

Supporting Information 1

Iodinated Meroditerpenes from a Red Alga *Callophycus* sp.

Serge Lavoie,^{†,‡} David Brumley,[†] Troy S. Alexander,[†] Christine Jasmin,^{†,‡} Franz A. Carranza,[‡]
Kate Nelson,[§] Cassandra L. Quave,^{§,¶,◇} and Julia Kubanek^{†,‡,*}

[†]School of Chemistry and Biochemistry and [‡]School of Biological Sciences, Aquatic Chemical Ecology Center, Institute for Bioengineering and Biosciences, Georgia Institute of Technology, Atlanta, Georgia 30332.

[§]Department of Dermatology, [¶]Center for the Study of Human Health, and [◇]Antibiotic Resistance Center, Emory University, Atlanta, Georgia 30322

*julia.kubanek@biosci.gatech.edu

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OTHER KNOWN IODINATED STRUCTURES

Refer to main article for references in [].

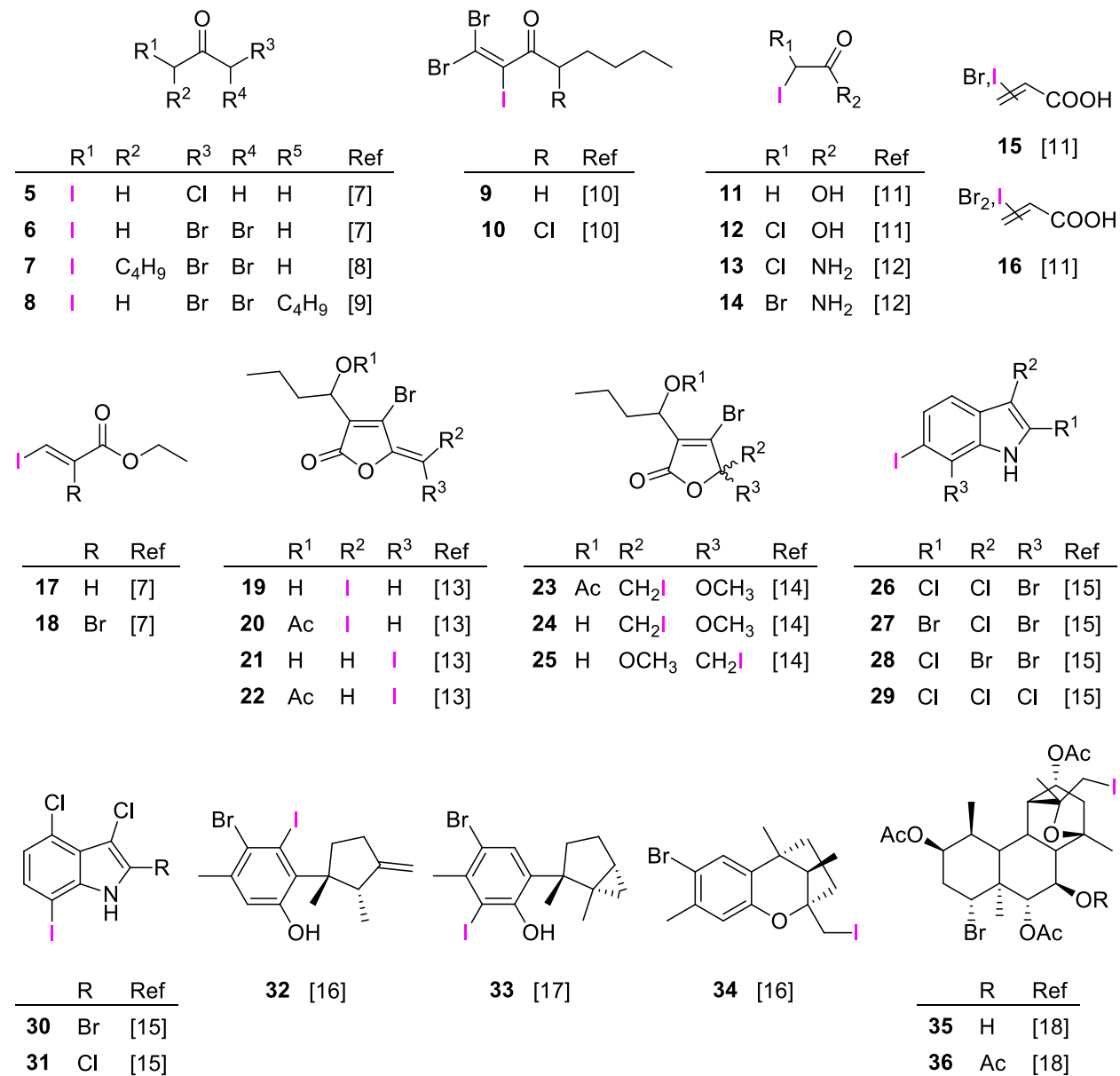


Figure S1. Iodinated natural products identified from members of the phylum Rhodophyta.

CHARACTERIZATION OF IODOCALLOPHYCOIC ACID A (1)

DFT Calculation in methanol

Table S1. Atomic coordinates for iodocallophycoic acid A (1), obtained through DFT calculations at the B3LYP/SVP level of theory in methanol.

Atom	2S,6S,7S,10S,14S-1a			2S,6S,7S,10S,14S-1b		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	2.8762	−2.6731	1.0968	2.8751	−2.6793	1.0943
C	2.9846	−1.4091	0.2871	2.9834	−1.4186	0.2793
C	1.6214	−0.7792	−0.0153	1.6205	−0.7875	−0.0214
C	0.7307	−1.7959	−0.8665	0.7256	−1.8057	−0.8662
C	0.6813	−3.1049	−0.0282	0.6759	−3.1113	−0.0225
C	2.0308	−3.7087	0.3351	2.0253	−3.7163	0.3394
H	2.3875	−2.4434	2.0603	2.3900	−2.4449	2.0584
H	3.8650	−3.0934	1.3250	3.8639	−3.1006	1.3210
Br	−0.4304	−4.5433	−0.8970	−0.4411	−4.5509	−0.8822
H	0.1183	−2.9180	0.8939	0.1159	−2.9194	0.9005
H	2.5662	−4.0328	−0.5707	2.5574	−4.0452	−0.5666
H	1.8797	−4.6009	0.9606	1.8742	−4.6056	0.9690
C	4.1300	−0.9055	−0.1899	4.1282	−0.9186	−0.2028
H	4.1888	−0.0154	−0.8099	4.1865	−0.0308	−0.8262
I	6.0818	−1.6989	0.1256	6.0797	−1.7141	0.1097
C	1.6719	0.6452	−0.6234	1.6718	0.6347	−0.6345
H	1.1213	−0.6879	0.9624	1.1233	−0.6920	0.9575
C	3.1448	3.8392	1.9409	3.1597	3.8344	1.9203
C	1.9799	3.1577	2.2740	1.9930	3.1542	2.2555
C	1.5056	2.1253	1.4498	1.5135	2.1218	1.4353
C	2.2047	1.7418	0.2809	2.2089	1.7328	0.2652
C	3.3598	2.4602	−0.0376	3.3633	2.4487	−0.0549
C	3.8455	3.5010	0.7735	3.8547	3.4905	0.7507
H	1.4187	3.4258	3.1735	1.4348	3.4255	3.1559
O	0.3527	1.4690	1.7326	0.3591	1.4698	1.7220
H	3.9027	2.2155	−0.9518	3.9145	2.2102	−0.9670
C	1.3696	−2.0247	−2.2497	1.3605	−2.0414	−2.2502
C	5.0763	4.2590	0.4356	5.0920	4.1903	0.3236
O	5.5374	5.1623	1.1044	5.7174	3.9359	−0.6867
O	5.6566	3.8488	−0.7083	5.4738	5.1608	1.1750
H	6.4482	4.3975	−0.8467	6.2845	5.5615	0.8156
H	0.6500	0.9263	−0.9125	0.6497	0.9168	−0.9216
H	2.2540	0.6447	−1.5562	2.2515	0.6304	−1.5687
H	3.5194	4.6440	2.5756	3.5271	4.6369	2.5607
H	−0.0533	1.8209	2.5392	−0.0447	1.8251	2.5281
H	0.8134	−2.7896	−2.8109	0.8008	−2.8068	−2.8072

Atom	2S,6S,7S,10S,14S-1a			2S,6S,7S,10S,14S-1b		
	x	y	z	x	y	z
H	2.4187	-2.3454	-2.1828	2.4088	-2.3648	-2.1847
H	1.3439	-1.0984	-2.8430	1.3359	-1.1172	-2.8468
C	-0.7107	-1.2573	-1.1054	-0.7153	-1.2652	-1.1036
C	-1.6221	-1.0278	0.1122	-1.6225	-1.0273	0.1156
C	-3.0574	-0.6370	-0.3005	-3.0585	-0.6368	-0.2948
C	-3.2291	0.7871	-0.8328	-3.2295	0.7837	-0.8371
C	-4.5508	0.9867	-1.5239	-4.5532	0.9804	-1.5252
C	-5.6994	0.6898	-0.5421	-5.6986	0.6936	-0.5367
C	-5.5271	-0.6858	0.0909	-5.5269	-0.6777	0.1058
C	-4.1669	-0.9394	0.8014	-4.1646	-0.9289	0.8132
H	-0.6450	-0.3368	-1.7033	-0.6492	-0.3479	-1.7064
H	-1.2085	-1.9870	-1.7637	-1.2167	-1.9971	-1.7566
H	-1.1922	-0.2805	0.7948	-1.1892	-0.2766	0.7923
H	-1.6822	-1.9613	0.6849	-1.6821	-1.9572	0.6940
H	-3.3213	-1.2971	-1.1480	-3.3267	-1.3026	-1.1365
C	-2.3200	1.7451	-0.6108	-2.3180	1.7417	-0.6251
H	-4.6171	0.2960	-2.3832	-4.6240	0.2829	-2.3787
H	-4.6550	2.0074	-1.9168	-4.6567	1.9981	-1.9257
H	-6.6635	0.7350	-1.0701	-6.6647	0.7370	-1.0613
H	-5.7233	1.4651	0.2398	-5.7176	1.4748	0.2394
H	-5.6711	-1.4661	-0.6693	-5.6754	-1.4633	-0.6479
Br	-7.1101	-0.9965	1.3001	-7.1061	-0.9762	1.3229
C	-4.0964	-2.4210	1.2193	-4.0954	-2.4075	1.2417
C	-3.9714	-0.0457	2.0376	-3.9626	-0.0266	2.0422
I	-2.4608	3.7738	-1.2483	-2.4569	3.7654	-1.2785
H	-1.4016	1.5907	-0.0464	-1.3982	1.5899	-0.0623
H	-4.9755	-2.6875	1.8229	-4.9725	-2.6677	1.8510
H	-3.2077	-2.6296	1.8309	-3.2046	-2.6135	1.8511
H	-4.0712	-3.0868	0.3413	-4.0753	-3.0799	0.3685
H	-2.9780	-0.2172	2.4797	-2.9678	-0.1967	2.4814
H	-4.7229	-0.2782	2.8064	-4.7113	-0.2523	2.8158
H	-4.0475	1.0253	1.7999	-4.0378	1.0427	1.7972

Table S2. Atomic coordinates for iodocallophycoic acid A (**1**), obtained through DFT calculation at the B3LYP/SVP level of theory in methanol (..contd).

Atom	2S,6S,7S,10S,14S-1c			2S,6S,7S,10S,14S-1d		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	3.4662	-2.0694	1.0249	3.4565	-2.0795	1.0035
C	3.3804	-0.8317	0.1719	3.3750	-0.8334	0.1625
C	1.9382	-0.4342	-0.1545	1.9339	-0.4245	-0.1536
C	1.1961	-1.6050	-0.9373	1.1857	-1.5822	-0.9499
C	1.3373	-2.8657	-0.0364	1.3206	-2.8534	-0.0626
C	2.7631	-3.2503	0.3346	2.7447	-3.2496	0.3035
H	2.9705	-1.8690	1.9919	2.9649	-1.8857	1.9739
H	4.5092	-2.3331	1.2462	4.4986	-2.3515	1.2190
Br	0.4437	-4.4938	-0.8168	0.4183	-4.4683	-0.8602
H	0.7569	-2.7181	0.8825	0.7411	-2.7129	0.8579
H	3.3263	-3.5478	-0.5632	3.3049	-3.5425	-0.5976
H	2.7468	-4.1194	1.0086	2.7238	-4.1247	0.9696
C	4.4317	-0.1463	-0.2960	4.4282	-0.1514	-0.3062
H	4.3575	0.7414	-0.9214	4.3559	0.7410	-0.9251
I	6.4822	-0.6038	0.0686	6.4774	-0.6250	0.0434
C	1.7818	0.9462	-0.8319	1.7809	0.9656	-0.8114
H	1.4352	-0.3719	0.8264	1.4337	-0.3738	0.8294
C	2.5703	4.3916	1.7121	2.6512	4.3713	1.7535
C	3.2854	4.2193	0.5316	3.3402	4.2092	0.5578
C	3.0445	3.1068	-0.2922	3.0716	3.1075	-0.2726
C	2.0809	2.1346	0.0654	2.1072	2.1406	0.0945
C	1.3747	2.3386	1.2518	1.4257	2.3344	1.2988
C	1.5994	3.4472	2.0835	1.6801	3.4325	2.1369
H	4.0401	4.9521	0.2331	4.0950	4.9387	0.2516
O	3.7235	2.9238	-1.4507	3.7256	2.9309	-1.4465
H	0.6097	1.6233	1.5600	0.6641	1.6151	1.6032
C	1.8450	-1.8158	-2.3176	1.8338	-1.7811	-2.3323
C	0.7879	3.5770	3.3193	0.9491	3.6380	3.4118
O	-0.0742	2.7934	3.6674	1.1316	4.5673	4.1725
O	1.0944	4.6691	4.0435	0.0366	2.6781	3.6635
H	0.5161	4.6731	4.8262	-0.3897	2.8955	4.5107
H	0.7431	1.0492	-1.1754	0.7379	1.0827	-1.1370
H	2.3960	1.0051	-1.7384	2.3815	1.0295	-1.7266
H	2.7609	5.2597	2.3441	2.8539	5.2263	2.4007
H	4.3730	3.6313	-1.5788	4.3781	3.6346	-1.5801
H	1.3714	-2.6568	-2.8448	1.3539	-2.6117	-2.8702
H	2.9225	-2.0212	-2.2466	2.9096	-1.9957	-2.2635
H	1.7197	-0.9204	-2.9442	1.7158	-0.8769	-2.9476
C	-0.3097	-1.2732	-1.1619	-0.3180	-1.2400	-1.1717
C	-1.1452	-0.8914	0.0727	-1.1531	-0.8674	0.0661
C	-2.6673	-0.9823	-0.1578	-2.6752	-0.9615	-0.1639
C	-3.2595	0.0515	-1.1175	-3.2712	0.0803	-1.1127

Atom	2S,6S,7S,10S,14S-1c			2S,6S,7S,10S,14S-1d		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	-4.6656	-0.2876	-1.5331	-4.6778	-0.2568	-1.5286
C	-5.5722	-0.3883	-0.2931	-5.5818	-0.3726	-0.2881
C	-4.9771	-1.3475	0.7303	-4.9832	-1.3420	0.7232
C	-3.5241	-1.0302	1.1852	-3.5301	-1.0267	1.1794
H	-0.3817	-0.4885	-1.9283	-0.3849	-0.4466	-1.9296
H	-0.7611	-2.1648	-1.6245	-0.7734	-2.1241	-1.6444
H	-0.8759	0.1122	0.4361	-0.8866	0.1354	0.4342
H	-0.8941	-1.5758	0.8923	-0.8993	-1.5550	0.8821
H	-2.8435	-1.9617	-0.6411	-2.8484	-1.9363	-0.6573
C	-2.5989	1.1613	-1.4717	-2.6121	1.1932	-1.4596
H	-4.6579	-1.2598	-2.0571	-4.6695	-1.2233	-2.0631
H	-5.0725	0.4559	-2.2319	-5.0873	0.4934	-2.2186
H	-6.5720	-0.7381	-0.5898	-6.5816	-0.7207	-0.5869
H	-5.6991	0.6102	0.1537	-5.7096	0.6207	0.1701
H	-5.0021	-2.3734	0.3376	-5.0066	-2.3634	0.3190
Br	-6.2723	-1.4688	2.2697	-6.2753	-1.4837	2.2636
C	-3.0228	-2.1779	2.0828	-3.0248	-2.1834	2.0631
C	-3.4267	0.3015	1.9494	-3.4338	0.2966	1.9580
I	-3.3225	2.6985	-2.7549	-3.3387	2.7394	-2.7299
H	-1.5970	1.4042	-1.1235	-1.6092	1.4335	-1.1121
H	-3.7207	-2.3397	2.9164	-3.7207	-2.3558	2.8962
H	-2.0411	-1.9522	2.5219	-2.0425	-1.9610	2.5026
H	-2.9390	-3.1224	1.5208	-2.9403	-3.1213	1.4903
H	-2.3835	0.5146	2.2278	-2.3903	0.5066	2.2377
H	-4.0139	0.2559	2.8783	-4.0207	0.2407	2.8866
H	-3.7906	1.1541	1.3580	-3.7981	1.1555	1.3759

Table S3. Atomic coordinates for iodocallophycoic acid A (**1**), obtained through DFT calculations at the B3LYP/SVP level of theory in methanol (..contd).

Atom	2S,6S,7S,10R,14R-1a			2S,6S,7S,10R,14R-1b		
	x	y	z	x	y	z
C	-3.1669	-1.7128	-1.6126	-3.1794	-1.6936	-1.6166
C	-3.3122	-0.9841	-0.3032	-3.3202	-0.9657	-0.3063
C	-1.9908	-0.3951	0.1983	-1.9956	-0.3834	0.1947
C	-0.9193	-1.5547	0.4243	-0.9304	-1.5493	0.4195
C	-0.8200	-2.2911	-0.9404	-0.8350	-2.2842	-0.9463
C	-2.1305	-2.8425	-1.4859	-2.1483	-2.8285	-1.4921
H	-2.8299	-0.9967	-2.3836	-2.8396	-0.9783	-2.3872
H	-4.1265	-2.1255	-1.9519	-4.1412	-2.1013	-1.9556
Br	0.5200	-3.7952	-0.9202	0.4983	-3.7942	-0.9286
H	-0.3793	-1.6142	-1.6822	-0.3914	-1.6082	-1.6873
H	-2.5191	-3.6329	-0.8255	-2.5405	-3.6179	-0.8326
H	-1.9559	-3.3006	-2.4707	-1.9764	-3.2860	-2.4776
C	-4.4498	-0.8786	0.3959	-4.4565	-0.8566	0.3943
H	-4.5367	-0.3678	1.3531	-4.5401	-0.3472	1.3526
I	-6.3449	-1.6647	-0.1819	-6.3556	-1.6335	-0.1827
C	-2.1203	0.5698	1.3991	-2.1184	0.5817	1.3960
H	-1.6095	0.1995	-0.6502	-1.6118	0.2092	-0.6542
C	-4.1739	4.3252	0.5918	-4.1650	4.3407	0.6072
C	-4.6361	3.4801	1.5951	-4.6285	3.4952	1.6075
C	-3.9855	2.2627	1.8574	-3.9786	2.2756	1.8633
C	-2.8566	1.8653	1.1030	-2.8527	1.8798	1.1048
C	-2.4119	2.7379	0.1089	-2.4054	2.7545	0.1114
C	-3.0478	3.9600	-0.1636	-3.0414	3.9790	-0.1529
H	-5.5104	3.7583	2.1901	-5.5012	3.7725	2.2052
O	-4.4162	1.4263	2.8333	-4.4085	1.4364	2.8372
H	-1.5341	2.4812	-0.487	-1.5285	2.4863	-0.4789
C	-1.3876	-2.4937	1.5516	-1.4040	-2.4872	1.5453
C	-2.4916	4.8197	-1.2375	-2.5602	4.9092	-1.2041
O	-1.5109	4.5492	-1.9033	-3.0743	5.9769	-1.4716
O	-3.1841	5.9597	-1.4183	-1.4708	4.4584	-1.8575
H	-2.7491	6.455	-2.1341	-1.2291	5.1295	-2.5192
H	-1.1096	0.8433	1.7334	-1.1058	0.8521	1.7267
H	-2.5915	0.0651	2.2514	-2.5877	0.0776	2.2498
H	-4.6830	5.2696	0.3964	-4.6642	5.2901	0.4060
H	-5.2044	1.7870	3.2660	-5.1949	1.7973	3.2730
H	-0.6962	-3.3421	1.6598	-0.7182	-3.3403	1.6513
H	-2.3954	-2.8949	1.3748	-2.4146	-2.8814	1.3687
H	-1.4084	-1.9599	2.5135	-1.4205	-1.9552	2.5083
C	0.4702	-0.9841	0.8351	0.4621	-0.9871	0.8313
C	1.1727	-0.0309	-0.1463	1.1706	-0.0390	-0.1508
C	2.4428	0.6225	0.4367	2.4396	0.6146	0.4339
C	3.6241	-0.3219	0.6762	3.6191	-0.3303	0.6794

Atom	2S,6S,7S,10R,14R-1a			2S,6S,7S,10R,14R-1b		
	x	y	z	x	y	z
C	4.7089	0.3084	1.5076	4.7031	0.3017	1.5106
C	5.2297	1.5831	0.8208	5.2263	1.5741	0.8212
C	4.0755	2.5220	0.4949	4.0737	2.5131	0.4902
C	2.9332	1.9108	-0.3652	2.9330	1.9001	-0.3708
H	0.3584	-0.474	1.8043	0.3526	-0.4757	1.8000
H	1.1207	-1.8451	1.0448	1.1074	-1.8517	1.0421
H	0.4781	0.7728	-0.4221	0.4785	0.7648	-0.4323
H	1.4152	-0.5489	-1.0875	1.4155	-0.5612	-1.0889
H	2.1648	1.0023	1.4380	2.1594	0.9978	1.4334
C	3.6826	-1.5439	0.1316	3.6764	-1.5550	0.1406
H	5.5413	-0.3867	1.6819	5.5347	-0.3936	1.6882
H	4.2921	0.5731	2.4958	4.2850	0.5695	2.4973
H	5.7685	1.3121	-0.1005	5.7669	1.3001	-0.0982
H	5.9490	2.0945	1.4774	5.9447	2.0867	1.4779
H	3.6400	2.9132	1.4248	3.6364	2.9072	1.4180
Br	4.8631	4.1883	-0.3214	4.8641	4.1765	-0.3292
C	3.4031	1.5308	-1.7797	3.4063	1.5152	-1.7828
C	1.7850	2.9339	-0.4608	1.7856	2.9235	-0.4728
I	5.2865	-2.9320	0.3339	5.2778	-2.9446	0.3521
H	2.8942	-1.9747	-0.4837	2.8884	-1.9873	-0.4742
H	2.5717	1.0997	-2.3574	2.5762	1.0822	-2.3611
H	4.2171	0.7917	-1.7689	4.2201	0.7759	-1.7676
H	3.7560	2.4209	-2.3210	3.7608	2.4033	-2.3263
H	2.1602	3.8929	-0.8447	2.1624	3.8810	-0.8589
H	1.3277	3.1203	0.5248	1.3255	3.1136	0.5109
H	0.9951	2.6018	-1.1481	0.9976	2.5887	-1.1609

Table S4. Atomic coordinates for iodocallophycoic acid A (**1**), obtained through DFT calculations at the B3LYP/SVP level of theory in methanol (..contd).

Atom	2S,6S,7S,10R,14R-1c			2S,6S,7S,10R,14R-1d		
	x	y	z	x	y	z
C	-2.7542	-2.1670	-1.6111	-2.7466	-2.1798	-1.6091
C	-3.0311	-1.2049	-0.4871	-3.0253	-1.2213	-0.4824
C	-1.7849	-0.4184	-0.0783	-1.7815	-0.4308	-0.0738
C	-0.6799	-1.4227	0.4831	-0.6713	-1.4321	0.4827
C	-0.4204	-2.4129	-0.6874	-0.4100	-2.4181	-0.6908
C	-1.6480	-3.1562	-1.2027	-1.6356	-3.1654	-1.2052
H	-2.4221	-1.5944	-2.4955	-2.4186	-1.6039	-2.4928
H	-3.6561	-2.7219	-1.9033	-3.6469	-2.7378	-1.9006
Br	0.9788	-3.7958	-0.2515	0.9964	-3.7958	-0.2614
H	0.0525	-1.8718	-1.5164	0.0586	-1.8729	-1.5196
H	-2.0311	-3.8378	-0.4277	-2.0142	-3.8503	-0.4308
H	-1.3653	-3.7770	-2.0657	-1.3522	-3.7831	-2.0702
C	-4.2042	-1.0712	0.1438	-4.1978	-1.0933	0.1507
H	-4.3704	-0.3892	0.9739	-4.3652	-0.4137	0.9826
I	-5.9987	-2.1285	-0.3039	-5.9892	-2.1560	-0.2968
C	-2.0250	0.8078	0.8342	-2.0245	0.7913	0.8433
H	-1.3788	-0.0235	-1.0221	-1.3791	-0.0313	-1.0173
C	-4.5933	3.9943	-0.6521	-4.6156	3.9750	-0.6202
C	-3.4745	3.6103	-1.3816	-3.4970	3.5959	-1.3554
C	-2.6421	2.5798	-0.9151	-2.6578	2.5676	-0.8979
C	-2.9323	1.8983	0.2911	-2.9387	1.8794	0.3074
C	-4.0551	2.3188	1.0093	-4.0592	2.2939	1.0295
C	-4.8934	3.3540	0.5594	-4.9049	3.3269	0.5903
H	-3.2270	4.1125	-2.3211	-3.2565	4.1025	-2.2943
O	-1.5316	2.2118	-1.6004	-1.5491	2.2071	-1.5900
H	-4.2894	1.8300	1.9567	-4.2994	1.8077	1.9779
C	-1.1950	-2.1473	1.7412	-1.1811	-2.1620	1.7399
C	-6.0878	3.7962	1.3212	-6.0721	3.6918	1.4312
O	-6.8434	4.6801	0.9691	-6.3559	3.1642	2.4884
O	-6.2699	3.1162	2.4694	-6.8125	4.6876	0.9083
H	-7.0696	3.4718	2.8946	-7.5482	4.8568	1.5223
H	-1.0473	1.2701	1.0356	-1.0484	1.2576	1.0429
H	-2.4138	0.4914	1.8134	-2.4089	0.4700	1.8227
H	-5.2421	4.7958	-1.0091	-5.2608	4.7762	-0.9821
H	-1.4382	2.7425	-2.4055	-1.4613	2.7421	-2.3929
H	-0.4380	-2.8503	2.1182	-0.4210	-2.8636	2.1129
H	-2.1208	-2.7101	1.5589	-2.1056	-2.7271	1.5582
H	-1.4012	-1.4245	2.5449	-1.3877	-1.4422	2.5462
C	0.6284	-0.6807	0.8834	0.6347	-0.6858	0.8824
C	1.3348	0.1822	-0.1750	1.3363	0.1810	-0.1760
C	2.5764	0.9122	0.3857	2.5745	0.9174	0.3838
C	3.7970	0.0229	0.6505	3.7986	0.0338	0.6511

Atom	2S,6S,7S,10R,14R-1c			2S,6S,7S,10R,14R-1d		
	x	y	z	x	y	z
C	4.8759	0.7256	1.4297	4.8740	0.7425	1.4297
C	5.3457	1.9772	0.6703	5.3391	1.9945	0.6681
C	4.1548	2.8686	0.3500	4.1448	2.8802	0.3447
C	3.0022	2.2004	-0.4517	2.9954	2.2054	-0.4564
H	0.4028	-0.0458	1.7550	0.4078	-0.0528	1.7551
H	1.3256	-1.4430	1.2609	1.3351	-1.4460	1.2582
H	0.6296	0.9333	-0.5516	0.6271	0.9288	-0.5517
H	1.6190	-0.4216	-1.0510	1.6231	-0.4212	-1.0523
H	2.2862	1.3061	1.3784	2.2822	1.3123	1.3755
C	3.8892	-1.2271	0.1790	3.8964	-1.2166	0.1818
H	5.7307	0.0636	1.6222	5.7314	0.0844	1.6242
H	4.4691	1.0281	2.4113	4.4652	1.0453	2.4104
H	5.8589	1.6780	-0.2570	5.8544	1.6954	-0.2582
H	6.0734	2.5347	1.2784	6.0639	2.5564	1.2756
H	3.7380	3.2760	1.2814	3.7255	3.2882	1.2748
Br	4.8632	4.5327	-0.5417	4.8472	4.5450	-0.5504
C	3.4258	1.8025	-1.8755	3.4220	1.8061	-1.8789
C	1.8232	3.1909	-0.5143	1.8124	3.1908	-0.5222
I	5.5377	-2.5512	0.4457	5.5502	-2.5333	0.4523
H	3.1076	-1.7257	-0.3907	3.1175	-1.7194	-0.3879
H	2.5800	1.3477	-2.4126	2.5787	1.3460	-2.4156
H	4.2509	1.0750	-1.8796	4.2505	1.0825	-1.8808
H	3.7458	2.6861	-2.4470	3.7381	2.6899	-2.4522
H	2.1440	4.1343	-0.9784	2.1300	4.1347	-0.9877
H	1.4460	3.4235	0.4955	1.4330	3.4238	0.4866
H	0.9835	2.8032	-1.1048	0.9752	2.7986	-1.1132

Table S5. Electronic energies (ΔE), free energies (ΔG), and Boltzmann distribution abundances for the conformers of iodocallophycoic acid A (**1**), obtained through DFT calculations at the B3LYP/SVP level of theory in methanol.

Conformers	Energies (Hartree)		Abundance (%)
	ΔE	ΔG	
2S,6S,7S,10S,14S-1a	-20261.620063	-20261.136105	11.34
2S,6S,7S,10S,14S-1a	-20261.620170	-20261.136008	10.24
2S,6S,7S,10S,14S-1c*	-20261.619932	-20261.137026	30.09
2S,6S,7S,10S,14S-1d	-20261.619771	-20261.136418	15.80
2S,6S,7S,10S,14S-1e	-20261.616524	-20261.133727	0.91
2S,6S,7S,10S,14S-1f	-20261.616361	-20261.133216	0.53
2S,6S,7S,10S,14S-1g	-20261.616496	-20261.132425	0.23
2S,6S,7S,10S,14S-1h	-20261.616371	-20261.132302	0.20
2S,6S,7S,10S,14S-1i	-20261.615654	-20261.132552	0.26
2S,6S,7S,10S,14S-1j	-20261.615757	-20261.132515	0.25
2S,6S,7S,10S,14S-1k*	-20261.619932	-20261.137026	30.09
2S,6S,7S,10S,14S-1l	-20261.613218	-20261.129865	0.02
2S,6S,7S,10S,14S-1m	-20261.613125	-20261.129444	0.01
2S,6S,7S,10S,14S-1n	-20261.612460	-20261.130213	0.02
2S,6S,7S,10R,14R-1a	-20261.620885	-20261.135784	18.63
2S,6S,7S,10R,14R-1b	-20261.620771	-20261.136651	46.66
2S,6S,7S,10R,14R-1c	-20261.620185	-20261.135421	12.68
2S,6S,7S,10R,14R-1d	-20261.620291	-20261.135535	14.31
2S,6S,7S,10R,14R-1e	-20261.615249	-20261.129950	0.04
2S,6S,7S,10R,14R-1f	-20261.617524	-20261.133842	2.38
2S,6S,7S,10R,14R-1g	-20261.617386	-20261.134323	3.96
2S,6S,7S,10R,14R-1h	-20261.615361	-20261.128153	0.01
2S,6S,7S,10R,14R-1i	-20261.615268	-20261.128116	0.01
2S,6S,7S,10R,14R-1j	-20261.614187	-20261.129645	0.03
2S,6S,7S,10R,14R-1k	-20261.615766	-20261.131476	0.19
2S,6S,7S,10R,14R-1l	-20261.614066	-20261.129824	0.03
2S,6S,7S,10R,14R-1m	-20261.615853	-20261.131924	0.31
2S,6S,7S,10R,14R-1n	-20261.615252	-20261.131964	0.33
2S,6S,7S,10R,14R-1o	-20261.615318	-20261.132224	0.43

*Convergent conformers.

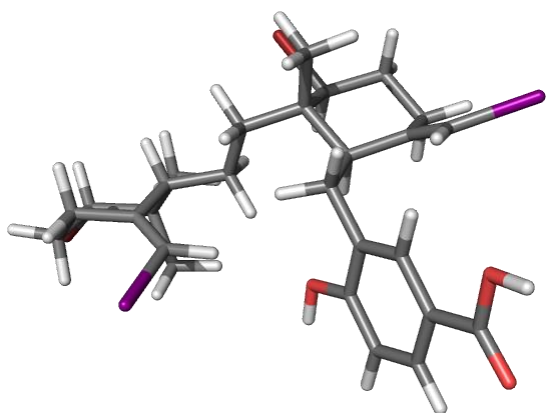
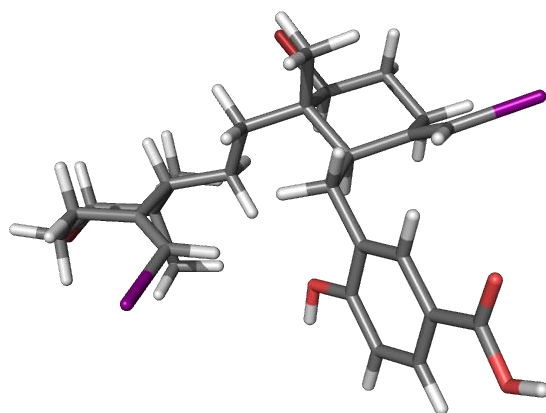
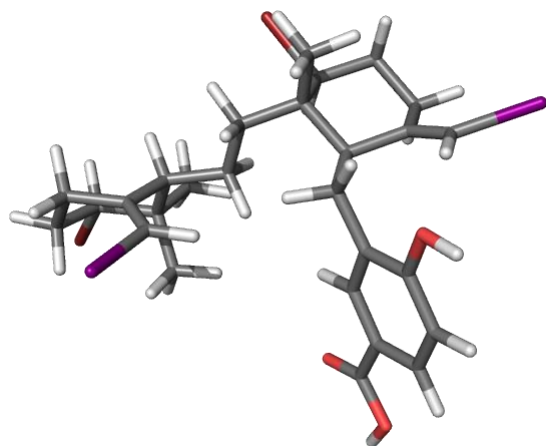
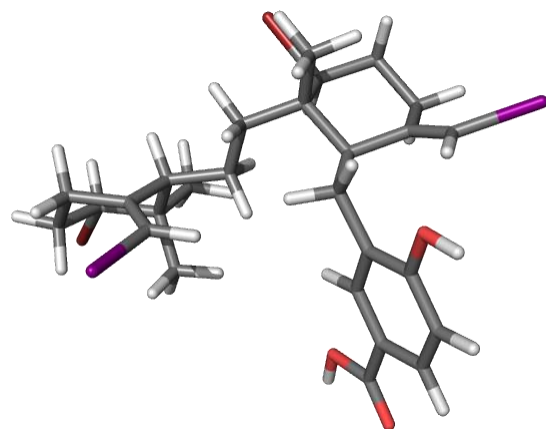
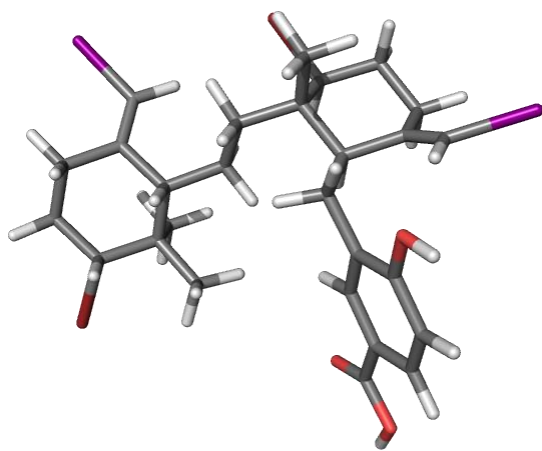
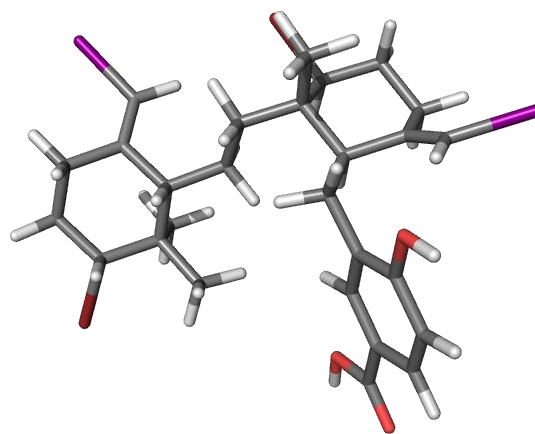
**2S,6S,7S,10S,14S-1a****2S,6S,7S,10S,14S-1b****2S,6S,7S,10S,14S-1c****2S,6S,7S,10S,14S-1d**

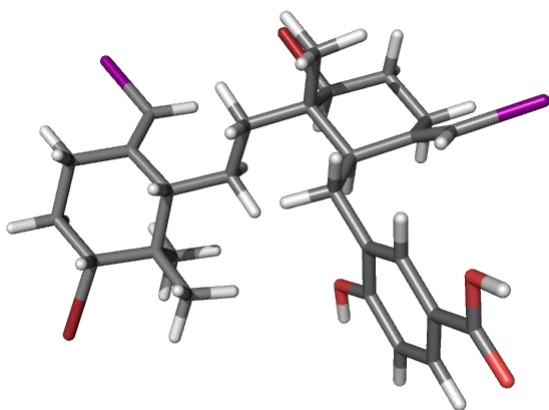
Figure S2. 3D structure of 2S,6S,7S,10S,14S-iodocallophycoic acid A (**1**) conformers optimized at the B3LYP/SVP level of theory in methanol.



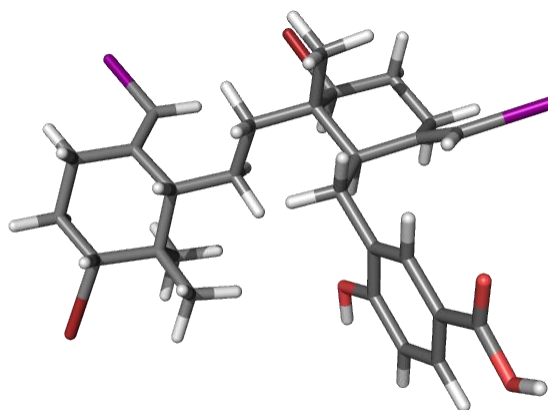
2S,6S,7S,10R,14R-1b



2S,6S,7S,10R,14R-1b



2S,6S,7S,10R,14R-1b



2S,6S,7S,10R,14R-1b

Figure S3. B3LYP/SVP in methanol optimized conformers of 2S,6S,7S,10R,14R-1.

DFT Calculation in acetonitrile

Table S6. Atomic coordinates for iodocallophycoic acid A (**1**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile.

