

Supplementary Material

Discovery of Andrastones from the Deep-Sea-Derived *Penicillium allii-sativi* MCCC 3A00580 by OSMAC Strategy

Chun-Lan Xie^{a,b}, Qingmei Liu^c, Zhi-Hui He^a, Ying-Bao Gai^a, Zheng-Biao Zou^a, Zongze Shao^a, Guang-Ming Liu^c, Hai-Feng Chen^{b,*}, Xian-Wen Yang^{a,*}

^a Key Laboratory of Marine Biogenetic Resources, Third Institute of Oceanography,
Ministry of Natural Sources, 184 Daxue Road, Xiamen, Fujian 361005, China

^b School of Pharmaceutical Sciences, Xiamen University, South Xiang'an Road, Xiamen,
Fujian 361102, China

^c College of Food and Biological Engineering, Jimei University, 43 Yindou Road,
Xiamen, Fujian 361021, China

* Correspondence: yangxianwen@tio.org.cn (X.-W.Y.); Tel.: +86-592-2195319;
haifeng@xmu.edu.cn (H.-F.C.); Tel.: +86-592-2181851

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Figure S54. COSY NMR spectrum of **9** in CDCl_3 .

Figure S55. HMBC NMR spectrum of **9** in CDCl_3 .

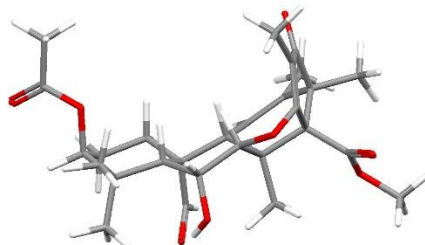
Figure S56. NOESY NMR spectrum of **9** in CDCl_3 .

Table S1 Energies analysis for **2**, **4**, **5**, and **7** at MMFF94x force field.

Configuration	Conformer	E (kcal/mol)	Configuration	Conformer	E (kcal/mol)
2a	1	173.34	4a	6	123.55
2a	2	174.04	4a	7	125.22
2a	3	174.91	4a	8	127.67
4a	1	121.65	4a	9	128.36
4a	2	121.9	5a	1	114.2
4a	3	122.29	5a	2	114.37
4a	4	122.53	7a	1	72.32
4a	5	122.72	7a	2	74.46

Table S2 Standard orientations of optimized coordinates for ECD calculations

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

Conformer 2a-1

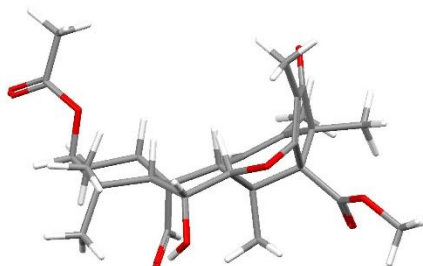
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2	1	0	3.681492	-1.257007	2.238520
3	1	0	4.185137	0.414223	2.415648
4	6	0	4.105596	-0.261964	0.378579
5	1	0	5.154792	-0.568823	0.380135
6	6	0	3.303693	-1.168141	-0.594753
7	6	0	1.780345	-0.773292	-0.471934
8	1	0	1.824091	0.291215	-0.731662
9	6	0	1.164479	-0.710322	1.002794
10	6	0	2.097480	0.190136	1.865231
11	1	0	2.010884	1.220425	1.501679

12	1	0	1.754039	0.199561	2.906501
13	6	0	0.834807	-1.366793	-1.595119
14	1	0	1.259847	-1.077927	-2.562405
15	6	0	-0.448162	-0.534967	-1.413153
16	1	0	-0.014097	0.465606	-1.356650
17	6	0	-1.199625	-0.755436	-0.073202
18	6	0	-0.264959	-0.014381	0.922104
19	1	0	0.003938	0.923460	0.417912
20	6	0	-2.546604	0.041190	-0.326503
21	6	0	-2.846794	1.277749	0.590556
22	6	0	-2.154040	1.175504	1.964991
23	6	0	-1.010881	0.483067	2.134442
24	1	0	-0.570357	0.418693	3.126702
25	6	0	-2.191895	0.610805	-1.680654
26	6	0	-2.177696	1.958980	-1.732350
27	6	0	-2.389402	2.454670	-0.345421
28	8	0	-2.196769	3.596410	0.032455
29	6	0	-2.777938	1.900398	3.132862
30	1	0	-3.794023	1.556791	3.357473
31	1	0	-2.839518	2.974957	2.918372
32	1	0	-2.172214	1.770626	4.034942
33	6	0	-1.534765	-2.218557	0.268730
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36	1	0	-2.170672	-2.643068	-0.513522
37	6	0	1.072104	-2.024122	1.752813
38	1	0	0.796170	-1.909329	2.823396
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42	8	0	-1.485874	-0.305870	-2.434021
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44	8	0	-4.328554	-1.069674	-1.554067
45	8	0	-4.234633	-1.351162	0.678575
46	6	0	-5.397628	-2.192942	0.579116
47	1	0	-5.623743	-2.498149	1.601016
48	1	0	-5.185568	-3.064273	-0.045900
49	1	0	-6.234742	-1.639998	0.145645
50	6	0	-1.728434	2.850094	-2.845818
51	1	0	-1.126707	3.674229	-2.449222
52	1	0	-2.586704	3.298206	-3.362140
53	1	0	-1.148134	2.290130	-3.585856

54	6	0	5.122068	1.903589	0.120181
55	8	0	6.091536	1.556363	0.757490
56	6	0	4.924751	3.266410	-0.501678
57	1	0	4.812123	3.172085	-1.586835
58	1	0	5.784011	3.897347	-0.272504
59	1	0	4.009822	3.729576	-0.117885
60	8	0	1.277840	-3.139257	1.311347
61	6	0	3.698632	-2.635449	-0.303431
62	1	0	3.137584	-3.318335	-0.944866
63	1	0	3.540333	-2.944191	0.729649
64	1	0	4.763454	-2.765757	-0.532242
65	6	0	3.778288	-0.878304	-2.039176
66	1	0	3.392318	-1.631583	-2.732569
67	1	0	4.872794	-0.921481	-2.085998
68	1	0	3.470574	0.110719	-2.390710
69	6	0	-4.367311	1.566579	0.754087
70	1	0	-4.849481	0.850078	1.420379
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72	1	0	-4.505144	2.573926	1.154385

Conformer 2a-2



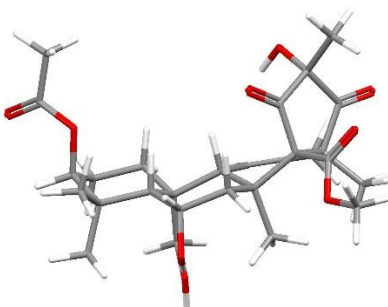
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5	1	0	5.178827	-0.508355	0.257753
6	6	0	3.280953	-1.242602	-0.512104
7	6	0	1.763992	-0.831288	-0.364996
8	1	0	1.785543	0.180713	-0.786316
9	6	0	1.229996	-0.542503	1.114791
10	6	0	2.202072	0.481990	1.772243
11	1	0	2.089363	1.441858	1.255576
12	1	0	1.916627	0.656487	2.816492

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17	6	0	-1.188646	-0.754498	0.192229
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23	6	0	-0.893948	0.794409	2.180147
24	1	0	-0.401120	0.874171	3.146167
25	6	0	-2.279043	0.361480	-1.539239
26	6	0	-2.287436	1.688249	-1.785956
27	6	0	-2.440968	2.378507	-0.475258
28	8	0	-2.256800	3.566450	-0.279739
29	6	0	-2.629028	2.320949	3.065541
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32	1	0	-1.972543	2.325612	3.941035
33	6	0	-1.495886	-2.146764	0.774503
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54	6	0	5.129627	1.887434	-0.391903

55	8	0	6.139181	1.631986	0.226192
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59	1	0	5.766065	3.789104	-1.131218
60	8	0	1.398092	-2.892457	1.788846
61	6	0	3.704134	-2.649002	-0.025672
62	1	0	3.107470	-3.420891	-0.516300
63	1	0	3.615974	-2.794212	1.050716
64	1	0	4.752892	-2.814406	-0.300930
65	6	0	3.670106	-1.174882	-2.008787
66	1	0	3.258522	-2.028938	-2.555069
67	1	0	4.760889	-1.216726	-2.111587
68	1	0	3.326878	-0.253905	-2.488831
69	6	0	-4.337702	1.634574	0.857125
70	1	0	-4.769770	0.989770	1.623475
71	1	0	-4.889832	1.476745	-0.076253
72	1	0	-4.471016	2.680393	1.143748

Conformer 4a-1



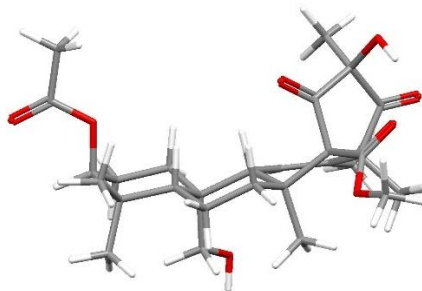
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5	1	0	5.371920	0.188931	0.282483
6	6	0	3.660804	-1.008989	-0.340255
7	6	0	2.097271	-0.848866	-0.309761
8	1	0	1.940470	0.076795	-0.883285
9	6	0	1.450663	-0.470818	1.081432
10	6	0	2.191557	0.816186	1.576161
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25	1	0	-0.213251	0.818377	2.817704
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31	8	0	-4.799570	1.935244	0.972478
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36	6	0	-1.303644	-2.313048	0.788632
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56	1	0	-2.875957	3.591447	-2.148885
57	1	0	-4.224913	3.824886	-0.997859
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60	6	0	4.487791	3.382074	-1.856694
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62	1	0	3.472885	3.741636	-1.659318
63	1	0	4.477472	2.905956	-2.843002
64	8	0	1.515017	-2.846288	1.888945
65	1	0	1.573084	-3.394556	2.685443
66	6	0	4.231219	-2.201548	0.461675
67	1	0	3.812802	-3.135849	0.083728
68	1	0	4.024919	-2.151938	1.532601
69	1	0	5.320921	-2.237290	0.337058
70	6	0	4.143020	-1.194186	-1.797685
71	1	0	3.886668	-2.191745	-2.165747
72	1	0	5.234514	-1.094172	-1.845432
73	1	0	3.710743	-0.450130	-2.472757
74	6	0	-4.175409	-0.801249	1.403730
75	1	0	-3.752648	-1.698352	1.858847
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Conformer 5a-1



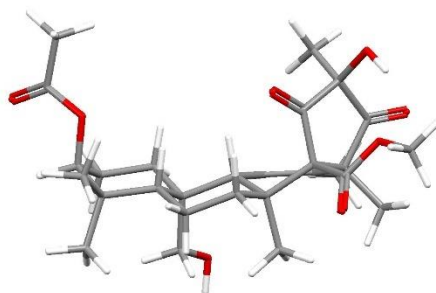
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4	6	0	4.375536	-0.040405	0.124793
5	1	0	5.454851	-0.217603	0.140730
6	6	0	3.659600	-1.214817	-0.590247
7	6	0	2.108657	-1.008127	-0.465851
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9	6	0	1.530637	-0.716515	0.970403

10	6	0	2.347652	0.449473	1.593078
11	1	0	2.111332	1.379056	1.059521
12	1	0	2.054939	0.594168	2.637649
13	6	0	1.255512	-2.055220	-1.205332
14	1	0	1.684085	-2.259737	-2.191852
15	1	0	1.262163	-3.015876	-0.675627
16	6	0	-0.184500	-1.559747	-1.425206
17	1	0	-0.150559	-0.703658	-2.103361
18	1	0	-0.764716	-2.343319	-1.921957
19	6	0	-0.901188	-1.140606	-0.111953
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21	1	0	0.239393	0.658750	0.064590
22	6	0	-2.188229	-0.261537	-0.389847
23	6	0	-2.982443	0.142892	0.928157
24	6	0	-2.000107	0.466141	2.065775
25	6	0	-0.668344	0.330007	1.933105
26	1	0	-0.055046	0.640094	2.773609
27	6	0	-1.873652	1.146309	-1.044209
28	6	0	-2.842080	2.230594	-0.532245
29	8	0	-3.665211	2.711130	-1.575585
30	1	0	-4.149843	1.938283	-1.919745
31	6	0	-3.644578	1.501244	0.552997
32	8	0	-4.654211	1.929477	1.064052
33	6	0	-2.597204	0.967689	3.363107
34	1	0	-3.160319	0.177516	3.876095
35	1	0	-3.297251	1.795019	3.205560
36	1	0	-1.808358	1.305096	4.041936
37	6	0	-1.298157	-2.424456	0.662351
38	1	0	-0.498038	-3.165062	0.617805
39	1	0	-2.178767	-2.891240	0.220451
40	1	0	-1.519548	-2.232108	1.715104
41	6	0	1.617817	-1.926704	1.941304
42	1	0	2.657628	-2.101059	2.216198
43	1	0	1.265885	-2.850641	1.471477
44	8	0	4.148773	1.161360	-0.673038
45	8	0	-1.020329	1.356105	-1.874609
46	6	0	-3.229120	-0.811168	-1.379128
47	8	0	-4.103114	-0.095551	-1.850718
48	8	0	-3.145176	-2.108187	-1.681379
49	6	0	-4.132214	-2.603735	-2.614260
50	1	0	-3.898060	-3.660189	-2.740154
51	1	0	-4.053872	-2.070242	-3.563686

52	1	0	-5.136800	-2.472505	-2.206630
53	6	0	-2.090094	3.439347	0.027682
54	1	0	-1.424748	3.160261	0.849505
55	1	0	-2.823482	4.167221	0.385523
56	1	0	-1.499951	3.881126	-0.780230
57	6	0	5.126574	2.098360	-0.683637
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59	6	0	4.733827	3.265832	-1.560136
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61	1	0	4.560752	2.925375	-2.586383
62	1	0	5.527767	4.013207	-1.546448
63	8	0	0.966595	-1.722246	3.192580
64	1	0	0.012867	-1.661376	3.029979
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66	1	0	3.624464	-3.395678	-0.403289
67	1	0	4.172916	-2.601321	1.075539
68	1	0	5.239093	-2.688687	-0.320918
69	6	0	4.065189	-1.192637	-2.084894
70	1	0	3.791982	-2.126841	-2.585717
71	1	0	5.152712	-1.083805	-2.176867
72	1	0	3.599711	-0.363899	-2.625311
73	6	0	-4.089982	-0.824295	1.395834
74	1	0	-3.682083	-1.738712	1.829649
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Conformer 5a-2



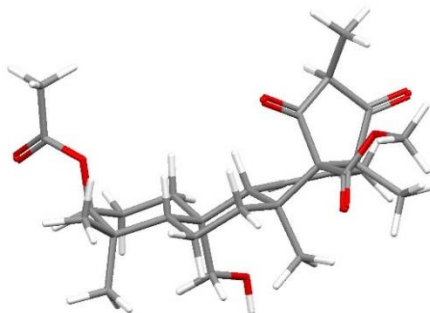
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4	6	0	4.402274	-0.002821	0.079789
5	1	0	5.486031	-0.144087	0.034529

6	6	0	3.711878	-0.886866	-0.990440
7	6	0	2.157015	-0.789009	-0.801712
8	1	0	1.954435	0.274612	-0.996165
9	6	0	1.589188	-1.012443	0.649489
10	6	0	2.377582	-0.097761	1.627075
11	1	0	2.109545	0.949256	1.435179
12	1	0	2.090493	-0.319420	2.659730
13	6	0	1.327406	-1.560311	-1.845061
14	1	0	1.749527	-1.413101	-2.844449
15	1	0	1.370454	-2.641105	-1.663415
16	6	0	-0.128640	-1.065859	-1.886298
17	1	0	-0.126226	-0.034319	-2.246128
18	1	0	-0.697556	-1.657828	-2.608990
19	6	0	-0.838810	-1.125972	-0.505639
20	6	0	0.093802	-0.494064	0.586703
21	1	0	0.243201	0.547131	0.266994
22	6	0	-2.157908	-0.247809	-0.478771
23	6	0	-2.946678	-0.322773	0.901889
24	6	0	-1.962069	-0.385980	2.083171
25	6	0	-0.628881	-0.432066	1.914330
26	1	0	-0.017620	-0.419682	2.811352
27	6	0	-1.901397	1.295543	-0.658884
28	6	0	-2.817701	2.133815	0.255355
29	8	0	-3.639204	3.007047	-0.495279
30	1	0	-4.165057	2.451588	-1.093993
31	6	0	-3.624742	1.071167	1.011377
32	8	0	-4.651921	1.290010	1.612823
33	6	0	-2.561785	-0.373175	3.473062
34	1	0	-3.110338	-1.300416	3.682112
35	1	0	-3.274893	0.446962	3.610818
36	1	0	-1.775223	-0.277598	4.227392
37	6	0	-1.201833	-2.604907	-0.213179
38	1	0	-0.378643	-3.265542	-0.488763
39	1	0	-2.059856	-2.913174	-0.811284
40	1	0	-1.439783	-2.786054	0.838422
41	6	0	1.723840	-2.475559	1.159386
42	1	0	2.771354	-2.694608	1.365071
43	1	0	1.400289	-3.201106	0.406494
44	8	0	4.135987	1.391454	-0.264453
45	8	0	-1.128396	1.791684	-1.446477
46	6	0	-3.131877	-0.600619	-1.618776
47	8	0	-3.107862	-1.562463	-2.347649

48	8	0	-4.110050	0.348137	-1.721443
49	6	0	-5.109148	0.106188	-2.737494
50	1	0	-5.811131	0.936344	-2.659748
51	1	0	-5.614611	-0.843550	-2.550916
52	1	0	-4.642518	0.082195	-3.724376
53	6	0	-2.005373	3.022599	1.201943
54	1	0	-1.335797	2.438007	1.837594
55	1	0	-2.701682	3.586196	1.829336
56	1	0	-1.416695	3.717126	0.595627
57	6	0	5.089870	2.302987	0.040242
58	8	0	6.140154	2.035515	0.582626
59	6	0	4.660530	3.686276	-0.393494
60	1	0	3.715200	3.957060	0.087913
61	1	0	4.491598	3.706448	-1.475228
62	1	0	5.433833	4.407073	-0.125887
63	8	0	1.073514	-2.723608	2.403202
64	1	0	0.116593	-2.676310	2.255991
65	6	0	4.296563	-2.315725	-0.904450
66	1	0	3.748963	-2.999025	-1.562024
67	1	0	4.285479	-2.742644	0.100527
68	1	0	5.340961	-2.309289	-1.238558
69	6	0	4.096227	-0.344079	-2.389286
70	1	0	3.843680	-1.060663	-3.177107
71	1	0	5.178689	-0.175010	-2.442041
72	1	0	3.598937	0.603427	-2.613840
73	6	0	-4.032500	-1.412890	1.021808
74	1	0	-3.601782	-2.408698	1.139800
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Conformer 7a-1

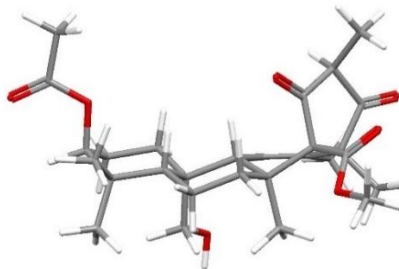


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4	6	0	-4.270634	0.071444	-0.098679
5	1	0	-5.355919	-0.039713	-0.023427
6	6	0	-3.586792	-0.573832	1.132569
7	6	0	-2.036087	-0.489003	0.932856
8	1	0	-1.850992	0.592227	0.844517
9	6	0	-1.464542	-1.078905	-0.410099
10	6	0	-2.255275	-0.425990	-1.581840
11	1	0	-1.953524	0.627248	-1.646518
12	1	0	-1.977558	-0.871765	-2.546713
13	6	0	-1.196225	-0.942151	2.139825
14	1	0	-1.621849	-0.539982	3.064506
15	1	0	-1.221715	-2.032961	2.254466
16	6	0	0.250089	-0.429997	2.039306
17	1	0	0.230738	0.661460	2.092314
18	1	0	0.828434	-0.780690	2.898926
19	6	0	0.961069	-0.874199	0.733467
20	6	0	0.029717	-0.564184	-0.491765
21	1	0	-0.098766	0.528695	-0.486704
22	6	0	2.279618	-0.043379	0.454195
23	6	0	3.051008	-0.499149	-0.862001
24	6	0	2.066010	-0.952359	-1.955350
25	6	0	0.736477	-0.933259	-1.774861
26	1	0	0.119499	-1.223478	-2.623133
27	6	0	2.015944	1.491721	0.215456
28	6	0	2.717126	1.980236	-1.043761
29	1	0	1.943435	2.005802	-1.829603
30	6	0	3.640562	0.830692	-1.406536
31	8	0	4.664038	0.925338	-2.046861
32	6	0	2.663049	-1.394167	-3.273675
33	1	0	3.177416	-2.358731	-3.177948
34	1	0	3.403430	-0.680597	-3.652315
35	1	0	1.879780	-1.511701	-4.028808
36	6	0	1.319398	-2.375749	0.868002
37	1	0	0.469701	-2.941424	1.254591
38	1	0	2.134870	-2.500307	1.581878
39	1	0	1.610783	-2.828852	-0.081543
40	6	0	-1.485985	-2.642529	-0.531519
41	1	0	-1.526547	-3.106036	0.455033
42	1	0	-0.553428	-2.975705	-1.002595

43	8	0	-3.984059	1.505984	-0.057711
44	8	0	1.384102	2.210828	0.957909
45	6	0	3.269283	-0.053116	1.634672
46	8	0	3.256723	-0.758323	2.615825
47	8	0	4.227115	0.885905	1.424440
48	6	0	5.237536	0.999493	2.445153
49	1	0	4.779533	1.263170	3.401187
50	1	0	5.906034	1.789577	2.104244
51	1	0	5.777985	0.055716	2.551228
52	6	0	3.371912	3.354718	-0.928377
53	1	0	4.142266	3.345364	-0.151918
54	1	0	2.624616	4.107480	-0.664165
55	1	0	3.843476	3.627772	-1.876118
56	6	0	-4.919384	2.344219	-0.559715
57	8	0	-5.964460	1.983807	-1.057246
58	6	0	-4.484007	3.783860	-0.399688
59	1	0	-3.485952	3.931751	-0.823787
60	1	0	-4.426360	4.038463	0.664252
61	1	0	-5.203161	4.438219	-0.893670
62	8	0	-2.581565	-3.227856	-1.239828
63	1	0	-2.477920	-3.016757	-2.179489
64	6	0	-4.130079	-2.009731	1.306989
65	1	0	-3.657667	-2.492457	2.170240
66	1	0	-3.971270	-2.645496	0.434263
67	1	0	-5.208179	-1.977203	1.509283
68	6	0	-4.006399	0.227075	2.388147
69	1	0	-3.744881	-0.306644	3.306941
70	1	0	-5.094437	0.367253	2.396039
71	1	0	-3.541441	1.216597	2.420085
72	6	0	4.184824	-1.526056	-0.672874
73	1	0	3.798901	-2.518913	-0.433214
74	1	0	4.871612	-1.219539	0.120115
75	1	0	4.774657	-1.587544	-1.589718

Conformer 7a-2



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3	1	0	-4.331634	0.962517	-2.015074
4	6	0	-4.298314	-0.059941	-0.130598
5	1	0	-5.373569	-0.260935	-0.134941
6	6	0	-3.558419	-1.168113	0.661582
7	6	0	-2.011561	-0.939239	0.523847
8	1	0	-1.866207	0.039570	1.004397
9	6	0	-1.437954	-0.728589	-0.927388
10	6	0	-2.279007	0.374117	-1.627671
11	1	0	-2.063911	1.343007	-1.158744
12	1	0	-1.987388	0.454061	-2.679424
13	6	0	-1.137726	-1.921509	1.325352
14	1	0	-1.563033	-2.075594	2.322525
15	1	0	-1.123013	-2.912173	0.854355
16	6	0	0.289944	-1.380707	1.514050
17	1	0	0.236173	-0.486542	2.139659
18	1	0	0.888509	-2.116707	2.058671
19	6	0	1.002284	-1.028049	0.178761
20	6	0	0.028898	-0.171675	-0.710966
21	1	0	-0.172590	0.733701	-0.120395
22	6	0	2.265644	-0.101139	0.400666
23	6	0	3.046596	0.245531	-0.939501
24	6	0	2.065199	0.441215	-2.106423
25	6	0	0.737489	0.286358	-1.967324
26	1	0	0.119120	0.511958	-2.830611
27	6	0	1.907645	1.328656	0.985242
28	6	0	2.674054	2.424088	0.262374
29	1	0	1.943729	2.936506	-0.385771
30	6	0	3.612510	1.668089	-0.660302
31	8	0	4.627170	2.112716	-1.148171
32	6	0	2.656779	0.858038	-3.436055
33	1	0	3.242183	0.046155	-3.886209
34	1	0	3.335689	1.712339	-3.338202
35	1	0	1.864090	1.124261	-4.141662
36	6	0	1.441146	-2.348418	-0.506088
37	1	0	0.657439	-3.104055	-0.429574
38	1	0	2.322813	-2.763487	-0.016340
39	1	0	1.680459	-2.217782	-1.564552
40	6	0	-1.497760	-2.004896	-1.812739
41	1	0	-2.533996	-2.222642	-2.069161

42	1	0	-1.121579	-2.884689	-1.280973
43	8	0	-4.099296	1.197394	0.585826
44	8	0	1.158787	1.528276	1.915253
45	6	0	3.326116	-0.547562	1.421176
46	8	0	4.189174	0.223733	1.802584
47	8	0	3.255289	-1.815954	1.847859
48	6	0	4.259289	-2.203466	2.810439
49	1	0	4.038687	-3.243259	3.050368
50	1	0	4.191662	-1.574624	3.700686
51	1	0	5.257391	-2.107489	2.377046
52	6	0	3.340234	3.450686	1.180678
53	1	0	4.062230	2.955307	1.834707
54	1	0	2.587147	3.947563	1.798122
55	1	0	3.867850	4.197085	0.580932
56	6	0	-5.097198	2.110969	0.533434
57	8	0	-6.135738	1.952946	-0.070958
58	6	0	-4.733271	3.341278	1.333450
59	1	0	-3.806240	3.780468	0.950673
60	1	0	-4.557039	3.071743	2.380052
61	1	0	-5.543140	4.068737	1.269482
62	8	0	-0.855333	-1.873635	-3.078062
63	1	0	0.097294	-1.781461	-2.923637
64	6	0	-4.066293	-2.546095	0.177144
65	1	0	-3.477087	-3.354882	0.622227
66	1	0	-4.040579	-2.674818	-0.906763
67	1	0	-5.106625	-2.689680	0.492821
68	6	0	-3.965521	-1.055339	2.151678
69	1	0	-3.675661	-1.950131	2.711504
70	1	0	-5.054882	-0.960309	2.236952
71	1	0	-3.514911	-0.185442	2.637143
72	6	0	4.209544	-0.688445	-1.329162
73	1	0	3.856141	-1.657780	-1.686356
74	1	0	4.889520	-0.846891	-0.487991
75	1	0	4.797628	-0.215221	-2.118079

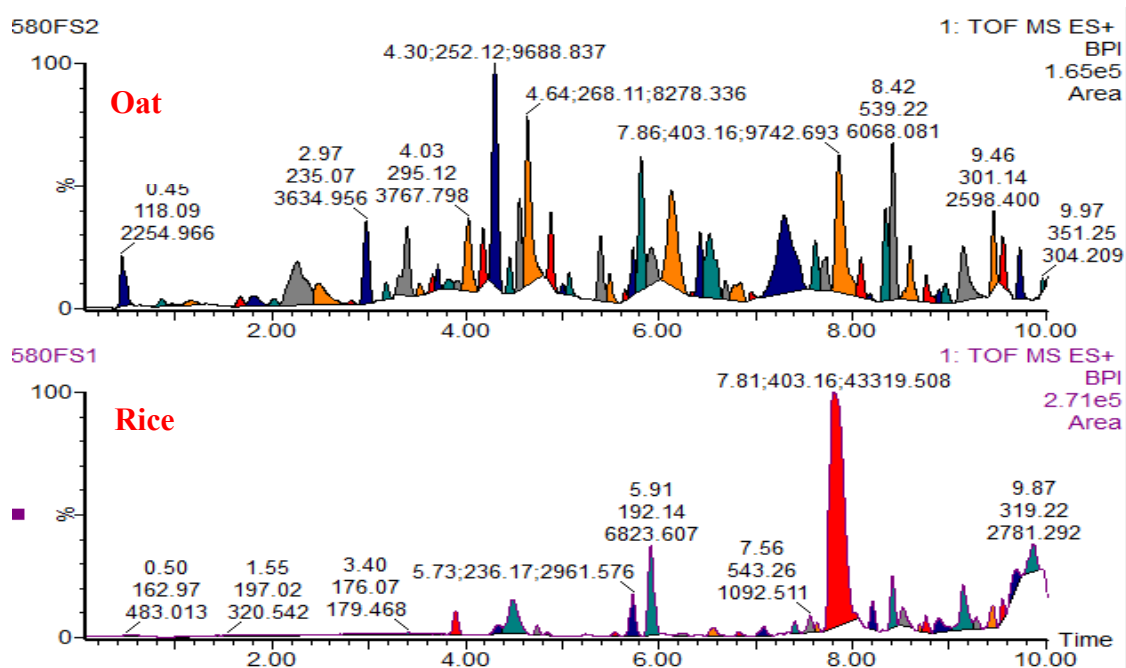


Figure S1 UPLC-MS-BPI spectra of *Penicillium allii-sativi* in oat and rice static culture.

