10.1071/CH19540_AC

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Supplementary Material

Arenaran Sesquiterpenes from the Nudibranch *Chromodoris Strigata* and its Dietary Sponge *Acanthodendrilla* sp. 2510: Spectroscopic and Computational Studies

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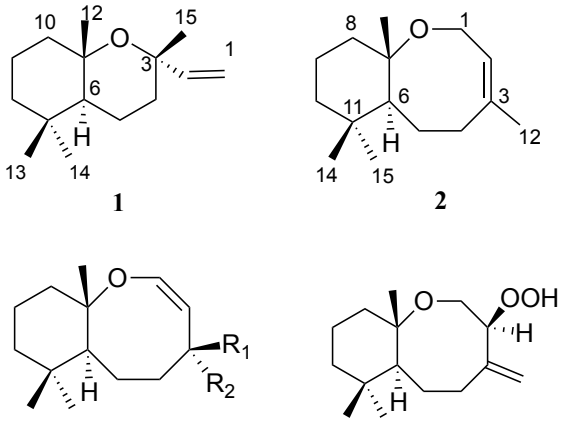
Figure S1. Image of two specimens of *Chromodoris strigata* on the sponge *Acanthodendrilla* sp. 2510.



1 **2**

3 R_1 = OOH; R_2 = Me
4 R_1 = Me; R_2 = OOH
6 R_1 = OH; R_2 = Me

5

Figure S2. Structures of isolated terpenes **1**-**5** and of alcohol **6**.

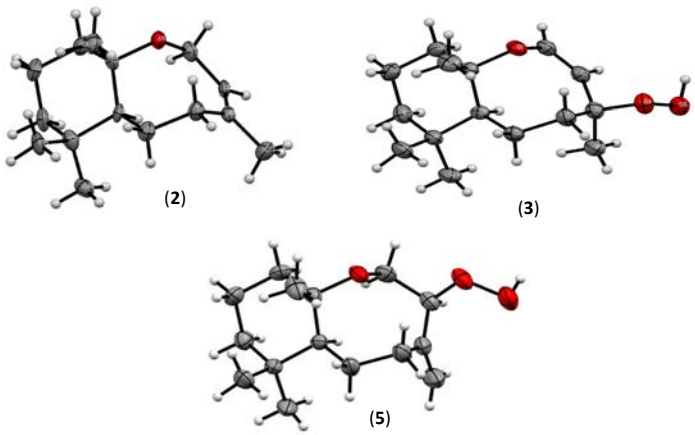


Figure S3. ORTEP views of crystal structures of **2, 3**, and **5**.

Figure S4. Comparison of ^{1}H NMR spectra of extracts of (a) *Acanthodendrilla* sp. 2510; (b) viscera of *C. strigata* #1613; (c) mantle of *C. strigata* #1613.

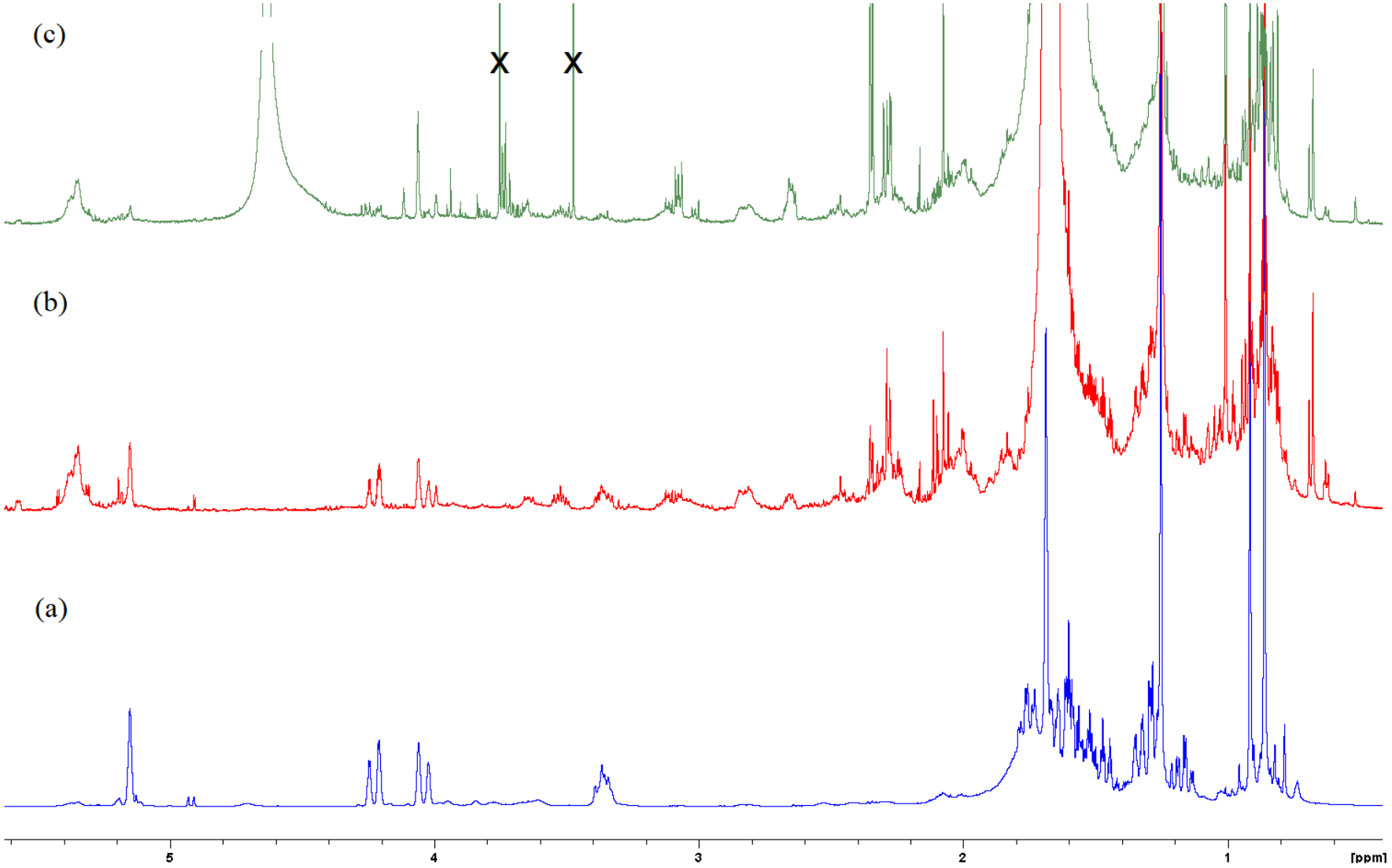


Figure S5. ^{1}H NMR spectrum of **1** (500 MHz, $CDCl_3$).

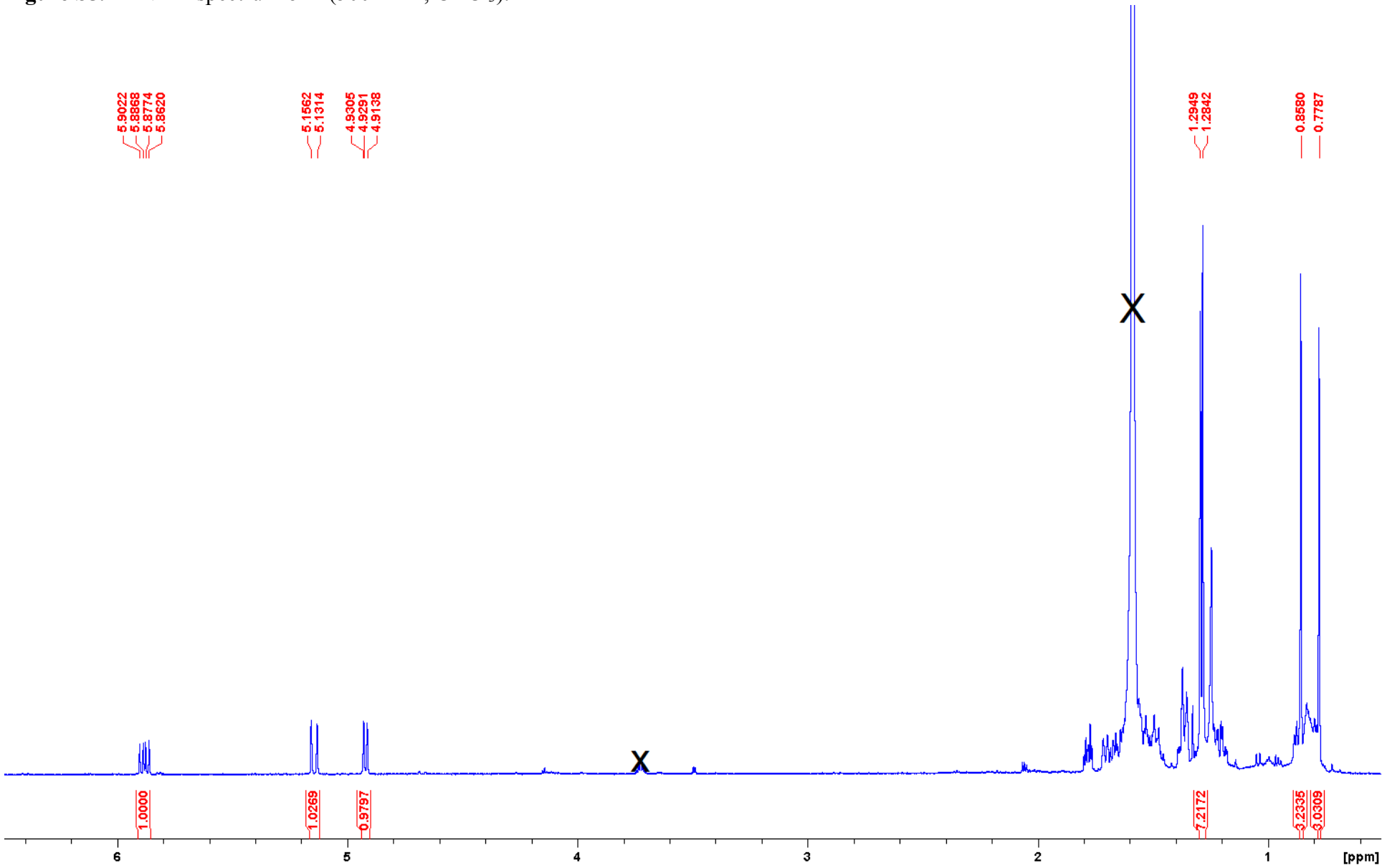


Figure S6. ^{1}H NMR spectrum of **2** (500 MHz, $CDCl_3$).

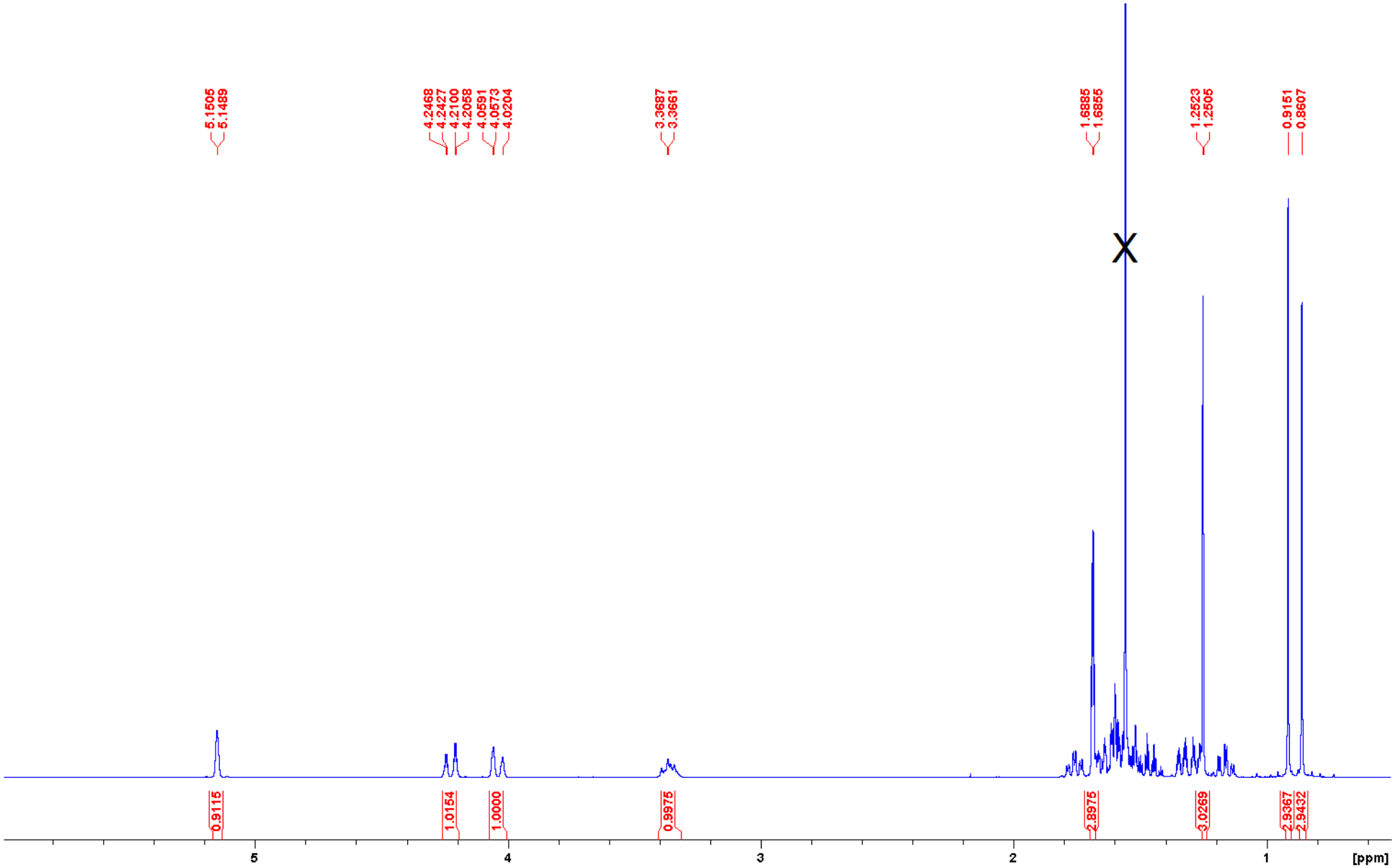


Figure S7. gCOSY spectrum of **2** (500 MHz, $CDCl_3$).

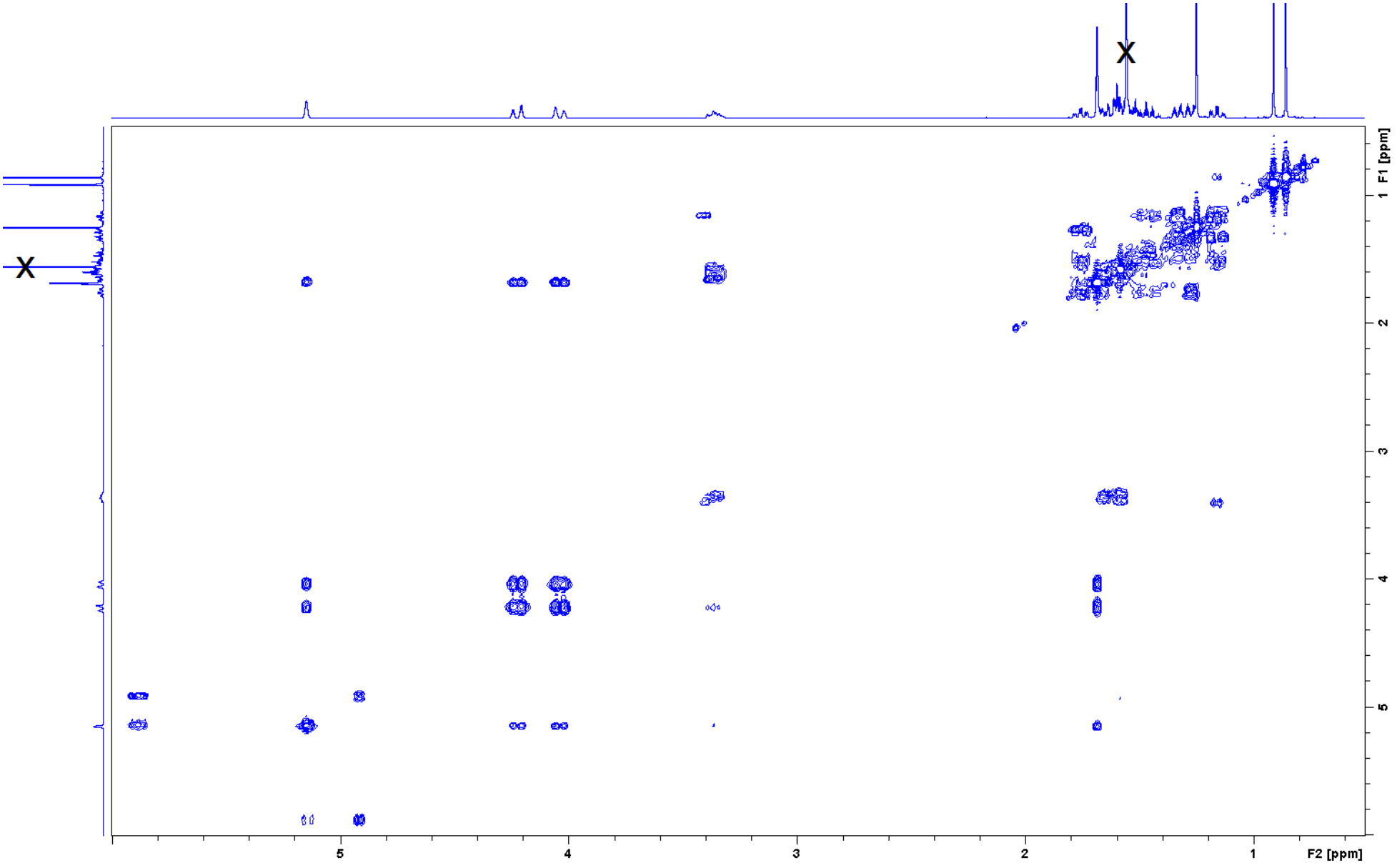


Figure S8. HSQC spectrum of **2** (500 MHz, $CDCl_3$).