Atom	2S,6S,7S,10S,14S-1a			2S,6S,7S,10S,14S-1b		
	x	y	z	x	y	z
C	2.8764	-2.6728	1.0969	2.8754	-2.6789	1.0944
C	2.9847	-1.4088	0.2870	2.9836	-1.4183	0.2793
C	1.6215	-0.7790	-0.0153	1.6206	-0.7874	-0.0214
C	0.7308	-1.7958	-0.8664	0.7258	-1.8057	-0.8661
C	0.6815	-3.1048	-0.0281	0.6762	-3.1111	-0.0223
C	2.0311	-3.7085	0.3353	2.0256	-3.7160	0.3397
H	2.3877	-2.4430	2.0603	2.3903	-2.4444	2.0585
H	3.8653	-3.0930	1.3251	3.8642	-3.1002	1.3211
Br	-0.4301	-4.5433	-0.8968	-0.4407	-4.5510	-0.8819
H	0.1184	-2.9179	0.8940	0.1161	-2.9193	0.9007
H	2.5665	-4.0327	-0.5704	2.5576	-4.0450	-0.5662
H	1.8800	-4.6006	0.9610	1.8745	-4.6052	0.9695
C	4.1300	-0.9053	-0.1902	4.1283	-0.9184	-0.2032
H	4.1887	-0.0153	-0.8104	4.1864	-0.0307	-0.8268
I	6.0820	-1.6986	0.1252	6.0798	-1.7138	0.1092
C	1.6719	0.6454	-0.6234	1.6718	0.6349	-0.6345
H	1.1214	-0.6878	0.9624	1.1234	-0.6918	0.9575
C	3.1443	3.8391	1.9415	3.1592	3.8343	1.9209
C	1.9793	3.1576	2.2743	1.9923	3.1541	2.2558
C	1.5052	2.1253	1.4499	1.5130	2.1218	1.4354
C	2.2045	1.7420	0.2810	2.2087	1.7330	0.2654
C	3.3597	2.4603	-0.0371	3.3631	2.4488	-0.0544
C	3.8452	3.5011	0.7742	3.8544	3.4905	0.7514
H	1.4180	3.4255	3.1737	1.4340	3.4253	3.1561
O	0.3523	1.4689	1.7323	0.3586	1.4697	1.7216
H	3.9027	2.2158	-0.9513	3.9145	2.2104	-0.9665
C	1.3697	-2.0247	-2.2497	1.3606	-2.0414	-2.2501
C	5.0760	4.2591	0.4366	5.0918	4.1904	0.3247
O	5.5370	5.1623	1.1056	5.7176	3.9360	-0.6854
O	5.6566	3.8490	-0.7073	5.4734	5.1609	1.1763
H	6.4482	4.3978	-0.8455	6.2842	5.5616	0.8172
H	0.6500	0.9264	-0.9125	0.6496	0.9169	-0.9216
H	2.2540	0.6450	-1.5562	2.2515	0.6307	-1.5687
H	3.5187	4.6438	2.5764	3.5264	4.6367	2.5615
H	-0.0540	1.8204	2.5390	-0.0454	1.8247	2.5279
H	0.8134	-2.7894	-2.8109	0.8008	-2.8067	-2.8071
H	2.4187	-2.3455	-2.1828	2.4089	-2.3649	-2.1846
H	1.3441	-1.0983	-2.8430	1.3362	-1.1172	-2.8466
C	-0.7106	-1.2574	-1.1054	-0.7152	-1.2653	-1.1036

Atom	2S,6S,7S,10S,14S-1a			2S,6S,7S,10S,14S-1b		
	x	y	z	x	y	z
C	-1.6220	-1.0278	0.1122	-1.6224	-1.0273	0.1156
C	-3.0574	-0.6372	-0.3004	-3.0585	-0.6370	-0.2947
C	-3.2292	0.7869	-0.8330	-3.2296	0.7834	-0.8372
C	-4.5509	0.9863	-1.5241	-4.5533	0.9799	-1.5254
C	-5.6994	0.6895	-0.5421	-5.6987	0.6932	-0.5368
C	-5.5270	-0.6861	0.0911	-5.5268	-0.6779	0.1061
C	-4.1668	-0.9394	0.8016	-4.1644	-0.9289	0.8134
H	-0.6450	-0.3368	-1.7034	-0.6492	-0.3480	-1.7064
H	-1.2084	-1.9871	-1.7636	-1.2166	-1.9972	-1.7565
H	-1.1922	-0.2804	0.7948	-1.1892	-0.2765	0.7923
H	-1.6820	-1.9612	0.6851	-1.6819	-1.9572	0.6942
H	-3.3213	-1.2974	-1.1478	-3.3267	-1.3029	-1.1363
C	-2.3201	1.7450	-0.6111	-2.3182	1.7415	-0.6255
H	-4.6173	0.2953	-2.3832	-4.6241	0.2823	-2.3787
H	-4.6552	2.0069	-1.9171	-4.6570	1.9976	-1.9261
H	-6.6635	0.7345	-1.0701	-6.6647	0.7365	-1.0613
H	-5.7233	1.4650	0.2396	-5.7177	1.4746	0.2392
H	-5.6711	-1.4665	-0.6688	-5.6753	-1.4637	-0.6475
Br	-7.1099	-0.9965	1.3005	-7.1060	-0.9762	1.3233
C	-4.0961	-2.4209	1.2198	-4.0951	-2.4074	1.2422
C	-3.9712	-0.0454	2.0377	-3.9624	-0.0263	2.0422
I	-2.4611	3.7735	-1.2490	-2.4572	3.7651	-1.2793
H	-1.4017	1.5907	-0.0468	-1.3984	1.5899	-0.0626
H	-4.9751	-2.6873	1.8236	-4.9721	-2.6674	1.8517
H	-3.2074	-2.6293	1.8314	-3.2043	-2.6132	1.8516
H	-4.0710	-3.0868	0.3419	-4.0752	-3.0800	0.3692
H	-2.9778	-0.2166	2.4796	-2.9675	-0.1962	2.4813
H	-4.7225	-0.2779	2.8066	-4.7109	-0.2519	2.8159
H	-4.0475	1.0255	1.7998	-4.0378	1.0430	1.7970

Table S7. Atomic coordinates for iodocallophycoic acid A (**1**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile (..contd).

Atom	2S,6S,7S,10S,14S-1c			2S,6S,7S,10S,14S-1d		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	3.4661	-2.0693	1.0250	3.4563	-2.0796	1.0036
C	3.3803	-0.8317	0.1720	3.3748	-0.8336	0.1625
C	1.9381	-0.4343	-0.1545	1.9337	-0.4247	-0.1535
C	1.1961	-1.6051	-0.9373	1.1855	-1.5824	-0.9498
C	1.3374	-2.8658	-0.0364	1.3205	-2.8536	-0.0626
C	2.7632	-3.2502	0.3347	2.7445	-3.2497	0.3036
H	2.9704	-1.8689	1.9919	2.9647	-1.8858	1.9739
H	4.5091	-2.3330	1.2464	4.4984	-2.3516	1.2190
Br	0.4440	-4.4940	-0.8170	0.4183	-4.4685	-0.8603
H	0.7570	-2.7183	0.8825	0.7409	-2.7131	0.8580
H	3.3265	-3.5477	-0.5631	3.3048	-3.5427	-0.5975
H	2.7470	-4.1193	1.0087	2.7236	-4.1248	0.9697
C	4.4317	-0.1461	-0.2958	4.4280	-0.1516	-0.3063
H	4.3574	0.7415	-0.9213	4.3557	0.7408	-0.9252
I	6.4821	-0.6036	0.0689	6.4772	-0.6252	0.0434
C	1.7817	0.9462	-0.8320	1.7807	0.9654	-0.8114
H	1.4351	-0.3719	0.8264	1.4335	-0.3739	0.8295
C	2.5702	4.3918	1.7118	2.6518	4.3712	1.7532
C	3.2853	4.2194	0.5313	3.3405	4.2091	0.5573
C	3.0444	3.1068	-0.2925	3.0715	3.1073	-0.2730
C	2.0808	2.1347	0.0652	2.1072	2.1405	0.0944
C	1.3745	2.3388	1.2515	1.4261	2.3343	1.2988
C	1.5992	3.4474	2.0832	1.6808	3.4325	2.1369
H	4.0400	4.9522	0.2328	4.0951	4.9385	0.2508
O	3.7234	2.9237	-1.4510	3.7252	2.9307	-1.4471
H	0.6094	1.6235	1.5597	0.6646	1.6150	1.6035
C	1.8451	-1.8158	-2.3176	1.8336	-1.7812	-2.3322
C	0.7876	3.5774	3.3188	0.9502	3.6379	3.4120
O	-0.0747	2.7940	3.6670	1.1329	4.5673	4.1726
O	1.0942	4.6694	4.0431	0.0377	2.6781	3.6640
H	0.5158	4.6737	4.8257	-0.3884	2.8955	4.5113
H	0.7431	1.0491	-1.1756	0.7377	1.0827	-1.1368
H	2.3960	1.0050	-1.7384	2.3812	1.0292	-1.7267
H	2.7607	5.2599	2.3437	2.8547	5.2262	2.4002
H	4.3729	3.6312	-1.5791	4.3777	3.6344	-1.5810
H	1.3715	-2.6568	-2.8449	1.3537	-2.6118	-2.8702
H	2.9226	-2.0212	-2.2466	2.9094	-1.9959	-2.2634
H	1.7198	-0.9204	-2.9442	1.7156	-0.8770	-2.9475
C	-0.3097	-1.2733	-1.1619	-0.3182	-1.2402	-1.1717
C	-1.1452	-0.8916	0.0727	-1.1533	-0.8676	0.0662
C	-2.6673	-0.9825	-0.1577	-2.6754	-0.9615	-0.1639
C	-3.2596	0.0513	-1.1175	-3.2713	0.0804	-1.1127

Atom	2S,6S,7S,10S,14S-1c			2S,6S,7S,10S,14S-1d		
	x	y	z	x	y	z
C	-4.6657	-0.2879	-1.5329	-4.6779	-0.2564	-1.5286
C	-5.5722	-0.3884	-0.2929	-5.5820	-0.3721	-0.2882
C	-4.9770	-1.3475	0.7305	-4.9835	-1.3418	0.7231
C	-3.5240	-1.0302	1.1854	-3.5304	-1.0267	1.1793
H	-0.3817	-0.4887	-1.9283	-0.3851	-0.4467	-1.9295
H	-0.7610	-2.1650	-1.6244	-0.7736	-2.1242	-1.6444
H	-0.8758	0.1121	0.4360	-0.8867	0.1351	0.4344
H	-0.8941	-1.5758	0.8923	-0.8996	-1.5554	0.8821
H	-2.8435	-1.9619	-0.6410	-2.8487	-1.9362	-0.6574
C	-2.5989	1.1610	-1.4719	-2.6120	1.1933	-1.4594
H	-4.6581	-1.2601	-2.0568	-4.6696	-1.2229	-2.0632
H	-5.0726	0.4556	-2.2318	-5.0873	0.4939	-2.2186
H	-6.5720	-0.7382	-0.5895	-6.5818	-0.7201	-0.5870
H	-5.6990	0.6102	0.1538	-5.7096	0.6210	0.1701
H	-5.0022	-2.3734	0.3380	-5.0071	-2.3632	0.3188
Br	-6.2722	-1.4685	2.2701	-6.2757	-1.4834	2.2634
C	-3.0227	-2.1779	2.0830	-3.0253	-2.1836	2.0629
C	-3.4264	0.3016	1.9494	-3.4339	0.2965	1.9581
I	-3.3226	2.6981	-2.7551	-3.3384	2.7397	-2.7296
H	-1.5970	1.4039	-1.1238	-1.6091	1.4335	-1.1119
H	-3.7205	-2.3395	2.9167	-3.7212	-2.3560	2.8960
H	-2.0409	-1.9522	2.5219	-2.0429	-1.9614	2.5025
H	-2.9390	-3.1224	1.5210	-2.9410	-3.1215	1.4900
H	-2.3832	0.5147	2.2276	-2.3903	0.5063	2.2377
H	-4.0135	0.2560	2.8784	-4.0206	0.2405	2.8867
H	-3.7905	1.1541	1.3580	-3.7981	1.1555	1.3761

Table S8. Atomic coordinates for iodocallophycoic acid A (**1**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile (..contd).

Atom	2S,6S,7S,10R,14R-1a			2S,6S,7S,10R,14R-1b		
	x	y	z	x	y	z
C	-3.1666	-1.7131	-1.6125	-3.1790	-1.6939	-1.6165
C	-3.3120	-0.9843	-0.3032	-3.3199	-0.9659	-0.3062
C	-1.9907	-0.3951	0.1983	-1.9954	-0.3834	0.1947
C	-0.9192	-1.5547	0.4245	-0.9301	-1.5492	0.4196
C	-0.8198	-2.2912	-0.9401	-0.8346	-2.2842	-0.9461
C	-2.1302	-2.8427	-1.4857	-2.1478	-2.8287	-1.4919
H	-2.8296	-0.9970	-2.3835	-2.8393	-0.9786	-2.3871
H	-4.1262	-2.1258	-1.9518	-4.1408	-2.1017	-1.9554
Br	0.5203	-3.7953	-0.9197	0.4988	-3.7942	-0.9281
H	-0.3790	-1.6144	-1.6820	-0.3909	-1.6083	-1.6871
H	-2.5189	-3.6330	-0.8252	-2.5400	-3.6181	-0.8324
H	-1.9556	-3.3008	-2.4704	-1.9759	-3.2862	-2.4773
C	-4.4497	-0.8787	0.3958	-4.4562	-0.8568	0.3944
H	-4.5366	-0.3679	1.3531	-4.5398	-0.3474	1.3527
I	-6.3447	-1.6650	-0.1820	-6.3552	-1.6340	-0.1825
C	-2.1203	0.5698	1.3990	-2.1183	0.5818	1.3958
H	-1.6094	0.1994	-0.6503	-1.6116	0.2092	-0.6543
C	-4.1744	4.3250	0.5917	-4.1661	4.3401	0.6070
C	-4.6363	3.4799	1.5952	-4.6290	3.4948	1.6078
C	-3.9856	2.2626	1.8575	-3.9787	2.2753	1.8635
C	-2.8568	1.8653	1.1028	-2.8531	1.8796	1.1046
C	-2.4124	2.7378	0.1085	-2.4065	2.7542	0.1108
C	-3.0485	3.9597	-0.1639	-3.0429	3.9785	-0.1536
H	-5.5105	3.7582	2.1904	-5.5015	3.7720	2.2059
O	-4.4159	1.4262	2.8335	-4.4080	1.4363	2.8377
H	-1.5348	2.4810	-0.4875	-1.5298	2.4861	-0.4800
C	-1.3874	-2.4936	1.5519	-1.4037	-2.4870	1.5456
C	-2.4925	4.8195	-1.2380	-2.5625	4.9086	-1.2053
O	-1.5120	4.5491	-1.9039	-3.0771	5.9759	-1.4729
O	-3.1853	5.9593	-1.4188	-1.4733	4.4578	-1.8590
H	-2.7506	6.4546	-2.1347	-1.2322	5.1287	-2.5212
H	-1.1096	0.8435	1.7333	-1.1057	0.8527	1.7264
H	-2.5913	0.0651	2.2514	-2.5873	0.0777	2.2498
H	-4.6836	5.2693	0.3964	-4.6657	5.2893	0.4060
H	-5.2041	1.7869	3.2663	-5.1943	1.7970	3.2739
H	-0.6960	-3.3419	1.6602	-0.7177	-3.3400	1.6517
H	-2.3952	-2.8949	1.3750	-2.4142	-2.8814	1.3689
H	-1.4084	-1.9597	2.5137	-1.4203	-1.9548	2.5085
C	0.4703	-0.9840	0.8353	0.4624	-0.9868	0.8314
C	1.1728	-0.0308	-0.1462	1.1708	-0.0387	-0.1506
C	2.4429	0.6226	0.4368	2.4398	0.6149	0.4341
C	3.6242	-0.3218	0.6761	3.6194	-0.3301	0.6793

Atom	2S,6S,7S,10R,14R-1a			2S,6S,7S,10R,14R-1b		
	x	y	z	x	y	z
C	4.7090	0.3085	1.5076	4.7034	0.3019	1.5106
C	5.2297	1.5833	0.8209	5.2265	1.5744	0.8214
C	4.0756	2.5222	0.4952	4.0738	2.5133	0.4907
C	2.9332	1.9111	-0.3650	2.9331	1.9005	-0.3704
H	0.3584	-0.4738	1.8044	0.3527	-0.4753	1.8001
H	1.1209	-1.8449	1.0451	1.1077	-1.8514	1.0424
H	0.4781	0.7729	-0.4220	0.4786	0.7651	-0.4321
H	1.4152	-0.5487	-1.0874	1.4156	-0.5608	-1.0888
H	2.1649	1.0023	1.4382	2.1596	0.9979	1.4337
C	3.6827	-1.5437	0.1313	3.6766	-1.5546	0.1402
H	5.5415	-0.3867	1.6817	5.5350	-0.3934	1.6880
H	4.2923	0.5730	2.4958	4.2853	0.5694	2.4974
H	5.7686	1.3124	-0.1005	5.7670	1.3005	-0.0981
H	5.9491	2.0946	1.4776	5.9449	2.0869	1.4782
H	3.6401	2.9134	1.4251	3.6366	2.9074	1.4185
Br	4.8630	4.1886	-0.3211	4.8642	4.1769	-0.3286
C	3.4029	1.5312	-1.7795	3.4062	1.5160	-1.7825
C	1.7849	2.9341	-0.4604	1.7857	2.9239	-0.4720
I	5.2867	-2.9318	0.3334	5.2781	-2.9443	0.3513
H	2.8943	-1.9744	-0.4840	2.8886	-1.9867	-0.4746
H	2.5715	1.1001	-2.3572	2.5762	1.0830	-2.3608
H	4.2170	0.7922	-1.7689	4.2201	0.7768	-1.7675
H	3.7557	2.4213	-2.3209	3.7606	2.4041	-2.3260
H	2.1601	3.8932	-0.8442	2.1624	3.8816	-0.8580
H	1.3276	3.1203	0.5253	1.3256	3.1138	0.5117
H	0.9950	2.6020	-1.1477	0.9976	2.5892	-1.1602

Table S9. Atomic coordinates for iodocallophycoic acid A (**1**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile (..contd).

Atom	2S,6S,7S,10R,14R-1c			2S,6S,7S,10R,14R-1d		
	x	y	z	x	y	z
C	-2.7542	-2.1672	-1.6109	-2.7464	-2.1797	-1.6090
C	-3.0311	-1.2050	-0.4870	-3.0252	-1.2212	-0.4823
C	-1.7848	-0.4185	-0.0783	-1.7815	-0.4306	-0.0737
C	-0.6799	-1.4228	0.4833	-0.6713	-1.4319	0.4830
C	-0.4204	-2.4130	-0.6871	-0.4100	-2.4180	-0.6904
C	-1.6480	-3.1564	-1.2024	-1.6355	-3.1654	-1.2048
H	-2.4221	-1.5947	-2.4953	-2.4182	-1.6039	-2.4927
H	-3.6561	-2.7222	-1.9030	-3.6466	-2.7377	-1.9006
Br	0.9788	-3.7961	-0.2509	0.9963	-3.7958	-0.2605
H	0.0526	-1.8721	-1.5162	0.0589	-1.8730	-1.5191
H	-2.0311	-3.8380	-0.4274	-2.0143	-3.8502	-0.4305
H	-1.3653	-3.7772	-2.0655	-1.3520	-3.7831	-2.0698
C	-4.2042	-1.0712	0.1439	-4.1978	-1.0932	0.1507
H	-4.3704	-0.3891	0.9740	-4.3652	-0.4137	0.9826
I	-5.9988	-2.1285	-0.3037	-5.9891	-2.1562	-0.2969
C	-2.0248	0.8078	0.8341	-2.0246	0.7915	0.8433
H	-1.3786	-0.0238	-1.0221	-1.3790	-0.0312	-1.0172
C	-4.5927	3.9945	-0.6526	-4.6156	3.9751	-0.6207
C	-3.4738	3.6105	-1.3819	-3.4969	3.5959	-1.3557
C	-2.6416	2.5799	-0.9153	-2.6577	2.5678	-0.8980
C	-2.9320	1.8984	0.2909	-2.9388	1.8796	0.3073
C	-4.0549	2.3190	1.0089	-4.0594	2.2940	1.0292
C	-4.8931	3.3541	0.5589	-4.9051	3.3270	0.5899
H	-3.2261	4.1127	-2.3214	-3.2563	4.1026	-2.2946
O	-1.5309	2.2119	-1.6002	-1.5489	2.2072	-1.5899
H	-4.2894	1.8301	1.9563	-4.2997	1.8078	1.9776
C	-1.1952	-2.1472	1.7414	-1.1813	-2.1616	1.7402
C	-6.0875	3.7965	1.3205	-6.0724	3.6919	1.4305
O	-6.8430	4.6804	0.9683	-6.3563	3.1643	2.4877
O	-6.2699	3.1165	2.4687	-6.8126	4.6877	0.9076
H	-7.0696	3.4722	2.8938	-7.5484	4.8570	1.5214
H	-1.0471	1.2700	1.0356	-1.0485	1.2578	1.0430
H	-2.4138	0.4915	1.8134	-2.4091	0.4702	1.8227
H	-5.2414	4.7960	-1.0098	-5.2608	4.7762	-0.9827
H	-1.4373	2.7425	-2.4055	-1.4610	2.7421	-2.3929
H	-0.4381	-2.8499	2.1188	-0.4211	-2.8630	2.1136
H	-2.1207	-2.7104	1.5590	-2.1056	-2.7269	1.5585
H	-1.4019	-1.4243	2.5449	-1.3880	-1.4416	2.5464
C	0.6284	-0.6808	0.8836	0.6346	-0.6855	0.8827
C	1.3346	0.1823	-0.1748	1.3361	0.1813	-0.1758
C	2.5762	0.9122	0.3859	2.5745	0.9174	0.3840
C	3.7969	0.0228	0.6504	3.7986	0.0337	0.6511

Atom	2S,6S,7S,10R,14R-1c			2S,6S,7S,10R,14R-1d		
	x	y	z	x	y	z
C	4.8758	0.7254	1.4297	4.8740	0.7422	1.4298
C	5.3455	1.9772	0.6706	5.3392	1.9942	0.6684
C	4.1547	2.8686	0.3504	4.1450	2.8801	0.3451
C	3.0019	2.2006	-0.4514	2.9956	2.2055	-0.4561
H	0.4028	-0.0461	1.7553	0.4077	-0.0525	1.7553
H	1.3257	-1.4432	1.2608	1.3351	-1.4457	1.2585
H	0.6293	0.9335	-0.5510	0.6270	0.9293	-0.5513
H	1.6186	-0.4213	-1.0510	1.6227	-0.4207	-1.0522
H	2.2862	1.3059	1.3787	2.2823	1.3122	1.3758
C	3.8890	-1.2271	0.1786	3.8962	-1.2166	0.1813
H	5.7307	0.0633	1.6220	5.7314	0.0840	1.6242
H	4.4691	1.0276	2.4114	4.4652	1.0447	2.4106
H	5.8588	1.6781	-0.2568	5.8546	1.6952	-0.2579
H	6.0733	2.5345	1.2788	6.0641	2.5559	1.2760
H	3.7379	3.2760	1.2819	3.7258	3.2881	1.2752
Br	4.8631	4.5328	-0.5412	4.8477	4.5449	-0.5499
C	3.4255	1.8030	-1.8752	3.4220	1.8064	-1.8786
C	1.8228	3.1909	-0.5137	1.8126	3.1910	-0.5217
I	5.5376	-2.5513	0.4450	5.5500	-2.5335	0.4514
H	3.1074	-1.7255	-0.3912	3.1173	-1.7191	-0.3885
H	2.5796	1.3483	-2.4124	2.5787	1.3463	-2.4153
H	4.2505	1.0754	-1.8797	4.2505	1.0828	-1.8807
H	3.7454	2.6867	-2.4466	3.7380	2.6902	-2.4519
H	2.1436	4.1345	-0.9774	2.1303	4.1349	-0.9871
H	1.4455	3.4231	0.4962	1.4332	3.4238	0.4872
H	0.9833	2.8033	-1.1045	0.9754	2.7990	-1.1128

Table S10. Electronic energies (ΔE), free energies (ΔG), and Boltzmann distribution abundances for the conformers of iodocallophycoic acid A (**1**), obtained through DFT calculations at the B3LYP/SVP level of theory in acetonitrile.

Conformers	Energies (Hartree)		Abundance (%)
	ΔE	ΔG	
2S,6S,7S,10S,14S-1a	-20261.620148	-20261.136193	11.34
2S,6S,7S,10S,14S-1b	-20261.620256	-20261.136095	10.22
2S,6S,7S,10S,14S-1c	-20261.620013	-20261.137114	30.07
2S,6S,7S,10S,14S-1d	-20261.619854	-20261.136509	15.85
2S,6S,7S,10S,14S-1e	-20261.616610	-20261.133813	0.91
2S,6S,7S,10S,14S-1f	-20261.616450	-20261.133314	0.54
2S,6S,7S,10S,14S-1g	-20261.616581	-20261.132517	0.23
2S,6S,7S,10S,14S-1h	-20261.616459	-20261.132398	0.20
2S,6S,7S,10S,14S-1i	-20261.615743	-20261.132642	0.26
2S,6S,7S,10S,14S-1j	-20261.615848	-20261.132612	0.26
2S,6S,7S,10S,14S-1k	-20261.620013	-20261.137114	30.07
2S,6S,7S,10S,14S-1l	-20261.613303	-20261.129973	0.02
2S,6S,7S,10S,14S-1m	-20261.613211	-20261.129544	0.01
2S,6S,7S,10S,14S-1n	-20261.612545	-20261.130293	0.02
2S,6S,7S,10R,14R-1a	-20261.620971	-20261.135879	18.69
2S,6S,7S,10R,14R-1b	-20261.620858	-20261.136722	45.63
2S,6S,7S,10R,14R-1c	-20261.620274	-20261.135508	12.62
2S,6S,7S,10R,14R-1d	-20261.620379	-20261.135628	14.32
2S,6S,7S,10R,14R-1e	-20261.615332	-20261.130046	0.04
2S,6S,7S,10R,14R-1f	-20261.617617	-20261.133993	2.54
2S,6S,7S,10R,14R-1g	-20261.617482	-20261.134607	4.86
2S,6S,7S,10R,14R-1h	-20261.615441	-20261.128215	0.01
2S,6S,7S,10R,14R-1i	-20261.615349	-20261.128197	0.01
2S,6S,7S,10R,14R-1j	-20261.614278	-20261.129742	0.03
2S,6S,7S,10R,14R-1k	-20261.615842	-20261.131557	0.19
2S,6S,7S,10R,14R-1l	-20261.614158	-20261.129835	0.03
2S,6S,7S,10R,14R-1m	-20261.615930	-20261.132005	0.31
2S,6S,7S,10R,14R-1n	-20261.615337	-20261.132058	0.33
2S,6S,7S,10R,14R-1o	-20261.615404	-20261.132271	0.41

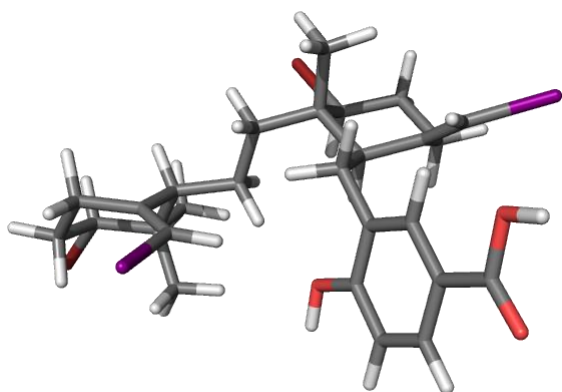
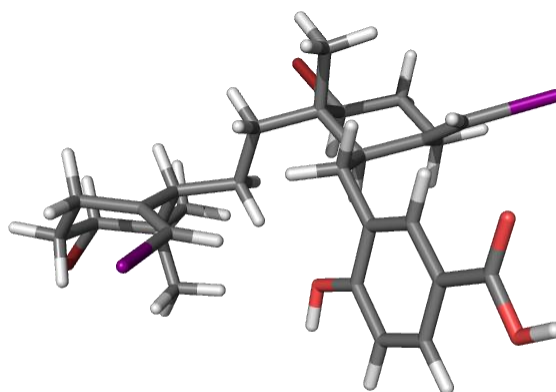
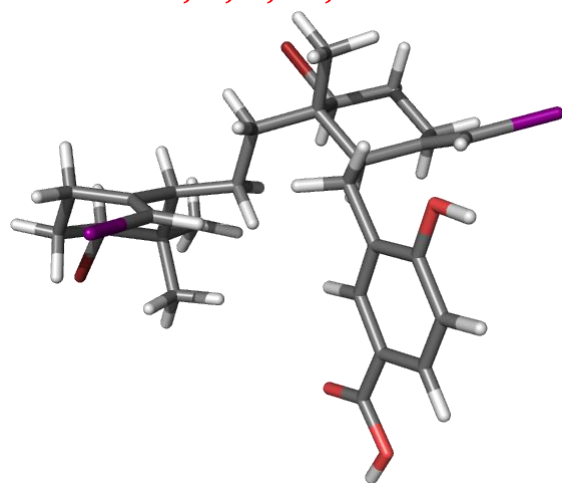
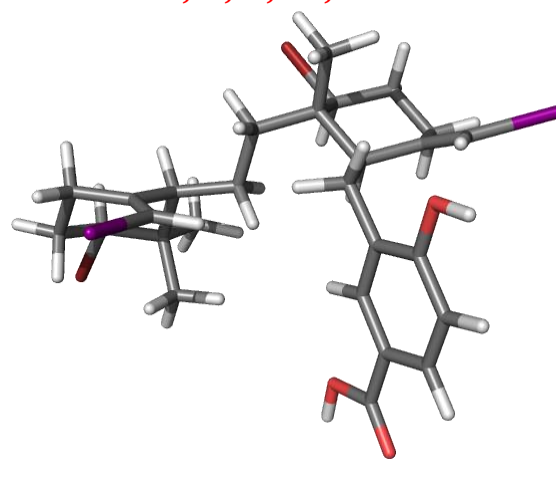
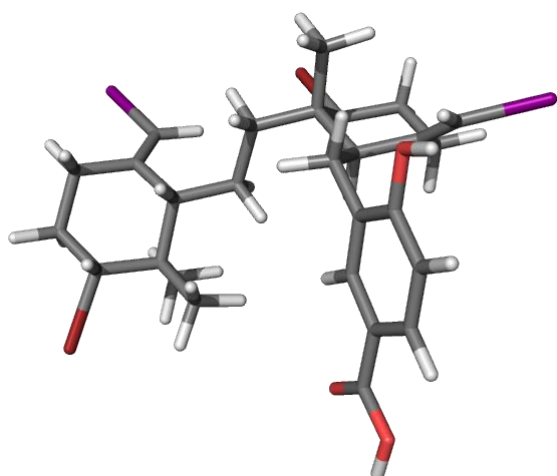
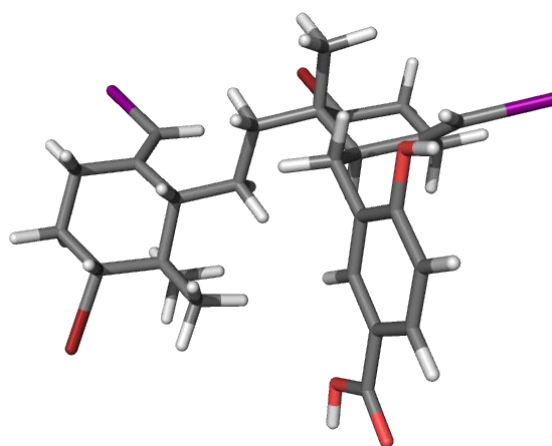
**2S,6S,7S,10S,14S-1a****2S,6S,7S,10S,14S-1b****2S,6S,7S,10S,14S-1c****2S,6S,7S,10S,14S-1d**

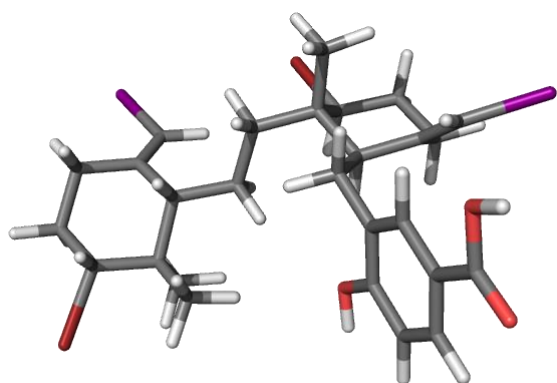
Figure S4. B3LYP/SVP optimized conformers of 2S,6S,7S,10S,14S-iodocallophycoic acid A (**1**) in acetonitrile.



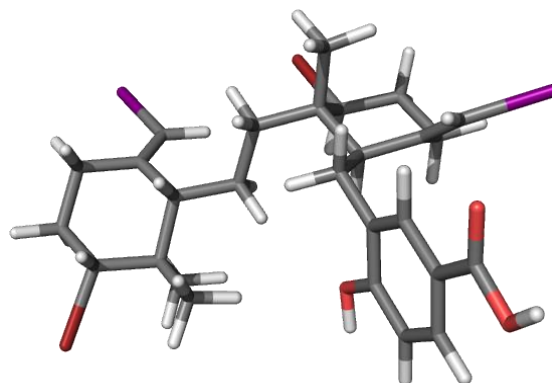
2S,6S,7S,10R,14R-1b



2S,6S,7S,10R,14R-1b



2S,6S,7S,10R,14R-1b



2S,6S,7S,10R,14R-1b

Figure S5. B3LYP/SVP optimized conformers of 2S,6S,7S,10R,14R-iodocallophycoic acid A (**1**) in acetonitrile.

CHARACTERIZATION OF BROMOPHYCOIC ACID F (6)**DFT Calculation****Table S11.** Atomic coordinates for bromophycoic acid F (6), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile.

Atom	6a			6b		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	1.5373	-0.2363	0.5746	1.5339	-0.2363	0.5661
C	0.7345	-2.2010	-0.8097	0.7387	-2.1983	-0.8260
C	3.1680	-1.6708	-0.6514	3.1717	-1.6716	-0.6496
C	2.1457	-2.7951	-0.7505	2.1486	-2.7942	-0.7573
C	3.0277	-0.7699	0.6027	3.0234	-0.7719	0.6046
C	0.3948	-1.2914	0.3901	0.3914	-1.2898	0.3725
H	0.6450	-1.6111	-1.7388	0.6564	-1.6073	-1.7550
H	3.1053	-1.0509	-1.5545	3.1168	-1.0506	-1.5525
H	2.2498	-3.4871	0.0994	2.2455	-3.4874	0.0924
H	1.4783	0.3681	-0.3471	1.4823	0.3690	-0.3554
H	-0.0086	-3.0127	-0.8877	-0.0048	-3.0091	-0.9102
H	2.3366	-3.3846	-1.6597	2.3453	-3.3830	-1.6658
Br	5.0137	-2.4682	-0.8457	5.0177	-2.4717	-0.8309
C	1.2126	0.7293	1.7308	1.2022	0.7288	1.7209
H	1.4286	0.2678	2.7117	1.4103	0.2659	2.7028
H	1.8695	1.6133	1.6862	1.8608	1.6117	1.6819
C	-0.8953	-0.5045	0.0442	-0.8955	-0.5012	0.0186
H	-0.8243	-0.1060	-0.9840	-0.8174	-0.1023	-1.0090
H	-1.7482	-1.2044	0.0213	-1.7491	-1.2000	-0.0103
C	0.1119	-2.1519	1.6409	0.0990	-2.1515	1.6202
H	-0.7801	-2.7747	1.4643	-0.7923	-2.7732	1.4368
H	0.9357	-2.8329	1.8882	0.9204	-2.8338	1.8722
H	-0.0894	-1.5369	2.5302	-0.1076	-1.5374	2.5089
C	-0.2146	1.2017	1.7230	-0.2241	1.2031	1.7031
H	-0.4572	2.0453	2.3797	-0.4703	2.0466	2.3587
C	-1.1844	0.6472	0.9793	-1.1895	0.6502	0.9524
C	-2.5951	1.1681	1.0453	-2.6001	1.1720	1.0101
C	-3.6645	0.1989	1.6266	-3.6728	0.2048	1.5884
H	-3.2981	-0.8407	1.6621	-3.3095	-0.8360	1.6214
H	-3.9347	0.4829	2.6540	-3.9427	0.4871	2.6163
C	-4.8027	0.3406	0.6458	-4.8093	0.3524	0.6064
C	-6.4440	0.8620	-1.5533	-6.4433	0.8801	-1.5916
C	-6.0986	-0.1475	0.6425	-6.1087	-0.1301	0.6055
C	-4.3342	1.0847	-0.4509	-4.3352	1.0925	-0.4899
C	-5.1377	1.3565	-1.5611	-5.1360	1.3677	-1.6019
C	-6.9353	0.1158	-0.4651	-6.9418	0.1382	-0.5044

Atom	6a			6b		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
H	−6.4915	−0.7337	1.4755	−6.4921	−0.7117	1.4450
H	−4.7523	1.9383	−2.4001	−4.7467	1.9462	−2.4415
H	−7.0989	1.0595	−2.4028	−7.1073	1.0736	−2.4362
O	−3.0566	1.4910	−0.3133	−3.0556	1.4923	−0.3509
C	−8.3193	−0.4161	−0.4387	−8.3431	−0.3433	−0.5666
O	−8.7958	−1.0630	0.4739	−9.1053	−0.1499	−1.4937
C	3.3847	−1.5434	1.8901	3.3699	−1.5477	1.8935
H	3.1149	−0.9667	2.7861	3.0950	−0.9716	2.7883
H	2.8931	−2.5211	1.9623	2.8760	−2.5245	1.9610
H	4.4689	−1.7222	1.9303	4.4534	−1.7285	1.9410
C	4.0205	0.4317	0.5311	4.0184	0.4285	0.5422
H	3.9788	0.9733	1.4900	3.9701	0.9685	1.5017
H	5.0366	0.0080	0.4822	5.0342	0.0035	0.5003
H	−2.6093	2.1168	1.6055	−2.6168	2.1217	1.5686
O	−9.0294	−0.1165	−1.5442	−8.7158	−1.0382	0.5268
H	−9.9143	−0.5057	−1.4343	−9.6404	−1.3110	0.3953
C	3.8681	1.4539	−0.6117	3.8758	1.4528	−0.6000
H	3.8567	0.9236	−1.5817	3.8708	0.9242	−1.5709
H	2.9040	1.9772	−0.5378	2.9119	1.9772	−0.5322
C	5.0066	2.4406	−0.6315	5.0157	2.4380	−0.6094
H	5.9933	1.9905	−0.8073	6.0029	1.9872	−0.7803
C	4.9684	3.7746	−0.4485	4.9781	3.7715	−0.4221
C	6.2331	4.5985	−0.4984	6.2441	4.5939	−0.4610
H	6.1731	5.3688	−1.2883	7.1347	3.9752	−0.6477
H	6.3884	5.1432	0.4504	6.1903	5.3668	−1.2489
H	7.1232	3.9804	−0.6890	6.3938	5.1353	0.4905
C	3.7156	4.5743	−0.1877	3.7247	4.5718	−0.1665
H	3.5724	5.3383	−0.9726	2.8129	3.9610	−0.1312
H	2.8051	3.9621	−0.1430	3.8040	5.1193	0.7895
H	3.8009	5.1264	0.7651	3.5884	5.3399	−0.9487

Table S12. Atomic coordinates for bromophycoic acid F (**6**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile (..contd).

