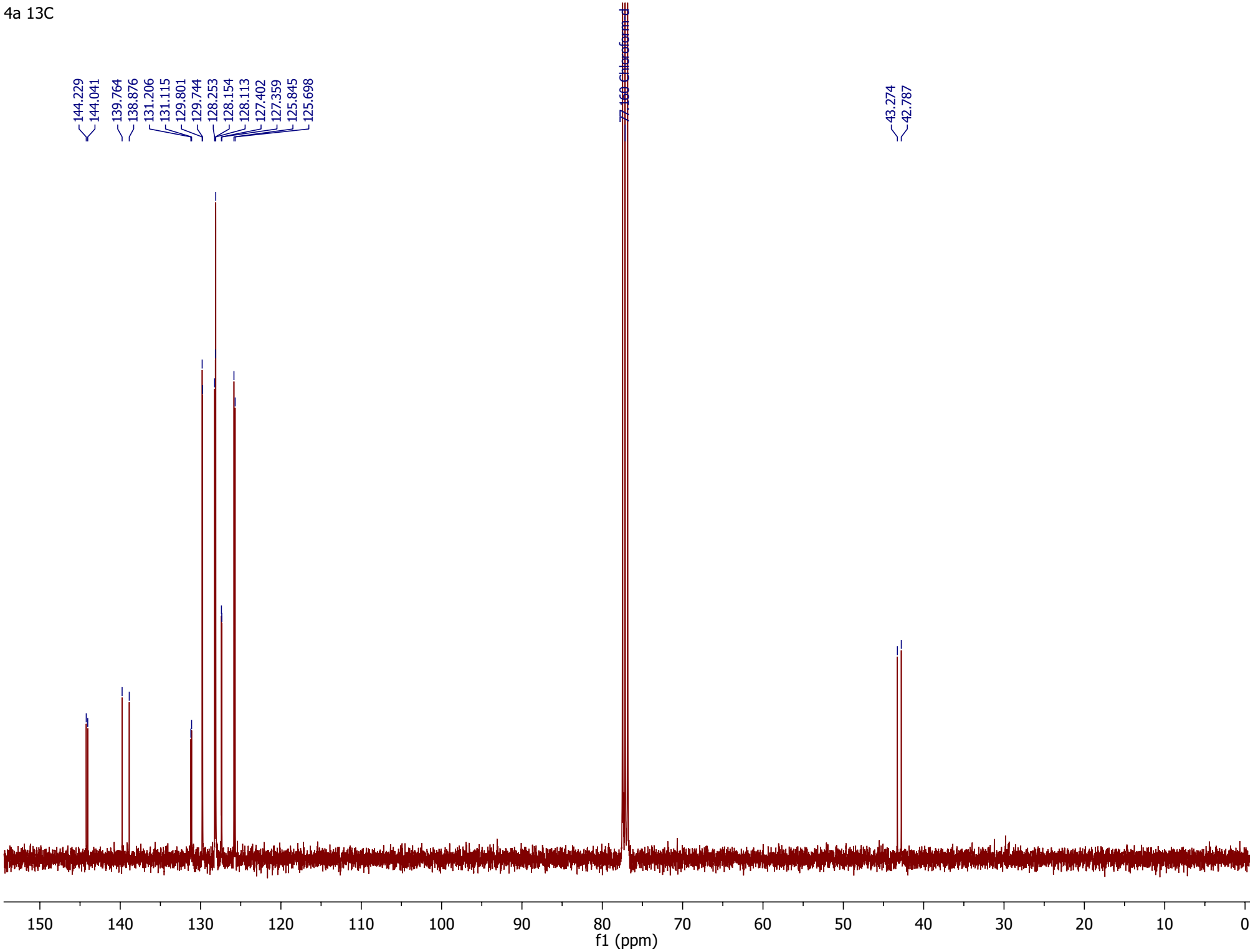

3b Proton
7.2600 Chloroform
7.2128
7.2086
7.1929
7.1812
7.1777
7.1635
7.1536
7.1449
7.1408
7.0680
7.0635
7.0342
7.0287
7.0241
7.0157
7.0114
7.0051
3.4764
3.4375
0.9256
0.2811
3.08
2.04
2.12
2.04
18.00
12.12
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


150.332
150.097
142.131
142.027
139.372
138.339
133.654
133.531
131.620
131.537
129.731
129.677
128.299
128.267
126.968
126.932
77.354
77.036
76.719
38.252
37.588
26.234
16.882
-5.023
-5.054
3b 13C
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