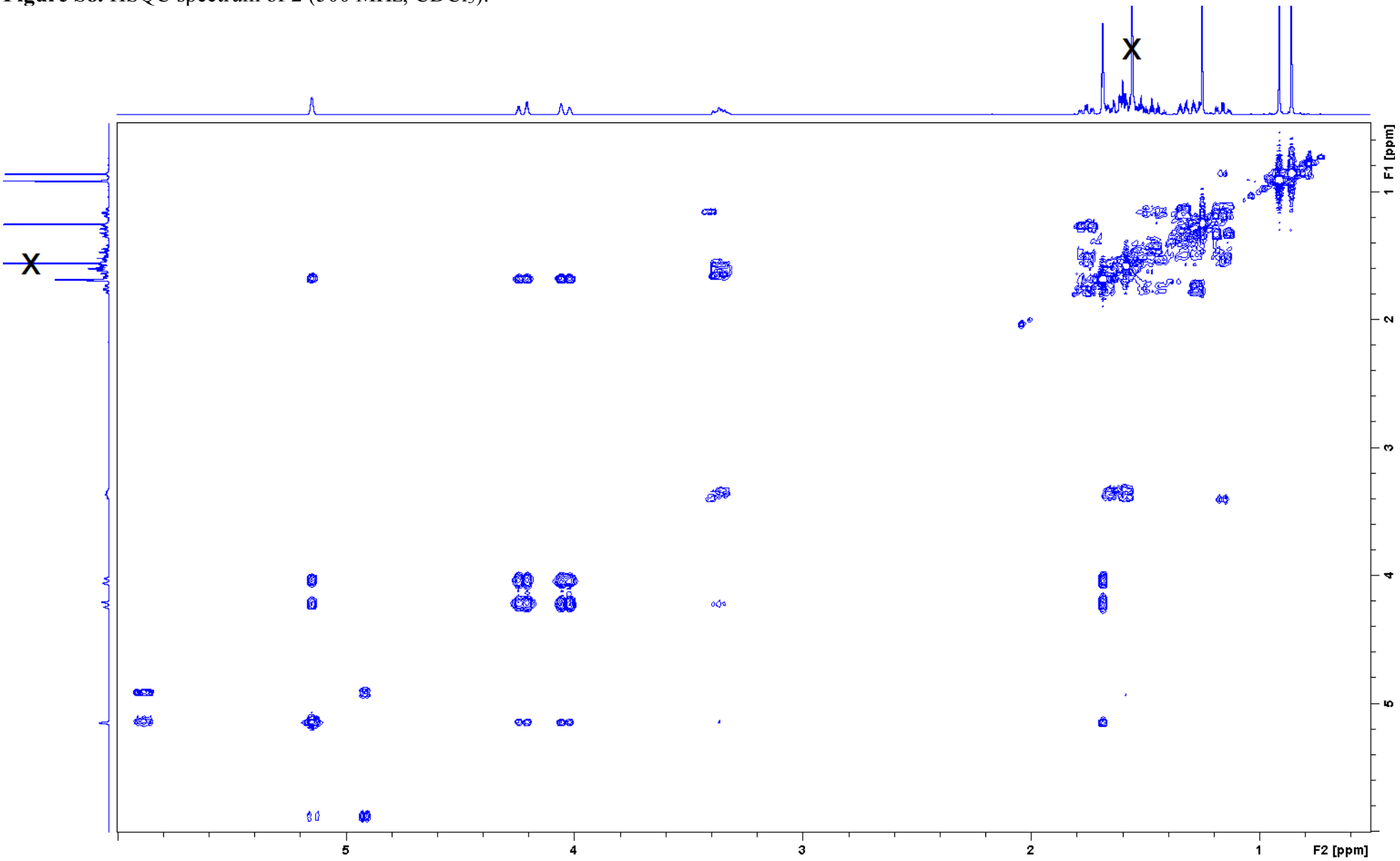


Figure S9. HMBC spectrum of **2** (700 MHz, $CDCl_3$).

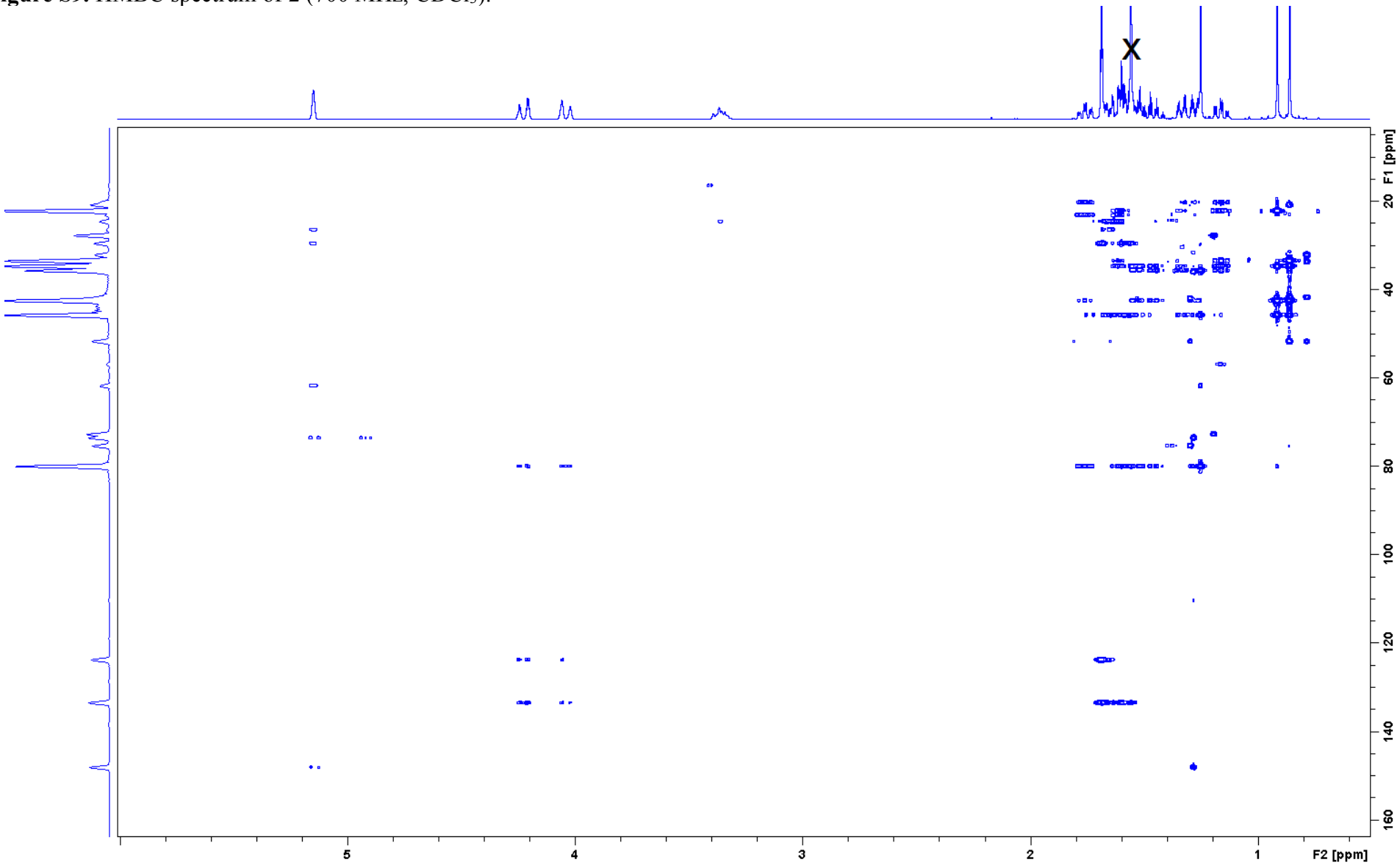


Figure S10. ^{1}H NMR spectrum of **3** (700 MHz, $CDCl_3$).

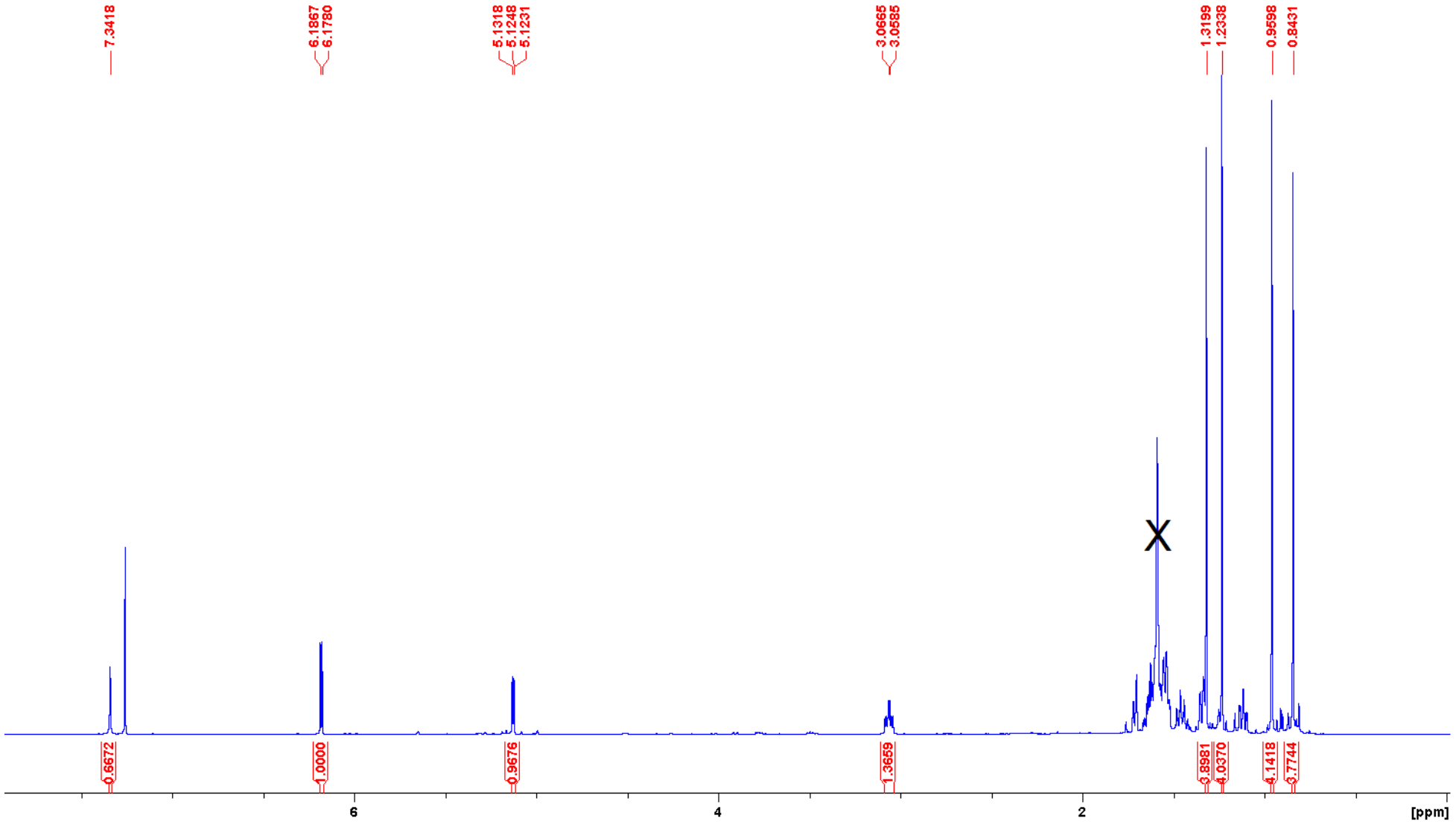


Figure S11. gCOSY spectrum of **3** (700 MHz, $CDCl_3$).

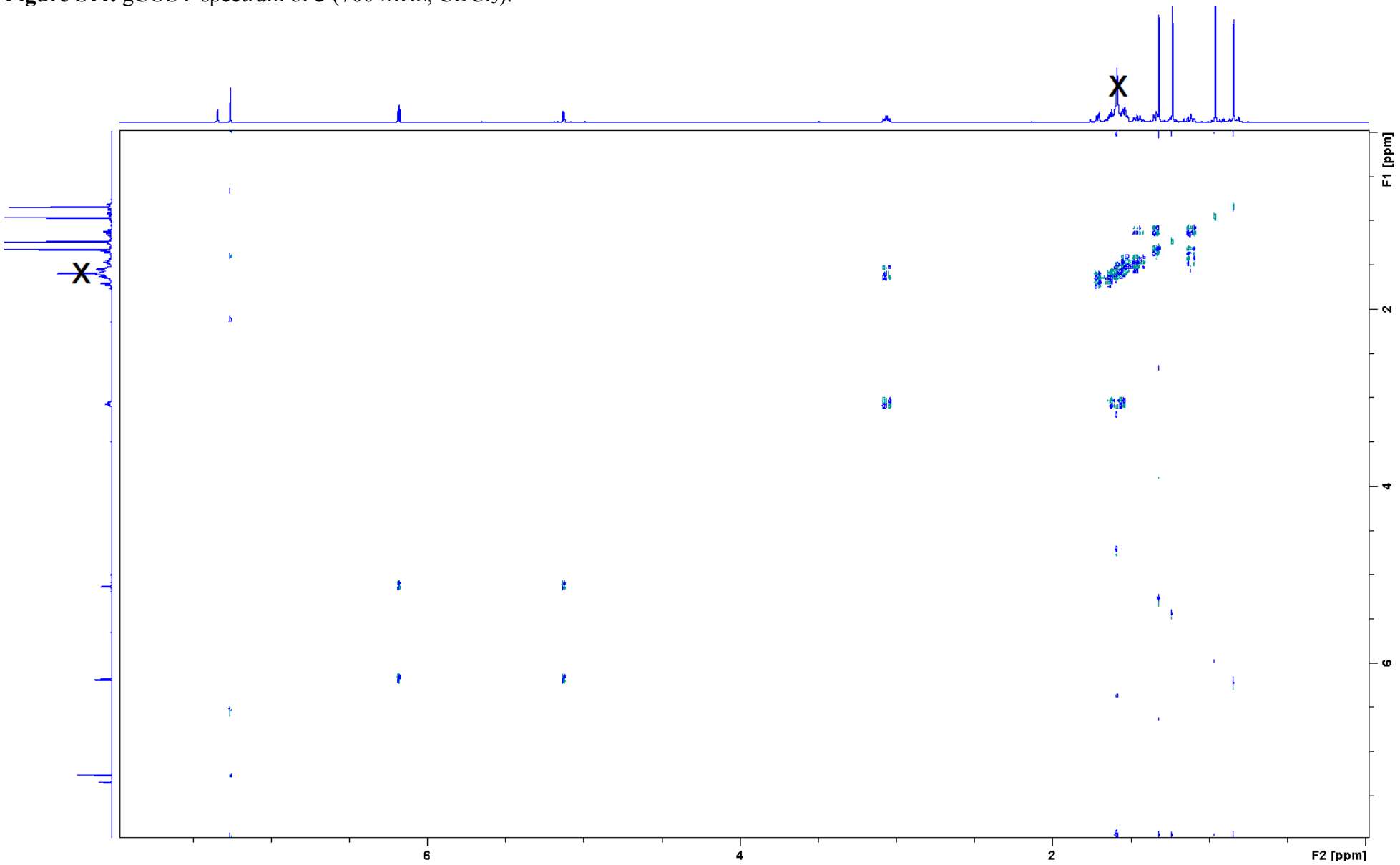


Figure S12. HSQC spectrum of **3** (700 MHz, $CDCl_3$).