Atom	6c			6d		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	1.3714	-0.1770	0.7015	1.3681	-0.1820	0.6979
C	0.6671	-1.9460	-0.9742	0.6731	-1.9408	-0.9925
C	3.0775	-1.4165	-0.6253	3.0814	-1.4130	-0.6277
C	2.0828	-2.5306	-0.9230	2.0886	-2.5257	-0.9371
C	2.8658	-0.7014	0.7328	2.8626	-0.7057	0.7333
C	0.2535	-1.2070	0.3158	0.2526	-1.2099	0.2998
H	0.6163	-1.2381	-1.8200	0.6271	-1.2276	-1.8342
H	3.0380	-0.6773	-1.4349	3.0456	-0.6694	-1.4334
H	2.1585	-3.3269	-0.1669	2.1605	-3.3264	-0.1853
H	1.3505	0.5482	-0.1303	1.3509	0.5485	-0.1292
H	-0.0597	-2.7453	-1.1976	-0.0525	-2.7386	-1.2249
H	2.3267	-2.9920	-1.8916	2.3377	-2.9814	-1.9071
Br	4.9471	-2.1476	-0.8487	4.9524	-2.1421	-0.8460
C	0.9757	0.6182	1.9599	0.9656	0.6047	1.9595
H	1.1469	0.0265	2.8778	1.1332	0.0073	2.8744
H	1.6231	1.5033	2.0696	1.6116	1.4897	2.0780
C	-1.0266	-0.3863	0.0113	-1.0260	-0.3873	-0.0062
H	-0.9050	0.1501	-0.9472	-0.8988	0.1563	-0.9599
H	-1.8692	-1.0799	-0.1544	-1.8673	-1.0799	-0.1822
C	-0.0854	-2.2252	1.4254	-0.0921	-2.2352	1.4011
H	-0.9538	-2.8297	1.1170	-0.9591	-2.8375	1.0845
H	0.7349	-2.9231	1.6330	0.7271	-2.9346	1.6081
H	-0.3499	-1.7322	2.3723	-0.3611	-1.7483	2.3498
C	-0.4551	1.0782	1.9412	-0.4655	1.0634	1.9372
H	-0.7429	1.8215	2.6939	-0.7577	1.8009	2.6939
C	-1.3781	0.6243	1.0791	-1.3839	0.6150	1.0673
C	-2.7989	1.1158	1.1521	-2.8050	1.1060	1.1365
C	-3.8681	0.0745	1.5896	-3.8786	0.0617	1.5548
H	-3.4943	-0.9587	1.4943	-3.5079	-0.9713	1.4448
H	-4.1528	0.2217	2.6414	-4.1659	0.1938	2.6079
C	-4.9922	0.3362	0.6175	-4.9986	0.3420	0.5829
C	-6.5973	1.1161	-1.5311	-6.5913	1.1573	-1.5565
C	-6.2906	-0.1387	0.5403	-6.3002	-0.1269	0.4990
C	-4.5035	1.1981	-0.3798	-4.5020	1.2133	-0.4013
C	-5.2883	1.5992	-1.4637	-5.2815	1.6329	-1.4829
C	-7.1096	0.2557	-0.5414	-7.1128	0.2874	-0.5807
H	-6.6993	-0.8128	1.2957	-6.7011	-0.8078	1.2513
H	-4.8876	2.2702	-2.2254	-4.8751	2.3112	-2.2350
H	-7.2381	1.4137	-2.3621	-7.2400	1.4617	-2.3800
O	-3.2266	1.5795	-0.1755	-3.2237	1.5852	-0.1885
C	-8.4980	-0.2627	-0.5916	-8.5165	-0.1688	-0.7252
O	-8.9917	-1.0020	0.2379	-9.2616	0.1485	-1.6318

Atom	6c			6d		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	3.1655	−1.6437	1.9183	3.1571	−1.6543	1.9150
H	2.8744	−1.1820	2.8726	2.8637	−1.1968	2.8706
H	2.6554	−2.6121	1.8486	2.6455	−2.6215	1.8389
H	4.2447	−1.8482	1.9702	4.2357	−1.8609	1.9693
C	3.8488	0.5008	0.8817	3.8440	0.4964	0.8932
H	3.7105	0.9351	1.8854	3.7011	0.9253	1.8986
H	4.8703	0.0895	0.8830	4.8659	0.0859	0.8966
H	−2.8481	1.9959	1.8133	−2.8581	1.9787	1.8074
O	−9.1912	0.1642	−1.6655	−8.9126	−0.9930	0.2651
H	−10.0806	−0.2262	−1.6098	−9.8372	−1.2373	0.0863
C	3.7990	1.6363	−0.1595	3.7978	1.6372	−0.1425
H	3.9746	1.2353	−1.1690	3.9745	1.2408	−1.1536
H	2.7904	2.0855	−0.1775	2.7898	2.0878	−0.1600
C	4.7905	2.7270	0.1539	4.7901	2.7251	0.1775
H	4.5518	3.3176	1.0490	4.5509	3.3123	1.0747
C	5.9211	3.0454	−0.5054	5.9221	3.0448	−0.4789
C	6.7975	4.1823	−0.0373	6.7994	4.1787	−0.0049
H	7.8181	3.8272	0.1934	7.8191	3.8212	0.2260
H	6.9099	4.9463	−0.8278	6.9141	4.9455	−0.7923
H	6.3937	4.6747	0.8601	6.3948	4.6682	0.8936
C	6.4233	2.3381	−1.7402	6.4252	2.3420	−1.7160
H	7.4563	1.9800	−1.5841	7.4577	1.9826	−1.5601
H	5.8106	1.4744	−2.0309	5.8122	1.4799	−2.0106
H	6.4663	3.0329	−2.5983	6.4695	3.0401	−2.5712

Table S13. Atomic coordinates for bromophycoic acid F (**6**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile (..contd).

Atom	6e			6f		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	1.6840	-0.6971	0.3885	1.6785	-0.6992	0.3917
C	2.0970	-2.6264	-1.2057	2.0792	-2.6263	-1.2084
C	3.8914	-0.9572	-0.7428	3.8793	-0.9615	-0.7520
C	3.6059	-2.4263	-1.0264	3.5894	-2.4295	-1.0367
C	3.2319	-0.4017	0.5450	3.2276	-0.4070	0.5403
C	1.2625	-2.1567	0.0047	1.2521	-2.1572	0.0074
H	1.7776	-2.0613	-2.0990	1.7562	-2.0590	-2.0989
H	3.5685	-0.3591	-1.6039	3.5530	-0.3612	-1.6103
H	3.9986	-3.0590	-0.2156	3.9851	-3.0644	-0.2290
H	1.3771	-0.1022	-0.4892	1.3679	-0.1019	-0.4831
H	1.8835	-3.6873	-1.4199	1.8625	-3.6865	-1.4234
H	4.1301	-2.7315	-1.9444	4.1082	-2.7341	-1.9580
Br	5.8905	-0.6725	-0.7905	5.8786	-0.6807	-0.8098
C	0.8402	-0.1744	1.5669	0.8421	-0.1773	1.5758
H	1.2086	-0.5740	2.5294	1.2145	-0.5804	2.5353
H	0.9495	0.9189	1.6563	0.9547	0.9154	1.6674
C	-0.2254	-2.0935	-0.4300	-0.2379	-2.0902	-0.4194
H	-0.2983	-1.6085	-1.4217	-0.3149	-1.6037	-1.4100
H	-0.6018	-3.1211	-0.5823	-0.6173	-3.1168	-0.5711
C	1.3805	-3.1796	1.1556	1.3741	-3.1826	1.1557
H	0.9468	-4.1417	0.8381	0.9371	-4.1432	0.8385
H	2.4193	-3.3769	1.4486	2.4140	-3.3823	1.4432
H	0.8361	-2.8555	2.0544	0.8348	-2.8593	2.0578
C	-0.6236	-0.4966	1.4410	-0.6231	-0.4956	1.4563
H	-1.3057	0.0010	2.1358	-1.3007	0.0026	2.1551
C	-1.1198	-1.3601	0.5439	-1.1258	-1.3561	0.5600
C	-2.5907	-1.6609	0.4200	-2.5979	-1.6526	0.4417
C	-3.2558	-1.1929	-0.9093	-3.2669	-1.1808	-0.8843
H	-2.6643	-0.3957	-1.3908	-2.6753	-0.3841	-1.3665
H	-3.3533	-2.0172	-1.6302	-3.3687	-2.0037	-1.6062
C	-4.5800	-0.6574	-0.4225	-4.5881	-0.6433	-0.3915
C	-6.7117	0.3700	1.0609	-6.7096	0.3848	1.0989
C	-5.7150	-0.2243	-1.0873	-5.7242	-0.2071	-1.0551
C	-4.5179	-0.5731	0.9786	-4.5203	-0.5613	1.0089
C	-5.5700	-0.0615	1.7408	-5.5689	-0.0486	1.7764
C	-6.7989	0.2913	-0.3420	-6.8036	0.3096	-0.3033
H	-5.7943	-0.2703	-2.1751	-5.7934	-0.2567	-2.1427
H	-5.4985	-0.0082	2.8285	-5.4937	0.0029	2.8639
H	-7.5544	0.7706	1.6257	-7.5578	0.7883	1.6551
O	-3.3553	-1.0317	1.4871	-3.3567	-1.0229	1.5126
C	-8.0048	0.7383	-1.0811	-8.0515	0.7844	-0.9499
O	-8.1331	0.6917	-2.2891	-9.0096	1.2437	-0.3594

Atom	6e			6f		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	3.8551	−1.0288	1.8101	3.8566	−1.0373	1.8009
H	3.2951	−0.7394	2.7106	3.3014	−0.7493	2.7048
H	3.8941	−2.1241	1.7806	3.8942	−2.1327	1.7689
H	4.8864	−0.6692	1.9375	4.8889	−0.6792	1.9239
C	3.4671	1.1359	0.6669	3.4664	1.1300	0.6633
H	3.0657	1.4701	1.6371	3.0742	1.4632	1.6376
H	4.5556	1.2930	0.7347	4.5558	1.2849	0.7218
H	−2.7438	−2.7504	0.5354	−2.7537	−2.7419	0.5561
O	−8.9775	1.2159	−0.2804	−8.0351	0.6609	−2.2919
H	−9.7190	1.4809	−0.8520	−8.8860	0.9956	−2.6242
C	2.9147	2.0635	−0.4327	2.9061	2.0607	−0.4298
H	3.2890	1.7299	−1.4179	3.2669	1.7254	−1.4194
H	1.8183	1.9974	−0.4829	1.8088	2.0003	−0.4670
C	3.3507	3.4906	−0.2254	3.3518	3.4856	−0.2275
H	4.4377	3.6438	−0.2694	4.4389	3.6335	−0.2862
C	2.5907	4.5757	0.0190	2.6005	4.5741	0.0280
C	3.2209	5.9351	0.2082	3.2397	5.9303	0.2091
H	2.8403	6.6555	−0.5383	4.3345	5.8892	0.1076
H	2.9659	6.3549	1.1979	2.8519	6.6531	−0.5315
H	4.3173	5.8990	0.1223	3.0007	6.3507	1.2026
C	1.0854	4.5679	0.1245	1.0968	4.5734	0.1543
H	0.6391	5.2296	−0.6393	0.6478	3.5773	0.0444
H	0.6426	3.5700	0.0068	0.7915	4.9776	1.1357
H	0.7647	4.9691	1.1023	0.6430	5.2359	−0.6044

Table S14. Atomic coordinates for bromophycoic acid F (**6**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile (..contd).

Atom	6g			6h		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	1.4291	-0.7962	0.4148	1.4245	-0.7987	0.4142
C	1.7781	-2.4750	-1.4547	1.7648	-2.4683	-1.4650
C	3.6497	-1.0113	-0.7008	3.6406	-1.0102	-0.7108
C	3.2898	-2.3985	-1.2154	3.2775	-2.3945	-1.2309
C	2.9866	-0.6238	0.6460	2.9829	-0.6289	0.6404
C	0.9369	-2.1506	-0.2026	0.9287	-2.1496	-0.2080
H	1.5176	-1.7594	-2.2542	1.5018	-1.7485	-2.2599
H	3.3859	-0.2697	-1.4650	3.3746	-0.2646	-1.4702
H	3.6206	-3.1723	-0.5056	3.6100	-3.1721	-0.5261
H	1.1822	-0.0552	-0.3653	1.1753	-0.0537	-0.3612
H	1.5107	-3.4747	-1.8370	1.4950	-3.4659	-1.8513
H	3.8226	-2.5899	-2.1589	3.8066	-2.5818	-2.1773
Br	5.6623	-0.8417	-0.6646	5.6534	-0.8426	-0.6813
C	0.5816	-0.4111	1.6425	0.5822	-0.4189	1.6471
H	0.9052	-0.9671	2.5415	0.9091	-0.9791	2.5422
H	0.7435	0.6498	1.8955	0.7457	0.6408	1.9043
C	-0.5314	-1.9292	-0.6506	-0.5412	-1.9248	-0.6490
H	-0.5484	-1.2857	-1.5504	-0.5613	-1.2764	-1.5452
H	-0.9590	-2.8944	-0.9765	-0.9708	-2.8880	-0.9784
C	0.9635	-3.3458	0.7750	0.9584	-3.3498	0.7634
H	0.4762	-4.2155	0.3050	0.4678	-4.2165	0.2914
H	1.9811	-3.6551	1.0440	1.9769	-3.6618	1.0259
H	0.4218	-3.1302	1.7073	0.4215	-3.1382	1.6993
C	-0.8932	-0.6310	1.4447	-0.8935	-0.6372	1.4544
H	-1.5644	-0.2141	2.2007	-1.5613	-0.2238	2.2154
C	-1.4114	-1.3128	0.4137	-1.4164	-1.3135	0.4222
C	-2.8916	-1.5125	0.2197	-2.8976	-1.5116	0.2340
C	-3.5014	-0.8048	-1.0271	-3.5131	-0.7972	-1.0061
H	-2.8656	0.0335	-1.3593	-2.8776	0.0416	-1.3381
H	-3.6133	-1.4950	-1.8755	-3.6305	-1.4834	-1.8571
C	-4.8149	-0.2978	-0.4840	-4.8230	-0.2906	-0.4537
C	-6.9406	0.5669	1.1077	-6.9355	0.5703	1.1507
C	-5.9157	0.2840	-1.0901	-5.9250	0.2970	-1.0550
C	-4.7832	-0.4418	0.9133	-4.7843	-0.4418	0.9420
C	-5.8330	-0.0155	1.7293	-5.8290	-0.0168	1.7662
C	-6.9966	0.7186	-0.2907	-7.0001	0.7299	-0.2461
H	-5.9700	0.4162	-2.1724	-5.9708	0.4288	-2.1369
H	-5.7861	-0.1404	2.8124	-5.7770	-0.1469	2.8485
H	-7.7809	0.9058	1.7148	-7.7794	0.9136	1.7519
O	-3.6514	-1.0241	1.3613	-3.6516	-1.0288	1.3816
C	-8.1662	1.3285	-0.9692	-8.2129	1.3579	-0.8254
O	-8.2673	1.4815	-2.1710	-9.1656	1.7540	-0.1827

Atom	6g			6h		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	3.5372	−1.4787	1.8074	3.5370	−1.4898	1.7956
H	2.9690	−1.3008	2.7313	2.9726	−1.3156	2.7225
H	3.5156	−2.5565	1.6064	3.5132	−2.5667	1.5898
H	4.5833	−1.2061	2.0083	4.5842	−1.2195	1.9938
C	3.3084	0.8578	1.0127	3.3077	0.8507	1.0132
H	2.8852	1.0636	2.0095	2.8889	1.0518	2.0128
H	4.3996	0.9344	1.1402	4.3995	0.9254	1.1364
H	−3.1000	−2.5971	0.1551	−3.1068	−2.5958	0.1649
O	−9.1387	1.7120	−0.1191	−8.1702	1.4572	−2.1687
H	−9.8556	2.0960	−0.6533	−8.9995	1.8780	−2.4547
C	2.8666	1.9753	0.0477	2.8629	1.9735	0.0559
H	3.2864	1.8031	−0.9543	3.2788	1.8063	−0.9486
H	1.7690	1.9560	−0.0712	1.7649	1.9554	−0.0590
C	3.2581	3.3395	0.5540	3.2572	3.3347	0.5678
H	2.7237	3.6620	1.4580	2.7259	3.6531	1.4752
C	4.1797	4.1854	0.0542	4.1779	4.1824	0.0695
C	4.4366	5.5231	0.7059	4.4381	5.5166	0.7273
H	3.7983	5.6829	1.5878	5.4940	5.6049	1.0405
H	5.4915	5.6142	1.0218	4.2564	6.3478	0.0221
H	4.2562	6.3506	−0.0040	3.8026	5.6725	1.6119
C	5.0253	3.9129	−1.1658	5.0194	3.9154	−1.1545
H	4.8220	4.6578	−1.9560	4.8635	2.9172	−1.5849
H	6.0974	4.0117	−0.9199	4.8135	4.6639	−1.9407
H	4.8710	2.9127	−1.5922	6.0923	4.0130	−0.9118

Table S15. Electronic energies (ΔE), free energies (ΔG), and Boltzmann distribution abundances for the conformers of bromophycoic acid F (**6**), obtained through DFT calculations at the B3LYP/SVP level of theory in acetonitrile.

Conformers	Energies (Hartree)		Abundance (%)
	ΔE	ΔG	
6a	−3848.596788	−3848.096045	8.1
6b	−3848.596732	−3848.096057	8.2
6c	−3848.596707	−3848.096972	21.6
6d	−3848.596679	−3848.096908	20.2
6e	−3848.595974	−3848.096257	10.1
6f	−3848.595943	−3848.096150	9.0
6g	−3848.596012	−3848.095758	6.0
6h	−3848.595984	−3848.095613	5.1

CHARACTERIZATION OF BROMOPHYCOIC ACID A METHYL ESTER (7)**DFT Calculation****Table S16.** Atomic coordinates for bromophycoic acid A methyl ester (7), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile.

Atom	7a			7b		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	-1.5803	-0.2419	0.1359	-1.4051	-0.0908	0.0944
C	-1.4597	-2.3932	1.4442	-1.3251	-2.2222	1.4391
C	-3.5953	-1.6882	0.3345	-3.4331	-1.5153	0.2808
C	-2.7325	-2.8775	0.7383	-2.5902	-2.7064	0.7187
C	-2.9145	-0.6554	-0.6025	-2.7264	-0.5089	-0.6656
C	-0.6332	-1.4032	0.5920	-0.4752	-1.2518	0.5871
H	-1.7463	-1.8995	2.3888	-1.6235	-1.7123	2.3714
H	-3.9414	-1.1753	1.2404	-3.7843	-0.9813	1.1723
H	-2.4881	-3.4887	-0.1441	-2.3364	-3.3348	-0.1489
H	-1.9226	0.1994	1.0885	-1.7645	0.3654	1.0338
H	-0.8388	-3.2612	1.7243	-0.7166	-3.0911	1.7425
H	-3.3049	-3.5280	1.4165	-3.1806	-3.3399	1.3977
Br	-5.3326	-2.3970	-0.4114	-5.1700	-2.2134	-0.4752
C	-0.7728	0.8677	-0.5614	-0.5772	1.0060	-0.5994
H	-0.2870	0.4862	-1.4744	-0.0785	0.6126	-1.5005
H	-1.4353	1.6783	-0.8969	-1.2283	1.8181	-0.9532
C	0.4449	-0.7816	1.5222	0.5914	-0.6246	1.5268
H	-0.0572	-0.4126	2.4312	0.0766	-0.2374	2.4211
H	1.1381	-1.5690	1.8597	1.2717	-1.4126	1.8885
C	0.0437	-2.1908	-0.5551	0.2175	-2.0630	-0.5343
H	0.9047	-2.7536	-0.1620	1.0735	-2.6170	-0.1182
H	-0.6308	-2.9272	-1.0089	-0.4502	-2.8098	-0.9810
H	0.4072	-1.5527	-1.3717	0.5914	-1.4418	-1.3590
C	0.2690	1.4659	0.3931	0.4515	1.6075	0.3670
H	-0.2525	1.9375	1.2423	-0.0816	2.0905	1.2025
H	0.8437	2.2609	-0.1077	1.0390	2.3943	-0.1319
C	1.2403	0.4348	1.0066	1.4058	0.5769	1.0062
O	1.8600	0.9895	2.1688	2.0154	1.1413	2.1690
H	2.3964	1.7397	1.8692	2.5636	1.8818	1.8666
C	2.3729	0.0759	0.0183	2.5468	0.1953	0.0366
H	1.9633	-0.2425	-0.9505	2.1460	-0.1360	-0.9315
C	3.4295	-0.9339	0.5240	3.5920	-0.8123	0.5692
H	3.3919	-1.0181	1.6223	3.5470	-0.8727	1.6689
H	3.2791	-1.9355	0.0979	3.4361	-1.8214	0.1634
C	4.7241	-0.2894	0.0941	4.8938	-0.1867	0.1334
C	6.7490	1.4540	-0.7027	6.9361	1.5246	-0.6887

Atom	7a			7b		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	6.0351	-0.7343	0.0952	6.2009	-0.6428	0.1462
C	4.4346	1.0254	-0.3037	4.6171	1.1235	-0.2882
C	5.4302	1.9184	-0.6995	5.6214	2.0007	-0.6969
C	7.0666	0.1360	-0.3241	7.2410	0.2109	-0.2858
H	6.2953	-1.7464	0.4102	6.4516	-1.6514	0.4797
H	5.1861	2.9407	-0.9921	5.3870	3.0196	-1.0084
H	7.5325	2.1600	-0.9912	7.7267	2.2182	-0.9883
O	3.1158	1.3145	-0.2511	3.3006	1.4247	-0.2447
C	8.4621	-0.3937	-0.3039	8.6319	-0.3304	-0.2526
O	8.7764	-1.4252	0.2492	8.9372	-1.3513	0.3243
O	9.4133	0.3198	-0.9414	9.5888	0.3603	-0.9064
H	9.0334	1.0610	-1.4362	9.2142	1.0915	-1.4197
C	-2.6757	-1.2237	-2.0167	-2.4608	-1.1096	-2.0614
H	-2.0225	-0.5559	-2.5976	-1.7951	-0.4557	-2.6440
H	-2.2188	-2.2203	-2.0157	-2.0061	-2.1065	-2.0306
H	-3.6296	-1.3036	-2.5583	-3.4041	-1.1999	-2.6196
C	-3.8346	0.5914	-0.7870	-3.6333	0.7383	-0.9011
H	-3.3964	1.2355	-1.5664	-3.1470	1.3792	-1.6546
H	-4.7846	0.2297	-1.2123	-4.5585	0.3821	-1.3805
C	-4.1563	1.4686	0.4391	-4.0312	1.6108	0.3052
H	-3.2438	1.9479	0.8221	-3.1256	2.0153	0.7909
H	-4.5376	0.8344	1.2603	-4.5412	1.0020	1.0669
C	-5.2059	2.5018	0.1206	-4.8981	2.7710	-0.1112
H	-6.1932	2.0854	-0.1221	-4.3858	3.5253	-0.7241
C	-5.0800	3.8422	0.0750	-6.2029	2.9794	0.1502
C	-6.2576	4.7186	-0.2795	-6.9092	4.2103	-0.3661
H	-7.1659	4.1307	-0.4800	-6.2356	4.8643	-0.9400
H	-6.4810	5.4307	0.5353	-7.7593	3.9357	-1.0163
H	-6.0399	5.3323	-1.1723	-7.3363	4.8000	0.4651
C	-3.8052	4.5971	0.3610	-7.0765	2.0508	0.9575
H	-2.9546	3.9454	0.6007	-6.5648	1.1322	1.2735

Table S17. Atomic coordinates for bromophycoic acid A methyl ester (**7**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile (..contd).

Atom	7c			7d		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	1.8064	−0.6170	0.5752	1.7883	−0.6358	0.5776
C	1.9226	−2.6625	−0.9104	1.8946	−2.6677	−0.9260
C	3.8594	−1.1069	−0.7508	3.8339	−1.1141	−0.7640
C	3.4522	−2.5666	−0.8957	3.4242	−2.5720	−0.9207
C	3.3792	−0.4262	0.5549	3.3607	−0.4451	0.5506
C	1.2451	−2.0584	0.3421	1.2256	−2.0750	0.3363
H	1.5568	−2.1270	−1.8033	1.5227	−2.1243	−1.8116
H	3.4820	−0.5457	−1.6143	3.4537	−0.5443	−1.6207
H	3.8865	−3.1730	−0.0862	3.8634	−3.1865	−0.1200
H	1.4532	−0.0708	−0.3114	1.4312	−0.0824	−0.3031
H	1.6140	−3.7147	−1.0343	1.5853	−3.7189	−1.0574
H	3.8536	−2.9688	−1.8381	3.8193	−2.9652	−1.8695
Br	5.8556	−0.9606	−1.0279	5.8293	−0.9700	−1.0492
C	1.1291	0.0737	1.7820	1.1184	0.0456	1.7937
H	1.6663	−0.1491	2.7164	1.6613	−0.1842	2.7230
H	1.2004	1.1623	1.6474	1.1891	1.1352	1.6669
C	−0.2864	−1.9269	0.0325	−0.3083	−1.9423	0.0389
H	−0.4329	−1.8527	−1.0554	−0.4628	−1.8622	−1.0475
H	−0.7868	−2.8553	0.3503	−0.8062	−2.8724	0.3555
C	1.4414	−3.0232	1.5347	1.4314	−3.0490	1.5197
H	2.4914	−3.3081	1.6786	0.8695	−3.9791	1.3365
H	1.0862	−2.6035	2.4867	2.4829	−3.3328	1.6546
H	0.8790	−3.9536	1.3551	1.0816	−2.6373	2.4771
C	−0.3525	−0.3078	1.9699	−0.3620	−0.3376	1.9881
H	−0.9072	0.5311	2.4178	−0.9139	0.4979	2.4459
H	−0.4535	−1.1478	2.6750	−0.4587	−1.1829	2.6873
C	−1.0207	−0.7180	0.6511	−1.0378	−0.7371	0.6699
O	−0.9499	0.3560	−0.2945	−0.9696	0.3435	−0.2680
H	−1.4230	1.1085	0.0934	−1.4305	1.0974	0.1317
C	−2.5035	−1.0671	0.8750	−2.5203	−1.0855	0.8980
H	−2.5832	−1.8395	1.6584	−2.5980	−1.8676	1.6718
C	−3.3093	−1.4760	−0.3806	−3.3314	−1.4768	−0.3605
H	−2.8041	−1.1256	−1.2953	−2.8215	−1.1278	−1.2731
H	−3.4357	−2.5651	−0.4530	−3.4715	−2.5639	−0.4389
C	−4.6060	−0.7294	−0.1832	−4.6183	−0.7150	−0.1592
C	−6.6236	1.0417	0.5719	−6.6264	1.0527	0.6241
C	−5.8232	−0.7751	−0.8410	−5.8349	−0.7400	−0.8241
C	−4.4061	0.2026	0.8484	−4.4150	0.1972	0.8871
C	−5.3958	1.1044	1.2380	−5.4039	1.0936	1.2960
C	−6.8586	0.1051	−0.4519	−6.8576	0.1550	−0.4354
H	−6.0085	−1.4793	−1.6540	−5.9854	−1.4707	−1.6239
H	−5.2149	1.8308	2.0317	−5.2243	1.7909	2.1159

Atom	7c			7d		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
H	−7.3932	1.7628	0.8604	−7.4347	1.7255	0.9156
O	−3.1741	0.1249	1.3977	−3.1856	0.1008	1.4391
C	−8.1529	0.0125	−1.1896	−8.2040	0.1818	−1.0796
O	−8.2857	−0.5909	−2.2321	−9.1619	0.7540	−0.6070
O	−9.2249	0.6333	−0.6545	−8.3470	−0.4660	−2.2548
H	−9.0332	0.9809	0.2292	−7.4986	−0.7908	−2.5909
C	4.0949	−1.0132	1.7894	4.0846	−1.0441	1.7747
H	3.6589	−0.6250	2.7207	5.1419	−0.7415	1.7697
H	5.1559	−0.7243	1.7798	4.0606	−2.1401	1.8024
H	4.0563	−2.1080	1.8367	3.6445	−0.6784	2.7132
C	3.7126	1.0974	0.5412	3.6947	1.0785	0.5490
H	3.3900	1.5259	1.5033	3.4023	1.4941	1.5265
H	4.8102	1.1965	0.5313	4.7918	1.1752	0.5075
C	3.1380	1.9611	−0.5982	3.0885	1.9600	−0.5594
H	2.0482	1.8392	−0.6651	1.9925	1.8830	−0.5594
H	3.5472	1.6094	−1.5631	3.4237	1.5885	−1.5454
C	3.4901	3.4163	−0.4385	3.5112	3.3995	−0.4301
H	4.5670	3.6331	−0.4517	4.5965	3.5641	−0.4758
C	2.6566	4.4613	−0.2703	2.7339	4.4864	−0.2580
C	3.1938	5.8649	−0.1212	3.3425	5.8639	−0.1448
H	2.7953	6.5276	−0.9106	2.9584	6.5331	−0.9358
H	2.8792	6.3091	0.8404	3.0728	6.3380	0.8161
H	4.2926	5.8953	−0.1706	4.4400	5.8391	−0.2196
C	1.1509	4.3627	−0.2180	1.2272	4.4630	−0.1677
H	0.7733	3.3343	−0.2959	0.7981	3.4538	−0.2267

Table S18. Atomic coordinates for bromophycoic acid A methyl ester (**7**), obtained through DFT calculation at the B3LYP/SVP level of theory in acetonitrile (..contd).

Atom	7e			7f		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
C	1.5324	-0.7881	0.6198	1.5293	-0.7841	0.6203
C	1.5802	-2.5260	-1.2168	1.5690	-2.5230	-1.2156
C	3.5795	-1.1103	-0.7614	3.5745	-1.1155	-0.7615
C	3.1124	-2.4961	-1.1869	3.1013	-2.4994	-1.1863
C	3.1114	-0.6721	0.6488	3.1087	-0.6748	0.6488
C	0.9172	-2.1383	0.1264	0.9083	-2.1320	0.1278
H	1.2417	-1.8189	-1.9935	1.2331	-1.8148	-1.9924
H	3.2384	-0.3771	-1.5025	3.2364	-0.3811	-1.5027
H	3.5168	-3.2654	-0.5116	3.5028	-3.2702	-0.5109
H	1.2199	-0.0745	-0.1566	1.2195	-0.0694	-0.1563
H	1.2315	-3.5236	-1.5349	1.2161	-3.5193	-1.5330
H	3.5031	-2.7236	-2.1901	3.4907	-2.7289	-2.1896
Br	5.5840	-1.0068	-0.9977	5.5793	-1.0211	-0.9985
C	0.8657	-0.2946	1.9258	0.8653	-0.2872	1.9264
H	1.3811	-0.7004	2.8096	1.3802	-0.6938	2.8102
H	0.9805	0.7972	1.9858	0.9836	0.8042	1.9854
C	-0.6074	-1.9020	-0.1532	-0.6153	-1.8895	-0.1512
H	-0.7497	-1.6493	-1.2146	-0.7570	-1.6350	-1.2123
H	-1.1450	-2.8488	0.0138	-1.1564	-2.8346	0.0147
C	1.0726	-3.3092	1.1238	1.0594	-3.3031	1.1257
H	0.4907	-4.1765	0.7719	0.4727	-4.1676	0.7754
H	2.1129	-3.6416	1.2259	2.0983	-3.6407	1.2261
H	0.7122	-3.0589	2.1318	0.7023	-3.0503	2.1341
C	-0.6333	-0.6417	2.0323	-0.6346	-0.6294	2.0348
H	-1.1605	0.1278	2.6174	-1.1586	0.1418	2.6204
H	-0.7785	-1.5884	2.5759	-0.7822	-1.5755	2.5788
C	-1.2956	-0.7833	0.6560	-1.2993	-0.7691	0.6594
O	-1.1555	0.4309	-0.0899	-1.1571	0.4448	-0.0866
H	-1.5932	1.1303	0.4197	-1.5921	1.1453	0.4238
C	-2.7982	-1.0910	0.7949	-2.8022	-1.0730	0.8013
H	-2.9341	-1.9764	1.4382	-2.9390	-1.9590	1.4435
C	-3.5838	-1.2463	-0.5294	-3.5918	-1.2253	-0.5210
H	-3.0224	-0.8023	-1.3672	-3.0332	-0.7782	-1.3593
H	-3.7821	-2.3002	-0.7694	-3.7899	-2.2787	-0.7635
C	-4.8329	-0.4450	-0.2583	-4.8397	-0.4251	-0.2423
C	-6.7587	1.3301	0.6991	-6.7733	1.3252	0.7410
C	-6.0137	-0.2875	-0.9634	-6.0287	-0.2741	-0.9396
C	-4.6215	0.2888	0.9201	-4.6257	0.3044	0.9366
C	-5.5663	1.1874	1.4152	-5.5776	1.1886	1.4475
C	-7.0038	0.5961	-0.4766	-7.0137	0.6135	-0.4497
H	-6.2037	-0.8329	-1.8895	-6.1890	-0.8666	-1.8449
H	-5.3771	1.7589	2.3251	-5.3908	1.7429	2.3688

Atom	7e			7f		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>x</i>	<i>y</i>	<i>z</i>
H	−7.4900	2.0518	1.0735	−7.5527	1.9953	1.1076
O	−3.4264	0.0315	1.4953	−3.4262	0.0497	1.5043
C	−8.2564	0.7311	−1.2769	−8.3306	0.8184	−1.1219
O	−8.3716	0.3195	−2.4109	−9.2741	1.3672	−0.5957
O	−9.3096	1.3415	−0.6947	−8.4619	0.3667	−2.3869
H	−9.1443	1.5233	0.2423	−7.6183	0.0504	−2.7426
C	3.7853	−1.5193	1.7495	3.7794	−1.5245	1.7494
H	3.7493	−2.5977	1.5550	3.7394	−2.6028	1.5548
H	4.8457	−1.2424	1.8382	4.8408	−1.2516	1.8384
H	3.3182	−1.3422	2.7287	3.3127	−1.3458	2.7286
C	3.5190	0.8064	0.9319	3.5230	0.8020	0.9310
H	3.2445	1.0436	1.9729	3.2507	1.0408	1.9723
H	4.6190	0.8551	0.9032	4.6231	0.8460	0.9011
C	2.9719	1.9153	0.0118	2.9795	1.9130	0.0112
H	1.8680	1.9054	0.0279	1.8756	1.9090	0.0305
H	3.2649	1.7247	−1.0314	3.2684	1.7195	−1.0326
C	3.4343	3.2819	0.4473	3.4507	3.2775	0.4438
H	3.0125	3.6230	1.4027	3.0350	3.6210	1.4011
C	4.2995	4.1101	−0.1690	4.3167	4.1014	−0.1771
C	4.6444	5.4544	0.4263	4.6708	5.4443	0.4159
H	5.7292	5.5360	0.6199	4.1440	5.6314	1.3637
H	4.3953	6.2725	−0.2737	5.7569	5.5208	0.6041
H	4.1120	5.6384	1.3716	4.4222	6.2633	−0.2832
C	4.9935	3.8091	−1.4748	5.0028	3.7967	−1.4862
H	4.7859	2.8011	−1.8573	6.0977	3.8902	−1.3772

Table S19. Electronic energies (ΔE), free energies (ΔG), and Boltzmann distribution abundances for the conformers of bromophycoic acid A methyl ester (**7**), obtained through DFT calculations at the B3LYP/SVP level of theory in acetonitrile.

Conformers	Energies (Hartree)		Abundance (%)
	ΔE	ΔG	
7a	−3924.974457	−3924.445987	41.2
7b	−3924.974442	−3924.445949	39.6
7c	−3924.971486	−3924.444208	6.3
7d	−3924.971318	−3924.444192	6.2
7e	−3924.971373	−3924.443598	3.3
7f	−3924.971174	−3924.443657	3.5

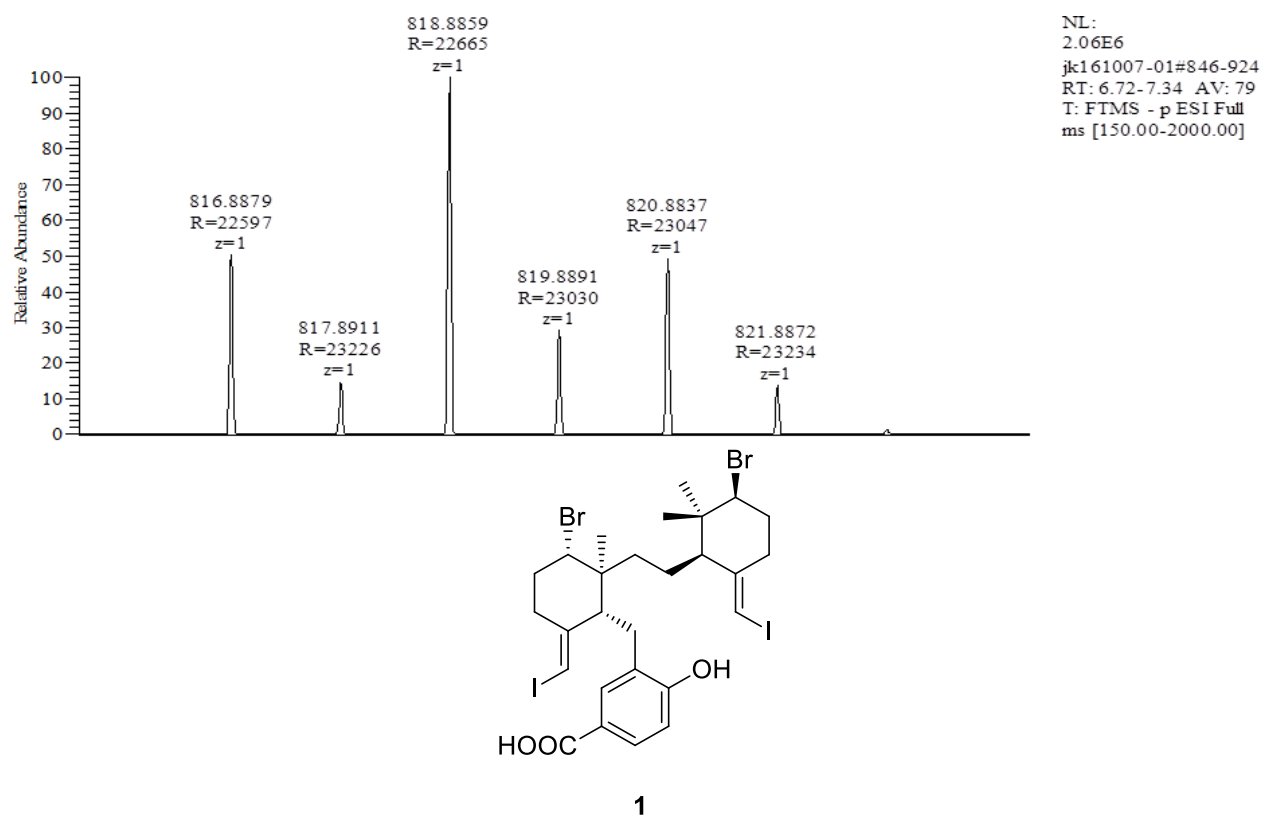
SPECTRA OF IODOCALLOPHYCOIC ACID A (1)**Figure S6.** Negative-mode HRESIMS spectrum of iodiccallophycoic acid A (1)

Figure S7. ^1H NMR spectrum of iodocallophycoic acid **1** at 800 MHz in CD_3OD .