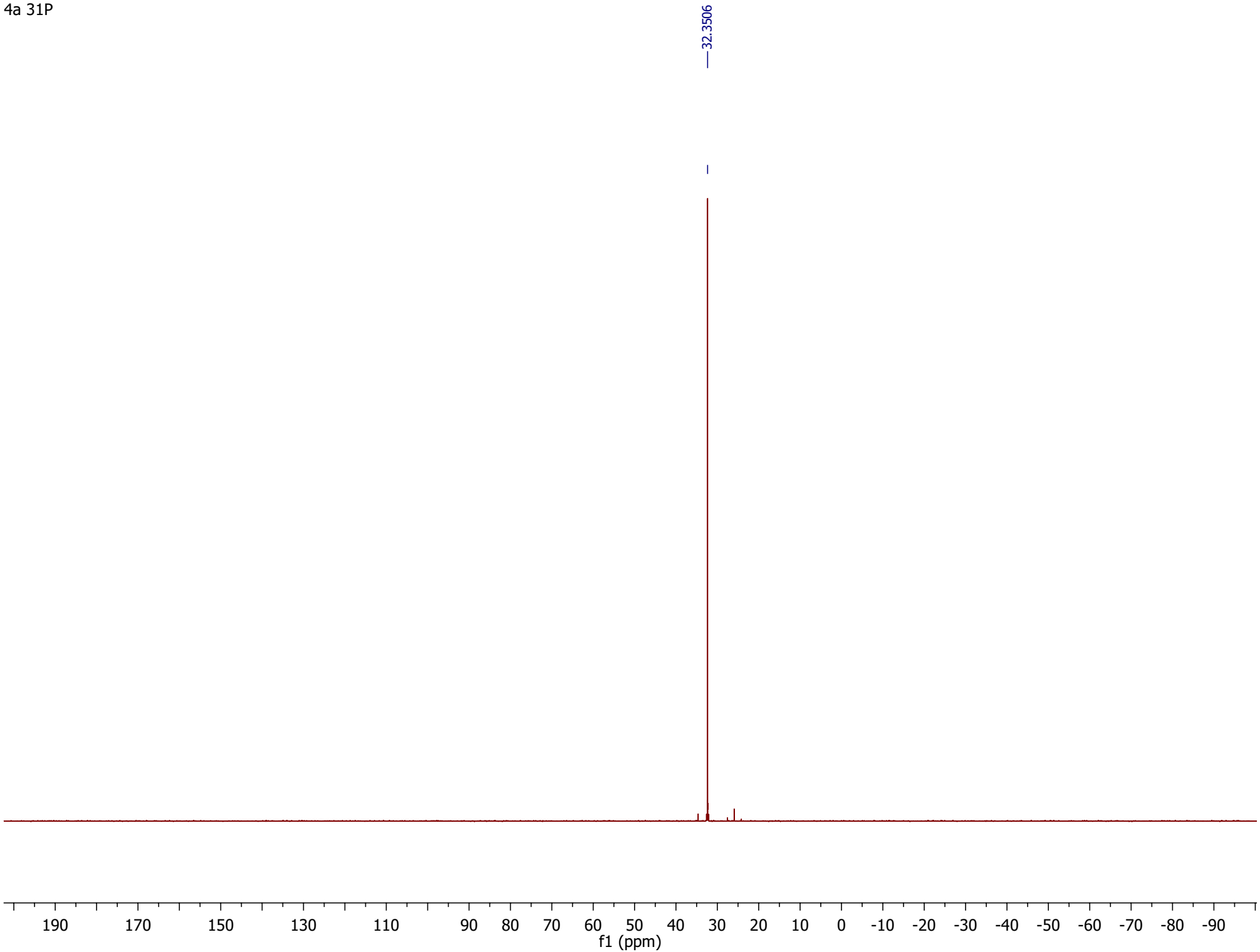
3b 31P

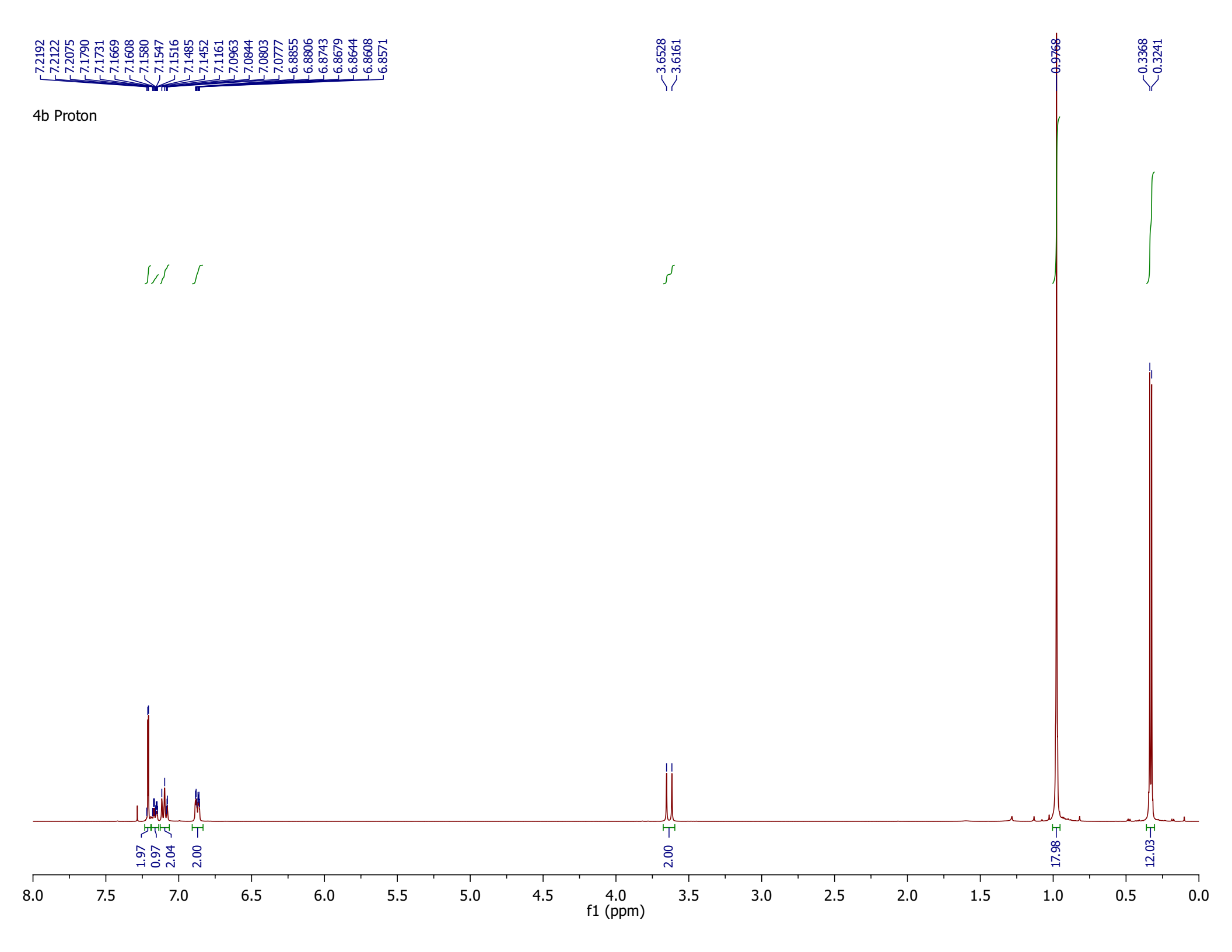

26.12
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

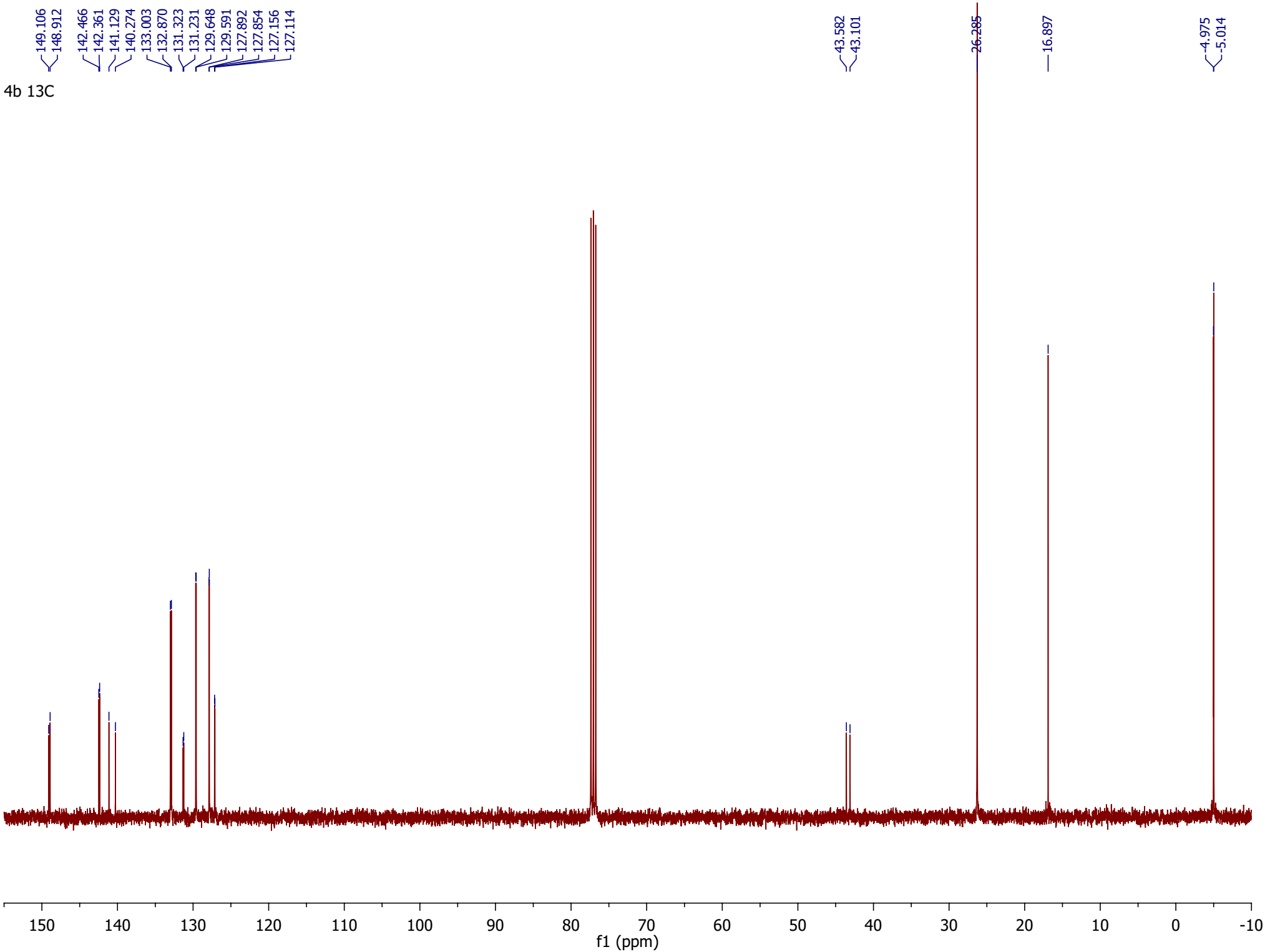

4a Proton
7.2488
7.2394
7.2372
7.2277
7.1375
7.1197
7.0748
7.0698
7.0625
7.0575
6.9052
6.8929
6.8882
5.2600 Dichloromethane
3.5884
3.5518
2.08
2.98
1.95
2.01
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

