BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Nomimicins B–D, new tetronate-class polyketides from a marine-derived actinomycete of the genus *Actinomadura*

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Copies of UV, IR, and NMR spectra for 1–4 as well as Cartesian coordinates and energies of the most stable conformers of 4a–d

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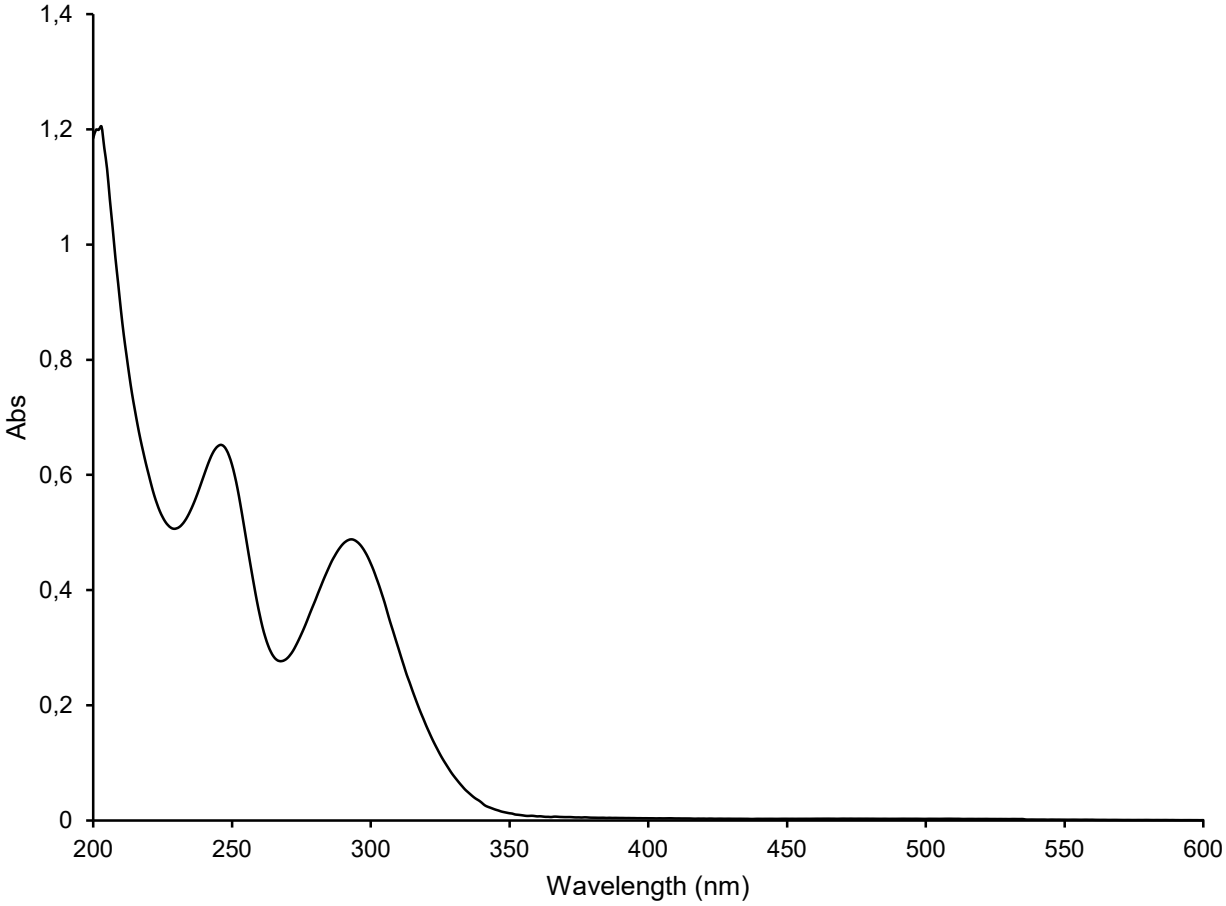


Figure S2. IR spectrum of **1.**

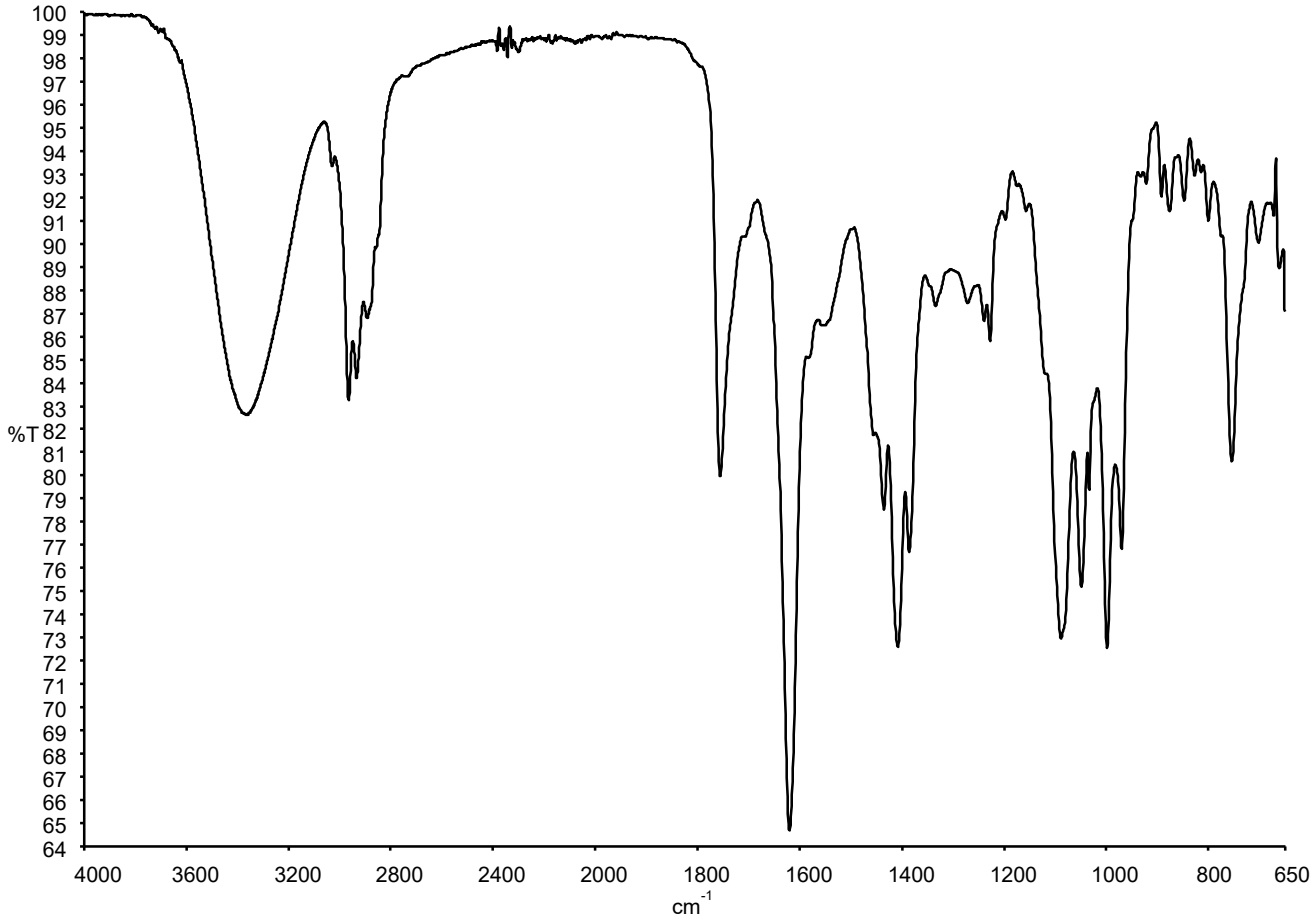


Figure S3. ^{1}H NMR spectrum of **1** (500 MHz, CD_3OD).

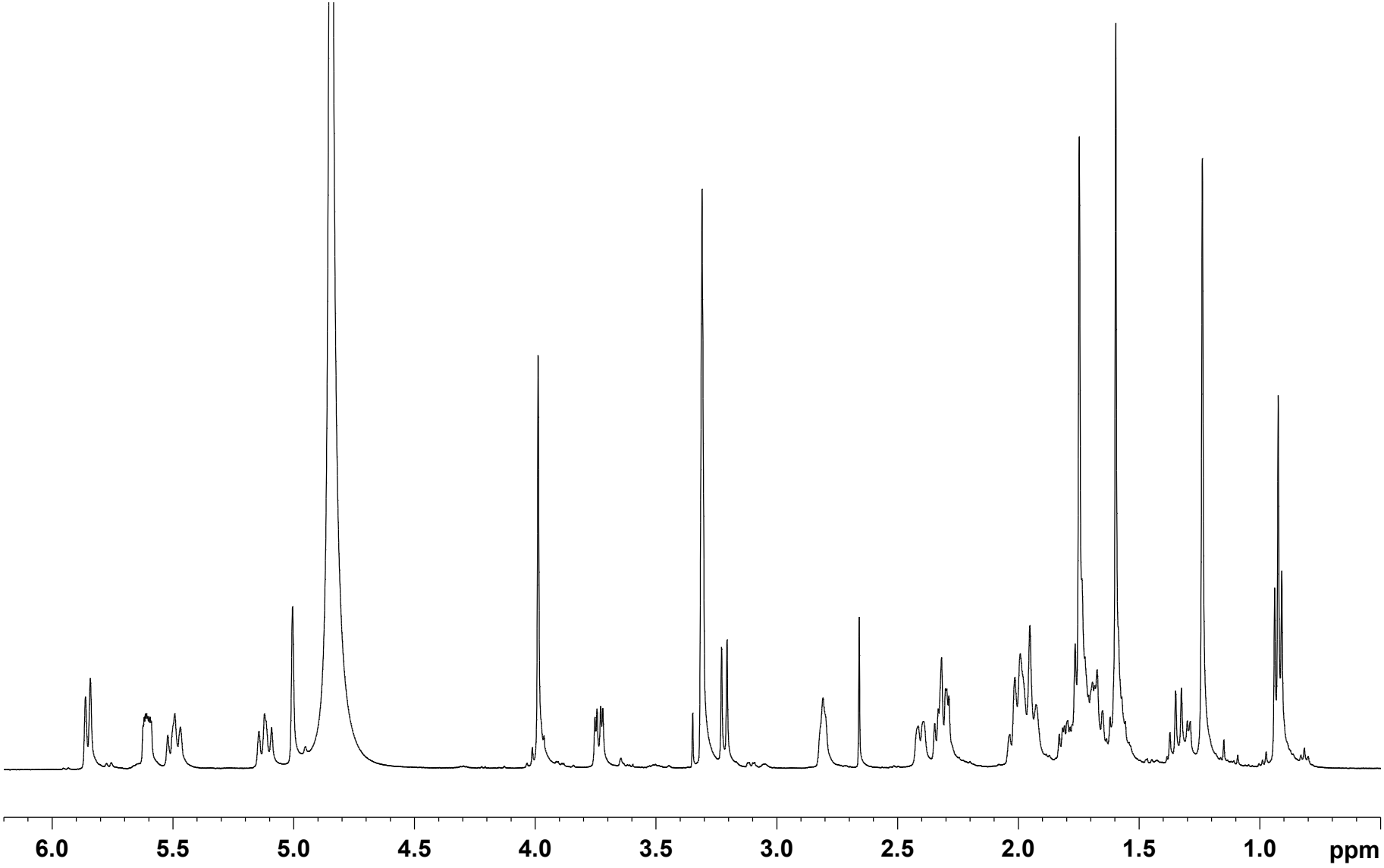


Figure S4. ^{13}C NMR spectrum of **1** (125 MHz, CD_3OD).

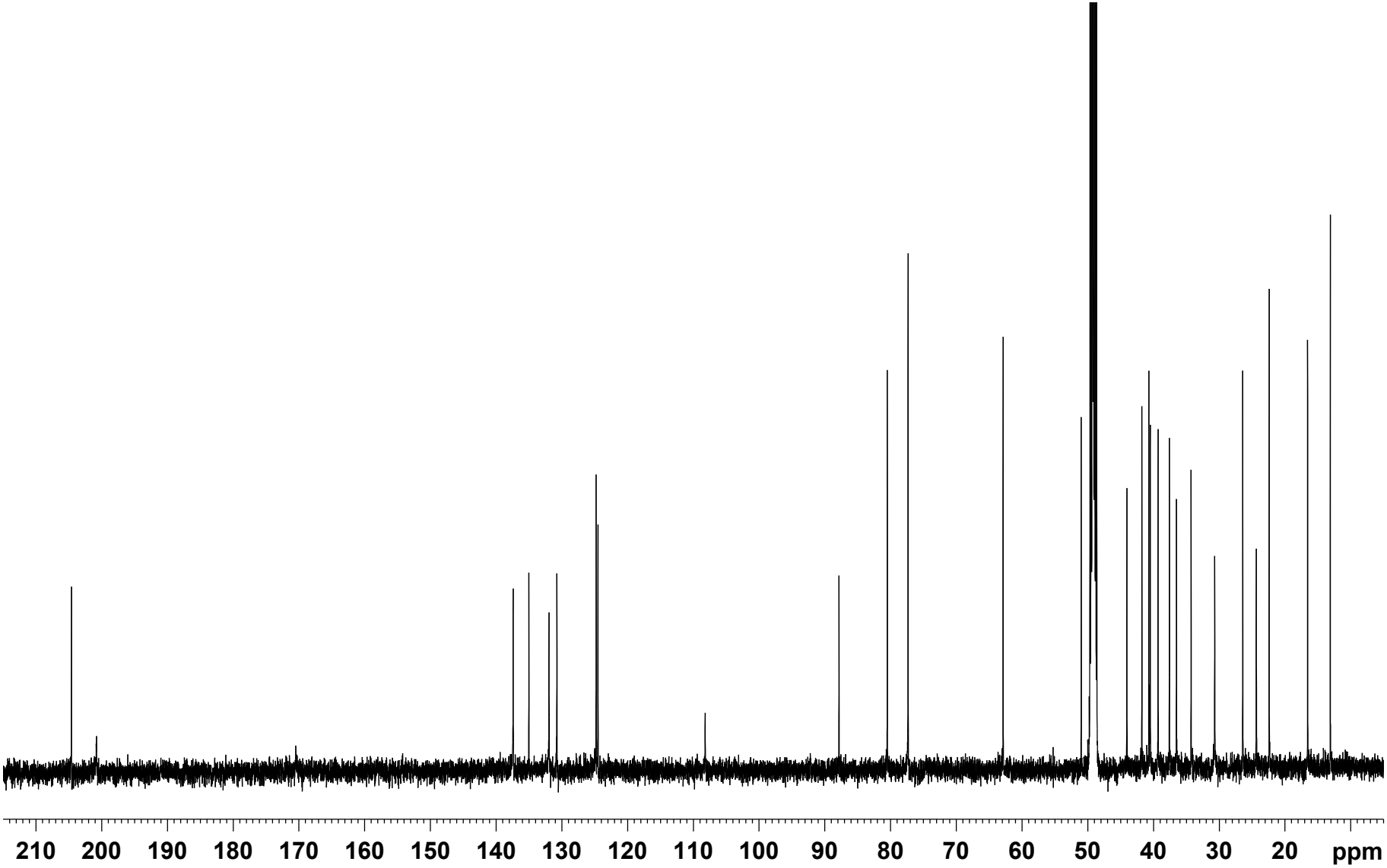


Figure S5. COSY spectrum of **1** (500 MHz, CD_3OD).

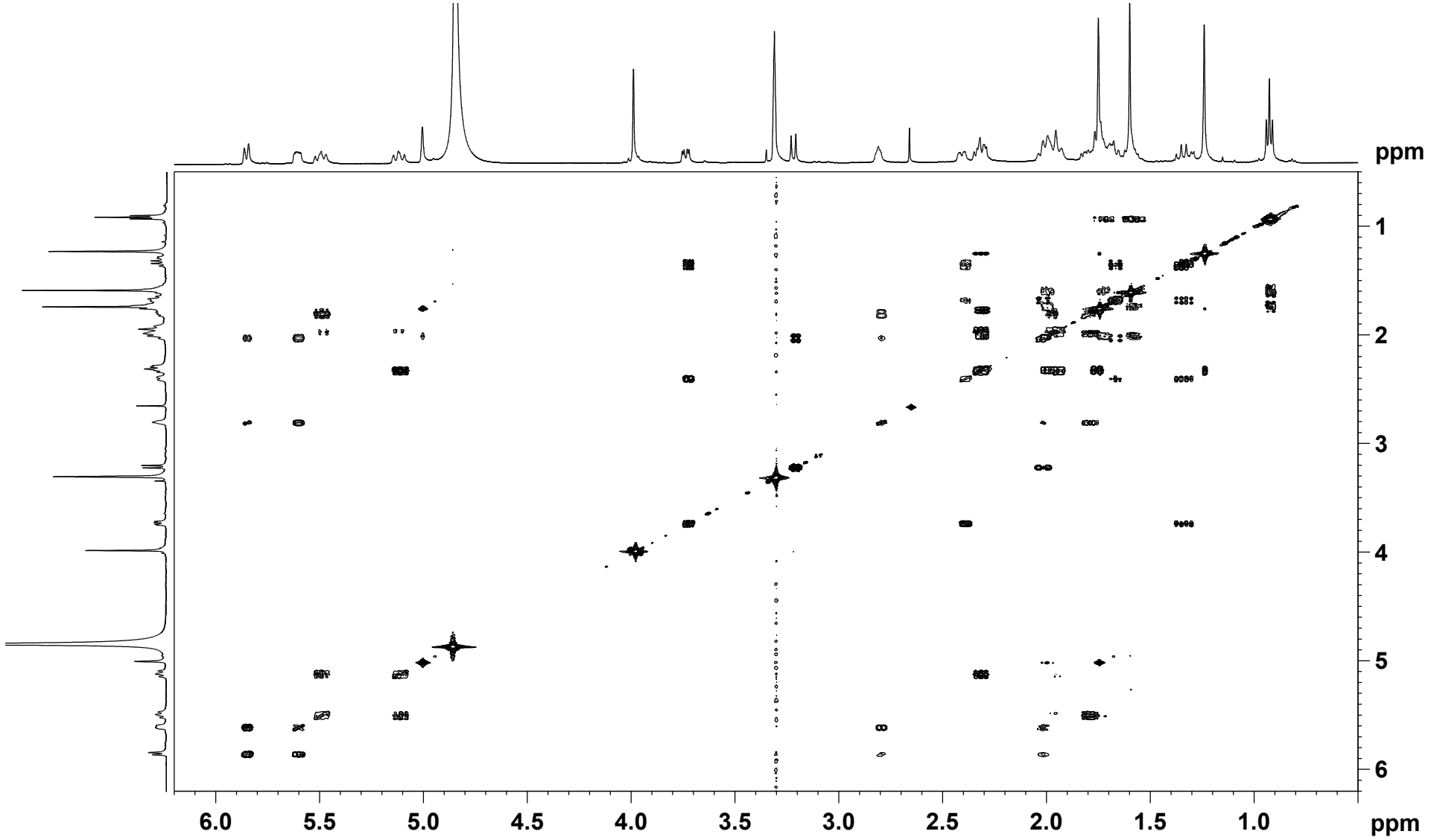


Figure S6. HSQC spectrum of **1** (500 MHz, CD_3OD).