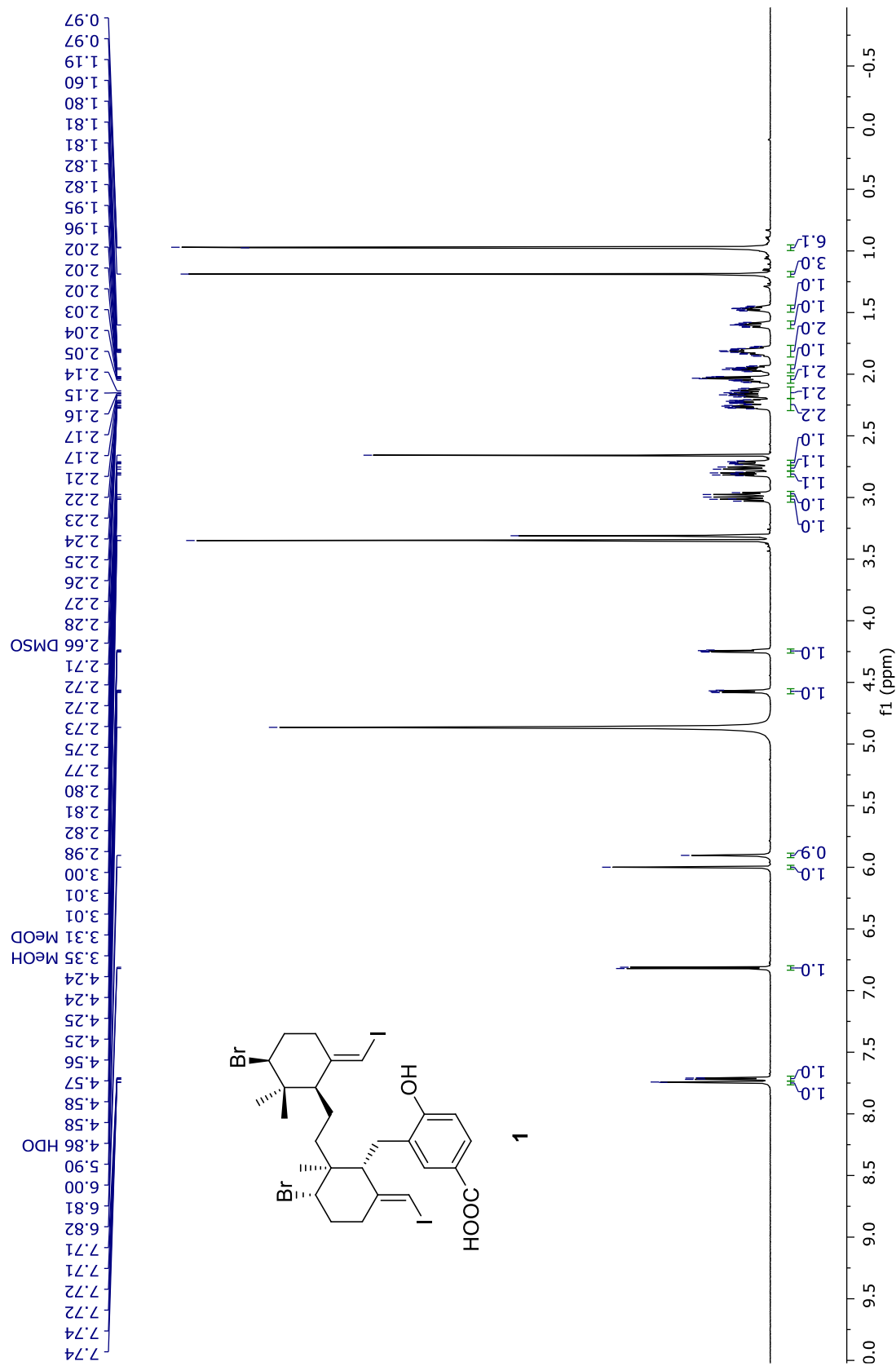


Figure S8. Enlarged ^1H NMR spectrum of iodocallophycoic acid **1** (**1**) at 800 MHz in CD_3OD .

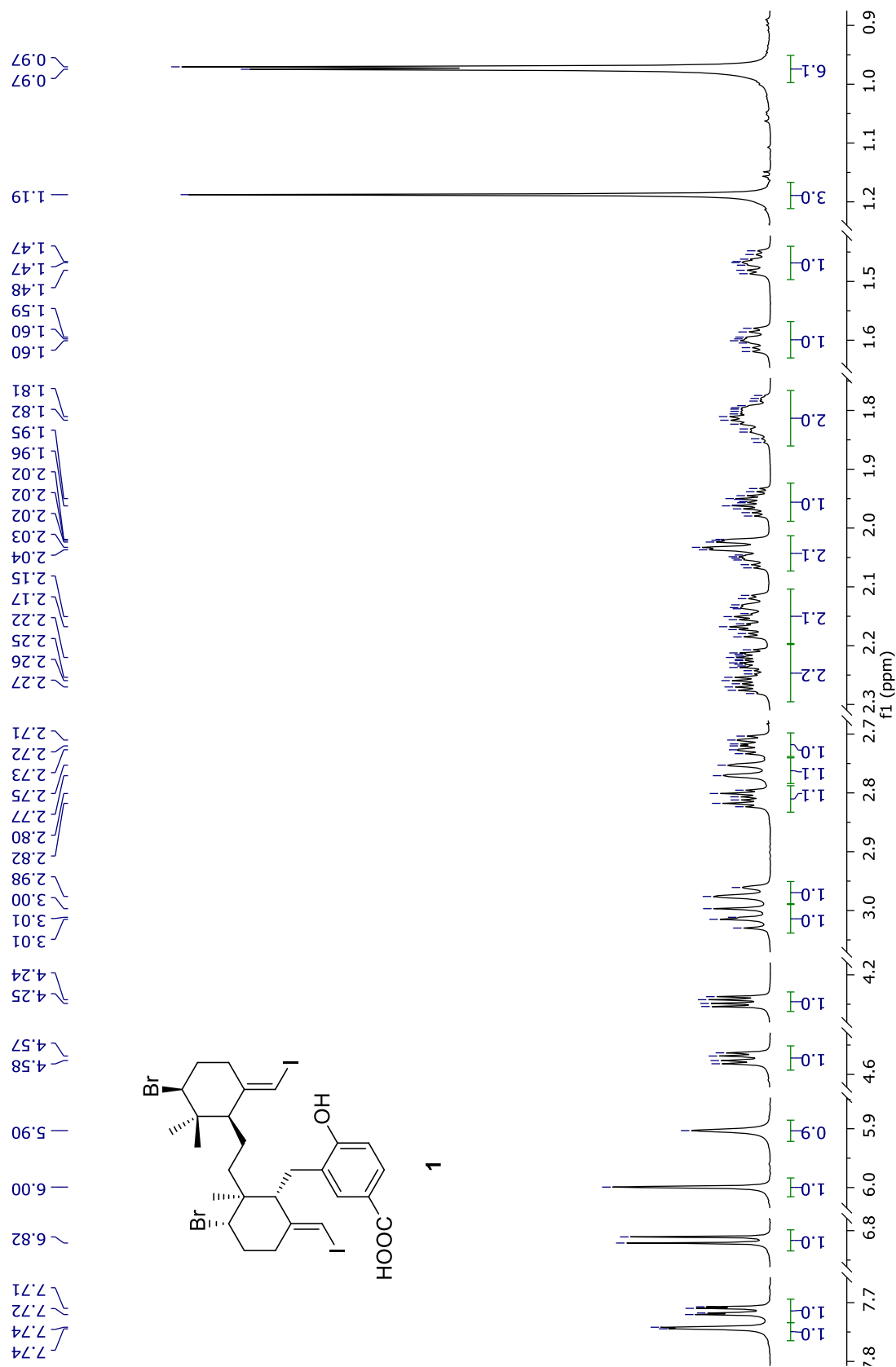


Figure S9. ^{13}C NMR spectrum of iodocallophycoic acid A (**1**) at 200 MHz in CD_3OD .

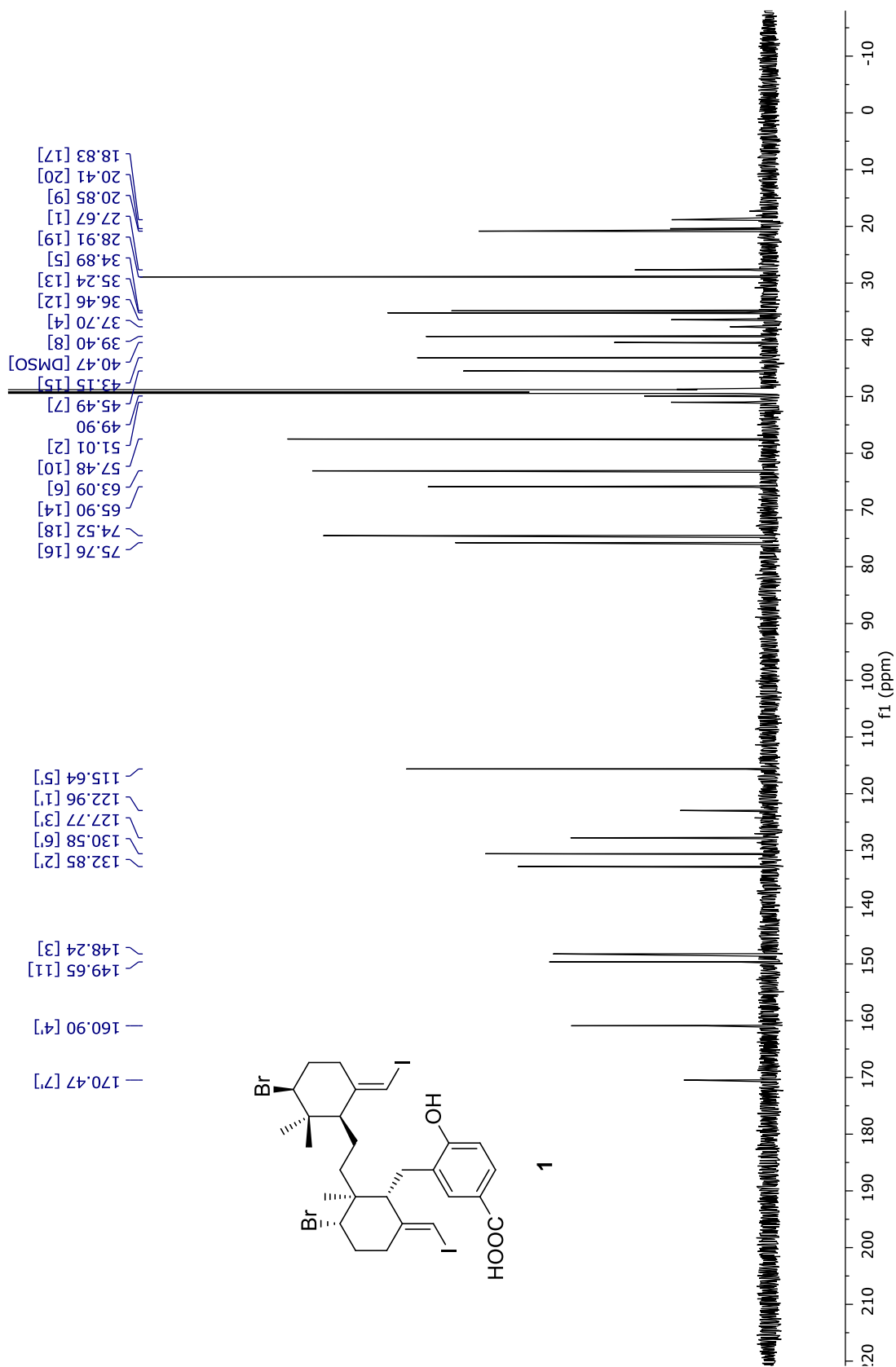


Figure S10. ^1H - ^1H DQF-COSY spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD .

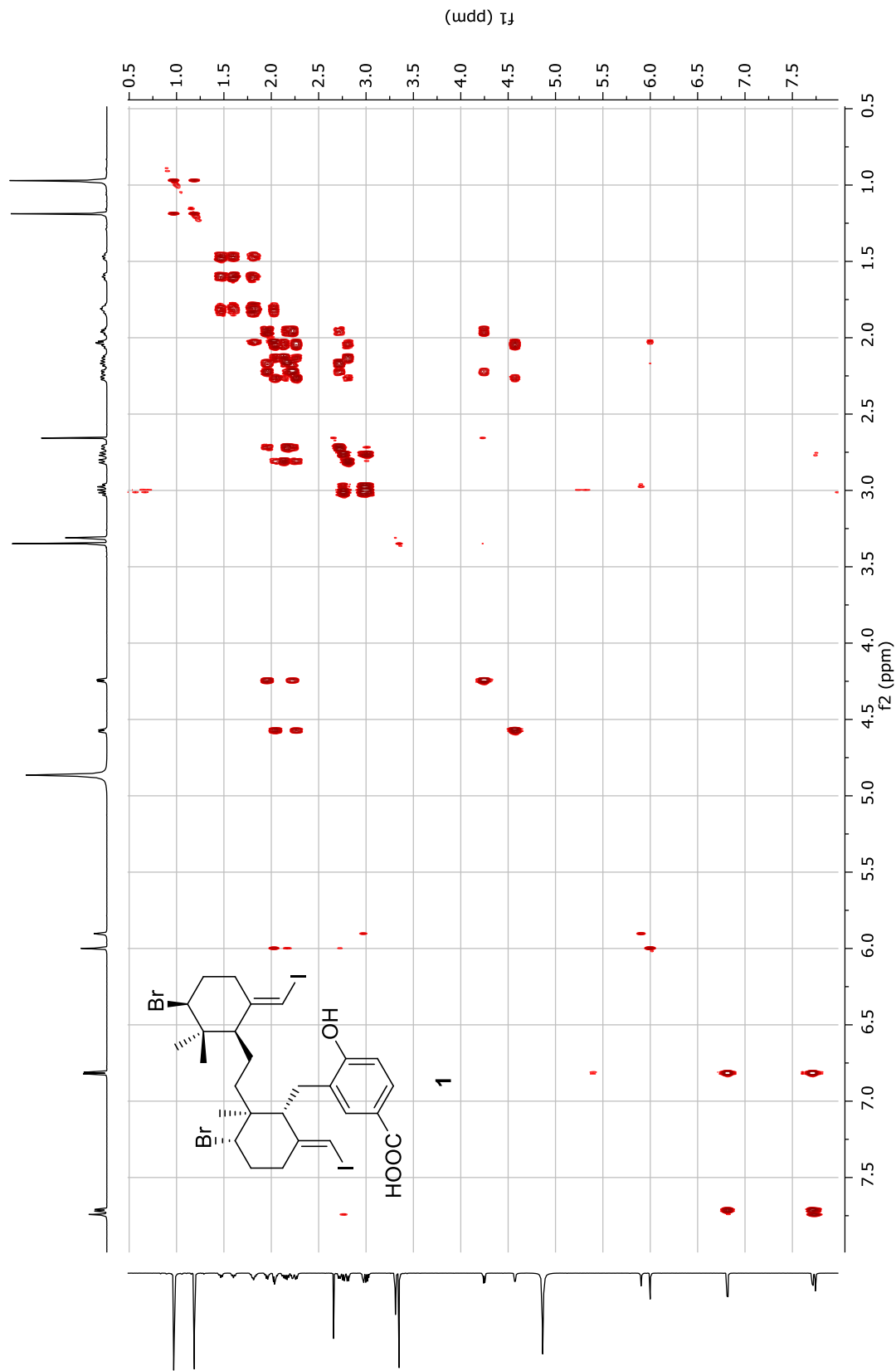


Figure S11. ^1H - ^{13}C edited-HSQC spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD .

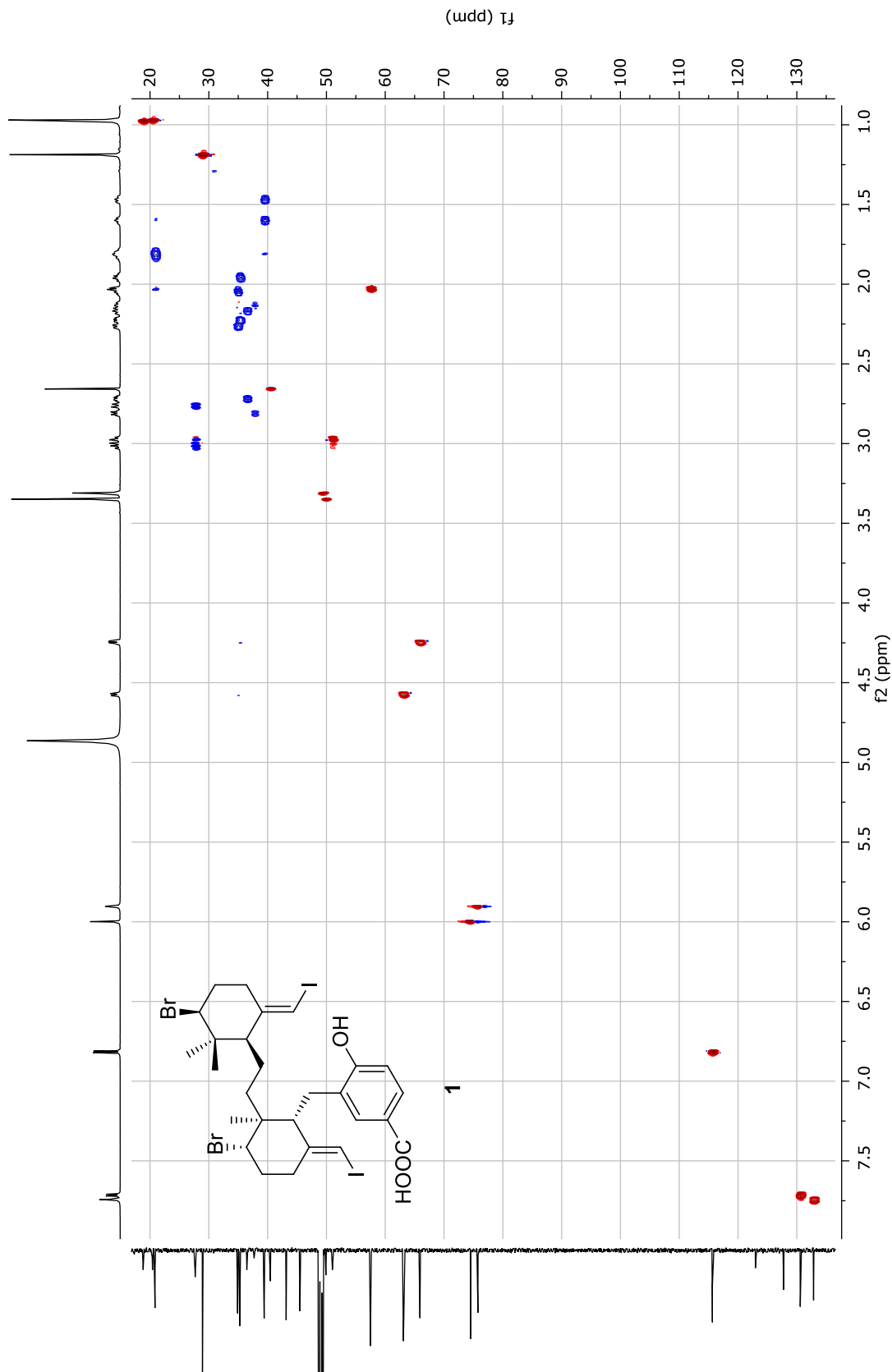


Figure S12. ^1H - ^{13}C HMBC spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD .

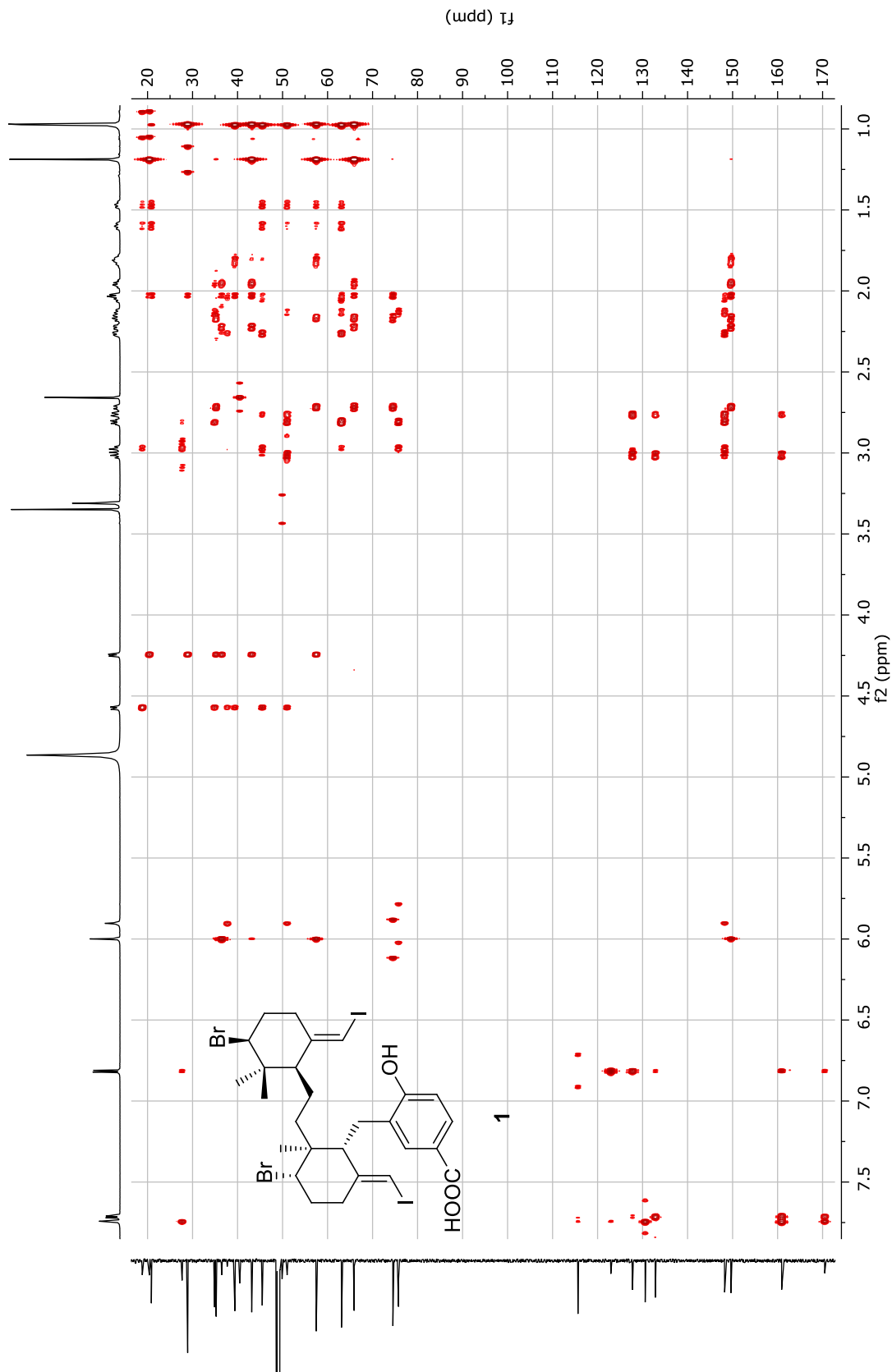
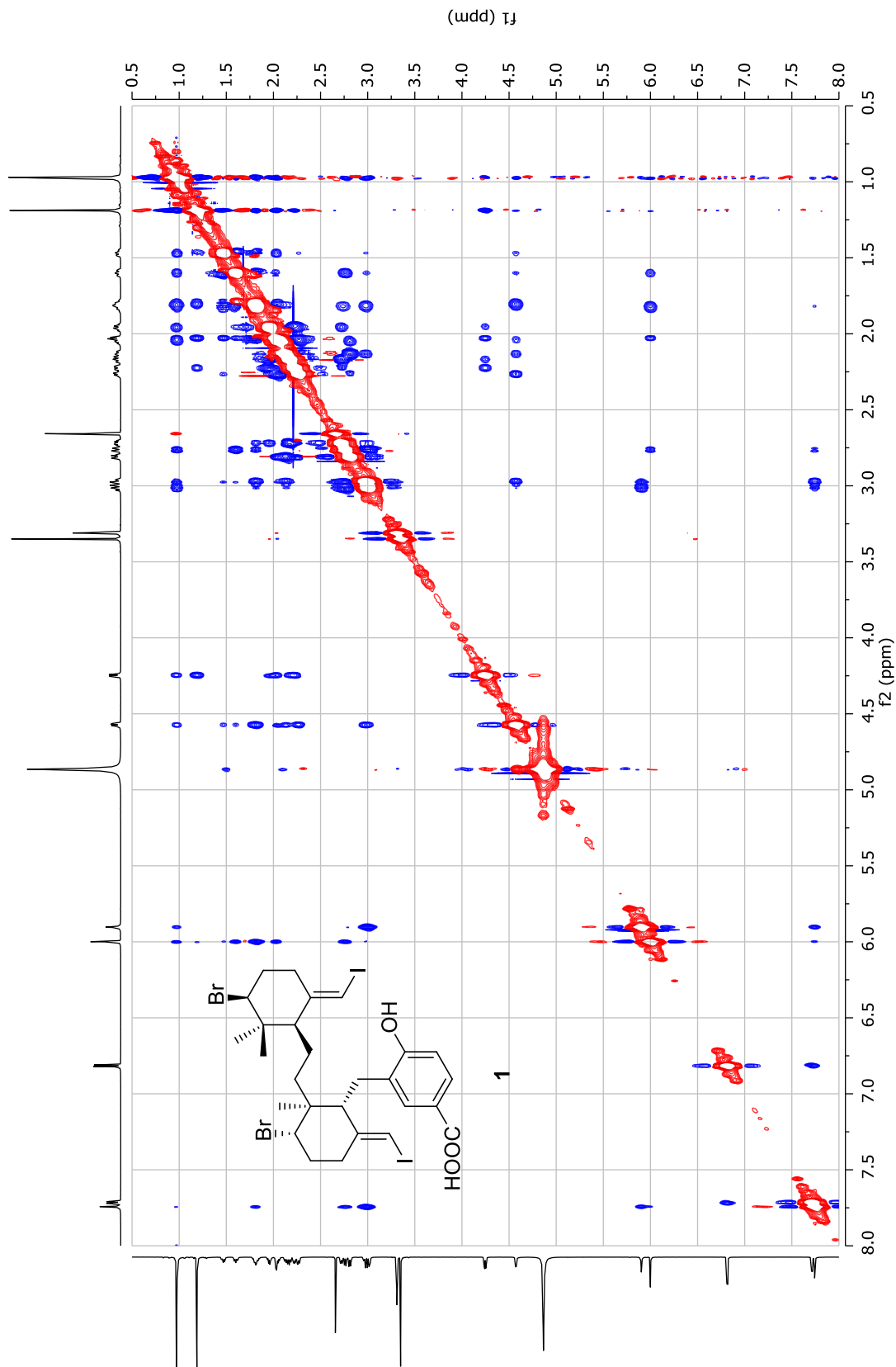
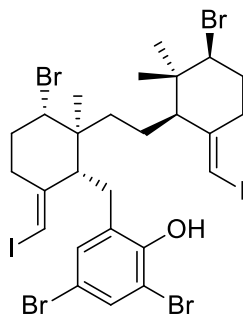
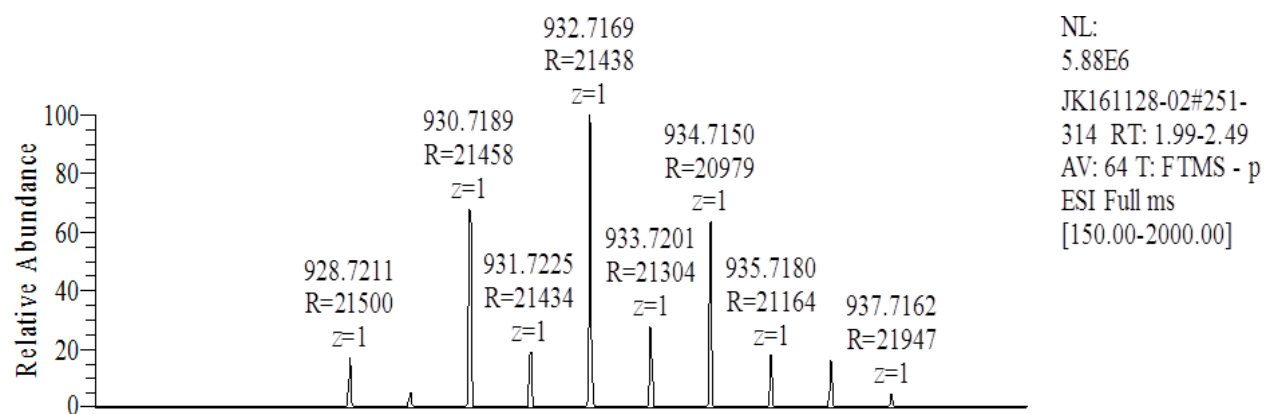


Figure S13. ^1H - ^1H NOESY spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD .



SPECTRA OF IODOCALLOPHYCOL A (2)**Figure S14.** Negative-mode HRESIMS spectrum of iodocallophycol A (2).**2**

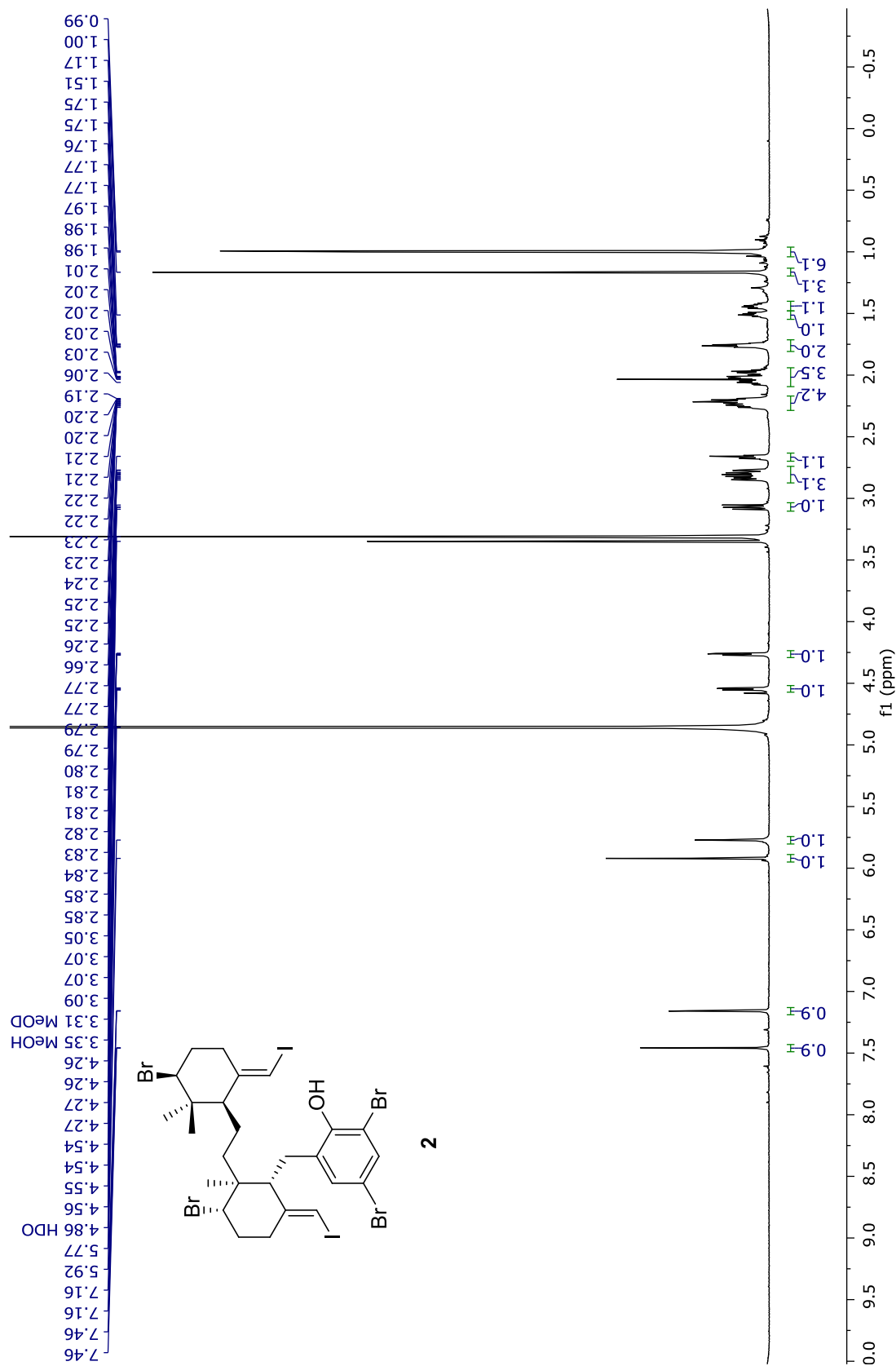


Figure S16. Enlarged ^1H NMR spectrum of iodocallophycol A (2) at 800 MHz in CD_3OD .

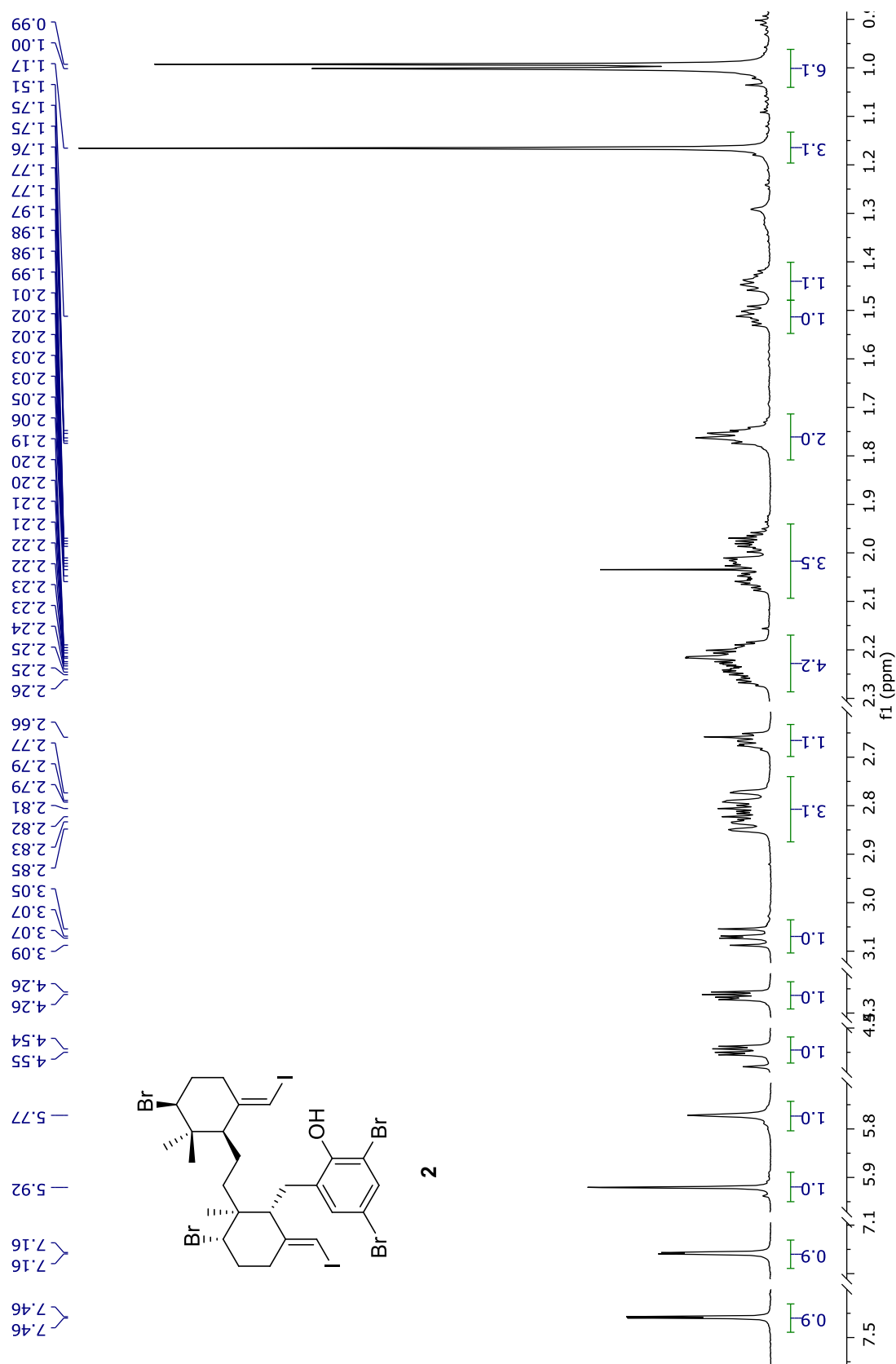
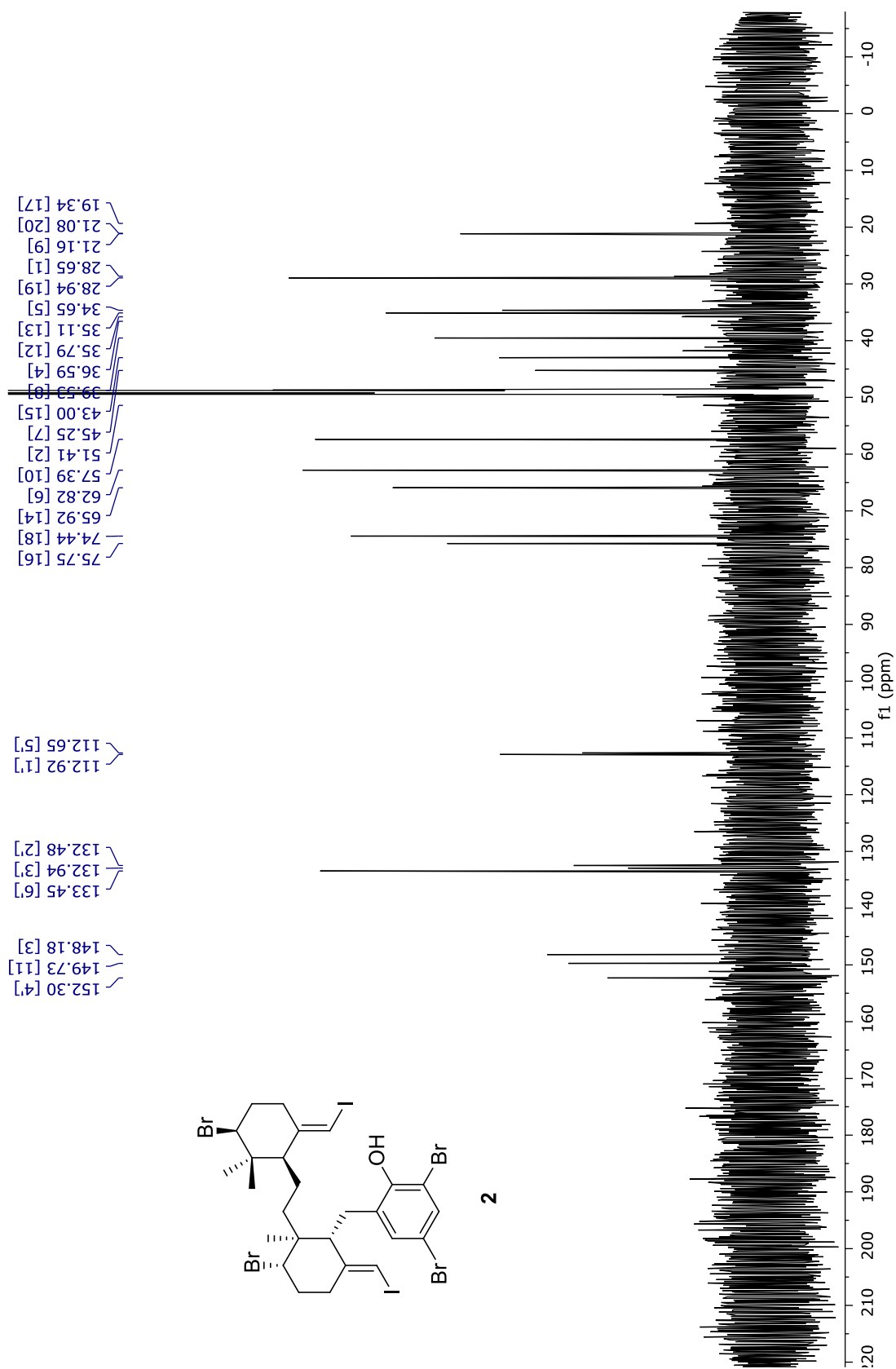


Figure S17. ^{13}C NMR spectrum of iodocallophycol A (2) at 200 MHz in CD_3OD .