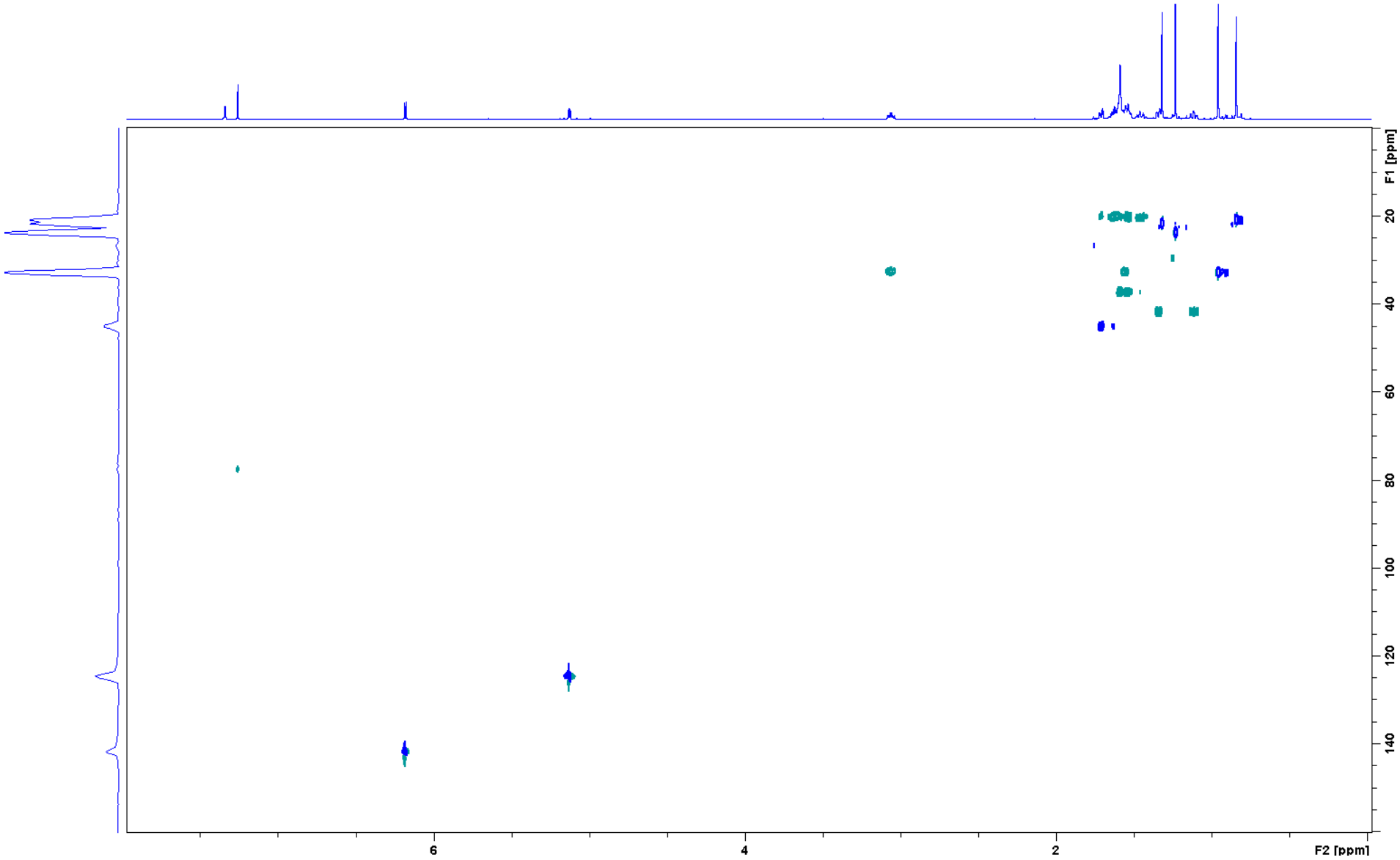


Figure S13. HMBC spectrum of **3** (700 MHz, $CDCl_3$).

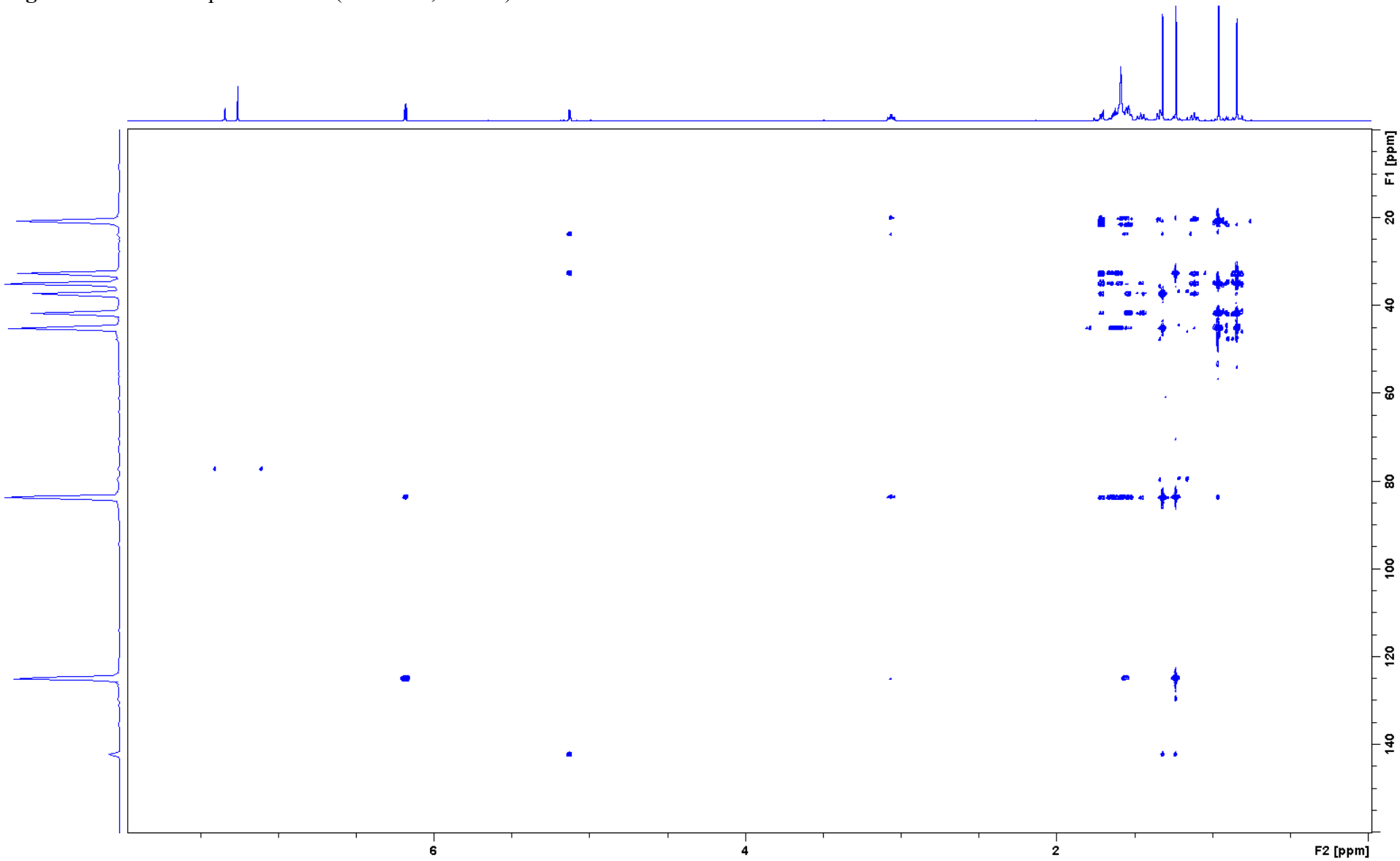


Figure S14. NOESY spectrum of **3** (700 MHz, $CDCl_3$).

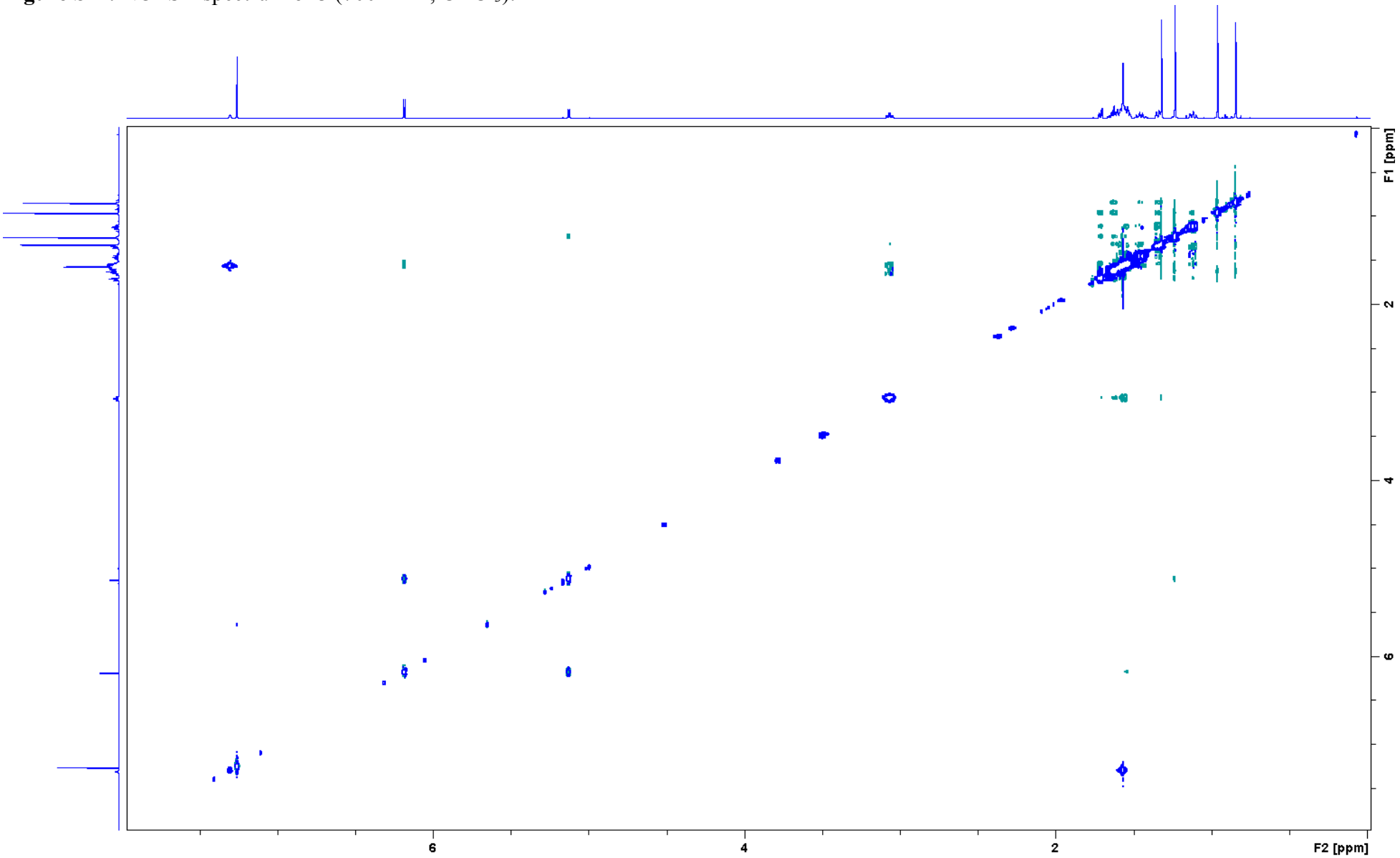


Figure S15. ^{1}H NMR spectrum of **4** (700 MHz, $CDCl_3$).

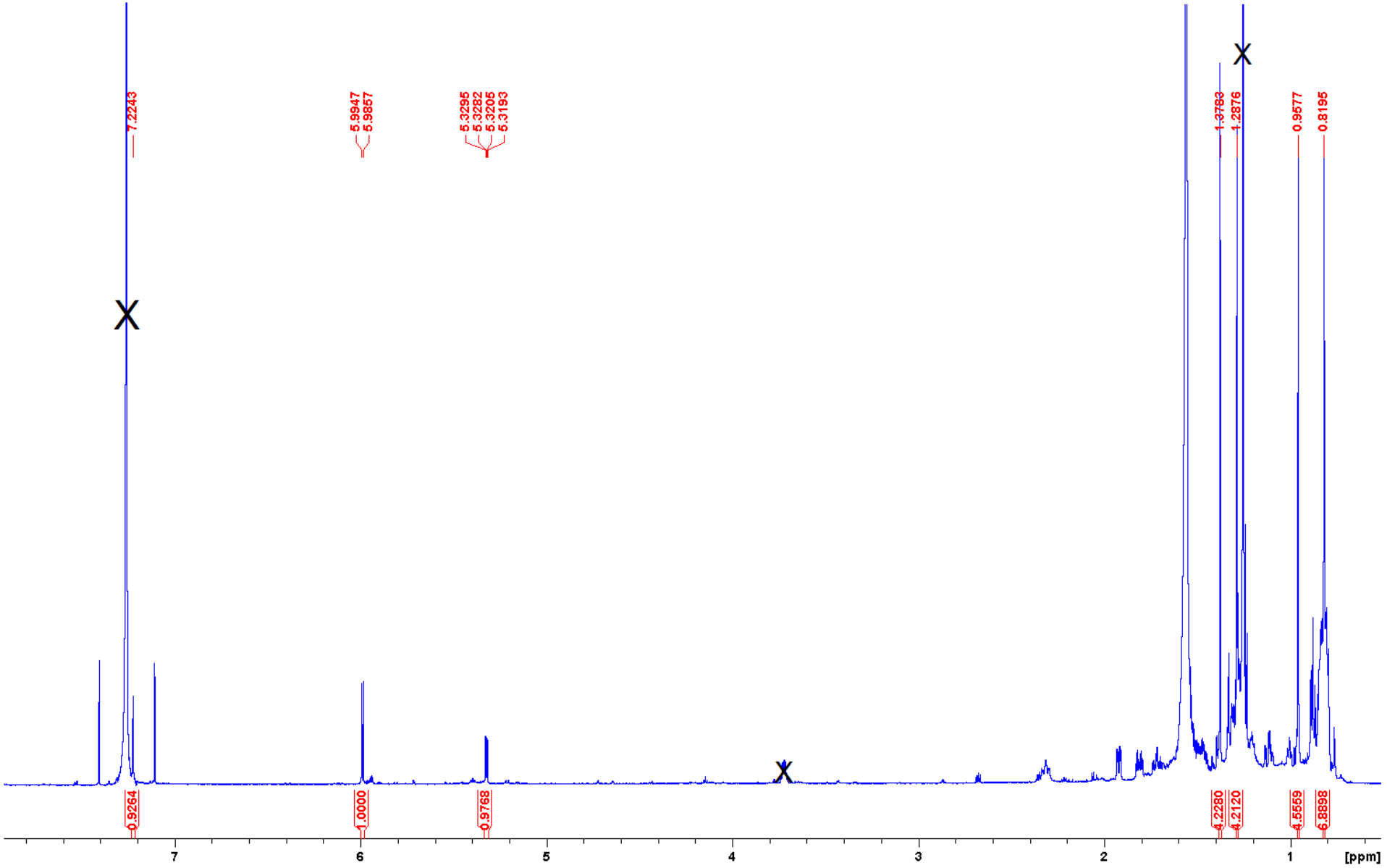


Figure S16. gCOSY spectrum of **4** (700 MHz, $CDCl_3$).

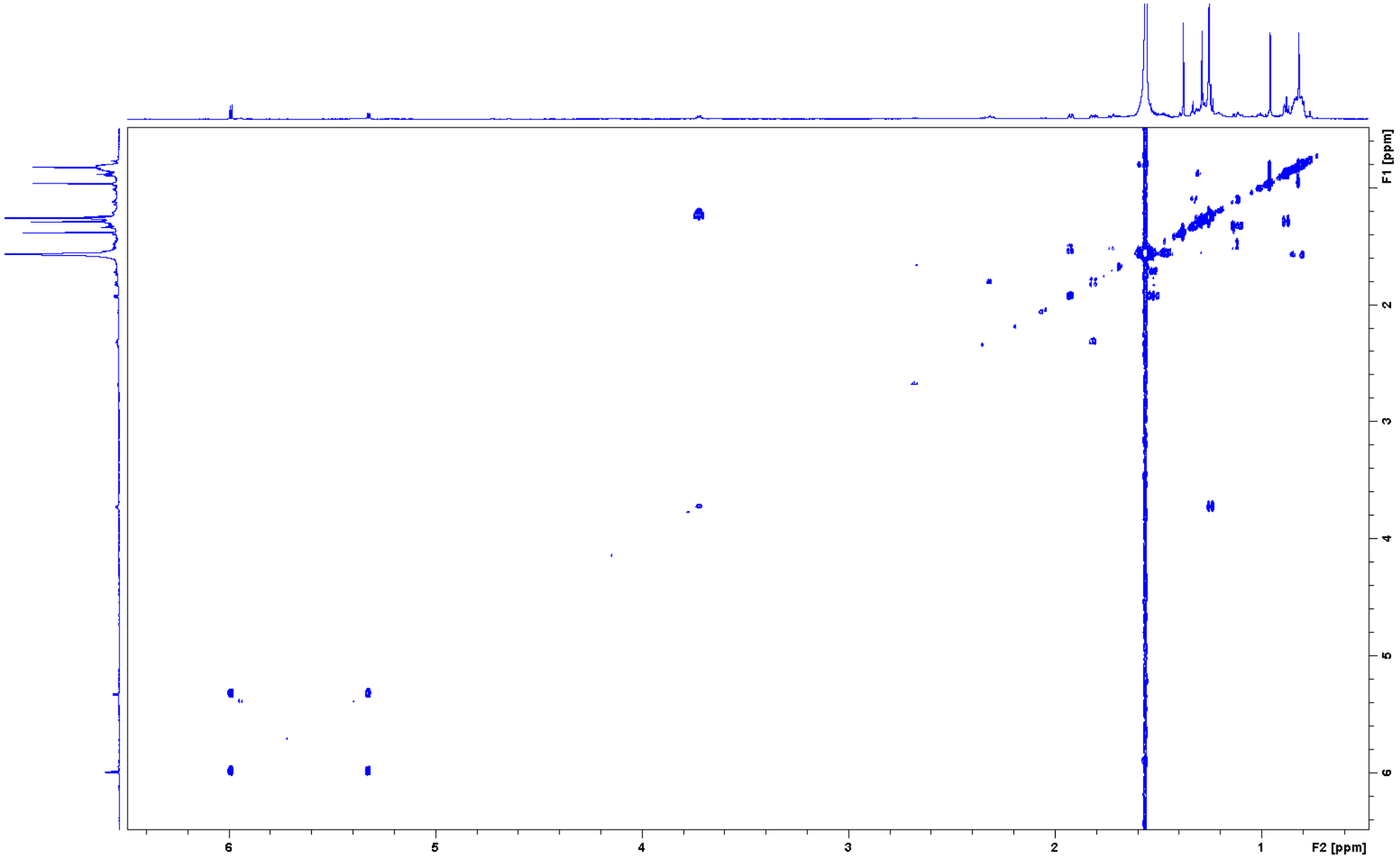


Figure S17. HSQC spectrum of **4** (700 MHz, $CDCl_3$).