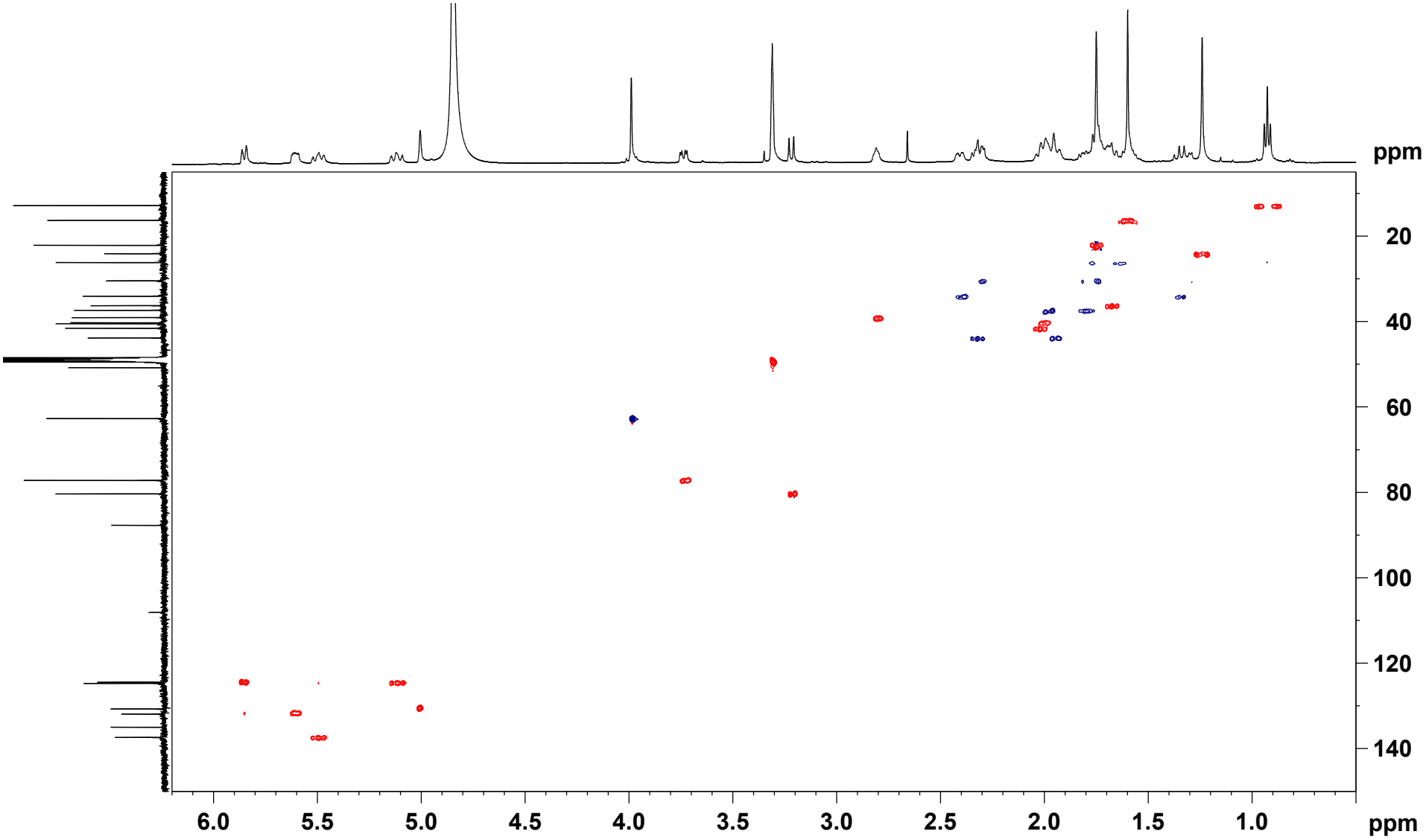


Figure S7. HMBC spectrum of **1** (500 MHz, CD_3OD).

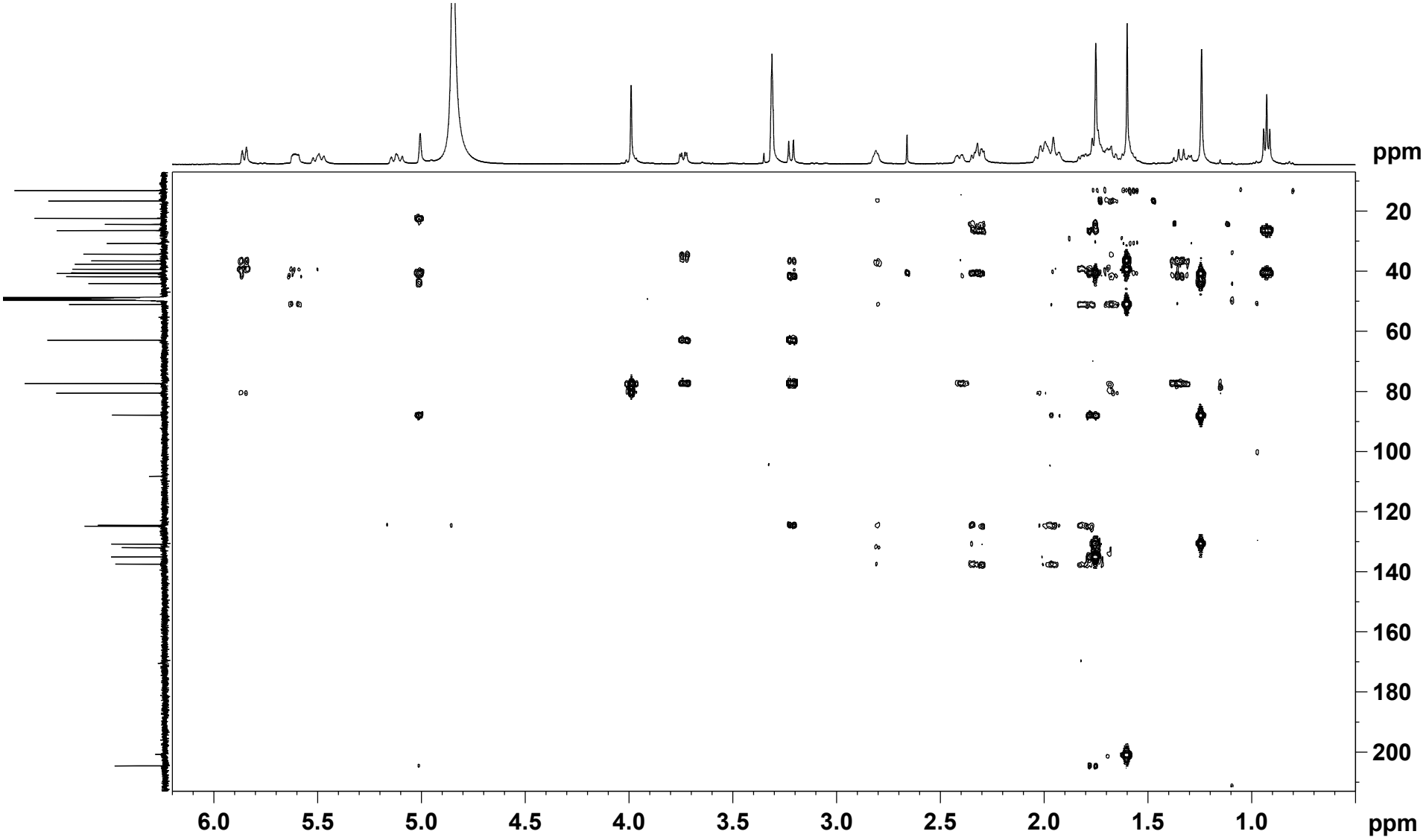


Figure S8. NOESY spectrum of **1** (500 MHz, CD_3OD).

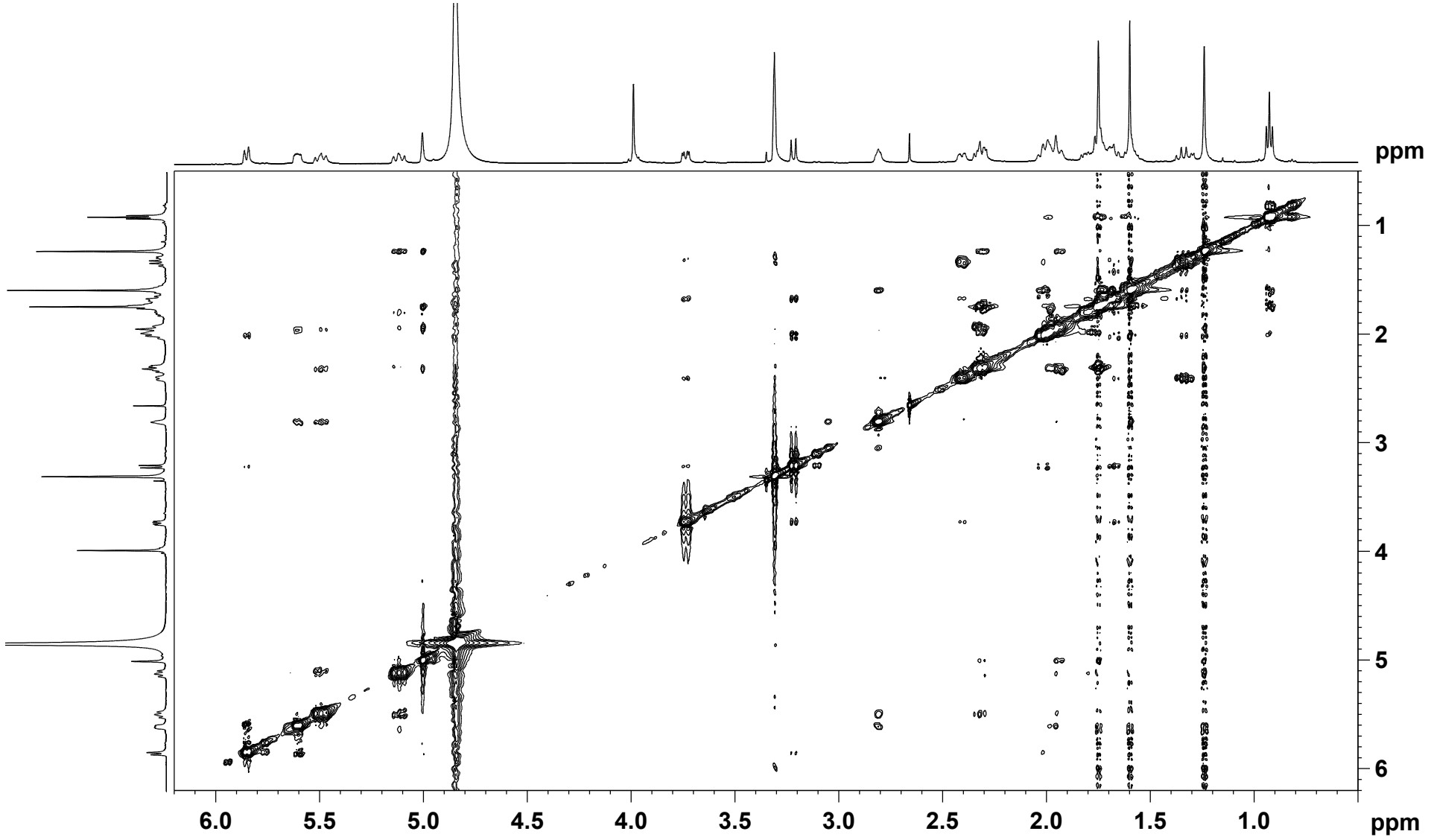


Figure S9. ROESY spectrum of **1** (500 MHz, CD_3OD).

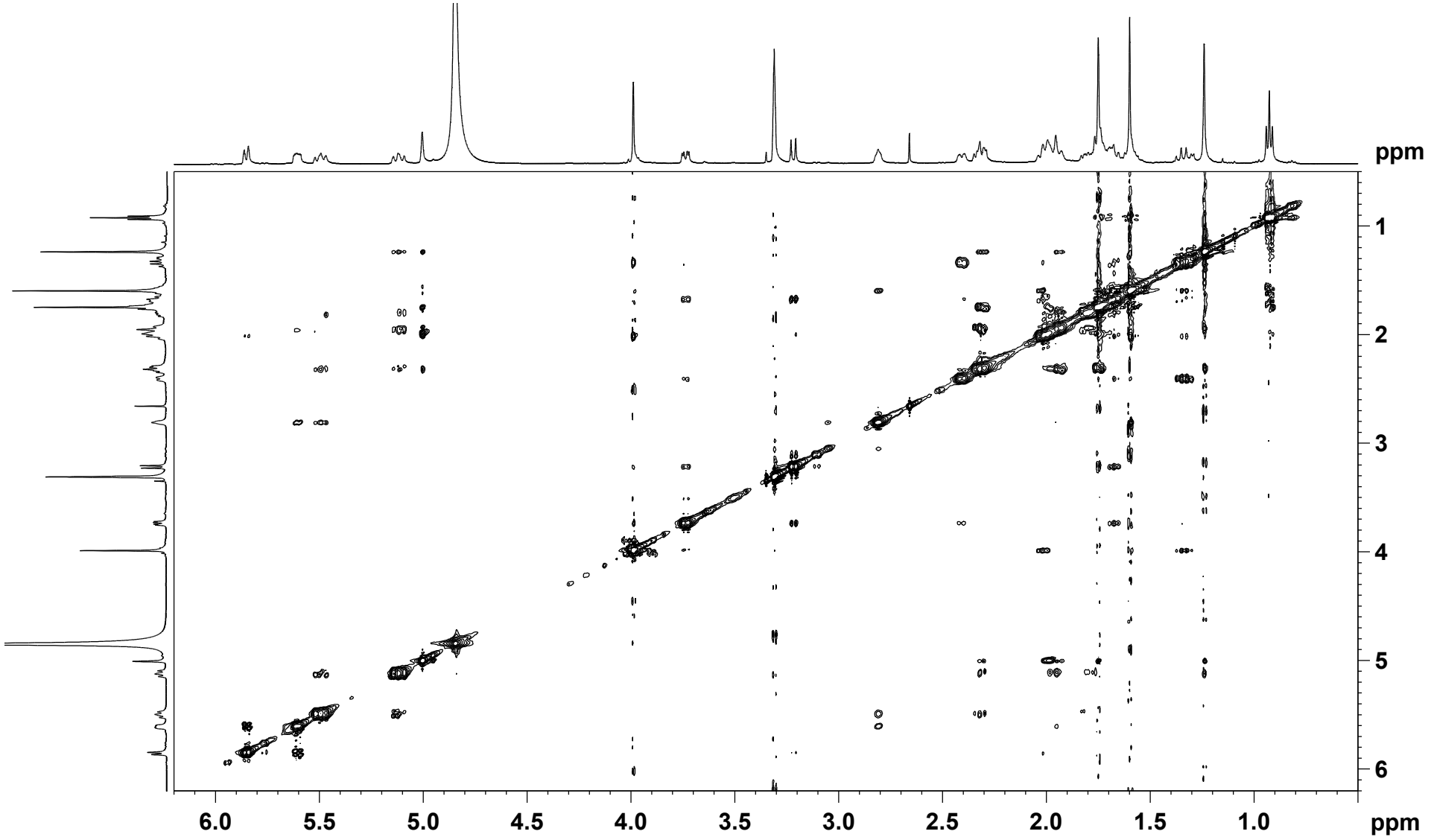


Figure S10. UV spectrum of nomimicin C (**2**).

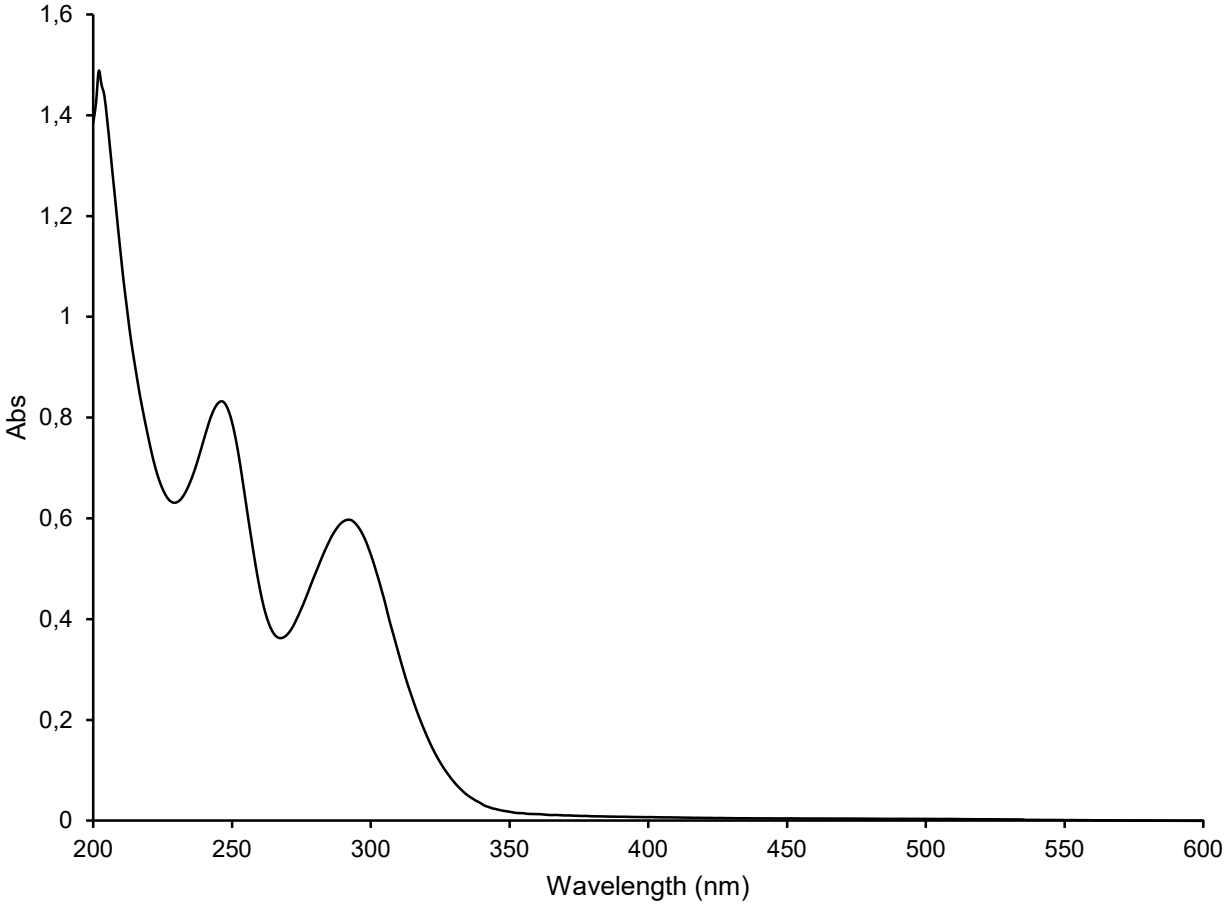


Figure S11. IR spectrum of **2.**

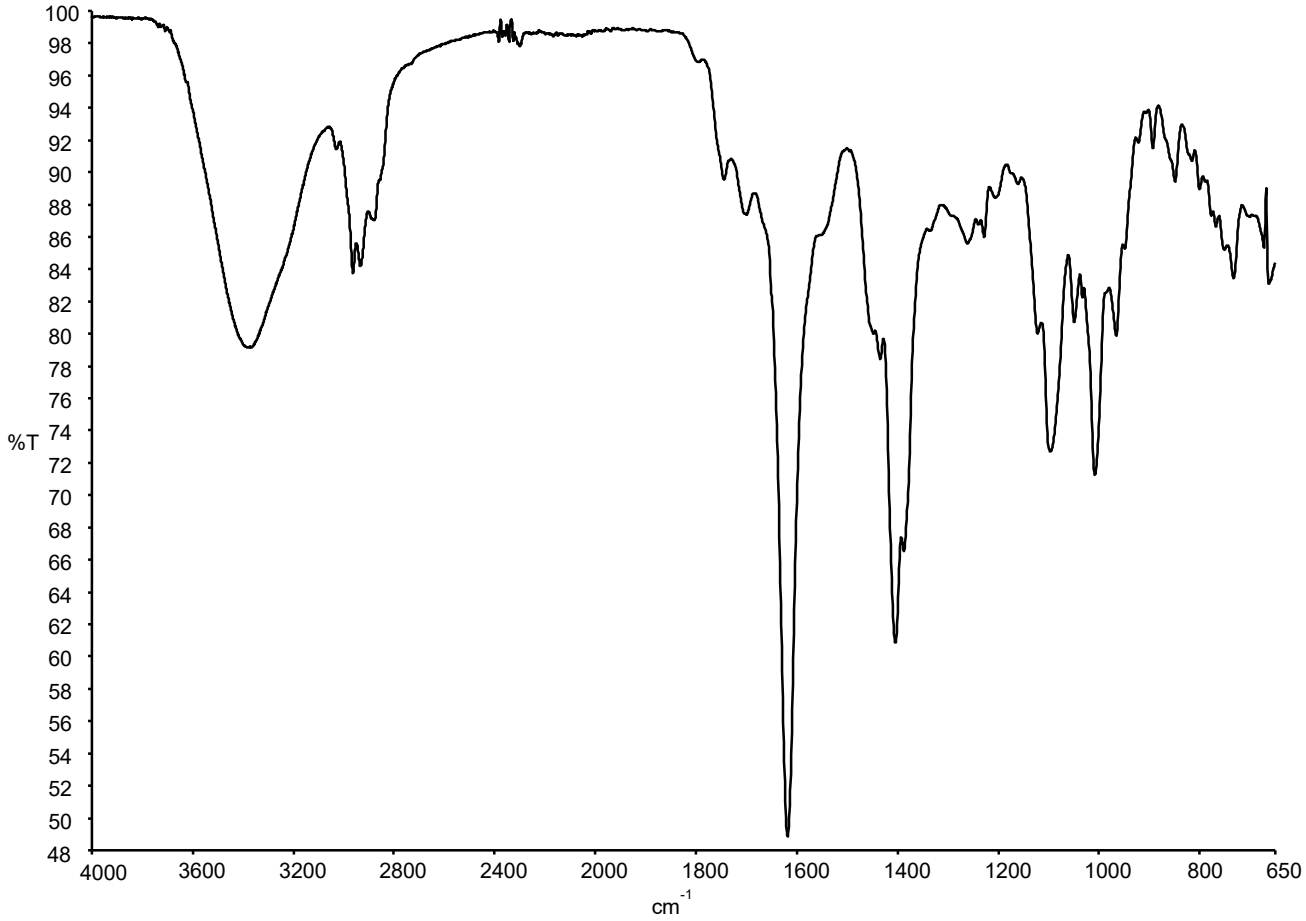


Figure S12. ^{1}H NMR spectrum of **2** (500 MHz, CD_3OD).

