Supporting Information 1

Iodinated Meroditerpenes from a Red Alga *Callophycus* sp.

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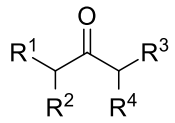
Contents

OTHER KNOWN IODINATED STRUCTURES

Refer to main article for references in [ ].



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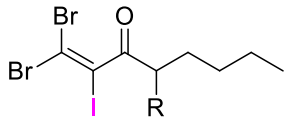
8	I	H	Br	Br	C_4H_9	[9]



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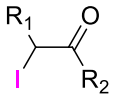

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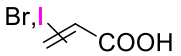
12	Cl	OH	[11]
13	Cl	NH_2	[12]
14	Br	NH_2	[12]



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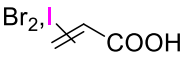

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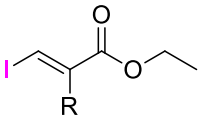

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17	H	[7]
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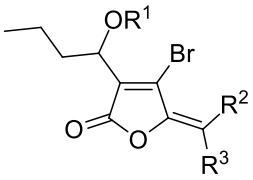
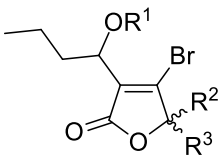


	R^1	R^2	R^3	Ref
19	H	I	H	[13]
20	Ac	I	H	[13]
21	H	H	I	[13]
22	Ac	H	I	[13]



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23	Ac	CH_2I	OCH_3	[14]
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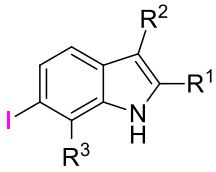
25	H	OCH_3	CH_2I	[14]



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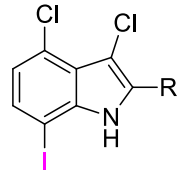
27	Br	Cl	Br	[15]
28	Cl	Br	Br	[15]
29	Cl	Cl	Cl	[15]



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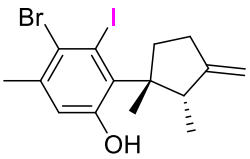
30	Br	[15]
31	Cl	[15]



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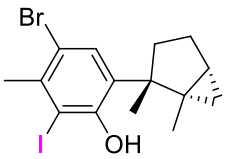

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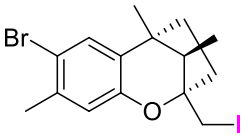

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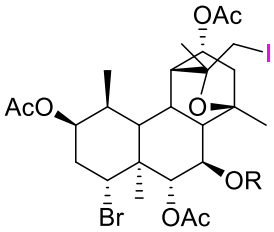


	R	Ref
35	H	[18]
36	Ac	[18]

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	**2*S*,6*S*,7*S*,10*S*,14*S*-1a**			**2*S*,6*S*,7*S*,10*S*,14*S*-1b**		
	x	*y*	*z*	*x*	*y*	*z*
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	**2*S*,6*S*,7*S*,10*S*,14*S*-1a**			**2*S*,6*S*,7*S*,10*S*,14*S*-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	**2*S*,6*S*,7*S*,10*S*,14*S*-1c**			**2*S*,6*S*,7*S*,10*S*,14*S*-1d**		
	x	*y*	*z*	*x*	*y*	*z*
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	**2*S*,6*S*,7*S*,10*S*,14*S*-1c**			**2*S*,6*S*,7*S*,10*S*,14*S*-1d**		
	x	*y*	*z*	*x*	*y*	*z*
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	**2*S*,6*S*,7*S*,10*R*,14*R*-1a**			**2*S*,6*S*,7*S*,10*R*,14*R*-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	**2*S*,6*S*,7*S*,10*R*,14*R*-1a**			**2*S*,6*S*,7*S*,10*R*,14*R*-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).

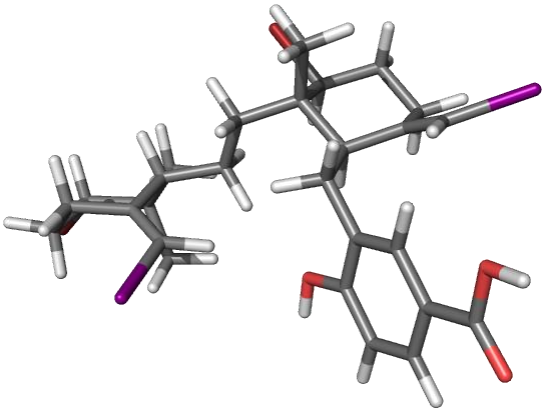
Atom	2*S*,6*S*,7*S*,10*R*,14*R*-1c			2*S*,6*S*,7*S*,10*R*,14*R*-1d		
	x	*y*	*z*	*x*	*y*	*z*
C	−2.7542	−2.1670	−1.6111	−2.7466	−2.1798	−1.6091
C	−3.0311	−1.2049	−0.4871	−3.0253	−1.2213	−0.4824
C	−1.7849	−0.4184	−0.0783	−1.7815	−0.4308	−0.0738
C	−0.6799	−1.4227	0.4831	−0.6713	−1.4321	0.4827
C	−0.4204	−2.4129	−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	**2*S*,6*S*,7*S*,10*R*,14*R*-1c**			**2*S*,6*S*,7*S*,10*R*,14*R*-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

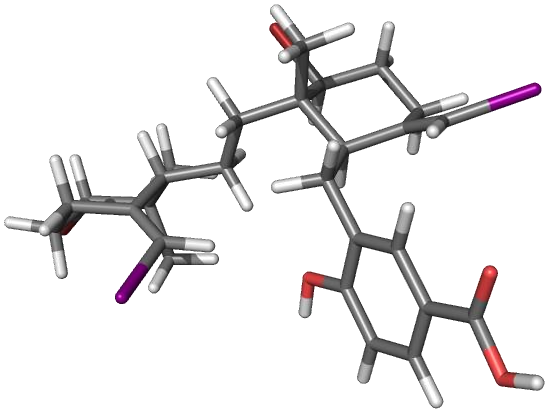
Table S5. Electronic energies (Δ*E*), free energies (Δ*G*), and Boltzmann distribution abundances for the conformers of iodocallophycoic acid A (**1**), obtained through DFT calculations at the B3LYP/SVP level of theory in methanol.