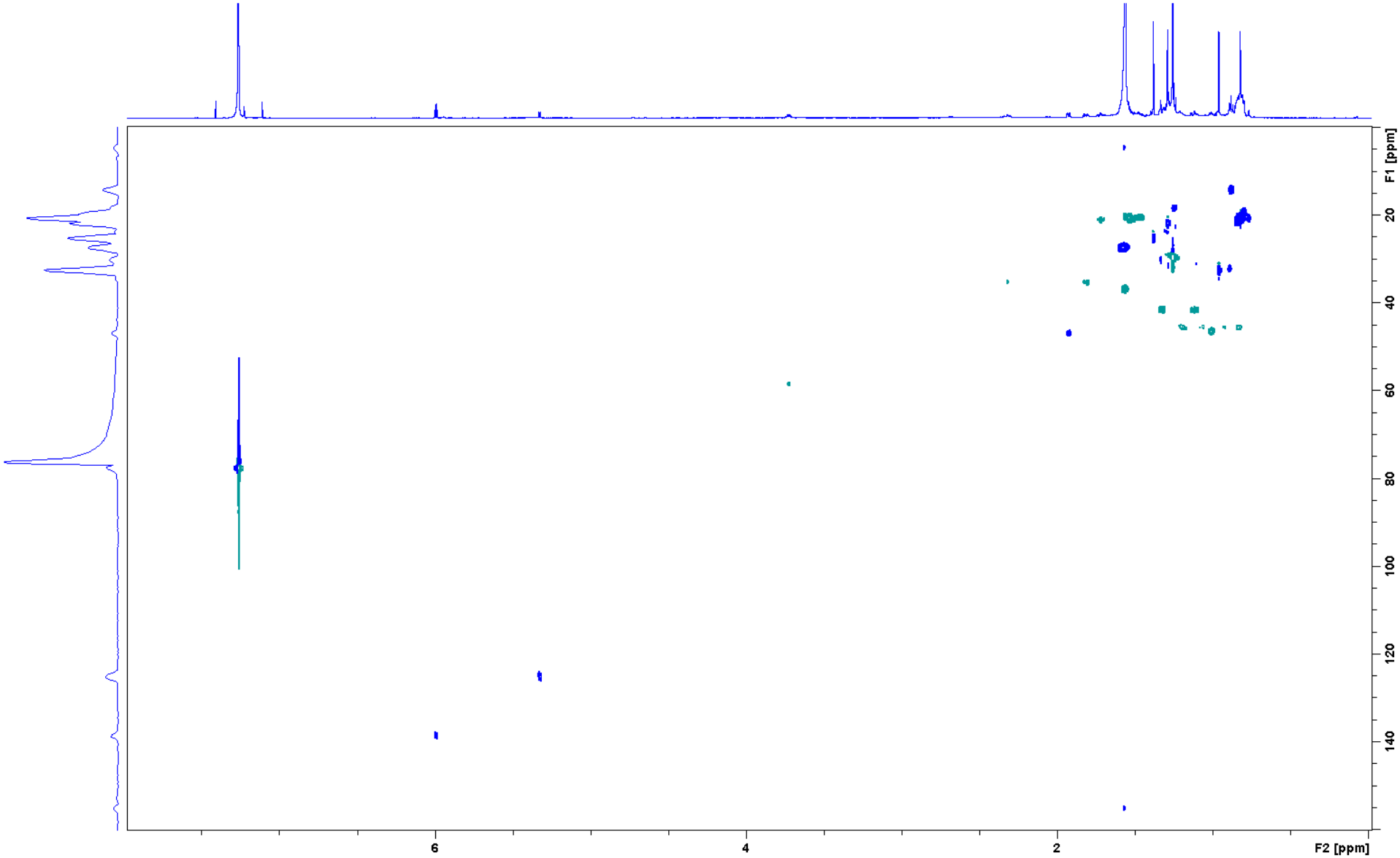


Figure S18. HMBC spectrum of **4** (700 MHz, $CDCl_3$).

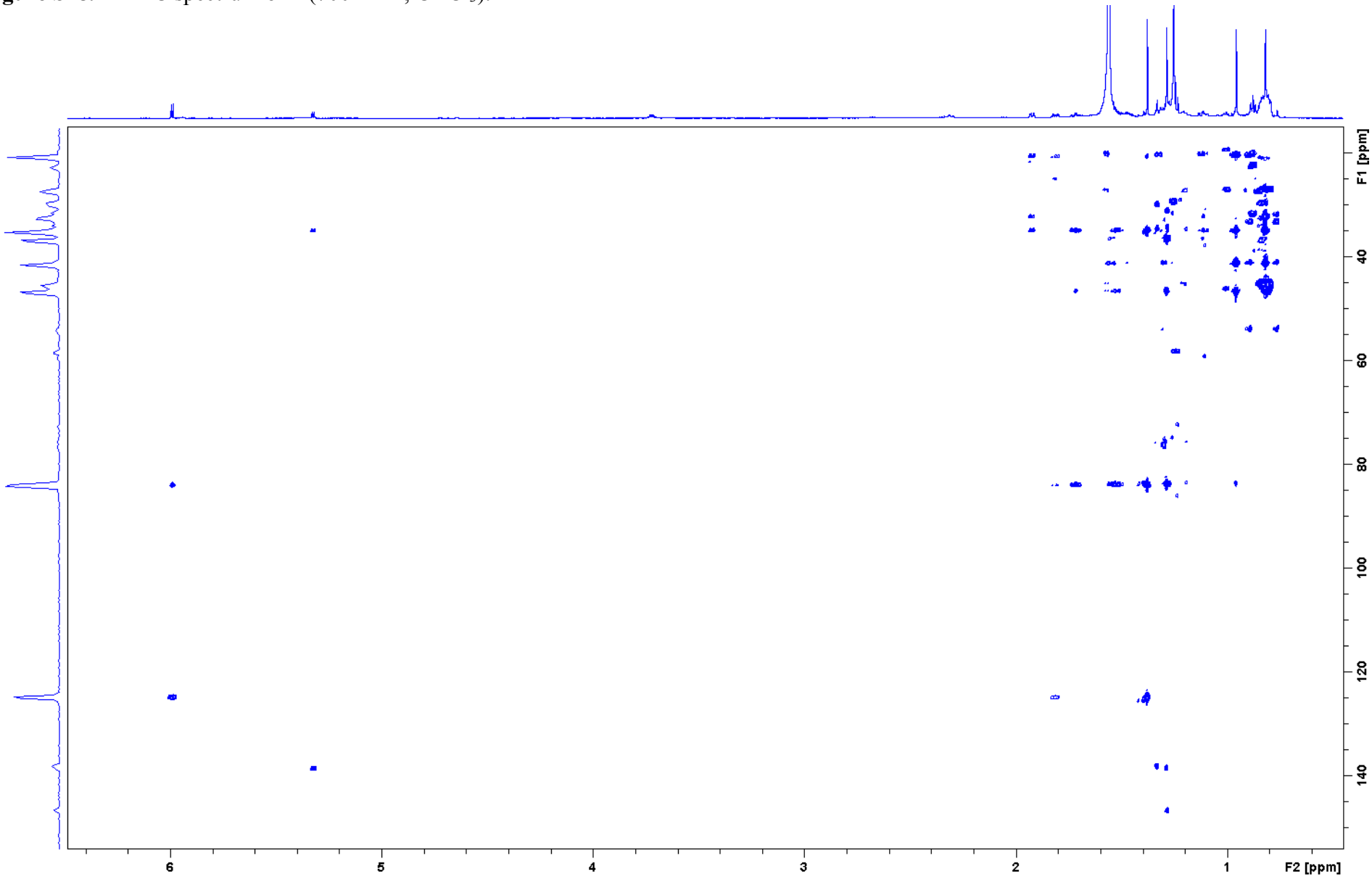


Figure S19. NOESY spectrum of **4** (700 MHz, $CDCl_3$).

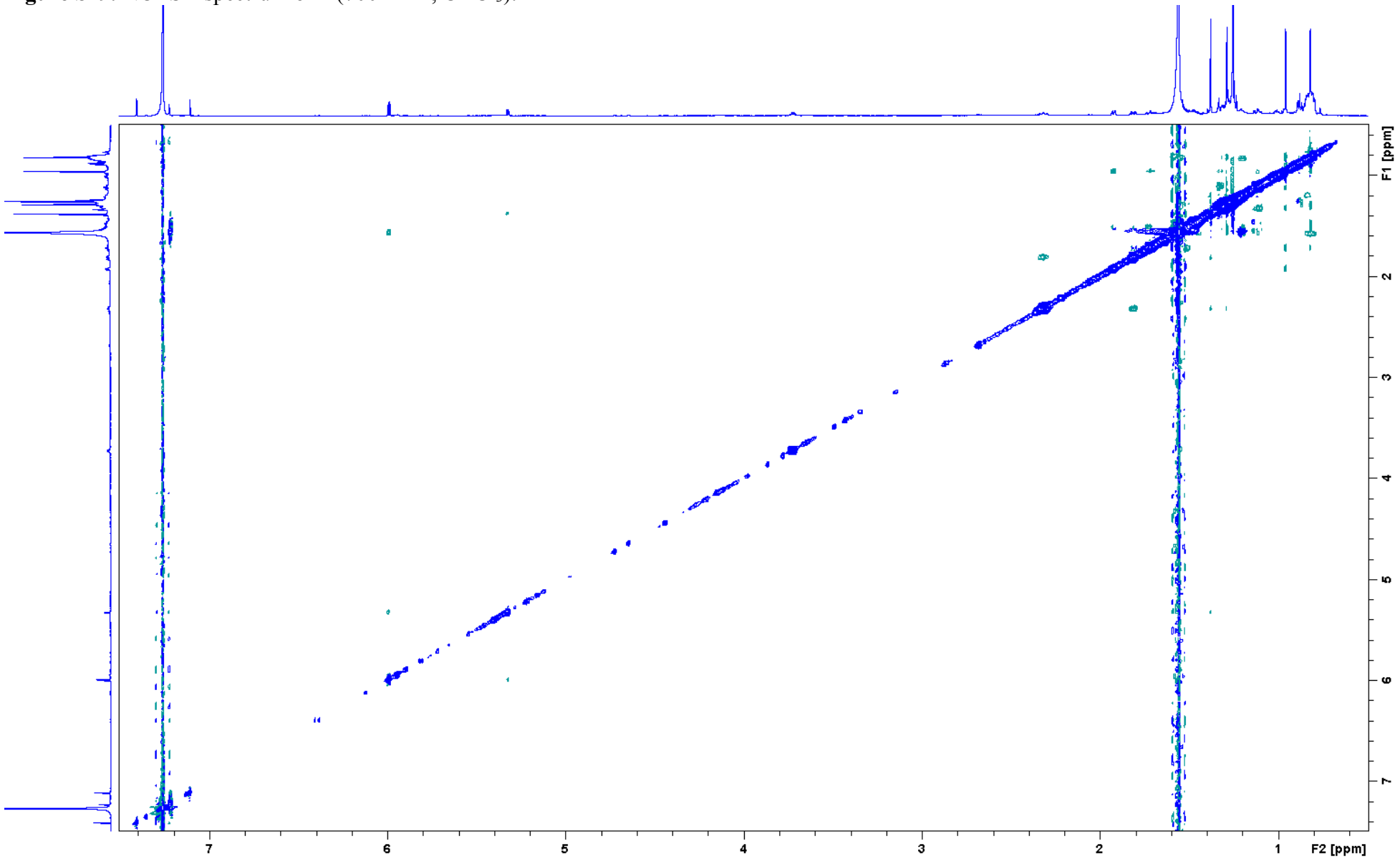


Figure S20. ^{1}H NMR spectrum of **5** (700 MHz, $CDCl_3$).

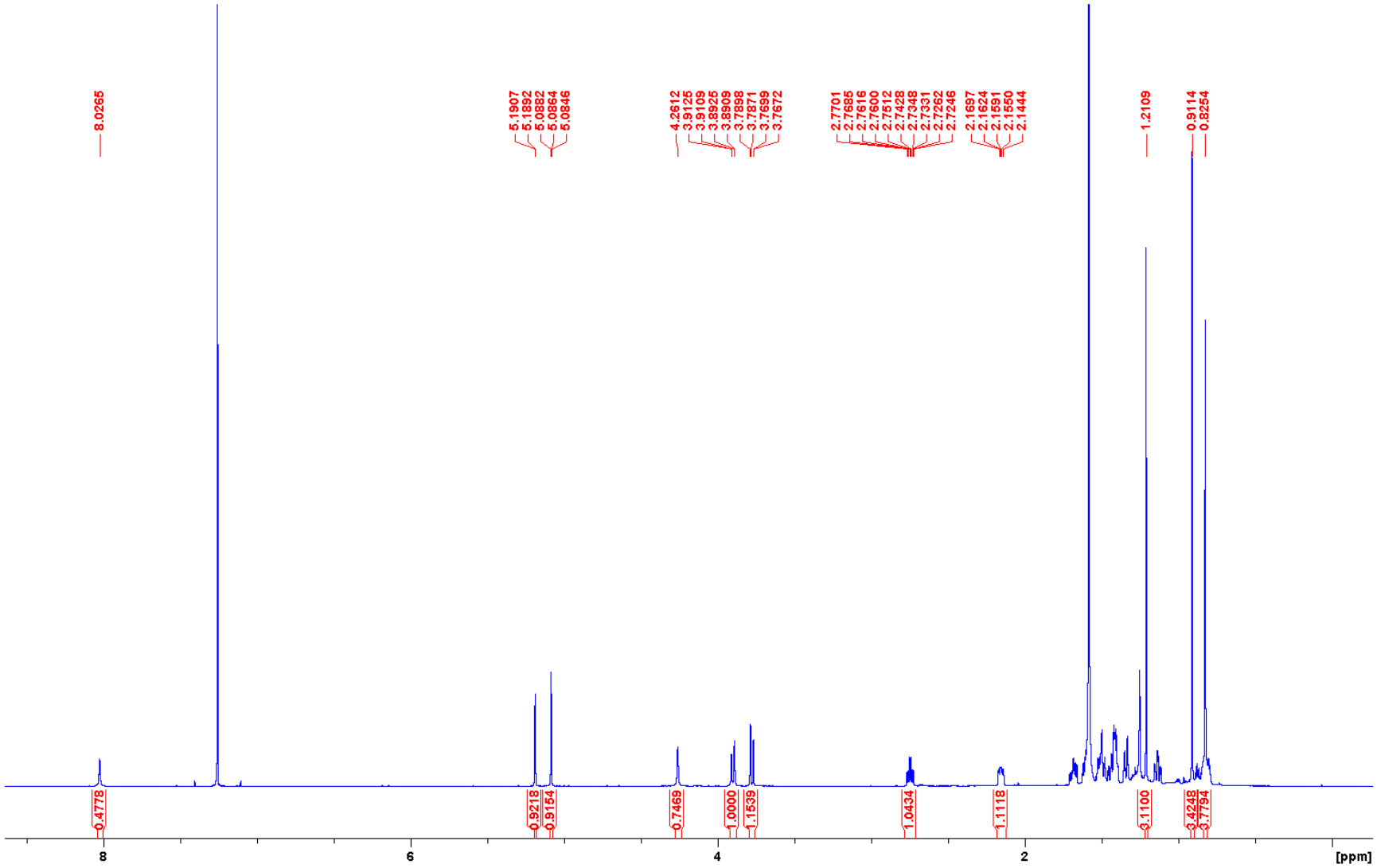


Figure S21. gCOSY spectrum of **5** (700 MHz, $CDCl_3$).