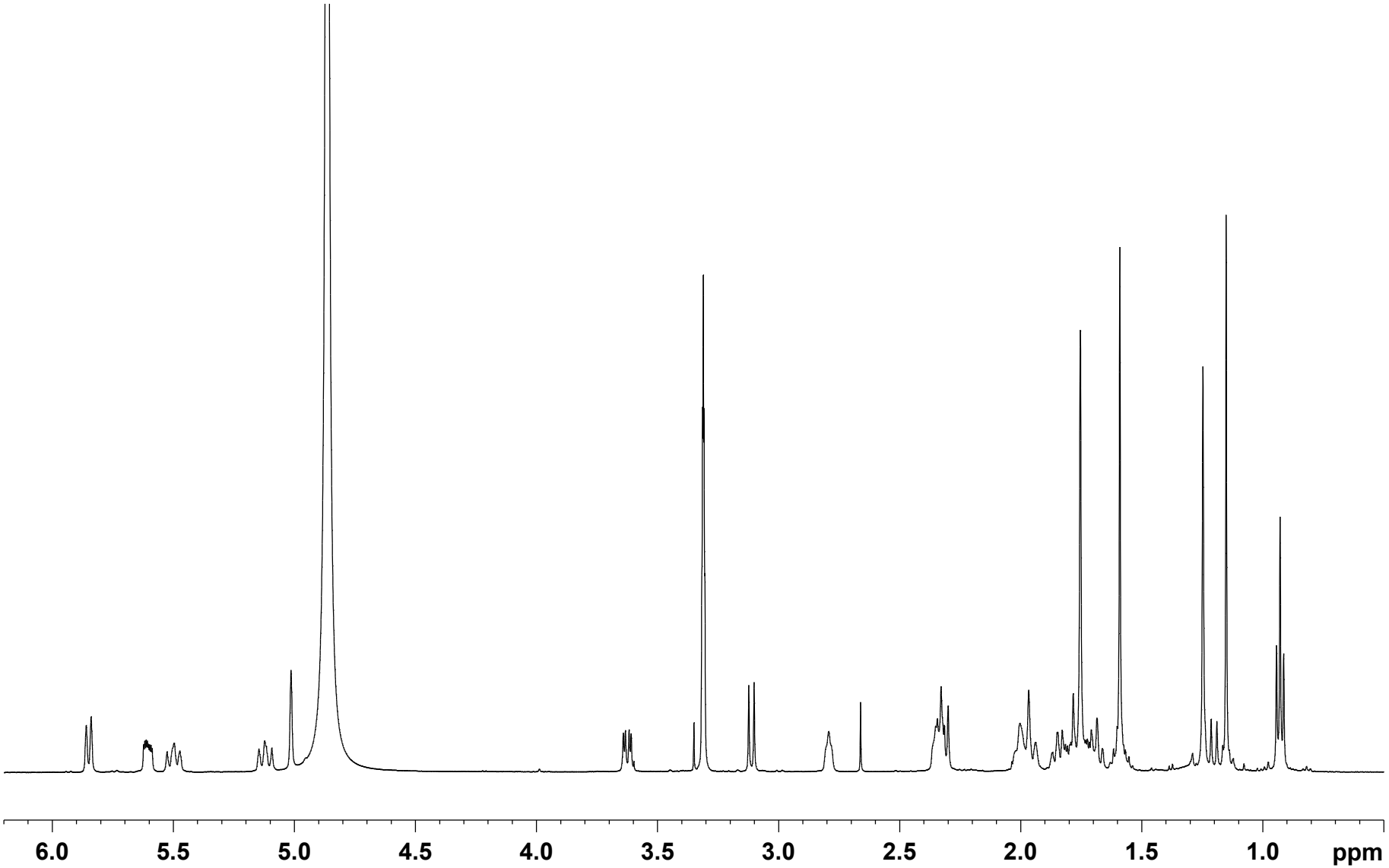


Figure S13. ^{13}C NMR spectrum of **2** (125 MHz, CD_3OD).

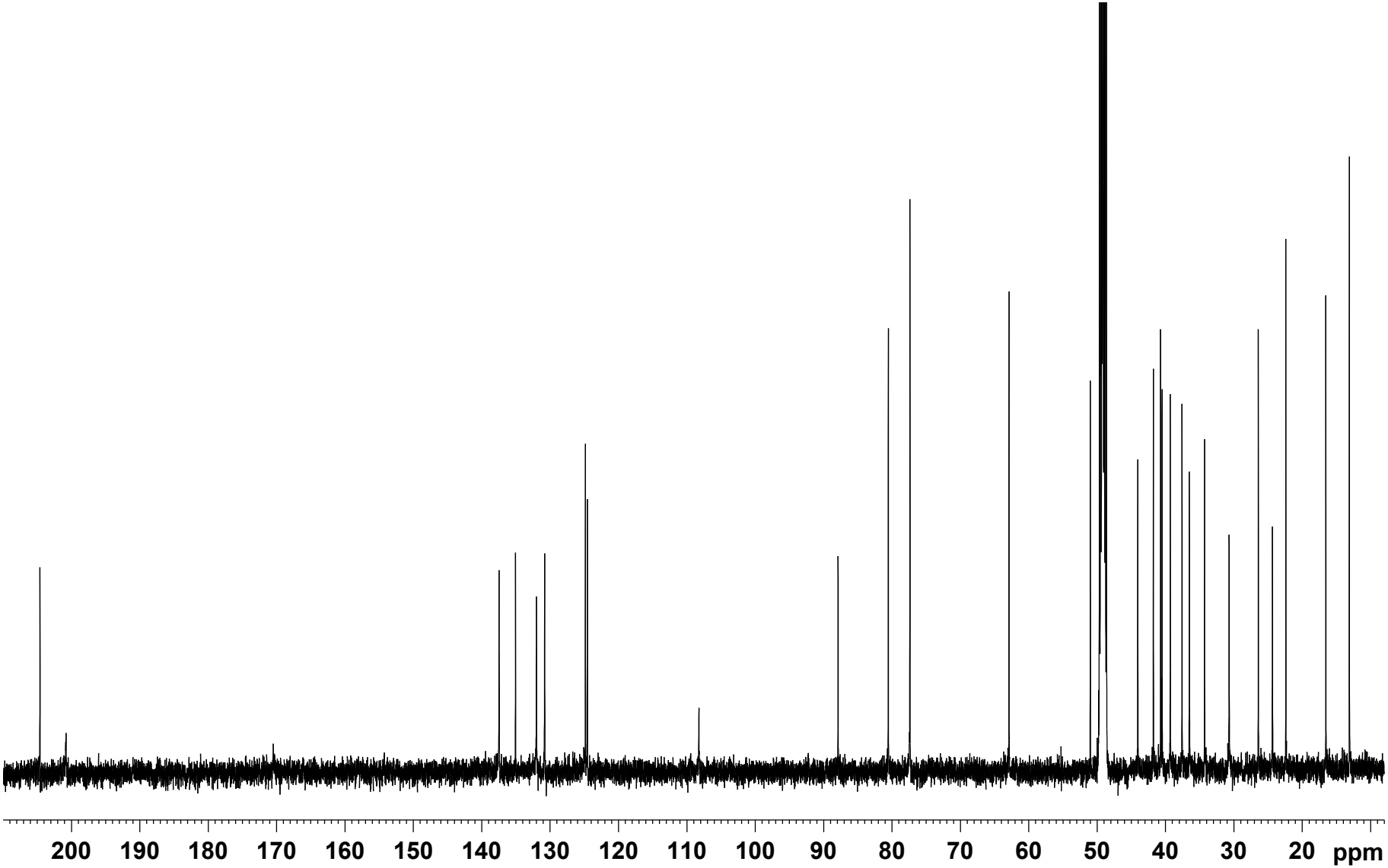


Figure S14. COSY spectrum of **2** (500 MHz, CD_3OD).

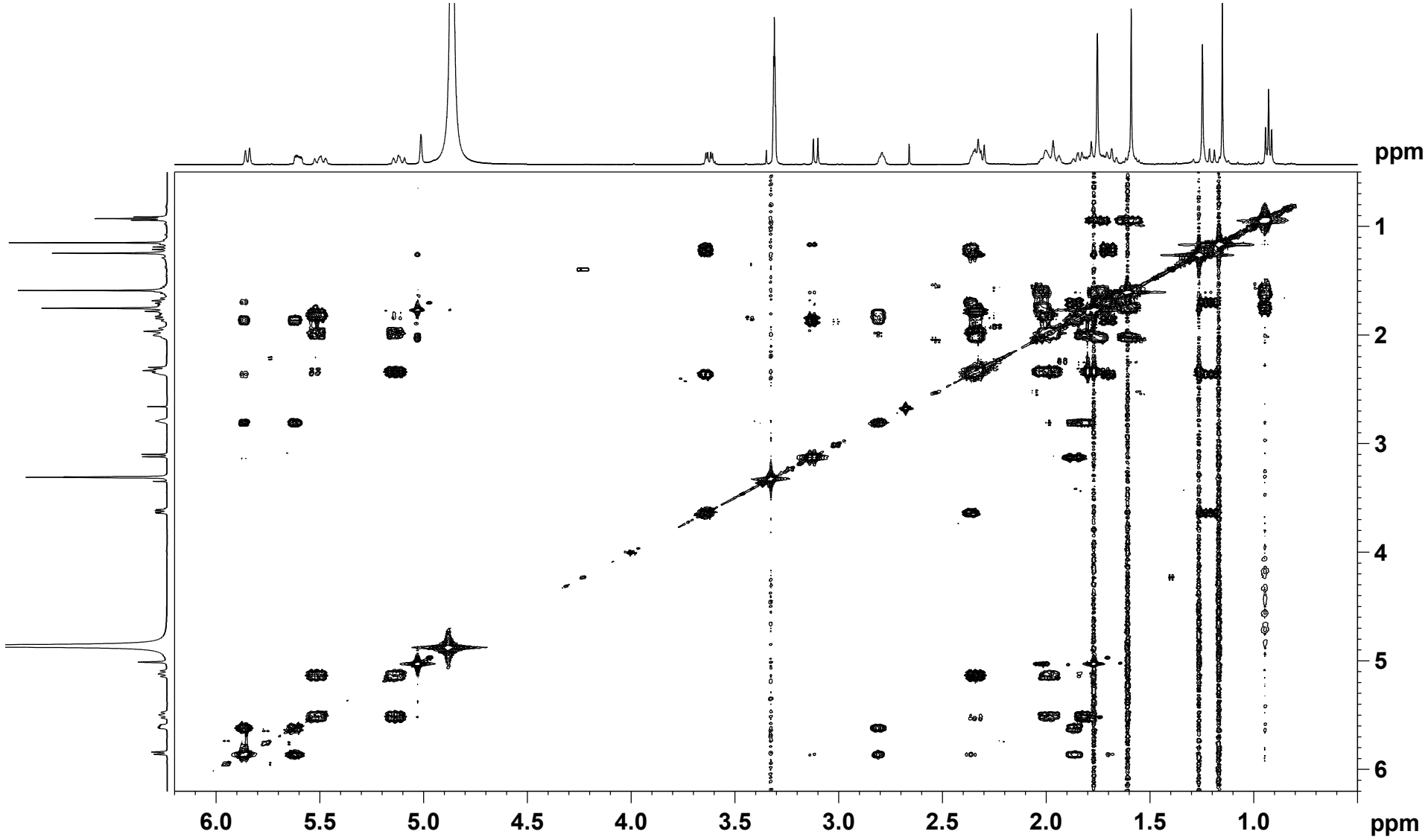


Figure S15. HSQC spectrum of **2** (500 MHz, CD_3OD).

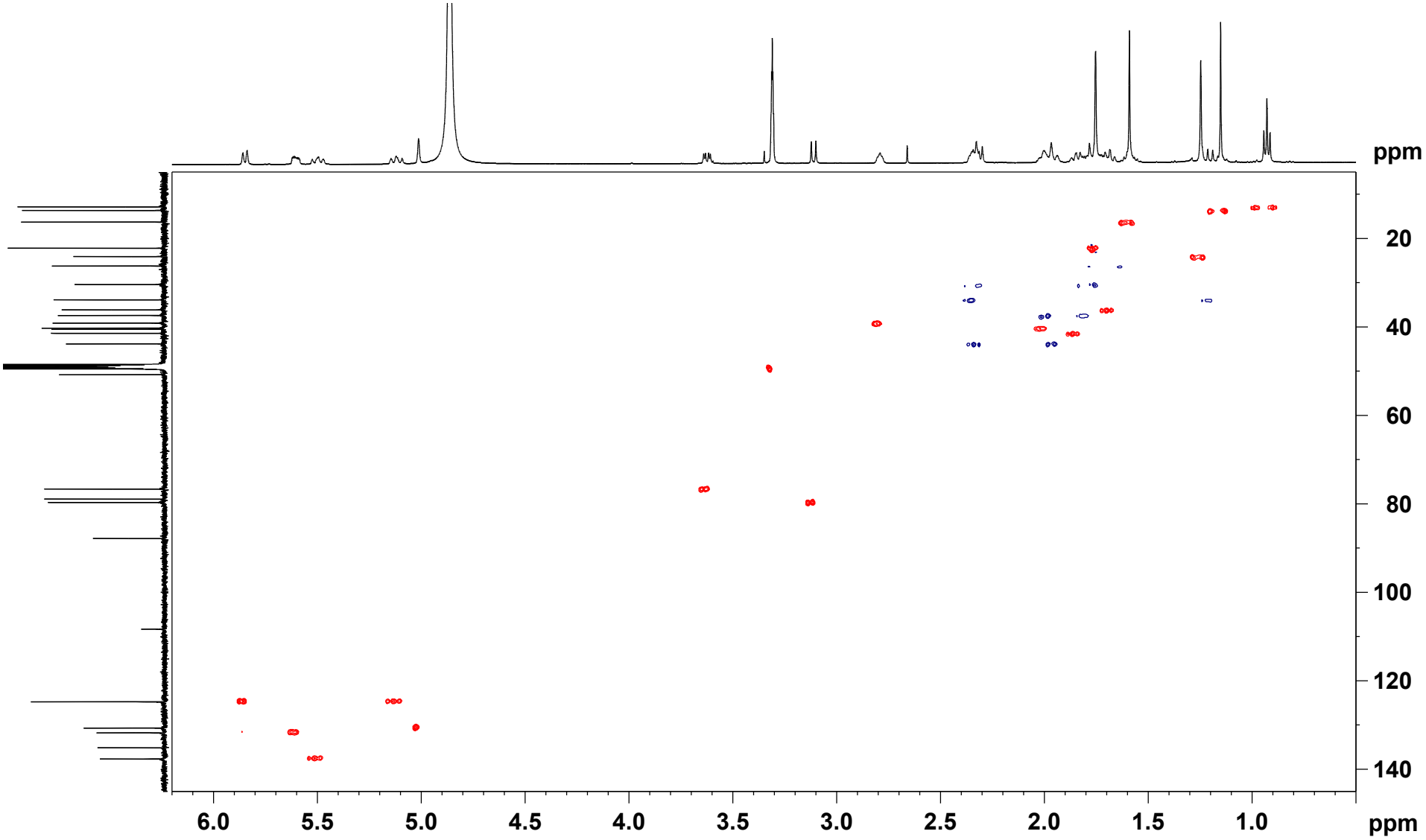


Figure S16. HMBC spectrum of **2** (500 MHz, CD_3OD).