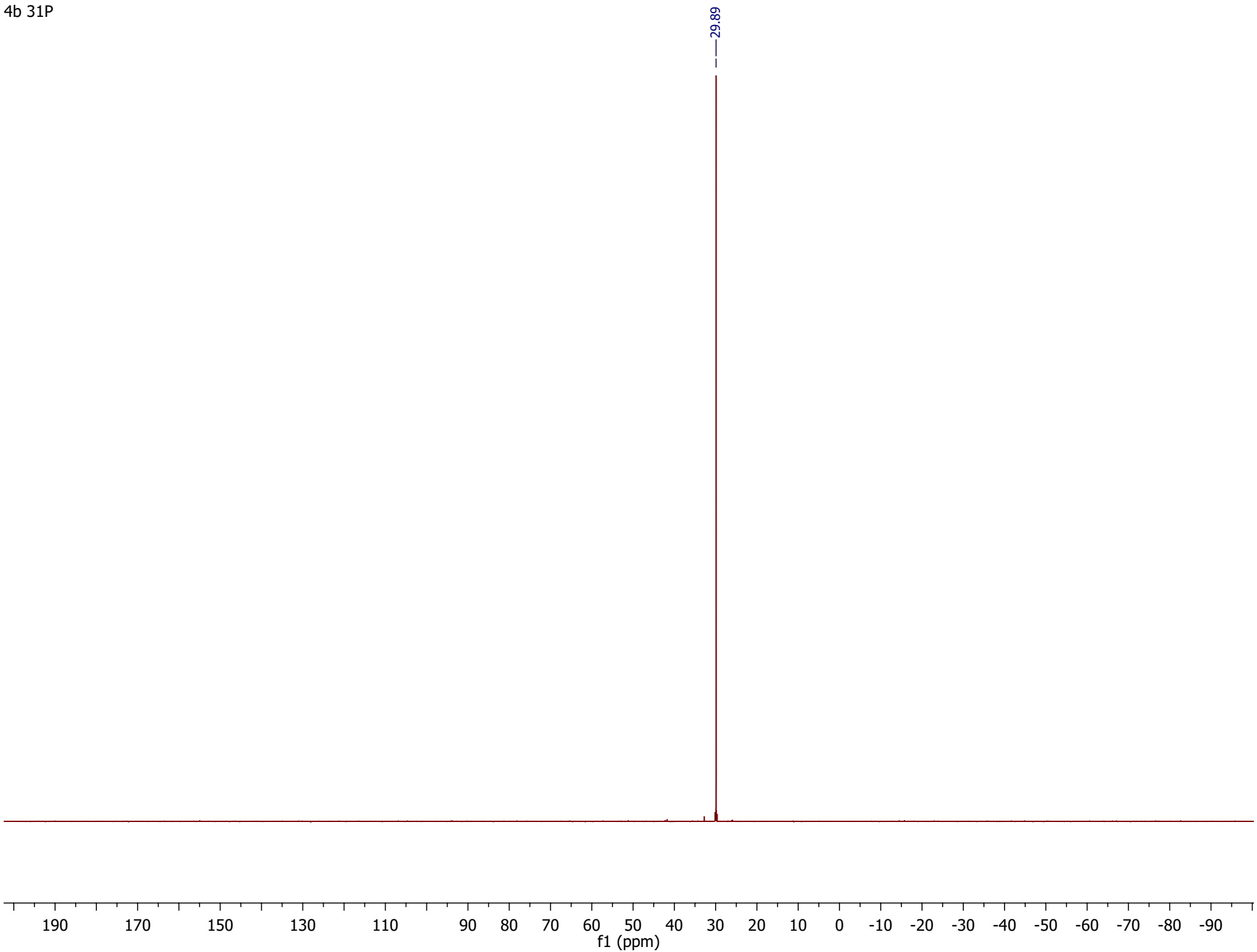

4a 13C
144.229
144.041
139.764
138.876
131.206
131.115
129.801
129.744
128.253
128.154
128.113
127.402
127.359
125.845
125.698
77.160 Chloroform-d
43.274
42.787
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