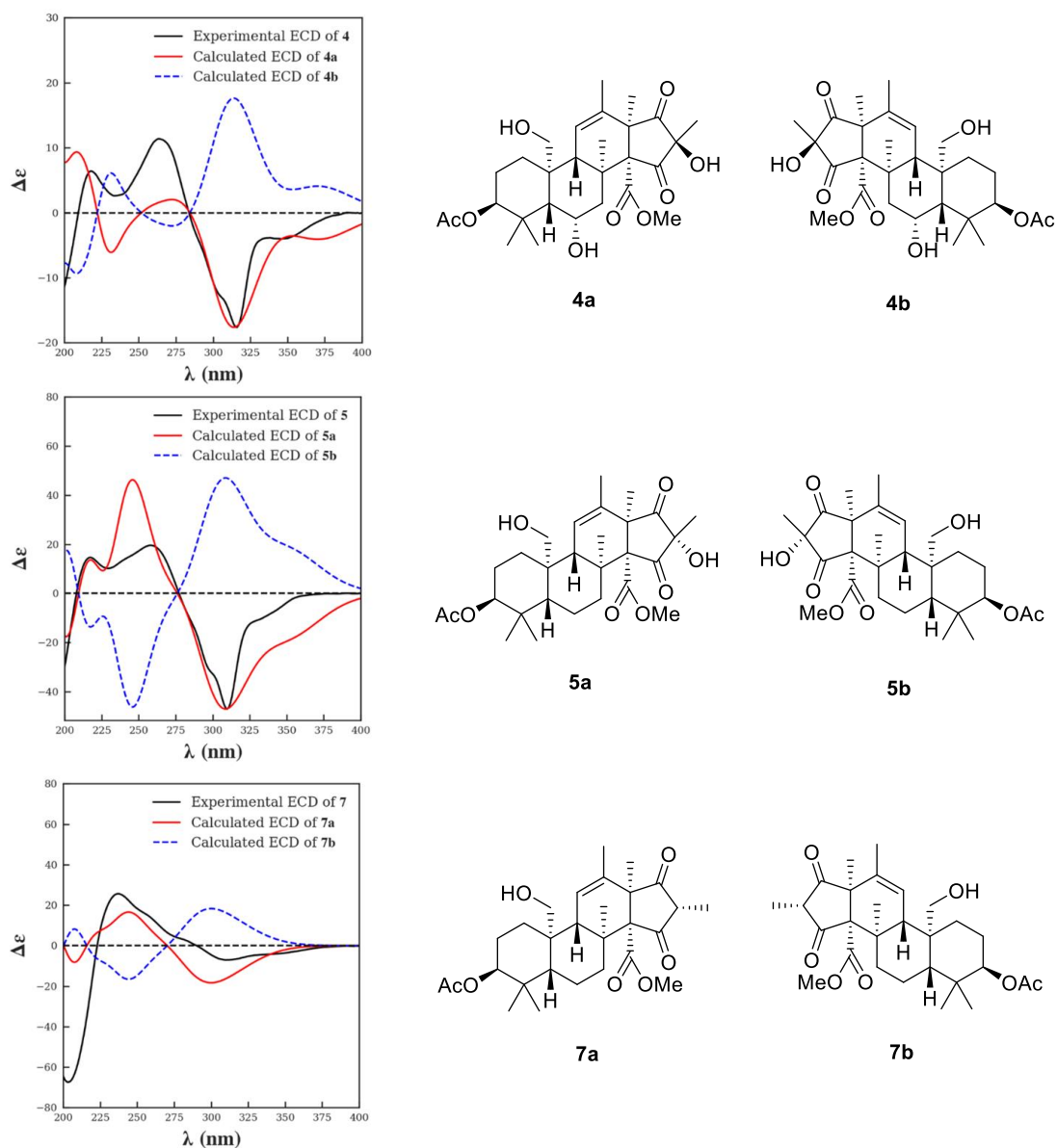


Figure S2. Calculated and experimental ECD spectra of **4**, **5** and **7** in MeOH.

4a: (3*S*,5*S*,6*S*,8*S*,9*R*,10*R*,13*R*,14*R*,16*R*)-**4**, **5a:** (3*S*,5*S*,8*S*,9*R*,10*R*,13*R*,14*R*,16*R*)-**5**, **7a:** (3*S*,5*S*,6*S*,8*S*,7*S*,9*R*,10*R*,13*R*,14*R*,16*R*)-**7**, and their enantiomers **4b**, **5b**, and **7b**.

Figure S3. ^1H NMR spectrum of **1** in CD_3OD .

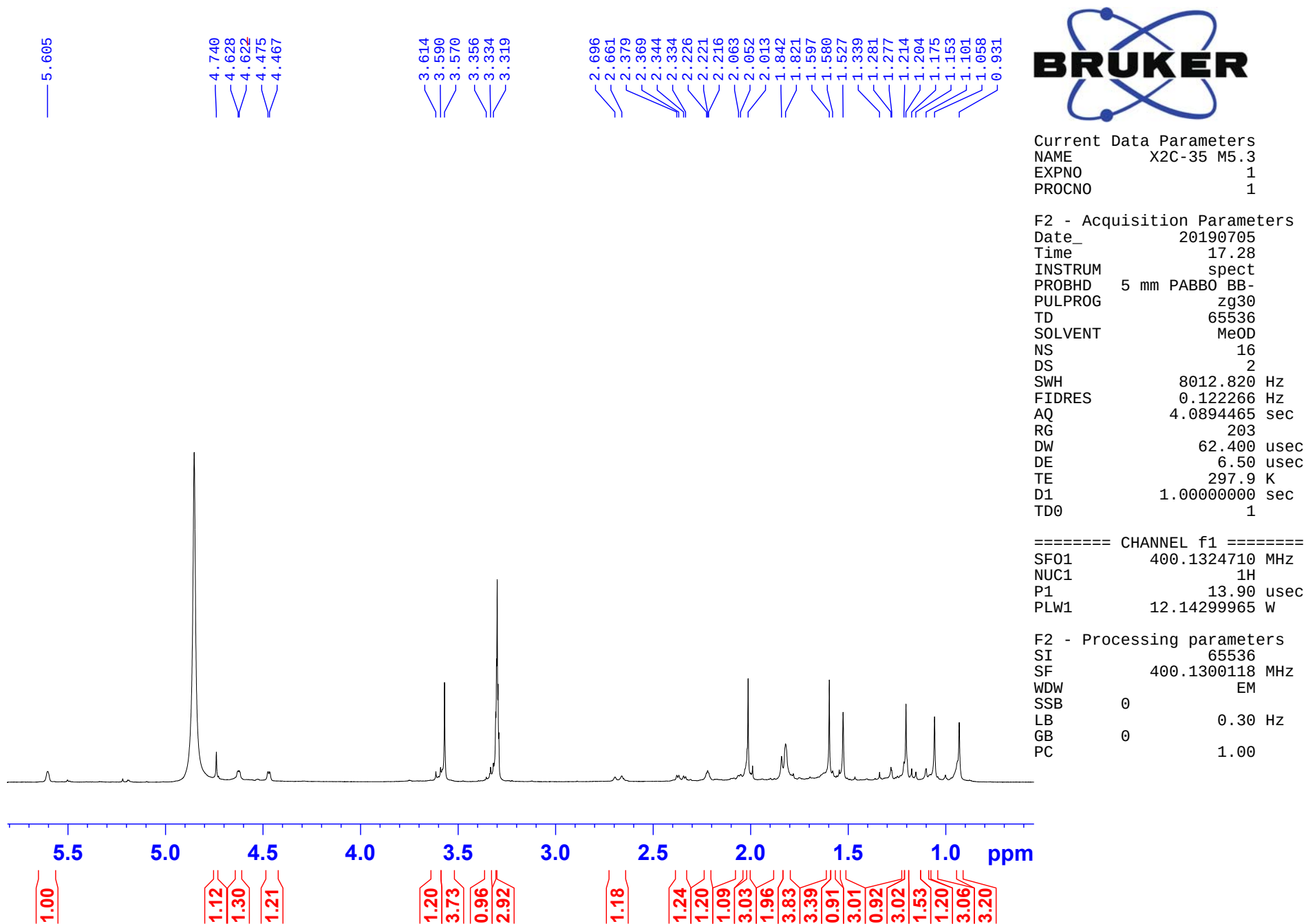


Figure S4. ^{13}C NMR spectrum of **1** in CD_3OD .

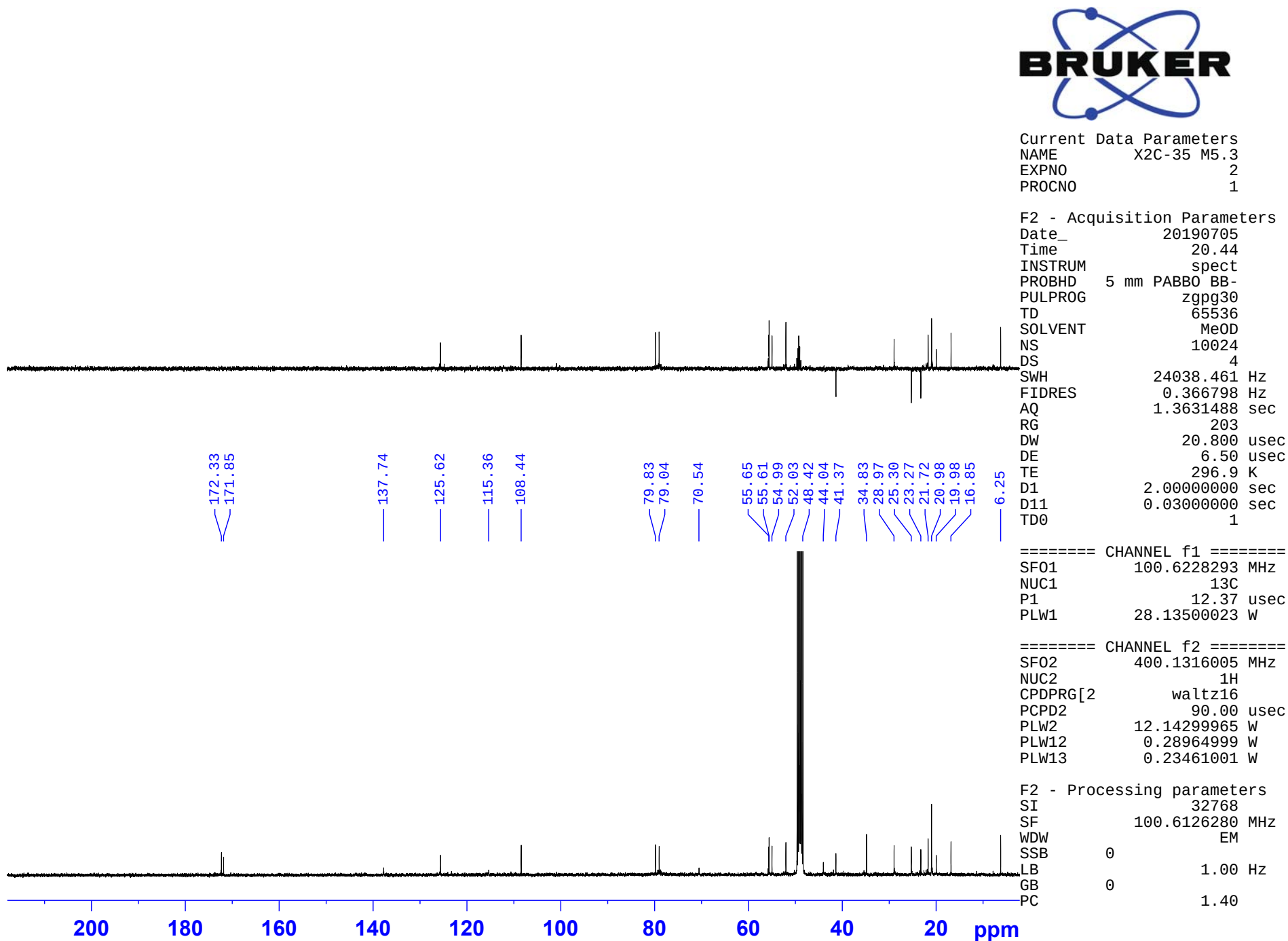


Figure S5. HSQC NMR spectrum of **1** in CD₃OD.

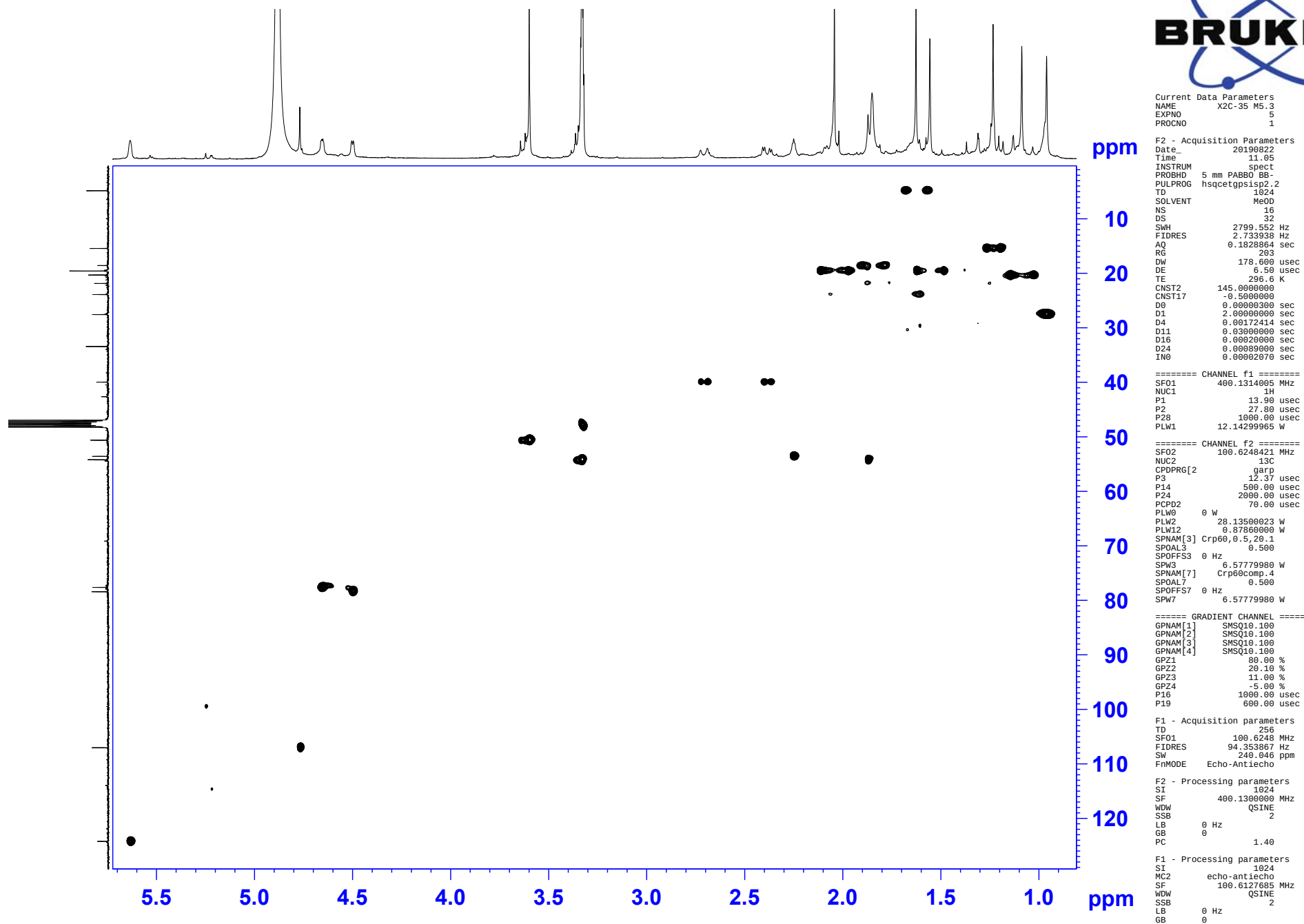
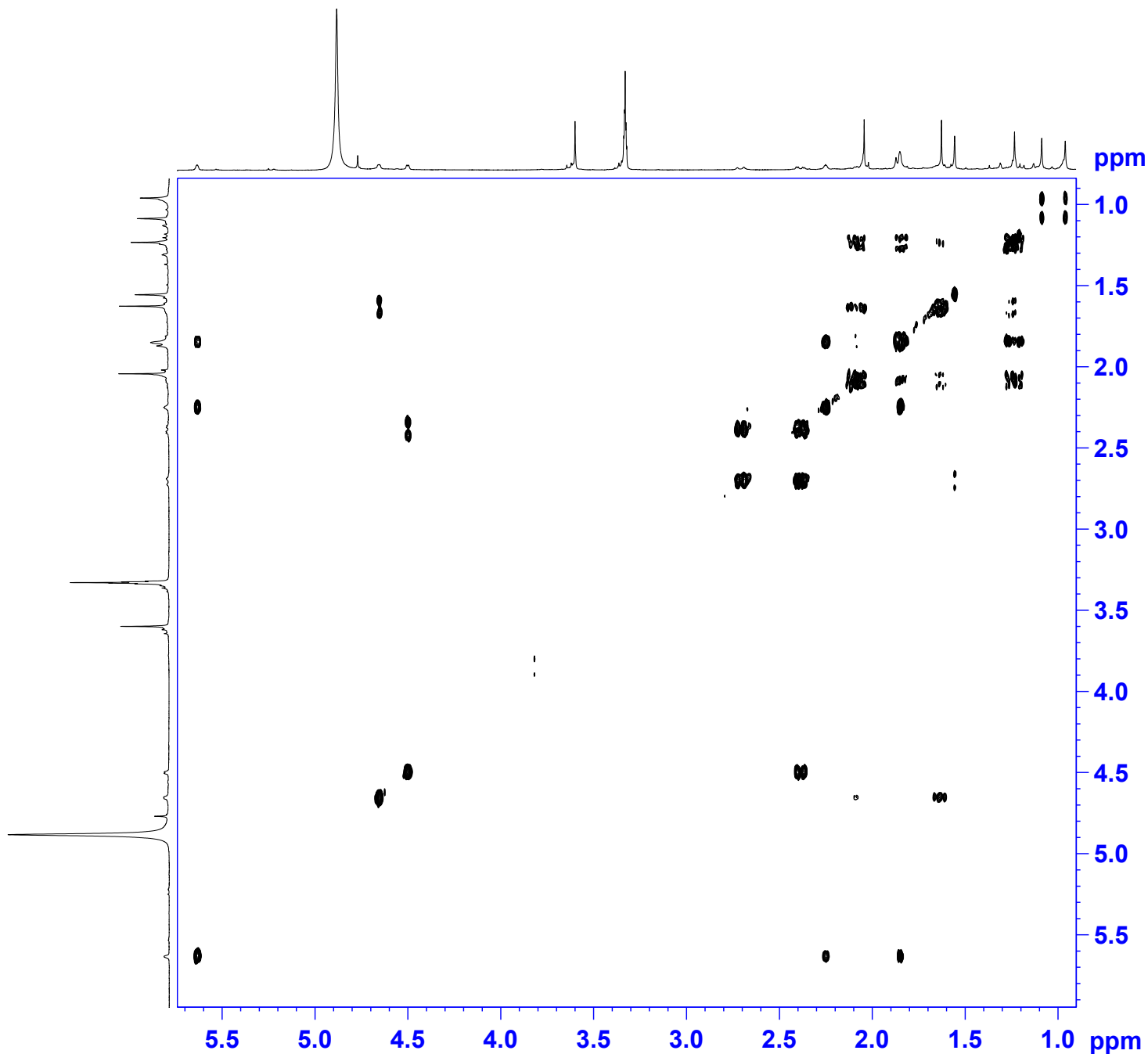


Figure S6. COSY NMR spectrum of **1** in CD₃OD.



Current Data Parameters
NAME X2C-35 M5.3
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190822
Time 13.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfqr
TD 2048
SOLVENT MeOD
NS 8
DS 8
SWH 2799.552 Hz
FIDRES 1.366969 Hz
AQ 0.3657728 sec
RG 203
DW 178.600 usec
DE 6.50 usec
TE 297.6 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00035700 sec

===== CHANNEL f1 =====
SF01 400.1314005 MHz
NUC1 1H
P1 13.90 usec
PLW1 12.14299965 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 400.1314 MHz
FIDRES 21.883753 Hz
SW 7.001 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S7. HMBC NMR spectrum of **1** in CD₃OD.

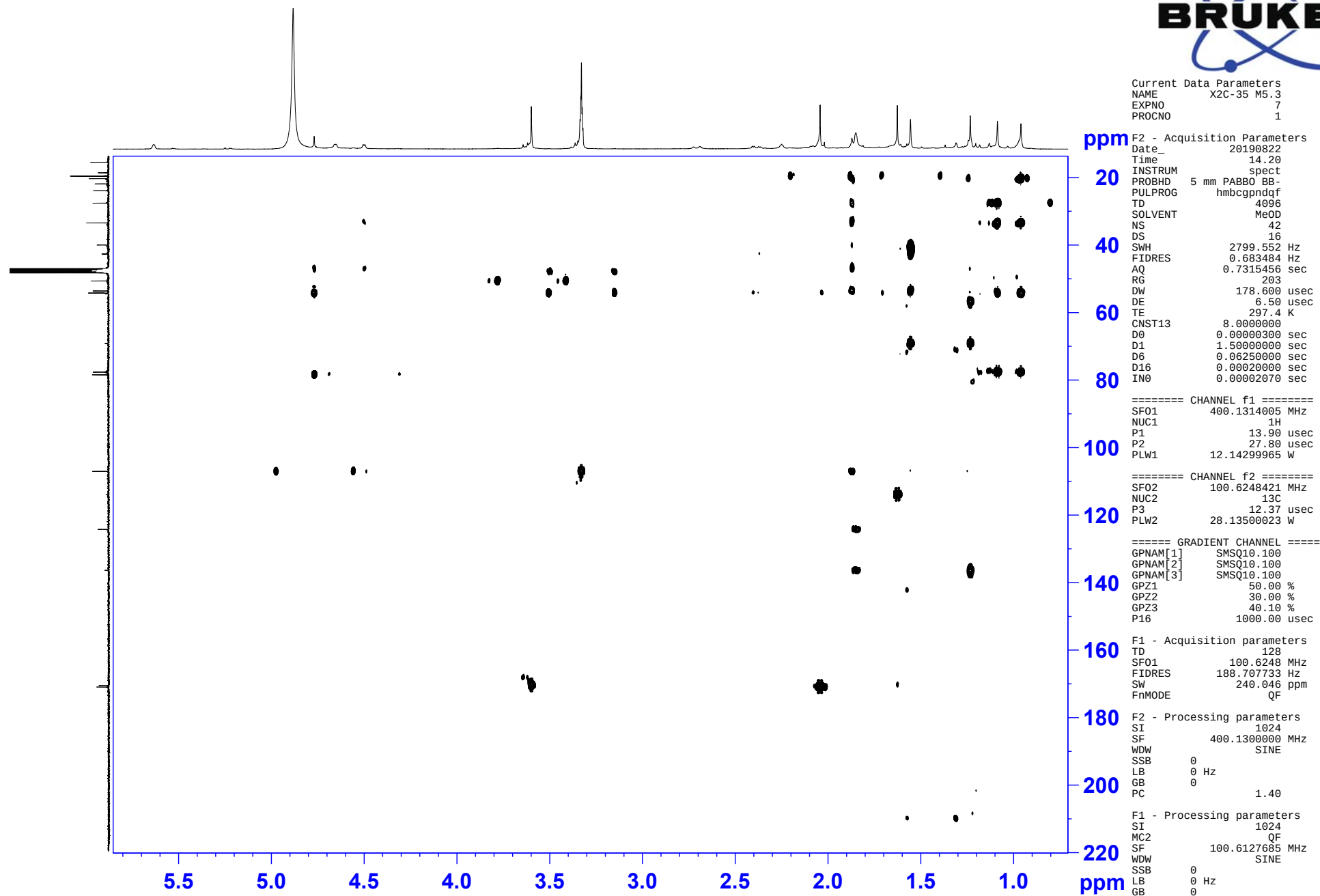
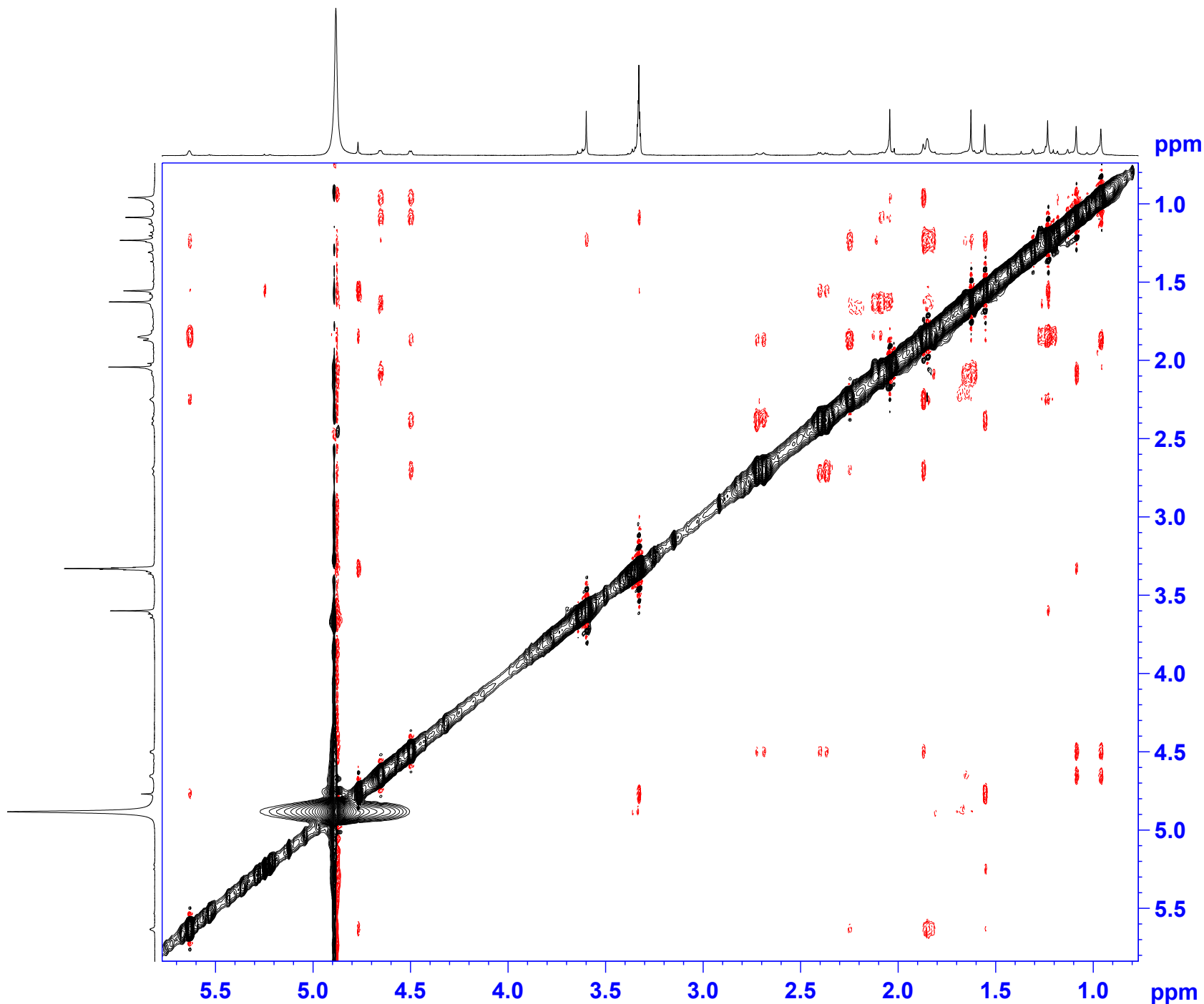


Figure S8. NOESY NMR spectrum of **1** in CD₃OD.



Current Data Parameters
NAME X2C-35 M5.3
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190823
Time 14.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesygpph
TD 2048
SOLVENT MeOD
NS 32
DS 32
SWH 2799.552 Hz
FIDRES 1.366969 Hz
AQ 0.3657728 sec
RG 203
DW 178.600 usec
DE 6.50 usec
TE 297.8 K
D0 0.00016080 sec
D1 2.00000000 sec
D8 0.30000001 sec
D11 0.03000000 sec
D12 0.00020000 sec
D16 0.00020000 sec
IN0 0.00035700 sec

===== CHANNEL f1 =====
SF01 400.1314005 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
P17 2500.00 usec
PLW1 12.14299965 W
PLW10 3.47059989 W

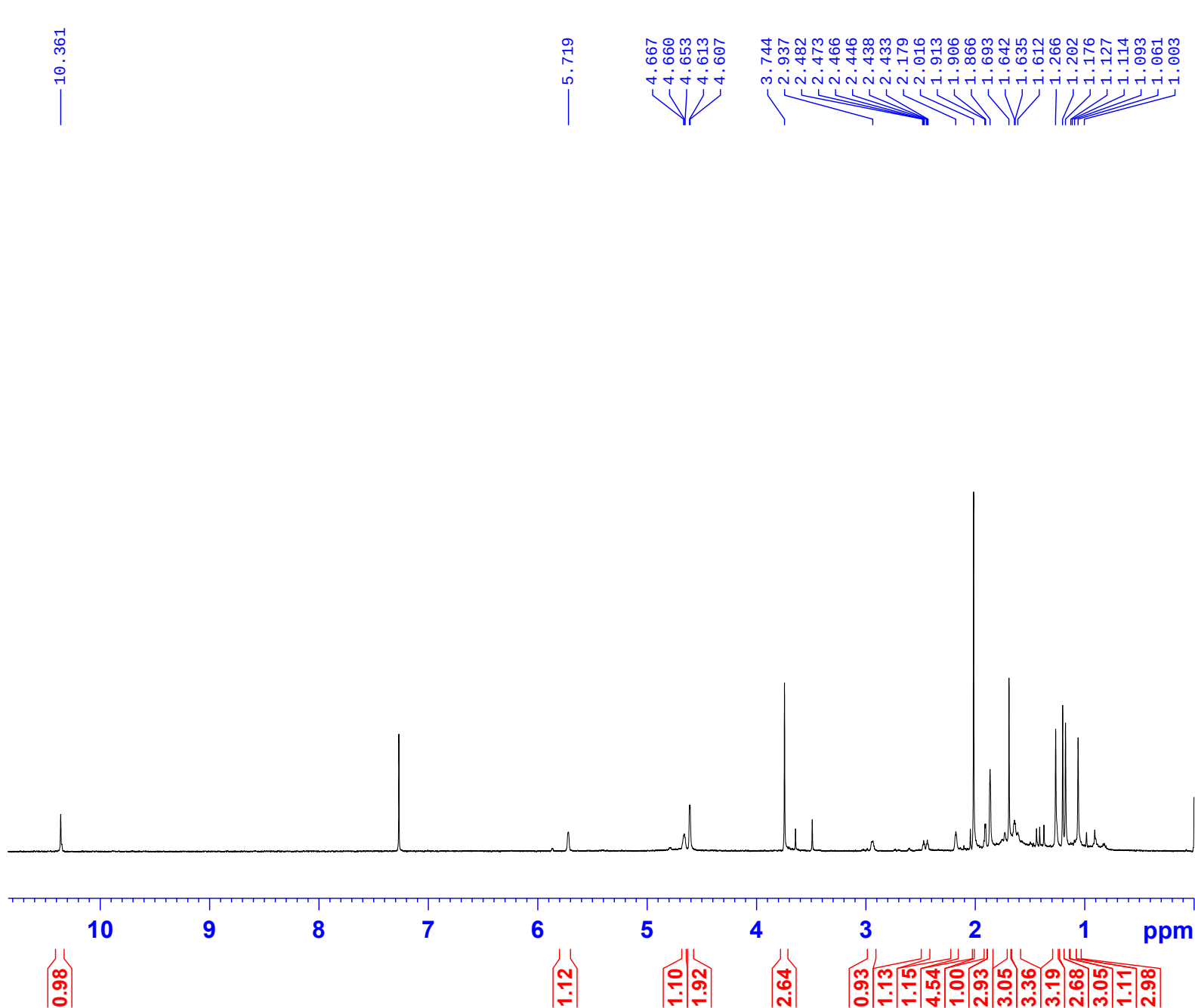
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 180
SF01 400.1314 MHz
FIDRES 15.561780 Hz
SW 7.001 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S9. ^1H NMR spectrum of **2** in CDCl_3 .