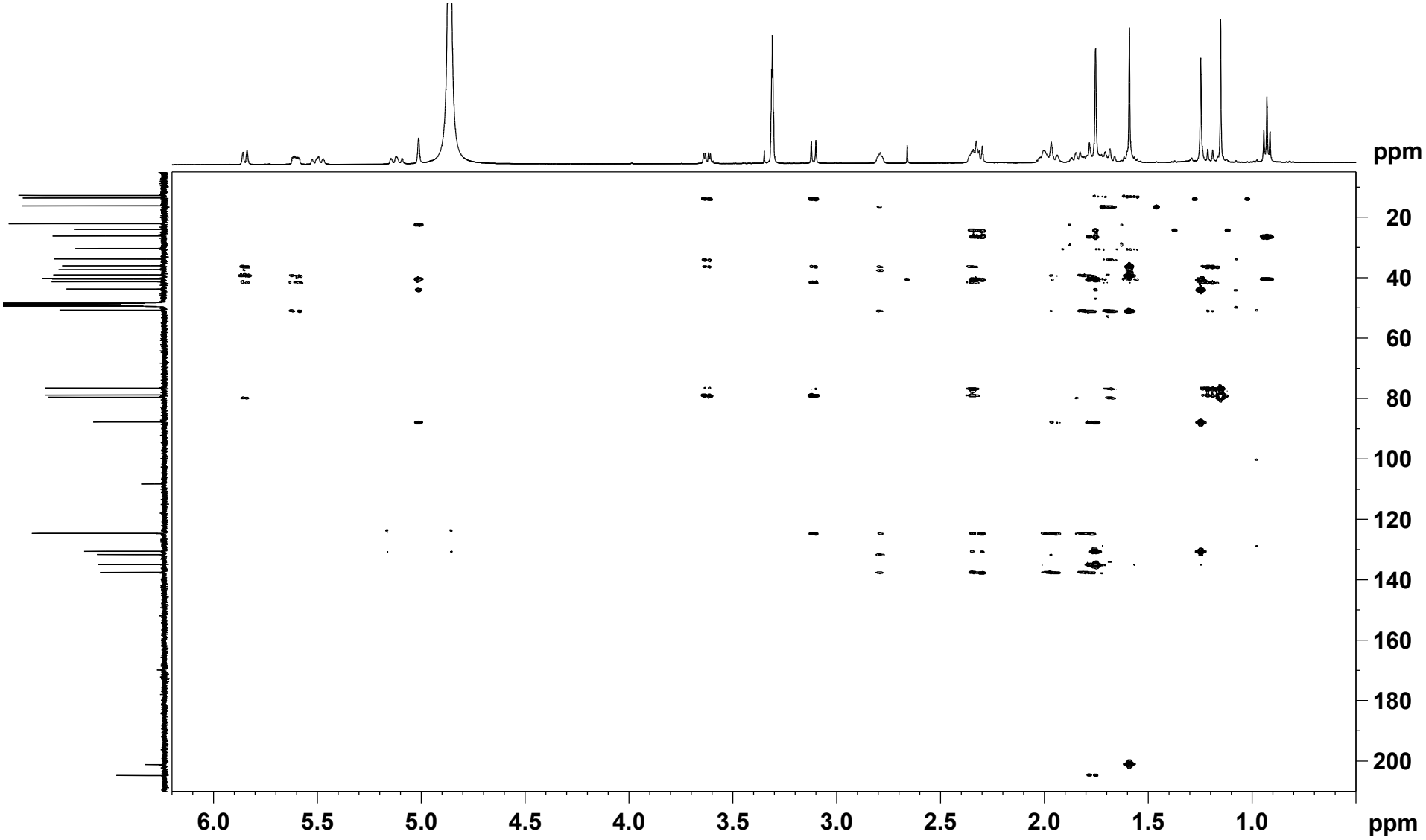


Figure S17. NOESY spectrum of **2** (500 MHz, CD_3OD).

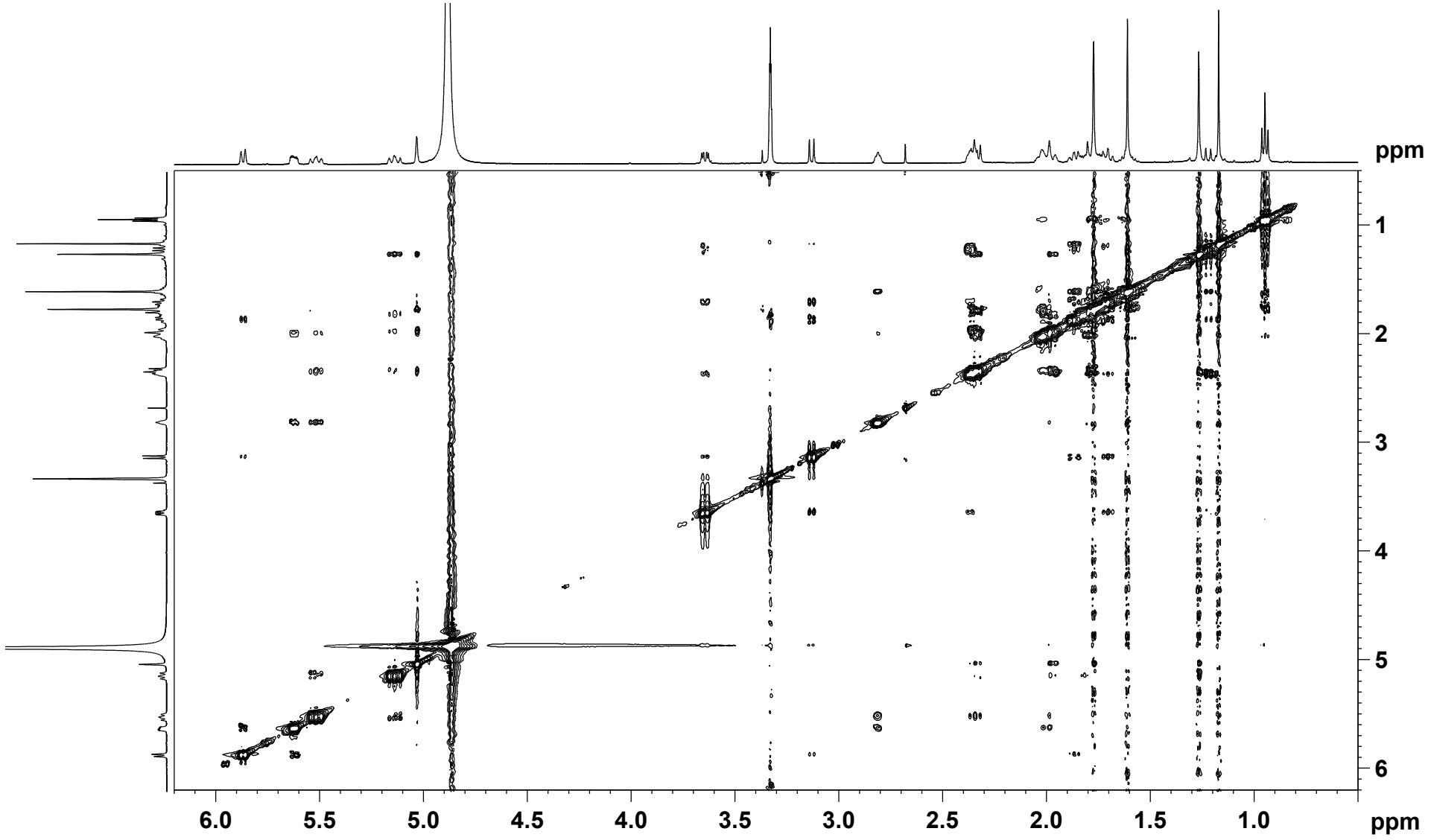


Figure S18. ROESY spectrum of **2** (500 MHz, CD_3OD).

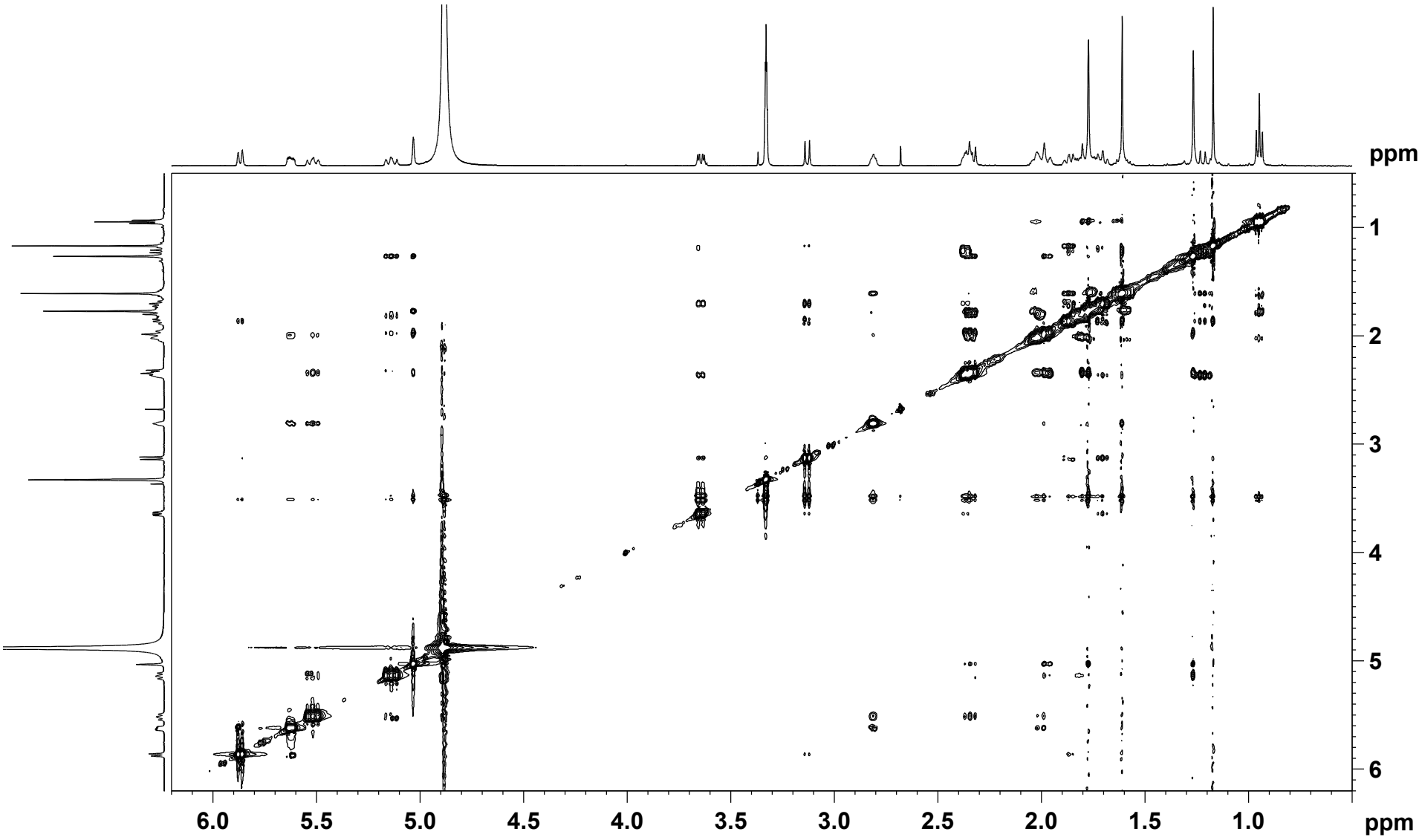


Figure S19. UV spectrum of nomimicin D (**3**).

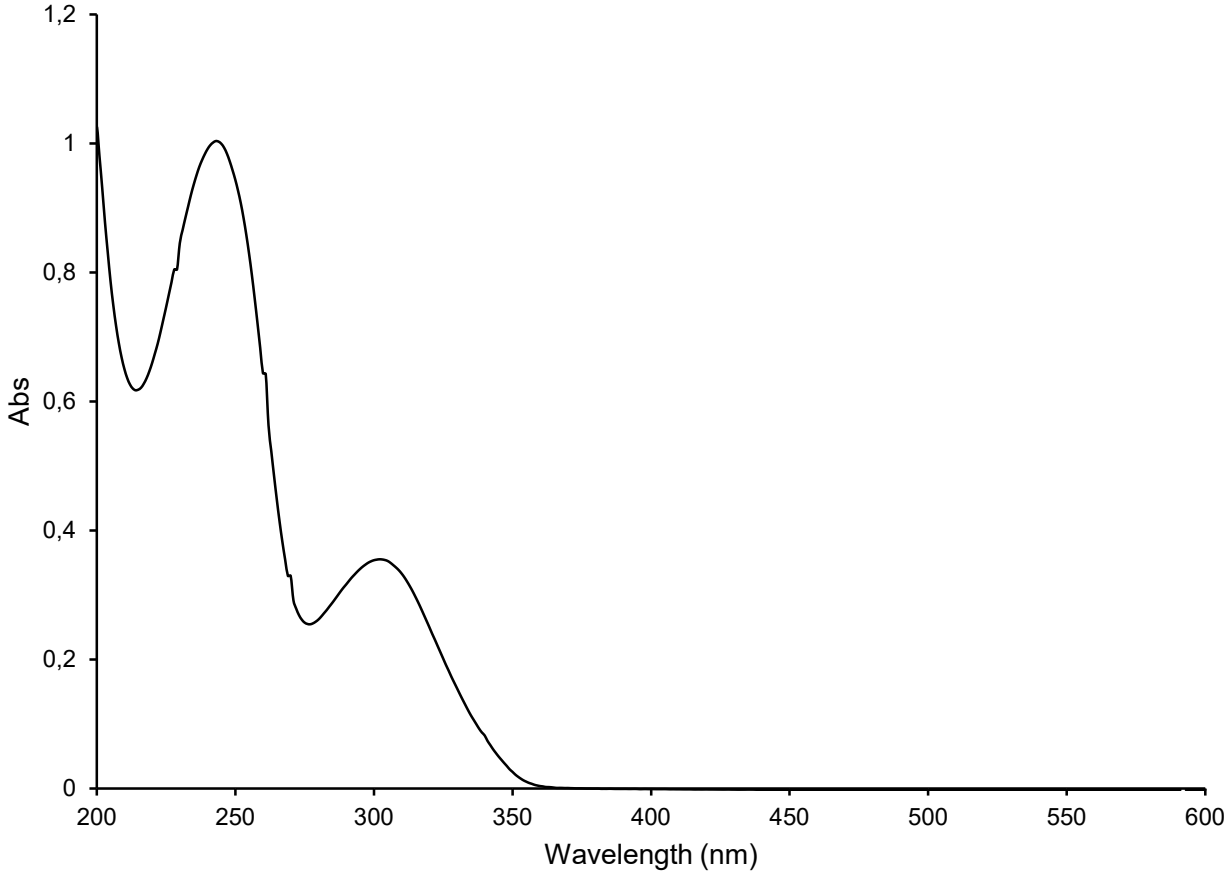


Figure S20. IR spectrum of **3.**

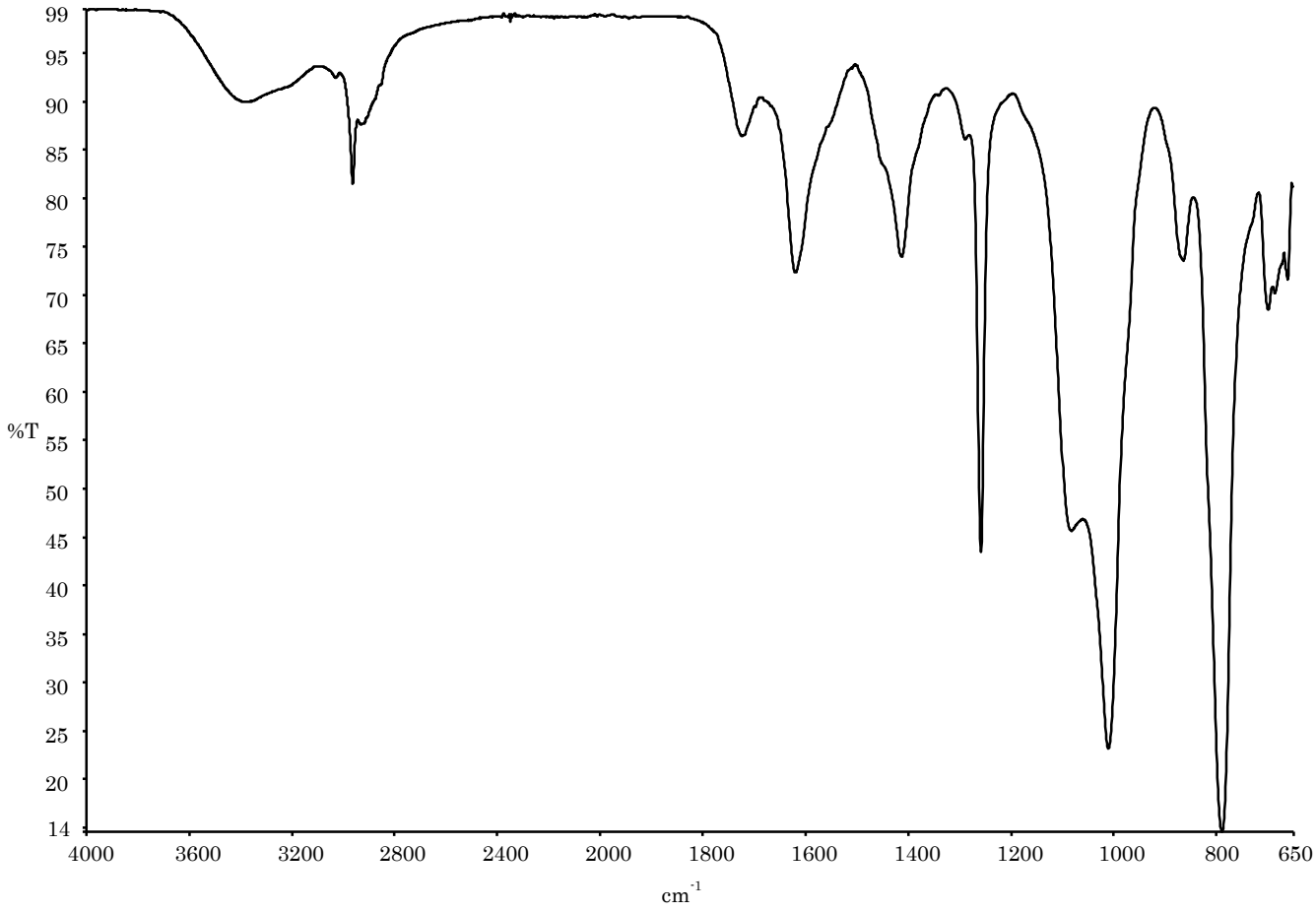


Figure S21. ^{1}H NMR spectrum of **3** (500 MHz, CD_3OD).

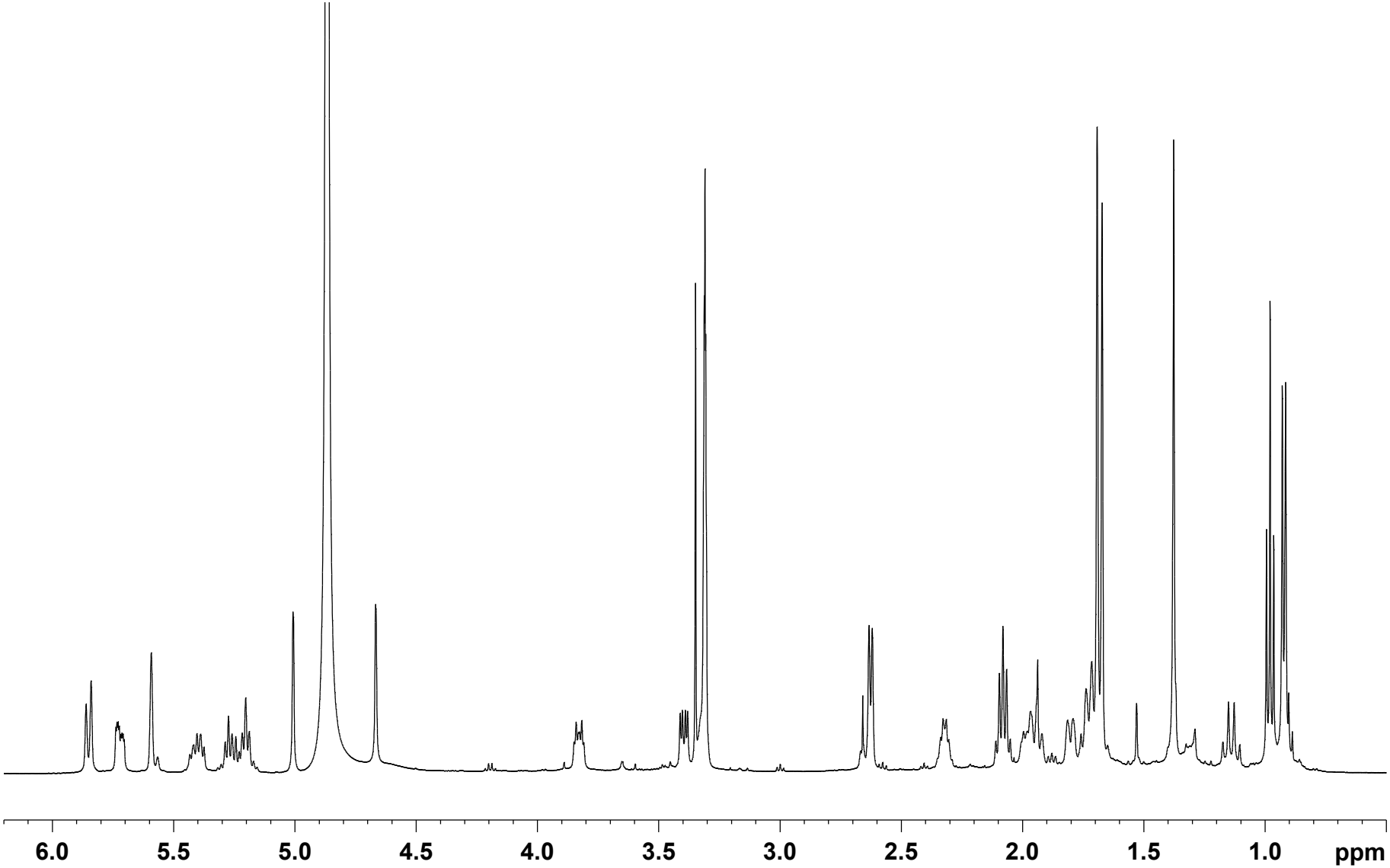


Figure S22. ^{13}C NMR spectrum of **3** (125 MHz, CD_3OD).