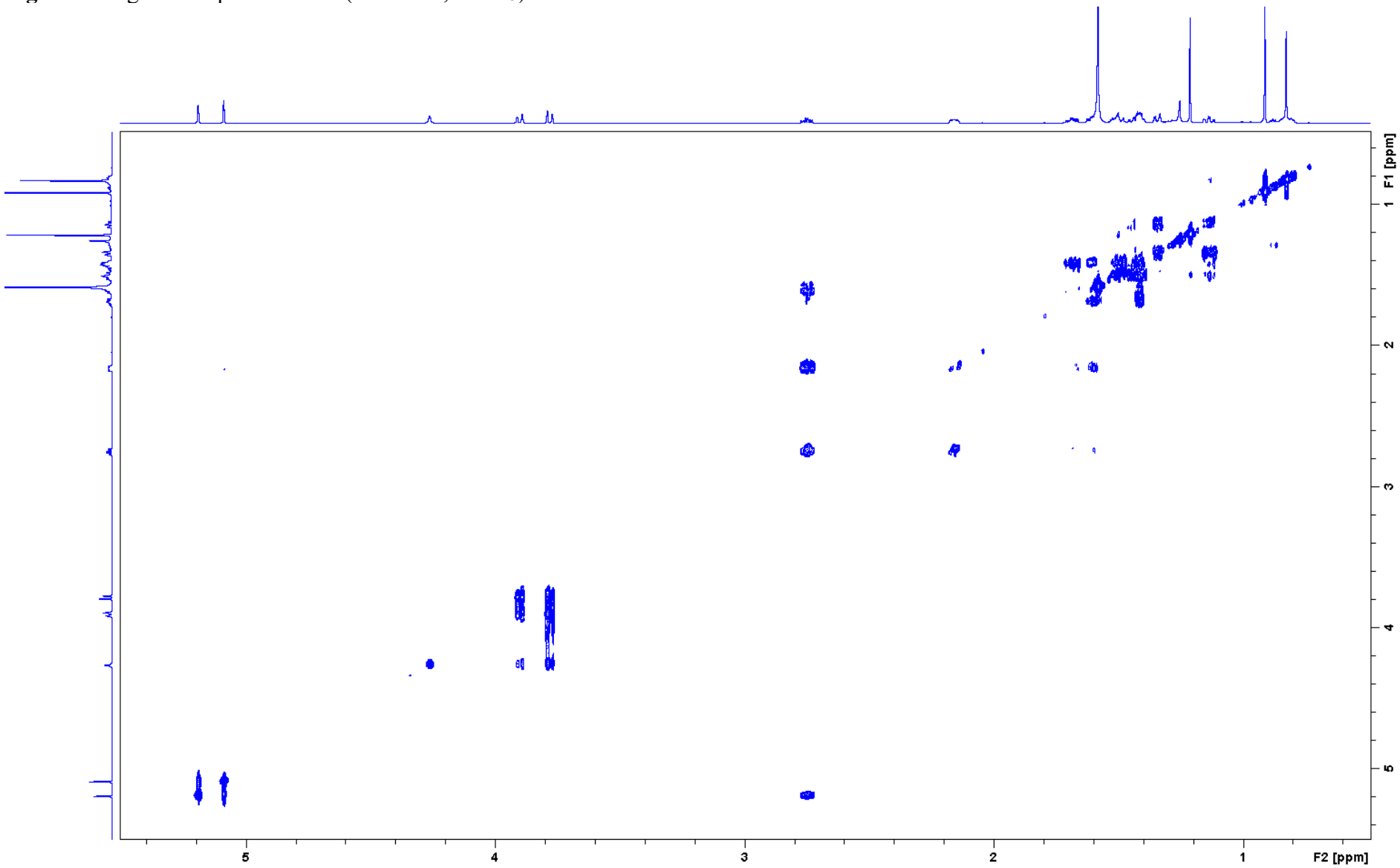


Figure S22. HSQC spectrum of **5** (700 MHz, $CDCl_3$).

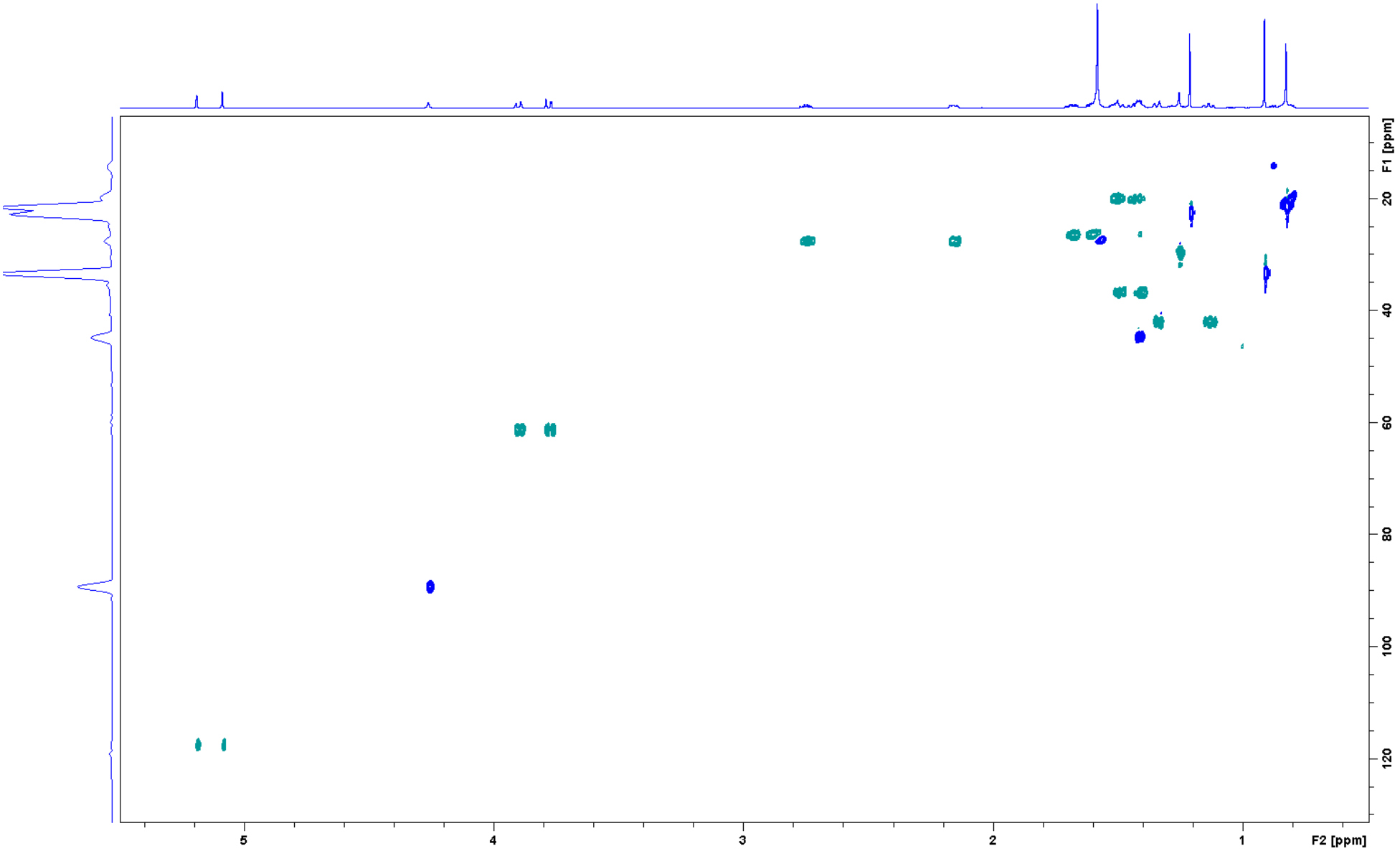


Figure S23. HMBC spectrum of **5** (700 MHz, $CDCl_3$).

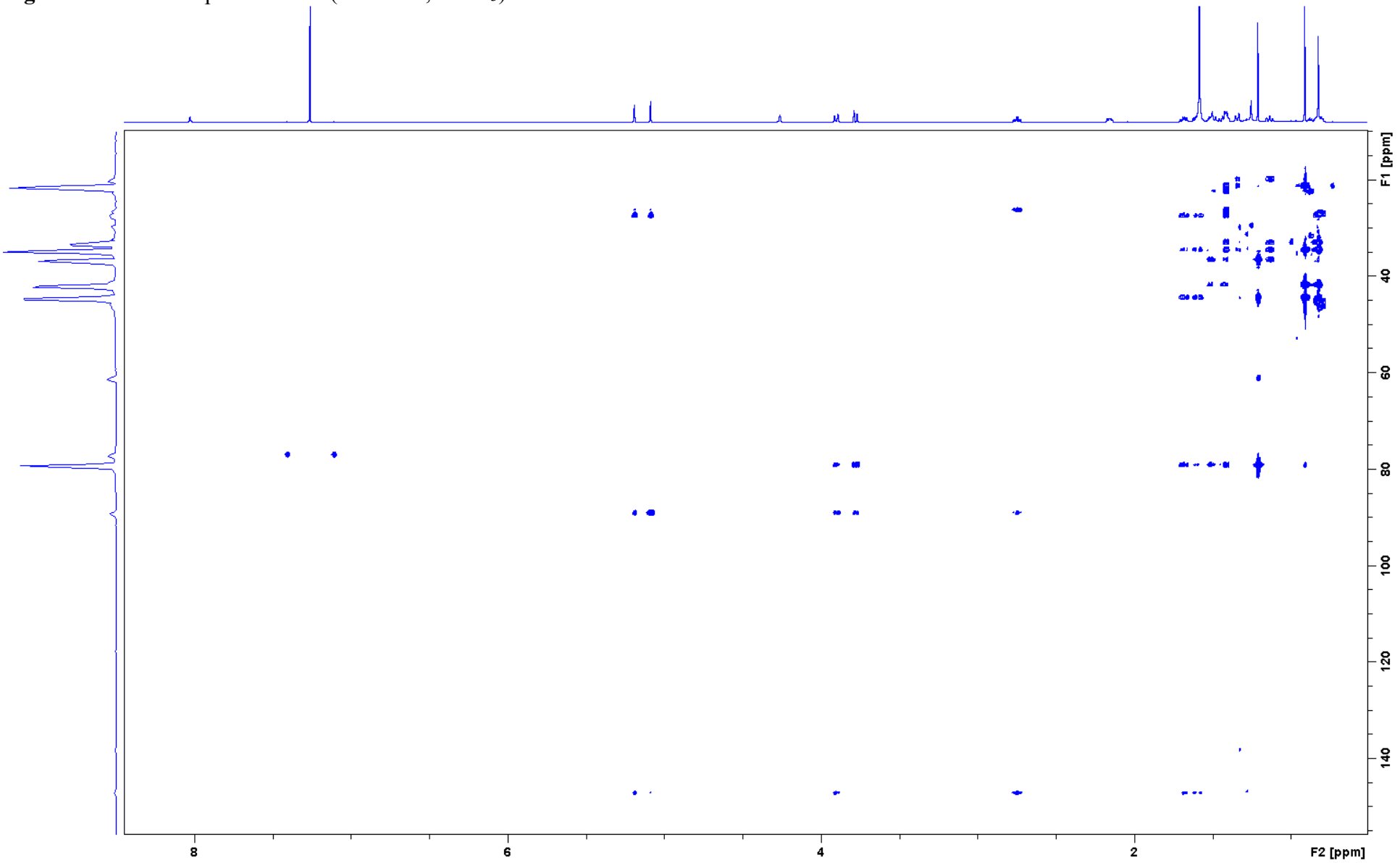


Figure S24. NOESY spectrum of **5** (700 MHz, $CDCl_3$).

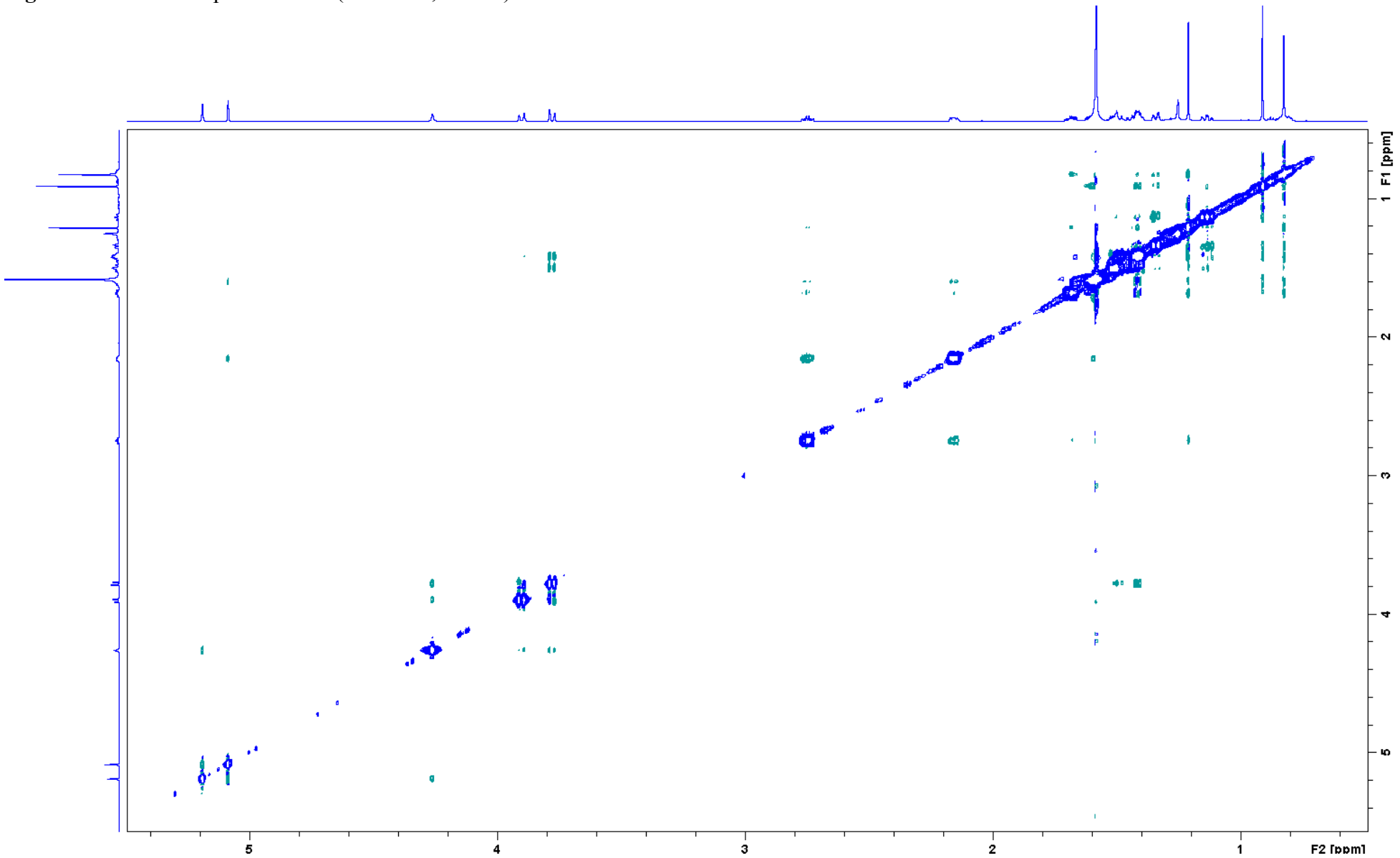


Table 1 Molecular modelling and DFT calculations for **2**.

Table A1.1. Proton experimental and calculated chemical shifts for compound **2**.

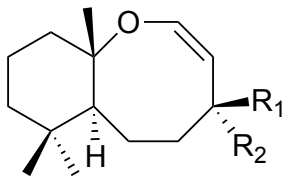
Position	^{1}H Expt.	Calculated
1a	4.22	4.2
1b	4.04	3.9
2	5.15	5.2
4a	3.36	3.4
4b	1.65	1.5
5	1.58	1.5
6	1.61	1.5
8a	1.76	1.8
8b	1.28	1.1
9a	1.54	1.5
9b	1.46	1.4
10a	1.34	1.3
10b	1.16	1.1
12	1.69	1.7
13	1.25	1.1
14	0.86	0.8
15	0.92	0.8

Table A1.2. Carbon experimental and calculated chemical shifts for compound **2**.

Position	^{13}C Expt.	Calculated
1	61.8	61.8
2	123.8	125.3
3	133.5	135.8
4	29.6	29.3
5	24.5	24.7
6	45.9	45.4
7	80	80.1
8	35.7	33.8
9	20.3	21.1
10	42.5	40.8
11	34.6	38.0
12	26.4	25.5
13	23.1	21.2
14	22.2	20.3
15	33.4	30.8

Table 2. Molecular modelling and DFT calculations for **3** and the corresponding alcohol **6**.

Table A2.1. Proton experimental and calculated chemical shifts for compounds **3** and alcohol **6**.



3 R_1 = OOH; R_2 = Me
6 R_1 = OH; R_2 = Me

Position	^{1}H Expt.	**3** Calculated	**6** Calculated
1	6.19	6.19	6.01
2	5.13	5.11	5.28
4a	3.07	2.91	2.11
4b	1.56	1.47	1.43
5	1.62	1.54	1.51
6	1.71	1.69	1.72
8a	1.59	1.55	1.61
8b	1.54	1.51	1.48
9a	1.54	1.46	1.48
9b	1.45	1.44	1.46
10a	1.34	1.23	1.26
10b	1.12	1.12	1.06
12	1.24	1.14	1.08
13	1.32	1.21	1.20
14	0.85	0.82	0.80
15	0.96	0.87	0.86
3-OOH	7.3	6.10	2.08

Table A2.2. Carbon experimental and calculated chemical shifts for compounds **3** and alcohol **6**.