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

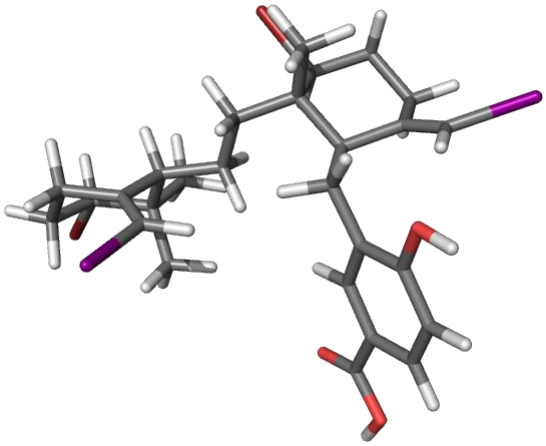
*Convergent conformers.



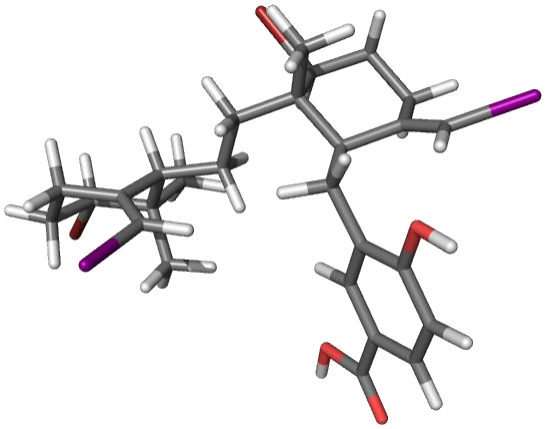
2*S*,6*S*,7*S*,10*S*,14*S*-1a



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

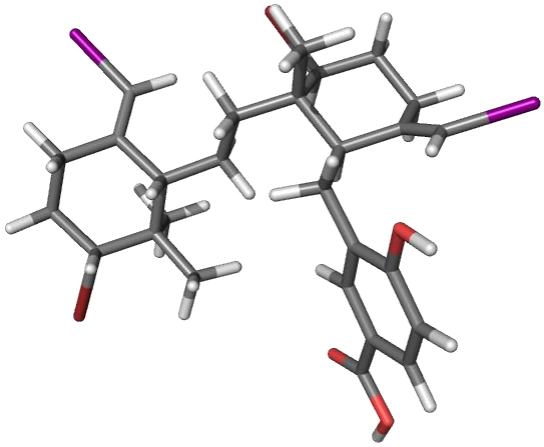


2*S*,6*S*,7*S*,10*S*,14*S*-1c

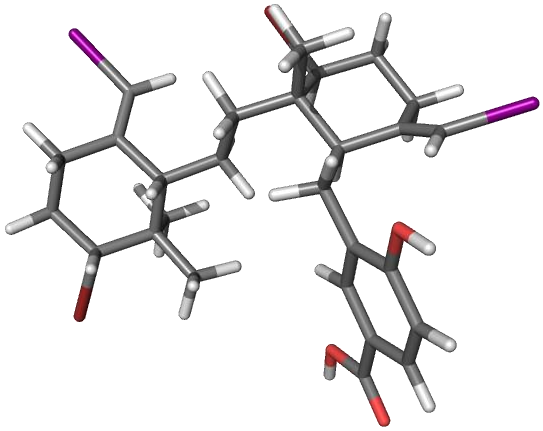


2*S*,6*S*,7*S*,10*S*,14*S*-1d

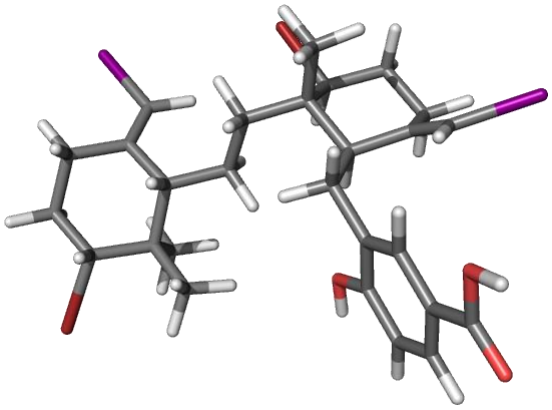
Figure S2. 3D structure of 2*S*,6*S*,7*S*,10*S*,14*S*-iodocallophycoic acid A (**1**) conformers optimized at the B3LYP/SVP level of theory in methanol.