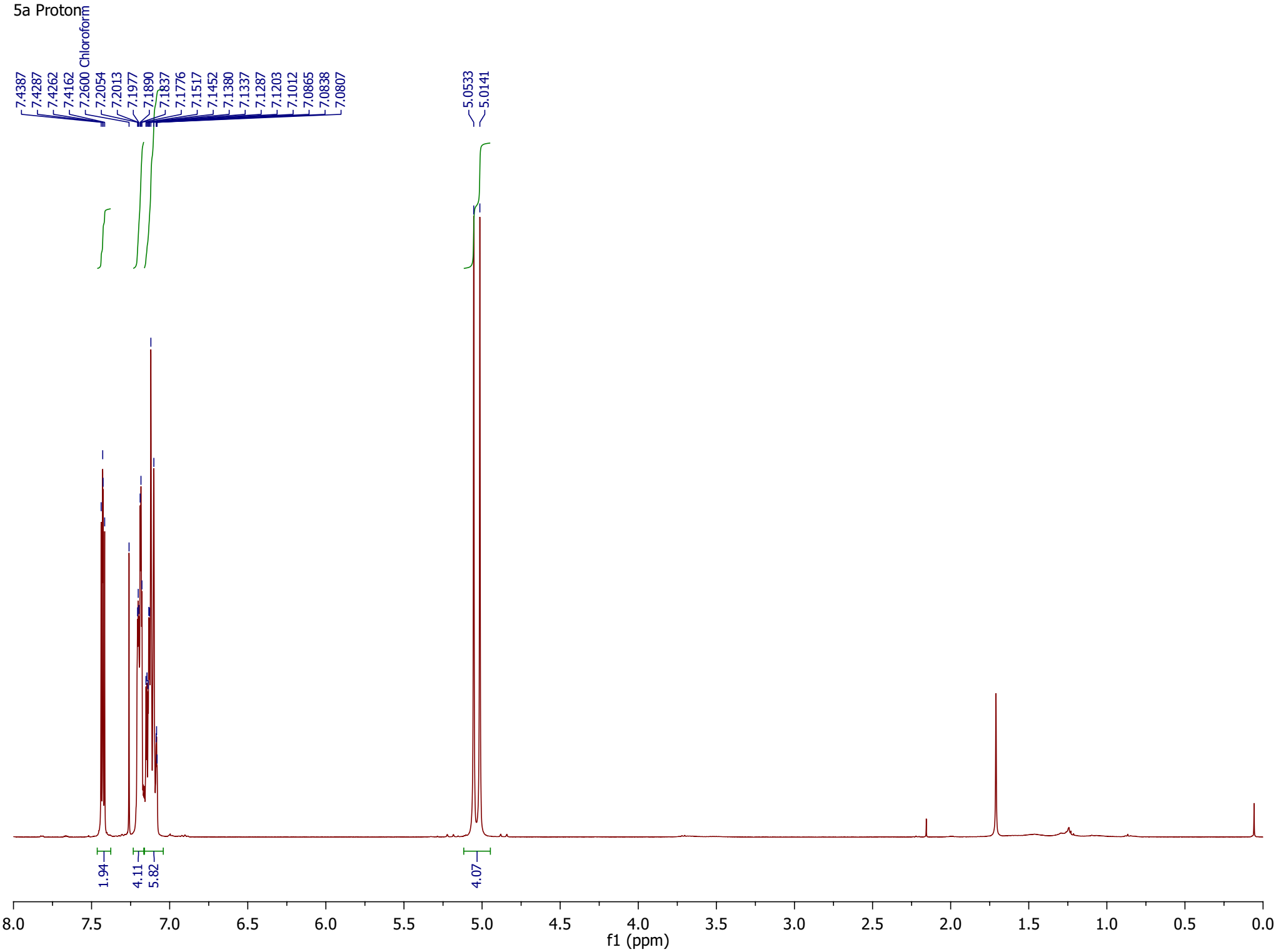
4a 31P

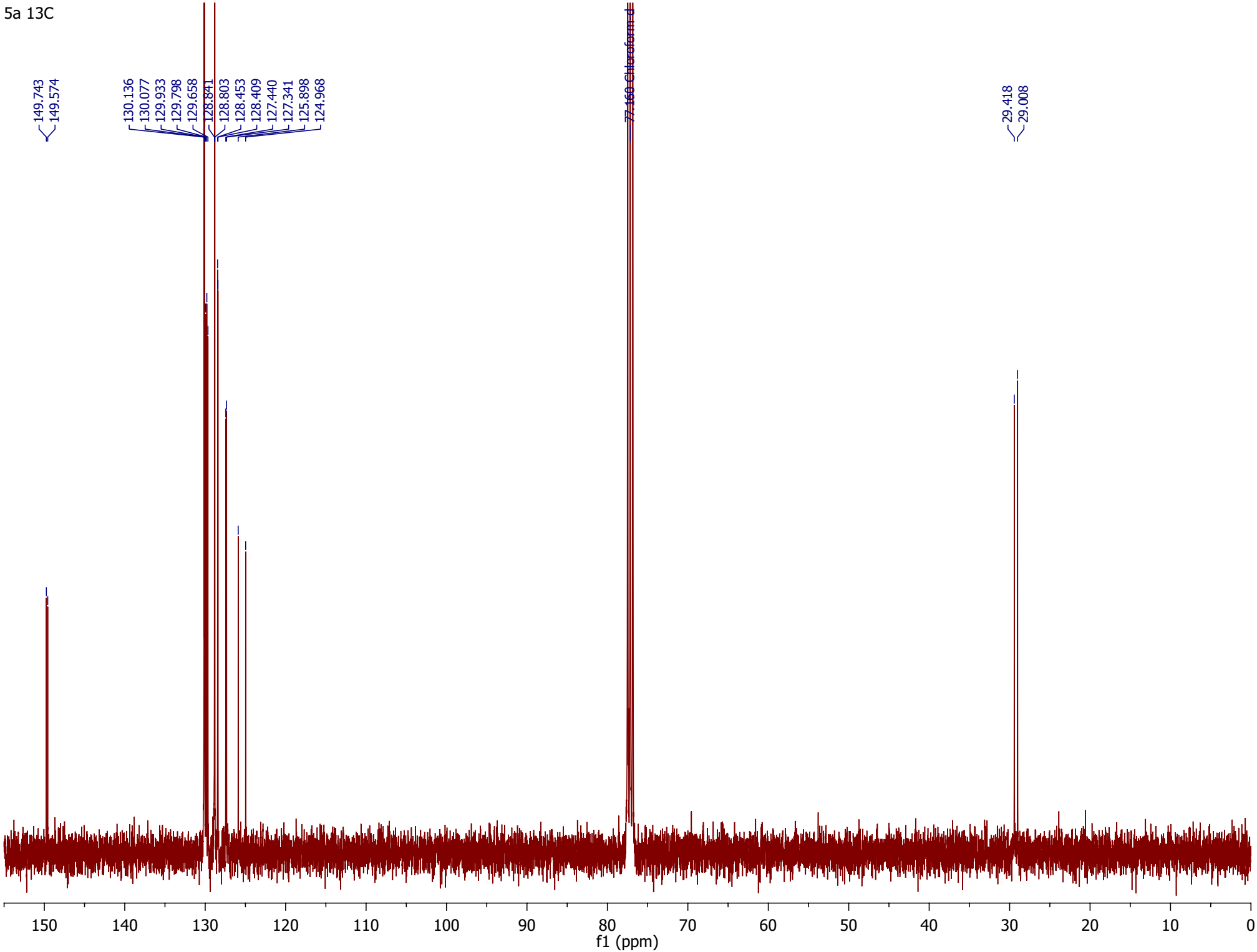

32.3506
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


7.2192
7.2122
7.2075
7.1790
7.1731
7.1669
7.1608
7.1580
7.1547
7.1516
7.1485
7.1452
7.1161
7.0963
7.0844
7.0803
7.0777
6.8855
6.8806
6.8743
6.8679
6.8644
6.8608
6.8571
3.6528
3.6161
0.9768
0.3368
0.3241
4b Proton
1.97
0.97
2.04
2.00
2.00
17.98
12.03
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
f1 (ppm)