Position	^{13}C Expt.	**3** Calculated	**6** Calculated
1	142.2	144.0	140.1
2	125.0	125.0	130.7
3	83.7	84.3	71.3
4	32.7	32.4	40.6
5	20.1	21.0	21.0
6	45.2	45.2	47.4

7	83.8	85.4	86.7
8	37.4	36.3	34.9
9	20.3	21.2	21.3
10	41.8	40.2	39.8
11	35.1	38.5	39.3
12	23.7	22.3	27.0
13	21.7	20.1	20.3
14	20.8	19.1	18.8
15	32.8	30.3	30.2

Table 3. Energies and XYZ Coordinates for conformers of **2**

Compound: Arenaran A, Conformer: 1, Energy:-662.309148 Hartree, Solvent: none, Boltzmann %: 99.233

Zero-point correction= 0.383128 (Hartree/Particle)
Thermal correction to Energy= 0.399475
Thermal correction to Enthalpy= 0.400419
Thermal correction to Gibbs Free Energy= 0.342076
Sum of electronic and zero-point Energies= -662.268096
Sum of electronic and thermal Energies= -662.251749
Sum of electronic and thermal Enthalpies= -662.250805
Sum of electronic and thermal Free Energies= -662.309148

C	-0.660755	1.118772	0.979670
C	0.298595	0.369087	0.031385
C	0.488450	-1.138338	0.403509
O	-0.781212	-1.851896	0.296303
C	-1.543411	-1.775810	-0.899158
C	-2.582597	-0.688137	-0.973226
C	-2.840934	0.296393	-0.110878
C	-2.068738	0.512722	1.176125
H	-2.049818	-2.745372	-0.979209
H	-2.633528	1.203388	1.810298
H	-1.992311	-0.425088	1.722541
H	-0.206658	1.225700	1.968031
H	-0.786828	2.135057	0.599109
H	-0.185057	0.349061	-0.950835
C	1.505470	-1.825246	-0.526365
H	1.072774	-1.912612	-1.527459
H	1.666202	-2.844919	-0.165071
C	1.627608	1.179565	-0.232579
C	2.824786	-1.065444	-0.651366
H	3.483222	-1.587595	-1.352024
H	3.354786	-1.049861	0.305757
C	2.564725	0.354856	-1.145035
H	2.115565	0.296609	-2.144308
H	3.507709	0.898602	-1.263415
C	-3.931771	1.298636	-0.391953
H	-4.696654	1.272166	0.392051
H	-3.532255	2.319059	-0.399913
H	-4.419417	1.116907	-1.351217
C	1.287215	2.475541	-0.999998
H	0.737447	3.192222	-0.387760
H	2.208028	2.967945	-1.324868
H	0.691119	2.263511	-1.891818
C	2.383973	1.592031	1.046601
H	1.762580	2.200932	1.705290
H	2.746208	0.743294	1.625252
H	3.255313	2.194602	0.774946
C	0.871209	-1.391360	1.864944

H	0.826527	-2.465162	2.055702
H	1.880674	-1.050636	2.087660
H	0.185101	-0.900448	2.554257
H	-0.897670	-1.710011	-1.784984
H	-3.186310	-0.751782	-1.878490

Compound: Arenaran A, Conformer: 2, Energy:-662.304557 Hartree, Solvent: none, Boltzmann %: 0.767

Zero-point correction= 0.382855 (Hartree/Particle)
Thermal correction to Energy= 0.399284
Thermal correction to Enthalpy= 0.400228
Thermal correction to Gibbs Free Energy= 0.341612
Sum of electronic and zero-point Energies= -662.263314
Sum of electronic and thermal Energies= -662.246885
Sum of electronic and thermal Enthalpies= -662.245941
Sum of electronic and thermal Free Energies= -662.304557

C	0.510651	-1.442012	-0.092286
C	-0.606057	-0.425320	-0.411984
C	-0.264645	1.041865	0.006516
O	0.817918	1.444423	-0.894837
C	2.084220	1.861966	-0.412944
C	3.008265	0.792301	0.104599
C	2.934892	-0.528174	-0.065756
C	1.850074	-1.240880	-0.852164
H	1.984123	2.641224	0.352489
H	1.655308	-0.721461	-1.790660
H	2.237646	-2.228779	-1.117355
H	0.706167	-1.475706	0.982968
H	0.137888	-2.433086	-0.352008
H	-0.650983	-0.359756	-1.506494
C	-1.425727	1.980911	-0.364955
H	-1.473425	2.022145	-1.457726
H	-1.182065	2.991348	-0.022798
C	-2.035384	-0.948113	0.002095
C	-2.777986	1.522542	0.175578
H	-3.557251	2.221117	-0.143773
H	-2.786050	1.543810	1.269920
C	-3.099656	0.122139	-0.340160
H	-3.198434	0.173997	-1.431310
H	-4.070087	-0.213608	0.040485
C	3.956324	-1.437211	0.571152
H	3.472091	-2.166991	1.230308
H	4.490677	-2.016048	-0.190225
H	4.690067	-0.883359	1.159010
C	-2.383998	-2.195933	-0.839551
H	-1.797958	-3.072066	-0.557037
H	-3.437022	-2.455116	-0.698559
H	-2.226674	-2.011525	-1.905738

C	-2.158018	-1.350850	1.485967
H	-1.391155	-2.072337	1.774256
H	-2.090096	-0.504515	2.168662
H	-3.129634	-1.823174	1.656388
C	0.099451	1.227714	1.481846
H	0.349888	2.270447	1.684656
H	-0.750841	0.980529	2.113297
H	0.938059	0.607533	1.791908
H	2.548648	2.355786	-1.275150
H	3.833344	1.188533	0.695466

Table 4. Energies and XYZ Coordinates for conformers of **3**

Compound: Arenaran C, Conformer: 01, Energy:-812.710732 Hartree, Solvent: none, Boltzmann %: 42.609
Zero-point correction= 0.390046 (Hartree/Particle)
Thermal correction to Energy= 0.408784
Thermal correction to Enthalpy= 0.409728
Thermal correction to Gibbs Free Energy= 0.346252
Sum of electronic and zero-point Energies= -812.666939
Sum of electronic and thermal Energies= -812.648200
Sum of electronic and thermal Enthalpies= -812.647256
Sum of electronic and thermal Free Energies= -812.710732

C	-0.169876	1.048988	1.033313
C	0.805163	0.340197	0.066300
C	0.854992	-1.204093	0.250245
O	-0.496064	-1.754596	0.013644
C	-1.170338	-1.450215	-1.134035
C	-2.040370	-0.449874	-1.258324
C	-2.430796	0.594345	-0.241756
C	-1.644325	0.596641	1.078885
H	-0.998425	-2.129901	-1.968314
H	-2.559518	-0.376612	-2.210733
H	-2.173580	1.292152	1.738330
H	-1.729199	-0.387959	1.529019
H	0.208428	0.972210	2.055757
H	-0.152129	2.115126	0.801111
H	0.407660	0.473732	-0.945127
C	1.814009	-1.849239	-0.759653
H	1.400144	-1.718473	-1.765184
H	1.854708	-2.925411	-0.569374
C	2.214029	1.047585	-0.003211
C	3.209123	-1.225567	-0.728687
H	3.838148	-1.698122	-1.488678
H	3.696509	-1.422636	0.230863
C	3.122324	0.276276	-0.990869
H	2.735413	0.426820	-2.006193
H	4.120895	0.724657	-0.973049
C	-2.458329	1.979757	-0.896353
H	-2.798279	2.731556	-0.181609
H	-1.461813	2.253138	-1.243768
H	-3.131847	1.983855	-1.755082
C	2.041757	2.469886	-0.578917
H	1.536818	3.144441	0.114421
H	3.022190	2.903607	-0.793573
H	1.475160	2.454683	-1.514140
C	2.923206	1.188830	1.358382
H	2.303359	1.716600	2.085351
H	3.207330	0.233232	1.796744
H	3.840034	1.771019	1.231137

O	-3.856708	0.405896	0.059049
C	1.143853	-1.694320	1.668237
H	0.967052	-2.770650	1.708122
H	2.176096	-1.511387	1.959030
H	0.492043	-1.219550	2.400894
O	-4.068598	-0.848950	0.749075
H	-4.192774	-1.470108	0.008571

Compound: Arenaran C, Conformer: 02, Energy:-812.709488 Hartree, Solvent: none, Boltzmann %: 11.41

Zero-point correction= 0.390123 (Hartree/Particle)
Thermal correction to Energy= 0.408823
Thermal correction to Enthalpy= 0.409767
Thermal correction to Gibbs Free Energy= 0.346376
Sum of electronic and zero-point Energies= -812.665740
Sum of electronic and thermal Energies= -812.647041
Sum of electronic and thermal Enthalpies= -812.646096
Sum of electronic and thermal Free Energies= -812.709488

C	-0.181975	1.023156	1.046683
C	0.801884	0.334369	0.074642
C	0.869053	-1.210476	0.248367
O	-0.476162	-1.769165	0.018760
C	-1.156311	-1.479071	-1.132538
C	-2.039827	-0.493079	-1.261854
C	-2.425480	0.568031	-0.262331
C	-1.656125	0.564974	1.069367
H	-0.982693	-2.168001	-1.958177
H	-2.572417	-0.440295	-2.207469
H	-2.193146	1.258225	1.726411
H	-1.736715	-0.424604	1.511889
H	0.188438	0.931350	2.070821
H	-0.168509	2.092904	0.832129
H	0.400874	0.468326	-0.935375
C	1.831319	-1.836506	-0.770502
H	1.411911	-1.701887	-1.773157
H	1.884960	-2.913771	-0.589604
C	2.201157	1.059447	0.008318
C	3.219541	-1.197374	-0.738630
H	3.851349	-1.655885	-1.504933
H	3.712510	-1.397645	0.217474
C	3.116172	0.305912	-0.987150
H	2.725908	0.461181	-2.000443
H	4.110006	0.764696	-0.967085
C	-2.407746	1.948778	-0.930308
H	-2.732967	2.718481	-0.227501
H	-1.401496	2.190822	-1.272024
H	-3.073981	1.960370	-1.794348
C	2.011425	2.483949	-0.556469

H	1.498737	3.147316	0.142086
H	2.986454	2.931143	-0.768155
H	1.444850	2.468998	-1.491669
C	2.910640	1.198878	1.369972
H	2.283873	1.710397	2.102817
H	3.209975	0.243660	1.798897
H	3.818283	1.796184	1.246866
O	-3.858937	0.427305	0.016640
C	1.173292	-1.706995	1.661446
H	1.007033	-2.785235	1.694881
H	2.205408	-1.515980	1.947343
H	0.521600	-1.244071	2.401995
O	-4.129918	-0.866060	0.616702
H	-4.282222	-0.617282	1.545442

Compound: Arenaran C, Conformer: 03, Energy:-812.708628 Hartree, Solvent: none, Boltzmann %: 4.589

Zero-point correction= 0.390094 (Hartree/Particle)
Thermal correction to Energy= 0.408821
Thermal correction to Enthalpy= 0.409765
Thermal correction to Gibbs Free Energy= 0.346225
Sum of electronic and zero-point Energies= -812.664759
Sum of electronic and thermal Energies= -812.646032
Sum of electronic and thermal Enthalpies= -812.645088
Sum of electronic and thermal Free Energies= -812.708628

C	-0.121469	1.015726	1.082286
C	0.828592	0.330340	0.075680
C	1.015475	-1.192607	0.333959
O	-0.302683	-1.849100	0.252000
C	-1.092495	-1.674212	-0.851211
C	-2.048441	-0.755824	-0.965979
C	-2.426738	0.341787	-0.000337
C	-1.549718	0.459882	1.261151
H	-0.938965	-2.401119	-1.647854
H	-2.647271	-0.798311	-1.869704
H	-2.075503	1.146891	1.932050
H	-1.528433	-0.509123	1.754118
H	0.333020	1.018236	2.076143
H	-0.205113	2.066840	0.802353
H	0.341538	0.373911	-0.903866
C	1.932919	-1.819837	-0.724598
H	1.425623	-1.776287	-1.694182
H	2.075021	-2.877730	-0.486522
C	2.165289	1.137279	-0.147757
C	3.271951	-1.092805	-0.847822
H	3.869450	-1.557487	-1.637534
H	3.853439	-1.200870	0.072719
C	3.046523	0.382517	-1.172245

H	2.566367	0.449380	-2.156180
H	4.005188	0.903536	-1.262104
C	-2.557093	1.677663	-0.734789
H	-2.869117	2.463027	-0.042015
H	-1.605524	1.968732	-1.181597
H	-3.291184	1.603315	-1.537672
C	1.834674	2.509355	-0.773885
H	1.338226	3.181705	-0.072286
H	2.756810	3.002073	-1.093761
H	1.195091	2.401401	-1.654244
C	2.970432	1.404482	1.139581
H	2.371251	1.919122	1.892950
H	3.367874	0.498359	1.594418
H	3.822299	2.049581	0.907428
O	-3.716748	0.001808	0.616074
C	1.464563	-1.577831	1.742965
H	1.372426	-2.659751	1.853600
H	2.501649	-1.307214	1.928900
H	0.845527	-1.108793	2.507262
O	-4.728467	-0.190567	-0.410040
H	-5.303281	0.577959	-0.248684

Compound: Arenaran C, Conformer: 04, Energy:-812.709853 Hartree, Solvent: none, Boltzmann %: 16.795

Zero-point correction= 0.390116 (Hartree/Particle)
Thermal correction to Energy= 0.408852
Thermal correction to Enthalpy= 0.409796
Thermal correction to Gibbs Free Energy= 0.346023
Sum of electronic and zero-point Energies= -812.665760
Sum of electronic and thermal Energies= -812.647024
Sum of electronic and thermal Enthalpies= -812.646080
Sum of electronic and thermal Free Energies= -812.709853

C	-0.111439	1.041823	1.063650
C	0.833155	0.332438	0.068390
C	0.996365	-1.191100	0.339707
O	-0.331665	-1.831768	0.249685
C	-1.109970	-1.642172	-0.857513
C	-2.055217	-0.711881	-0.972906
C	-2.429102	0.382701	-0.001876
C	-1.543327	0.500331	1.253078
H	-0.952698	-2.360027	-1.661969
H	-2.634040	-0.733252	-1.890946
H	-2.060214	1.195991	1.921694
H	-1.527343	-0.465319	1.753012
H	0.343830	1.057011	2.057037
H	-0.186941	2.088653	0.766012
H	0.352745	0.376365	-0.914371
C	1.912510	-1.840588	-0.706390

H	1.413294	-1.798674	-1.680212
H	2.037986	-2.898166	-0.457812
C	2.183447	1.117431	-0.153586
C	3.262445	-1.133616	-0.826867
H	3.858521	-1.614158	-1.608092
H	3.836110	-1.241205	0.098601
C	3.059551	0.341512	-1.166403
H	2.585988	0.406050	-2.153691
H	4.025885	0.848237	-1.255423
C	-2.570574	1.718015	-0.734944
H	-2.859744	2.504070	-0.034073
H	-1.630301	2.002249	-1.210176
H	-3.333378	1.644792	-1.510100
C	1.876042	2.489059	-0.792350
H	1.385496	3.173898	-0.098775
H	2.806908	2.965838	-1.111045
H	1.239443	2.383346	-1.675115
C	2.985375	1.383080	1.136137
H	2.390816	1.914905	1.881094
H	3.365160	0.474847	1.601849
H	3.849211	2.011630	0.902892
O	-3.716889	0.052153	0.626162
C	1.427006	-1.571981	1.755324
H	1.317834	-2.651465	1.874130
H	2.466605	-1.315545	1.947207
H	0.809504	-1.086807	2.510668
O	-4.747617	-0.107425	-0.382781
H	-4.828908	-1.077258	-0.417626

Compound: Arenaran C, Conformer: 05, Energy:-812.709158 Hartree, Solvent: none, Boltzmann %: 8.045

Zero-point correction= 0.390108 (Hartree/Particle)
Thermal correction to Energy= 0.408801
Thermal correction to Enthalpy= 0.409745
Thermal correction to Gibbs Free Energy= 0.346263
Sum of electronic and zero-point Energies= -812.665314
Sum of electronic and thermal Energies= -812.646621
Sum of electronic and thermal Enthalpies= -812.645676
Sum of electronic and thermal Free Energies= -812.709158

C	-0.282997	0.985022	0.937651
C	0.792538	0.330952	0.041379
C	1.050886	-1.167940	0.370139
O	-0.211696	-1.915337	0.193117
C	-0.909790	-1.820939	-0.974972
C	-1.913507	-0.974576	-1.197895
C	-2.442914	0.117637	-0.299515
C	-1.681927	0.340089	1.017643
H	-0.633408	-2.544444	-1.741451