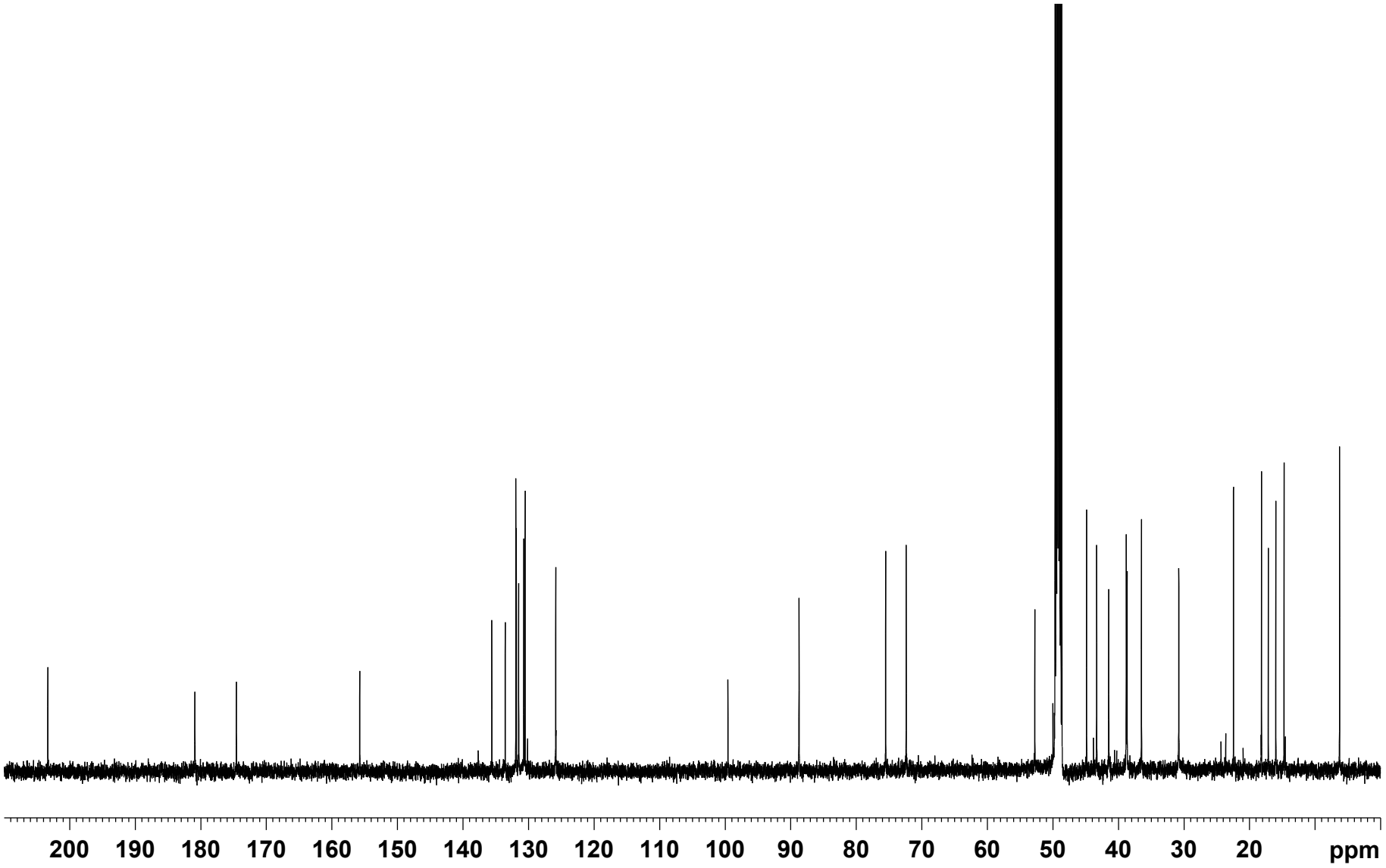


Figure S23. COSY spectrum of **3** (500 MHz, CD_3OD).

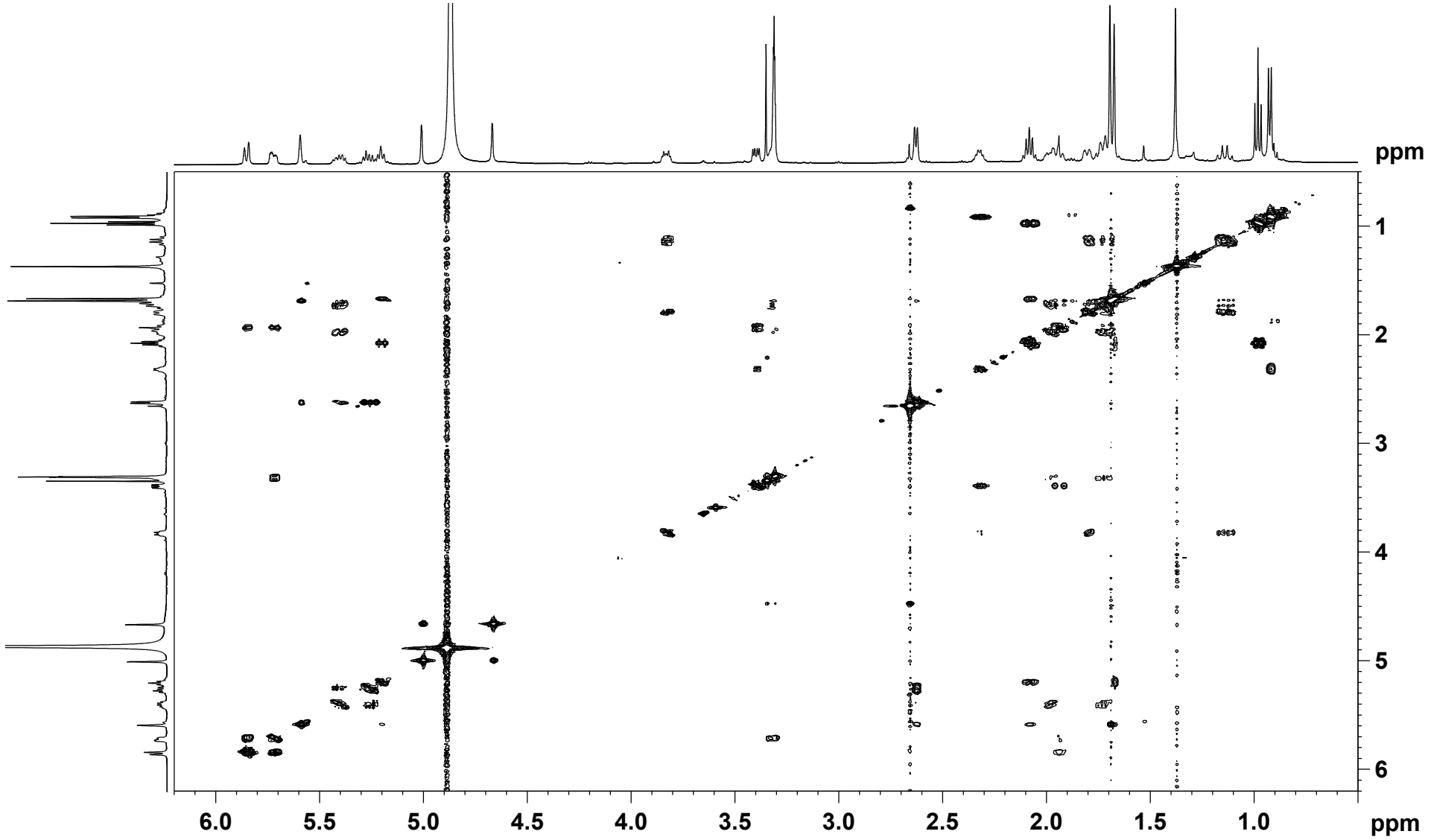


Figure S24. HSQC spectrum of **3** (500 MHz, CD_3OD).

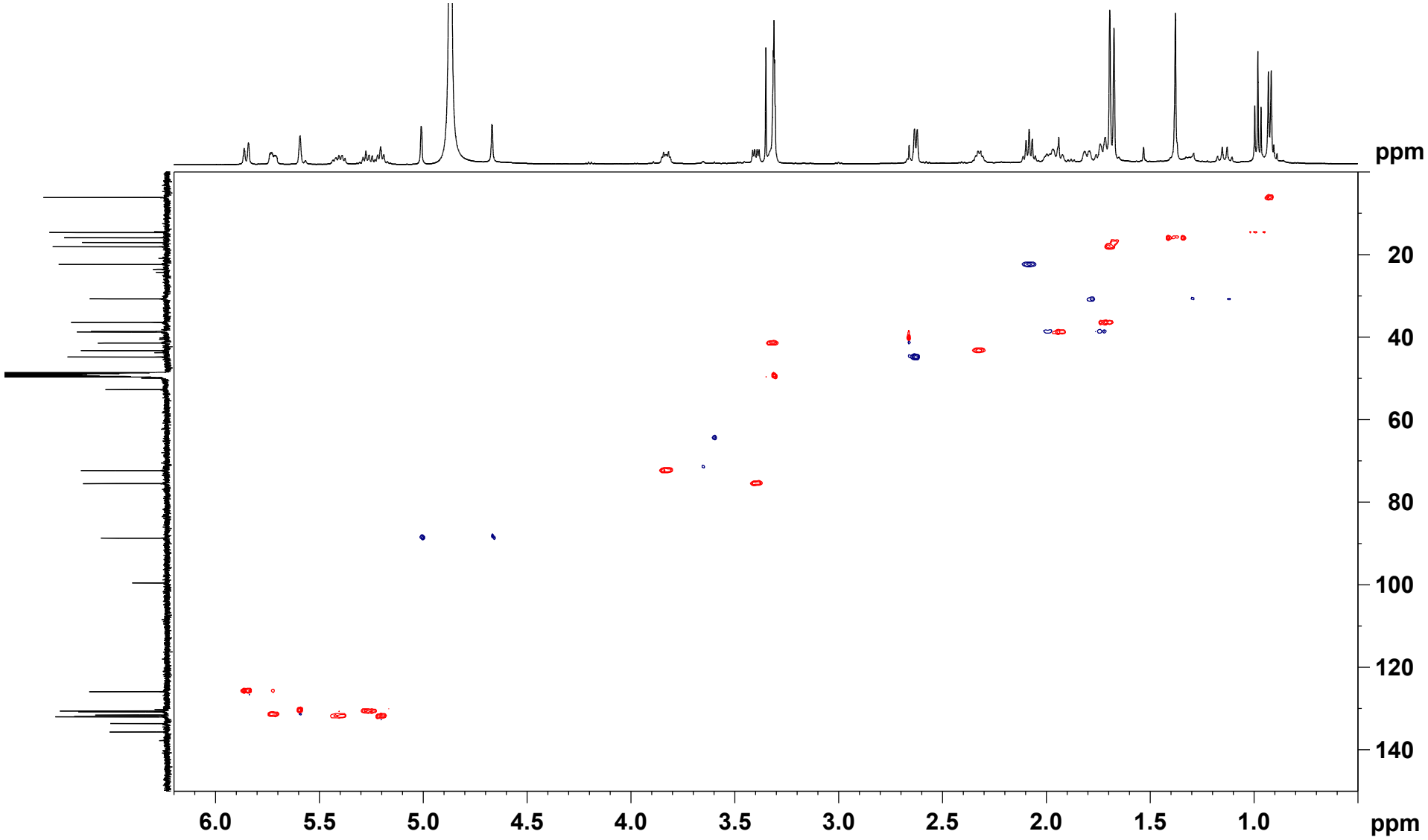


Figure S25. HMBC spectrum of **3** (500 MHz, CD_3OD).

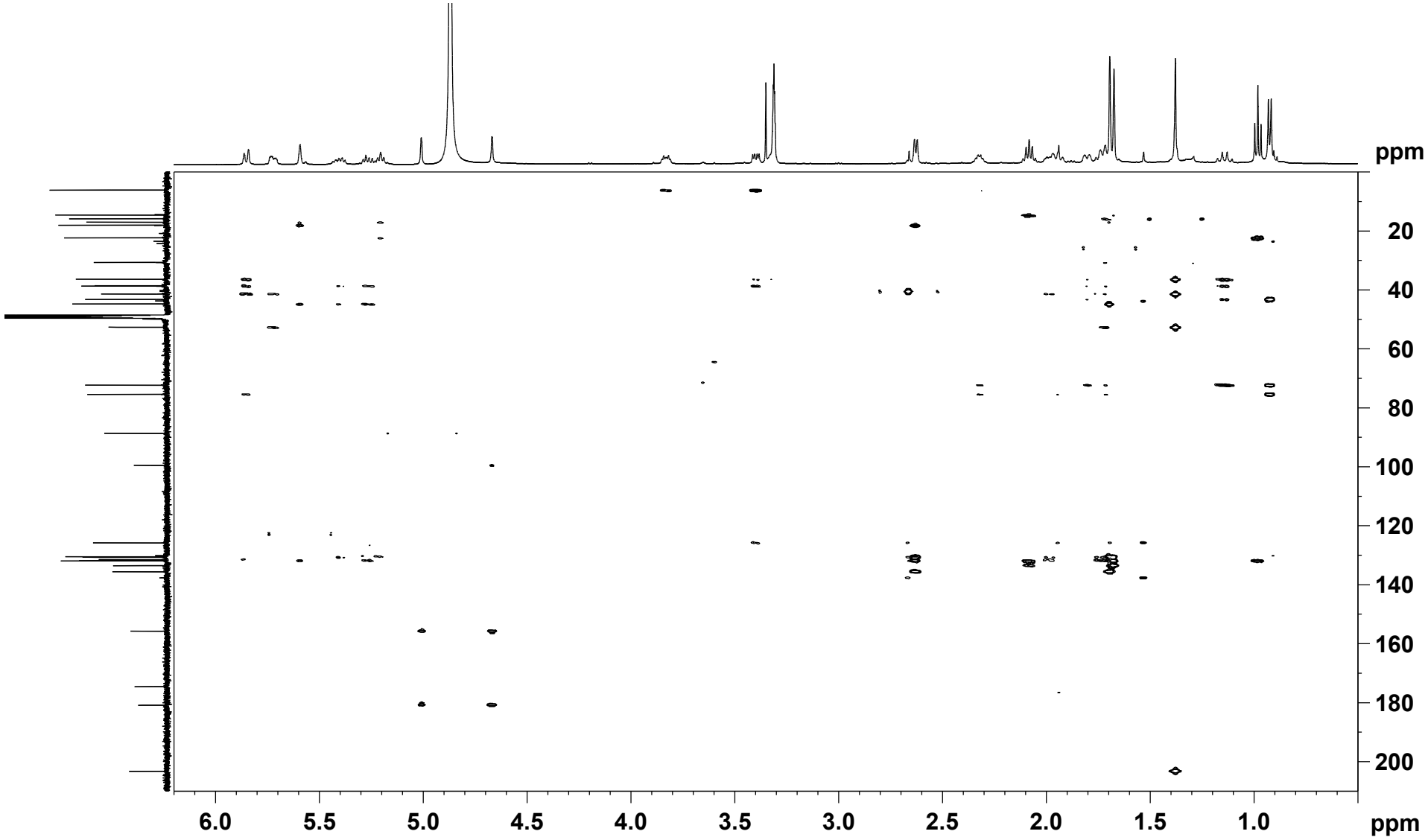


Figure S26. NOESY spectrum of **3** (500 MHz, CD_3OD).

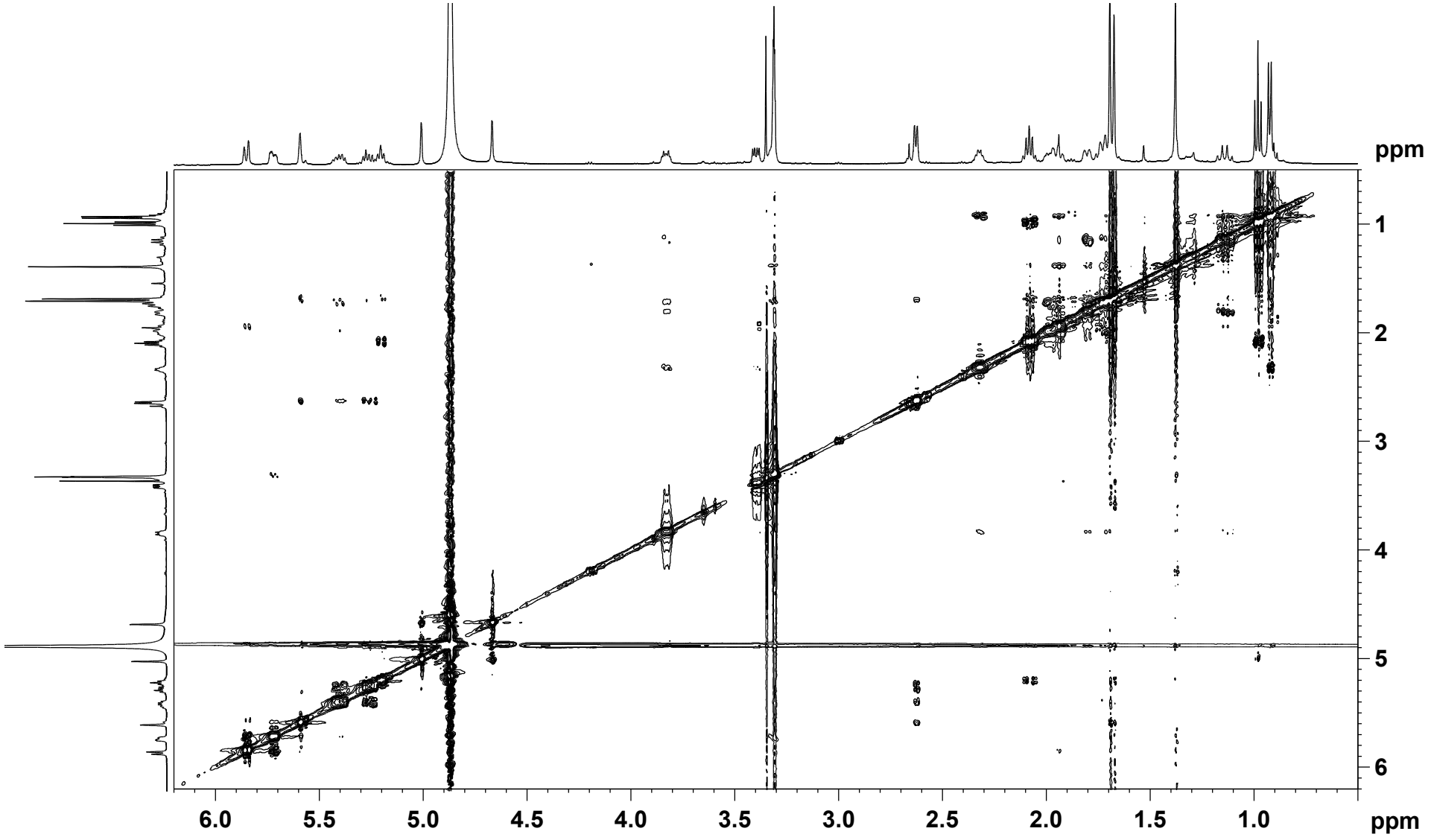


Figure S27. ROESY spectrum of **3** (500 MHz, CD_3OD).