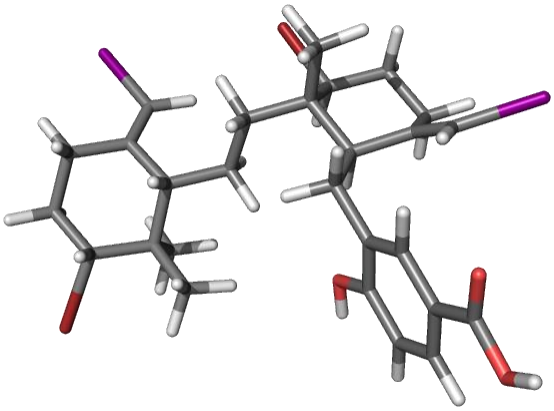
2*S*,6*S*,7*S*,10*R*,14*R*-1b



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



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



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

Figure S3. B3LYP/SVP in methanol optimized conformers of 2*S*,6*S*,7*S*,10*R*,14*R*-**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	**2*S*,6*S*,7*S*,10*S*,14*S*-1a**			**2*S*,6*S*,7*S*,10*S*,14*S*-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	**2*S*,6*S*,7*S*,10*S*,14*S*-1a**			**2*S*,6*S*,7*S*,10*S*,14*S*-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	**2*S*,6*S*,7*S*,10*S*,14*S*-1c**			**2*S*,6*S*,7*S*,10*S*,14*S*-1d**		
	x	*y*	*z*	*x*	*y*	*z*
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	**2*S*,6*S*,7*S*,10*S*,14*S*-1c**			**2*S*,6*S*,7*S*,10*S*,14*S*-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	**2*S*,6*S*,7*S*,10*R*,14*R*-1a**			**2*S*,6*S*,7*S*,10*R*,14*R*-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	**2*S*,6*S*,7*S*,10*R*,14*R*-1a**			**2*S*,6*S*,7*S*,10*R*,14*R*-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	2*S*,6*S*,7*S*,10*R*,14*R*−1c			2*S*,6*S*,7*S*,10*R*,14*R*−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	**2*S*,6*S*,7*S*,10*R*,14*R*−1c**			**2*S*,6*S*,7*S*,10*R*,14*R*−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 (Δ*E*), free energies (Δ*G*), 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 (%)
	Δ*E*	Δ*G*	
2*S*,6*S*,7*S*,10*S*,14*S*-1a	−20261.620148	−20261.136193	11.34
2*S*,6*S*,7*S*,10*S*,14*S*-1b	−20261.620256	−20261.136095	10.22
2*S*,6*S*,7*S*,10*S*,14*S*-1c	−20261.620013	−20261.137114	30.07
2*S*,6*S*,7*S*,10*S*,14*S*-1d	−20261.619854	−20261.136509	15.85
2*S*,6*S*,7*S*,10*S*,14*S*-1e	−20261.616610	−20261.133813	0.91
2*S*,6*S*,7*S*,10*S*,14*S*-1f	−20261.616450	−20261.133314	0.54
2*S*,6*S*,7*S*,10*S*,14*S*-1g	−20261.616581	−20261.132517	0.23
2*S*,6*S*,7*S*,10*S*,14*S*-1h	−20261.616459	−20261.132398	0.20
2*S*,6*S*,7*S*,10*S*,14*S*-1i	−20261.615743	−20261.132642	0.26
2*S*,6*S*,7*S*,10*S*,14*S*-1j	−20261.615848	−20261.132612	0.26
2*S*,6*S*,7*S*,10*S*,14*S*-1k	−20261.620013	−20261.137114	30.07
2*S*,6*S*,7*S*,10*S*,14*S*-1l	−20261.613303	−20261.129973	0.02
2*S*,6*S*,7*S*,10*S*,14*S*-1m	−20261.613211	−20261.129544	0.01
2*S*,6*S*,7*S*,10*S*,14*S*-1n	−20261.612545	−20261.130293	0.02
2*S*,6*S*,7*S*,10*R*,14*R*-1a	−20261.620971	−20261.135879	18.69
2*S*,6*S*,7*S*,10*R*,14*R*-1b	−20261.620858	−20261.136722	45.63
2*S*,6*S*,7*S*,10*R*,14*R*-1c	−20261.620274	−20261.135508	12.62
2*S*,6*S*,7*S*,10*R*,14*R*-1d	−20261.620379	−20261.135628	14.32
2*S*,6*S*,7*S*,10*R*,14*R*-1e	−20261.615332	−20261.130046	0.04
2*S*,6*S*,7*S*,10*R*,14*R*-1f	−20261.617617	−20261.133993	2.54
2*S*,6*S*,7*S*,10*R*,14*R*-1g	−20261.617482	−20261.134607	4.86
2*S*,6*S*,7*S*,10*R*,14*R*-1h	−20261.615441	−20261.128215	0.01
2*S*,6*S*,7*S*,10*R*,14*R*-1i	−20261.615349	−20261.128197	0.01
2*S*,6*S*,7*S*,10*R*,14*R*-1j	−20261.614278	−20261.129742	0.03
2*S*,6*S*,7*S*,10*R*,14*R*-1k	−20261.615842	−20261.131557	0.19
2*S*,6*S*,7*S*,10*R*,14*R*-1l	−20261.614158	−20261.129835	0.03
2*S*,6*S*,7*S*,10*R*,14*R*-1m	−20261.615930	−20261.132005	0.31
2*S*,6*S*,7*S*,10*R*,14*R*-1n	−20261.615337	−20261.132058	0.33
2*S*,6*S*,7*S*,10*R*,14*R*-1o	−20261.615404	−20261.132271	0.41