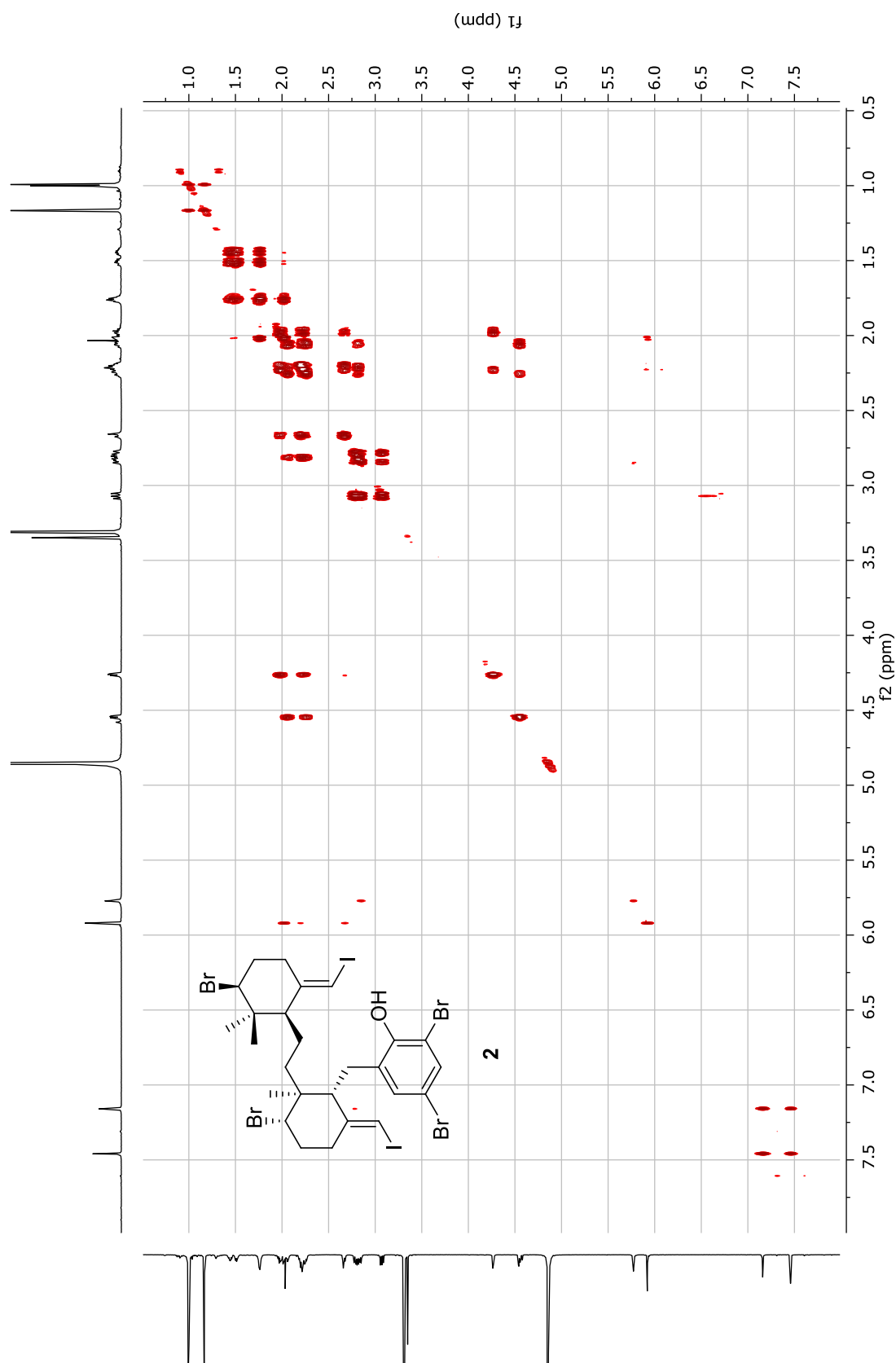


Figure S19. ^1H - ^{13}C edited-HSQC spectrum of iodocallophycol A (**2**) at 800 MHz in CD_3OD .

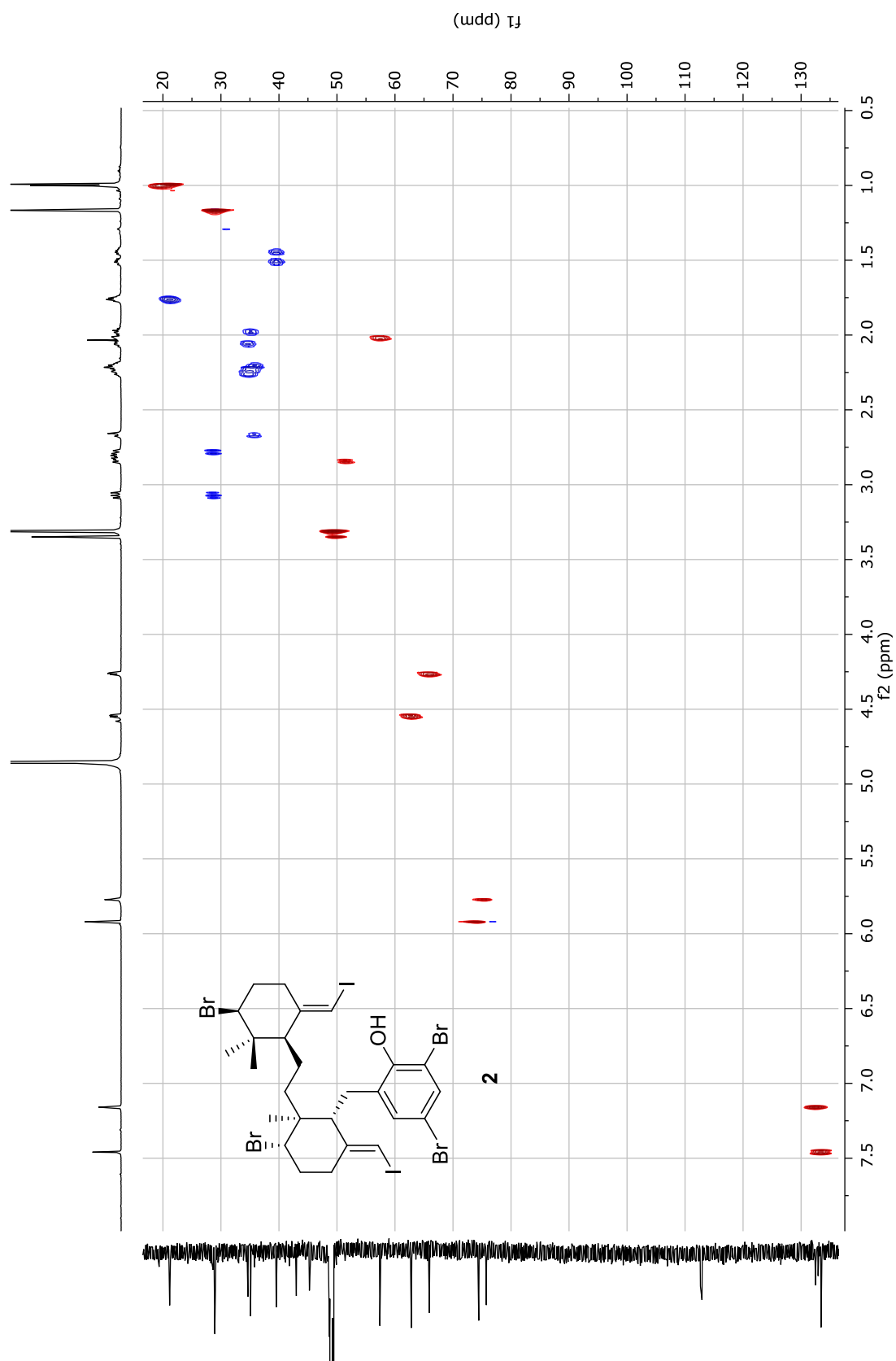
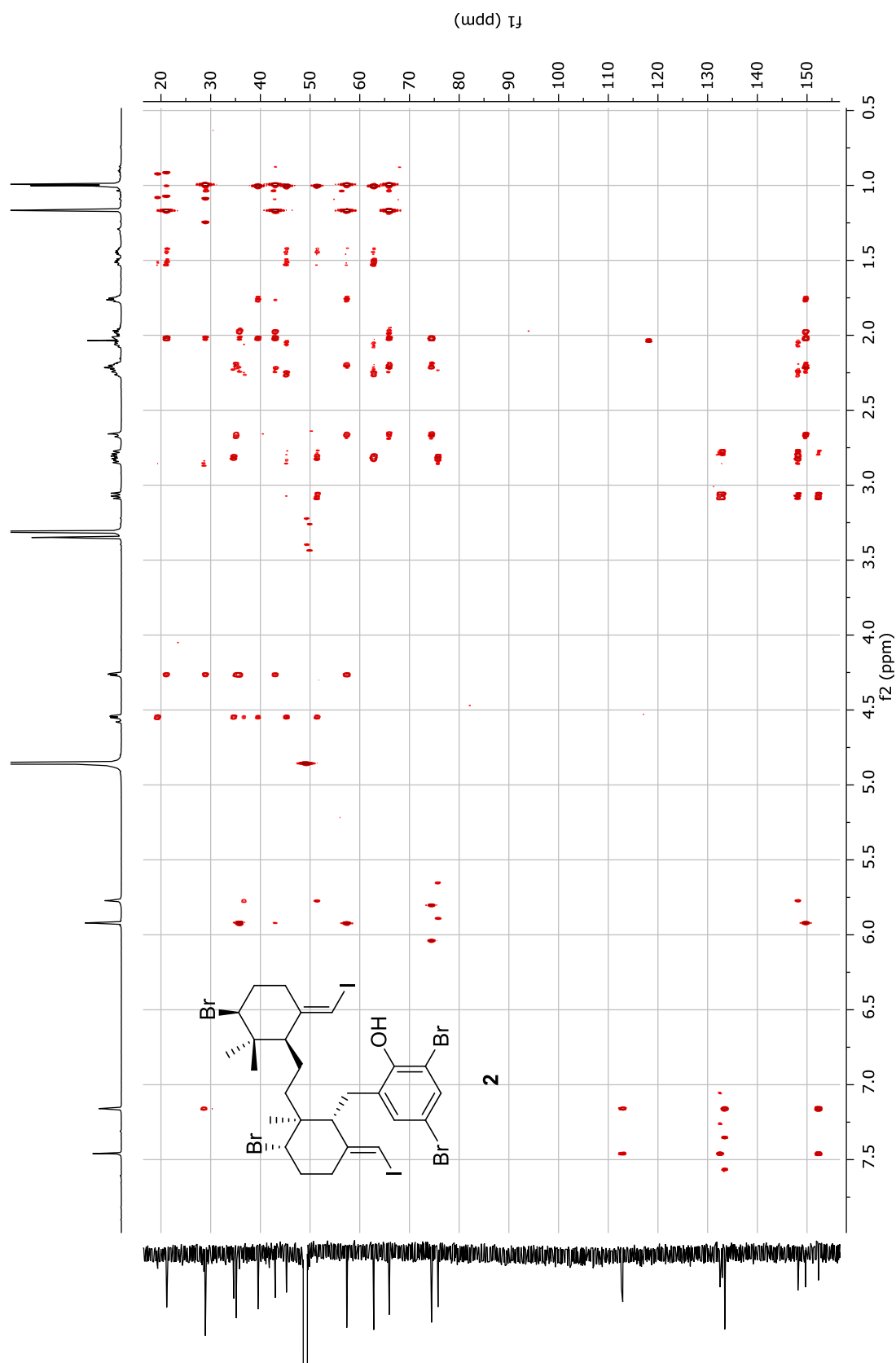
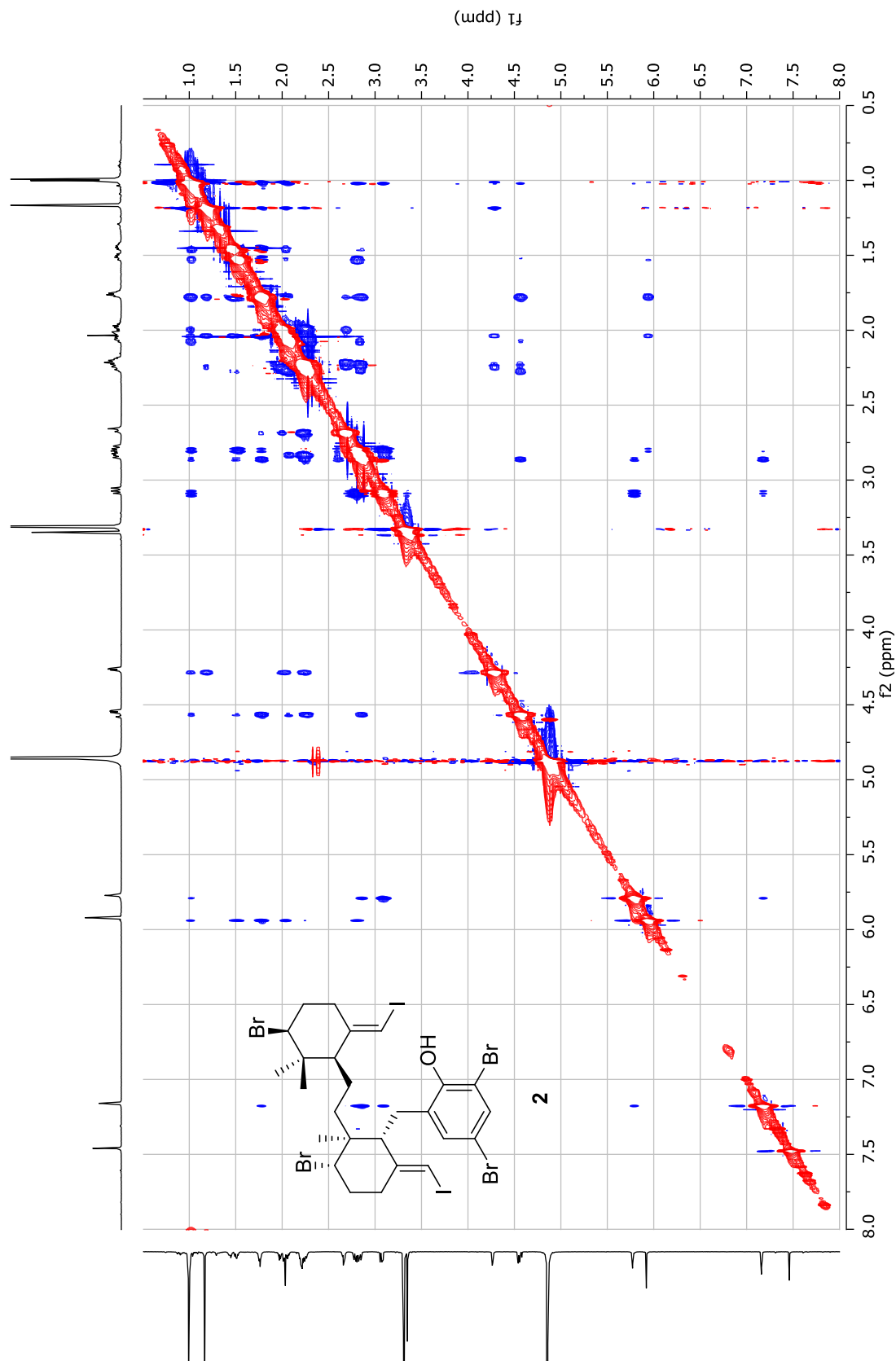


Figure S20. ^1H - ^{13}C HMBC spectrum of iodocallophycol A (2) at 800 MHz in CD_3OD .





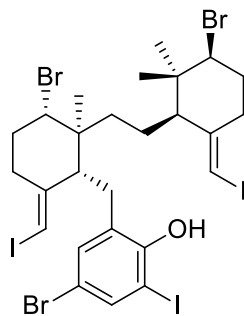
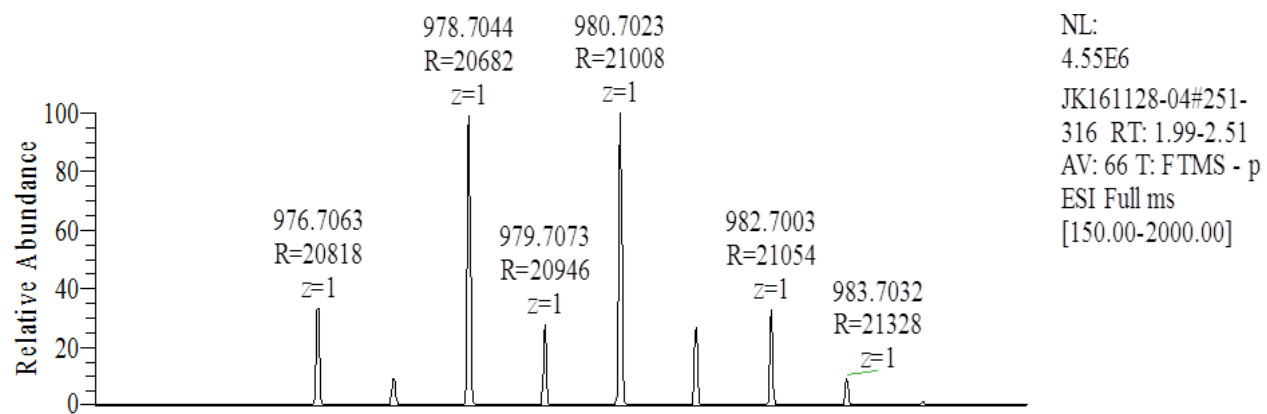
SPECTRA OF IODOCALLOPHYCOL B (3)**Figure S22.** Negative-mode HRESIMS spectrum of iodocallophycol B (3).**3**

Figure S23. ^1H NMR spectrum of iodocallophycol B (3) at 800 MHz in CD_3OD .

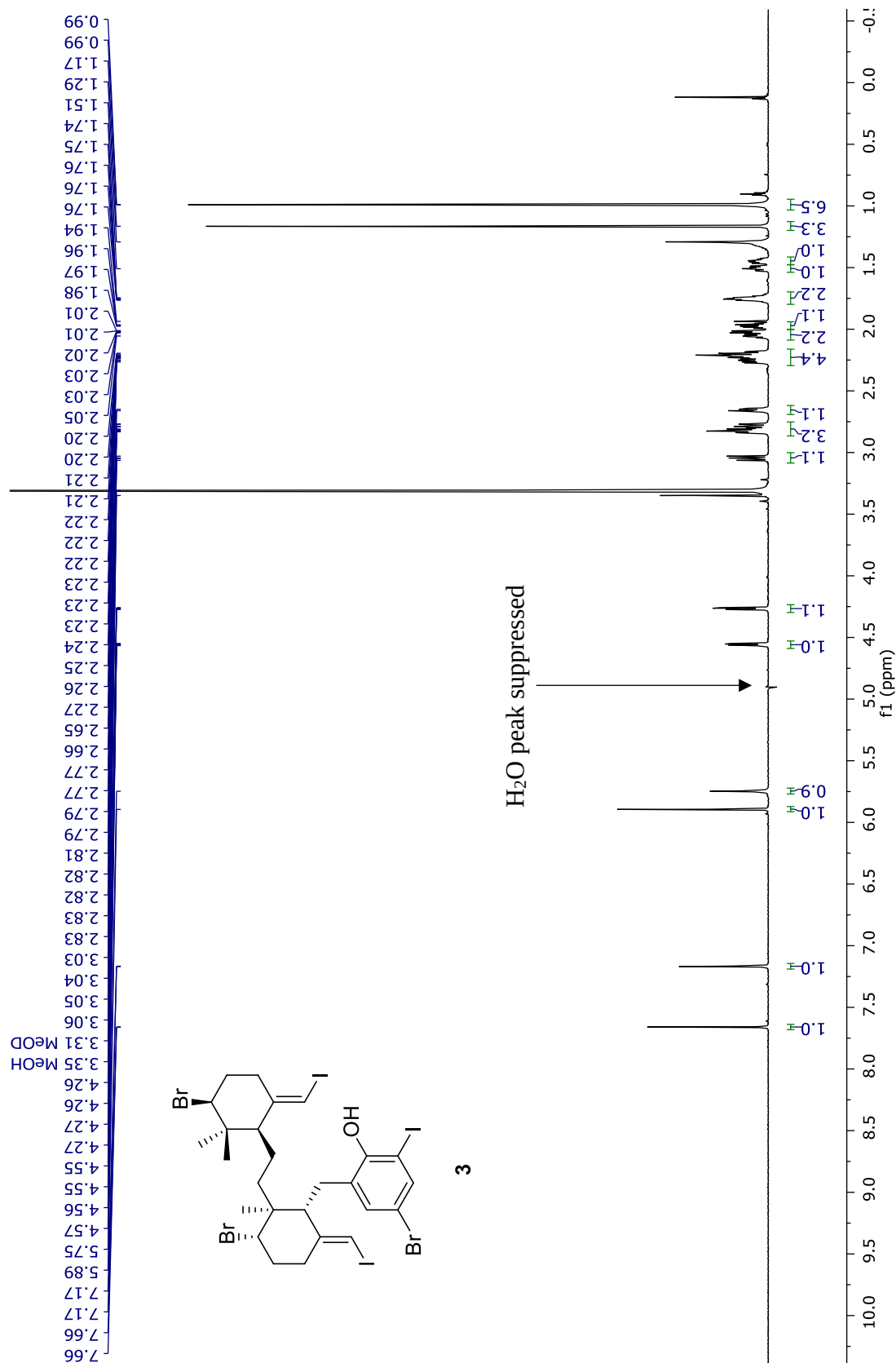


Figure S24. Enlarged ^1H NMR spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD .

Figure S25. ^{13}C NMR spectrum of iodocallophycol B (3) at 200 MHz in CD_3OD .

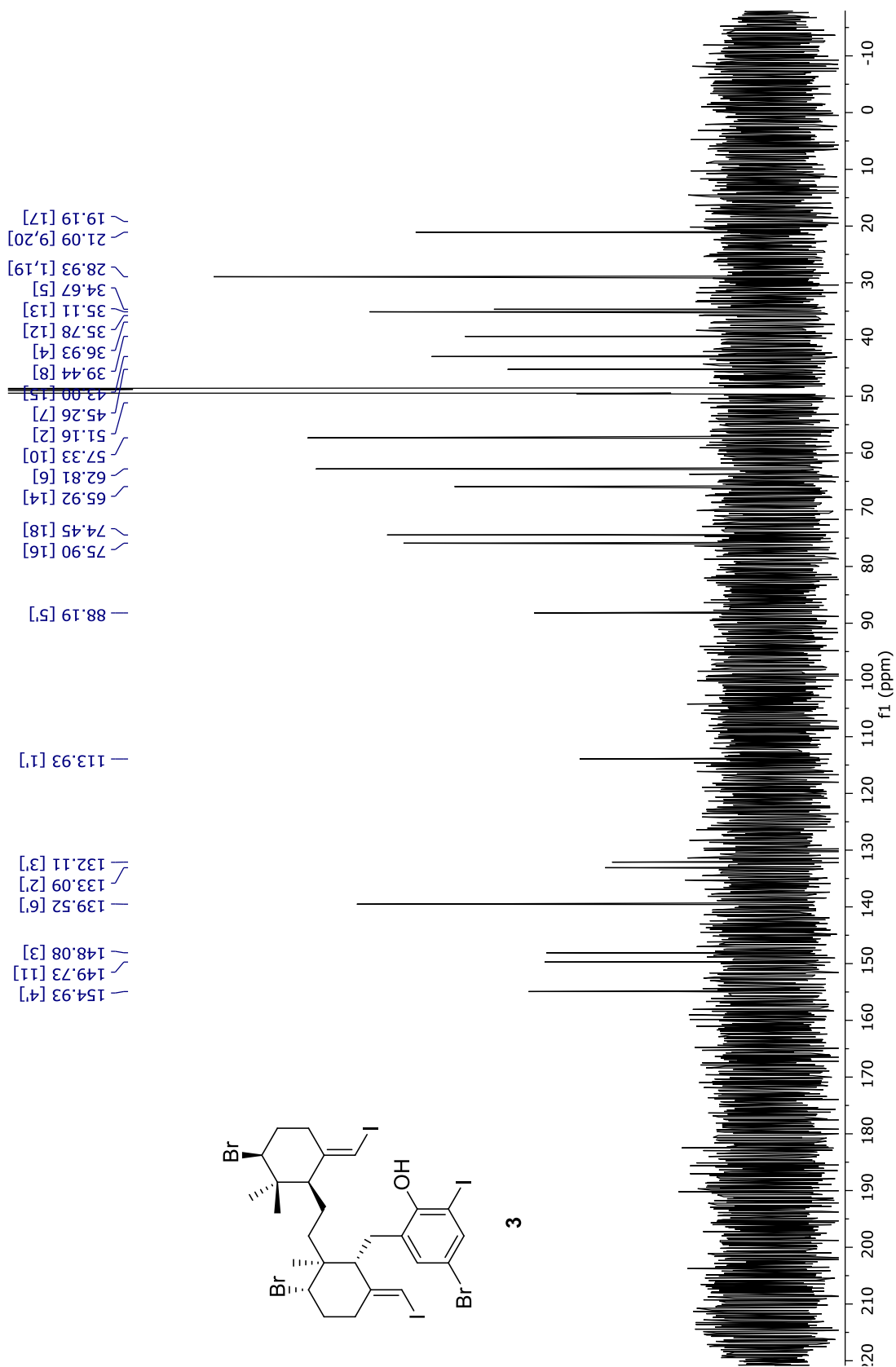


Figure S26. ^1H - ^1H DQF-COSY spectrum of iodocallophycol B (3) at 800 MHz in CD_3OD .

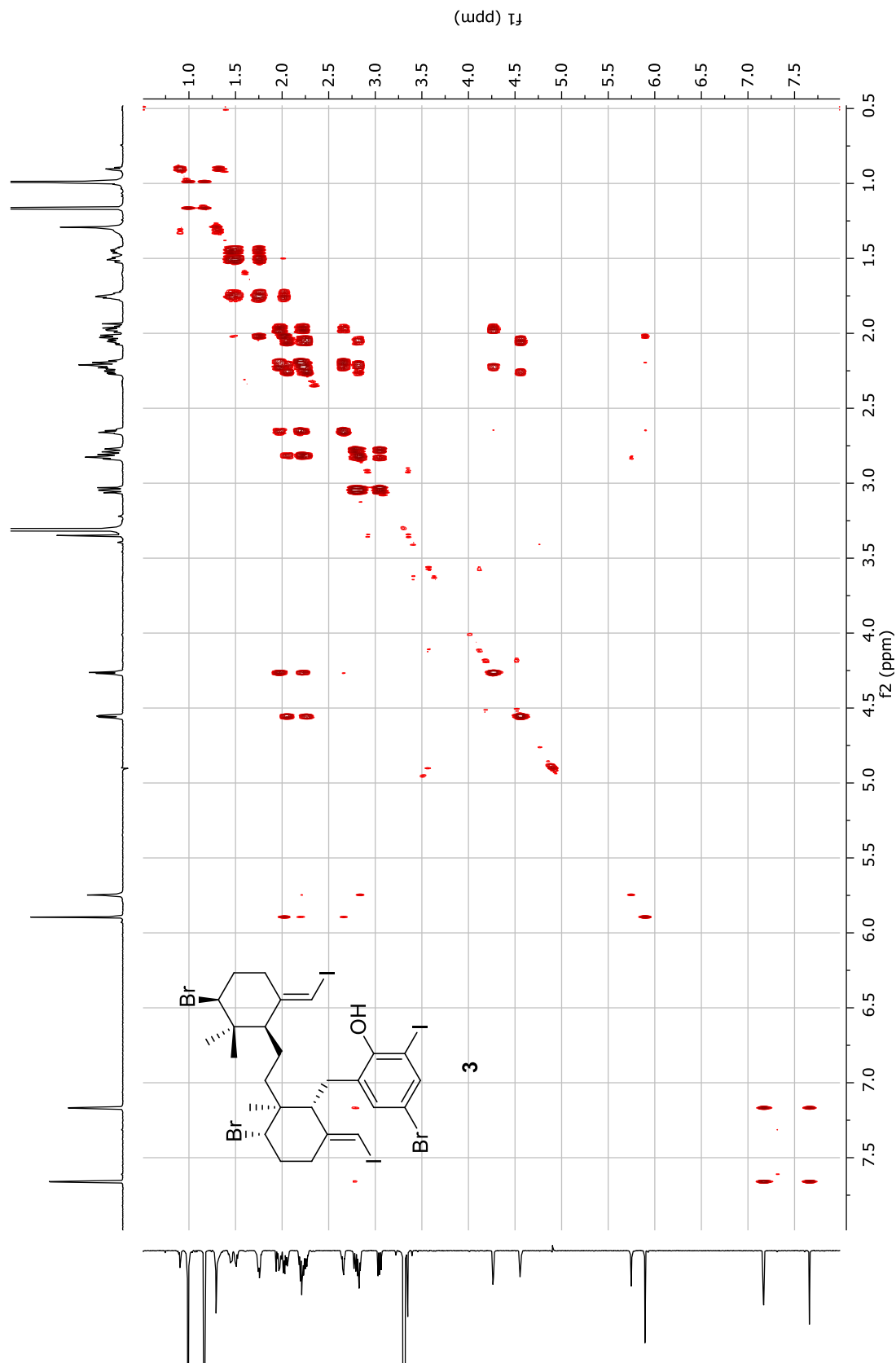


Figure S27. ^1H - ^{13}C edited-HSQC spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD .

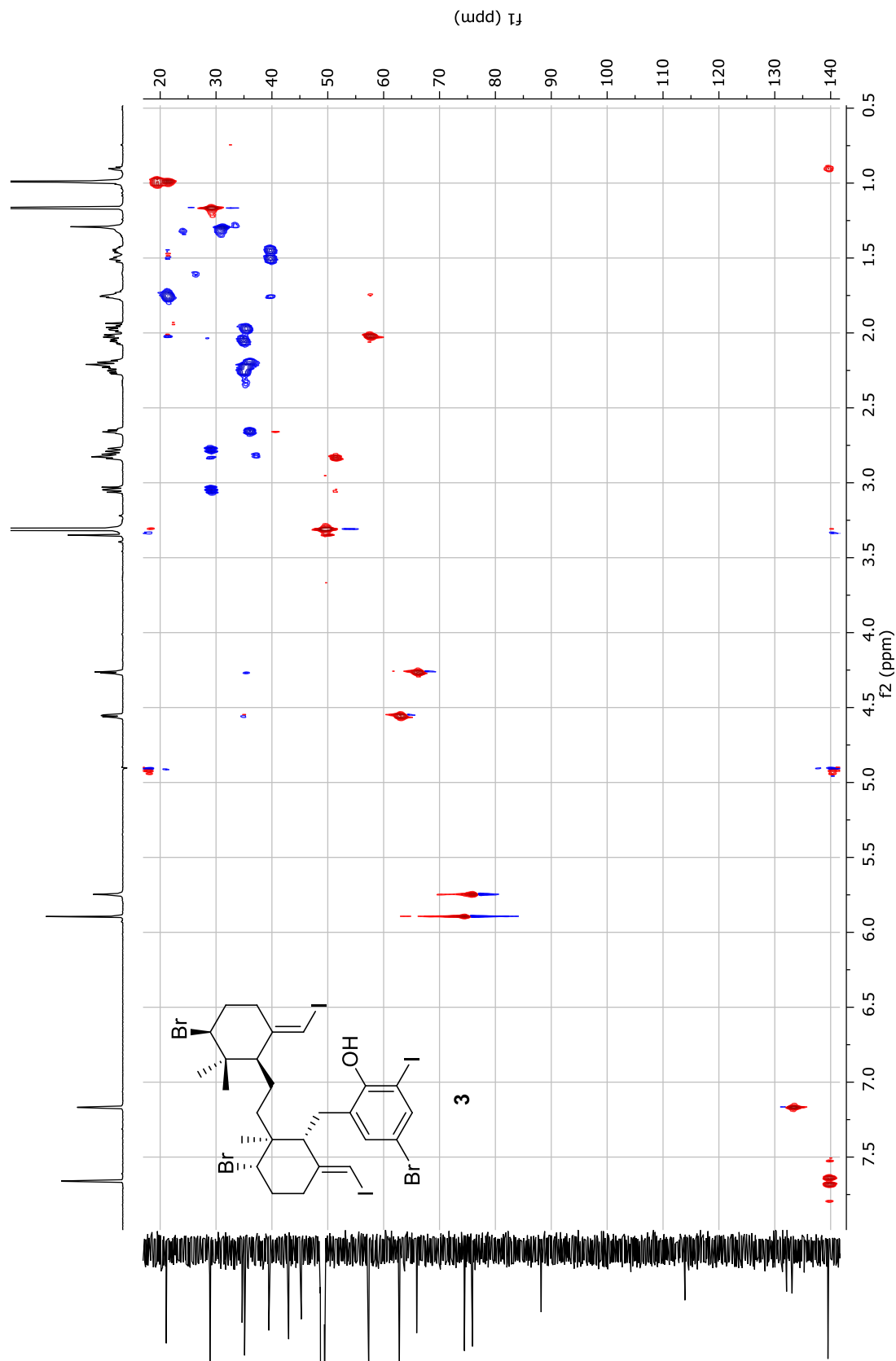


Figure S28. ^1H - ^{13}C HMBC spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD .

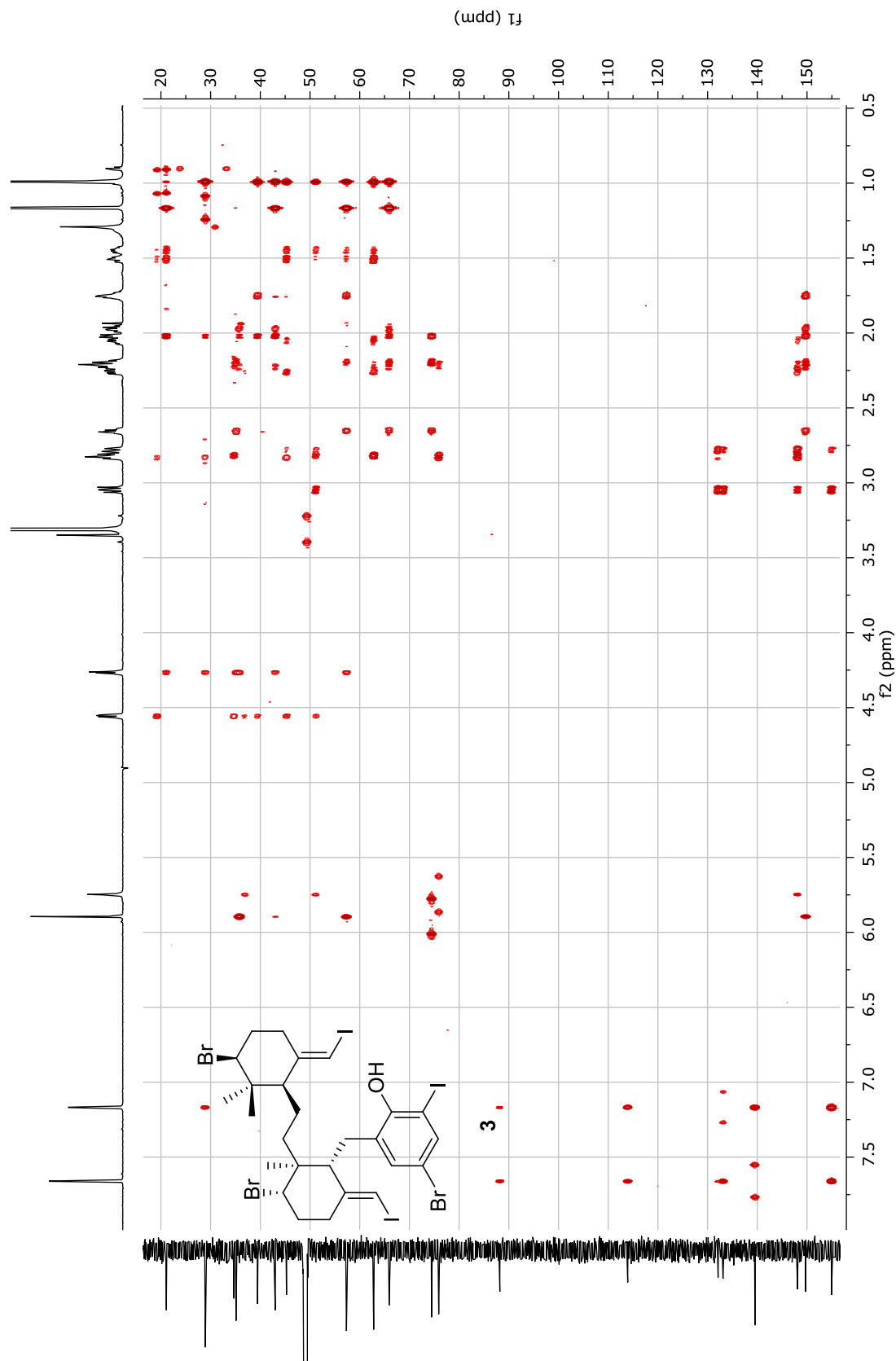
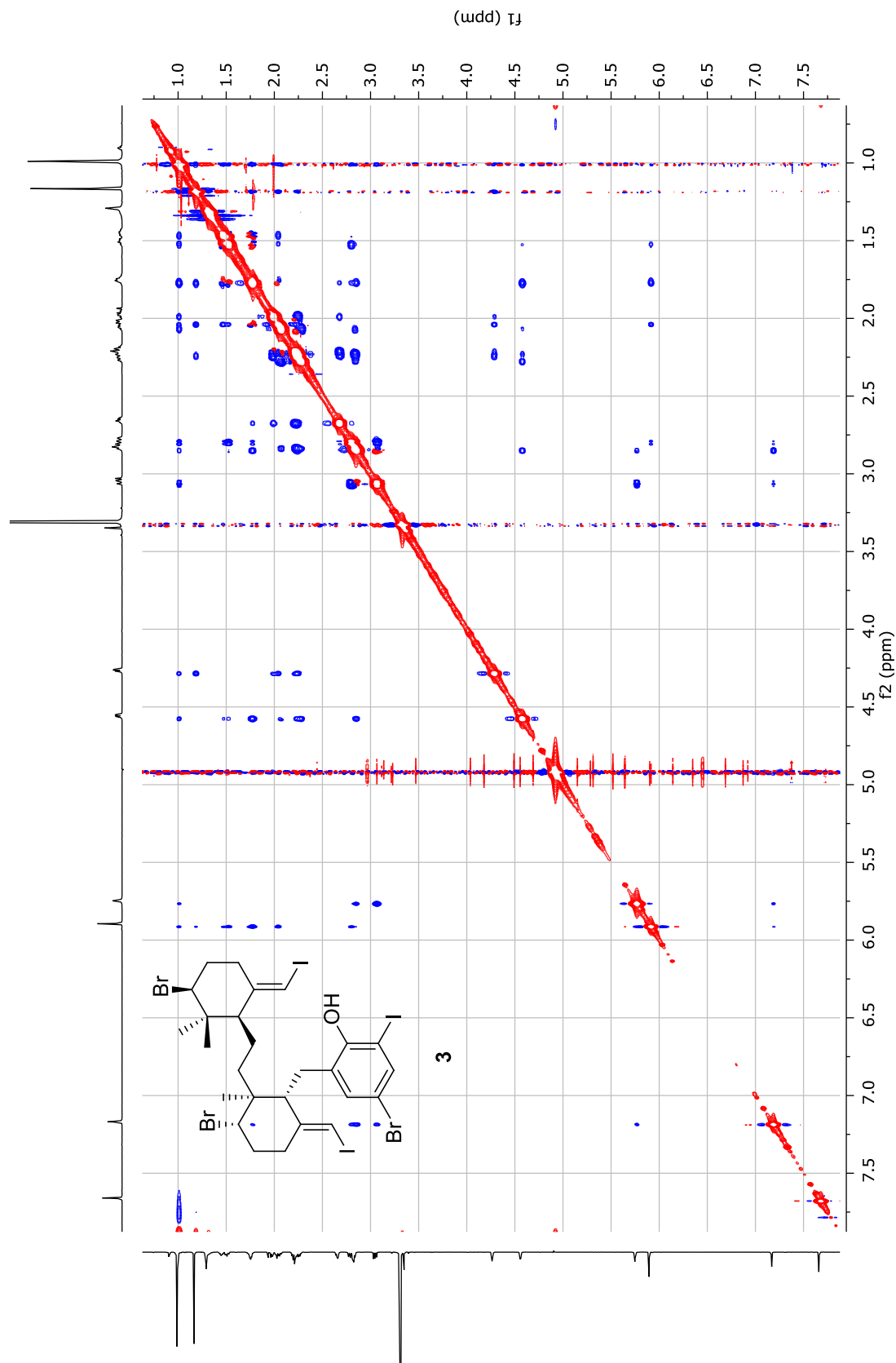


Figure S29. ^1H - ^1H NOESY spectrum of iodocallophycol B (3) at 800 MHz in CD_3OD .