Current Data Parameters
NAME X2C-19 C2.5 NEW D
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190312
Time 11.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
SF01 400.1324710 MHz
NUC1 ^1H
P1 13.90 usec
PLW1 12.14299965 W

F2 - Processing parameters
SI 65536
SF 400.1300062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S10. ^{13}C NMR spectrum of **2** in CDCl_3 .

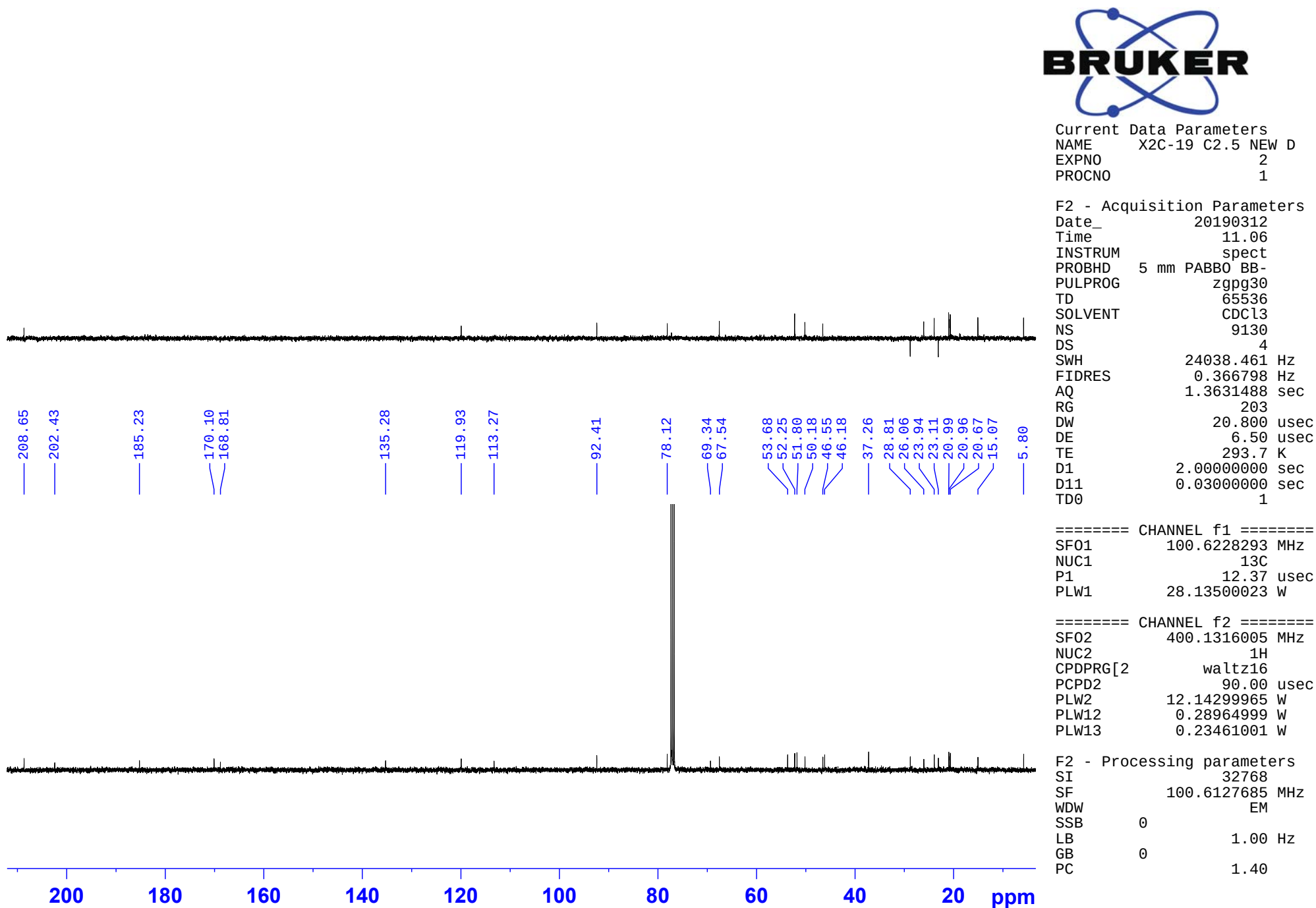


Figure S11. HSQC NMR spectrum of **2** in CDCl₃.

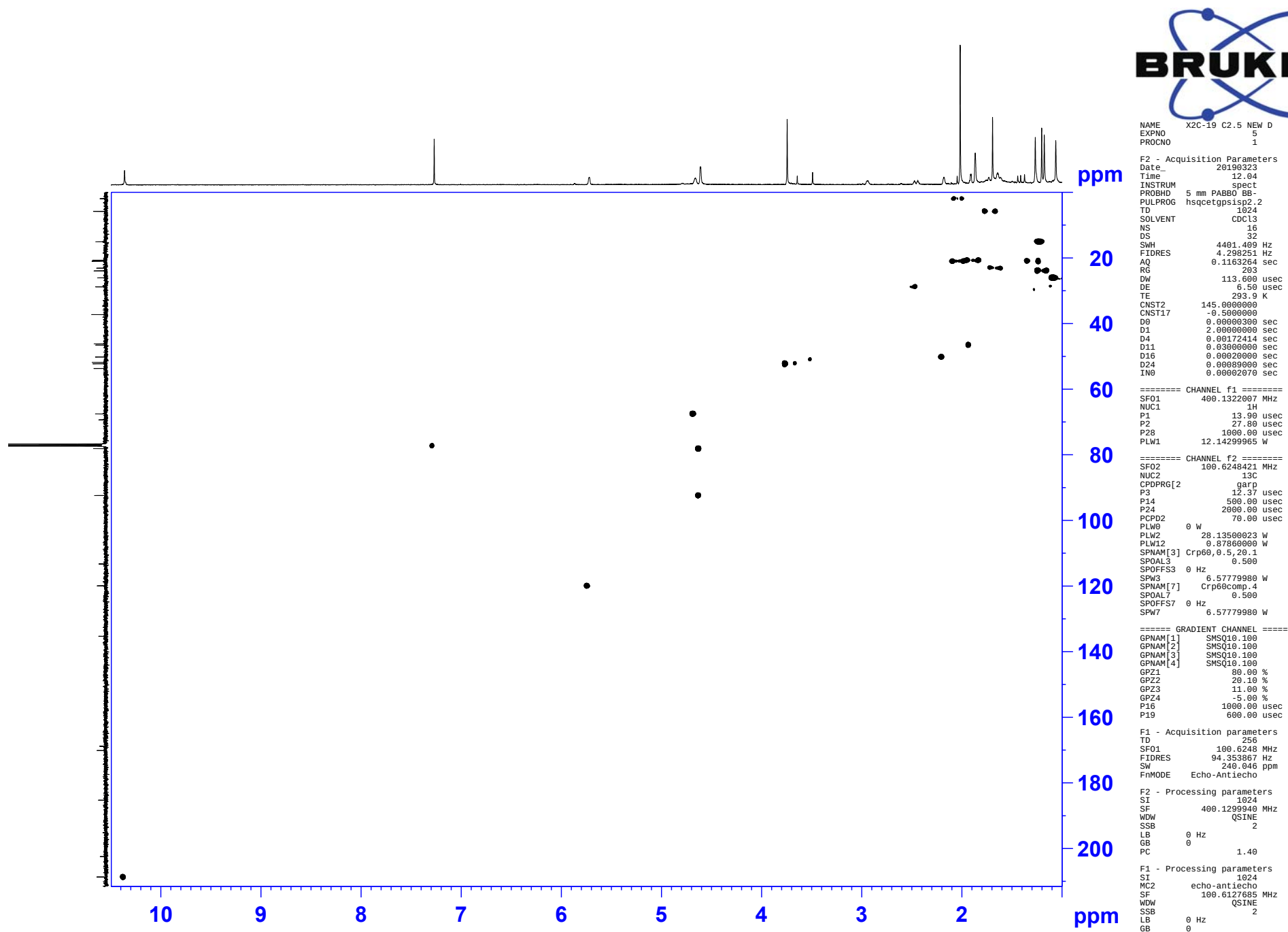


Figure S12. COSY NMR spectrum of **2** in CDCl₃.

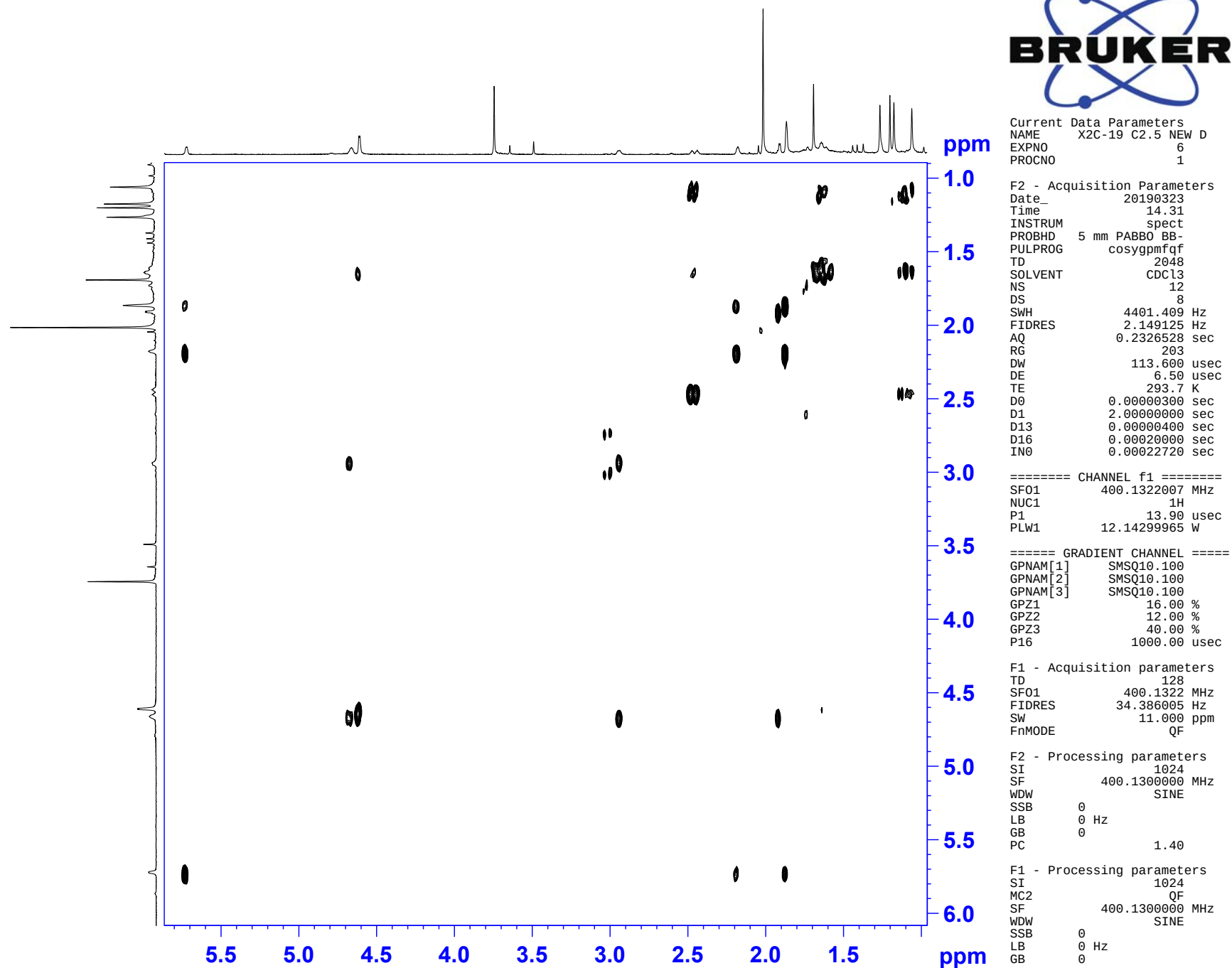


Figure S13. HMBC NMR spectrum of **2** in CDCl₃.



Current Data Parameters
NAME X2C-19 C2.5 NEW D
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190323
Time 15.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 64
DS 16
SWH 4401.409 Hz
FIDRES 1.074563 Hz
AQ 0.4653056 sec
RG 203
DW 113.600 usec
DE 6.50 usec
TE 293.5 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1322007 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
P3 12.37 usec
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 100.6248 MHz
FIDRES 188.707733 Hz
SW 240.046 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127685 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

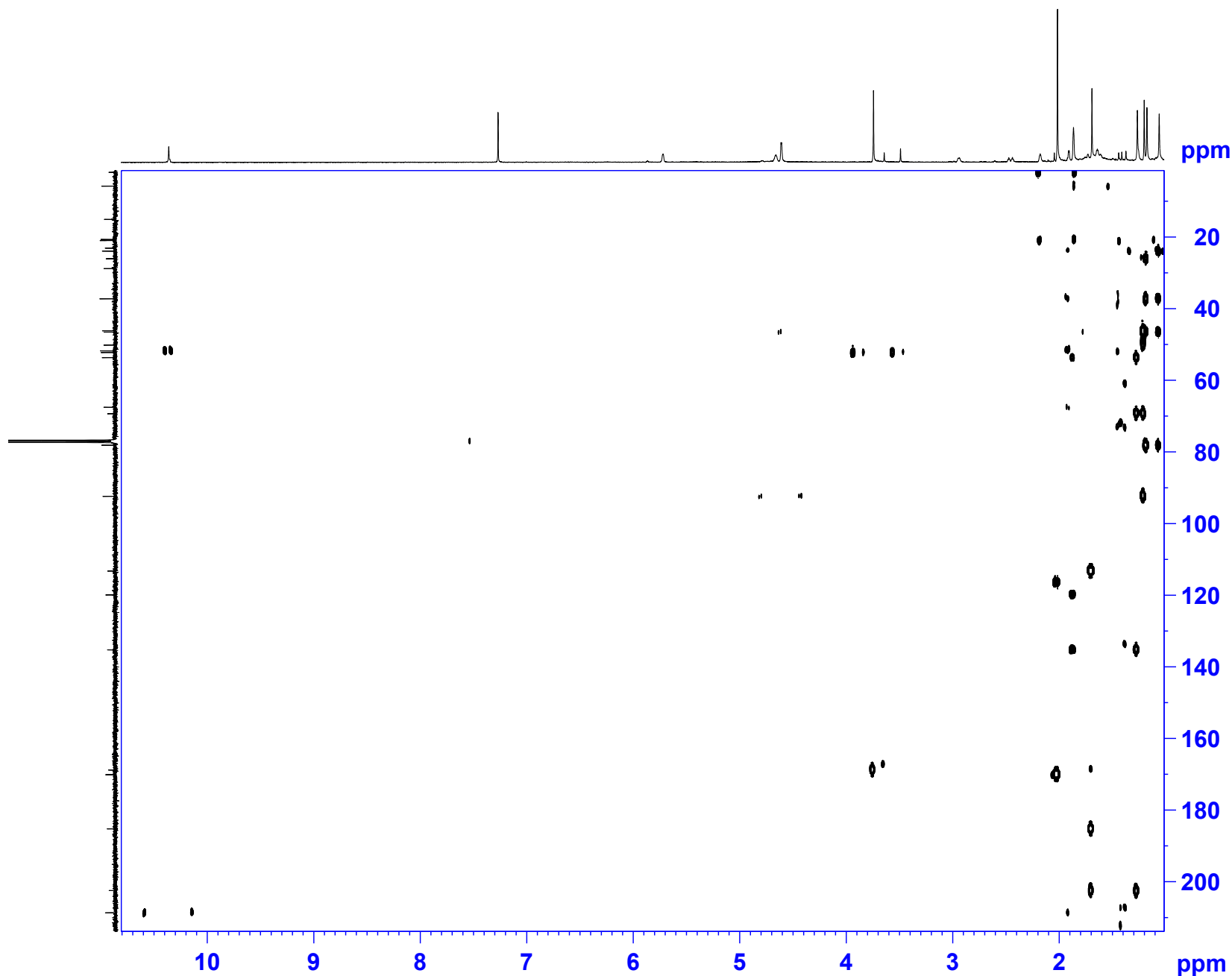


Figure S14. NOESY NMR spectrum of **2** in CDCl₃.

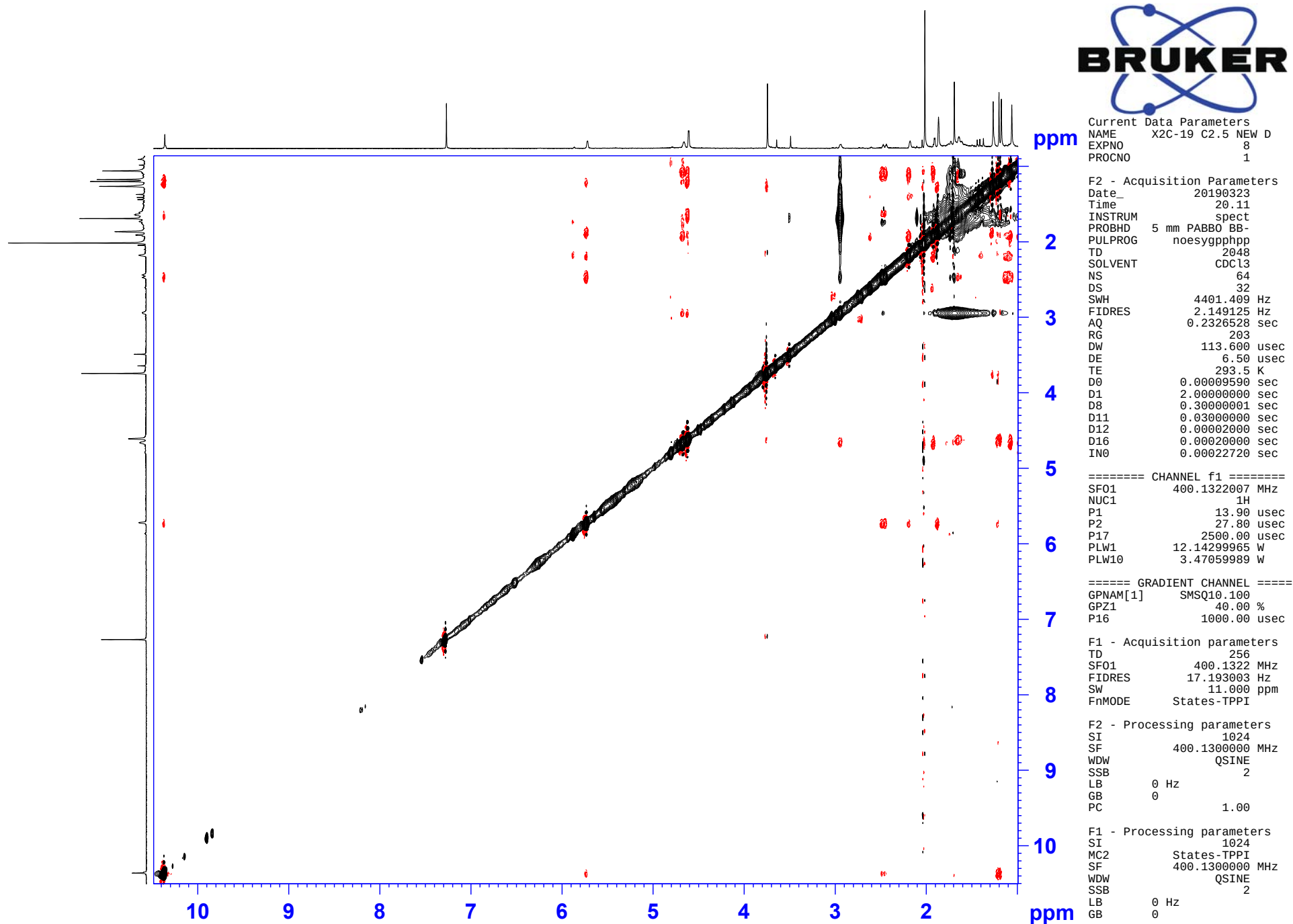


Figure S15. ^1H NMR spectrum of **3** in CDCl_3 .

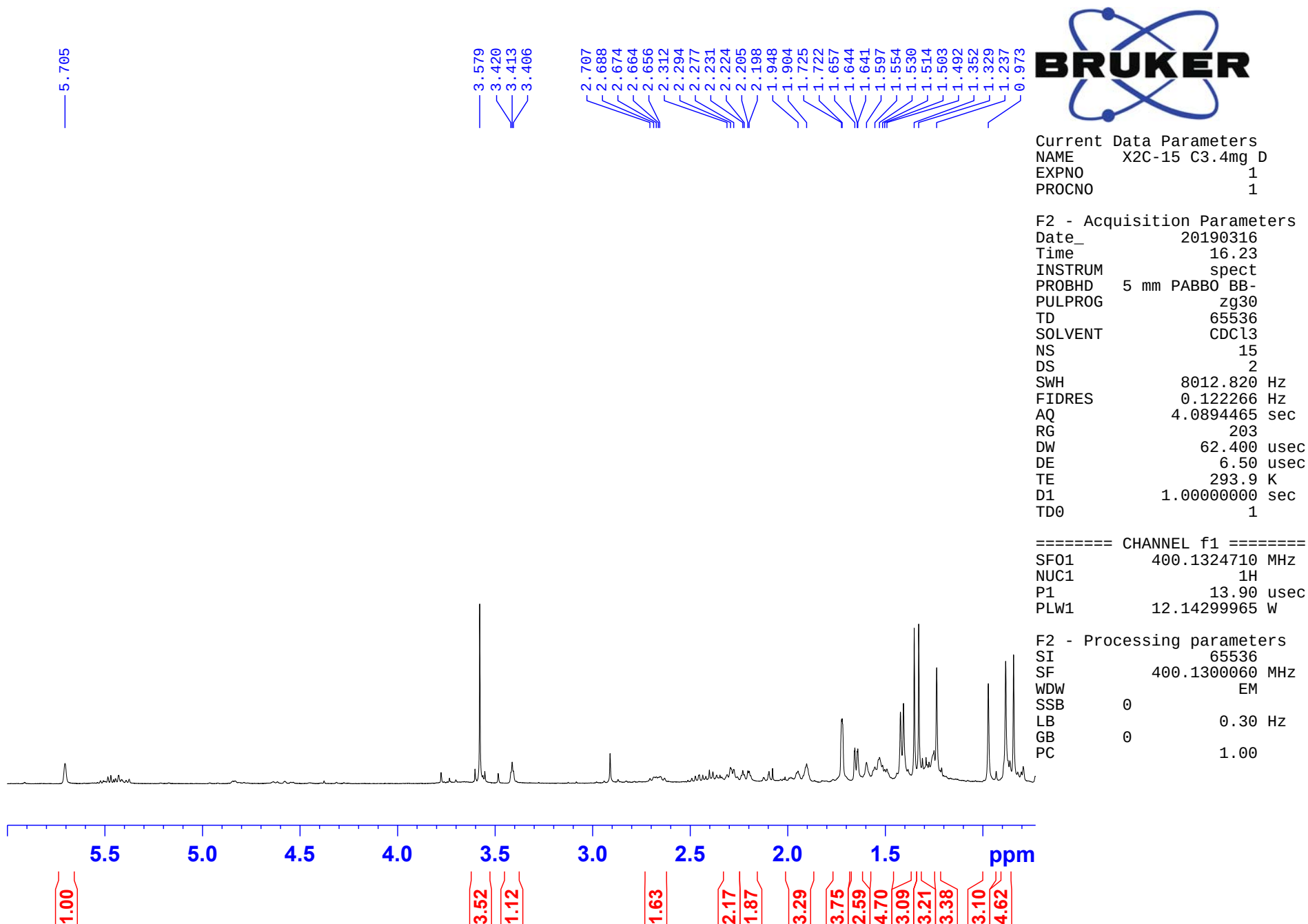
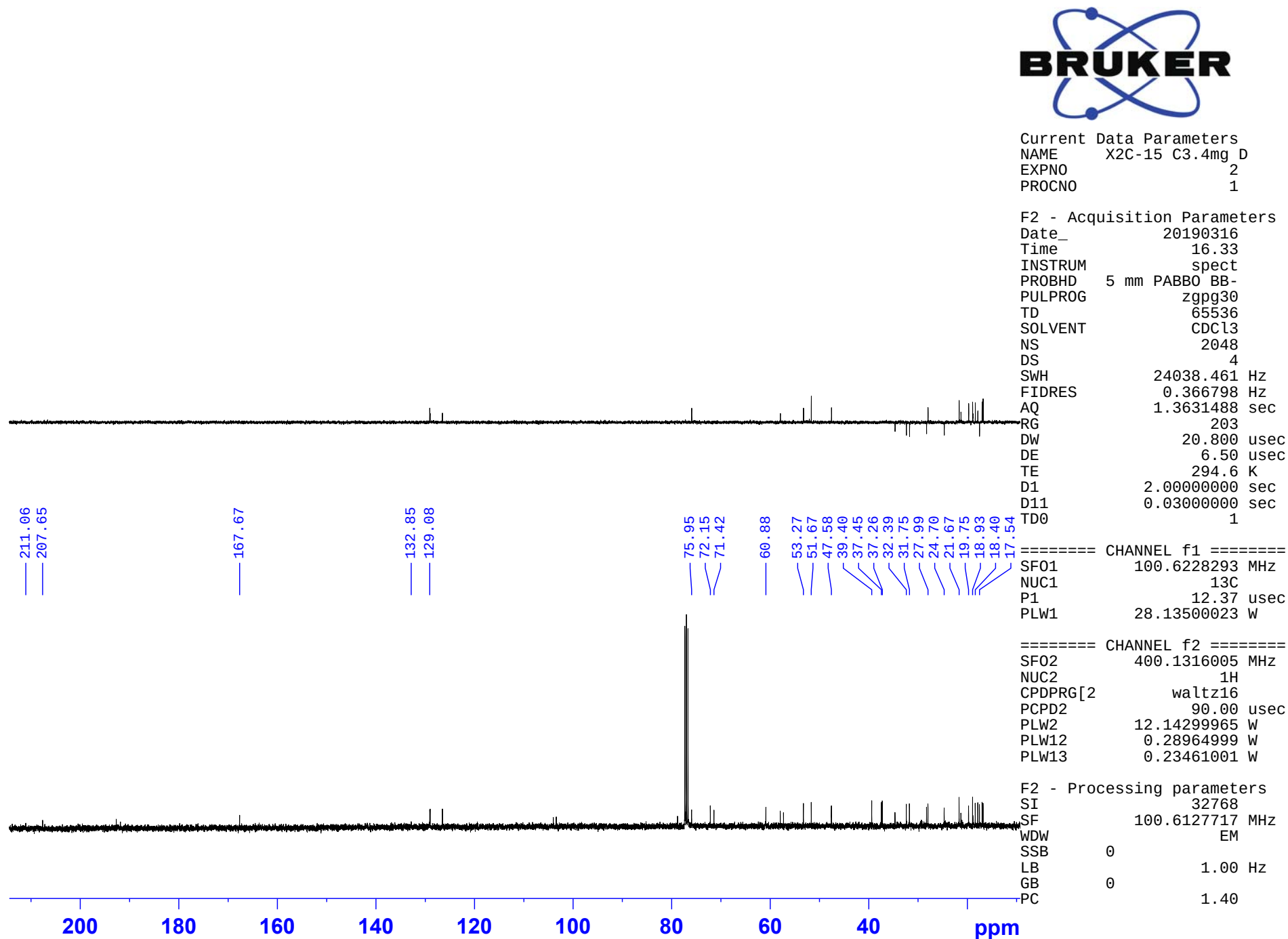


Figure S16. ^{13}C NMR spectrum of **3** in CDCl_3 .