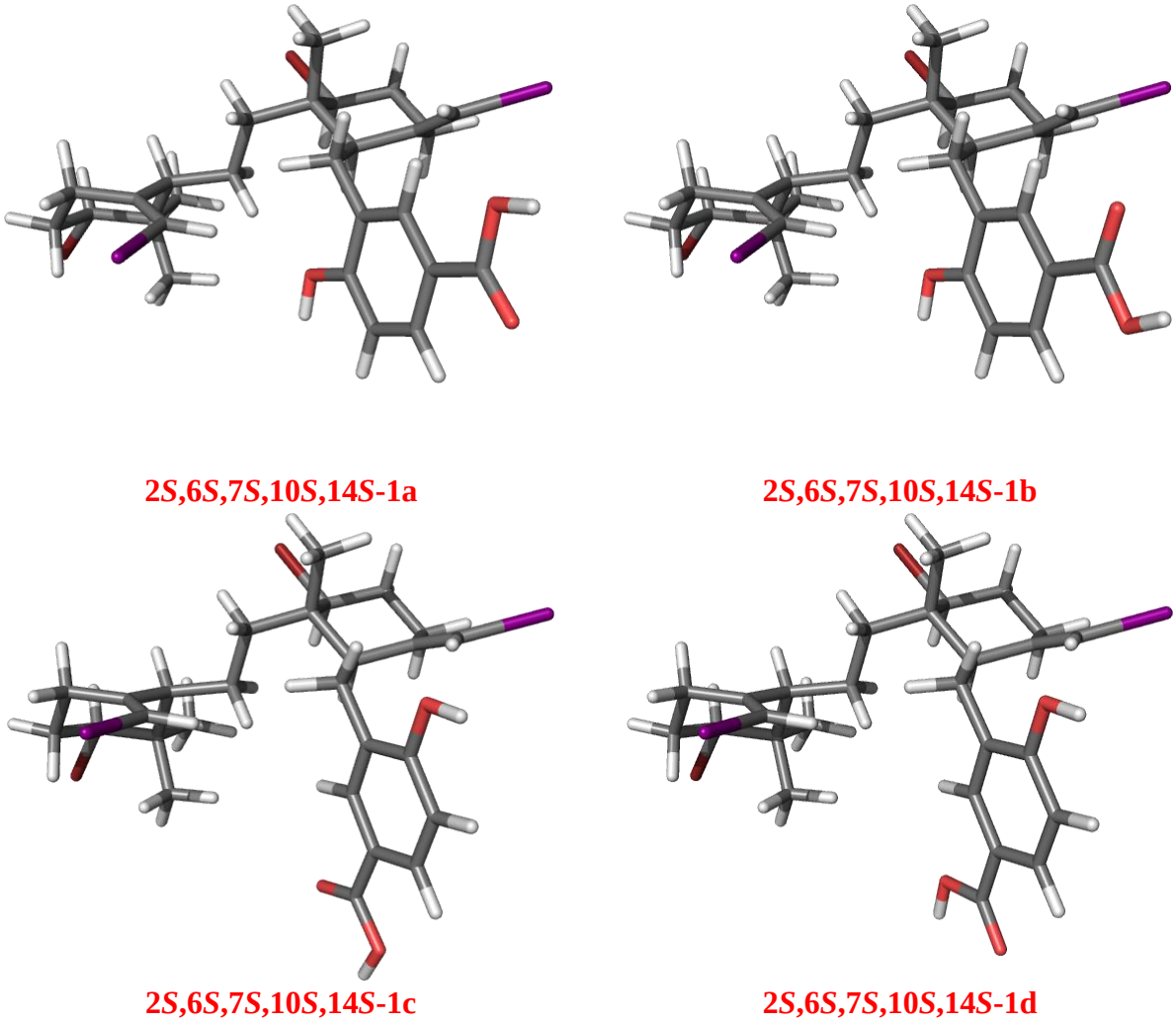


Figure S4. B3LYP/SVP optimized conformers of 2*S*,6*S*,7*S*,10*S*,14*S*-iodocallophycoic acid A (**1**) in acetonitrile.

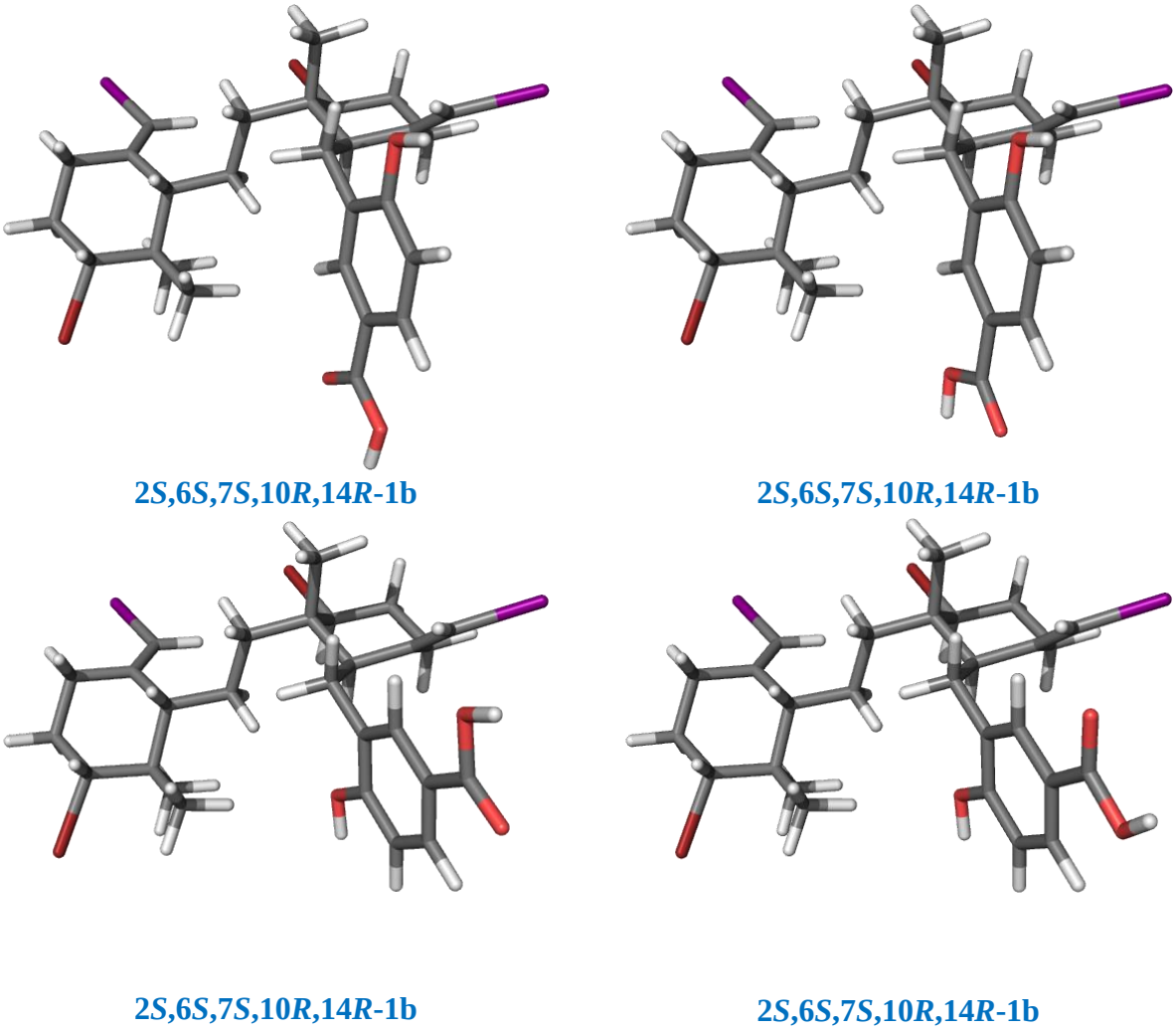


Figure S5. B3LYP/SVP optimized conformers of 2*S*,6*S*,7*S*,10*R*,14*R*-iodocallophycoic acid A (**1**) in acetonitrile.