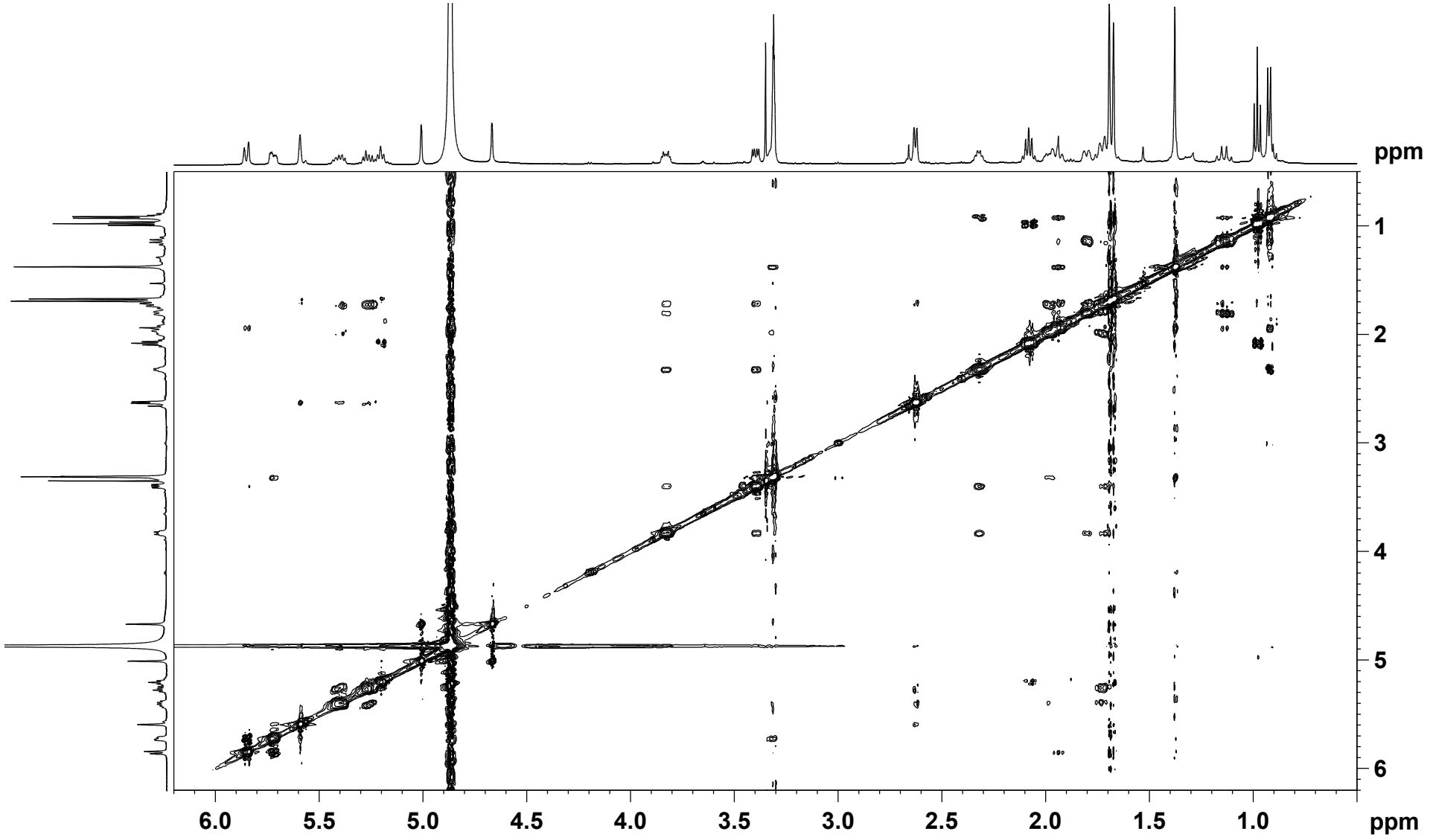


Figure S28. UV spectrum of nomimicin (**4**).

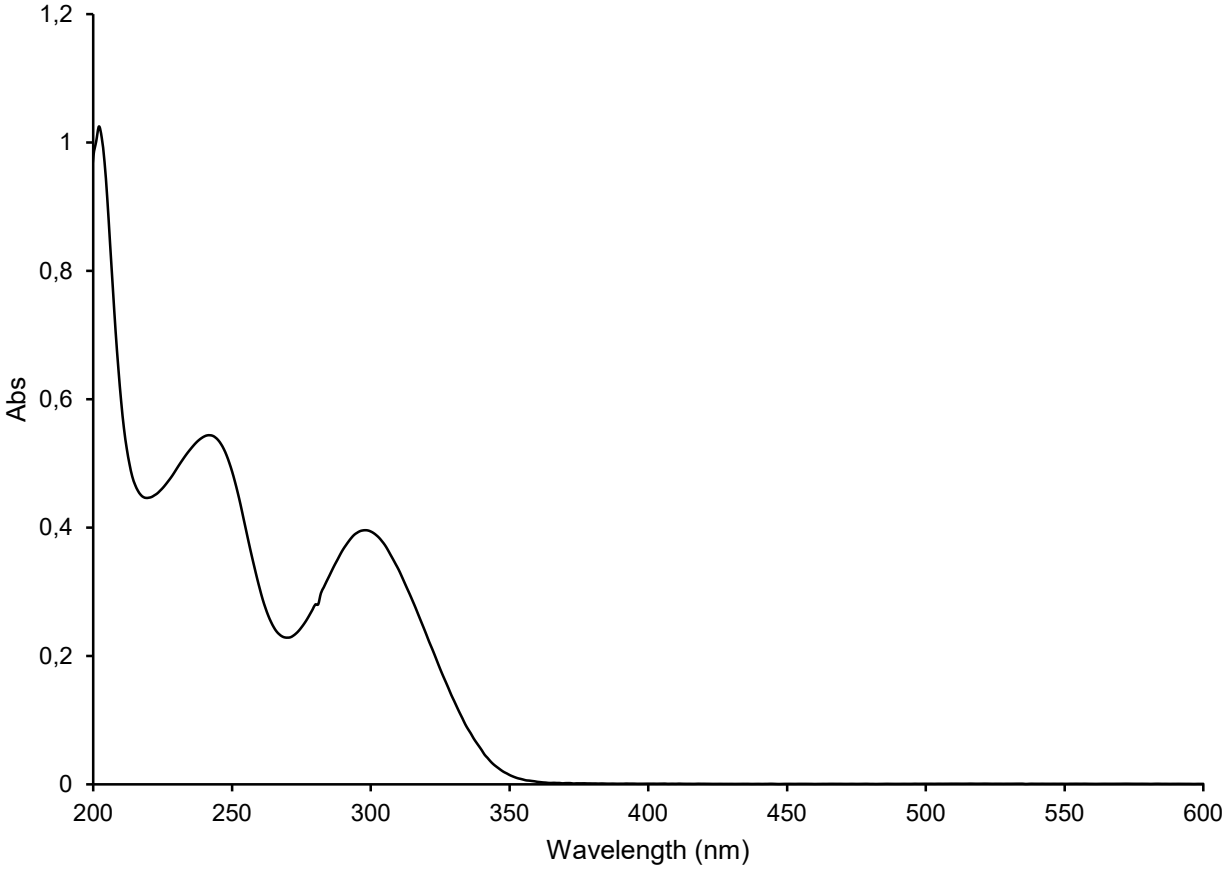


Figure S29. IR spectrum of **4.**

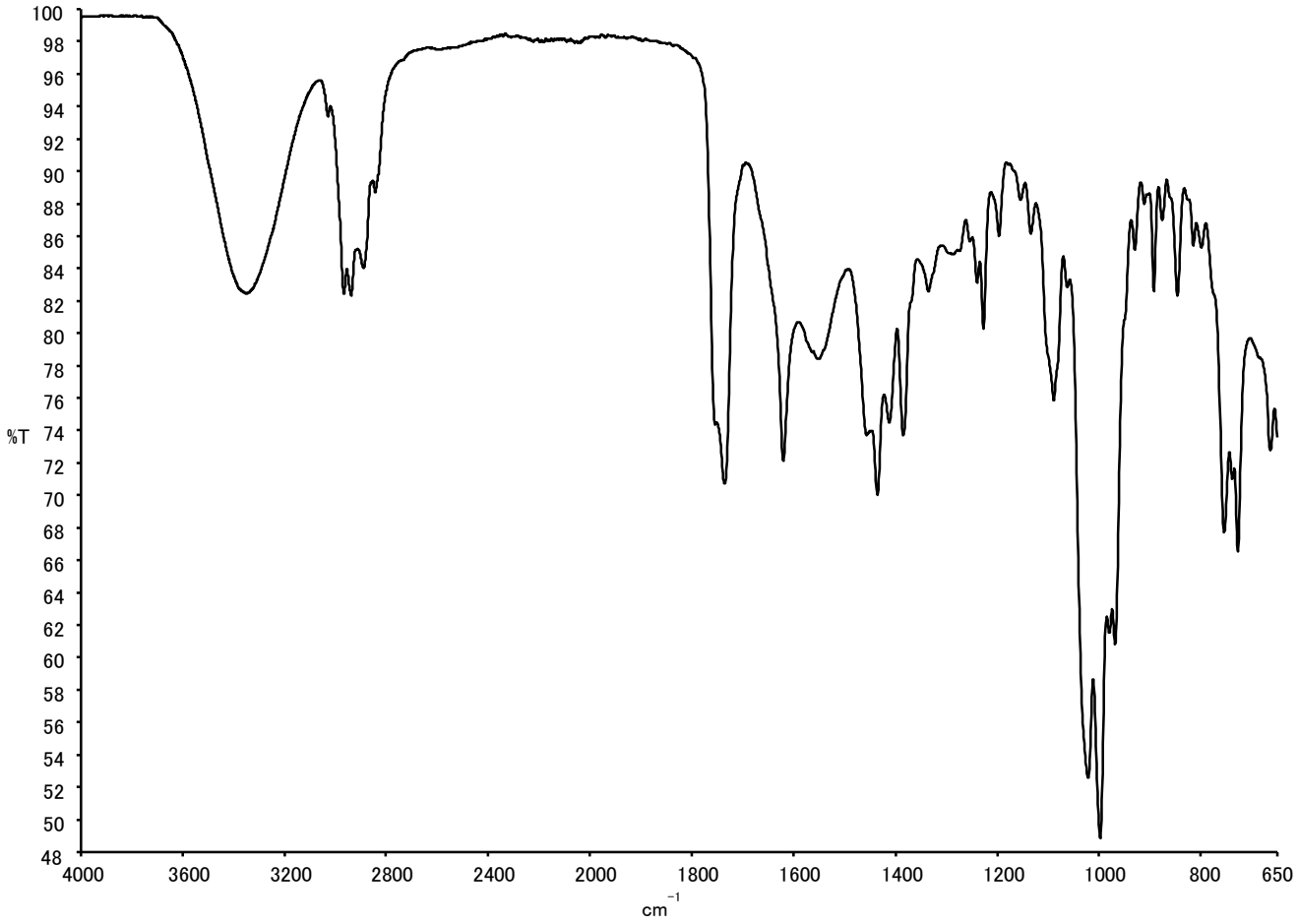


Figure S30. ^{1}H NMR spectrum of **4** (500 MHz, CD_3OD).

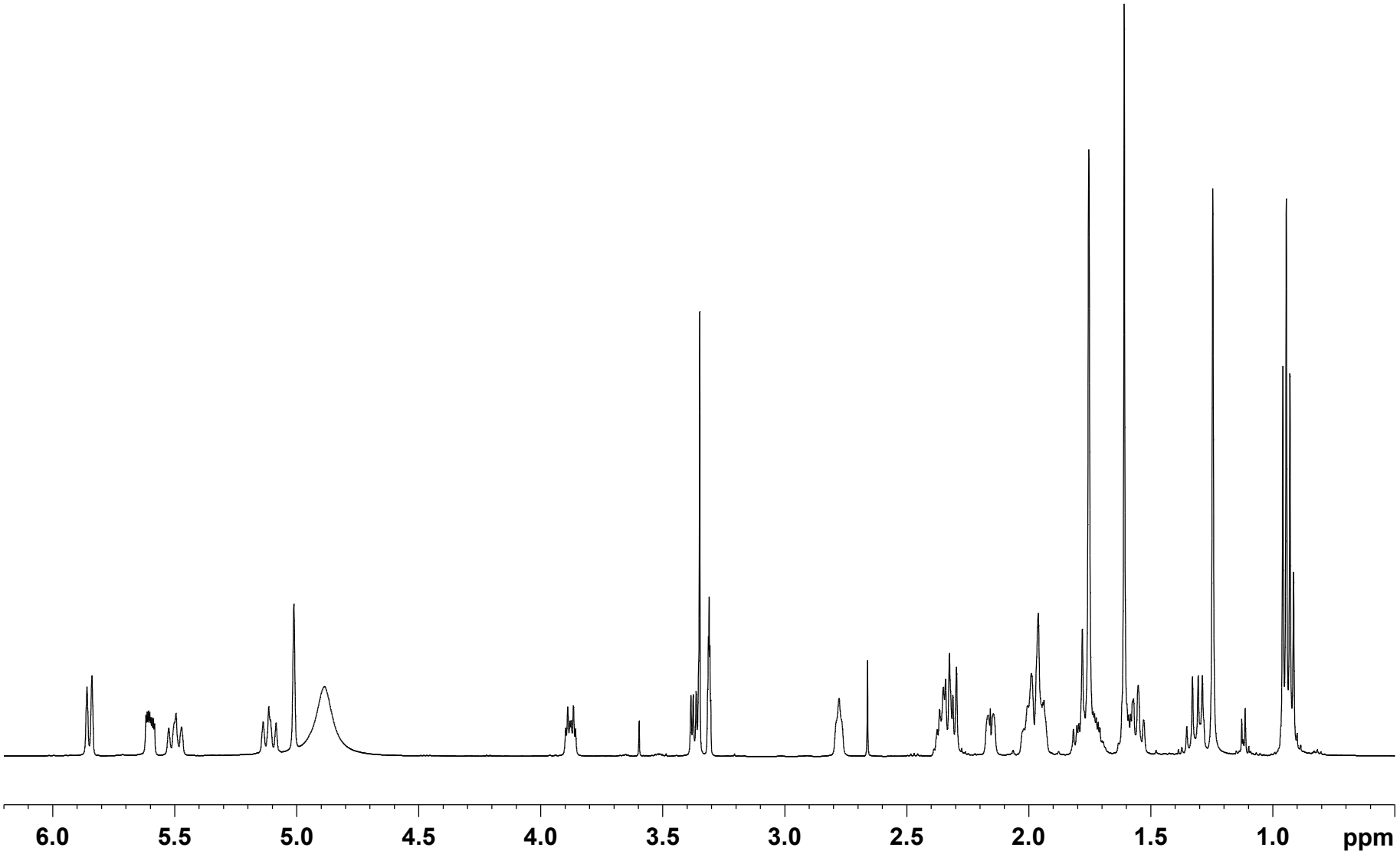


Figure S31. ^{13}C NMR spectrum of **4** (125 MHz, CD_3OD).

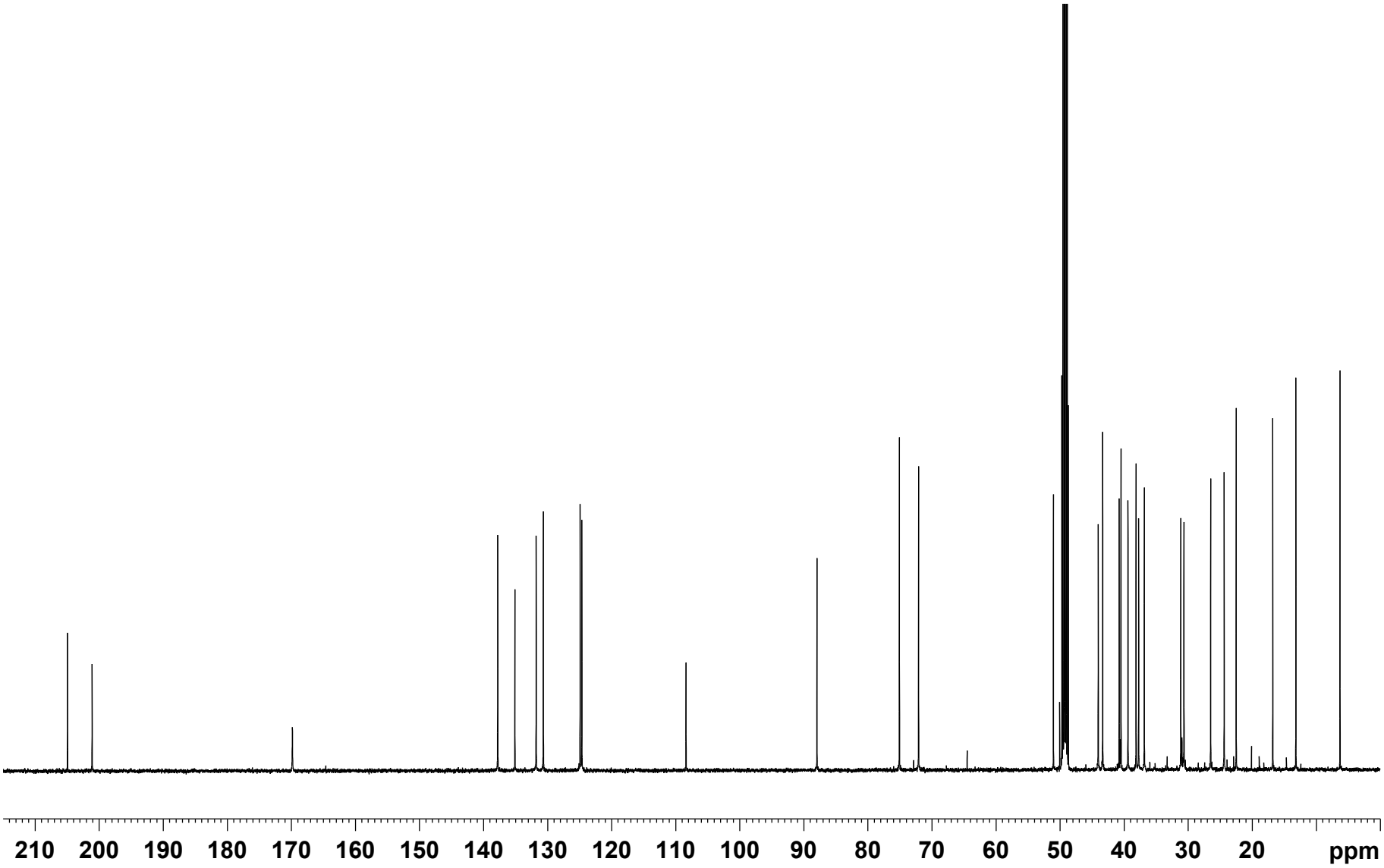


Figure S32. COSY spectrum of **4** (500 MHz, CD_3OD).