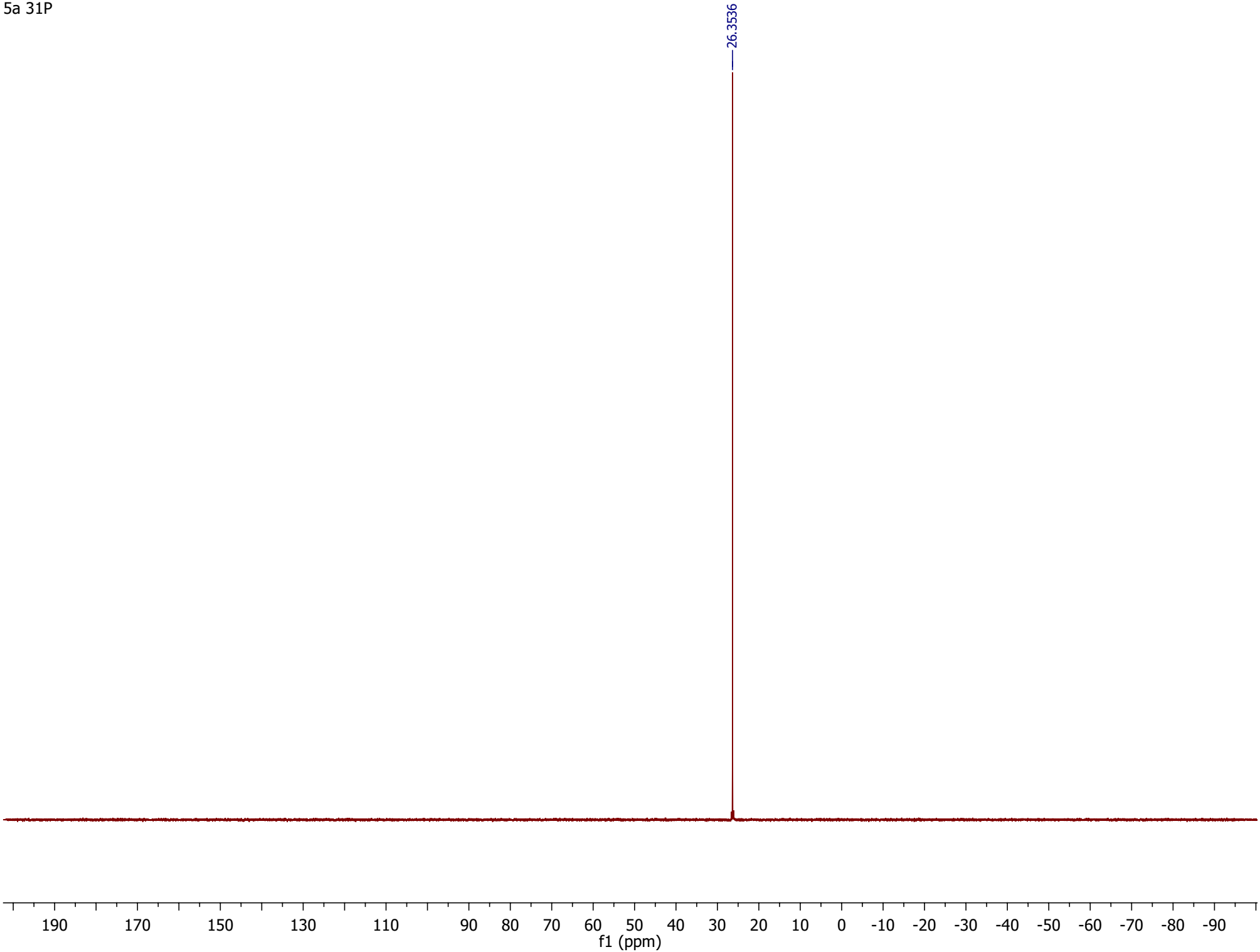

149.106
148.912
142.466
142.361
141.129
140.274
133.003
132.870
131.323
131.231
129.648
129.591
127.892
127.854
127.156
127.114
43.582
43.101
26.285
16.897
4.975
-5.014
4b 13C
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