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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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 (Δ*E*), free energies (Δ*G*), 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 (%)
	Δ*E*	Δ*G*	
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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**		
	x	*y*	*z*	*x*	*y*	*z*
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

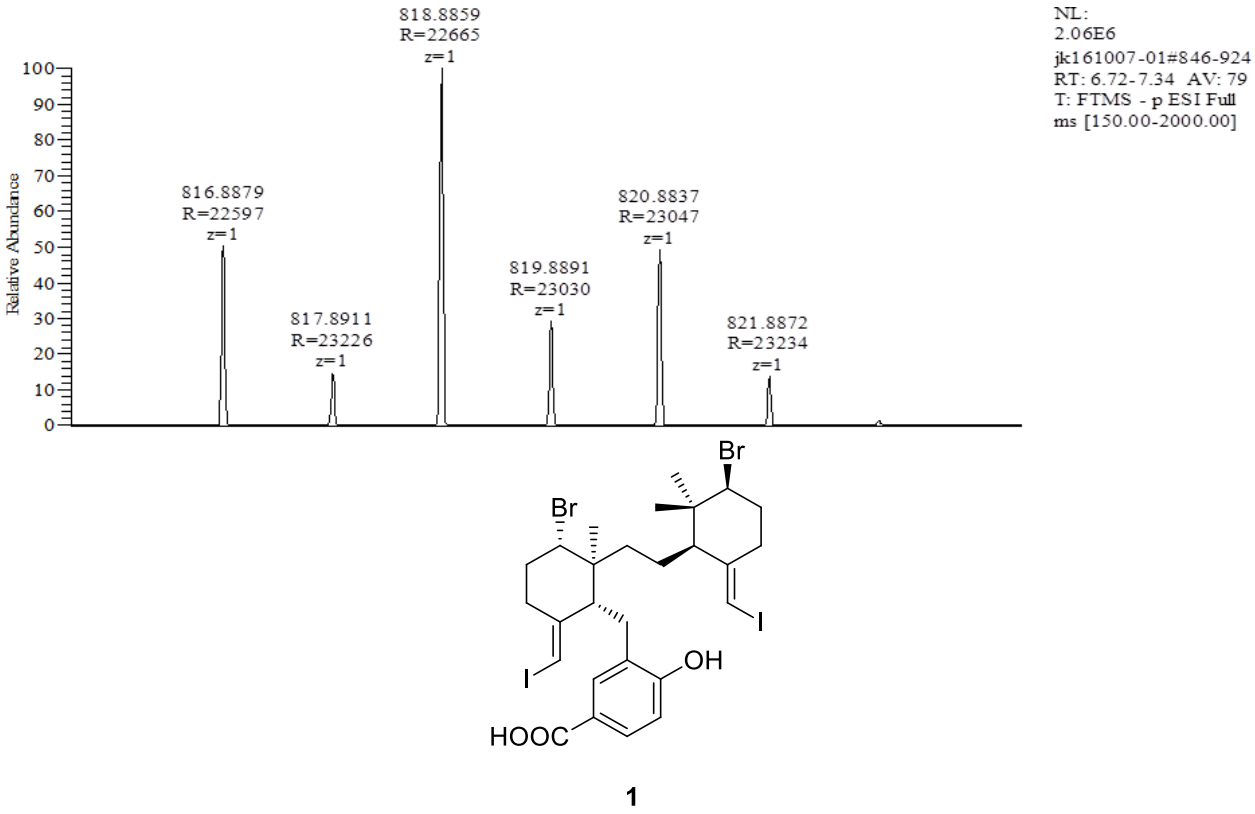
Atom	**7e**			**7f**		
	x	*y*	*z*	*x*	*y*	*z*
H	−7.4900	2.0518	1.0735	−7.5527	1.9953	1.1076
O	−3.4264	0.0315	1.4953	−3.4262	0.0497	1.5043
C	−8.2564	0.7311	−1.2769	−8.3306	0.8184	−1.1219
O	−8.3716	0.3195	−2.4109	−9.2741	1.3672	−0.5957
O	−9.3096	1.3415	−0.6947	−8.4619	0.3667	−2.3869
H	−9.1443	1.5233	0.2423	−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 (Δ*E*), free energies (Δ*G*), 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 (%)
	Δ*E*	Δ*G*	
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 iodocallophycoic acid A (**1**)