Current Data Parameters
NAME X2C-15 C3.4mg D
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date 20190322
Time 9.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgpsisp2.2
TD 1024
SOLVENT CDCl3
NS 8
DS 32
SWH 3201.024 Hz
FIDRES 3.126000 Hz
AQ 0.1599488 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 294.3 K
CNST2 145.0000000
CNST17 -0.5000000
D0 0.00000300 sec
D1 2.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
P28 1000.00 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.37 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 70.00 usec
PLW0 0 W
PLW2 28.13500023 W
PLW12 0.87800000 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 6.57779980 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 6.57779980 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SF01 100.6248 MHz
FIDRES 94.353867 Hz
SW 240.046 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6127685 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

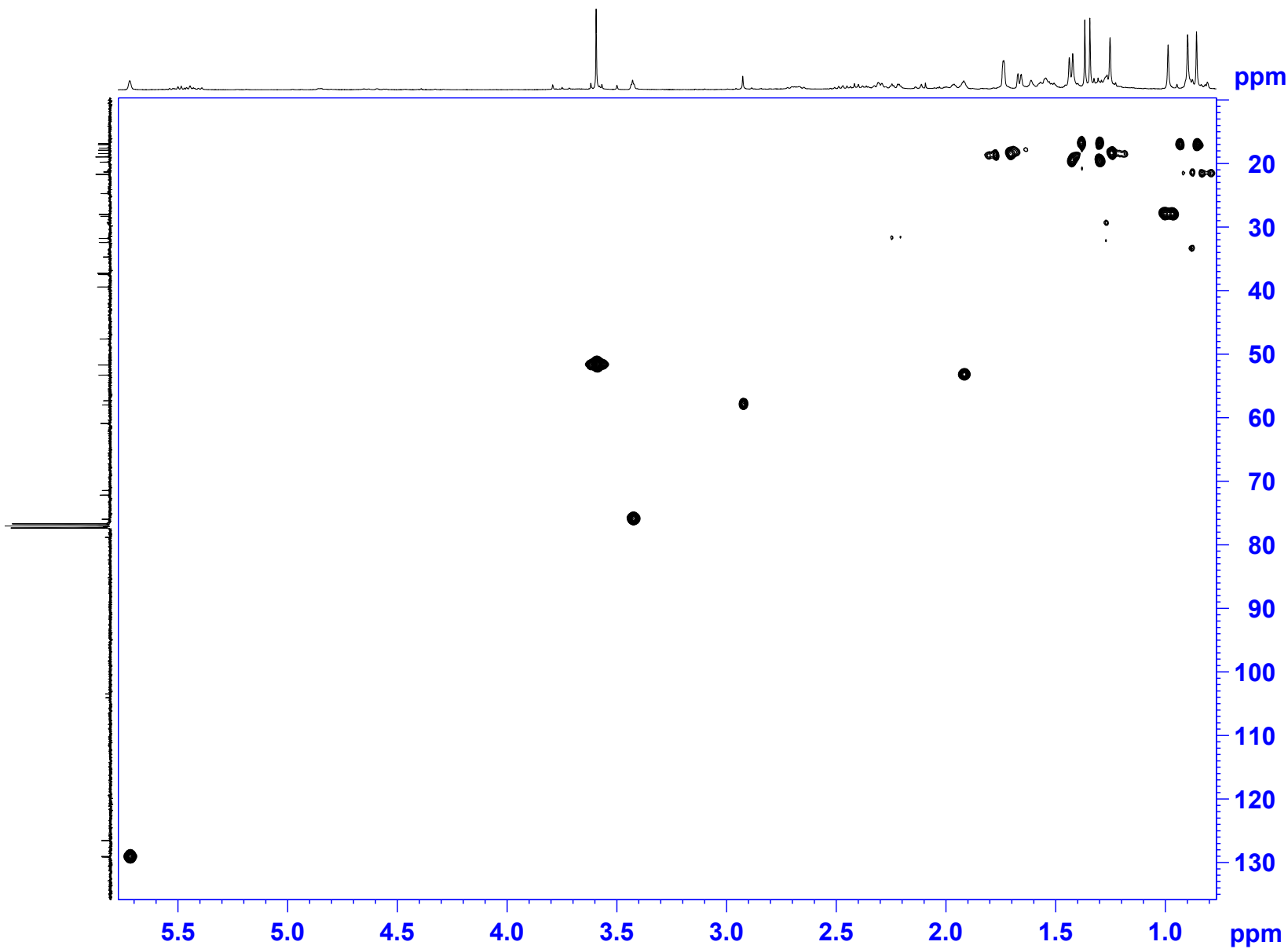
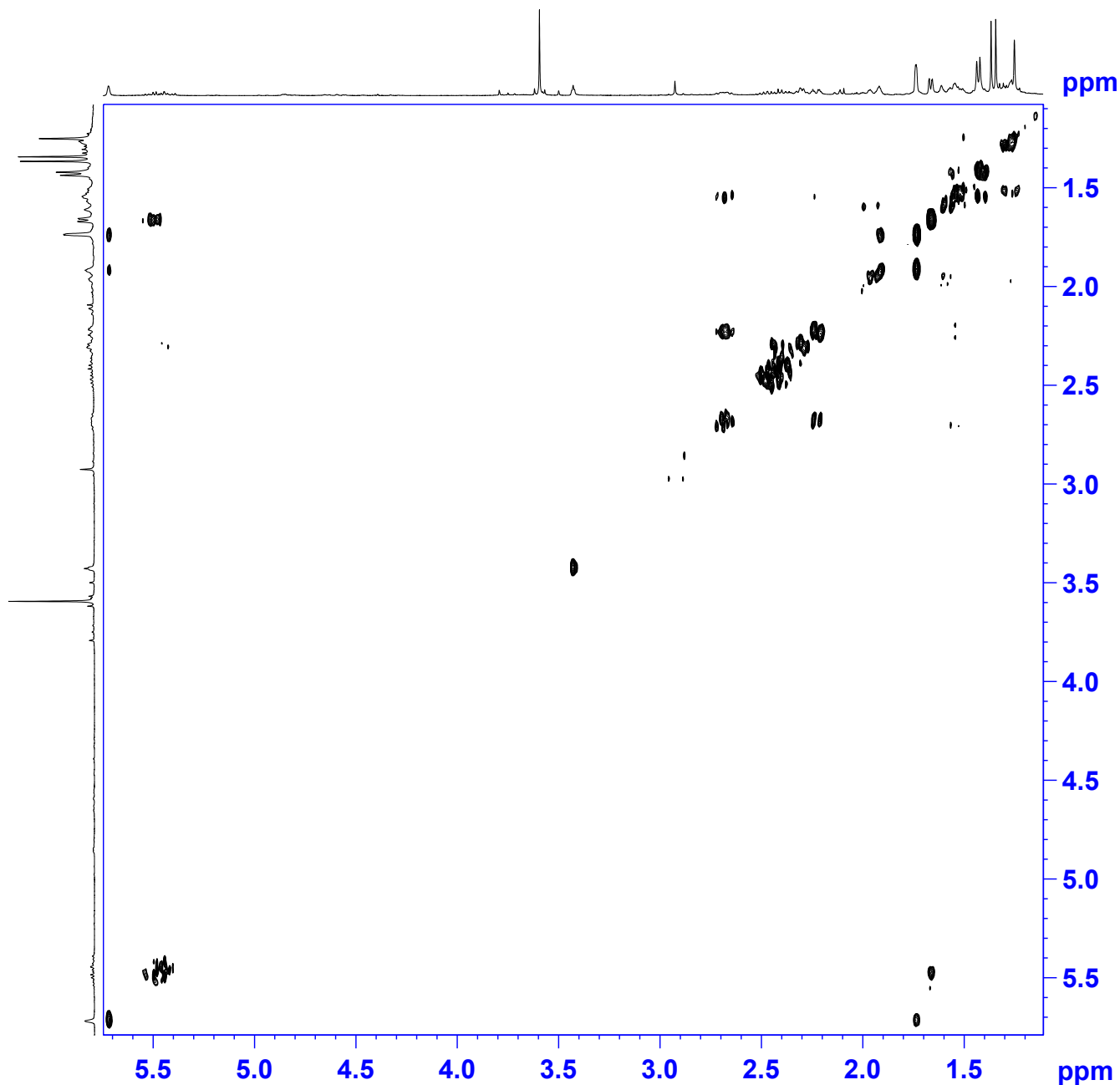


Figure S18. COSY NMR spectrum of **3** in CDCl₃.



Current Data Parameters
NAME X2C-15 C3.4mg D
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190322
Time 11.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfzf
TD 2048
SOLVENT CDCl3
NS 8
DS 8
SWH 3201.024 Hz
FIDRES 1.563000 Hz
AQ 0.3198976 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 294.2 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00031240 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.90 usec
PLW1 12.14299965 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 400.1316 MHz
FIDRES 25.008003 Hz
SW 8.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S19. HMBC NMR spectrum of **3** in CDCl₃.



C
NAME x2C-1b C3.4mg D
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190322
Time 11.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 3201.024 Hz
FIDRES 0.781500 Hz
AQ 0.6397952 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 293.9 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
P3 12.37 usec
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 100.6248 MHz
FIDRES 188.707733 Hz
SW 240.046 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127524 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

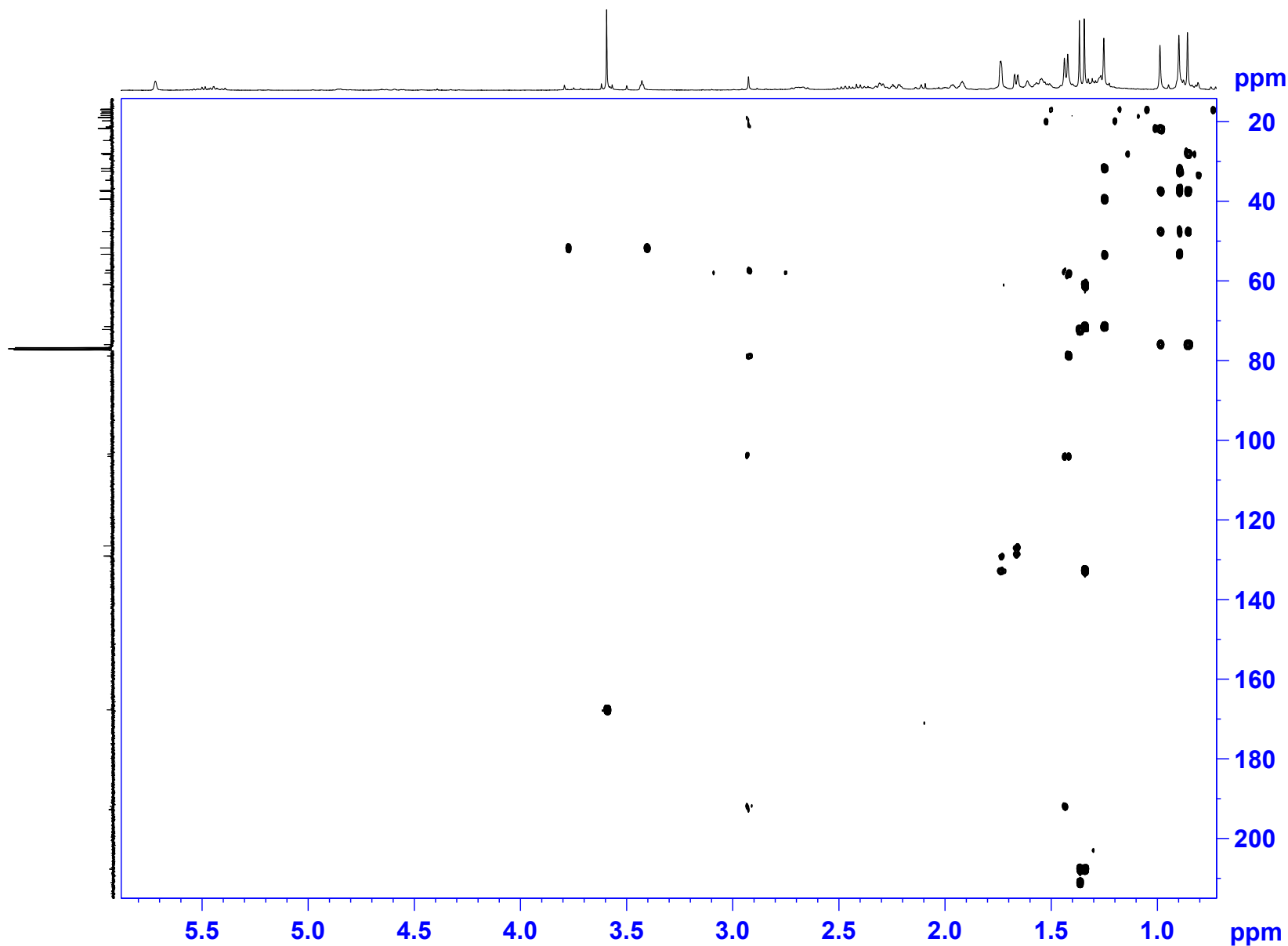


Figure S20. NOESY NMR spectrum of **3** in CDCl₃.

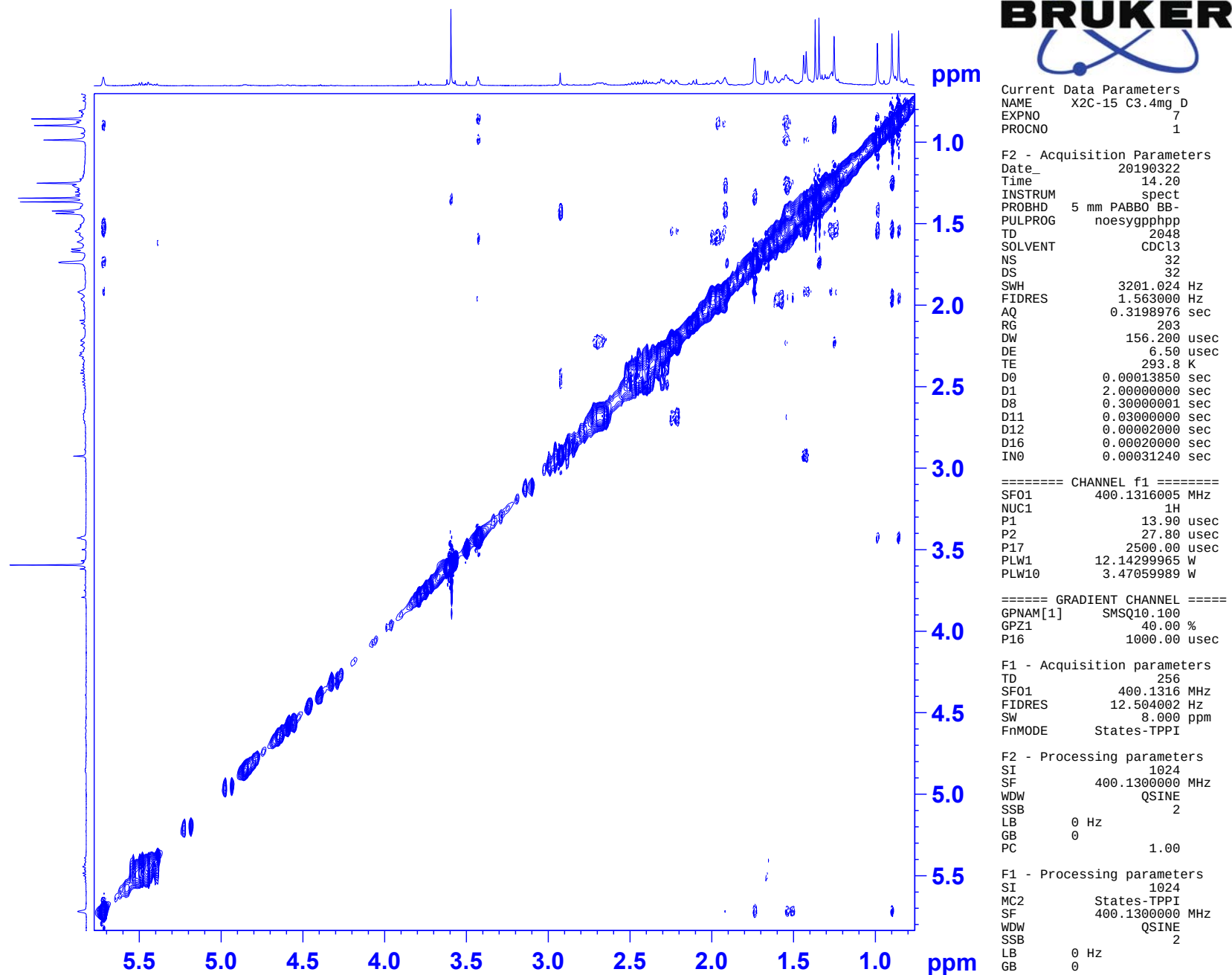
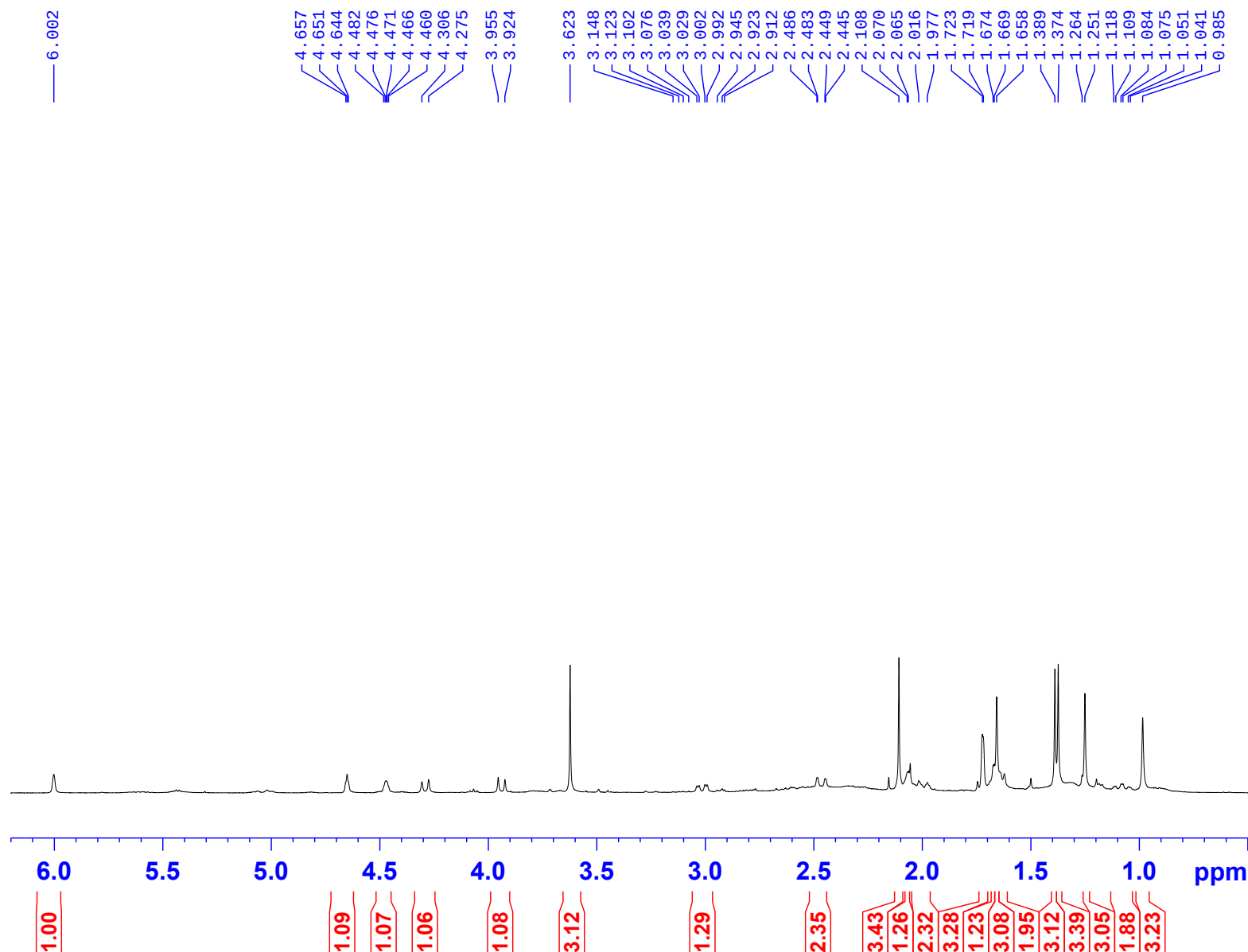


Figure S21. ^1H NMR spectrum of **4** in CDCl_3 .

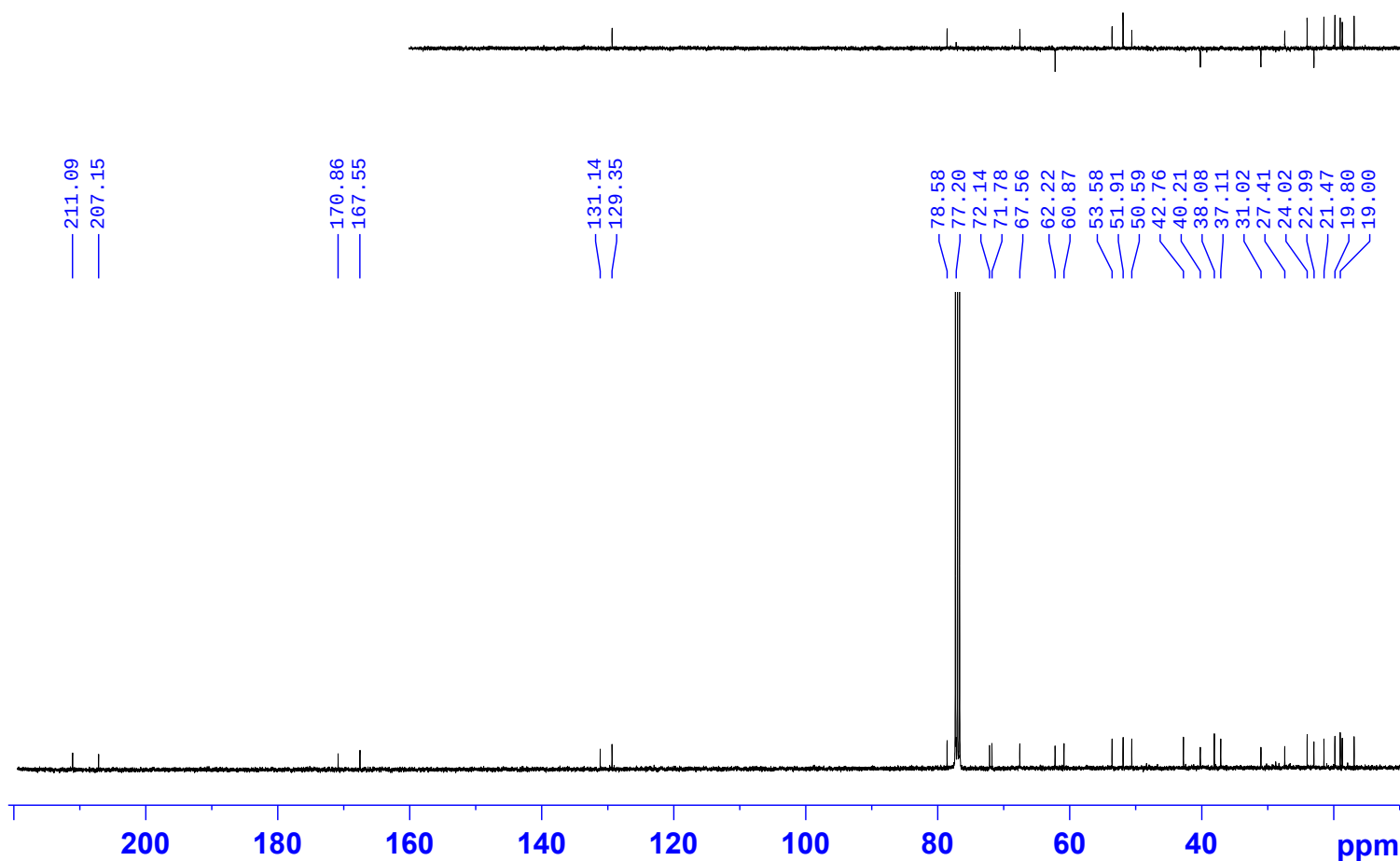


Current Data Parameters
NAME X2C-24 C6.8 NEW D
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190320
Time 17.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl_3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
SF01 400.1324710 MHz
NUC1 ^1H
P1 13.90 usec
PLW1 12.14299965 W

F2 - Processing parameters
SI 65536
SF 400.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S22. ^{13}C NMR spectrum of **4** in CDCl_3 .



Current Data Parameters
NAME X2C-24 C6.8 NEW D
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190320
Time 17.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl_3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6228293 MHz
NUC1 ^{13}C
P1 12.37 usec
PLW1 28.13500023 W

===== CHANNEL f2 =====
SF02 400.1316005 MHz
NUC2 ^1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 12.14299965 W
PLW12 0.28964999 W
PLW13 0.23461001 W

F2 - Processing parameters
SI 32768
SF 100.6127720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S23. HSQC NMR spectrum of **4** in CDCl₃.

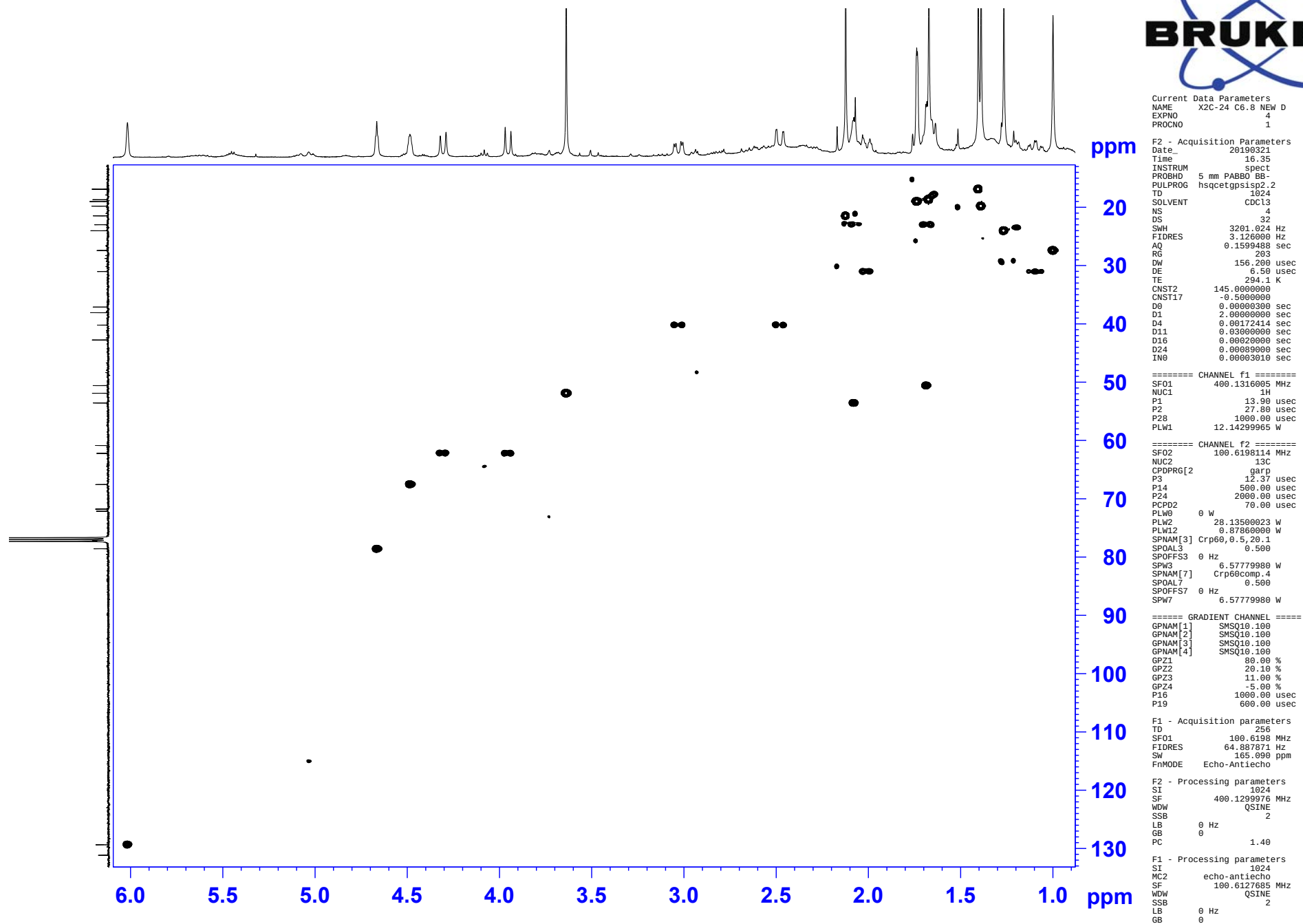
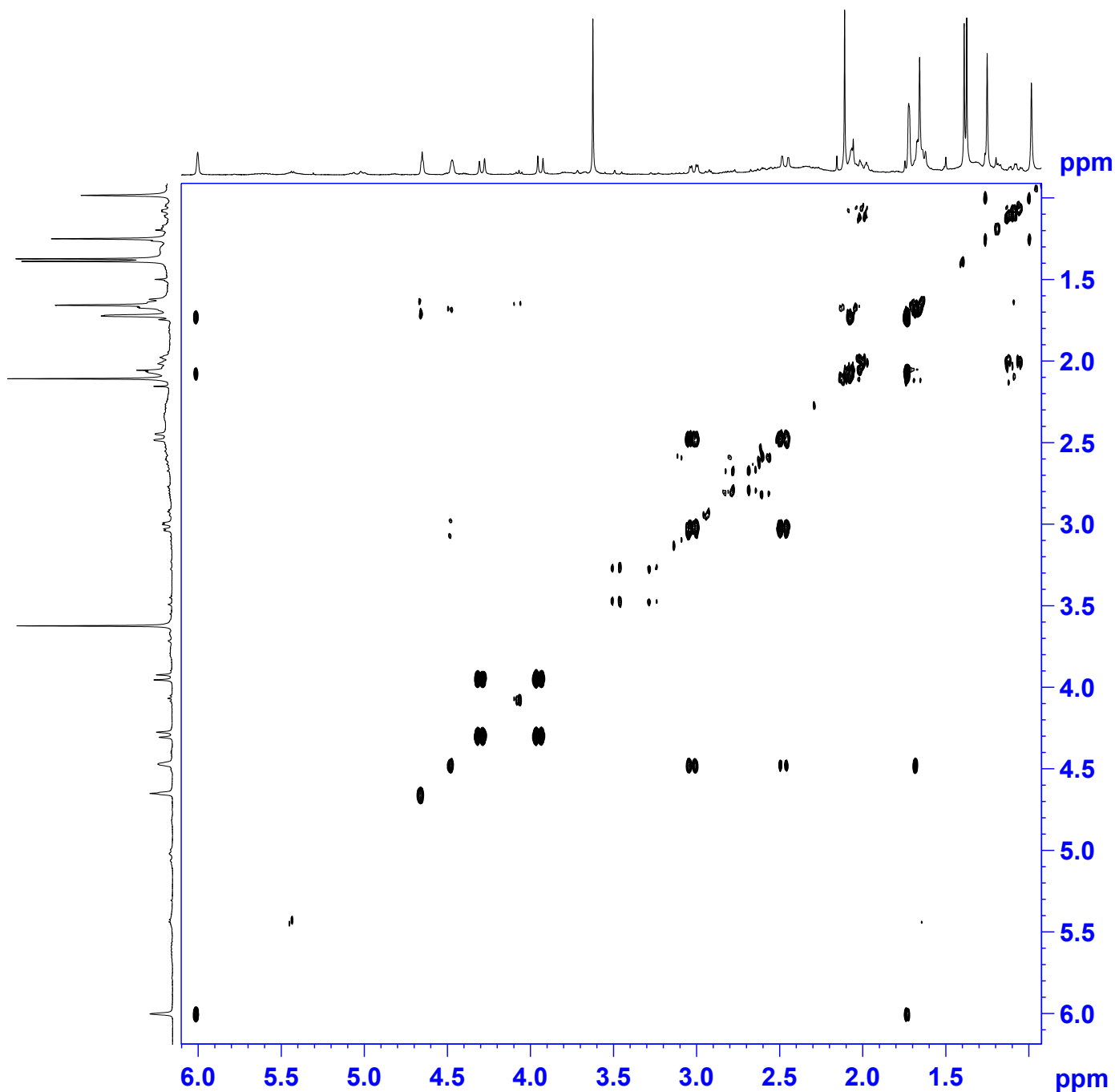


Figure S24. COSY NMR spectrum of **4** in CDCl₃.