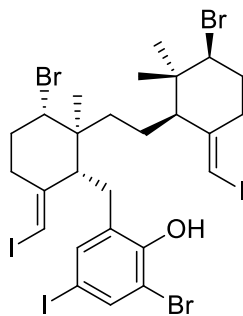
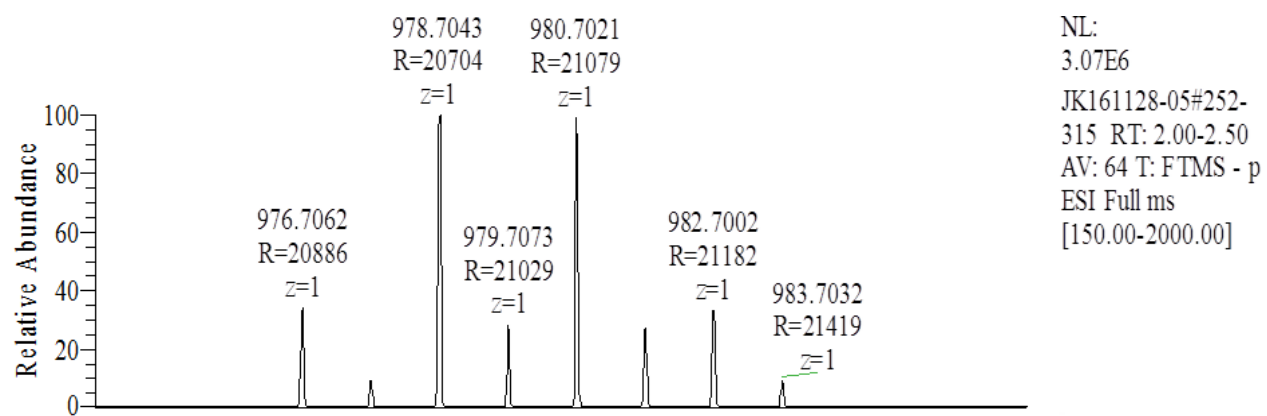
SPECTRA OF IODOCALLOPHYCOL C (4)**Figure S30.** Negative-mode HRESIMS spectrum of iodocallophycol C (4).**4**

Figure S31. ^1H NMR spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD .

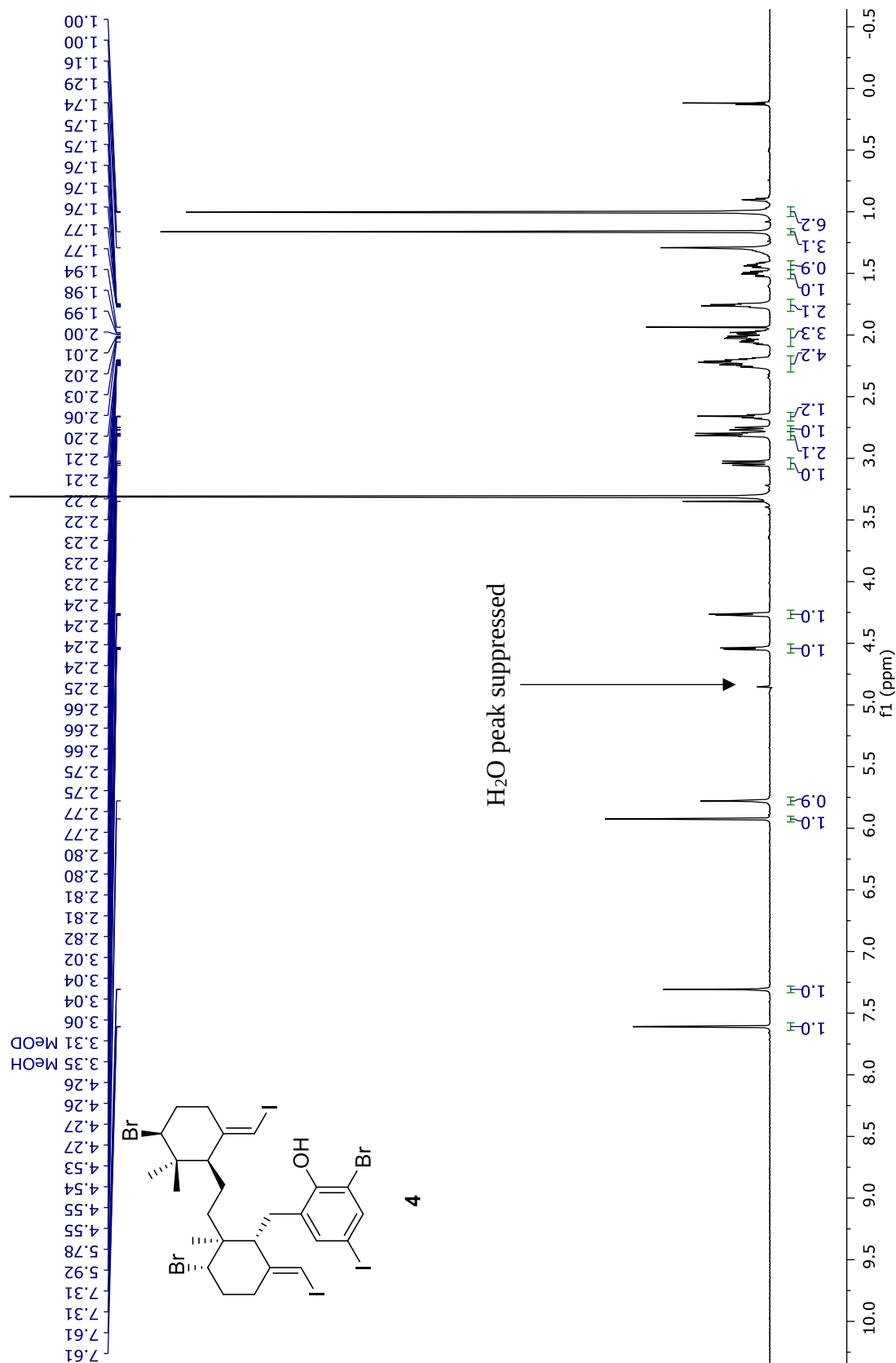
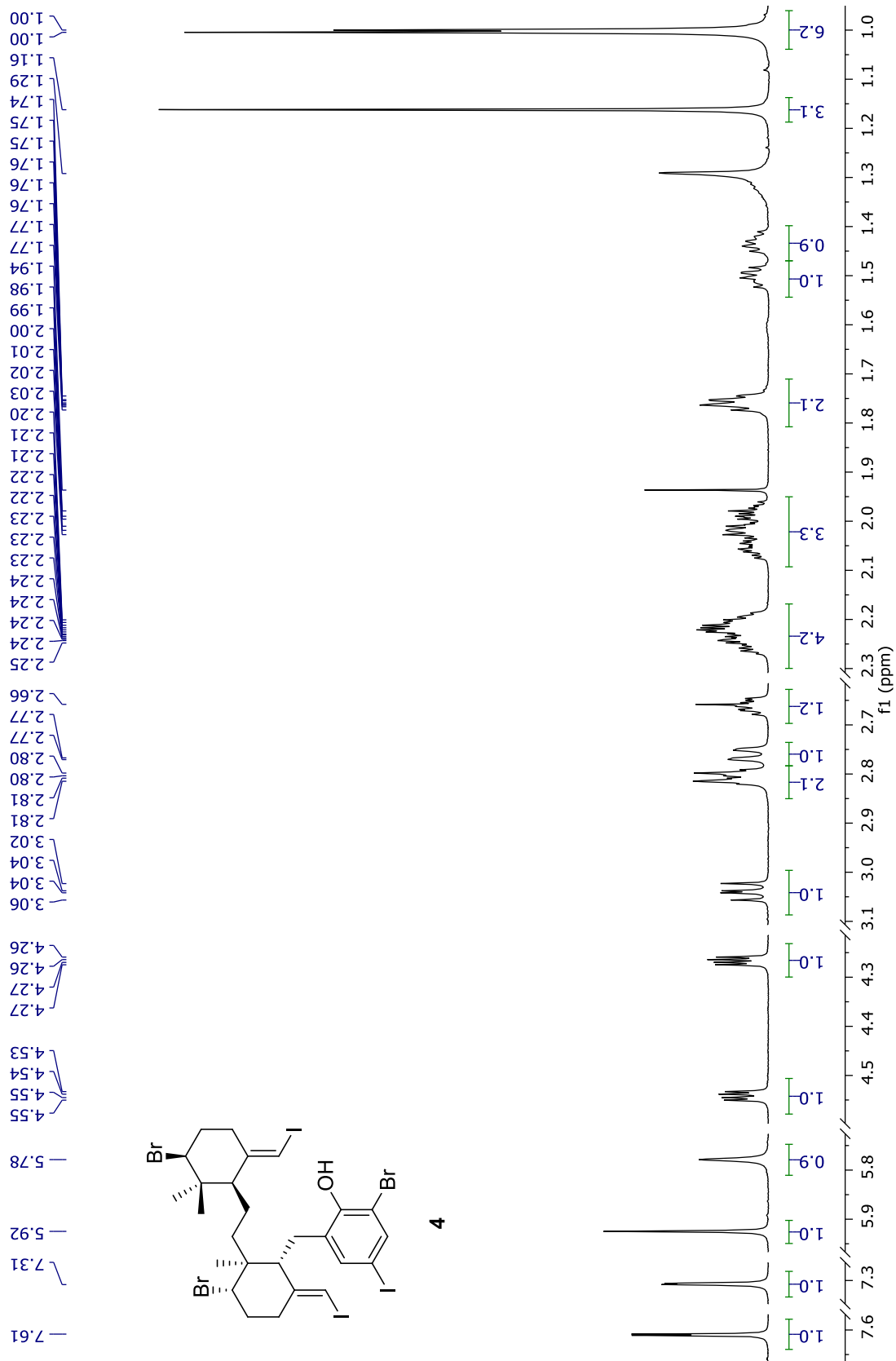


Figure S32. Enlarged ^1H NMR spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD .



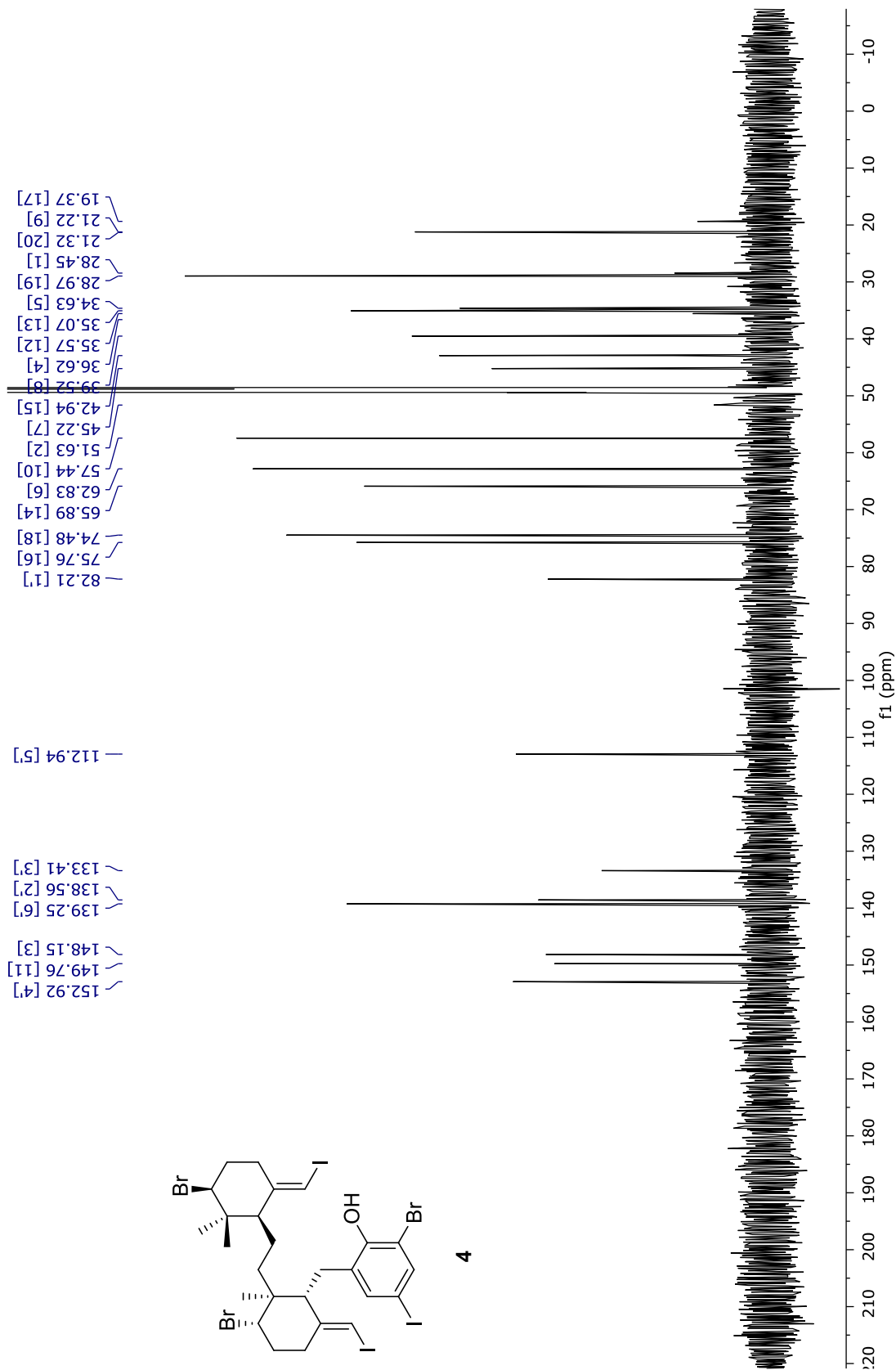


Figure S33. ^{13}C NMR spectrum of iodocallophycol C (**4**) at 200 MHz in CD_3OD .

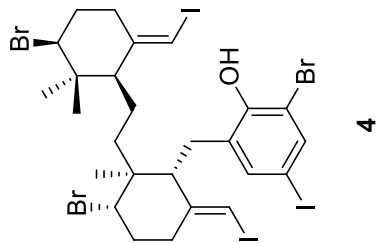


Figure S34. ^1H - ^1H DQF-COSY spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD .

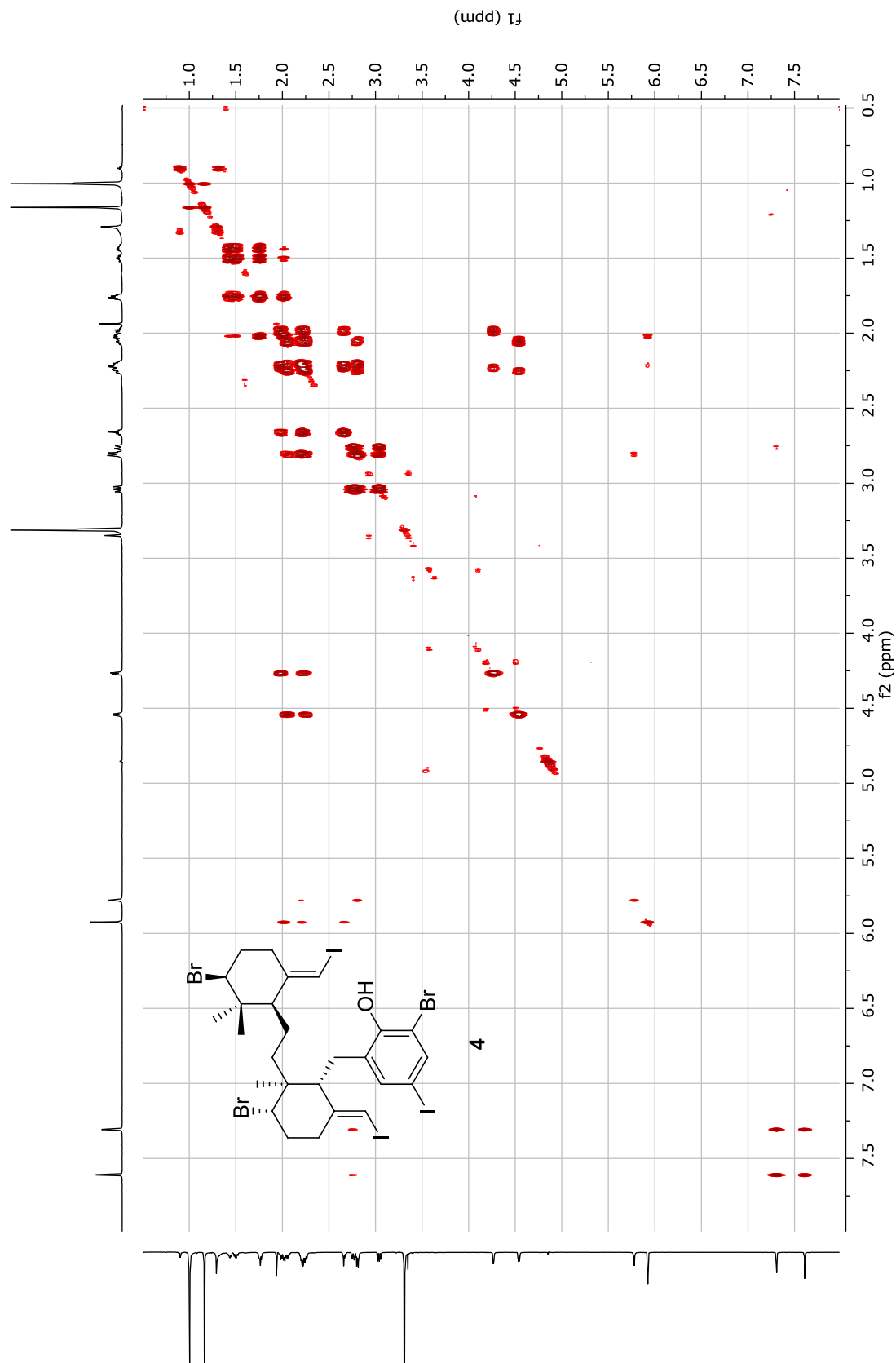


Figure S35. ^1H - ^{13}C edited-HSQC spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD .

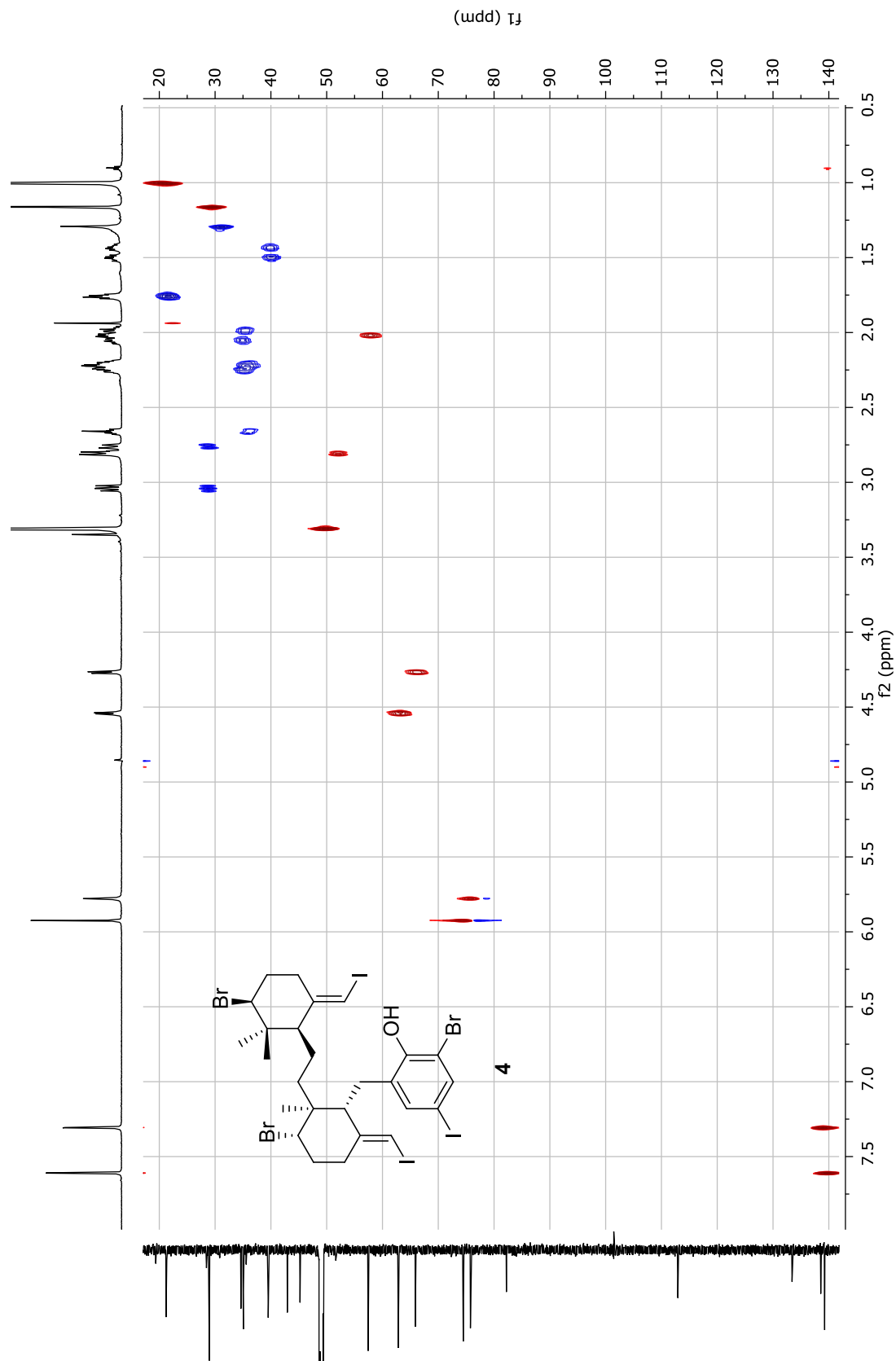


Figure S36. ^1H - ^{13}C HMBC spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD .

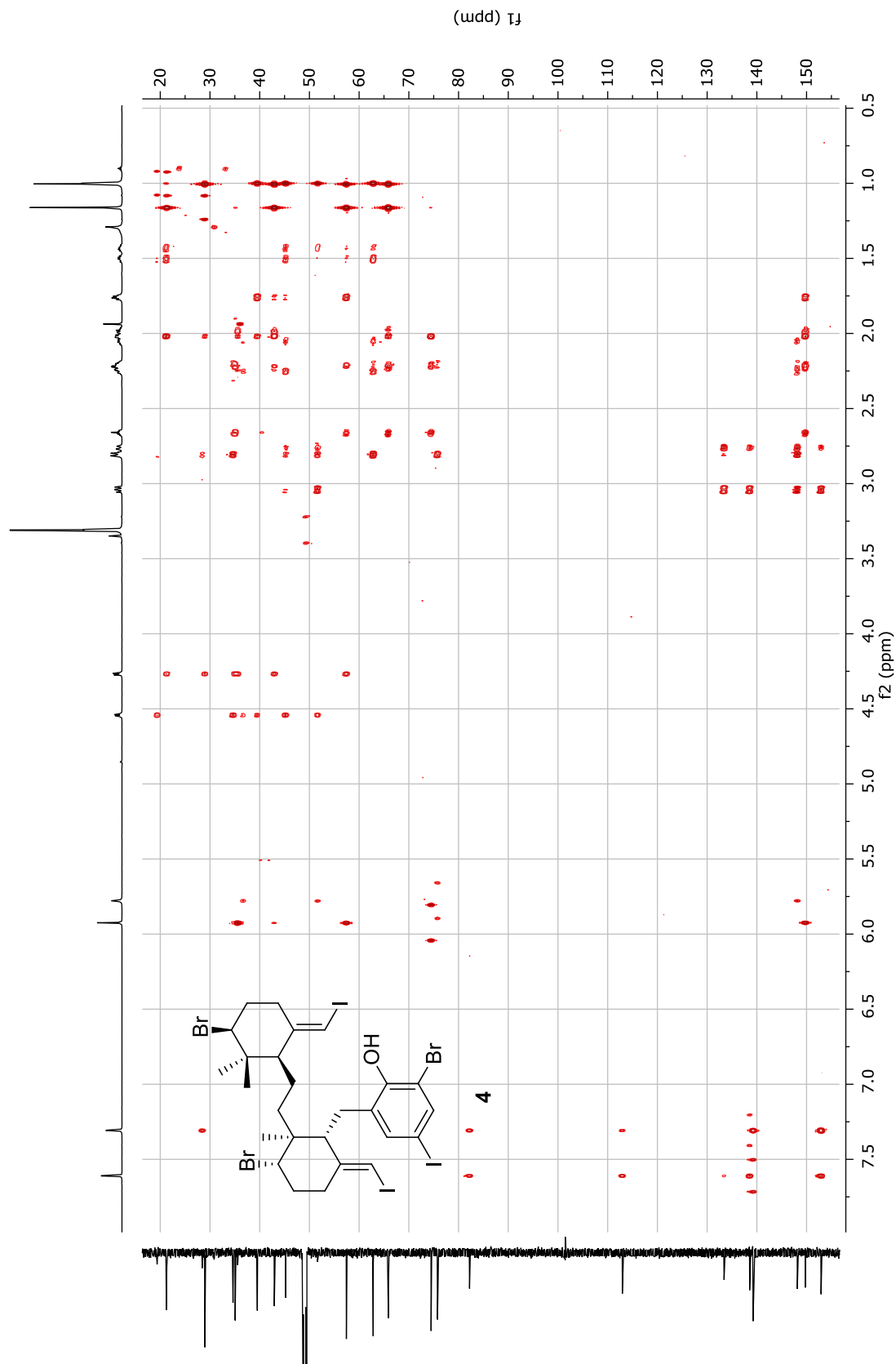
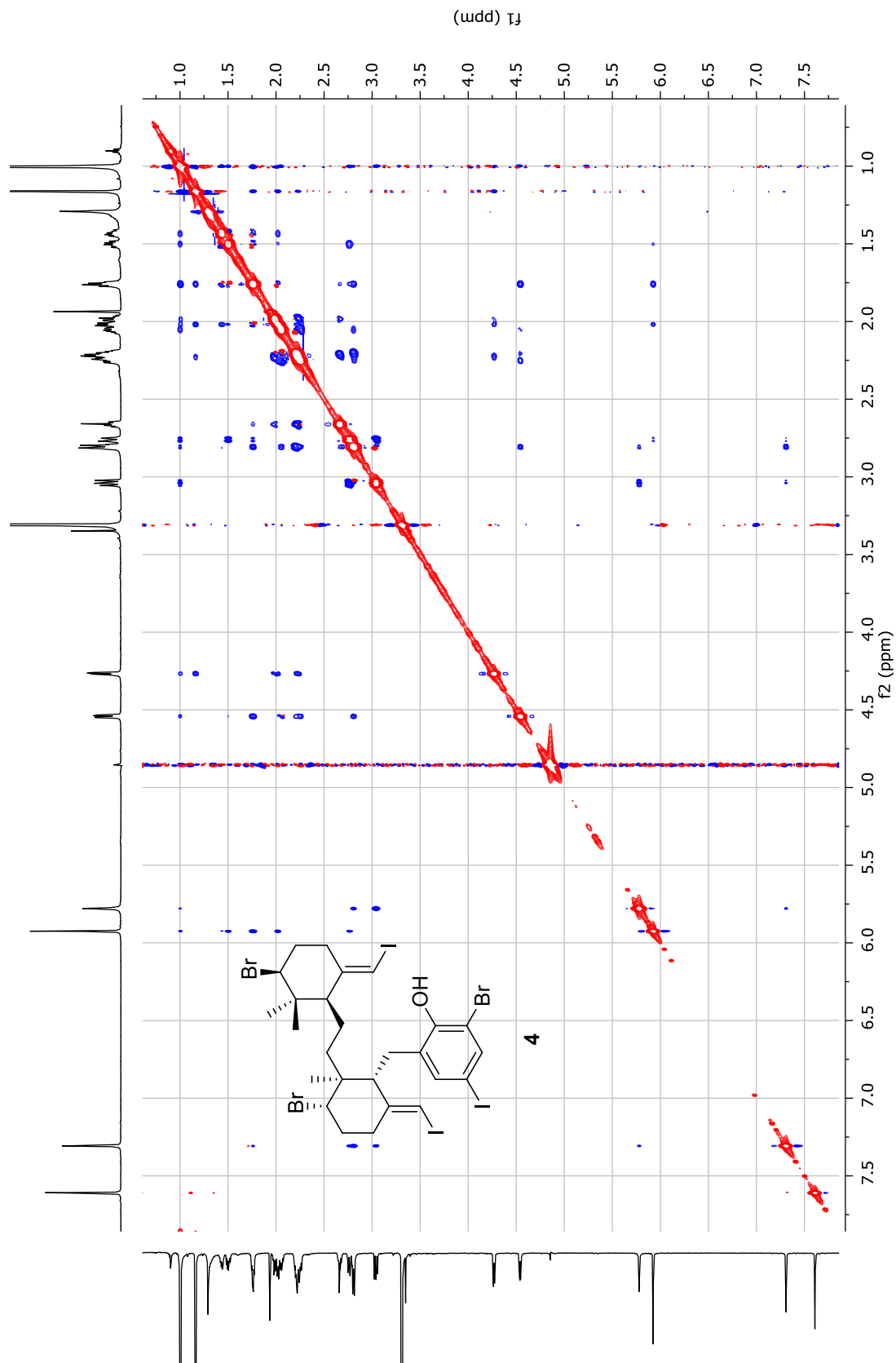
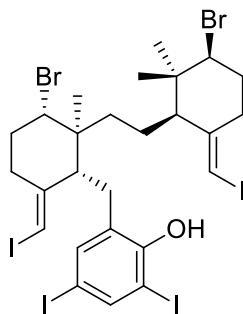
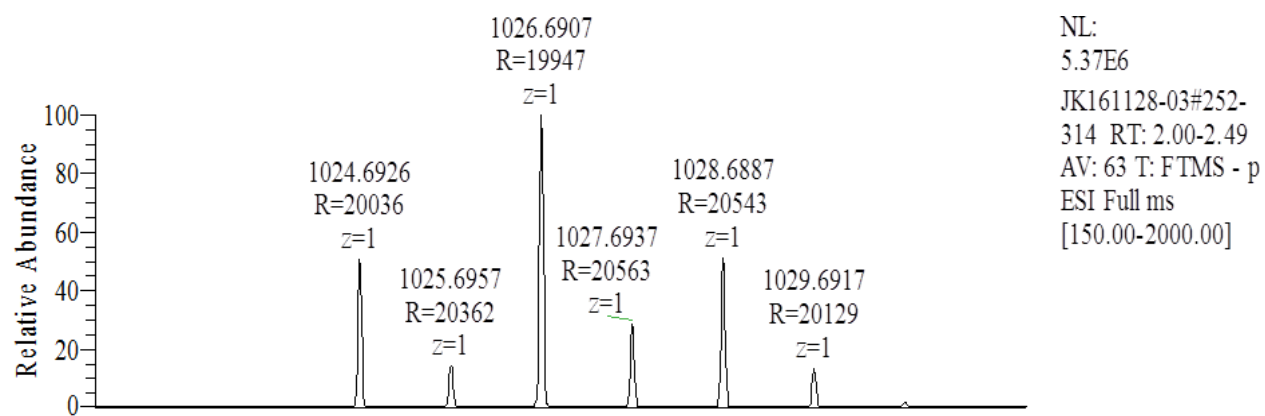


Figure S37. ^1H - ^1H NOESY spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD .



SPECTRA OF IODOCALLOPHYCOL D (5)**Figure S38.** Negative-mode HRESIMS spectrum of iodocallophycol D (5).**5**

Chemical structure of compound 5 is shown. The structure is a complex molecule with two bromine atoms, two iodine atoms, and a hydroxyl group. The spectrum includes integration values and a label "H₂O peak suppressed" with an arrow pointing to a peak at 2.20 ppm.

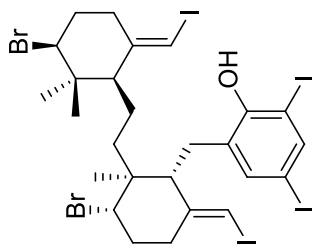


Figure S40. Enlarged ^1H NMR spectrum of iodocallophycol D (5) at 800 MHz in CD_3OD .

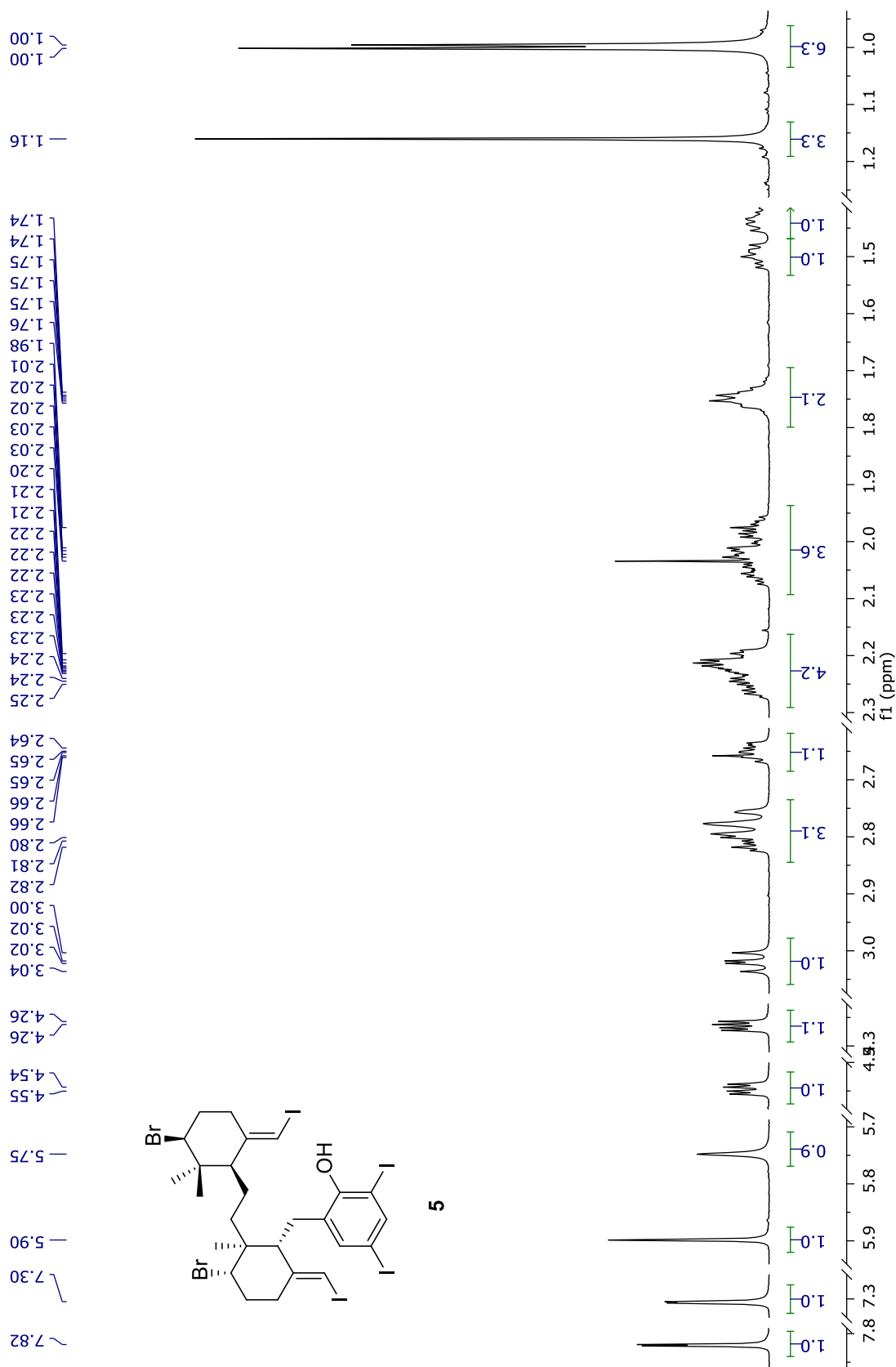


Figure S41. ^{13}C NMR spectrum of iodocallophycol D (5) at 200 MHz in CD_3OD .