1

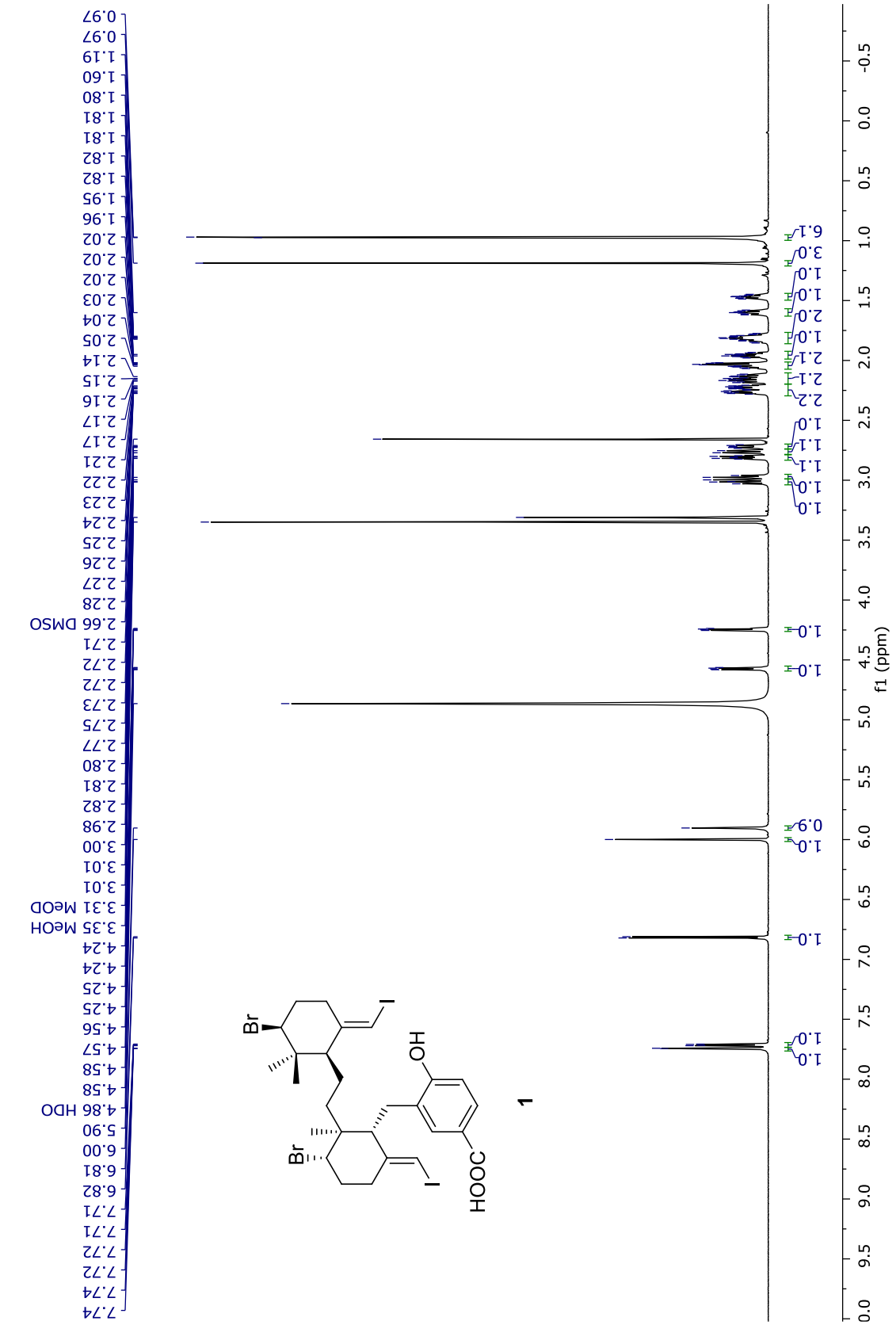


Figure S7. ^{1}H NMR spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD.

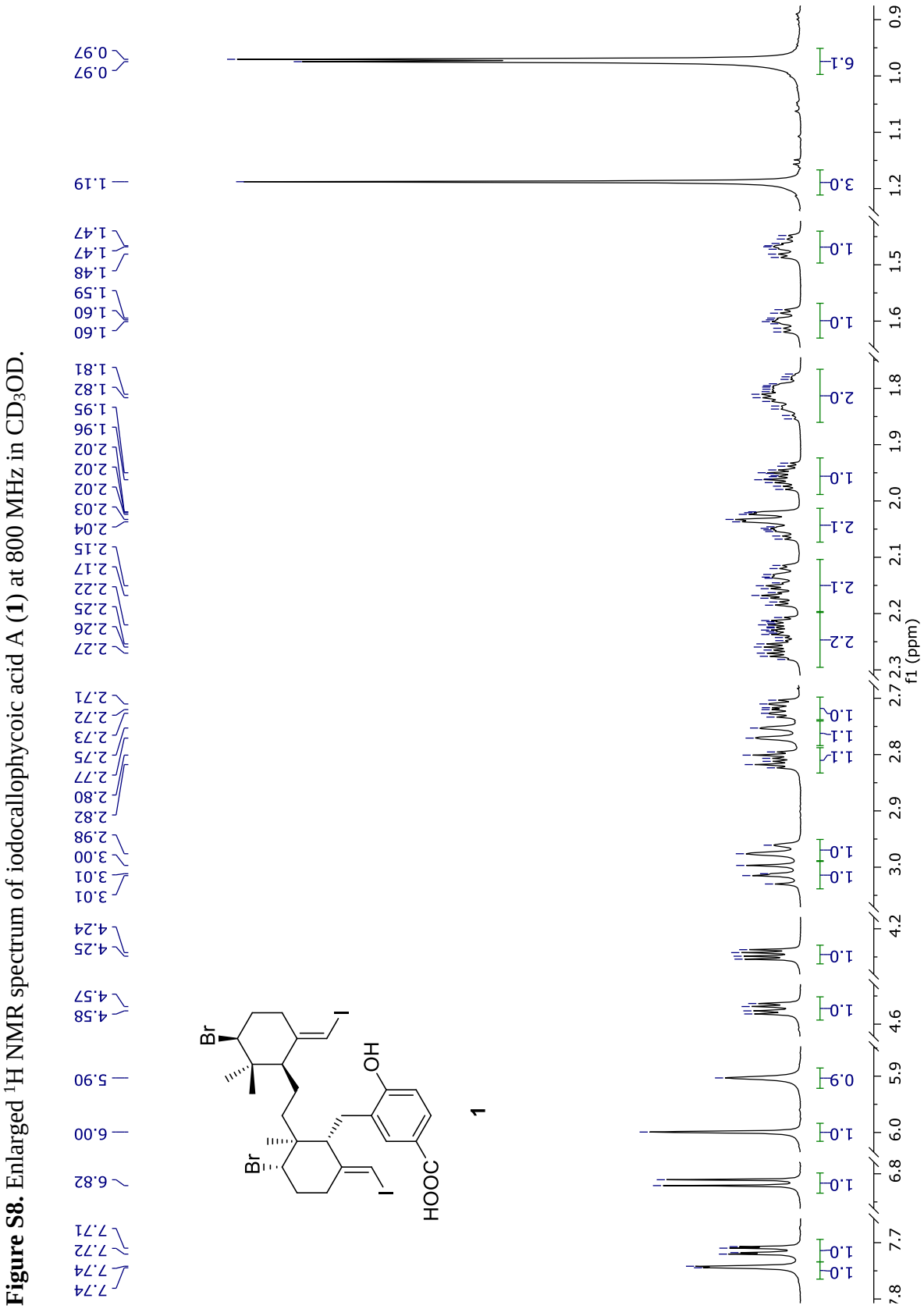


Figure S8. Enlarged ^{1}H NMR spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD.