Current Data Parameters
NAME X2C-24 C6.8 NEW D
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190321
Time 17.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfqr
TD 2048
SOLVENT CDCl3
NS 2
DS 8
SWH 3201.024 Hz
FIDRES 1.563000 Hz
AQ 0.3198976 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 293.8 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00031240 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.90 usec
PLW1 12.14299965 W

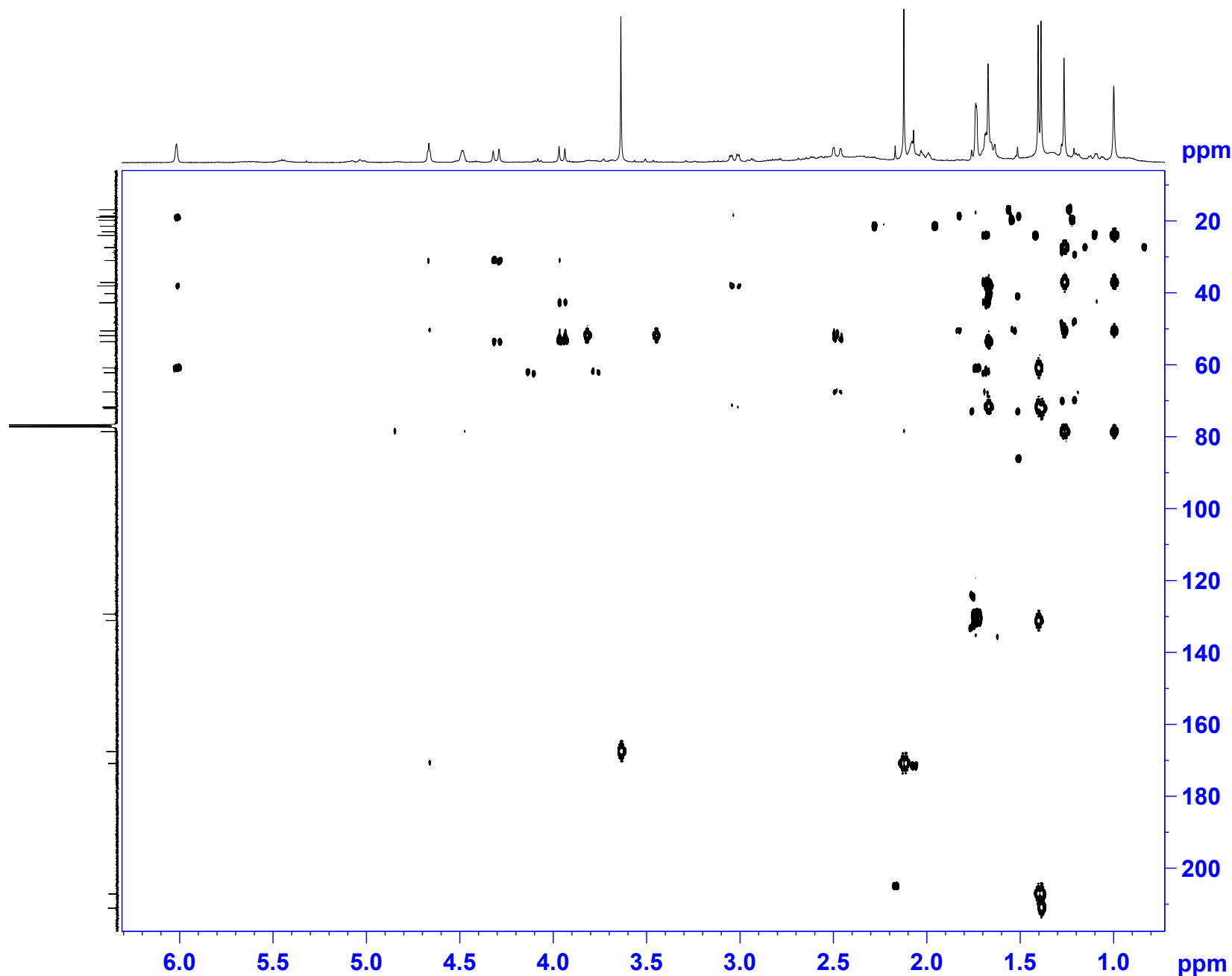
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 400.1316 MHz
FIDRES 25.008003 Hz
SW 8.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S25. HMBC NMR spectrum of **4** in CDCl₃.



Current Data Parameters
NAME X2C-24 C6.8 NEW D
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190326
Time 18.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 16
DS 16
SWH 3201.024 Hz
FIDRES 0.781500 Hz
AQ 0.6397952 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 293.8 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
P3 12.37 usec
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 100.6248 MHz
FIDRES 188.707733 Hz
SW 240.046 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127685 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

Figure S26. NOESY NMR spectrum of **4** in CDCl₃.

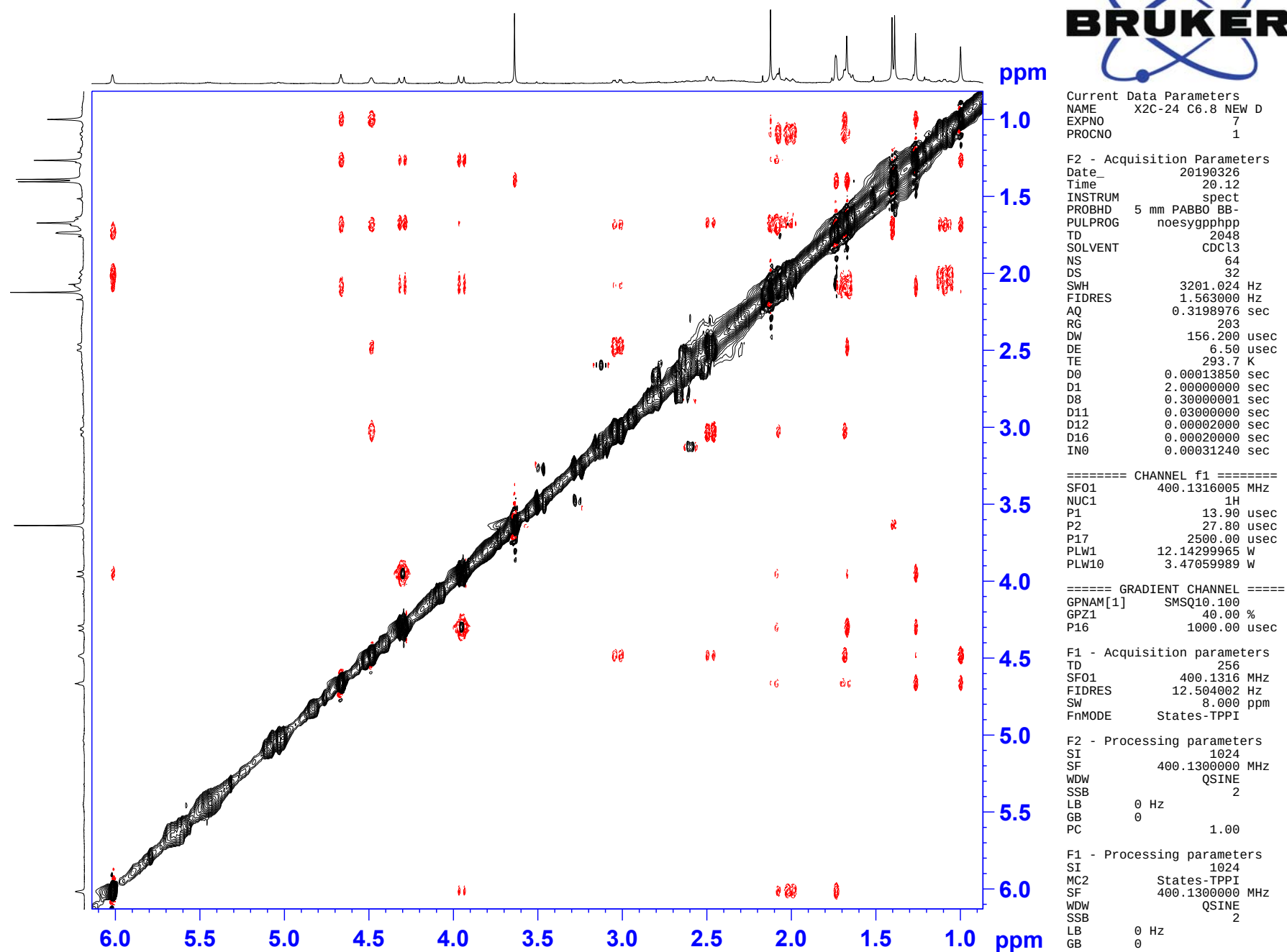
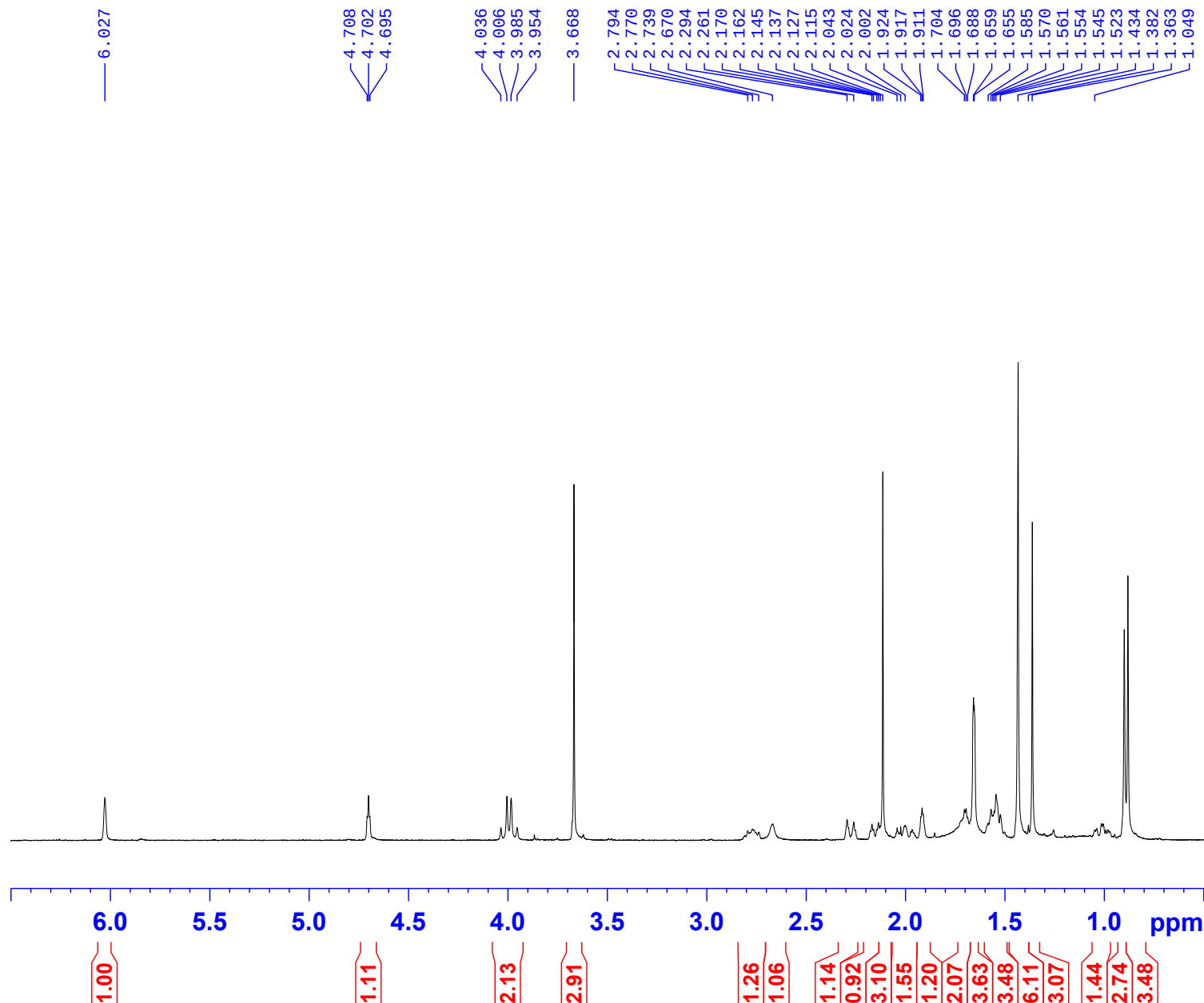


Figure S27. ^1H NMR spectrum of **5** in CDCl_3 .



Current Data Parameters
NAME X2C-9 M10mg NEW
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190309
Time 17.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 13.90 usec
PLW1 12.14299965 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S28. ^{13}C NMR spectrum of **5** in CDCl_3 .

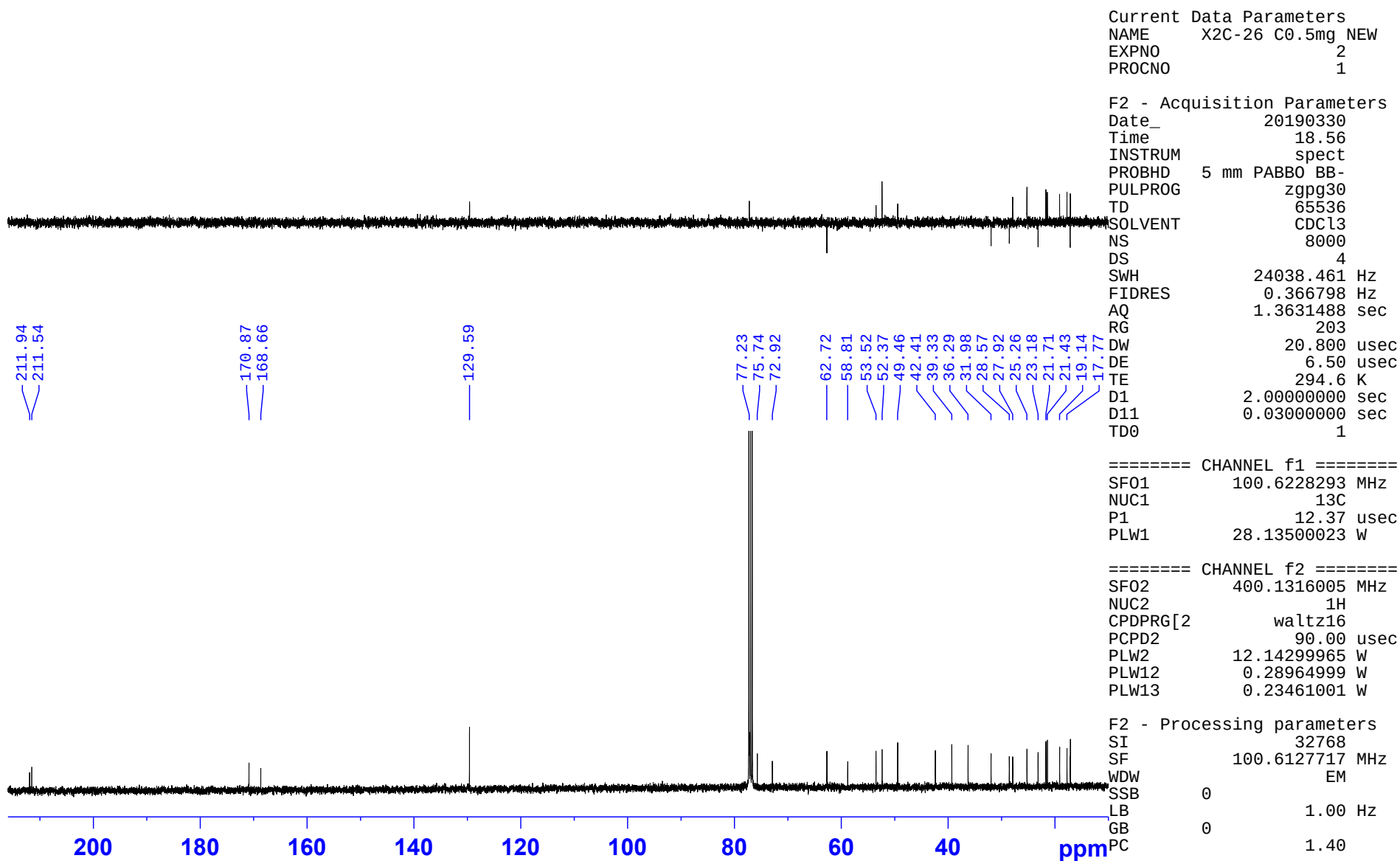


Figure S29. HSQC NMR spectrum of **5** in CDCl₃.



Current Data Parameters
NAME XZC-26 C0.5m0 NEW
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190331
Time 2.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgpsis2.2
TD 1024
SOLVENT CDCl3
NS 16
DS 32
SWH 3201.024 Hz
FIDRES 3.126000 Hz
AQ 0.1599488 sec
RG 203
DW 156.200 usec
DE 0.50 usec
TE 294.3 K
CNST2 145.000000
CNST17 -0.500000
D0 0.00000000 sec
D1 2.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.0002070 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.00 usec
P2 27.80 usec
P28 1000.00 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
CPDPRG2 garrp
P3 12.37 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 70.00 usec
PLW0 0 W
PLW2 28.13500023 W
PLW12 0.87860000 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 6.57779980 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 6.57779980 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SF01 100.6248 MHz
FIDRES 94.353867 Hz
SW 240.046 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1299977 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6127685 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

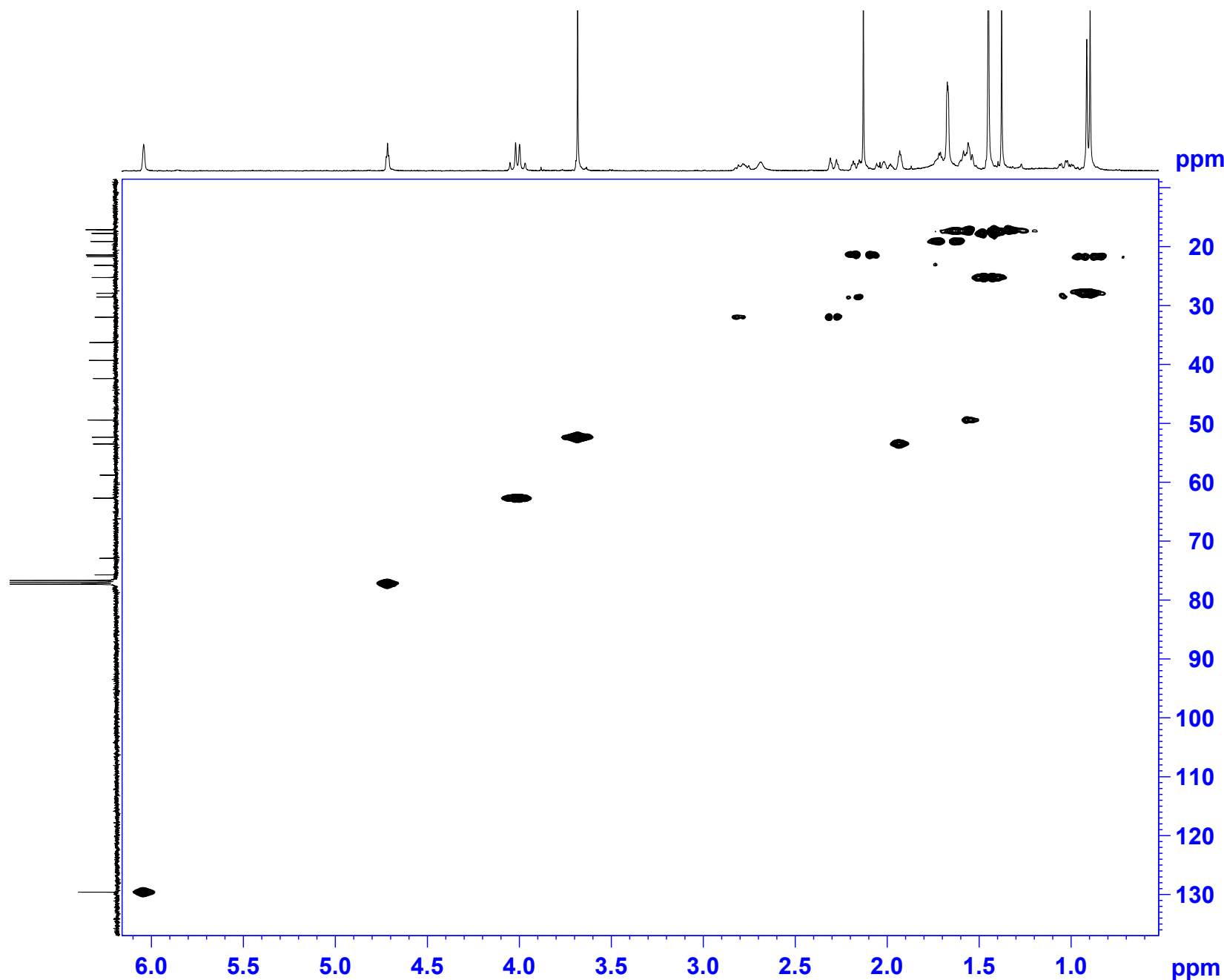


Figure S30. COSY NMR spectrum of **5** in CDCl₃.

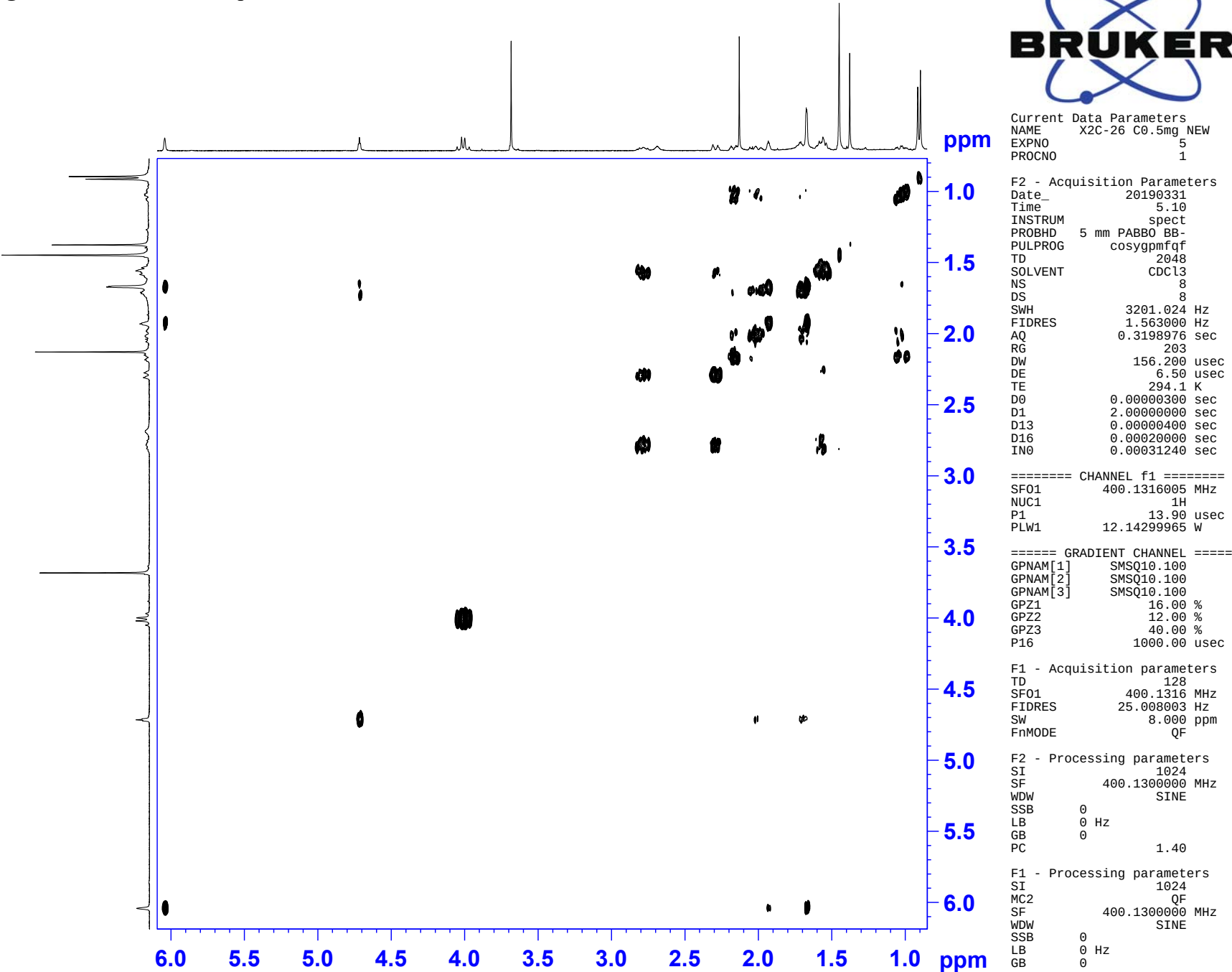


Figure S31. HMBC NMR spectrum of **5** in CDCl₃.



Current Data Parameters
NAME X2C-26 C0.5mg NEW
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190331
Time 5.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 3201.024 Hz
FIDRES 0.781500 Hz
AQ 0.6397952 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 293.8 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
P3 12.37 usec
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 100.6248 MHz
FIDRES 188.707733 Hz
SW 240.046 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127685 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

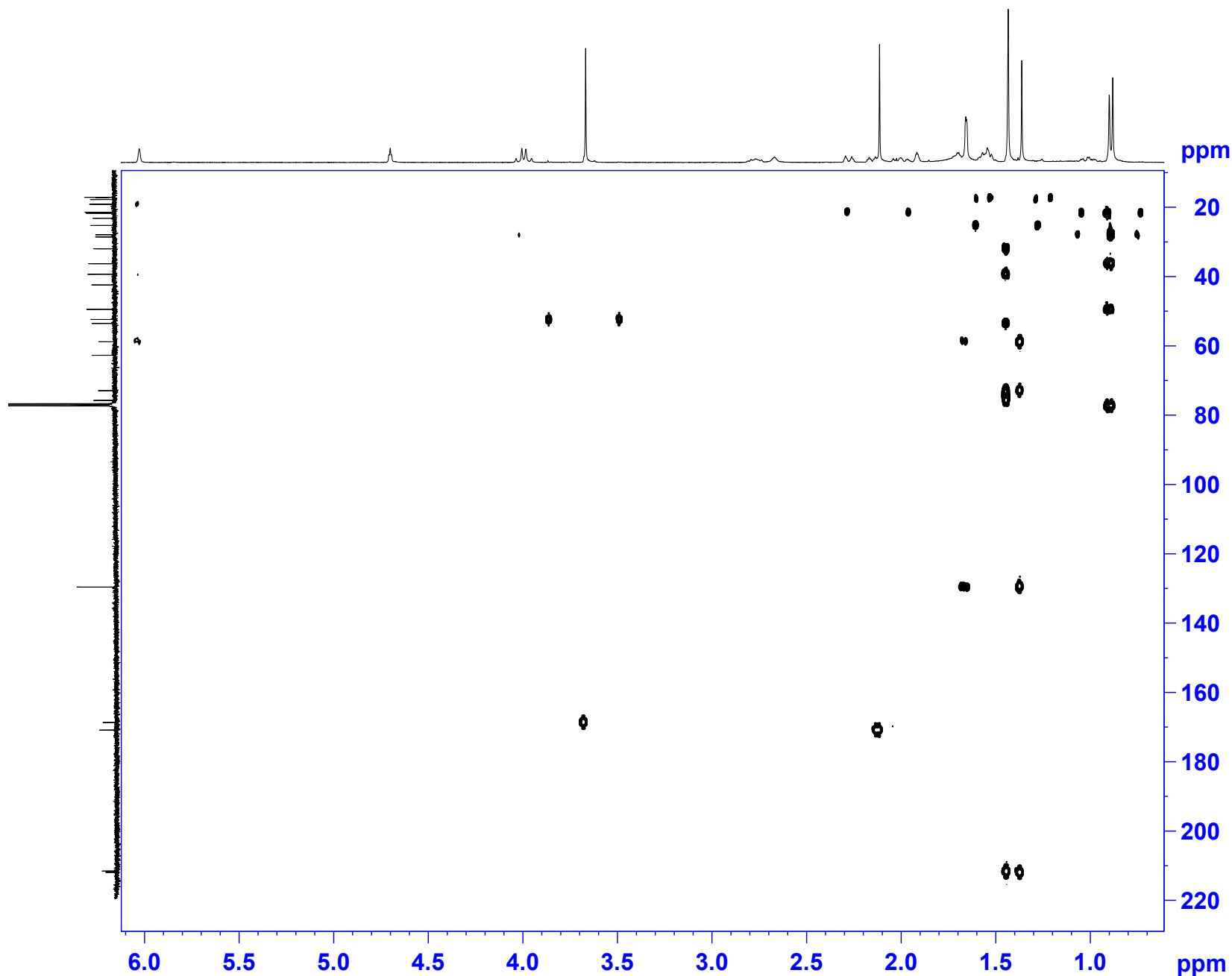


Figure S32. NOESY NMR spectrum of **5** in CDCl₃.

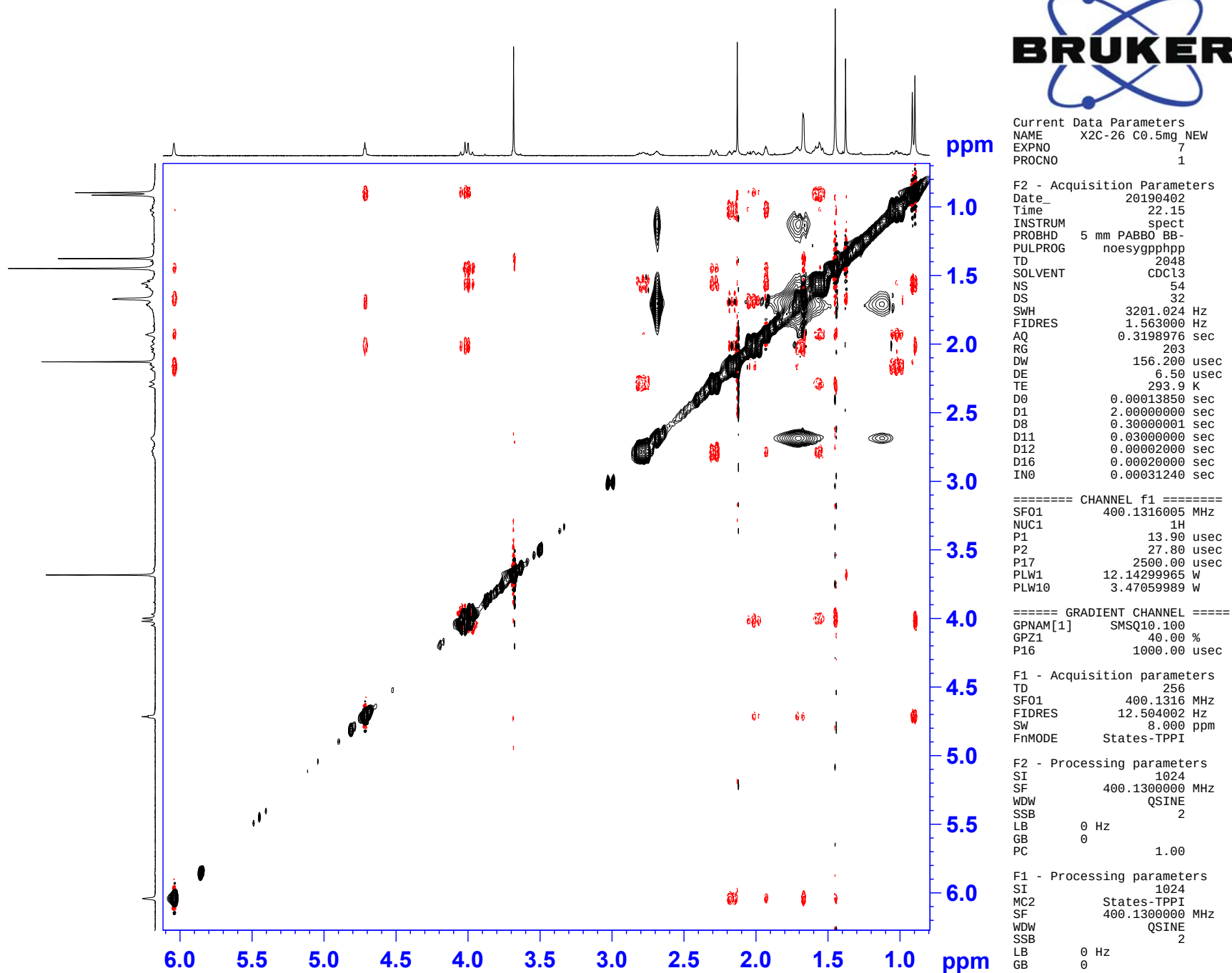


Figure S33. ^1H NMR spectrum of **6** in CD_3OD .