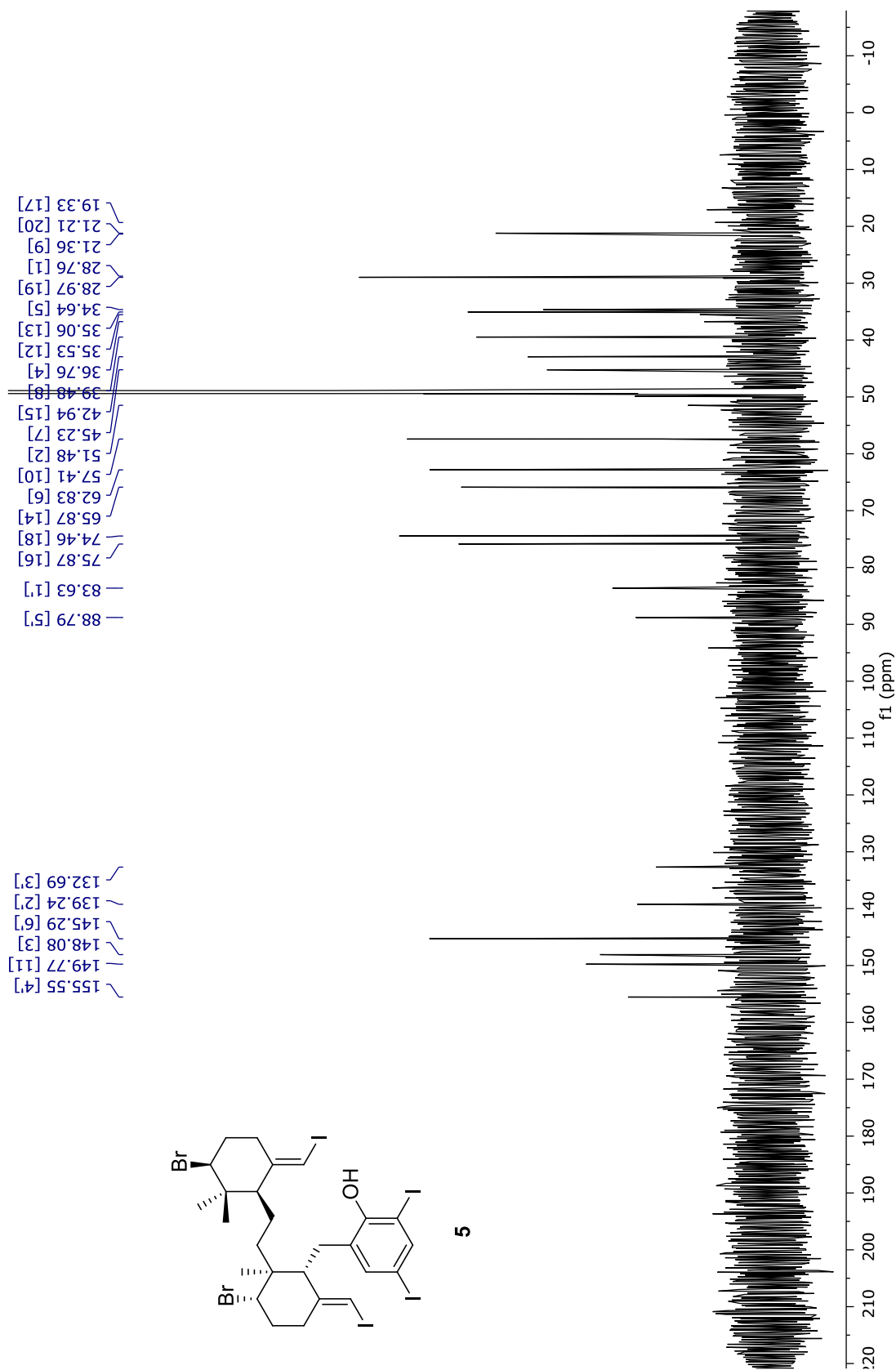


Figure S42. ^1H - ^1H DQF-COSY spectrum of iodocallophycol D (5) at 800 MHz in CD_3OD .

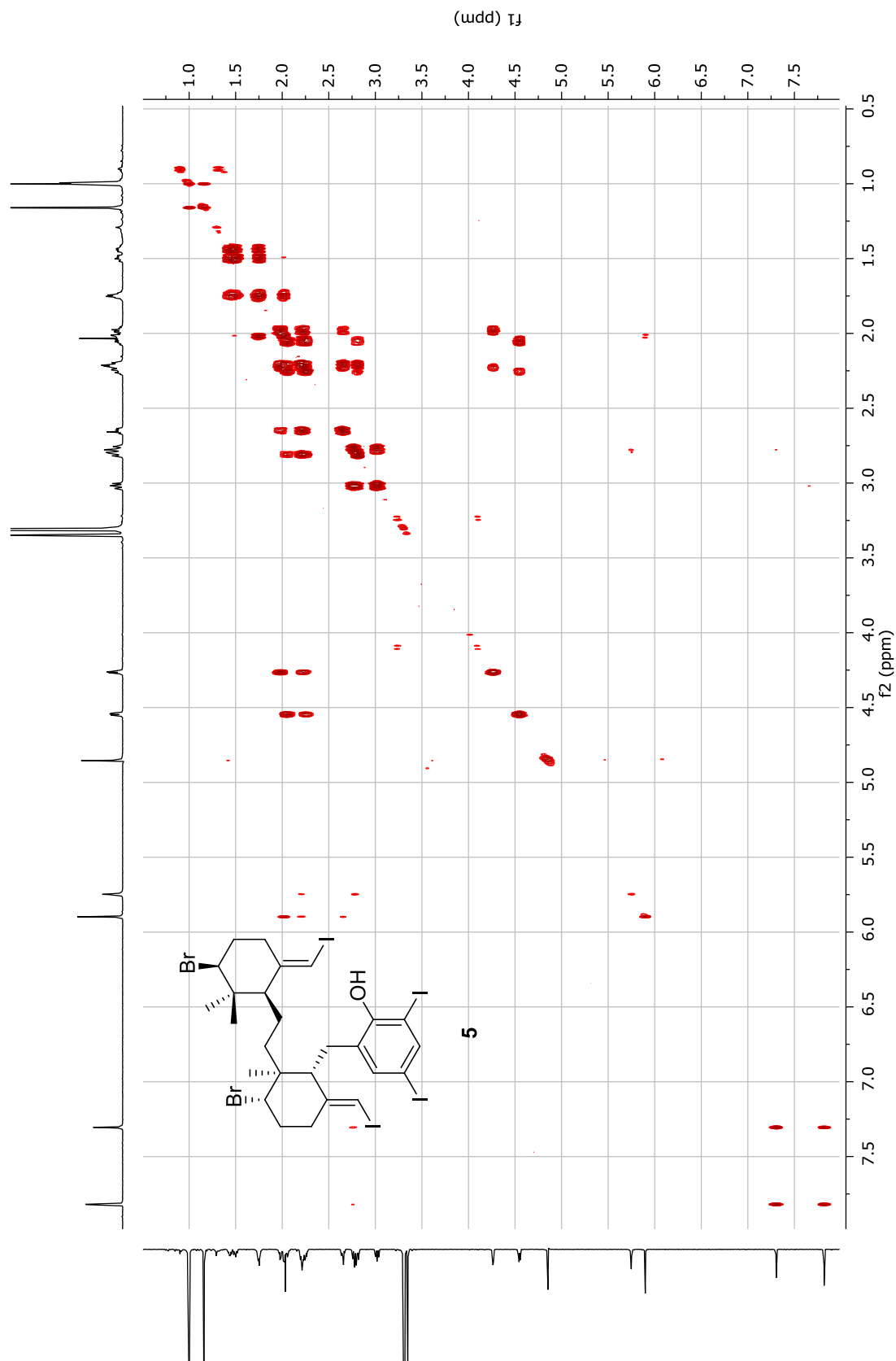


Figure S43. ^1H - ^{13}C edited-HSQC spectrum of iodocallophycol D (5) at 800 MHz in CD_3OD .

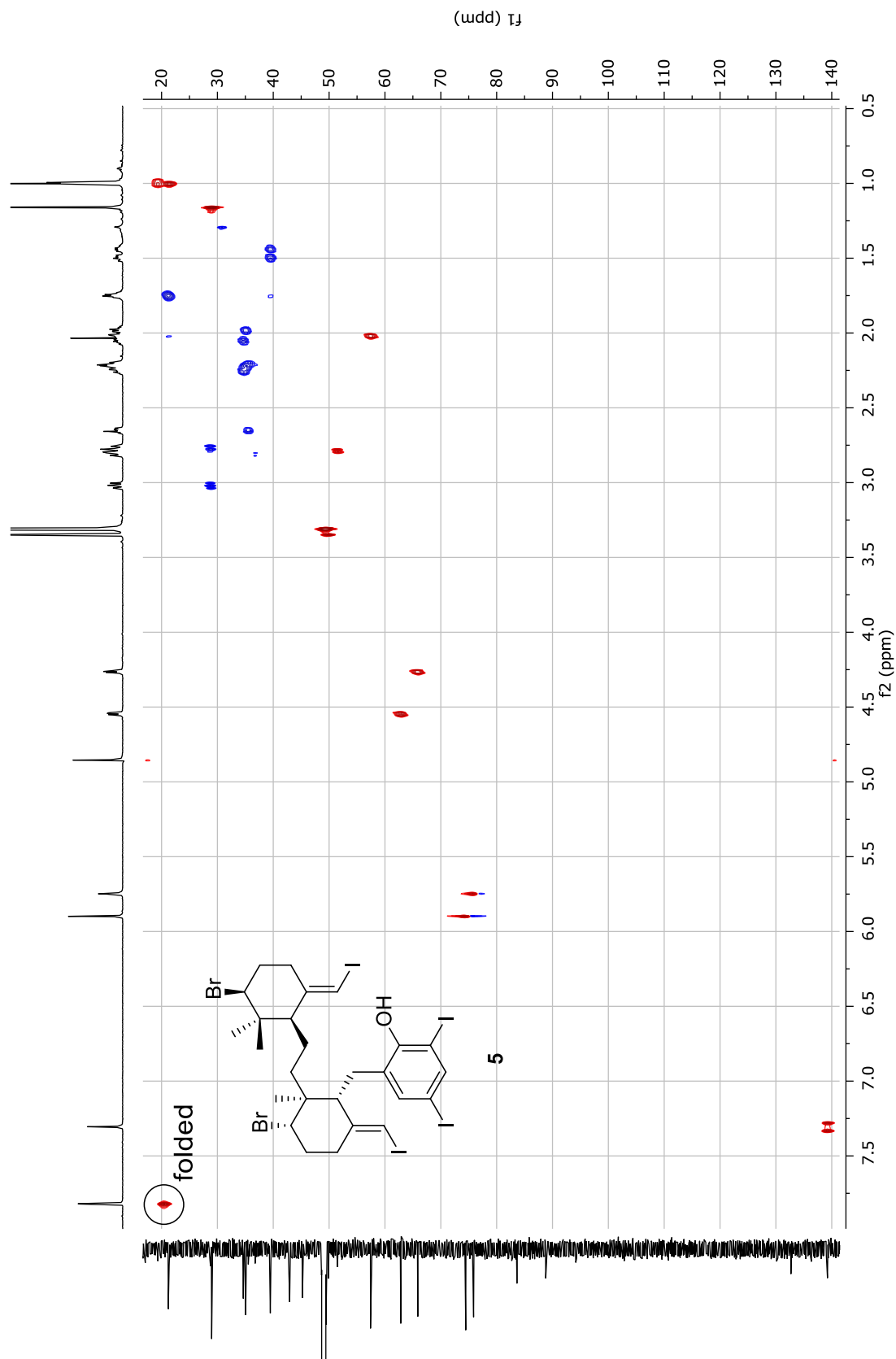


Figure S44. ^1H - ^{13}C HMBC spectrum of iodocallophycol D (5) at 800 MHz in CD_3OD .

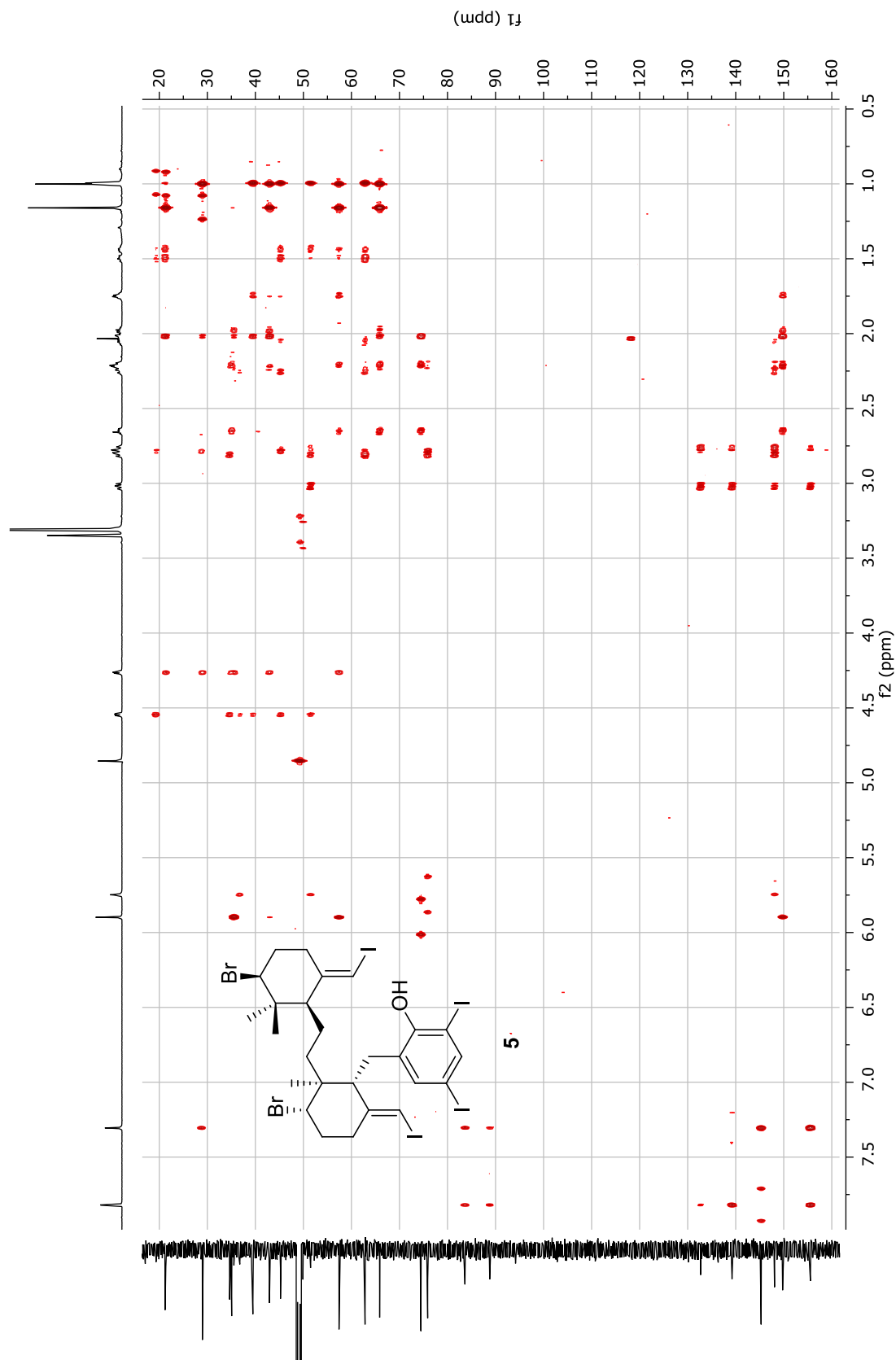
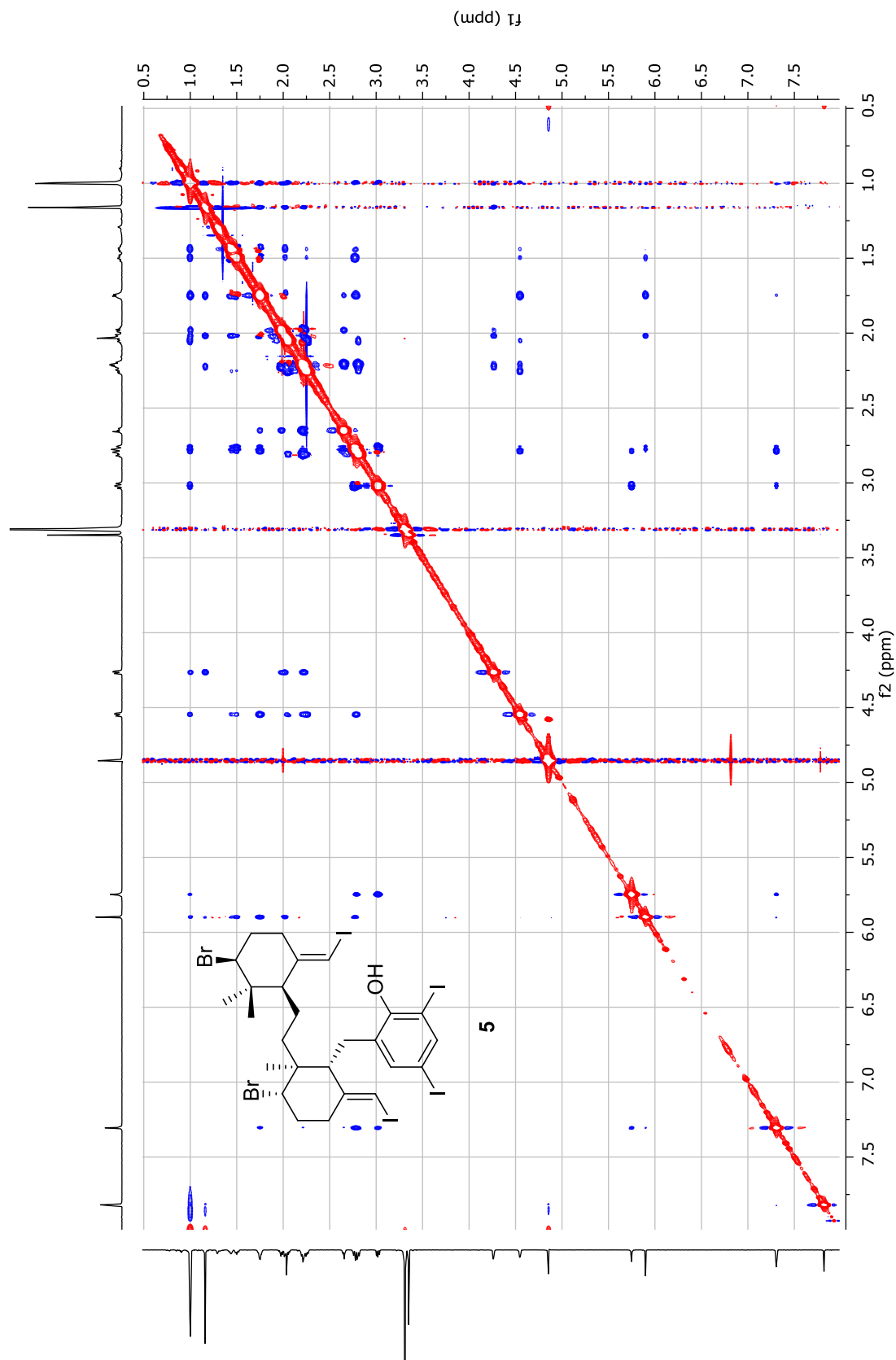


Figure S45. ^1H - ^1H NOESY spectrum of iodocallophycol D (5) at 800 MHz in CD_3OD .



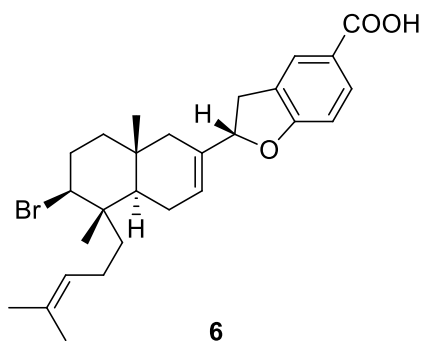
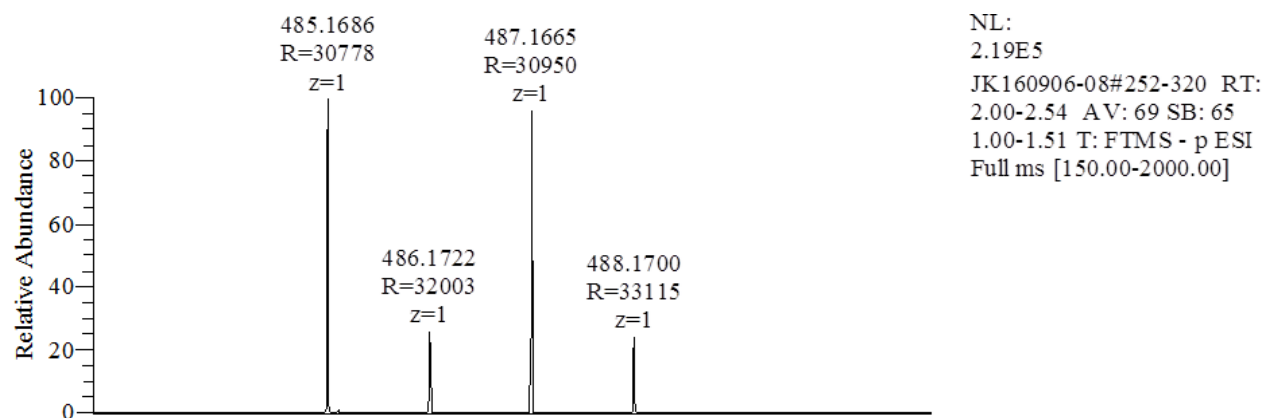
SPECTRA OF BROMOPHYCOIC ACID F (6)**Figure S46.** Negative-mode HRESIMS spectrum of bromophycoic acid F (**6**).

Figure S47. ^1H NMR spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD .

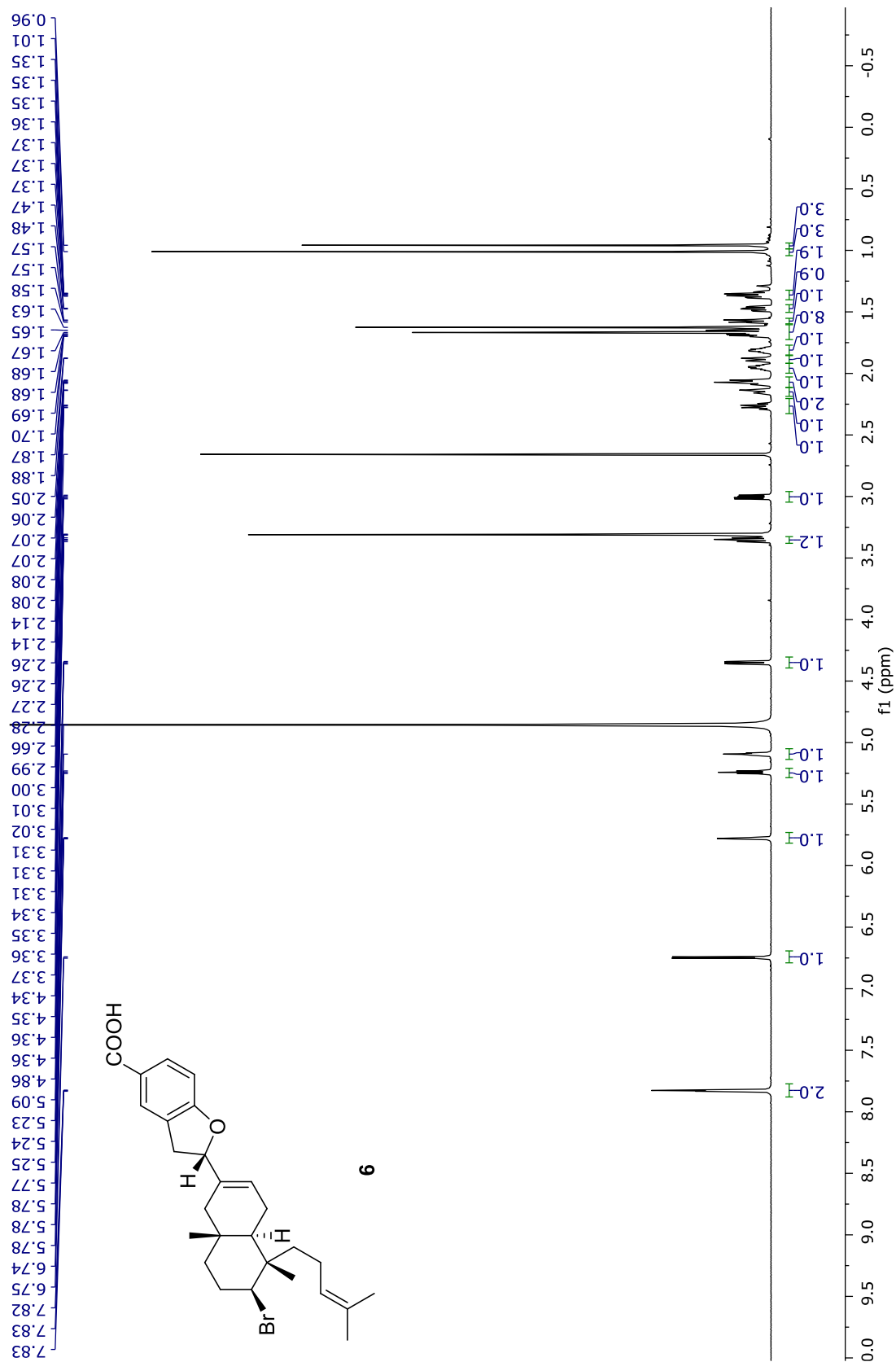


Figure S48. Enlarged ^1H NMR spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD .

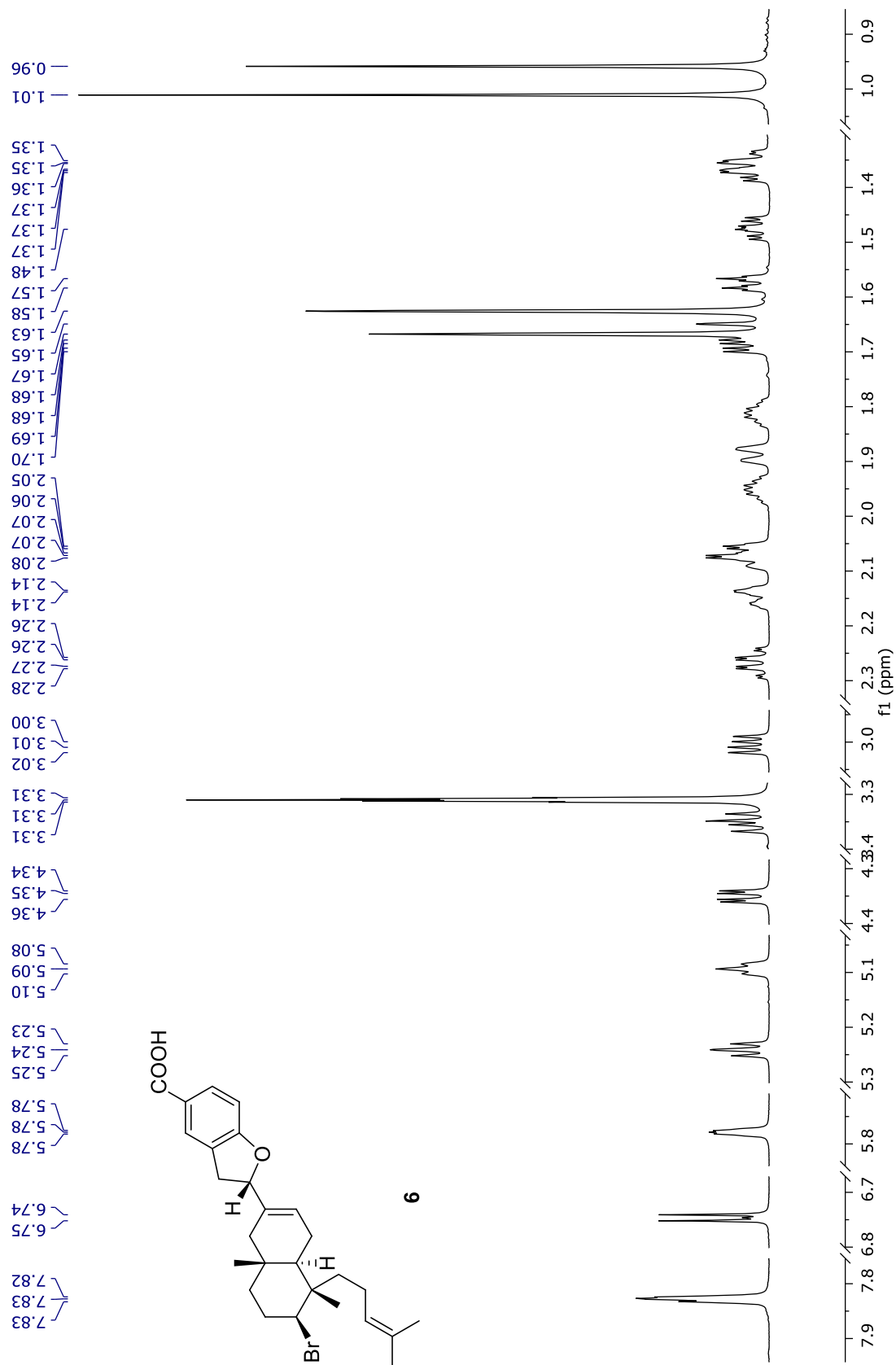


Figure S49. ^{13}C NMR spectrum of bromophycoic acid F (**6**) at 200 MHz in CD_3OD .

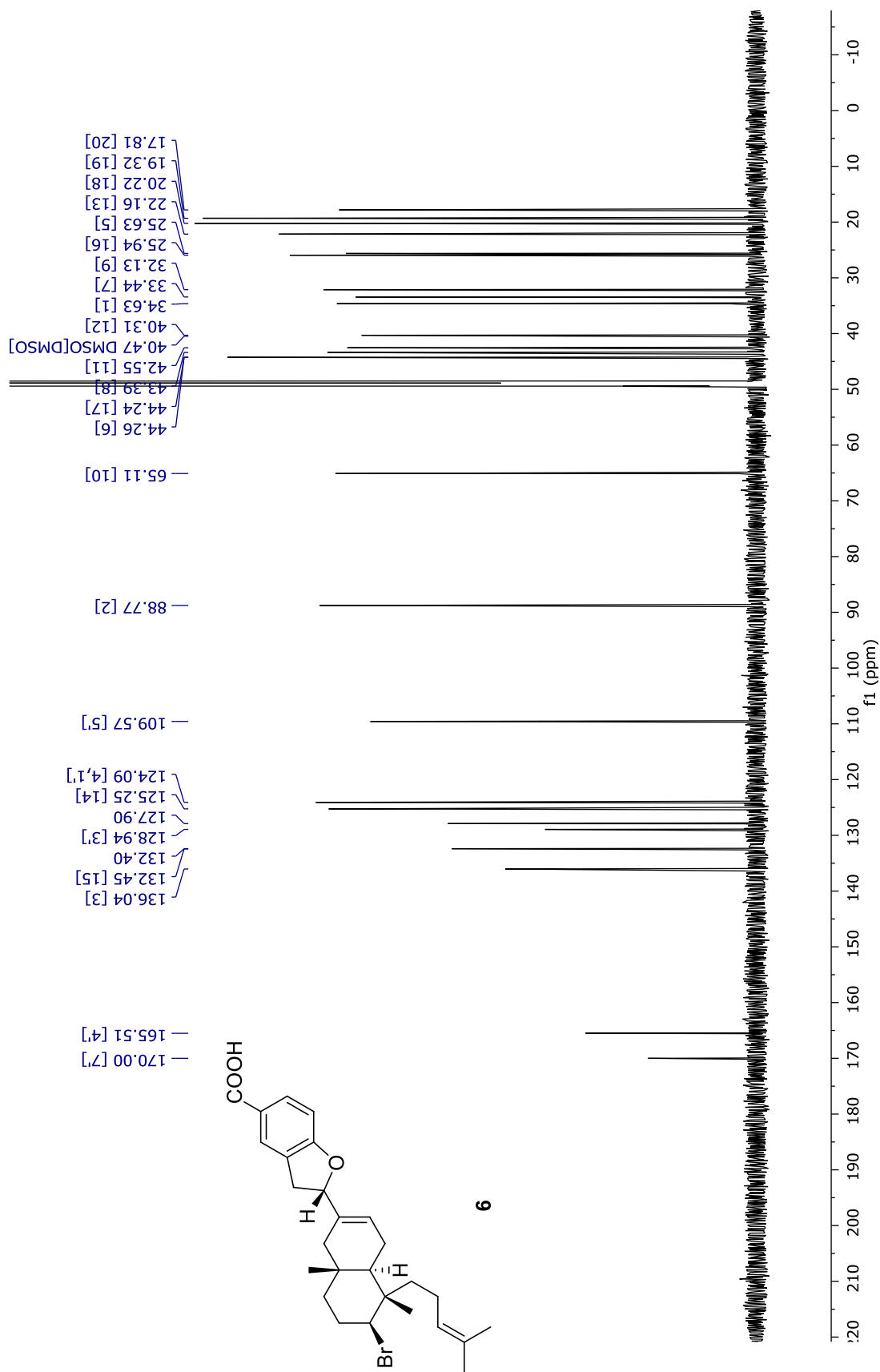


Figure S50. ^1H - ^1H DQF-COSY spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD .

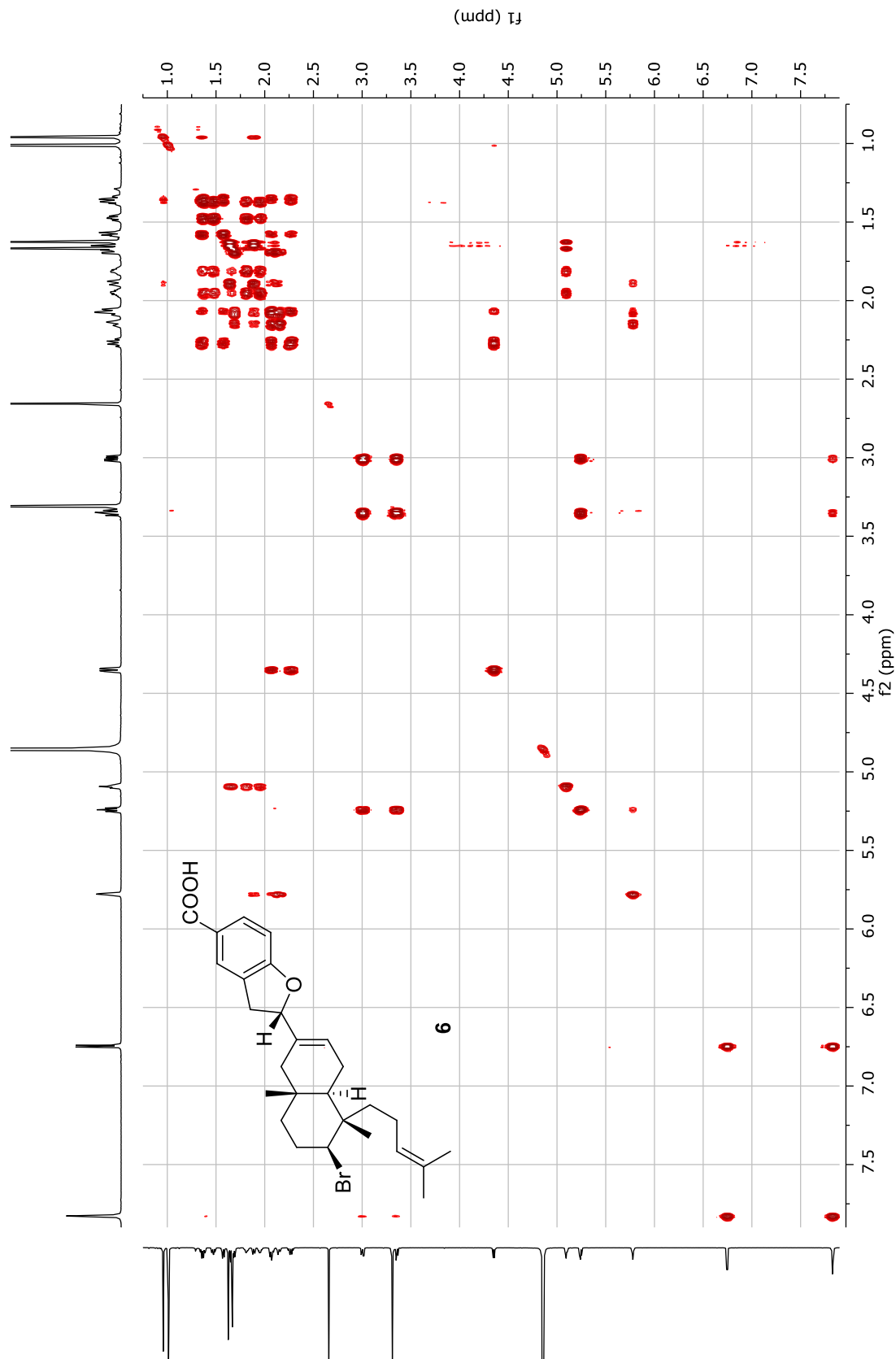


Figure S51. ^1H - ^{13}C edited-HSQC spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD .

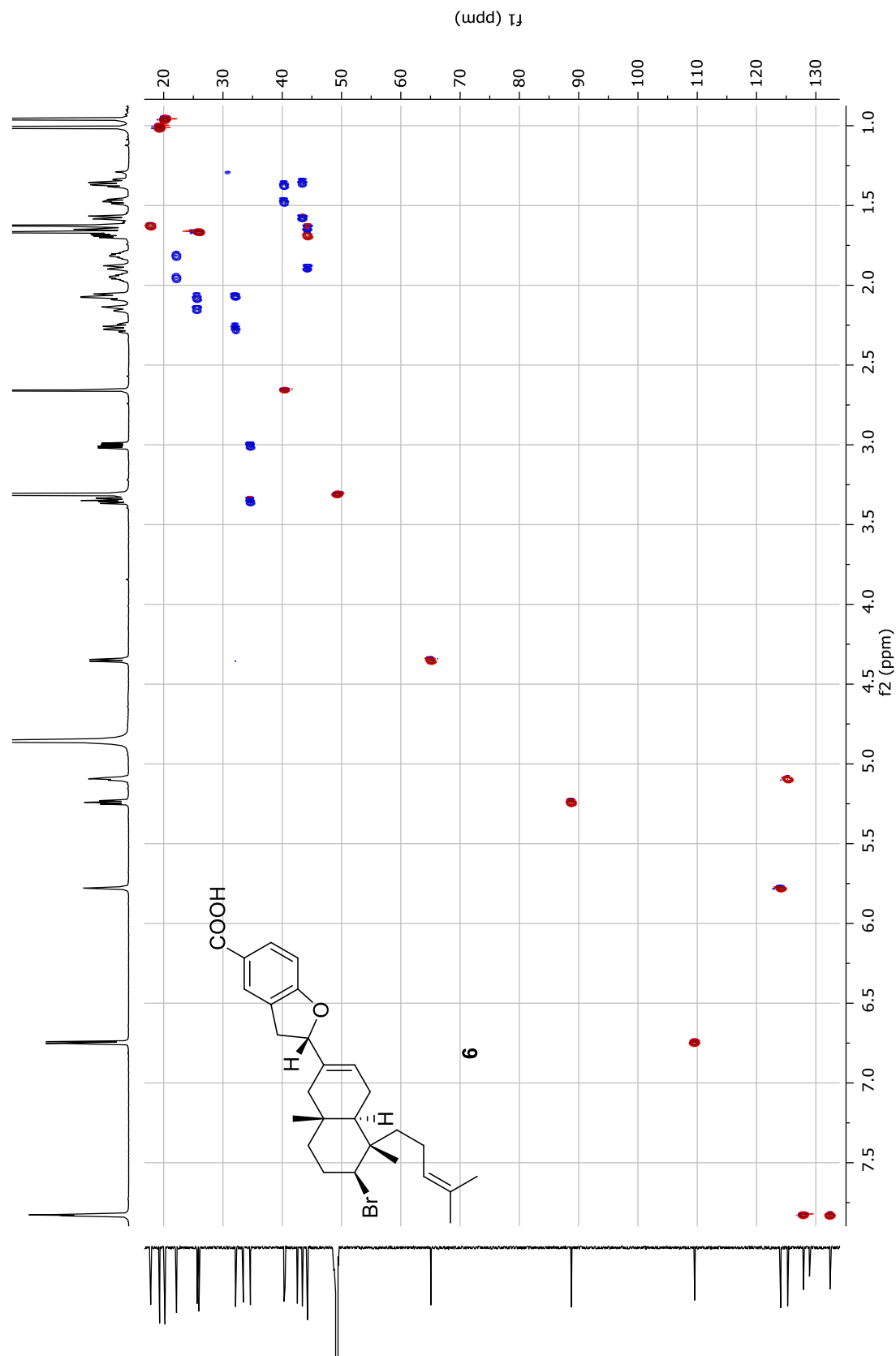


Figure S52. ^1H - ^{13}C HMBC spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD .