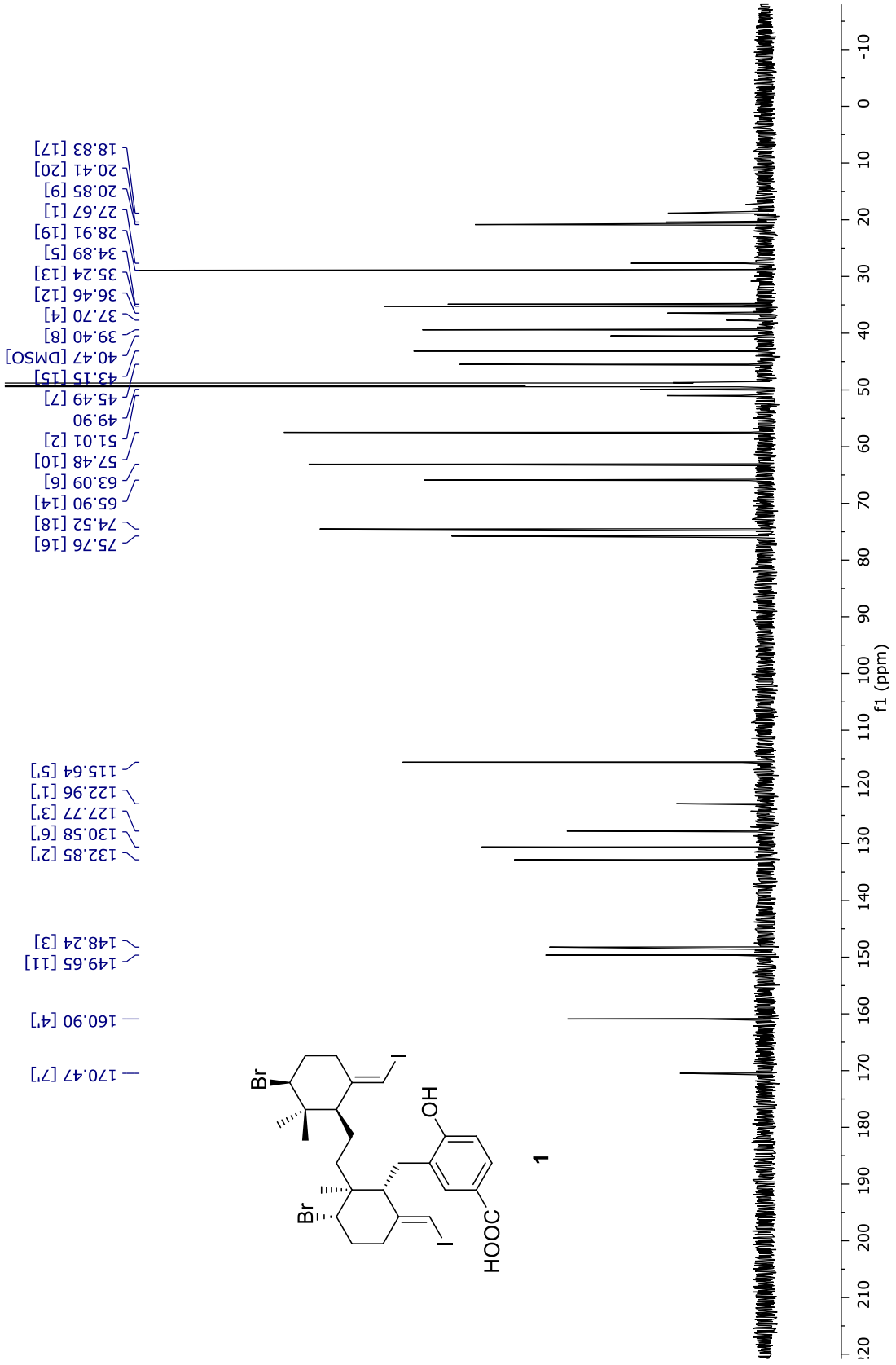


Figure S9. ^{13}C NMR spectrum of iodocallophycoic acid A (**1**) at 200 MHz in CD_3OD.