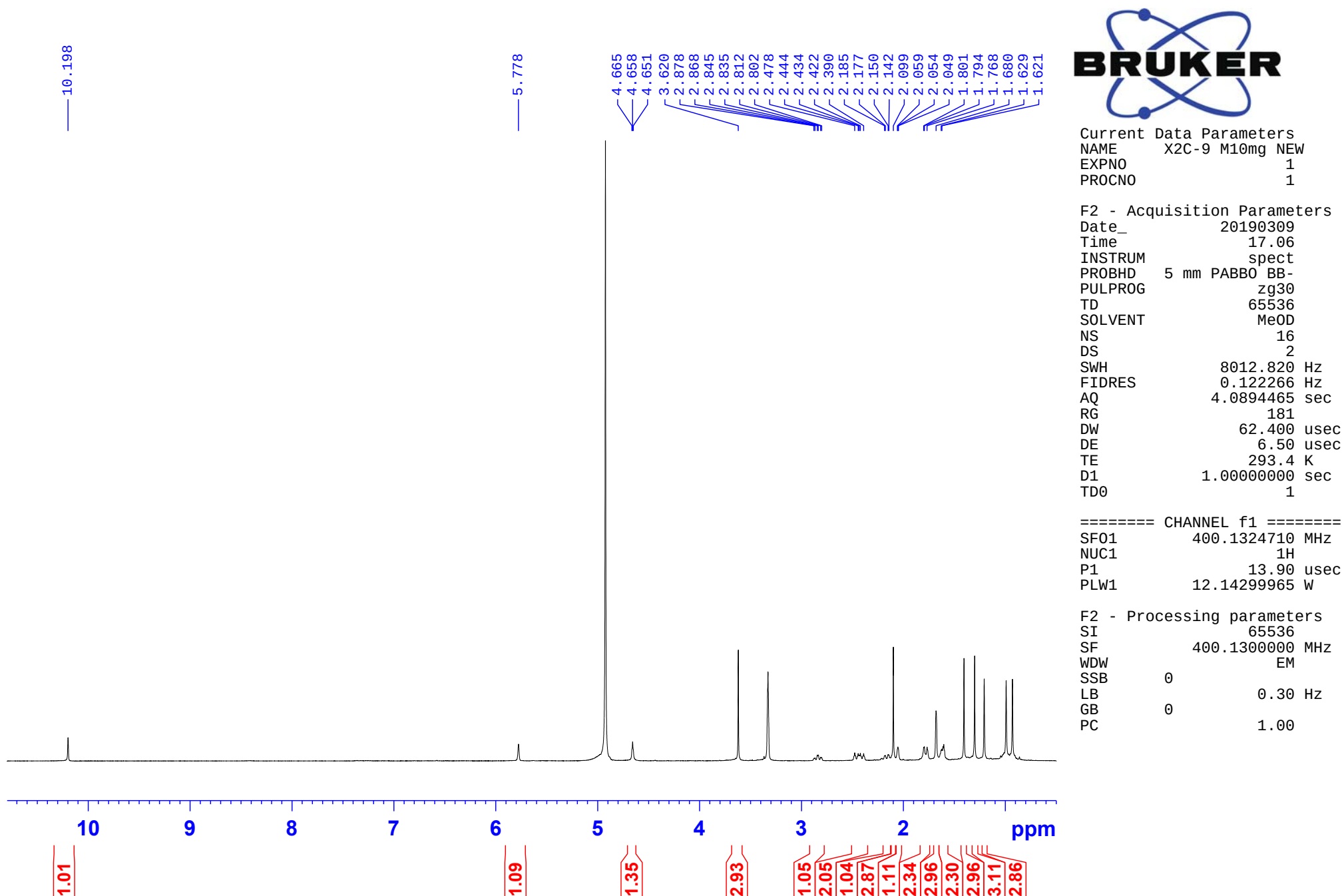


Figure S34. ^{13}C NMR spectrum of **6** in CD_3OD .

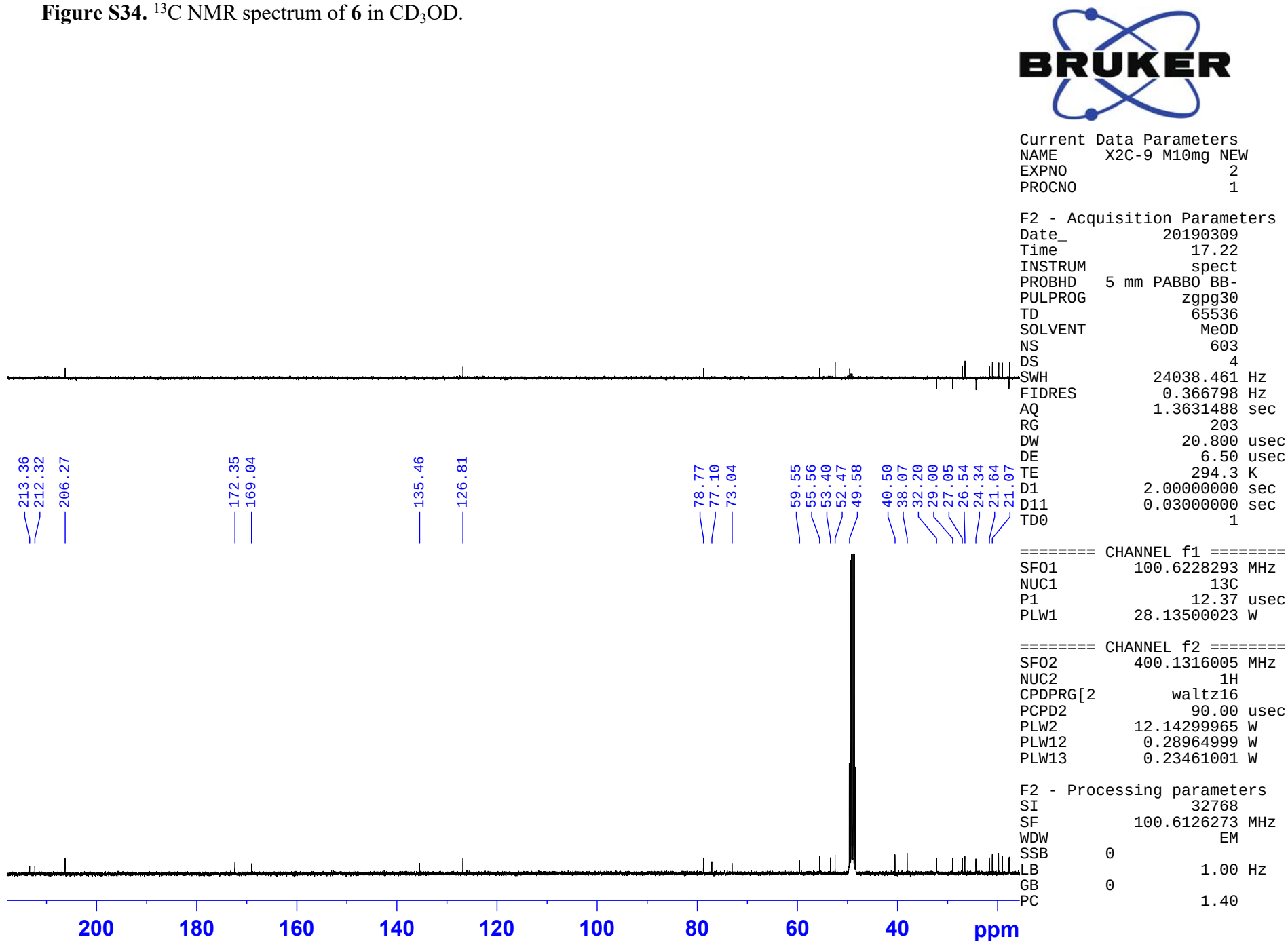
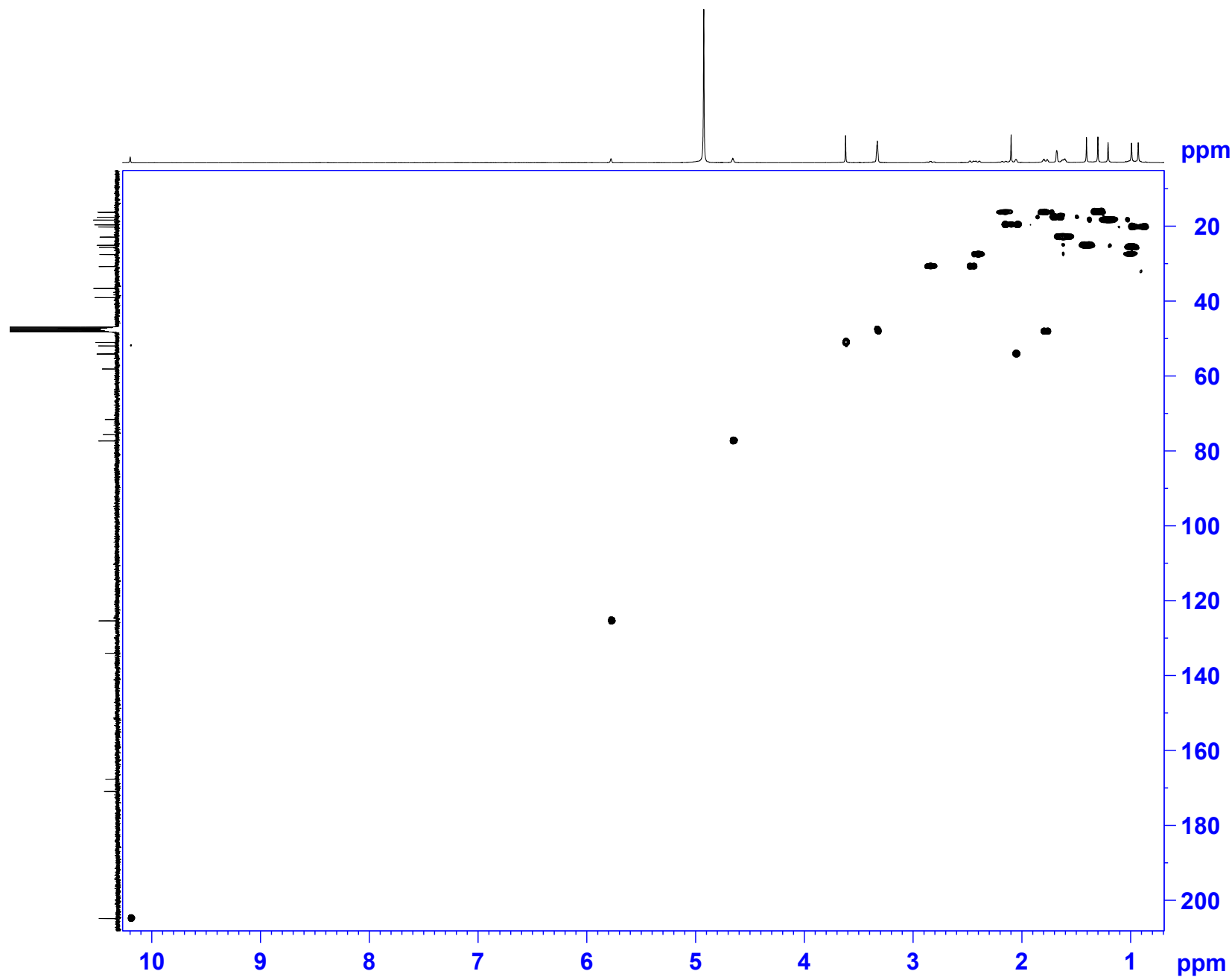


Figure S35. HSQC NMR spectrum of **6** in CD₃OD.



Current Data Parameters
NAME X2C-9 M10mg NEW
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190321
Time 8.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgpsisp2.2
TD 1024
SOLVENT MeOD
NS 8
DS 32
SWH 4401.409 Hz
FIDRES 4.298251 Hz
AQ 0.1163264 sec
RG 203
DM 113.600 usec
DE 6.50 usec
TE 294.0 K
CNST2 145.000000
CNST17 -0.500000
D0 0.00000000 sec
D1 2.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00000000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1322007 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
P28 1000.00 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
CPDPRG2 gard
P3 12.37 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 70.00 usec
PLW0 0 W
PLW2 28.13500023 W
PLW12 0.87860000 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 6.57779980 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 6.57779980 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SF01 100.6248 MHz
FIDRES 94.353867 Hz
SW 240.046 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6127685 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S36. COSY NMR spectrum of **6** in CD₃OD.

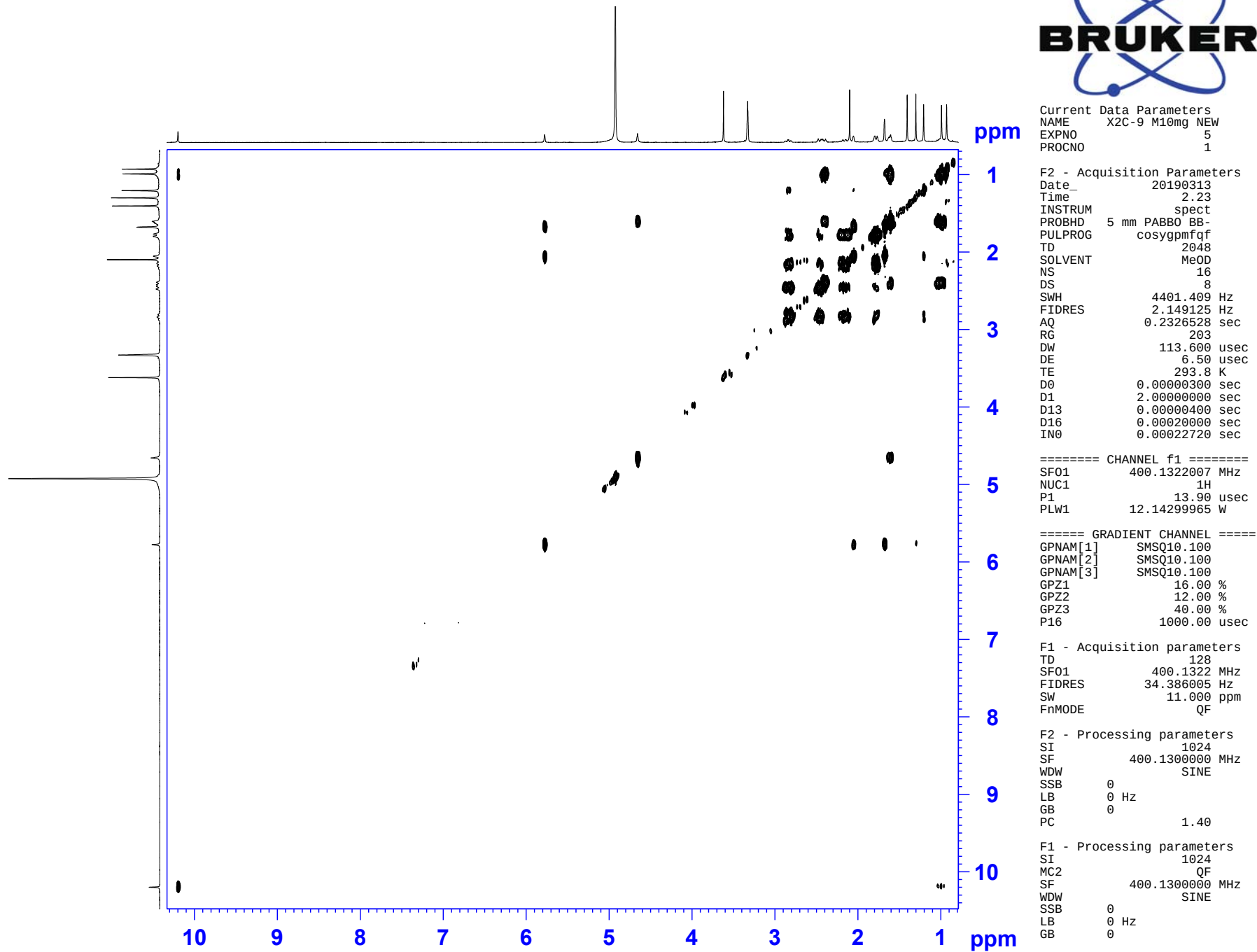


Figure S37. HMBC NMR spectrum of **6** in CD₃OD.



Current Data Parameters
NAME X2C-9 M10mg NEW
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190313
Time 3.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 4096
SOLVENT MeOD
NS 64
DS 16
SWH 4401.409 Hz
FIDRES 1.074563 Hz
AQ 0.4653056 sec
RG 203
DW 113.600 usec
DE 6.50 usec
TE 293.5 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1322007 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6238359 MHz
NUC2 13C
P3 12.37 usec
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 428
SF01 100.6238 MHz
FIDRES 188.707733 Hz
SW 240.048 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127685 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

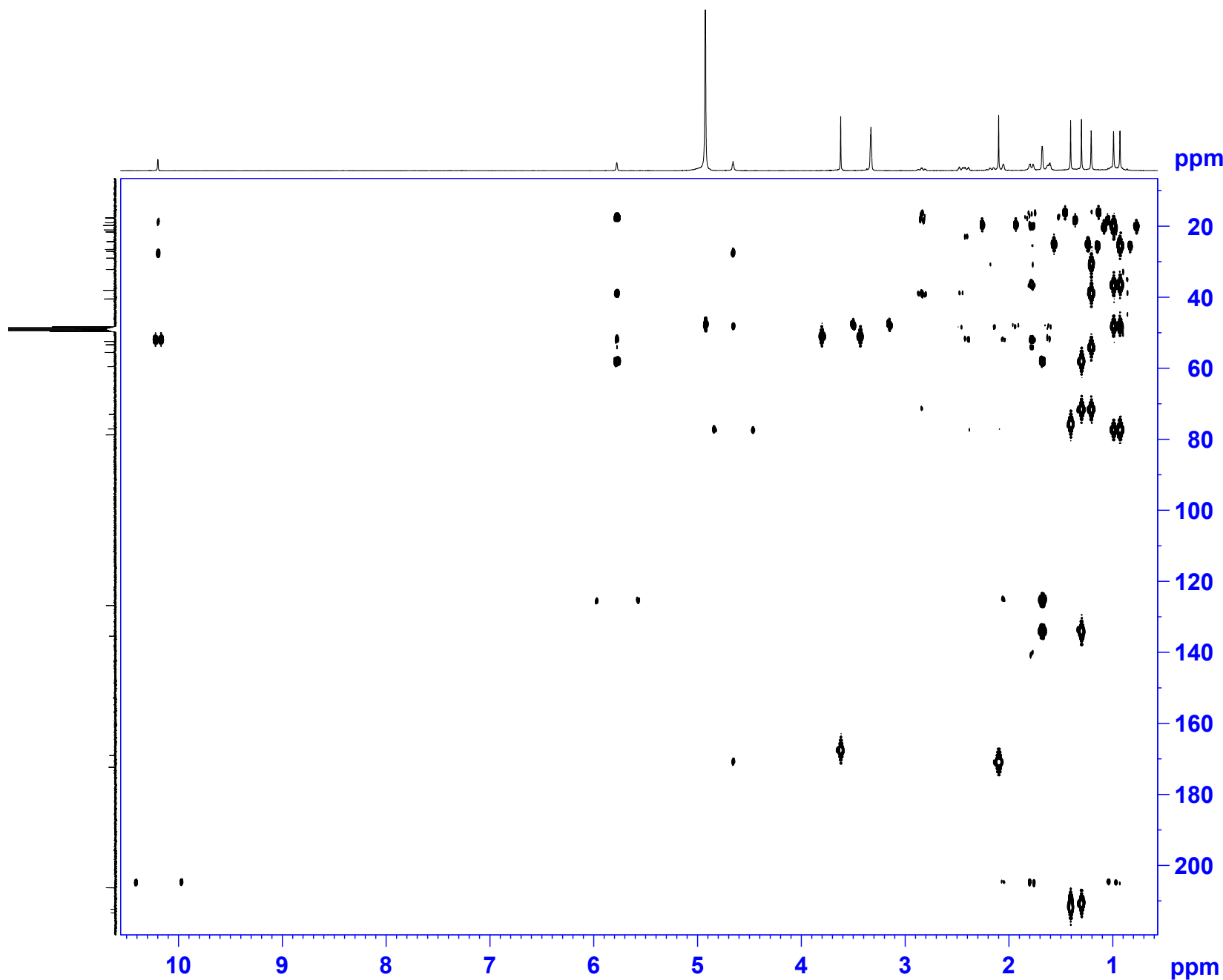


Figure S38. NOESY NMR spectrum of **6** in CD₃OD.



Current Data Parameters
NAME X2C-9 M10mg NEW
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190321
Time_ 10.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG noesyggpphpp
TD 2048
SOLVENT MeOD
NS 32
DS 32
SWH 4401.409 Hz
FIDRES 2.149125 Hz
AQ 0.2326528 sec
RG 203
DW 113.600 usec
DE 6.50 usec
TE 294.0 K
D0 0.00009590 sec
D1 2.00000000 sec
D8 0.30000001 sec
D11 0.03000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
IN0 0.00022720 sec

===== CHANNEL f1 =====
SF01 400.1322007 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
P17 2500.00 usec
PLW1 12.14299965 W
PLW10 3.47059989 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SF01 400.1322 MHz
FIDRES 17.193003 Hz
SW 11.000 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

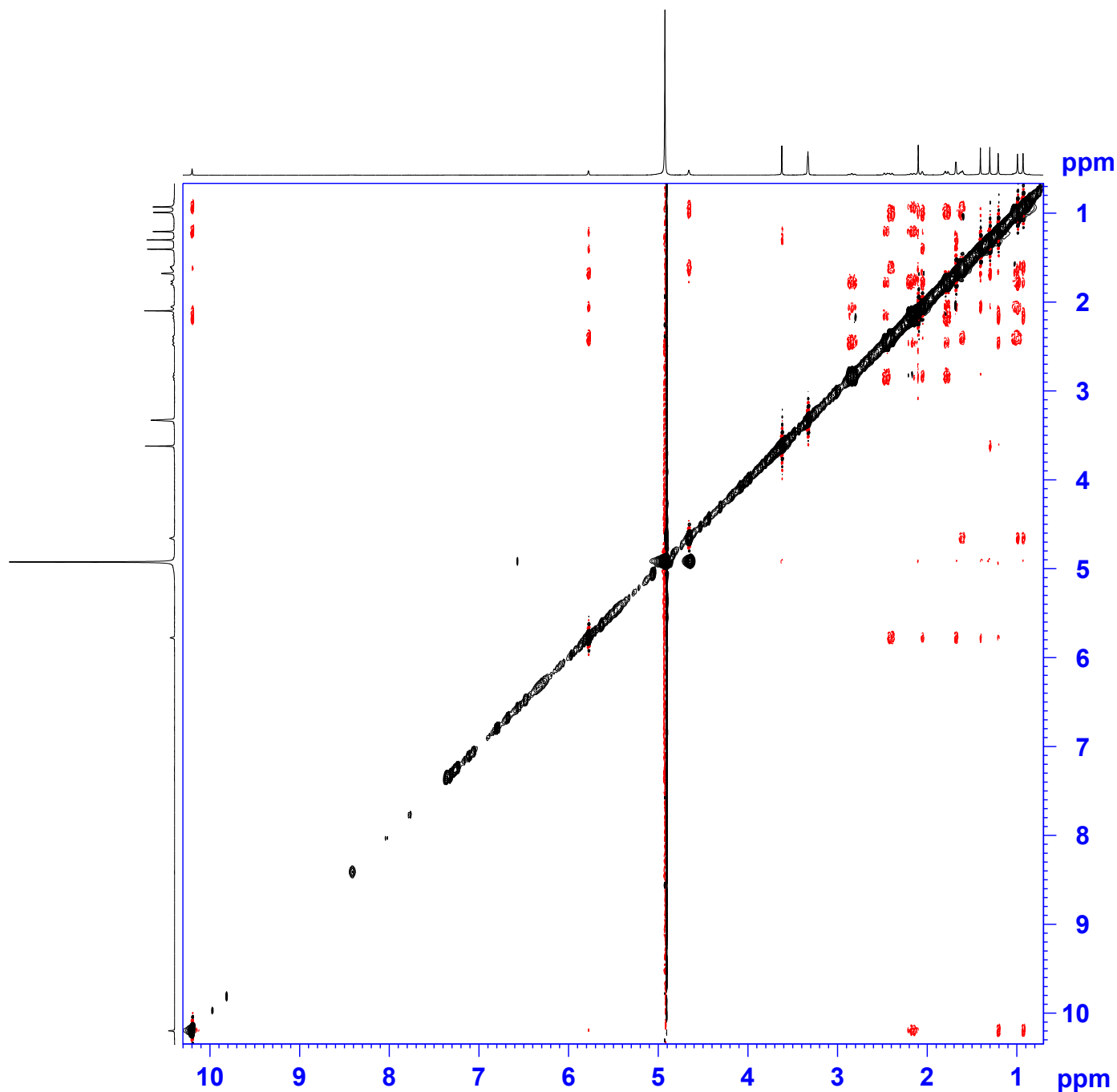


Figure S39. ^1H NMR spectrum of **7** in CDCl_3 .

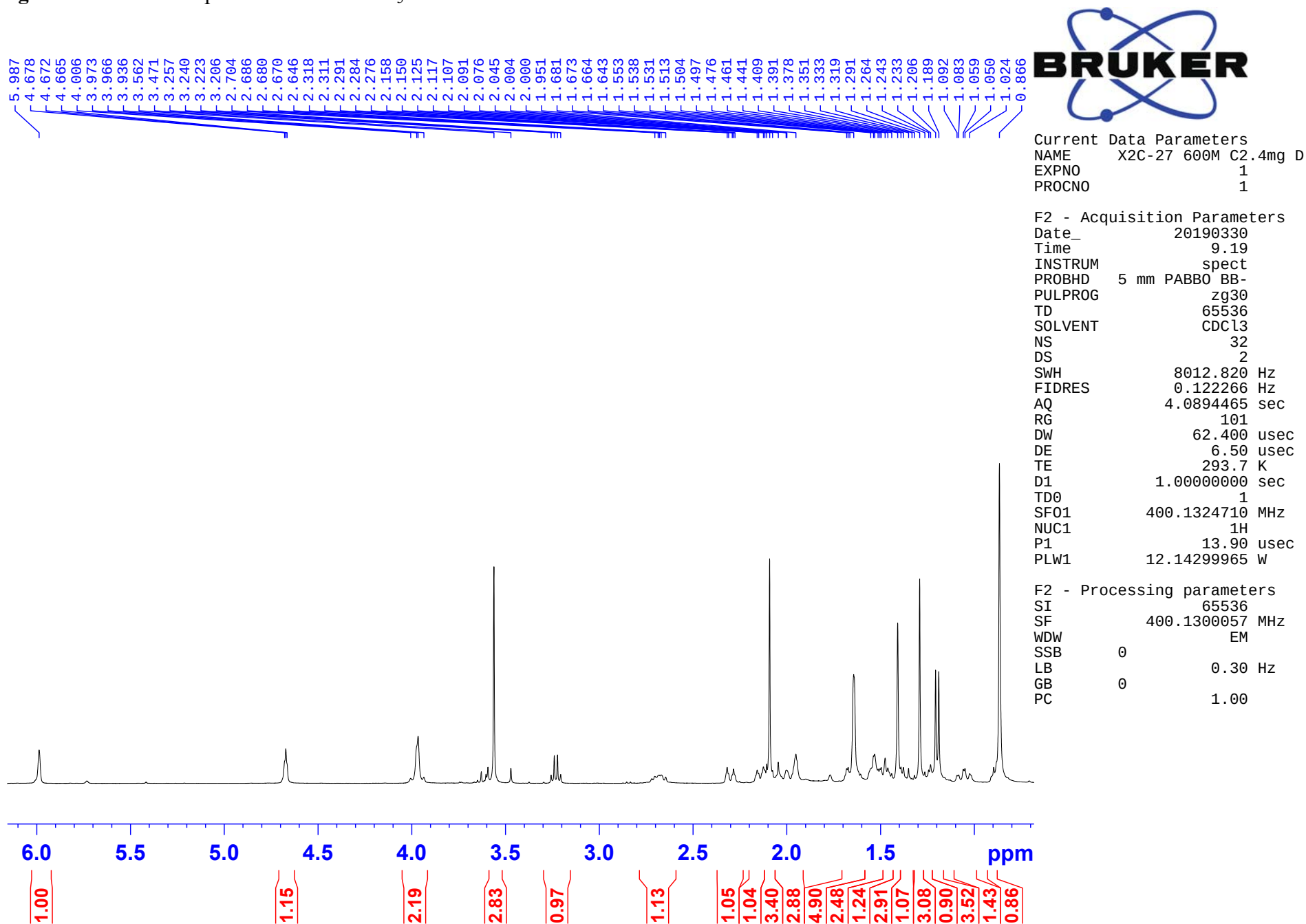


Figure S40. ^{13}C NMR spectrum of **7** in CDCl_3 .

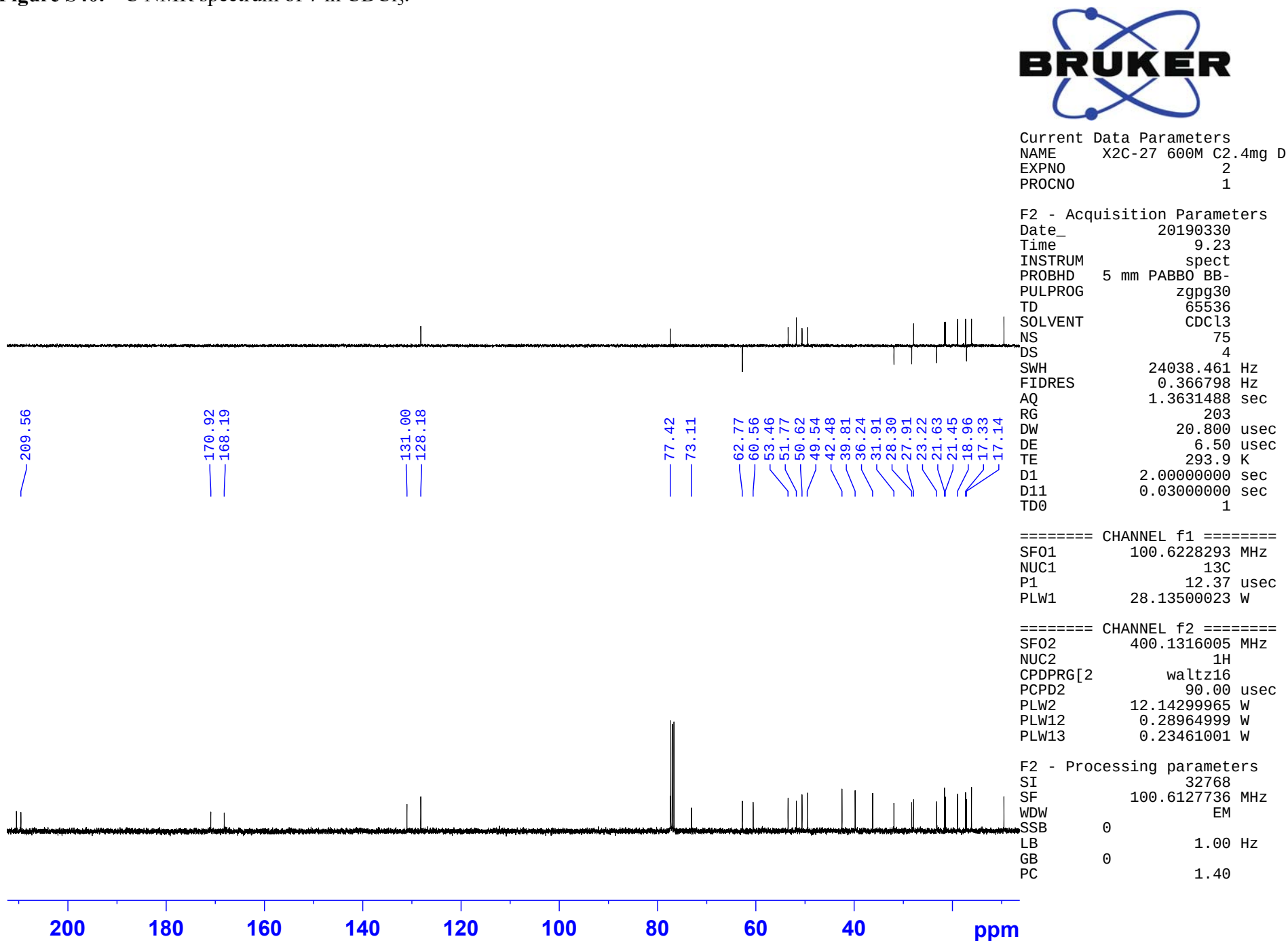


Figure S41. HSQC NMR spectrum of **7** in CDCl₃.