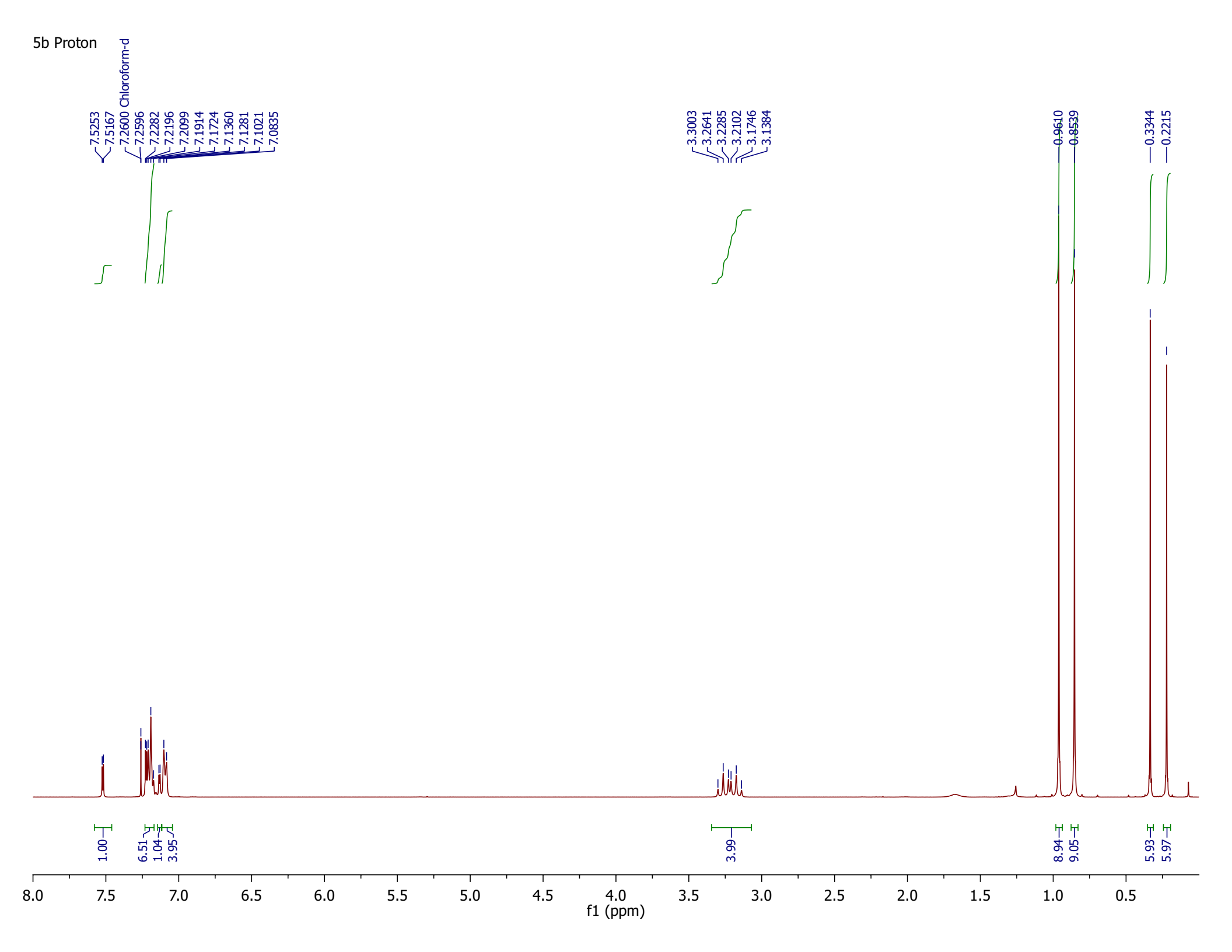

4b 31P
29.89
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

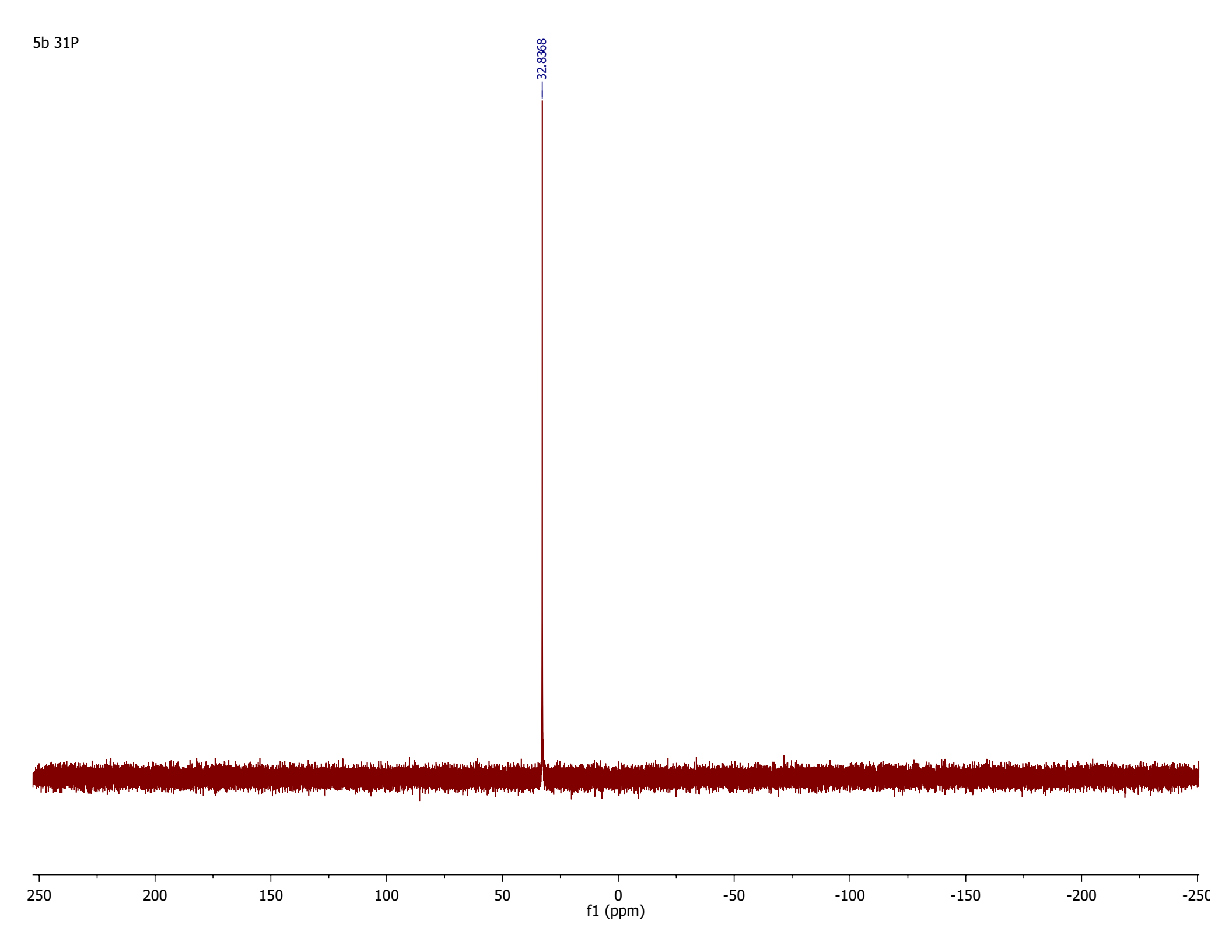

5a Proton
Chloroform
7.4387
7.4287
7.4262
7.4162
7.2600
7.2054
7.2013
7.1977
7.1890
7.1837
7.1776
7.1517
7.1452
7.1380
7.1337
7.1287
7.1203
7.1012
7.0865
7.0838
7.0807
5.0533
5.0141
1.94
4.11
5.82
4.07
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