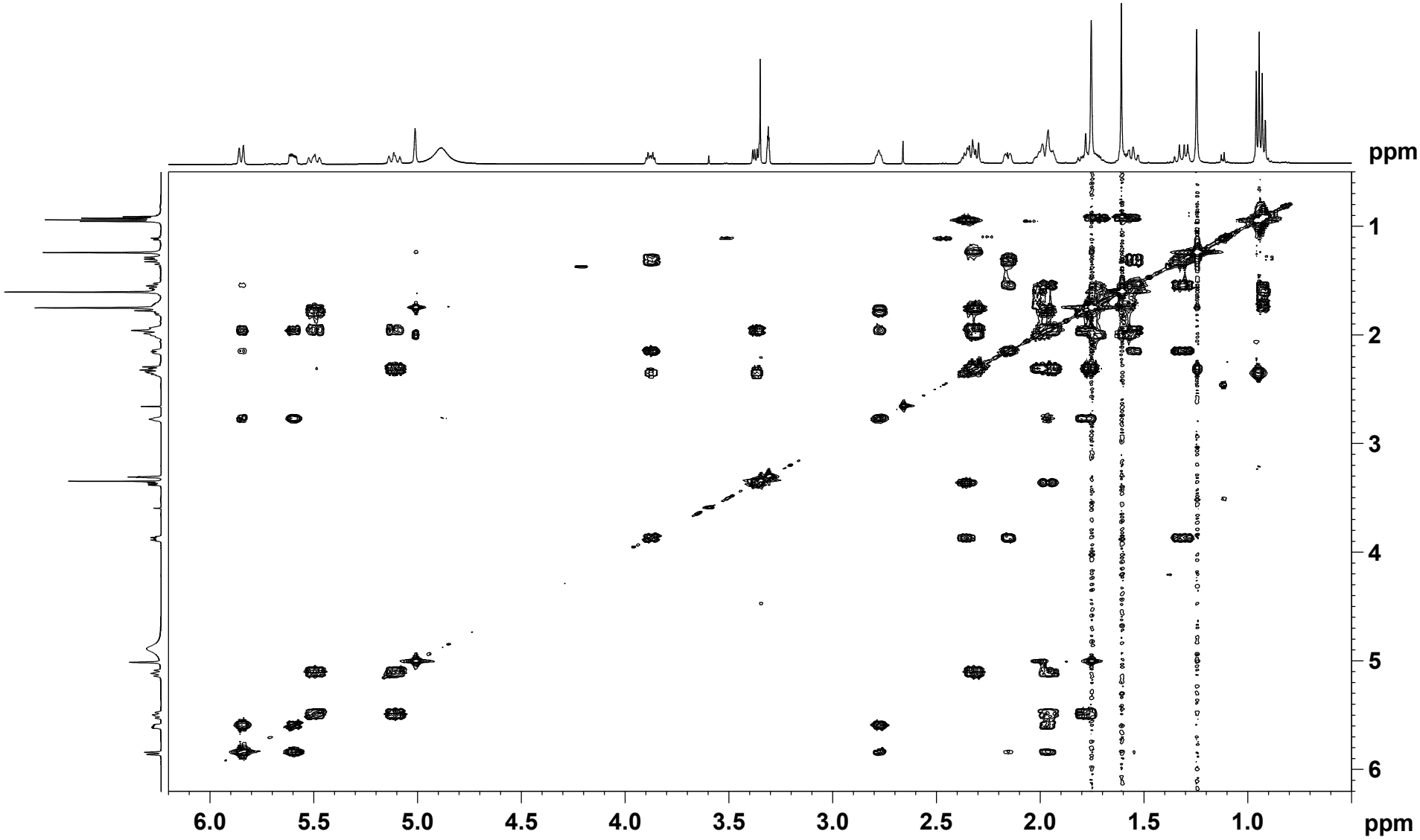


Figure S33. HSQC spectrum of **4** (500 MHz, CD_3OD).

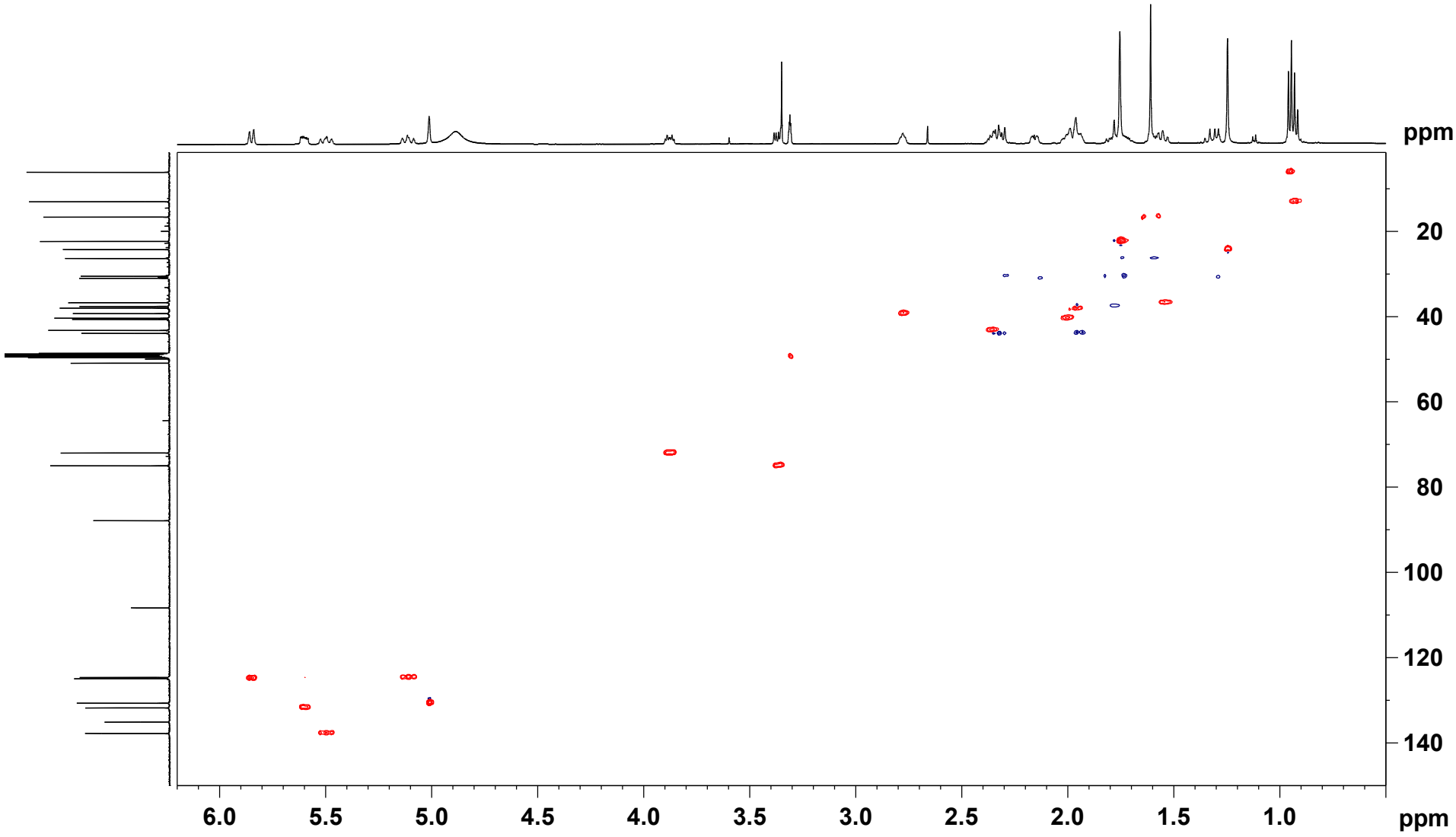
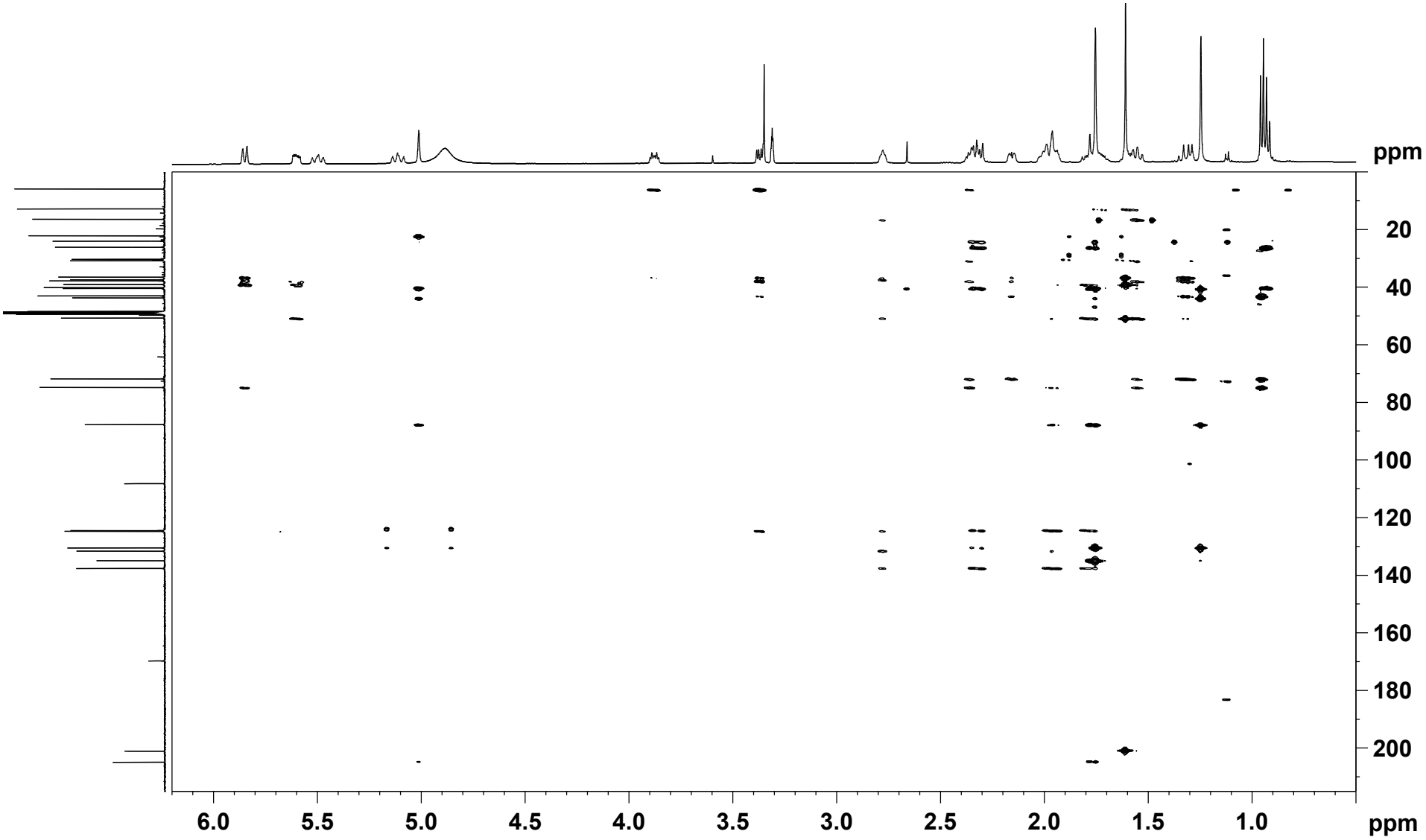


Figure S34. HMBC spectrum of **4** (500 MHz, CD_3OD).



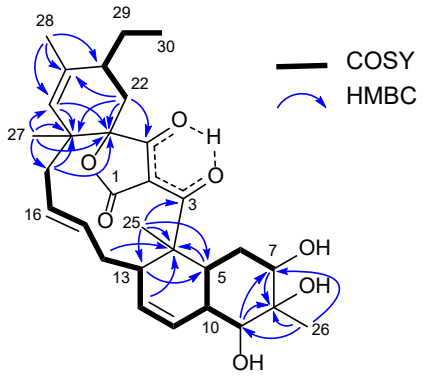


Figure S35. COSY and key HMBC correlations for **2**.

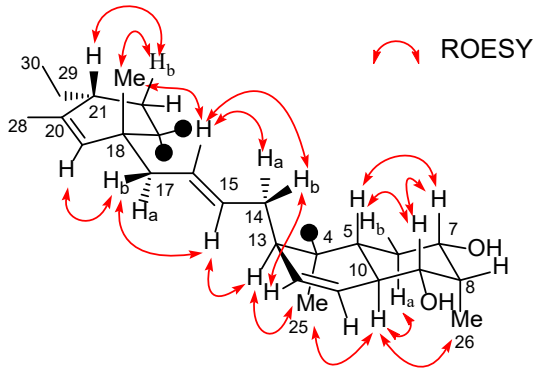


Figure S36. Relative correlations for **2** determined by ROESY analysis.

Table S1. NOESY and ROESY correlations of nomimicin B (**1**).

	nomimicin B (**1**)		
atom no.	δ_H, mult (*J* in Hz)[a]	NOESY[a]	ROESY[a]
5	1.66[b]	6b, 7, 9, 10	6b, 7, 9, 10
6ax	1.34, ddd (12.0, 12.0, 12.0)	6b, 10, 25,	6b, 10, 25, 26
6eq	2.41, brd (12.0)	5, 6a, 7	5, 6a, 7
7	3.74, dd (12.0, 4.3)	5, 6a, 9	5, 6a, 9
9	3.21, d (11.2)	5, 7	5, 7
10	2.02[b]	6a, 11, 25	6a, 11, 25, 26
11	5.85, d (10.1)	9, 10, 12	9, 10, 12
12	5.61, ddd (10.0, 5.3, 2.6)	11, 13, 14b	11, 13, 14b
13	2.81, m	12, 15, 25	12, 15, 23
14a	1.80[b]	15, 16	15, 16
14b	1.98[b]	12, 15, 16	12, 13, 15, 16
15	5.49, dd (14.7, 11.5)	13, 14a, 14b, 16, 17b	13, 14a, 14b, 16, 17b
16	5.12, dd (14.8, 11.3)	14a, 15, 17a, 17b, 27	14a, 14b, 15 17b, 27
17a	1.95[b]	27, 17b, 19	27, 17b, 19
17b	2.32[b]	15, 16, 17a, 19	17a, 19, 16, 15
19	5.00, s	17a, 17b, 27, 28	27, 28, 17a, 17b
21	2.00[b]	22b, 30	22b, 30
22a	1.78[b]	30	30
22b	2.34[b]	21, 27, 29b	21, 27, 29b
25	1.60, s	10, 13	10, 13
26	3.99, s		6b, 10
27	1.24, s		16, 17b, 19, 22b
28	1.75, s	19, 22a, 29b, 30	19
29a	1.58[d]	30	22b, 30
29b	1.72[b]	21	21, 22b
30	0.93, t (7.4)	21, 22a, 29a, 29b	21, 22a, 29a, 29b

[a]Recorded at 500 MHz. [b]Overlapping signals.

Table S2. NOESY and ROESY correlations of nomimicin C (**2**).

	nomimicin C (**2**)		
atom no.	δ_H, mult (*J* in Hz)[a]	NOESY[a]	ROESY[a]
5	1.68[b]	6b, 7, 9	6b, 7, 9
6ax	1.20, ddd (11.9, 11.9, 11.9)	6b, 10, 25	6b, 10, 25
6eq	2.35[b]	5, 6a, 7	5, 6a, 7
7	3.62, dd (11.8, 4.2)	5, 6a, 6b, 9	5, 6a, 6b, 9
9	3.11, d (11.0)	5, 7, 10	5, 7, 10
10	1.85[b]	6a, 9, 11, 25, 26	6a, 9, 11, 25, 26
11	5.84, d (10.0)	9, 10, 12	9, 10, 12
12	5.60, ddd (10.0, 5.1, 2.5)	11, 13, 14b	11, 13, 14b
13	2.79, m	12, 14a, 14b, 15, 25	12, 14a, 14b, 15, 25
14a	1.80[b]	13, 16	13, 16
14b	1.98[b]	12, 13, 15, 16	12, 13, 15, 16
15	5.48, dd (14.5, 11.9)	13, 14b, 16, 17b	13, 14b, 16, 17b
16	5.12, dd (14.8, 11.6)	14a, 14b, 15, 17b, 27	14a, 14b, 17b, 27
17a	1.95[b]	16, 19, 17b, 27	16, 19, 17b, 27
17b	2.32[b]	15, 19, 17a, 27	15, 16, 17b, 19, 27
19	5.01, s	17b, 21, 27, 28	17b, 21, 27, 28
21	2.01[b]	22b, 28, 30	22b, 28, 30
22a	1.79[b]	30	30
22b	2.34[b]	21, 22a, 27, 29b	21, 22a, 27, 29b
25	1.59, s	6b, 10, 13	6b, 10, 13
26	1.15, s	10	10
27	1.25, s	16, 17b, 19, 22b	16, 7b, 19, 22b
28	1.75, s	19, 21, 30	19, 21, 30
29a	1.62[b]	30	30
29b	1.75[b]	21, 22b, 30	21, 22b, 30
30	0.93, t (7.4)	21, 22a, 28, 29a, 29b	21, 22a, 28, 29a, 29b

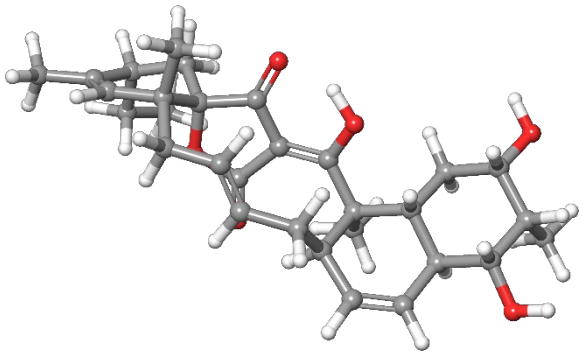
[a]Recorded at 500 MHz. [b]Overlapping signals.

Table S3. ROESY and NOESY correlations of nomimicin D (**3**).

nomimicin D (**3**)			
atom no.	δ_H, mult (*J* in Hz)[a]	NOESY[a]	ROESY[a]
5	1.72[b]	7	7, 9
6ax	1.14, ddd (11.7, 11.7, 11.7)	6eq, 10, 25, 26	6eq, 10, 25, 26
6eq	1.80, brd (11.7)	6ax, 7	6ax, 7
7	3.83, ddd (11.6, 4.5, 4.5)	5, 6ax, 6eq, 8	5, 6eq, 8, 9
8	2.32, m	9, 26	7, 9, 26
9	3.40, dd (10.8, 4.7)	5, 8, 10	5, 6eq, 7, 8
10	1.94[b]	6ax, 9, 11, 25, 26	6ax, 11, 26, 29
11	5.85, d (10.2)	10, 12	9, 10, 12
12	5.72, ddd (10.2, 4.8, 2.5)	11, 13	11, 13
13	3.32[b]	12, 14b, 15, 25	12, 14b, 15, 25
14a	1.75[b]	14b, 15	14b, 15, 16
14b	2.00[b]	13, 14a, 15	13, 14a, 15, 16
15	5.40, dt (15.0, 7.2)	13, 14a, 14b, 17	14a, 14b, 17
16	5.26, dt (15.2, 7.0)	17	14a, 14b, 17
17	2.63, d (6.9)	15, 16, 19, 27	15, 16, 19, 27
19	5.59, s	17, 27, 28	17, 27, 28
21	5.20, t (7.3)	28, 29	28, 29
22a	4.66, d (1.5)	22b	22b
22b	5.00, d (1.5)	22a	22a
25	1.38, s	6ax, 10, 13	6ax, 10, 13
26	0.92, d (6.9)	6ax, 8, 10	6ax, 8, 10
27	1.69, s	17, 19	17, 19
28	1.67, s	19, 21	19, 21
29	2.08, q (7.5)	21, 30	21, 30
30	0.98, t (7.5)	29	29

[a]Recorded at 500 MHz. [b]Overlapping signals.