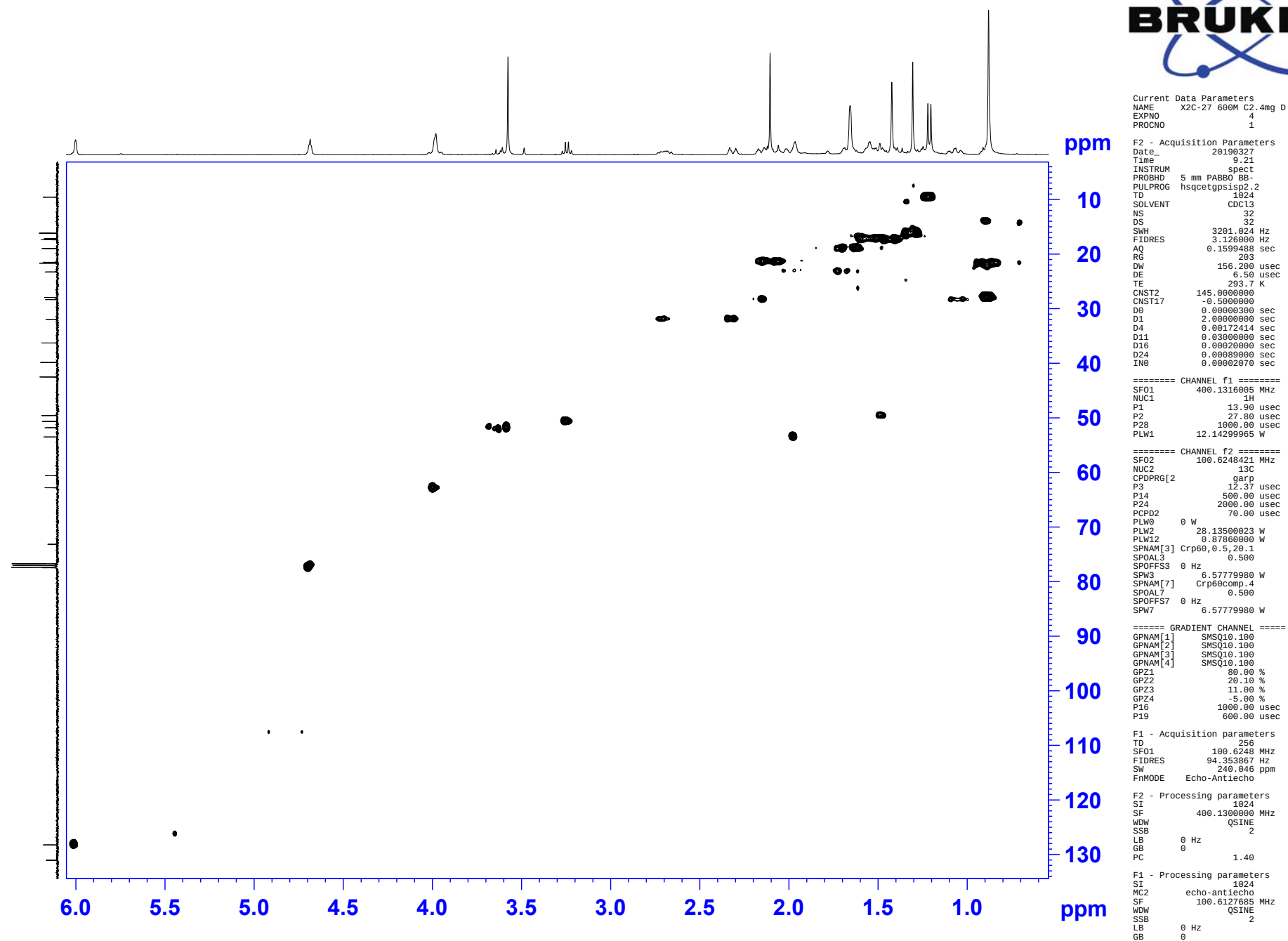


Figure S42. COSY NMR spectrum of **7** in CDCl₃.

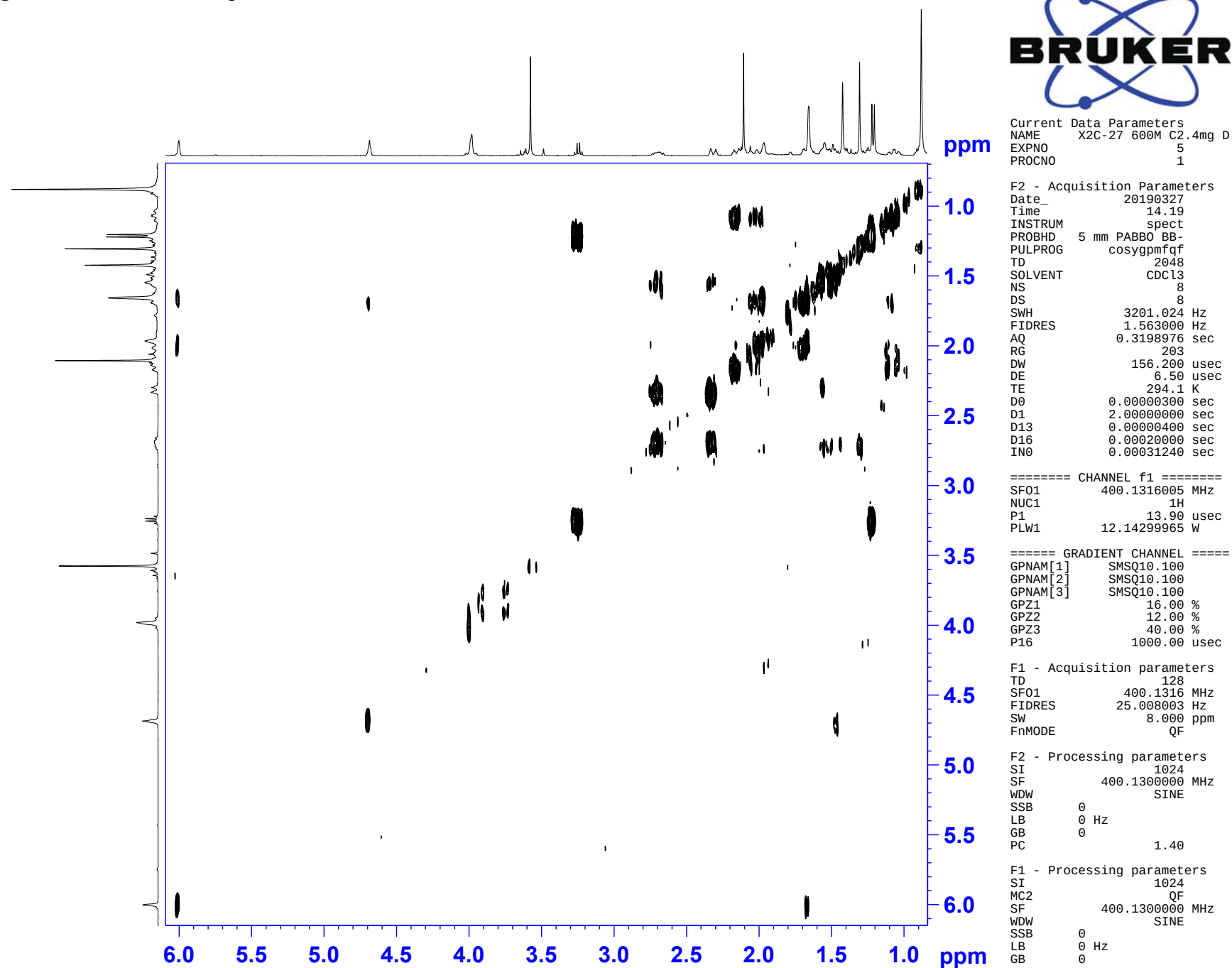


Figure S43. HMBC NMR spectrum of 7 in CDCl₃.

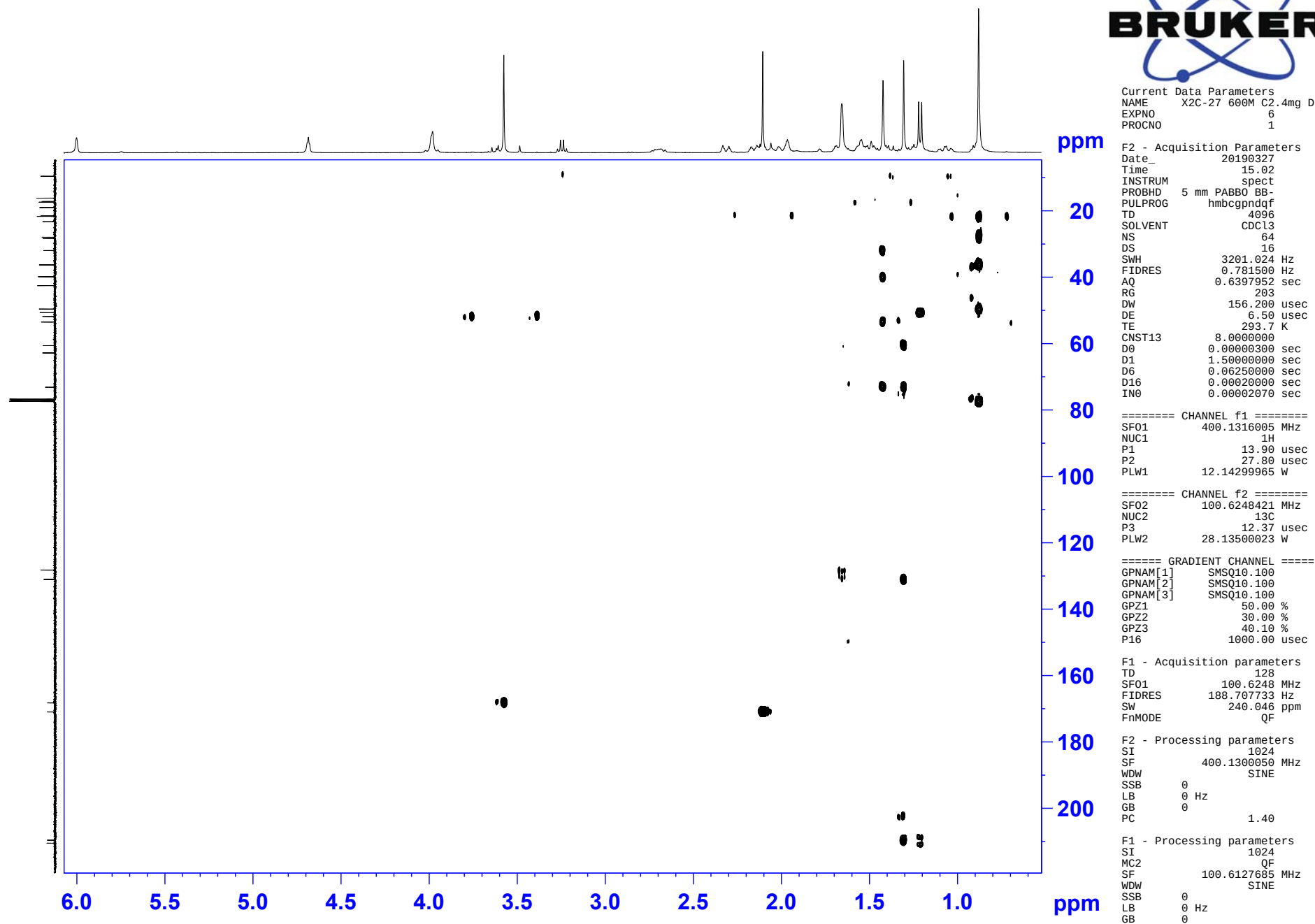


Figure S44. NOESY NMR spectrum of **7** in CDCl₃.

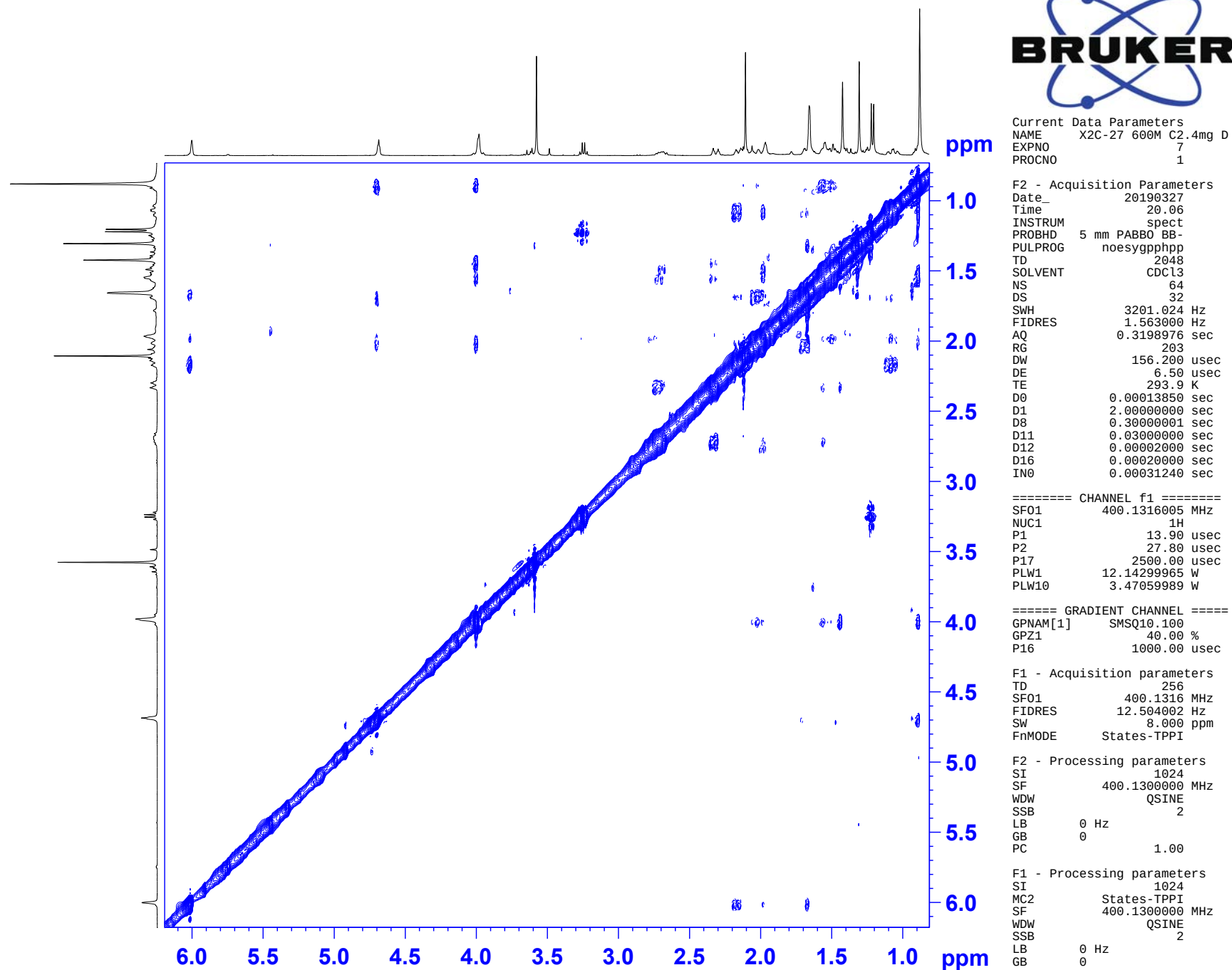
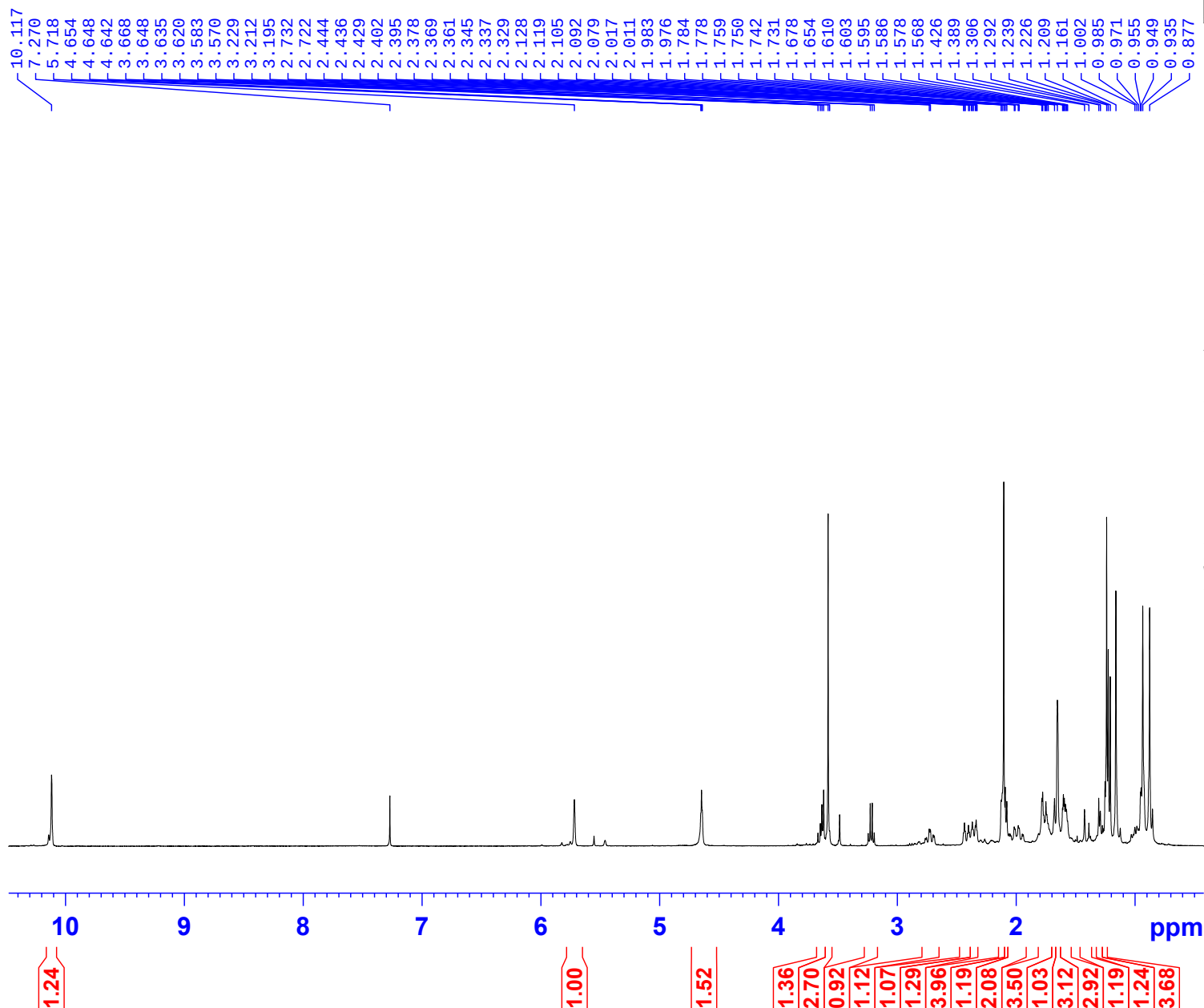


Figure S45. ^1H NMR spectrum of **8** in CDCl_3 .



Current Data Parameters
 NAME X2C-31 =x2c-30 C11.9mg new
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190402
 Time 20.32
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl_3
 NS 32
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 144
 DW 62.400 usec
 DE 6.50 usec
 TE 294.0 K
 D1 1.00000000 sec
 TD0 1
 SF01 400.1324710 MHz
 NUC1 ^1H
 P1 13.90 usec
 PLW1 12.14299965 W

F2 - Processing parameters
 SI 65536
 SF 400.1300058 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S46. ^{13}C NMR spectrum of **8** in CDCl_3 .

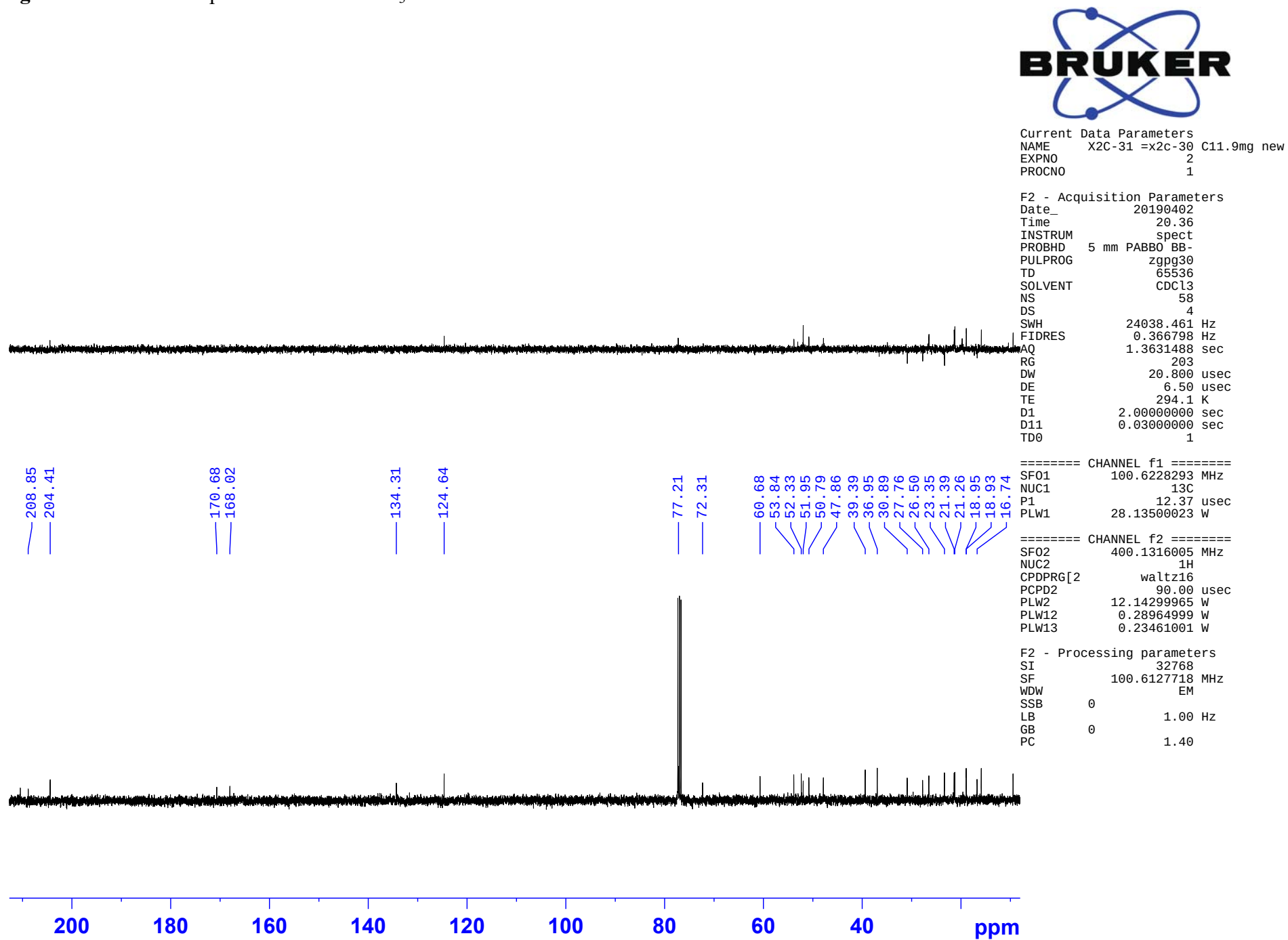


Figure S47. HSQC NMR spectrum of **8** in CDCl₃.



Current Data Parameters
NAME X2C-31 =x2c-30 C11.9mg new
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190410
Time 21.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgpsisp2.2
TD 1024
SOLVENT CDCl3
NS 8
DS 32
SWH 4401.409 Hz
FIDRES 4.298251 Hz
AQ 0.1163264 sec
RG 203
DW 113.600 usec
DE 6.50 usec
TE 294.4 K
CNST2 145.000000
CNST17 -0.500000
D0 0.00000300 sec
D1 2.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.0002070 sec

===== CHANNEL f1 =====
SF01 400.1322007 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
P28 1000.00 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
CPDPRG2 gfp
P3 12.37 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 70.00 usec
PLW0 0 W
PLW2 28.13500023 W
PLW12 0.87860000 W
SPNAM[3] Crp60, 0.5, 20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 6.57779980 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 6.57779980 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SF01 100.6248 MHz
FIDRES 94.353867 Hz
SW 240.046 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6127605 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

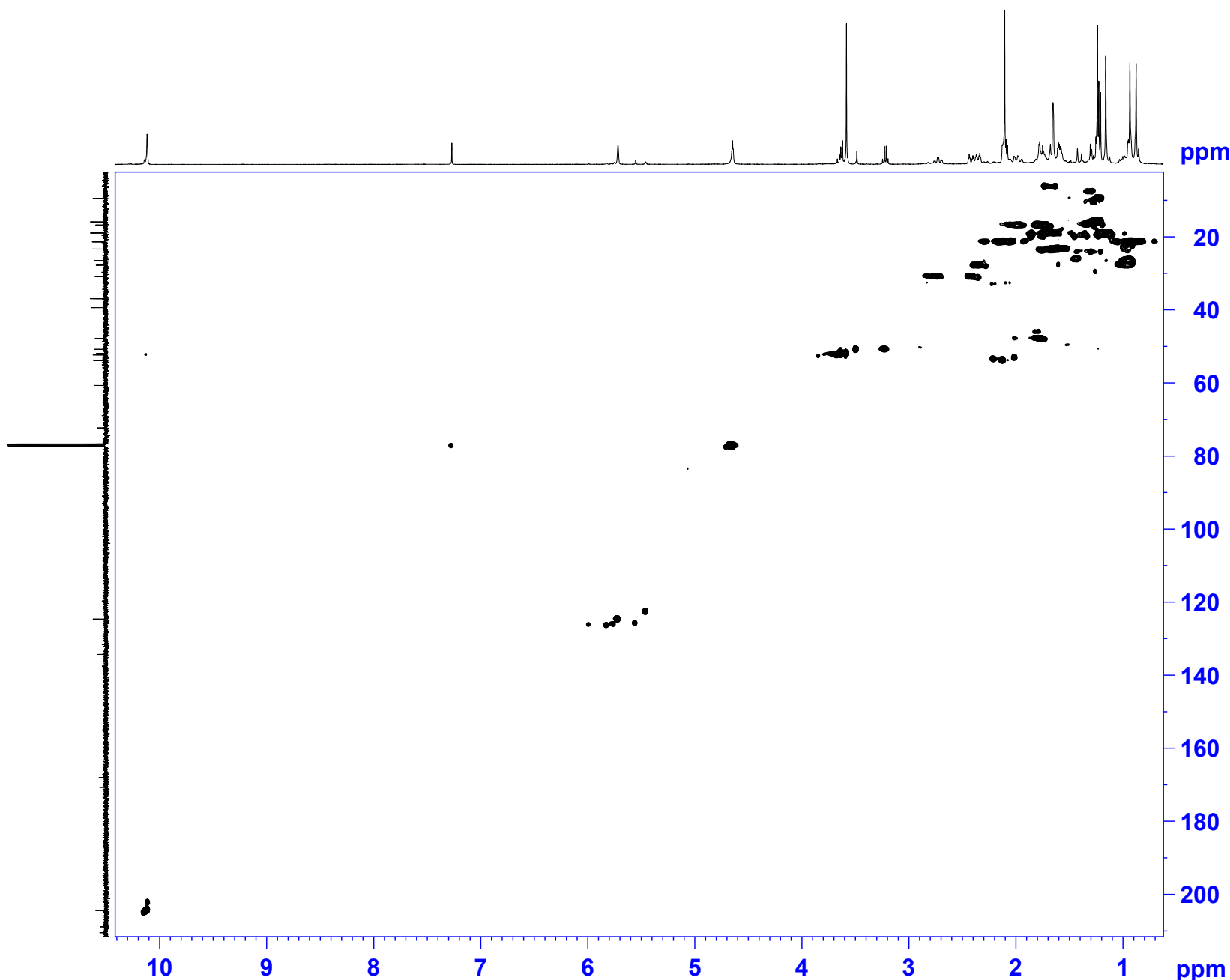


Figure S48. COSY NMR spectrum of **8** in CDCl₃.