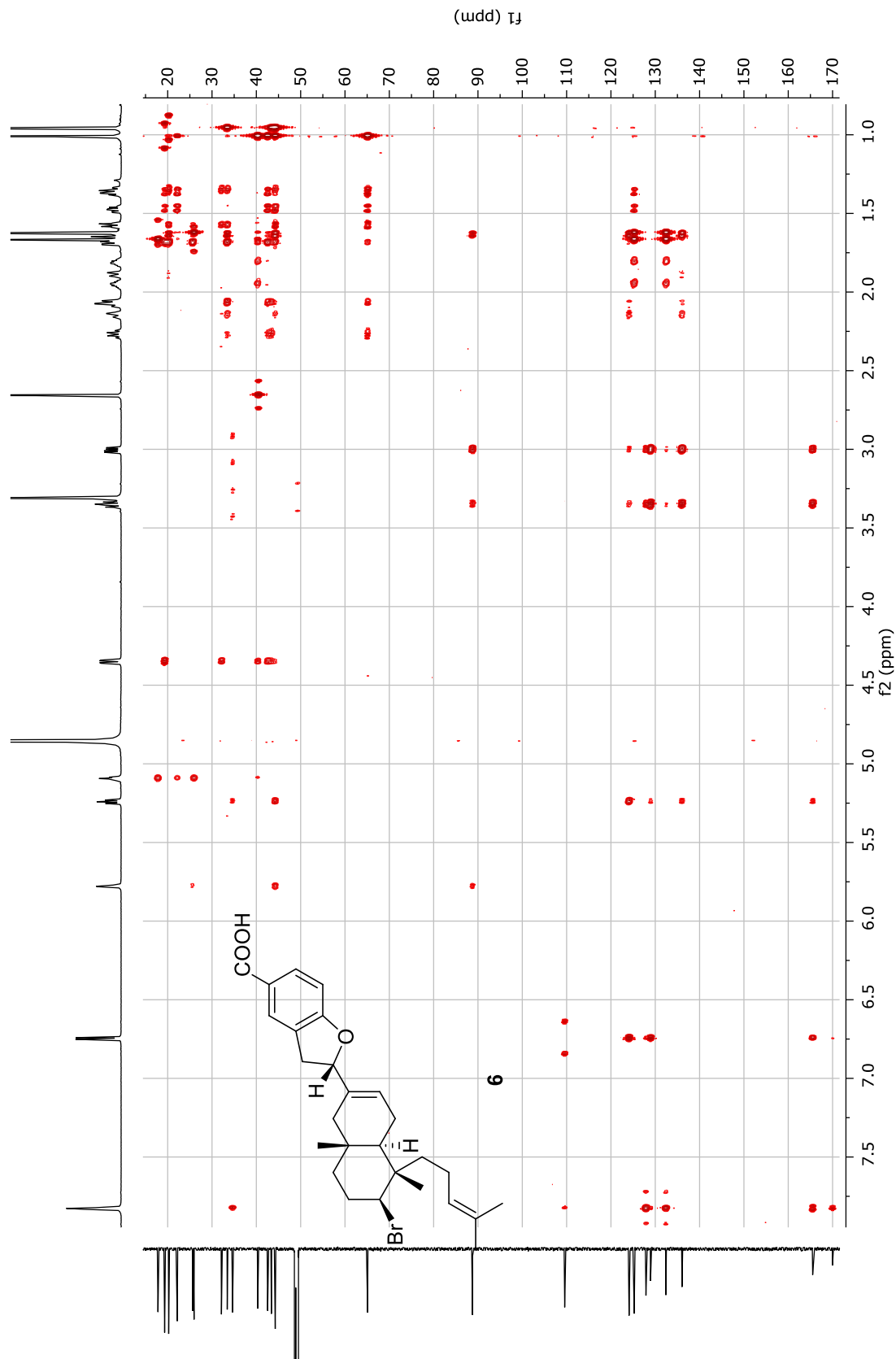
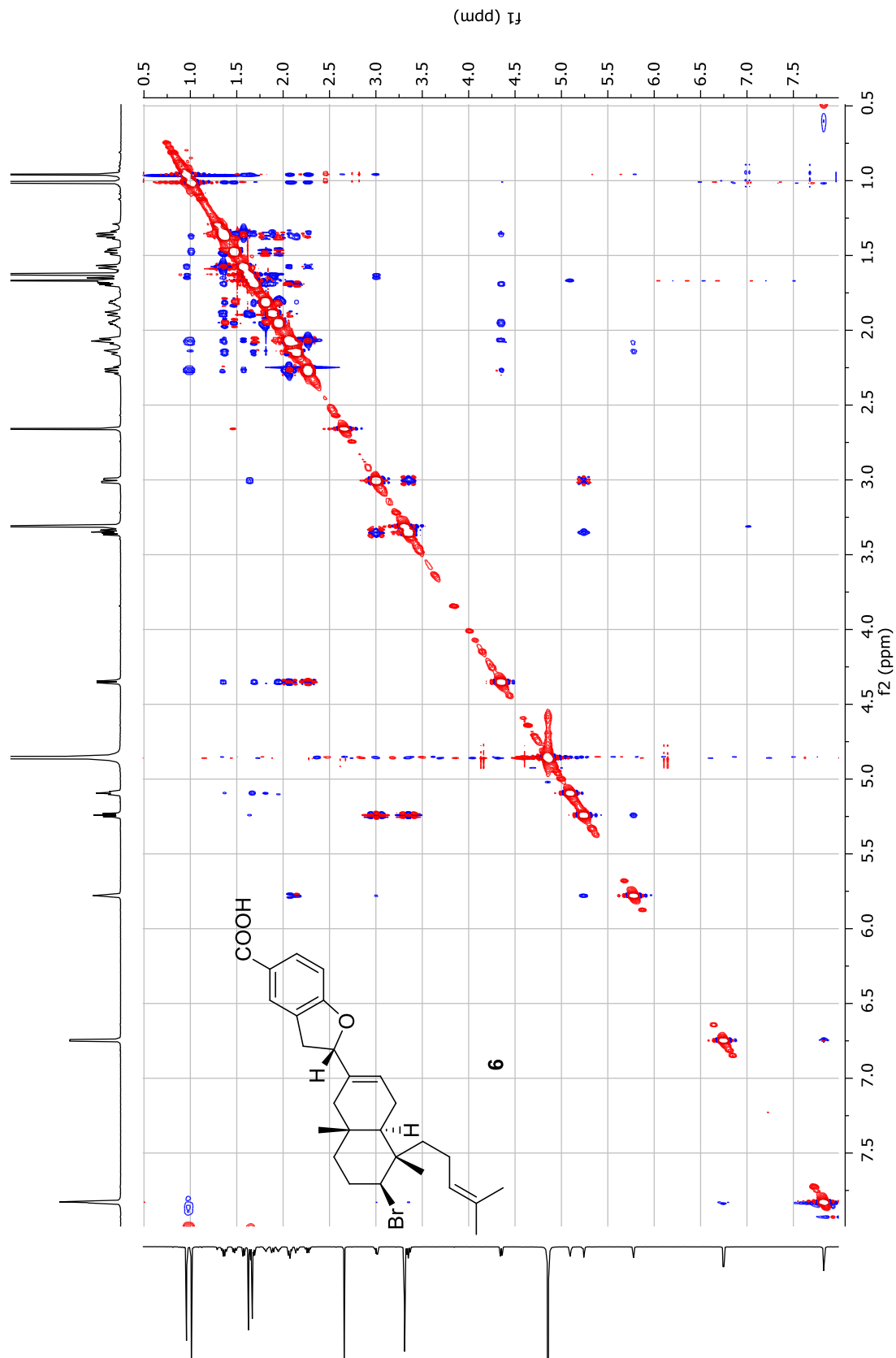


Figure S53. ^1H - ^1H NOESY spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD .



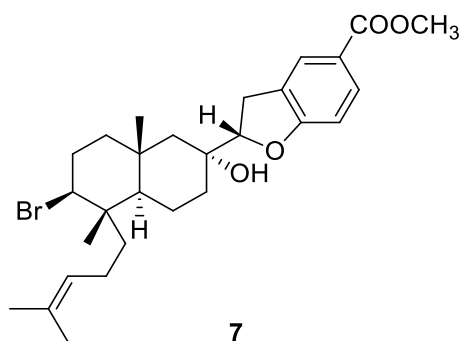
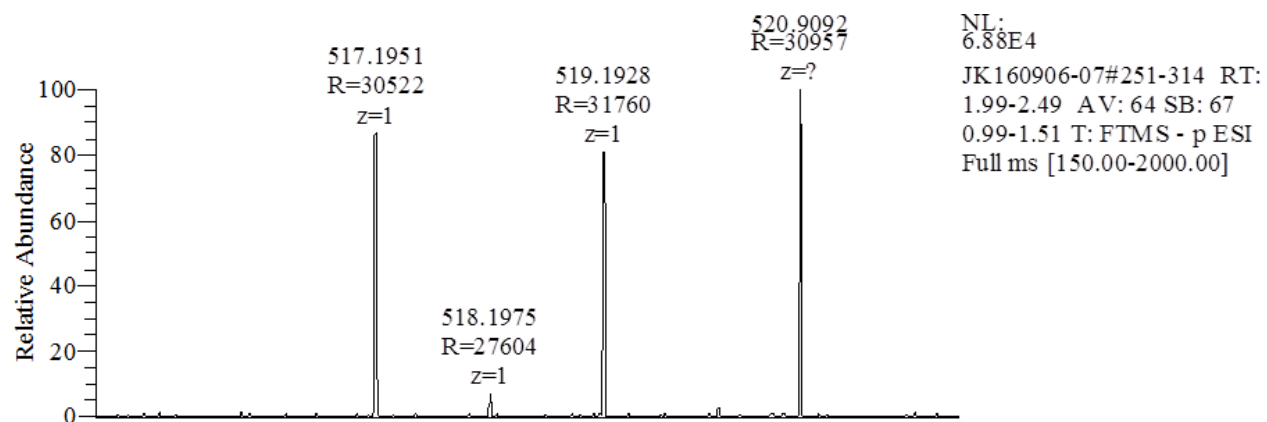
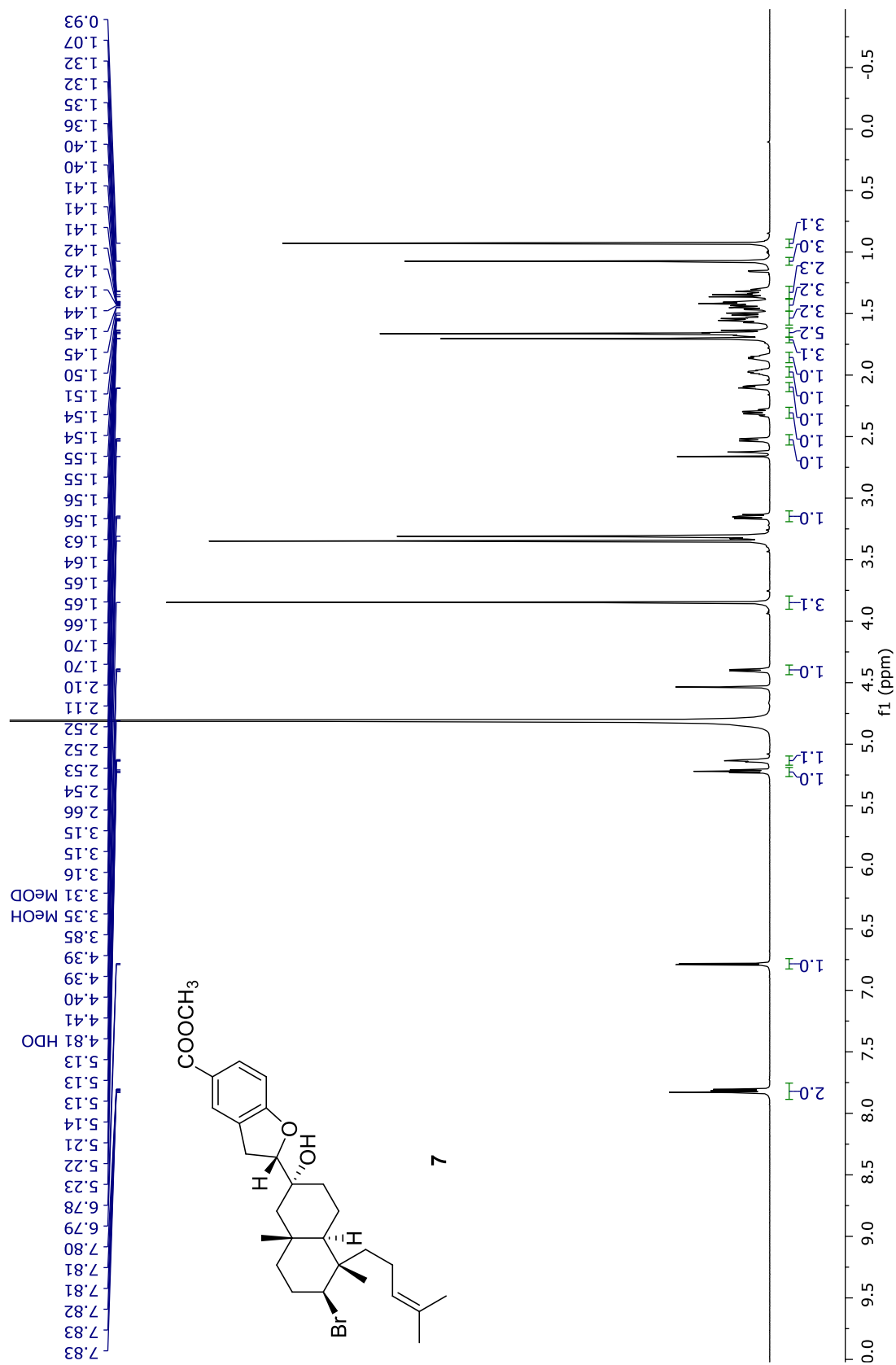
SPECTRA OF BROMOPHYCOIC ACID A METHYL ESTER (7)**Figure S54.** Negative-mode HRESIMS spectrum of bromophycoic Acid A methyl ester (7).

Figure S55. ^1H NMR spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD .



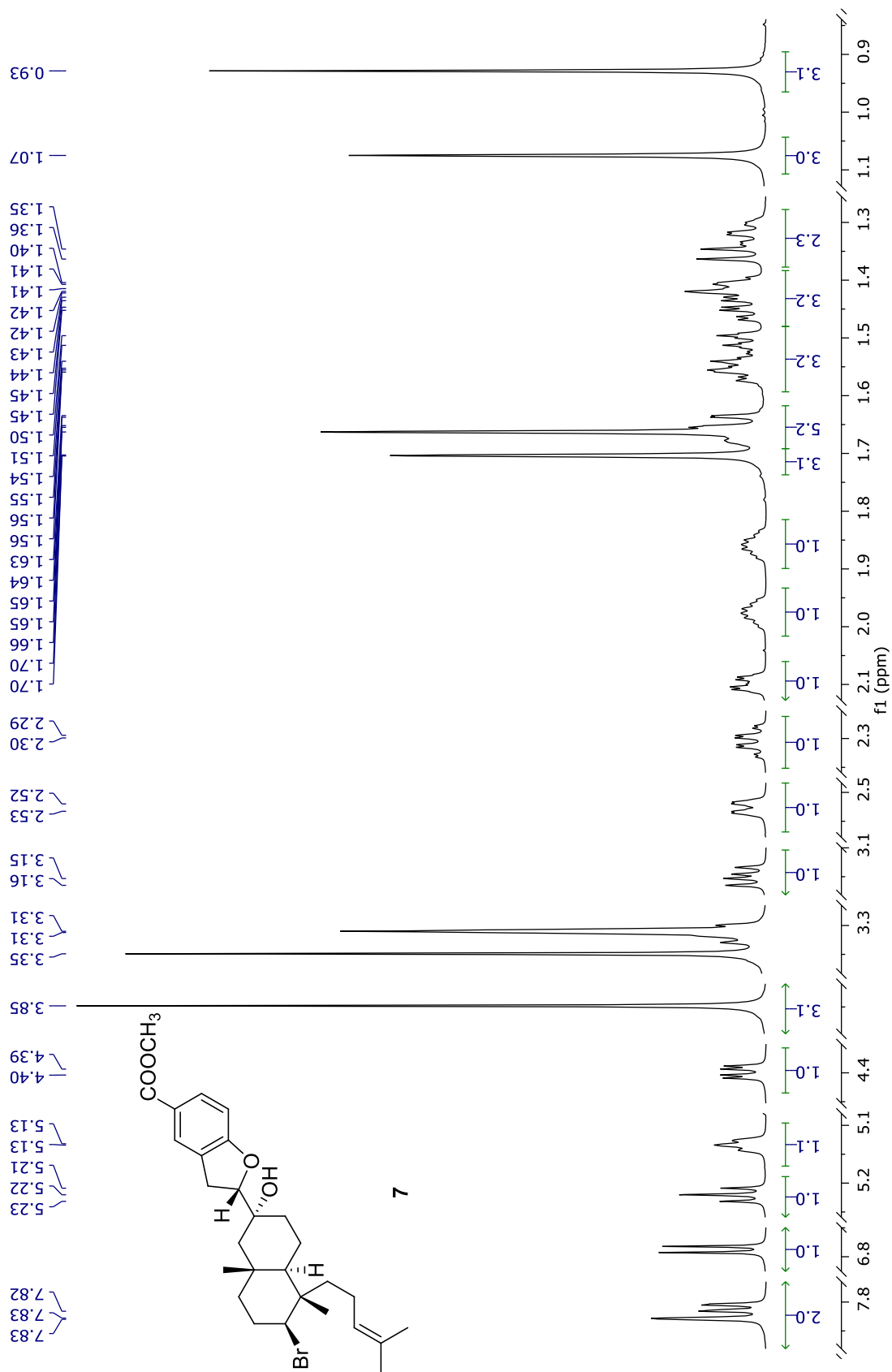


Figure S56. Enlarged ^1H NMR spectrum of bromophycoic acid **7** at 800 MHz in CD_3OD .

Figure S57. ^{13}C NMR spectrum of bromophycoic acid A methyl ester (**7**) at 200 MHz in CD_3OD .

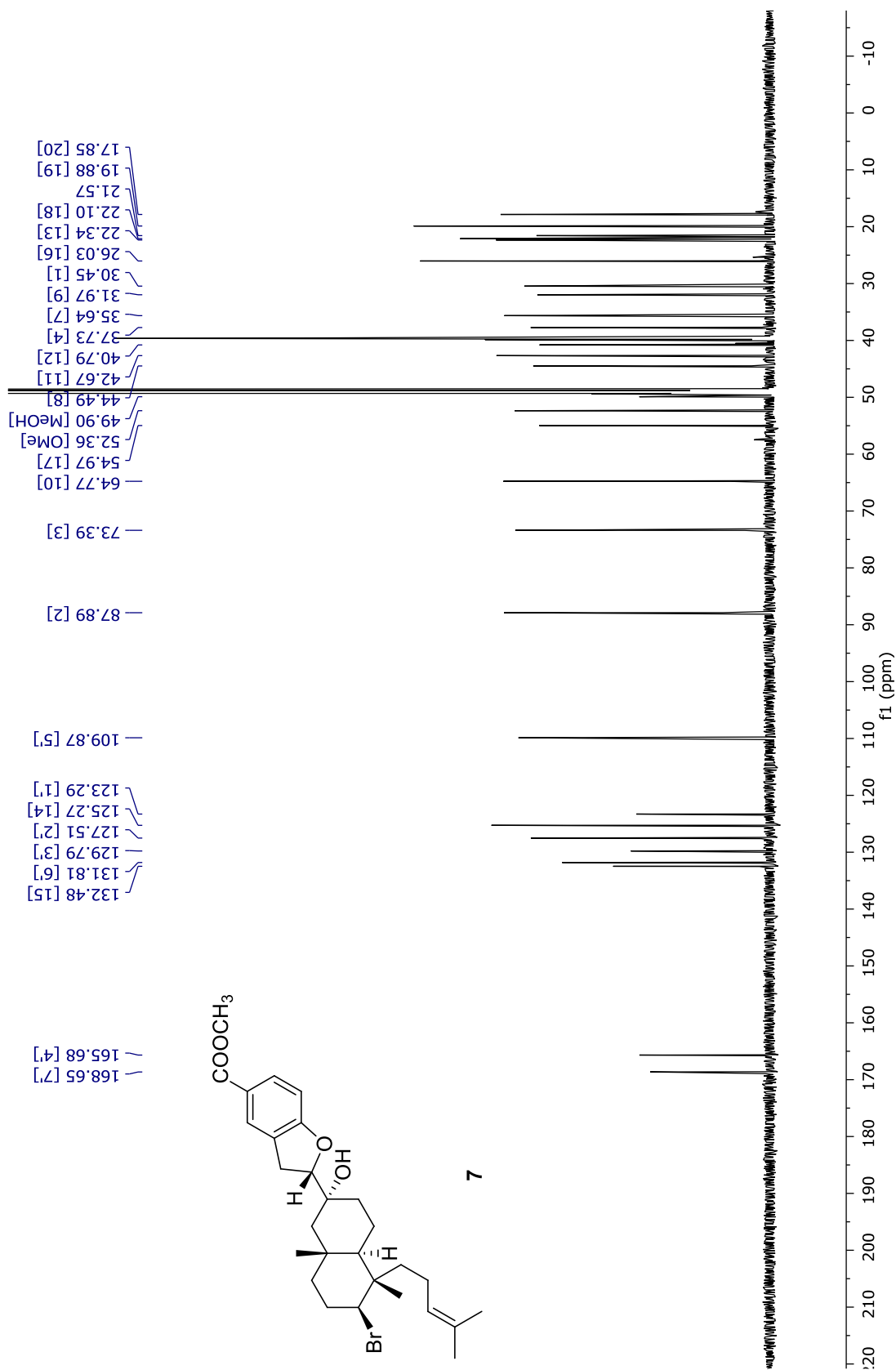


Figure S58. ^1H - ^1H DQF-COSY spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD .

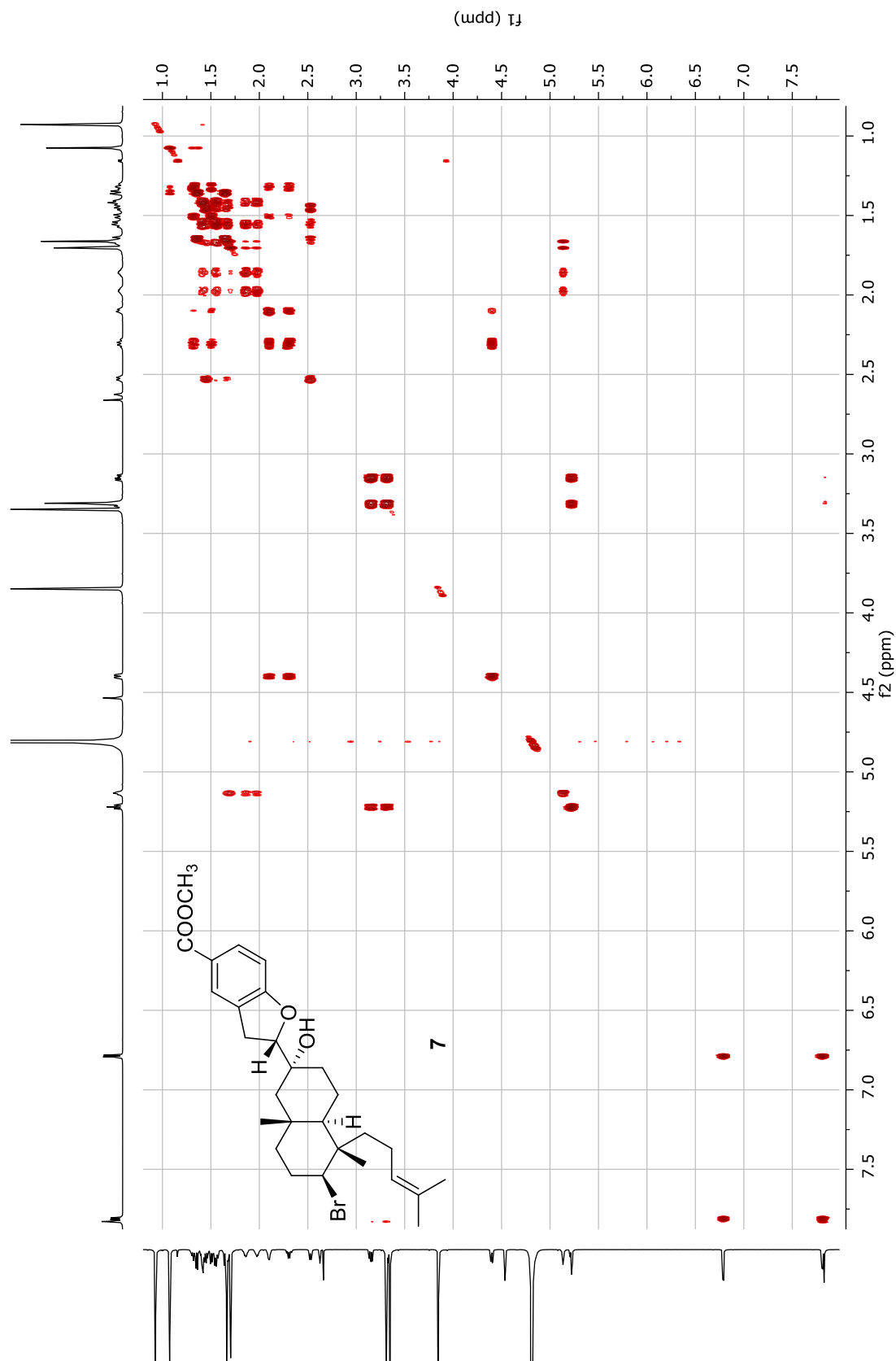


Figure S59. ^1H - ^{13}C edited-HSQC spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD .

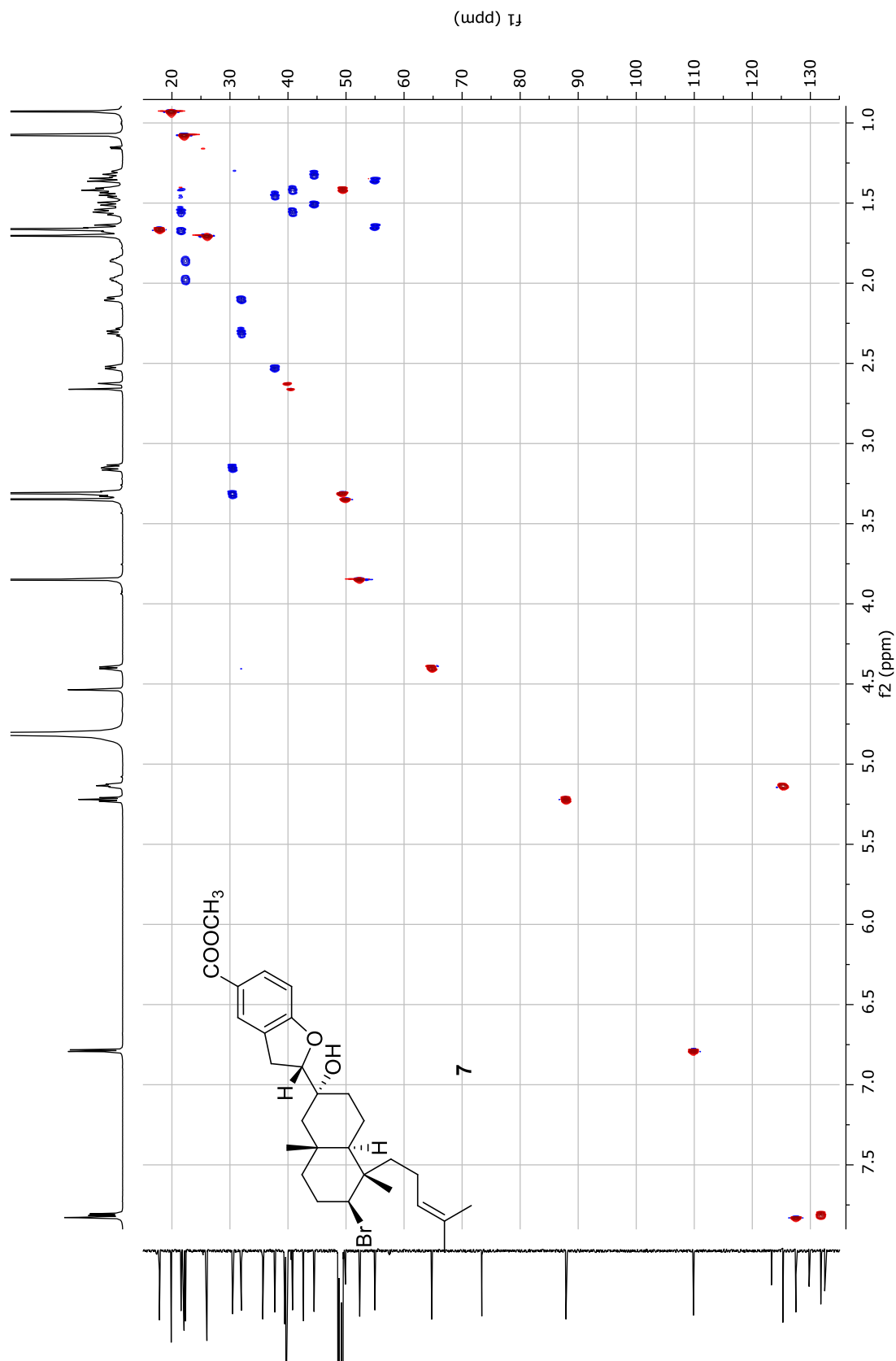


Figure S60. ^1H - ^{13}C HMBC spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD .

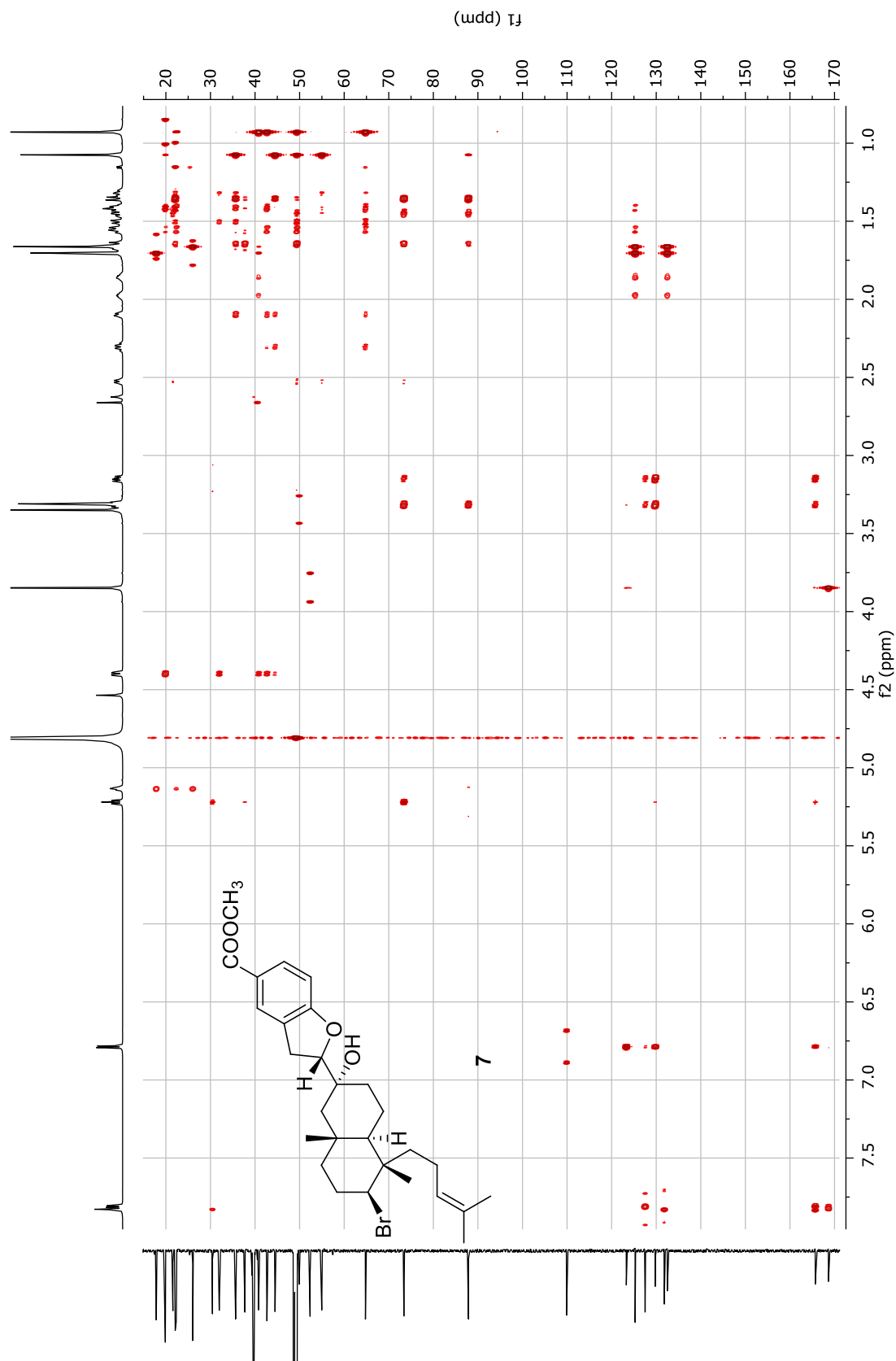
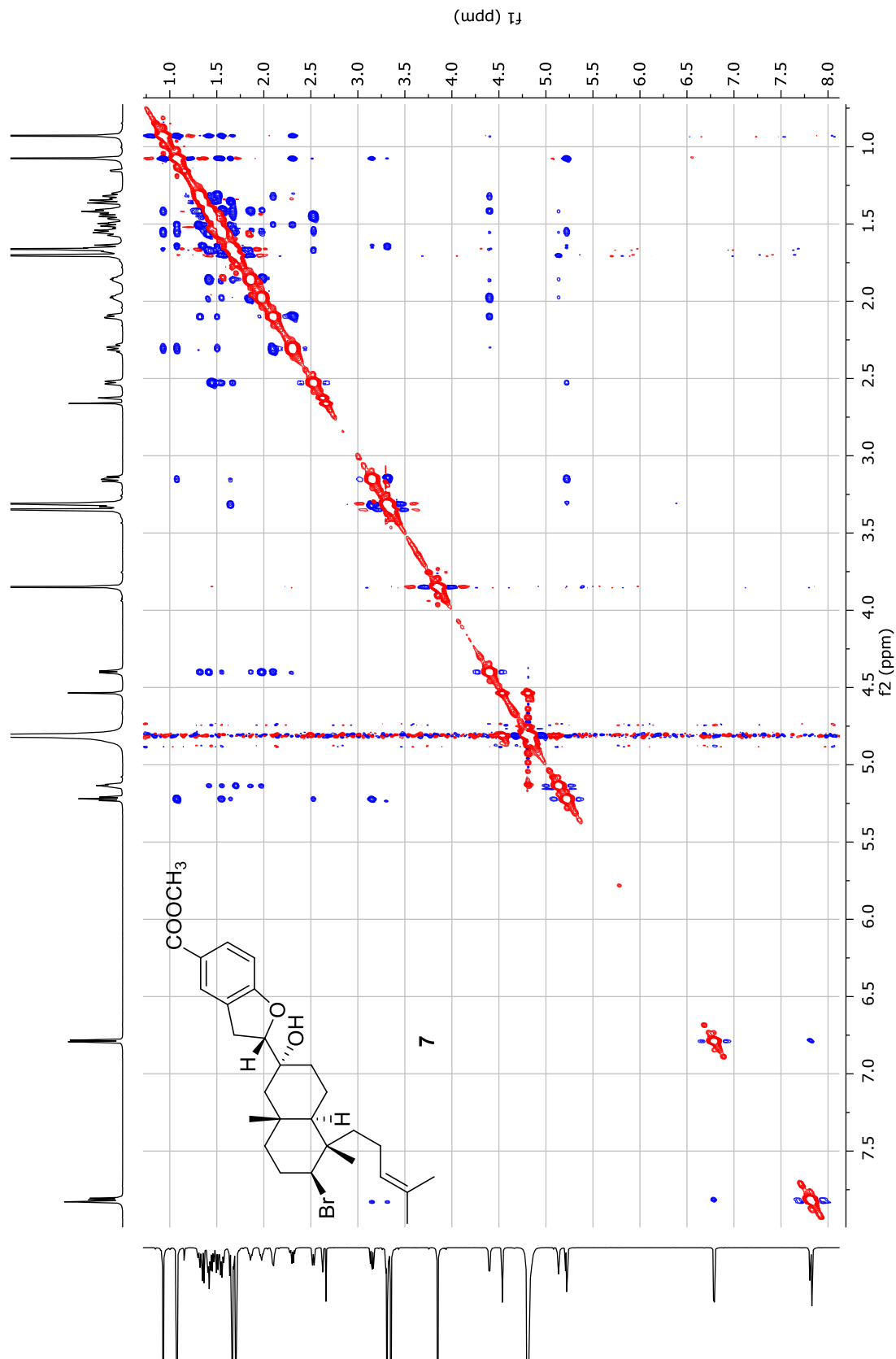


Figure S61. ^1H - ^1H NOESY spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD .



SPECTRA OF 3-GERANYLGERANYL-4-HYDROXYBENZOIC ACID (8)**Figure S62.** ^1H NMR spectrum of 3-geranylgeranyl-4-hydroxybenzoic acid (**8**) at 500 MHz in CD_3OD .