H	-2.427821	-1.075054	-2.149114
H	-2.305755	1.008226	1.616960
H	-1.640786	-0.610527	1.544779
H	0.086886	1.054570	1.963732
H	-0.408740	2.017929	0.608528
H	0.392314	0.312972	-0.977736
C	2.097313	-1.767986	-0.578588
H	1.678846	-1.788958	-1.590442
H	2.282525	-2.806098	-0.288809
C	2.092439	1.214439	-0.096598
C	3.394243	-0.959643	-0.610711
H	4.088455	-1.410272	-1.325933
H	3.895282	-0.999237	0.361148
C	3.107166	0.486013	-1.010565
H	2.713933	0.488539	-2.034558
H	4.035565	1.065605	-1.036616
C	-2.614497	1.408245	-1.105985
H	-3.042375	2.198202	-0.487887
H	-1.651259	1.753287	-1.483825
H	-3.269942	1.235662	-1.962518
C	1.734121	2.540595	-0.801474
H	1.134988	3.200832	-0.172400
H	2.648554	3.082384	-1.057829
H	1.184467	2.361986	-1.729802
C	2.761788	1.576235	1.244252
H	2.067830	2.076922	1.921765
H	3.171224	0.713325	1.767424
H	3.590450	2.265909	1.061518
O	-3.763394	-0.441408	0.026282
C	1.390761	-1.479506	1.826724
H	1.359799	-2.561261	1.968544
H	2.386404	-1.132770	2.094728
H	0.674571	-1.029922	2.513729
O	-4.554094	0.530413	0.772297
H	-5.232270	0.761028	0.113599

Compound: Arenaran C, Conformer: 06, Energy:-812.709322 Hartree, Solvent: none, Boltzmann %: 9.571

Zero-point correction= 0.390124 (Hartree/Particle)
Thermal correction to Energy= 0.408819
Thermal correction to Enthalpy= 0.409763
Thermal correction to Gibbs Free Energy= 0.346371
Sum of electronic and zero-point Energies= -812.665569
Sum of electronic and thermal Energies= -812.646874
Sum of electronic and thermal Enthalpies= -812.645930
Sum of electronic and thermal Free Energies= -812.709322

C	-0.286215	0.990204	0.927246
C	0.792383	0.330599	0.039199

C	1.042022	-1.168871	0.371169
O	-0.224020	-1.908770	0.188488
C	-0.912474	-1.812607	-0.986019
C	-1.911381	-0.962899	-1.216412
C	-2.444373	0.131188	-0.322181
C	-1.689381	0.352134	0.998374
H	-0.631662	-2.536728	-1.750122
H	-2.420364	-1.061338	-2.170510
H	-2.307922	1.031597	1.591629
H	-1.654892	-0.596811	1.530173
H	0.076862	1.059663	1.955789
H	-0.406165	2.022766	0.595478
H	0.398580	0.313598	-0.982338
C	2.090775	-1.774491	-0.571341
H	1.677911	-1.794321	-1.585455
H	2.269962	-2.813180	-0.279829
C	2.096565	1.208625	-0.090534
C	3.391424	-0.971690	-0.596808
H	4.087297	-1.425560	-1.308305
H	3.887271	-1.013406	0.377616
C	3.113263	0.475280	-0.998397
H	2.726093	0.479618	-2.024642
H	4.044483	1.050503	-1.018964
C	-2.611483	1.422375	-1.128675
H	-3.059919	2.203949	-0.515183
H	-1.644962	1.776018	-1.490273
H	-3.255557	1.245162	-1.991781
C	1.748343	2.536412	-0.797338
H	1.148501	3.199361	-0.171749
H	2.666710	3.074113	-1.048046
H	1.203359	2.360572	-1.728875
C	2.759233	1.567156	1.254515
H	2.063447	2.071056	1.927815
H	3.161654	0.702445	1.780154
H	3.592019	2.253178	1.077050
O	-3.772269	-0.422010	-0.016958
C	1.372821	-1.480961	1.829817
H	1.332200	-2.562227	1.972915
H	2.370098	-1.142334	2.101875
H	0.657664	-1.024253	2.513311
O	-4.587949	0.566699	0.677751
H	-4.617893	0.184488	1.572310

Compound: Arenaran C, Conformer: 11, Energy:-812.709024 Hartree, Solvent: none, Boltzmann %: 6.98

Zero-point correction= 0.389954 (Hartree/Particle)
Thermal correction to Energy= 0.408654
Thermal correction to Enthalpy= 0.409598
Thermal correction to Gibbs Free Energy= 0.346447

Sum of electronic and zero-point Energies= -812.665517
Sum of electronic and thermal Energies= -812.646817
Sum of electronic and thermal Enthalpies= -812.645873
Sum of electronic and thermal Free Energies= -812.709024

C	-0.195566	1.093350	0.893228
C	0.858639	0.371816	0.014658
C	0.859244	-1.167455	0.234575
O	-0.525999	-1.632325	0.041152
C	-1.155605	-1.363754	-1.140980
C	-2.077604	-0.416291	-1.287891
C	-2.540135	0.605111	-0.263092
C	-1.446129	1.614898	0.161696
H	-0.909411	-2.025097	-1.970760
H	-2.560206	-0.370723	-2.259023
H	-1.152037	2.161799	-0.739212
H	-1.940472	2.341364	0.814154
H	-0.520134	0.449029	1.708902
H	0.261135	1.961811	1.371299
H	0.529860	0.482443	-1.024319
C	1.791146	-1.846411	-0.778486
H	1.390237	-1.698312	-1.786250
H	1.803270	-2.924425	-0.593856
C	2.279449	1.038138	0.008171
C	3.207874	-1.264422	-0.731726
H	3.823006	-1.744851	-1.498052
H	3.683940	-1.499527	0.224634
C	3.189395	0.247587	-0.964053
H	4.206005	0.650226	-0.907271
H	2.841685	0.434525	-1.987249
C	-3.743533	1.372511	-0.818943
H	-4.101241	2.096507	-0.085533
H	-3.465248	1.906663	-1.730526
H	-4.556155	0.685846	-1.057361
C	2.149391	2.470195	-0.550137
H	1.583405	3.124643	0.116041
H	3.140081	2.914918	-0.677852
H	1.655231	2.471794	-1.525490
C	2.942062	1.138233	1.396093
H	2.277849	1.598925	2.130501
H	3.251973	0.172728	1.792250
H	3.837219	1.762662	1.330419
O	-2.908146	-0.009447	1.000512
C	1.157666	-1.658027	1.651322
H	0.880607	-2.711879	1.715621
H	2.213121	-1.573327	1.898216
H	0.584977	-1.115066	2.402382
O	-3.941489	-1.001946	0.793018
H	-3.411393	-1.815807	0.714273

Table 5. Energies and XYZ Coordinates for conformers of **4**

Compound: Arenaran D, Conformer: 01, Energy:-812.710032 Hartree, Solvent: none, Boltzmann %: 9.827

Zero-point correction=	0.390011 (Hartree/Particle)
Thermal correction to Energy=	0.408746
Thermal correction to Enthalpy=	0.409690
Thermal correction to Gibbs Free Energy=	0.346163
Sum of electronic and zero-point Energies=	-812.666185
Sum of electronic and thermal Energies=	-812.647450
Sum of electronic and thermal Enthalpies=	-812.646506
Sum of electronic and thermal Free Energies=	-812.710032

C	-0.237466	0.741918	1.247470
C	0.737627	0.295040	0.136781
C	1.077625	-1.222547	0.172855
O	-0.174064	-1.991832	0.008631
C	-1.005067	-1.704675	-1.041142
C	-2.053986	-0.891038	-0.969590
C	-2.538609	-0.082627	0.210317
C	-1.581883	0.004926	1.415016
H	-0.792182	-2.243252	-1.963485
H	-2.673325	-0.814656	-1.856841
H	-2.130356	0.527049	2.205648
H	-1.423702	-1.013860	1.764591
H	0.261736	0.689954	2.219011
H	-0.461433	1.796411	1.087361
H	0.213588	0.431124	-0.813762
C	2.023093	-1.604194	-0.974608
H	1.487382	-1.481346	-1.921592
H	2.275112	-2.664850	-0.886304
C	1.984105	1.252997	0.005568
C	3.280079	-0.735572	-1.018016
H	3.896071	-1.026105	-1.874089
H	3.896994	-0.907857	-0.130834
C	2.900061	0.739327	-1.131297
H	2.382475	0.889831	-2.086516
H	3.799396	1.362712	-1.166977
C	-3.895678	-0.625246	0.675563
H	-4.599315	-0.688532	-0.154733
H	-3.770427	-1.627440	1.089208
H	-4.317586	0.020431	1.449754
C	1.501929	2.658837	-0.412791
H	0.972273	3.174513	0.389751
H	2.360616	3.279170	-0.684156
H	0.837687	2.609711	-1.279541
C	2.803598	1.417077	1.301270
H	2.185784	1.767414	2.130017
H	3.295557	0.499004	1.619687
H	3.586205	2.164355	1.143049

O	-2.672258	1.318278	-0.184186
C	1.596626	-1.755406	1.507561
H	1.604451	-2.846274	1.468939
H	2.610490	-1.418452	1.712905
H	0.961290	-1.452580	2.339547
O	-3.609415	1.445129	-1.287784
H	-4.365210	1.868013	-0.843652

Compound: Arenaran D, Conformer: 02, Energy:-812.710576 Hartree, Solvent: none, Boltzmann %: 17.484

Zero-point correction= 0.389894 (Hartree/Particle)
Thermal correction to Energy= 0.408701
Thermal correction to Enthalpy= 0.409645
Thermal correction to Gibbs Free Energy= 0.345772
Sum of electronic and zero-point Energies= -812.666454
Sum of electronic and thermal Energies= -812.647647
Sum of electronic and thermal Enthalpies= -812.646703
Sum of electronic and thermal Free Energies= -812.710576

C	-0.237718	0.718295	1.273207
C	0.729487	0.287697	0.149553
C	1.071556	-1.229430	0.163054
O	-0.181170	-1.997625	0.002563
C	-1.022820	-1.710118	-1.036942
C	-2.069971	-0.893654	-0.956996
C	-2.542371	-0.074687	0.220547
C	-1.588288	-0.010423	1.428785
H	-0.826335	-2.257969	-1.957706
H	-2.704331	-0.837120	-1.835822
H	-2.134282	0.507421	2.223450
H	-1.439815	-1.034713	1.766588
H	0.264619	0.642039	2.241443
H	-0.453981	1.777758	1.137100
H	0.198175	0.434572	-0.795602
C	2.005535	-1.595180	-0.998724
H	1.460692	-1.458866	-1.938818
H	2.258176	-2.656961	-0.928114
C	1.974066	1.248400	0.020416
C	3.262249	-0.725992	-1.041143
H	3.870706	-1.004365	-1.906570
H	3.886808	-0.910956	-0.161969
C	2.881815	0.750502	-1.130067
H	2.357626	0.914768	-2.079565
H	3.780981	1.374200	-1.163556
C	-3.914207	-0.585666	0.678387
H	-4.617627	-0.611495	-0.153400
H	-3.817645	-1.596424	1.079419
H	-4.317309	0.065460	1.456852
C	1.487861	2.659140	-0.375884

H	0.960490	3.162973	0.435516
H	2.344151	3.284666	-0.642664
H	0.820606	2.621146	-1.241125
C	2.802581	1.397083	1.312164
H	2.189552	1.733413	2.150175
H	3.299967	0.476332	1.613797
H	3.581530	2.149143	1.158806
O	-2.652310	1.330954	-0.165399
C	1.603802	-1.778987	1.485593
H	1.615645	-2.869123	1.431352
H	2.617834	-1.440775	1.687650
H	0.973600	-1.490667	2.326536
O	-3.637316	1.488517	-1.221872
H	-3.064930	1.708895	-1.977816

Compound: Arenaran D, Conformer: 03, Energy:-812.711057 Hartree, Solvent: none, Boltzmann %: 29.099

Zero-point correction= 0.389940 (Hartree/Particle)
Thermal correction to Energy= 0.408718
Thermal correction to Enthalpy= 0.409662
Thermal correction to Gibbs Free Energy= 0.345817
Sum of electronic and zero-point Energies= -812.666934
Sum of electronic and thermal Energies= -812.648156
Sum of electronic and thermal Enthalpies= -812.647212
Sum of electronic and thermal Free Energies= -812.711057

C	-0.392589	0.791522	1.067993
C	0.676788	0.277715	0.080359
C	1.096241	-1.199250	0.322470
O	-0.098229	-2.063288	0.183875
C	-0.875368	-1.977139	-0.935181
C	-1.949501	-1.201322	-1.062093
C	-2.536457	-0.228657	-0.067150
C	-1.715681	0.016115	1.208682
H	-0.607263	-2.662326	-1.738572
H	-2.513413	-1.302028	-1.984807
H	-2.349206	0.597724	1.883852
H	-1.557464	-0.949990	1.686420
H	0.035159	0.867451	2.071474
H	-0.649837	1.809883	0.777516
H	0.210215	0.267564	-0.908863
C	2.130353	-1.657597	-0.714827
H	1.648872	-1.679424	-1.698212
H	2.431996	-2.683341	-0.484399
C	1.875967	1.287354	-0.095840
C	3.339870	-0.726085	-0.792154
H	4.023991	-1.078711	-1.569551
H	3.906447	-0.754827	0.143483
C	2.890363	0.699364	-1.105974

H	2.429127	0.704238	-2.101107
H	3.755830	1.367358	-1.164835
C	-3.954291	-0.692154	0.293511
H	-4.545171	-0.866510	-0.608133
H	-3.906496	-1.625211	0.857737
H	-4.458066	0.054222	0.909120
C	1.345912	2.600479	-0.710783
H	0.737368	3.173855	-0.009982
H	2.185531	3.235973	-1.005903
H	0.742884	2.407295	-1.601685
C	2.599006	1.656654	1.215040
H	1.907973	2.055387	1.959788
H	3.127485	0.818770	1.667919
H	3.341051	2.434135	1.012915
O	-2.602711	0.989114	-0.880164
C	1.555592	-1.536388	1.739768
H	1.636130	-2.620927	1.833536
H	2.529121	-1.105677	1.963784
H	0.845951	-1.184958	2.488230
O	-3.218453	2.061709	-0.112382
H	-4.070304	2.156135	-0.573294

Compound: Arenaran D, Conformer: 04, Energy:-812.710403 Hartree, Solvent: none, Boltzmann %: 14.557

Zero-point correction= 0.389933 (Hartree/Particle)
Thermal correction to Energy= 0.408692
Thermal correction to Enthalpy= 0.409636
Thermal correction to Gibbs Free Energy= 0.346023
Sum of electronic and zero-point Energies= -812.666493
Sum of electronic and thermal Energies= -812.647734
Sum of electronic and thermal Enthalpies= -812.646790
Sum of electronic and thermal Free Energies= -812.710403

C	-0.386924	0.828399	1.018615
C	0.695245	0.286570	0.058844
C	1.088592	-1.193279	0.328867
O	-0.115108	-2.039472	0.177339
C	-0.872863	-1.942419	-0.955530
C	-1.947567	-1.168692	-1.083358
C	-2.551071	-0.222331	-0.073407
C	-1.712060	0.058626	1.182725
H	-0.586684	-2.611783	-1.765709
H	-2.503492	-1.253560	-2.012250
H	-2.340878	0.652418	1.852690
H	-1.546830	-0.894108	1.683696
H	0.032562	0.940780	2.022035
H	-0.632309	1.841103	0.693408
H	0.249102	0.268910	-0.939714
C	2.136862	-1.679201	-0.681590

H	1.674671	-1.709272	-1.673868
H	2.419882	-2.705341	-0.430512
C	1.912660	1.277060	-0.104791
C	3.360157	-0.765300	-0.748323
H	4.053460	-1.137170	-1.508314
H	3.909249	-0.789210	0.197790
C	2.936404	0.661797	-1.089047
H	2.493368	0.660053	-2.092394
H	3.812003	1.316970	-1.140472
C	-3.938565	-0.747295	0.322161
H	-4.540656	-0.944483	-0.566524
H	-3.834894	-1.677416	0.883718
H	-4.460297	-0.019466	0.943538
C	1.416554	2.591827	-0.744659
H	0.811055	3.186996	-0.058916
H	2.271833	3.207766	-1.035584
H	0.823588	2.398831	-1.642571
C	2.617622	1.649659	1.214995
H	1.921542	2.071838	1.942003
H	3.120675	0.807680	1.688381
H	3.378471	2.409738	1.017004
O	-2.702718	0.987232	-0.886884
C	1.516180	-1.517223	1.759337
H	1.567977	-2.601728	1.871426
H	2.496658	-1.107574	1.992421
H	0.804054	-1.136664	2.491109
O	-3.462540	1.984585	-0.147805
H	-2.778535	2.656737	0.017375

Compound: Arenaran D, Conformer: 06, Energy:-812.707851 Hartree, Solvent: none, Boltzmann %: 0.976

Zero-point correction= 0.389946 (Hartree/Particle)
Thermal correction to Energy= 0.408725
Thermal correction to Enthalpy= 0.409669
Thermal correction to Gibbs Free Energy= 0.346175
Sum of electronic and zero-point Energies= -812.664079
Sum of electronic and thermal Energies= -812.645301
Sum of electronic and thermal Enthalpies= -812.644357
Sum of electronic and thermal Free Energies= -812.707851