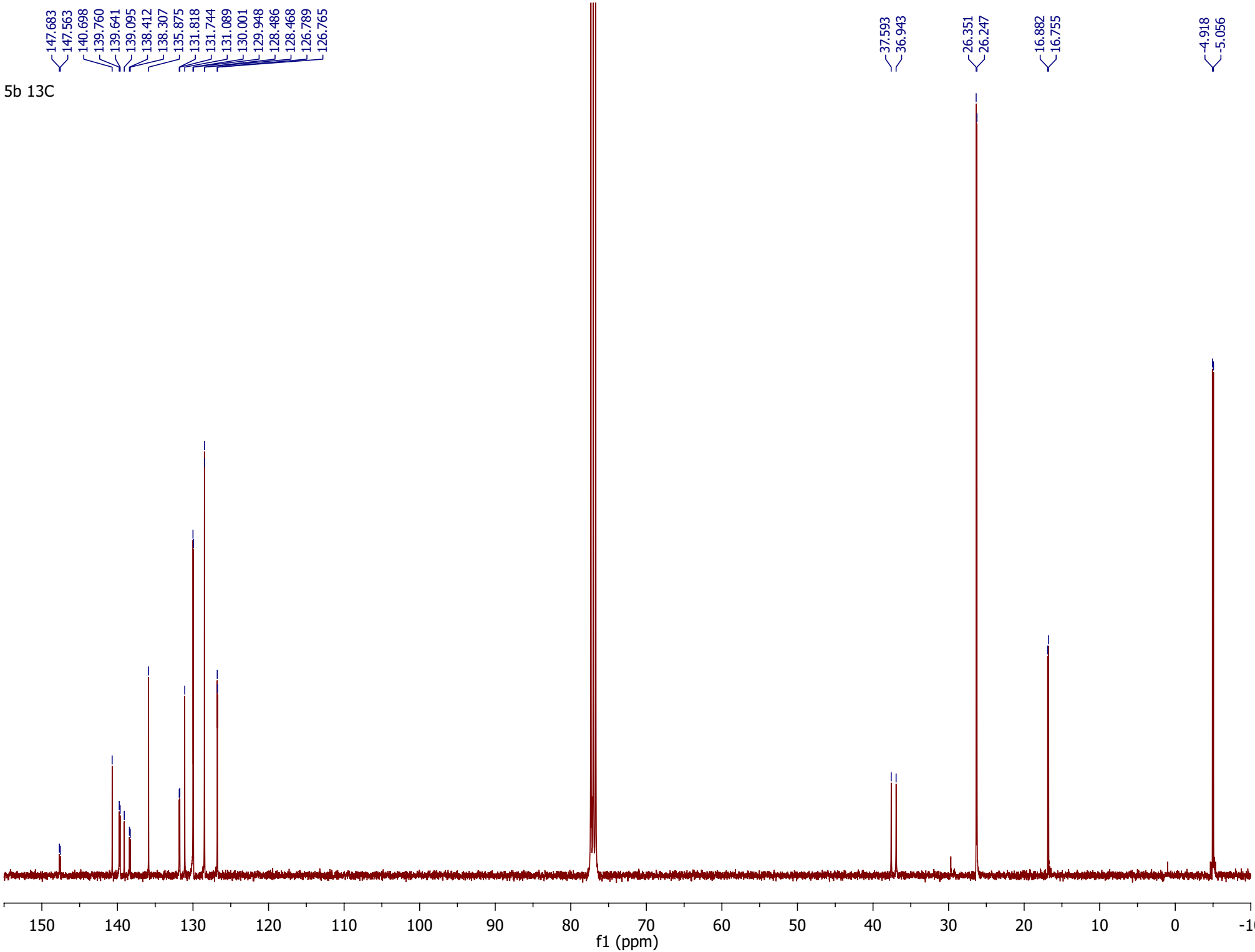

5a 13C
149.743
149.574
130.136
130.077
129.933
129.798
129.658
128.841
128.803
128.453
128.409
127.440
127.341
125.898
124.968
77.160 Chloroform-d
29.418
29.008
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5a 31P


26.3536
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


5b Proton
Chloroform-d
7.5253
7.5167
7.2600
7.2596
7.2282
7.2196
7.2099
7.1914
7.1724
7.1360
7.1281
7.1021
7.0835
3.3003
3.2641
3.2285
3.2102
3.1746
3.1384
0.9610
0.8539
0.3344
0.2215
1.00
6.51
1.04
3.95
3.99
8.94
9.05
5.93
5.97
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
f1 (ppm)


5b 31P
32.8368
250
200
150
100
50
0
-50
-100
-150
-200
-250
f1 (ppm)


147.683
147.563
140.698
139.760
139.641
139.095
138.412
138.307
135.875
131.818
131.744
131.089
130.001
129.948
128.486
128.468
126.789
126.765
37.593
36.943
26.351
26.247
16.882
16.755
4.918
-5.056
5b 13C
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)