Table S4. Cartesian coordinates and energies of the most stable conformer of **4a**.



4a (ΔG = 0.0 kcal/mol)

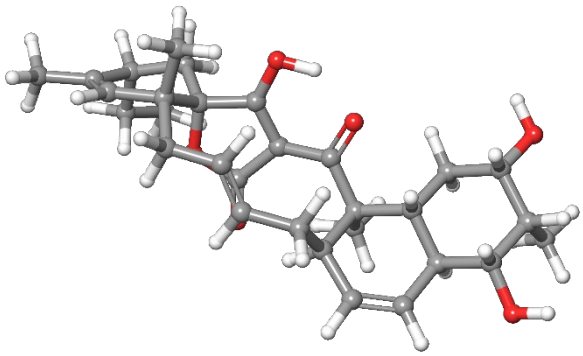
M06-2X/def2-TZVP-SMD(MeOH)//M06-2X/6-31G(d)-SMD(MeOH):		
Gibbs Free Energy (a.u.)	=	−1617.990463
M06-2X/def2-TZVP-SMD(MeOH):		
Electronic energy (a.u.)	=	−1618.593138
M06-2X/6-31G(d)-SMD(MeOH):		
Zero-point correction (a.u.)	=	0.663531
Thermal correction to Energy (a.u.)	=	0.697126
Thermal correction to Enthalpy (a.u.)	=	0.698070
Thermal correction to Gibbs Free Energy (a.u.)	=	0.602675

C	−3.503719	−2.346714	2.018768	C	−3.645152	−0.928348	2.483653
C	−2.842684	0.059614	1.614795	C	−1.406663	−0.467423	1.327473
C	−1.478556	−1.858223	0.592342	C	−2.535046	−2.744197	1.197996
C	−5.114423	−0.482563	2.517646	C	−5.279711	0.929994	3.107325
C	−4.385326	1.900074	2.329127	C	−2.928249	1.436913	2.295338
H	−3.357511	0.126062	0.644467	H	−3.275366	−0.872508	3.519517
C	−5.025003	0.971896	4.615534	O	−5.838844	−1.443966	3.275191
O	−4.511032	3.183884	2.931226	C	−0.628314	−0.610233	2.647818
C	−0.659504	0.477094	0.398921	C	0.661656	0.373915	−0.030811
O	−1.393789	1.424828	−0.127383	C	1.639477	−0.706686	0.113186
O	2.586816	−0.577666	−0.849731	C	2.365451	0.552627	−1.719717
C	1.091115	1.157639	−1.160964	O	0.536366	2.160395	−1.624592
C	3.524265	1.533137	−1.535198	O	1.725959	−1.631641	0.893988
C	−1.689680	−1.808606	−0.957891	C	−0.406444	−1.965046	−1.729979
C	0.043227	−1.135931	−2.672441	C	1.404868	−1.243425	−3.302139
C	2.266578	0.047683	−3.188329	C	1.683546	1.118875	−4.130266

C	3.662248	−0.283699	−3.677645
C	4.887106	0.905325	−1.852568
C	5.512444	0.066671	−0.711618
H	−4.220916	−3.069641	2.399844
H	−2.480596	−3.789269	0.893961
H	−6.322708	1.233321	2.937115
H	−2.550962	1.377486	3.322789
H	−3.989715	0.728106	4.874078
H	−5.672929	0.256624	5.129063
H	−3.988011	3.806797	2.401920
H	0.400098	−0.923285	2.472441
H	−0.845789	1.972098	−0.768030
H	3.499613	1.926940	−0.514148
H	−2.207474	−0.885844	−1.250439
H	−0.577815	−0.283741	−2.958990
H	1.318885	−1.457654	−4.376482
H	0.619692	1.297559	−3.956449
H	3.681631	−0.872176	−4.596844
H	5.999076	−0.804052	−4.700691
H	6.676972	−1.020392	−3.079586
H	6.565455	−0.099793	−0.966336
H	5.792408	1.755548	0.637118

C	4.821642	0.087611	−3.125828
C	6.139258	−0.320159	−3.729921
C	5.437464	0.718326	0.666353
H	−0.513522	−2.347953	0.765753
H	−5.489581	−0.477409	1.481599
H	−4.751292	1.947582	1.290979
H	−2.335827	2.192927	1.774845
H	−5.241348	1.967971	5.010081
H	−6.770566	−1.171176	3.284207
H	−1.108293	−1.368329	3.274221
H	−0.614276	0.335119	3.197890
H	3.343562	2.379927	−2.204942
H	−2.362498	−2.633450	−1.225418
H	0.219027	−2.810432	−1.431182
H	1.944444	−2.082350	−2.849352
H	2.210249	2.072954	−4.037394
H	1.805293	0.771193	−5.161667
H	5.577214	1.743265	−2.030130
H	6.791306	0.551283	−3.866927
H	5.039526	−0.920376	−0.677361
H	6.060169	0.172370	1.382180
H	4.415026	0.722727	1.058638

Table S5. Cartesian coordinates and energies of the most stable conformer of **4b**.



4b (ΔG = 0.4 kcal/mol)

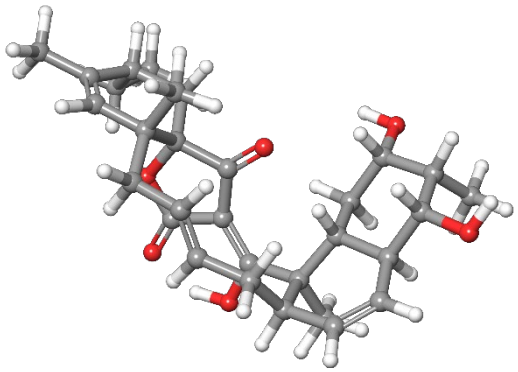
M06-2X/def2-TZVP-SMD(MeOH)//M06-2X/6-31G(d)-SMD(MeOH):			
Gibbs Free Energy (a.u.)	=	−1617.989748	
M06-2X/def2-TZVP-SMD(MeOH):			
Electronic energy (a.u.)	=	−1618.592155	
M06-2X/6-31G(d)-SMD(MeOH):			
Zero-point correction (a.u.)	=	0.663404	
Thermal correction to Energy (a.u.)	=	0.697073	
Thermal correction to Enthalpy (a.u.)	=	0.698017	
Thermal correction to Gibbs Free Energy (a.u.)	=	0.602407	

C	3.618438	−2.909456	−0.579758	C	3.596050	−2.596963	0.886760
C	2.246516	−2.007607	1.341583	C	1.744913	−0.909585	0.363405
C	1.574001	−1.515065	−1.078718	C	2.729540	−2.413072	−1.436418
C	3.919407	−3.832798	1.738119	C	4.018140	−3.495126	3.236562
C	2.724025	−2.801589	3.672159	C	2.405109	−1.579392	2.810437
H	1.506189	−2.821987	1.306460	H	4.389366	−1.859668	1.088091
C	5.268592	−2.681520	3.576455	O	5.138024	−4.385086	1.254332
O	2.861065	−2.450254	5.045375	C	2.738885	0.264248	0.324390
C	0.375484	−0.398696	0.810911	C	−0.358178	0.669337	0.118117
O	−0.219862	−0.956279	1.743585	C	−0.133183	1.376208	−1.147617
O	−1.298307	1.950198	−1.549630	C	−2.383160	1.661905	−0.649570
C	−1.691651	0.841546	0.399706	O	−2.367565	0.368997	1.407338
C	−2.894037	2.981673	−0.067781	O	0.855282	1.518871	−1.836063
C	0.236993	−2.284458	−1.351032	C	−0.766837	−1.451250	−2.103366
C	−2.006901	−1.178225	−1.698225	C	−2.919243	−0.192170	−2.376254
C	−3.499885	0.907016	−1.437439	C	−4.542970	0.261648	−0.504280

C	−4.225278	1.915965	−2.305660
C	−3.363629	3.958870	−1.152301
C	−2.242858	4.779816	−1.835195
H	4.416873	−3.553661	−0.940213
H	2.794035	−2.675314	−2.492315
H	4.082399	−4.448033	3.781395
H	3.219561	−0.852265	2.910908
H	5.263195	−1.689580	3.113726
H	6.165481	−3.203811	3.232878
H	2.022055	−2.053943	5.329490
H	2.368992	1.081147	−0.295383
H	−1.734714	−0.221670	1.908174
H	−2.106467	3.424195	0.549511
H	−0.195437	−2.653647	−0.411959
H	−2.362485	−1.633739	−0.770359
H	−3.789946	−0.705525	−2.807762
H	−4.154491	−0.614174	0.020779
H	−4.847764	1.463781	−3.079838
H	−5.641434	3.529251	−3.777741
H	−4.314530	4.701212	−3.791520
H	−2.723787	5.600685	−2.379436
H	−1.694869	5.890488	−0.041819

C	−4.198722	3.247720	−2.196414
C	−4.980385	4.122875	−3.139989
C	−1.211742	5.364777	−0.874187
H	1.602124	−0.670138	−1.775574
H	3.106877	−4.563318	1.595092
H	1.896101	−3.520285	3.561892
H	1.498088	−1.110394	3.197653
H	5.350434	−2.544297	4.657764
H	5.332275	−5.177042	1.781278
H	3.690265	−0.070811	−0.101061
H	2.929024	0.652284	1.329640
H	−3.727638	2.745672	0.601172
H	0.479290	−3.173280	−1.947303
H	−0.396145	−0.983866	−3.019317
H	−2.383595	0.282214	−3.205743
H	−4.919434	0.969573	0.239730
H	−5.393040	−0.060747	−1.114758
H	−4.013156	4.688077	−0.646375
H	−5.590130	4.846452	−2.585113
H	−1.737548	4.161791	−2.584728
H	−0.568568	6.082041	−1.393859
H	−0.563519	4.589250	−0.452792

Table S6. Cartesian coordinates and energies of the most stable conformer of **4c**.



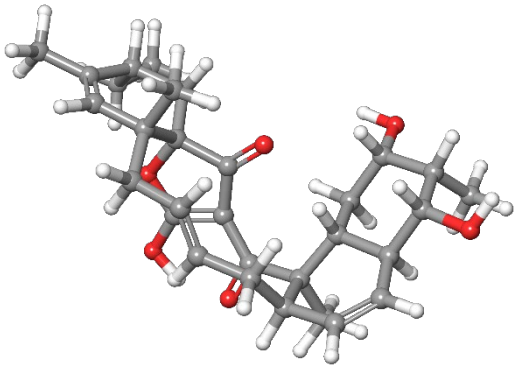
4c (ΔG = 3.5 kcal/mol)

M06-2X/def2-TZVP-SMD(MeOH)//M06-2X/6-31G(d)-SMD(MeOH):			
Gibbs Free Energy (a.u.)	=	−1617.984871	
M06-2X/def2-TZVP-SMD(MeOH):			
Electronic energy (a.u.)	=	−1618.586628	
M06-2X/6-31G(d)-SMD(MeOH):			
Zero-point correction (a.u.)	=	0.663069	
Thermal correction to Energy (a.u.)	=	0.696797	
Thermal correction to Enthalpy (a.u.)	=	0.697741	
Thermal correction to Gibbs Free Energy (a.u.)	=	0.601757	

C	1.860459	−3.459310	−2.831985	C	2.192833	−1.993084	−2.859413
C	1.197889	−1.132826	−2.052228	C	−0.251763	−1.602591	−2.299214
C	−0.397974	−3.086560	−1.796580	C	0.682014	−3.934794	−2.429161
C	3.612081	−1.676168	−2.374454	C	3.961273	−0.191477	−2.601203
C	2.903567	0.685037	−1.919253	C	1.480742	0.340058	−2.363188
H	1.415731	−1.295168	−0.991161	H	2.161243	−1.680349	−3.914794
C	4.147735	0.154664	−4.080021	O	4.512152	−2.530782	−3.068664
O	3.221913	2.045455	−2.197232	C	−0.570394	−1.573346	−3.814119
C	−1.344627	−0.781702	−1.620529	C	−1.334381	0.041244	−0.494802
O	−2.502099	−0.999269	−2.203615	C	−2.617691	0.454941	0.056409
O	−2.496049	0.957098	1.285166	C	−1.117345	0.929387	1.731912
C	−0.347569	0.355626	0.533365	O	0.868793	0.270088	0.544045
C	−0.695930	2.371282	2.000210	O	−3.731874	0.363810	−0.458461
C	−0.295529	−3.391619	−0.274381	C	−1.229319	−2.685563	0.669919
C	−0.820582	−2.195345	1.841232	C	−1.643751	−1.358336	2.779778
C	−1.054727	0.061423	3.016344	C	0.384052	−0.061543	3.556985

C	−1.876495	0.775743	4.069110
C	−1.571302	3.060906	3.068040
C	−2.699898	3.912004	2.446892
H	2.611150	−4.140192	−3.226940
H	0.488758	−5.006254	−2.460316
H	4.918040	−0.003764	−2.092933
H	1.373687	0.533681	−3.438007
H	3.214072	0.091985	−4.647964
H	4.867138	−0.526239	−4.542819
H	2.599991	2.595456	−1.694684
H	−1.522805	−2.061216	−4.026022
H	−3.234325	−0.509748	−1.722967
H	−0.745179	2.919170	1.052934
H	0.735084	−3.218691	0.057057
H	0.222227	−2.350860	2.121294
H	−1.692504	−1.838057	3.766809
H	1.077931	−0.486199	2.829223
H	−2.256280	0.143831	4.873184
H	−3.013864	1.981457	6.063707
H	−3.902115	2.996720	4.921281
H	−3.336836	4.291939	3.252575
H	−1.556937	5.749962	2.267190
C	−2.106078	2.091865	4.110946
C	−2.898741	2.695141	5.243048
C	−2.190515	5.107404	1.644890
H	−1.381654	−3.435593	−2.136929
H	3.665526	−1.890851	−1.295217
H	2.965445	0.510769	−0.835070
H	0.781958	1.002806	−1.841389
H	4.531124	1.173008	−4.184646
H	5.409371	−2.331953	−2.755270
H	0.201758	−2.095590	−4.377998
H	−0.627951	−0.542631	−4.178704
H	0.356037	2.356798	2.297764
H	−0.457608	−4.476815	−0.198116
H	−2.268453	−2.554477	0.356545
H	−2.673820	−1.276961	2.412699
H	0.769758	0.911027	3.873369
H	0.368726	−0.711604	4.439169
H	−0.924534	3.766509	3.612048
H	−2.404578	3.593578	5.632692
H	−3.333373	3.274692	1.818785
H	−3.027840	5.713157	1.283832
H	−1.604970	4.807807	0.770002

Table S7. Cartesian coordinates and energies of the most stable conformer of **4d**.



4d (ΔG = 6.6 kcal/mol)

M06-2X/def2-TZVP-SMD(MeOH)//M06-2X/6-31G(d)-SMD(MeOH):		
Gibbs Free Energy (a.u.)	=	−1617.979974
M06-2X/def2-TZVP-SMD(MeOH):		
Electronic energy (a.u.)	=	−1618.580947
M06-2X/6-31G(d)-SMD(MeOH):		
Zero-point correction (a.u.)	=	0.662219
Thermal correction to Energy (a.u.)	=	0.695993
Thermal correction to Enthalpy (a.u.)	=	0.696937
Thermal correction to Gibbs Free Energy (a.u.)	=	0.600973

C	4.798129	0.356612	−0.661757	C	3.865655	−0.611239	−1.337749
C	2.478207	−0.672378	−0.665771	C	2.621313	−0.693659	0.870177
C	3.296870	0.647454	1.332342	C	4.576705	0.857650	0.553923
C	3.674606	−0.330715	−2.832130	C	2.852422	−1.444172	−3.511003
C	1.516062	−1.602040	−2.775862	C	1.697146	−1.840457	−1.275720
H	1.948008	0.249241	−0.931338	H	4.335913	−1.605337	−1.274884
C	3.620670	−2.762442	−3.625970	O	4.962624	−0.206470	−3.423002
O	0.804306	−2.670629	−3.393564	C	3.534305	−1.859581	1.311313
C	1.320249	−0.869455	1.671112	C	−0.037871	−0.515583	1.282252
O	1.468333	−1.303555	2.834544	C	−1.001361	−0.508034	2.302151
O	−2.154086	0.042689	2.009603	C	−2.081994	0.579029	0.653163
C	−0.683430	0.158578	0.171270	O	−0.316574	0.384584	−0.973036
C	−3.177513	−0.099993	−0.157614	O	−0.880587	−0.951894	3.507228
C	2.526872	1.990994	1.182403	C	1.173362	2.120588	1.823974
C	0.151547	2.728125	1.218604	C	−1.265044	2.772635	1.720726
C	−2.290452	2.111794	0.754683	C	−2.204751	2.786596	−0.629176

C	−3.693033	2.329702	1.282666
C	−4.589757	0.146532	0.414789
C	−5.076852	−1.025825	1.293403
H	5.721491	0.596044	−1.184682
H	5.303092	1.534682	1.001980
H	2.625469	−1.101816	−4.531012
H	2.229221	−2.786784	−1.115883
H	3.807702	−3.226634	−2.652466
H	4.587486	−2.598744	−4.109578
H	−0.071990	−2.711056	−2.978506
H	4.498901	−1.813103	0.805816
H	0.094087	−1.261776	3.549185
H	−2.957884	−1.172475	−0.189347
H	2.433893	2.234842	0.117487
H	0.331531	3.174889	0.239878
H	−1.588853	3.815716	1.838684
H	−1.255279	2.601946	−1.134733
H	−3.864129	3.288546	1.773680
H	−6.142328	2.894263	1.917785
H	−6.338219	1.256490	2.553936
H	−6.032211	−0.749527	1.751485
H	−5.994464	−2.174091	−0.305060
C	−4.714940	1.480821	1.134440
C	−6.084489	1.833650	1.657514
C	−5.283535	−2.323622	0.515721
H	3.532826	0.523239	2.397973
H	3.132288	0.622443	−2.938194
H	0.948354	−0.667932	−2.898276
H	0.706718	−1.942932	−0.817550
H	3.057212	−3.477479	−4.231171
H	4.837256	−0.014227	−4.366424
H	3.068909	−2.824437	1.084137
H	3.717337	−1.820720	2.385965
H	−3.093032	0.265730	−1.184575
H	3.202828	2.748388	1.605874
H	1.030825	1.666621	2.808126
H	−1.331710	2.305737	2.711026
H	−3.014094	2.448215	−1.281310
H	−2.320806	3.867898	−0.494541
H	−5.283593	0.195608	−0.438423
H	−6.857140	1.618341	0.909306
H	−4.367923	−1.183707	2.114935
H	−5.687249	−3.103498	1.169287
H	−4.353556	−2.708892	0.085761