C	-0.334402	0.767986	1.193964
C	0.669674	0.263174	0.134481
C	0.924184	-1.270900	0.190654
O	-0.359221	-1.968713	-0.028274
C	-1.120106	-1.646391	-1.120551
C	-2.146766	-0.803515	-1.085414
C	-2.660400	-0.015460	0.092698
C	-1.723954	0.105150	1.310745
H	-0.875112	-2.178619	-2.038268

H	-2.727451	-0.689351	-1.995742
H	-2.282181	0.678027	2.059300
H	-1.612279	-0.900770	1.714781
H	0.114511	0.692884	2.188732
H	-0.482154	1.834962	1.027894
H	0.199636	0.424941	-0.839130
C	1.899700	-1.708709	-0.910864
H	1.417815	-1.558377	-1.882412
H	2.086956	-2.781610	-0.810375
C	1.974302	1.148019	0.066351
C	3.204396	-0.912625	-0.894291
H	3.842835	-1.239064	-1.720438
H	3.767978	-1.117567	0.020927
C	2.914086	0.580901	-1.024798
H	2.452881	0.758325	-2.003944
H	3.847891	1.152467	-1.016233
C	-3.994870	-0.629999	0.557724
H	-4.686176	-0.725938	-0.280138
H	-3.812505	-1.619988	0.976086
H	-4.456997	-0.003925	1.323997
C	1.598564	2.579241	-0.374658
H	1.061975	3.127377	0.401943
H	2.505303	3.147284	-0.600063
H	0.979119	2.567393	-1.275064
C	2.737965	1.268795	1.400664
H	2.100505	1.651831	2.199625
H	3.164693	0.326303	1.740798
H	3.565954	1.973288	1.281991
O	-3.123144	1.284854	-0.376361
C	1.352175	-1.825801	1.548633
H	1.297641	-2.915457	1.513431
H	2.374119	-1.548104	1.797439
H	0.700063	-1.482153	2.351280
O	-2.064489	1.968078	-1.107977
H	-1.937475	2.752894	-0.547546

Compound: Arenaran D, Conformer: 09, Energy:-812.708797 Hartree, Solvent: none, Boltzmann %: 2.657

Zero-point correction= 0.389983 (Hartree/Particle)
Thermal correction to Energy= 0.408732
Thermal correction to Enthalpy= 0.409676
Thermal correction to Gibbs Free Energy= 0.346295
Sum of electronic and zero-point Energies= -812.665109
Sum of electronic and thermal Energies= -812.646361
Sum of electronic and thermal Enthalpies= -812.645417
Sum of electronic and thermal Free Energies= -812.708797

C	-0.338891	0.769611	1.193591
C	0.667201	0.263042	0.136775

C	0.920881	-1.270545	0.185595
O	-0.363025	-1.969374	-0.037707
C	-1.133377	-1.644426	-1.119850
C	-2.161472	-0.802253	-1.074012
C	-2.660708	-0.007185	0.104905
C	-1.720607	0.094268	1.320136
H	-0.902378	-2.180802	-2.039256
H	-2.757630	-0.704824	-1.977547
H	-2.274921	0.660078	2.076442
H	-1.605392	-0.916000	1.712481
H	0.113831	0.709164	2.187671
H	-0.505863	1.829290	1.007602
H	0.200852	0.430074	-0.837688
C	1.895007	-1.705407	-0.918196
H	1.411795	-1.551223	-1.888712
H	2.081565	-2.778885	-0.822208
C	1.973632	1.145810	0.074236
C	3.200458	-0.910470	-0.900119
H	3.837160	-1.233500	-1.729030
H	3.765251	-1.121216	0.013011
C	2.911762	0.584286	-1.021118
H	2.450053	0.768598	-1.998931
H	3.846456	1.154391	-1.010233
C	-4.009360	-0.589818	0.566308
H	-4.699690	-0.679524	-0.273416
H	-3.850387	-1.579705	0.994731
H	-4.461322	0.052947	1.324528
C	1.599370	2.580999	-0.354023
H	1.060791	3.121558	0.425566
H	2.507528	3.148883	-0.575014
H	0.976660	2.578630	-1.251705
C	2.739132	1.255078	1.408636
H	2.102554	1.632107	2.210943
H	3.166428	0.310001	1.740962
H	3.566956	1.960536	1.294296
O	-3.086032	1.313267	-0.352035
C	1.346961	-1.832003	1.541306
H	1.286014	-2.921280	1.503847
H	2.370955	-1.560834	1.788805
H	0.698400	-1.485178	2.345360
O	-1.990988	2.011523	-1.003733
H	-2.245242	1.927450	-1.939709

Compound: Arenaran D, Conformer: 11, Energy:-812.707459 Hartree, Solvent: none, Boltzmann %: 0.644

Zero-point correction= 0.390047 (Hartree/Particle)
Thermal correction to Energy= 0.408627
Thermal correction to Enthalpy= 0.409571
Thermal correction to Gibbs Free Energy= 0.346281

Sum of electronic and zero-point Energies= -812.663694
Sum of electronic and thermal Energies= -812.645114
Sum of electronic and thermal Enthalpies= -812.644169
Sum of electronic and thermal Free Energies= -812.707459

C	-0.162097	1.150670	1.083258
C	0.739181	0.390502	0.069288
C	0.771267	-1.158996	0.286088
O	-0.578372	-1.690410	-0.001030
C	-1.570793	-1.613534	0.945680
C	-2.503751	-0.668481	0.951539
C	-2.543805	0.566773	0.083017
C	-1.534728	1.631805	0.582338
H	-1.608470	-2.443708	1.648364
H	-3.292886	-0.764184	1.690075
H	-1.409837	2.355035	-0.230574
H	-2.019901	2.172765	1.400523
H	-0.312664	0.554916	1.983389
H	0.356694	2.046576	1.427586
H	0.267612	0.487620	-0.911027
C	1.620163	-1.823752	-0.804714
H	1.098236	-1.686216	-1.757066
H	1.657105	-2.900084	-0.615766
C	2.152303	1.060368	-0.116829
C	3.024902	-1.233851	-0.914105
H	3.561359	-1.726534	-1.730070
H	3.601294	-1.443150	-0.007668
C	2.956693	0.269409	-1.174877
H	2.489459	0.428612	-2.153948
H	3.965078	0.690786	-1.242296
C	-3.960575	1.141136	0.024683
H	-4.632617	0.432923	-0.462159
H	-4.340054	1.343239	1.028915
H	-3.964443	2.072905	-0.543673
C	1.948455	2.483134	-0.678721
H	1.468379	3.152163	0.038224
H	2.915272	2.924861	-0.935069
H	1.337989	2.465687	-1.585285
C	2.975479	1.184078	1.181328
H	2.405256	1.655826	1.984331
H	3.335209	0.225237	1.552410
H	3.854972	1.807598	0.998710
O	-2.084975	0.335509	-1.278078
C	1.197486	-1.651126	1.670521
H	1.026819	-2.727924	1.735511
H	2.257070	-1.474360	1.841835
H	0.647618	-1.171602	2.480105
O	-2.740993	-0.812508	-1.860482
H	-2.090913	-1.508521	-1.649615

Compound: Arenaran D, Conformer: 12, Energy:-812.709615 Hartree, Solvent: none, Boltzmann %: 6.318

Zero-point correction= 0.389887 (Hartree/Particle)
Thermal correction to Energy= 0.408611
Thermal correction to Enthalpy= 0.409555
Thermal correction to Gibbs Free Energy= 0.346350
Sum of electronic and zero-point Energies= -812.666078
Sum of electronic and thermal Energies= -812.647354
Sum of electronic and thermal Enthalpies= -812.646410
Sum of electronic and thermal Free Energies= -812.709615

C	-0.143730	1.054914	0.946922
C	0.887735	0.359375	0.020498
C	1.032391	-1.159505	0.321472
O	-0.317902	-1.744250	0.276691
C	-1.067606	-1.599237	-0.862944
C	-2.082366	-0.747550	-0.958051
C	-2.519860	0.258698	0.085730
C	-1.500126	1.403192	0.304602
H	-0.820640	-2.268829	-1.684167
H	-2.659914	-0.759226	-1.874725
H	-1.332952	1.890660	-0.659810
H	-2.001532	2.137518	0.942568
H	0.268910	1.999952	1.303127
H	-0.313781	0.463166	1.846484
H	0.462777	0.381381	-0.988570
C	1.931606	-1.823479	-0.730322
H	1.438192	-1.768449	-1.705679
H	2.046938	-2.884095	-0.489133
C	2.243139	1.132757	-0.147189
C	3.294505	-1.132139	-0.838222
H	3.882027	-1.609121	-1.628010
H	3.865825	-1.270482	0.084334
C	3.132017	0.356604	-1.150031
H	2.686922	0.452839	-2.147641
H	4.112906	0.840114	-1.203871
C	-2.946427	-0.394466	1.400689
H	-3.765639	-1.092505	1.226984
H	-2.118917	-0.955691	1.830348
H	-3.272425	0.368615	2.112207
C	1.951671	2.513089	-0.771361
H	1.394514	3.165540	-0.095842
H	2.889597	3.020877	-1.012151
H	1.377733	2.416501	-1.696821
C	3.007000	1.369680	1.170449
H	2.370385	1.825634	1.932008
H	3.424481	0.457284	1.593082
H	3.840902	2.054082	0.992392
O	-3.632403	1.028325	-0.464156

C	1.489500	-1.538330	1.730799
H	1.296584	-2.602288	1.879461
H	2.553552	-1.367172	1.874520
H	0.949084	-0.989554	2.501636
O	-4.732010	0.142871	-0.807931
H	-5.373708	0.356051	-0.107813

Compound: Arenaran D, Conformer: 15, Energy:-812.709658 Hartree, Solvent: none, Boltzmann %: 6.613

Zero-point correction= 0.389916 (Hartree/Particle)
Thermal correction to Energy= 0.408642
Thermal correction to Enthalpy= 0.409586
Thermal correction to Gibbs Free Energy= 0.346309
Sum of electronic and zero-point Energies= -812.666051
Sum of electronic and thermal Energies= -812.647325
Sum of electronic and thermal Enthalpies= -812.646381
Sum of electronic and thermal Free Energies= -812.709658

C	-0.252180	0.777180	1.158996
C	0.795443	0.327720	0.107066
C	1.074682	-1.200746	0.160953
O	-0.226177	-1.883381	0.065605
C	-1.027289	-1.646640	-1.022821
C	-2.102299	-0.867622	-0.976938
C	-2.583604	-0.055910	0.207653
C	-1.652430	1.109168	0.608729
H	-0.768881	-2.189255	-1.929784
H	-2.709949	-0.803540	-1.871655
H	-1.545347	1.768904	-0.255433
H	-2.196029	1.673935	1.373925
H	-0.343547	0.033728	1.951216
H	0.099262	1.681763	1.658020
H	0.329347	0.467675	-0.874136
C	1.978384	-1.614217	-1.008613
H	1.440232	-1.452062	-1.947767
H	2.189948	-2.685277	-0.941380
C	2.074808	1.232085	0.024788
C	3.275029	-0.798706	-1.046809
H	3.864161	-1.094656	-1.919642
H	3.895356	-1.028936	-0.175652
C	2.980078	0.700906	-1.113908
H	2.486559	0.912091	-2.070181
H	3.915770	1.269530	-1.119335
C	-2.943256	-0.945156	1.403138
H	-3.715335	-1.660591	1.117071
H	-2.064961	-1.500185	1.725470
H	-3.313715	-0.338360	2.232119
C	1.645625	2.662012	-0.363790
H	1.065641	3.149248	0.422905

H	2.527831	3.281411	-0.547252
H	1.043368	2.660891	-1.276256
C	2.872224	1.327721	1.340392
H	2.232953	1.600834	2.182950
H	3.381971	0.401470	1.600320
H	3.637964	2.102879	1.249140
O	-3.892999	0.498600	-0.122976
C	1.620378	-1.751623	1.479072
H	1.520186	-2.838406	1.464550
H	2.672422	-1.513641	1.616121
H	1.071070	-1.376372	2.342119
O	-3.800123	1.348213	-1.299075
H	-3.895443	2.232425	-0.903355

Compound: Arenaran D, Conformer: 16, Energy:-812.709528 Hartree, Solvent: none, Boltzmann %: 5.762

Zero-point correction= 0.389760 (Hartree/Particle)
Thermal correction to Energy= 0.408568
Thermal correction to Enthalpy= 0.409513
Thermal correction to Gibbs Free Energy= 0.346055
Sum of electronic and zero-point Energies= -812.665823
Sum of electronic and thermal Energies= -812.647014
Sum of electronic and thermal Enthalpies= -812.646070
Sum of electronic and thermal Free Energies= -812.709528

C	-0.142479	1.055435	0.947236
C	0.887129	0.358962	0.019262
C	1.032244	-1.159982	0.319953
O	-0.318353	-1.745533	0.276531
C	-1.071107	-1.596304	-0.859061
C	-2.086995	-0.744646	-0.946995
C	-2.522272	0.261230	0.097779
C	-1.499824	1.405338	0.307573
H	-0.825667	-2.260965	-1.684952
H	-2.657443	-0.756460	-1.868879
H	-1.333444	1.890127	-0.658637
H	-1.998795	2.141602	0.944700
H	-0.312466	0.463559	1.846644
H	0.271993	1.999686	1.303305
H	0.460880	0.381195	-0.989322
C	1.929805	-1.824399	-0.732957
H	1.435152	-1.769476	-1.707767
H	2.045108	-2.884987	-0.491700
C	2.242748	1.131702	-0.150655
C	3.292722	-1.133445	-0.842880
H	3.879111	-1.610776	-1.633309
H	3.865154	-1.271742	0.078966
C	3.130045	0.355257	-1.154672
H	2.683603	0.451436	-2.151747

H	4.110936	0.838577	-1.210019
C	-2.941459	-0.389054	1.416877
H	-3.778352	-1.065902	1.249472
H	-2.117322	-0.964011	1.834798
H	-3.247923	0.378937	2.130935
C	1.950805	2.512062	-0.774578
H	1.394384	3.164621	-0.098600
H	2.888532	3.019700	-1.016446
H	1.375937	2.415459	-1.699525
C	3.008555	1.368548	1.165847
H	2.373180	1.824746	1.928254
H	3.426333	0.456045	1.587955
H	3.842446	2.052627	0.986496
O	-3.642343	1.029901	-0.435326
C	1.490494	-1.538927	1.728769
H	1.297742	-2.602883	1.877616
H	2.554699	-1.367746	1.871378
H	0.950712	-0.990127	2.499975
O	-4.782364	0.155771	-0.659660
H	-4.842469	0.174972	-1.630941

Compound: Arenaran D, Conformer: 17, Energy:-812.709576 Hartree, Solvent: none, Boltzmann %: 6.063

Zero-point correction= 0.389792 (Hartree/Particle)
Thermal correction to Energy= 0.408588
Thermal correction to Enthalpy= 0.409532
Thermal correction to Gibbs Free Energy= 0.346081
Sum of electronic and zero-point Energies= -812.665865
Sum of electronic and thermal Energies= -812.647069
Sum of electronic and thermal Enthalpies= -812.646125
Sum of electronic and thermal Free Energies= -812.709576

C	-0.245331	0.776616	1.166802
C	0.796845	0.327068	0.109522
C	1.074439	-1.201534	0.160526
O	-0.228907	-1.882419	0.071131
C	-1.034023	-1.644393	-1.012613
C	-2.104805	-0.859266	-0.963713
C	-2.582602	-0.042763	0.218616
C	-1.645683	1.117341	0.623704
H	-0.783362	-2.190506	-1.919834
H	-2.710614	-0.802243	-1.860718
H	-2.187336	1.677820	1.392259
H	-1.546674	1.783909	-0.235093
H	-0.335658	0.030364	1.956681
H	0.111720	1.677752	1.668126
H	0.326386	0.469138	-0.869309
C	1.970926	-1.615897	-1.014218
H	1.428022	-1.452021	-1.950396

H	2.181295	-2.687355	-0.949048
C	2.077494	1.229186	0.021630
C	3.268590	-0.802228	-1.058879
H	3.852426	-1.098350	-1.935236
H	3.893288	-1.034394	-0.191385
C	2.975624	0.697940	-1.122637
H	2.477189	0.911122	-2.075944
H	3.912249	1.264974	-1.132663
C	-2.948523	-0.931551	1.413098
H	-3.718719	-1.648879	1.125999
H	-2.071128	-1.485353	1.740224
H	-3.322691	-0.322720	2.238596
C	1.648545	2.660367	-0.362341
H	1.073505	3.147182	0.428082
H	2.530836	3.278500	-0.549811
H	1.040763	2.661890	-1.271073
C	2.882309	1.321398	1.332975
H	2.247898	1.593659	2.179418
H	3.392649	0.394171	1.588431
H	3.648309	2.095973	1.238901
O	-3.884393	0.529107	-0.105626
C	1.625403	-1.754905	1.475266
H	1.523525	-2.841550	1.460244
H	2.678466	-1.518624	1.607231
H	1.080951	-1.379293	2.341180
O	-3.759267	1.454505	-1.222604
H	-4.298013	1.001014	-1.894499