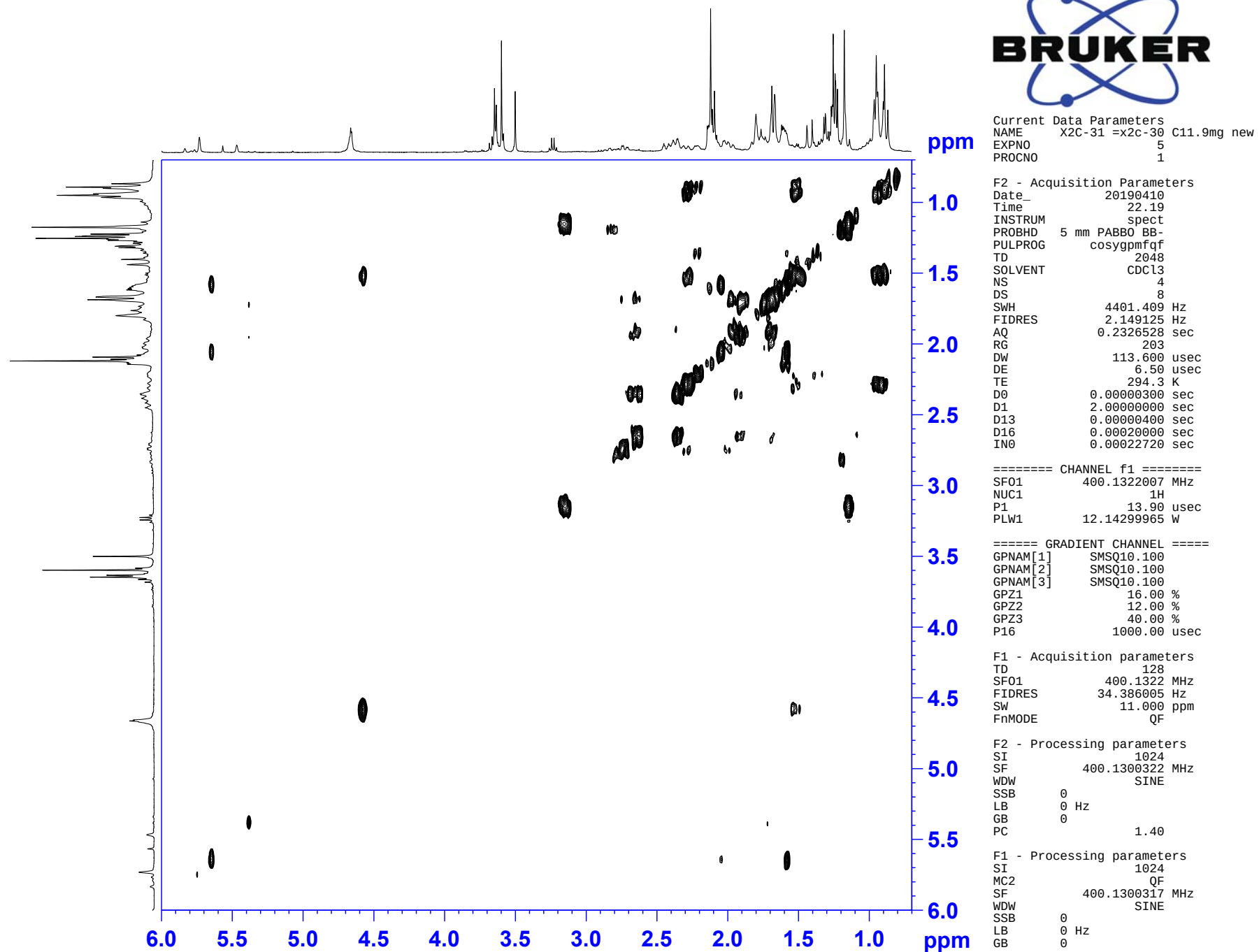


Figure S49. HMBC NMR spectrum of **8** in CDCl₃.



Current Data Parameters
NAME X2C-31 =x2c-30 C11.9mg new
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190410
Time 22.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 16
DS 16
SWH 4401.409 Hz
FIDRES 1.074563 Hz
AQ 0.4653056 sec
RG 203
DW 113.600 usec
DE 6.50 usec
TE 294.1 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1322007 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
P3 12.37 usec
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 100.6248 MHz
FIDRES 188.707733 Hz
SW 240.046 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300339 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127685 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

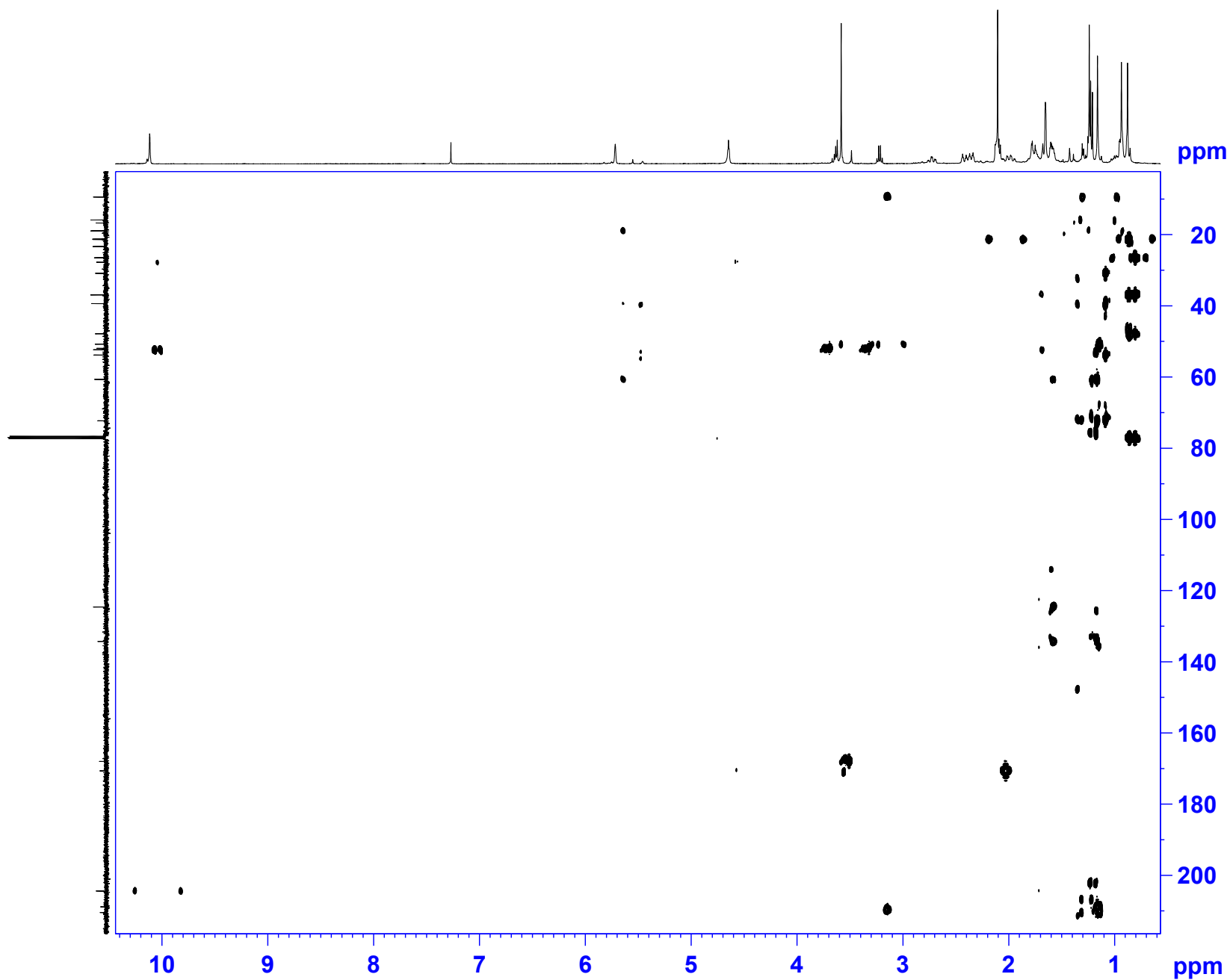


Figure S50. NOESY NMR spectrum of **8** in CDCl₃.

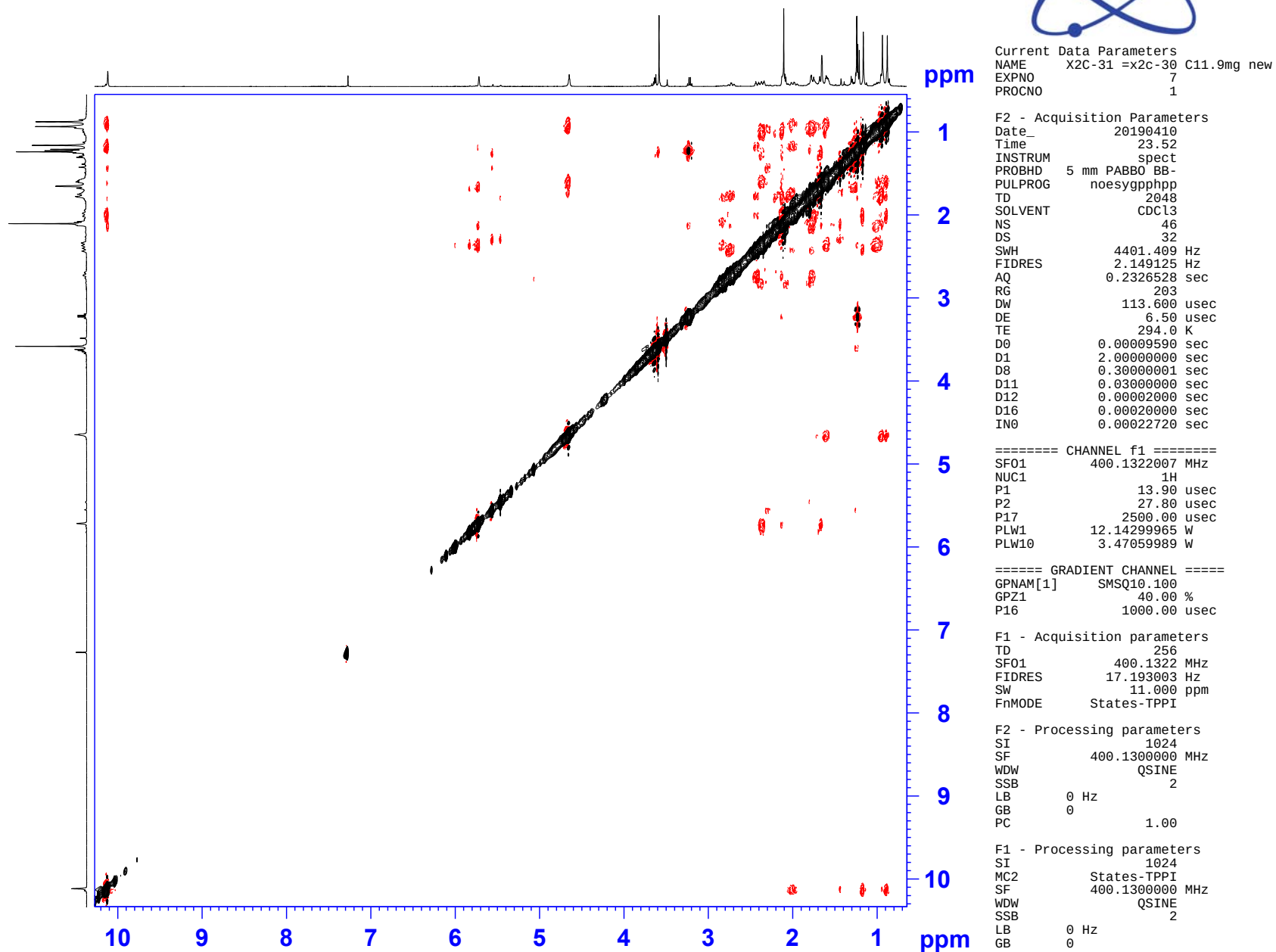


Figure S51. ^1H NMR spectrum of **9** in CDCl_3 .

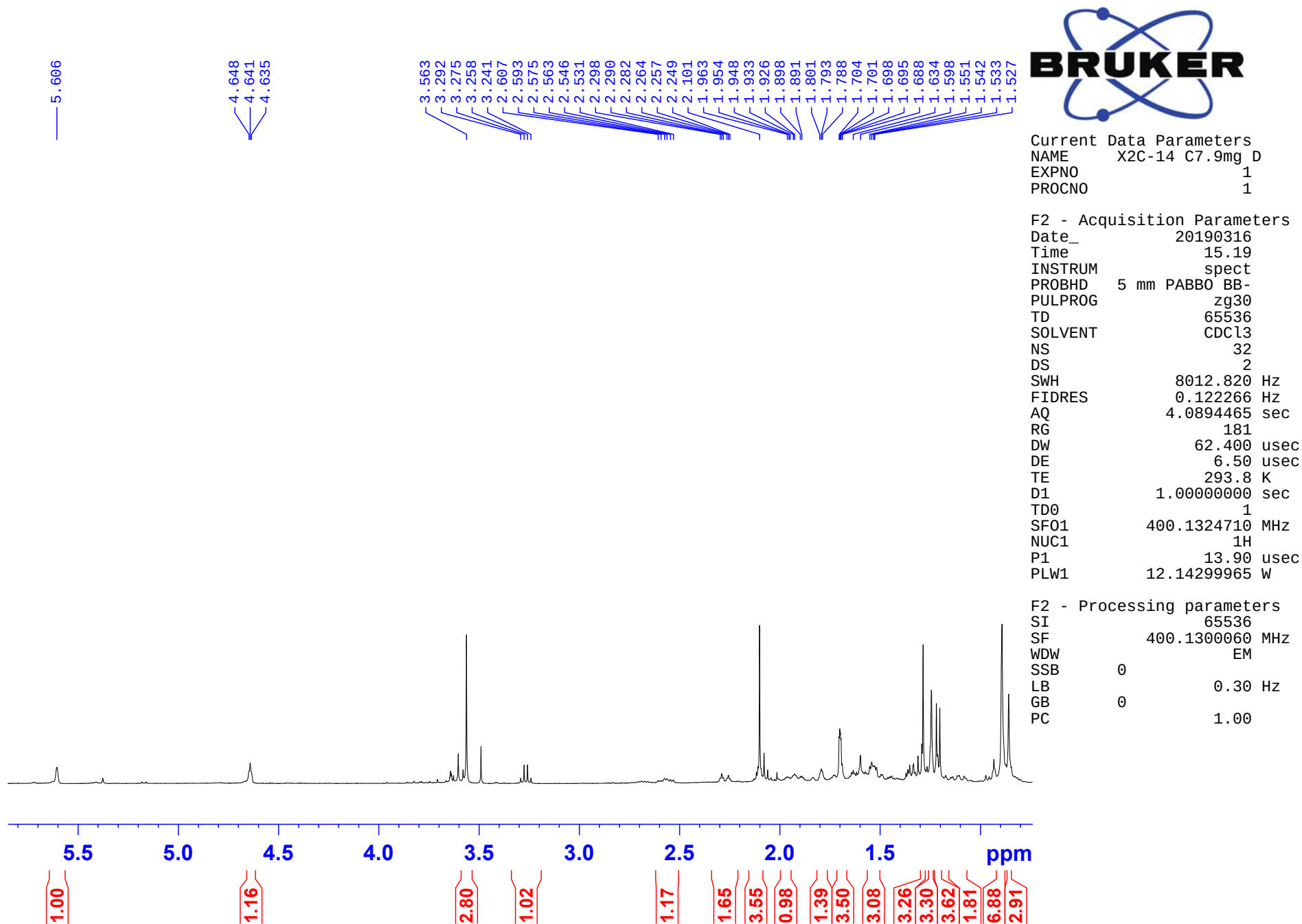


Figure S52. ^{13}C NMR spectrum of **9** in CDCl_3 .



Current Data Parameters
NAME X2C-14 C7.9mg D
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190316
Time 15.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl_3
NS 1558
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SF01 100.6228293 MHz
NUC1 ^{13}C
P1 12.37 usec
PLW1 28.13500023 W
SF02 400.1316005 MHz
NUC2 ^1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 12.14299965 W
PLW12 0.28964999 W
PLW13 0.23461001 W

F2 - Processing parameters
SI 32768
SF 100.6127714 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

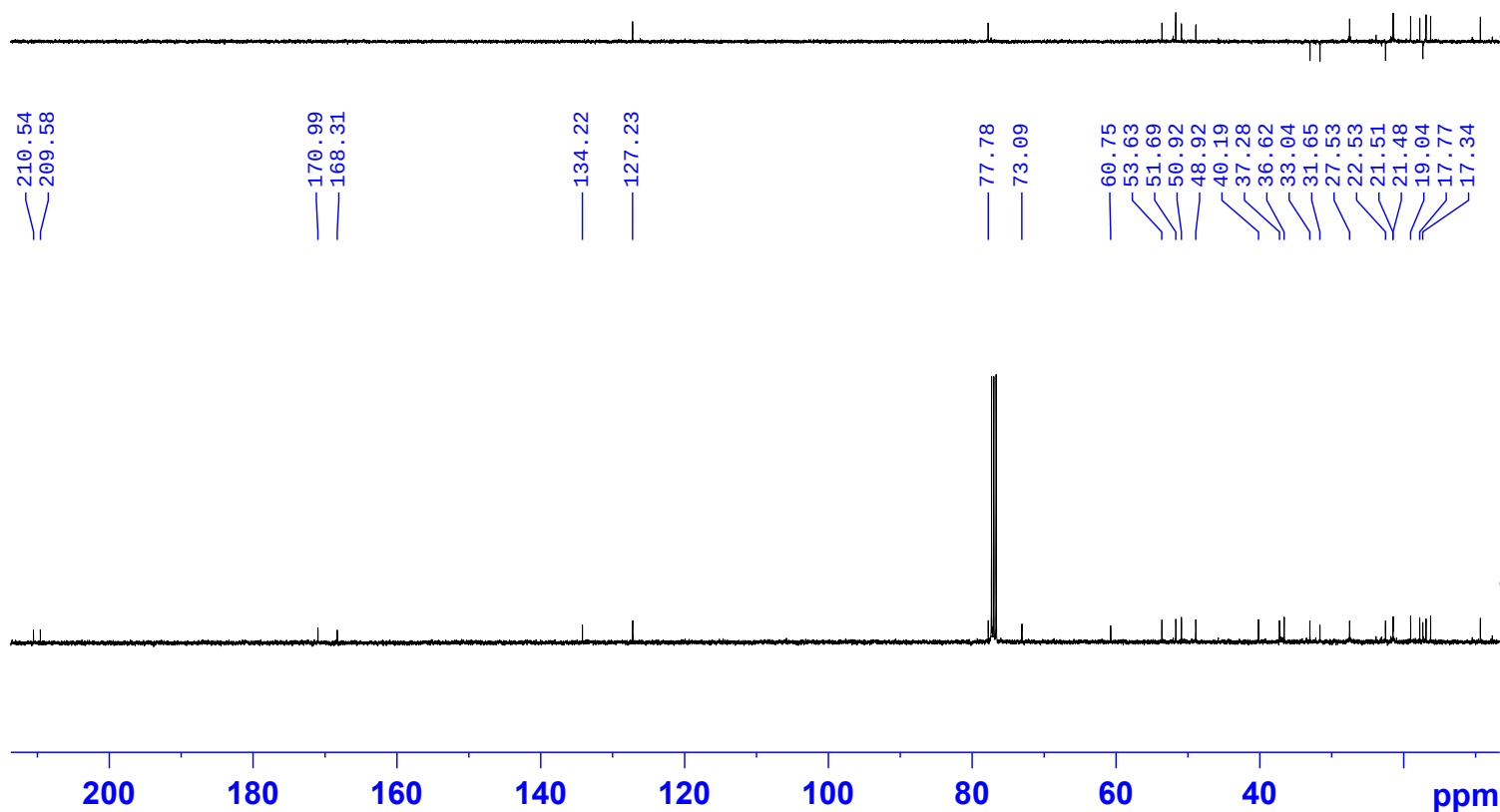


Figure S53. HSQC NMR spectrum of **9** in CDCl₃.

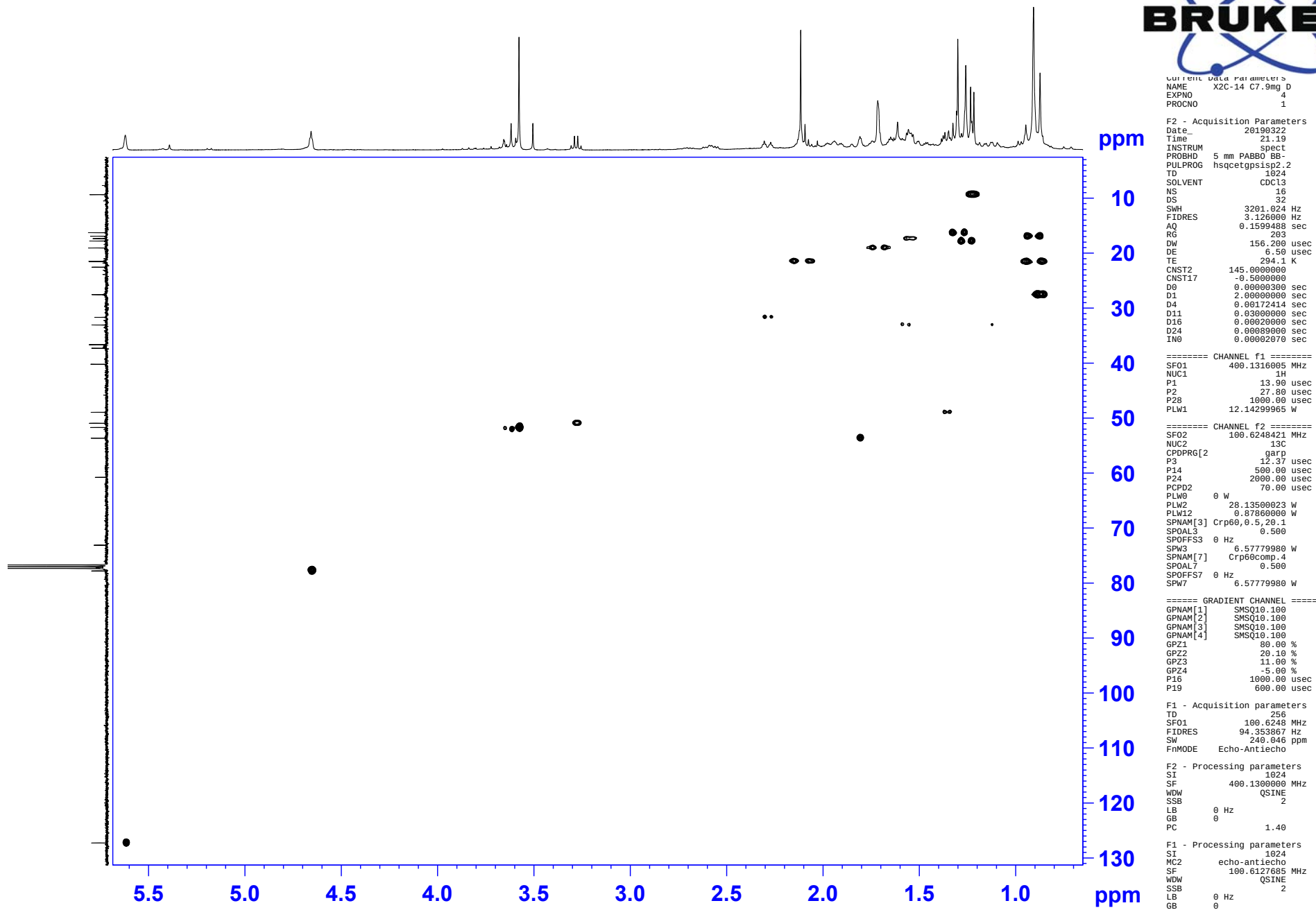


Figure S54. COSY NMR spectrum of **9** in CDCl₃.

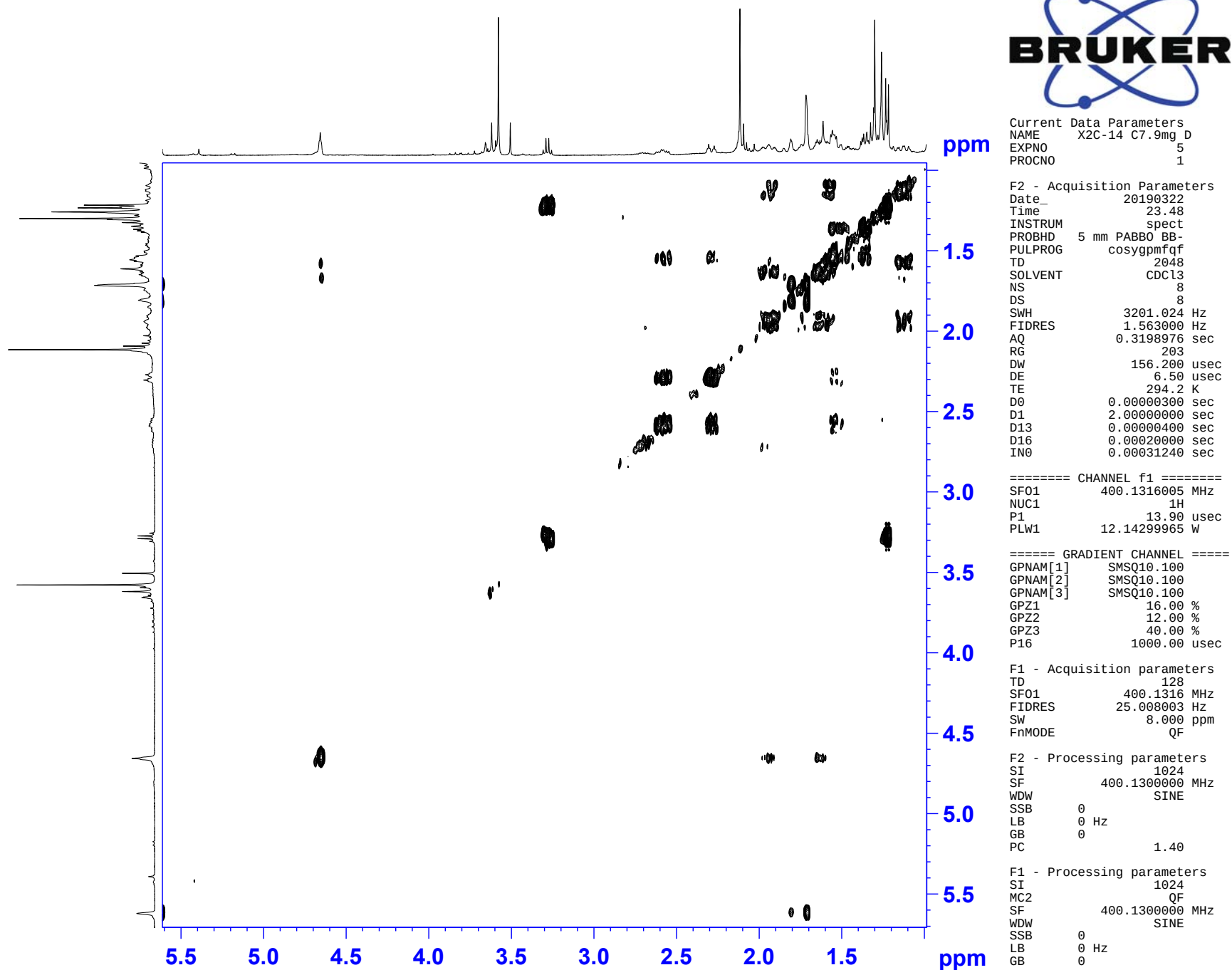


Figure S55. HMBC NMR spectrum of **9** in CDCl₃.



Current Data Parameters
NAME X2C-14 C7.9mg D
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190323
Time 0.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 3201.024 Hz
FIDRES 0.781500 Hz
AQ 0.6397952 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 293.9 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002070 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SF02 100.6248421 MHz
NUC2 13C
P3 12.37 usec
PLW2 28.13500023 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 100.6248 MHz
FIDRES 188.707733 Hz
SW 240.046 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 100.6127799 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

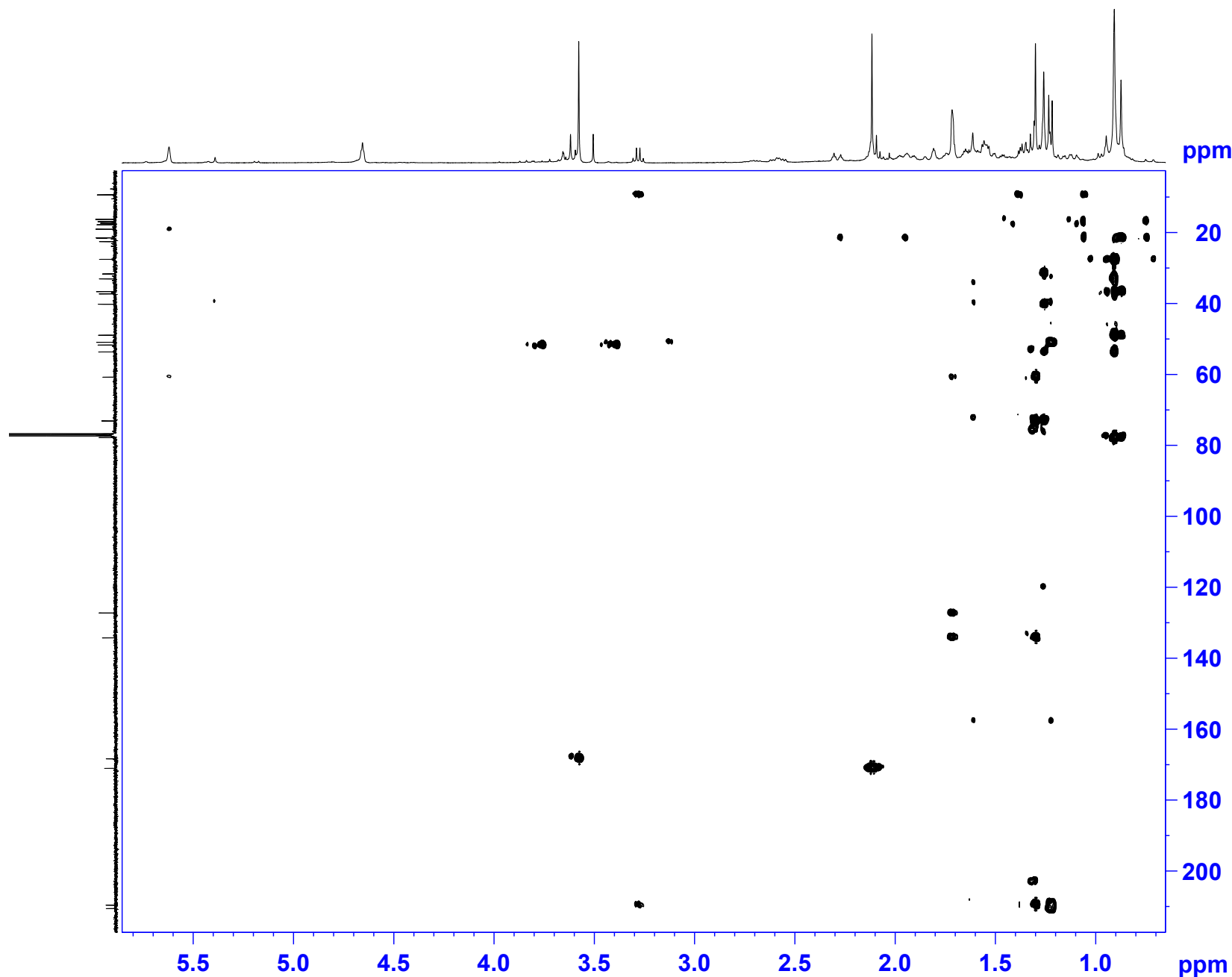


Figure S56. NOESY NMR spectrum of **9** in CDCl₃.