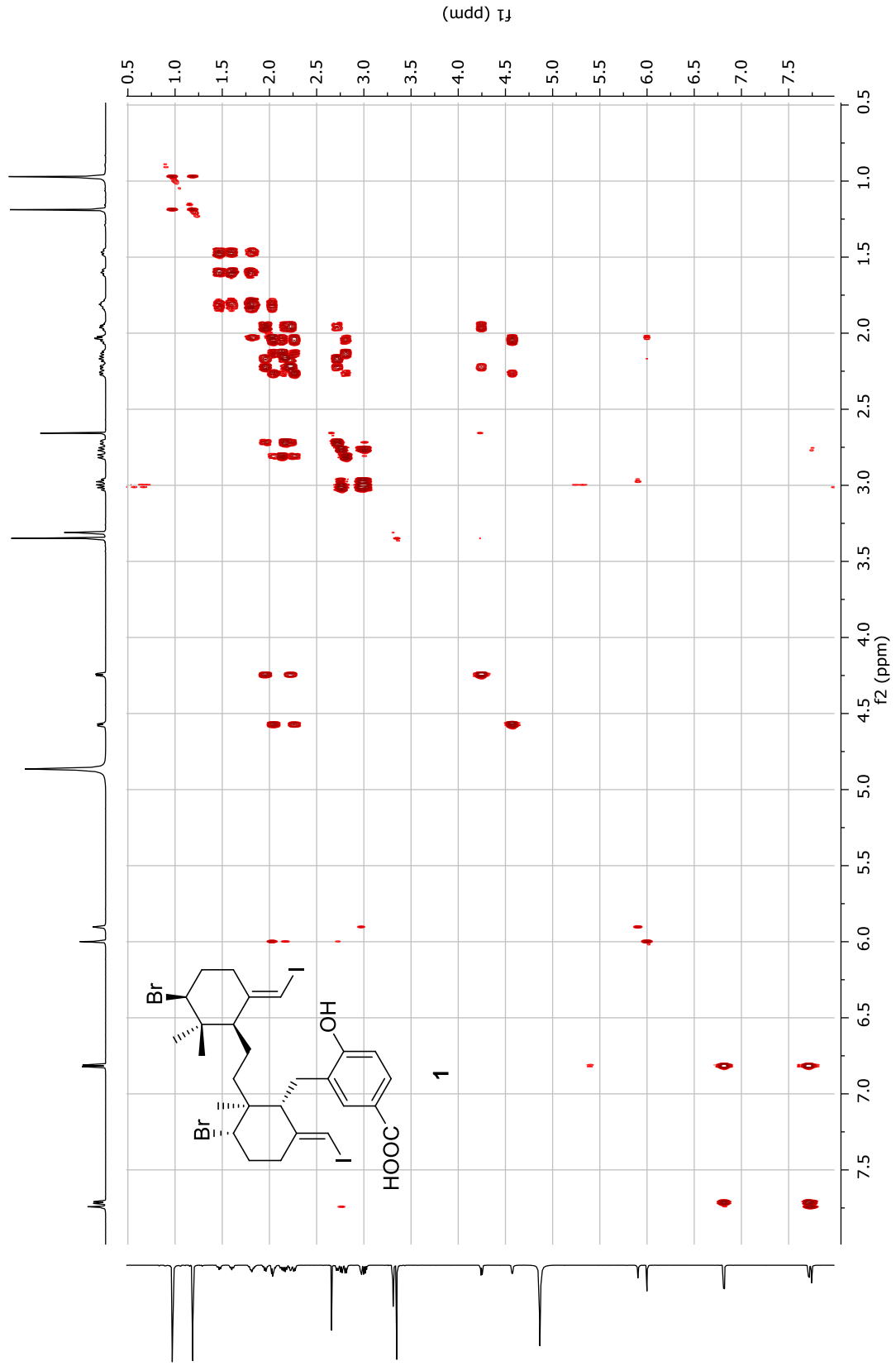


Figure S10. ^{1}H-^{1}H DQF-COSY spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD.

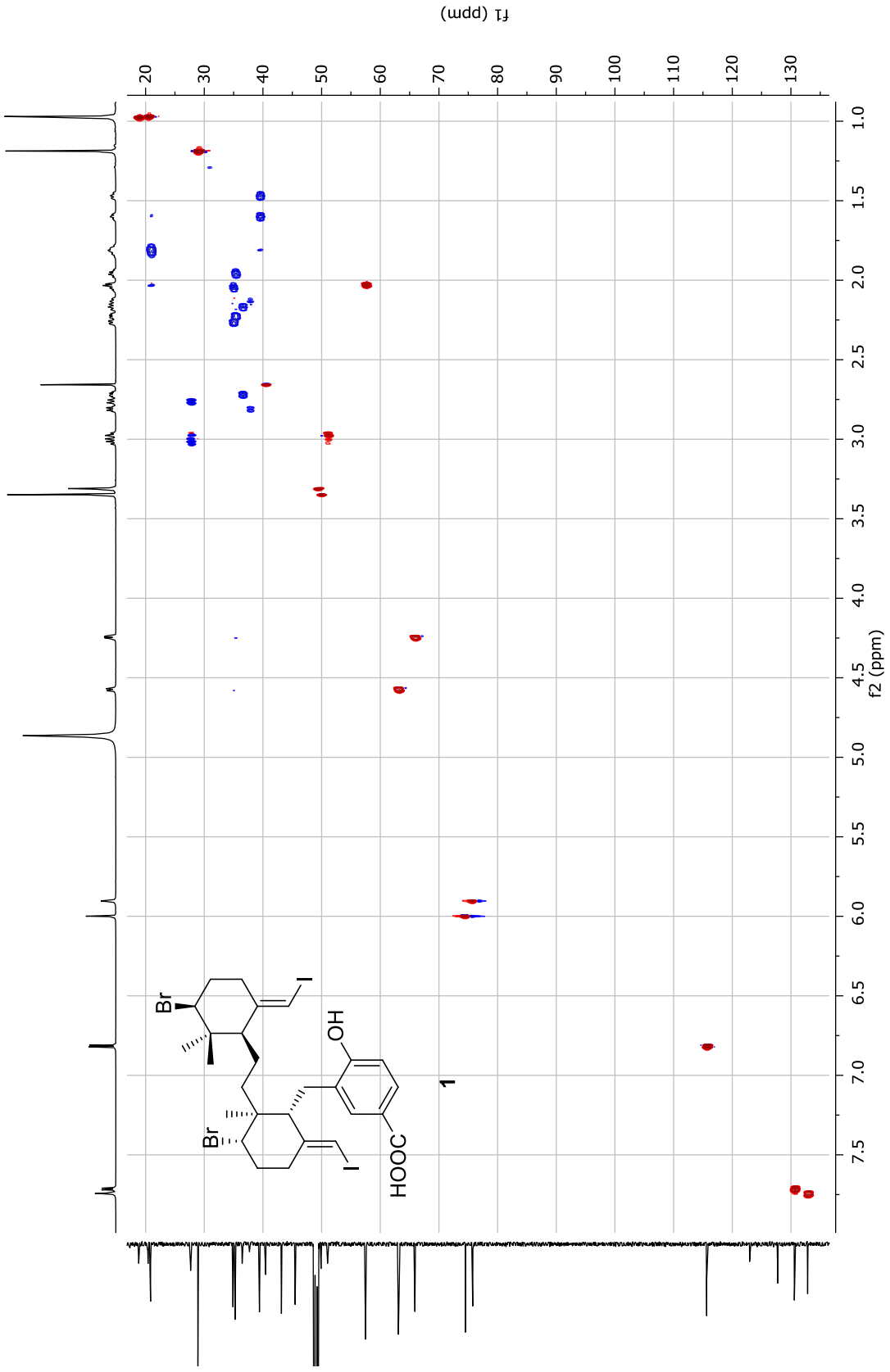


Figure S11. ^{1}H-^{13}C edited-HSQC spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD.

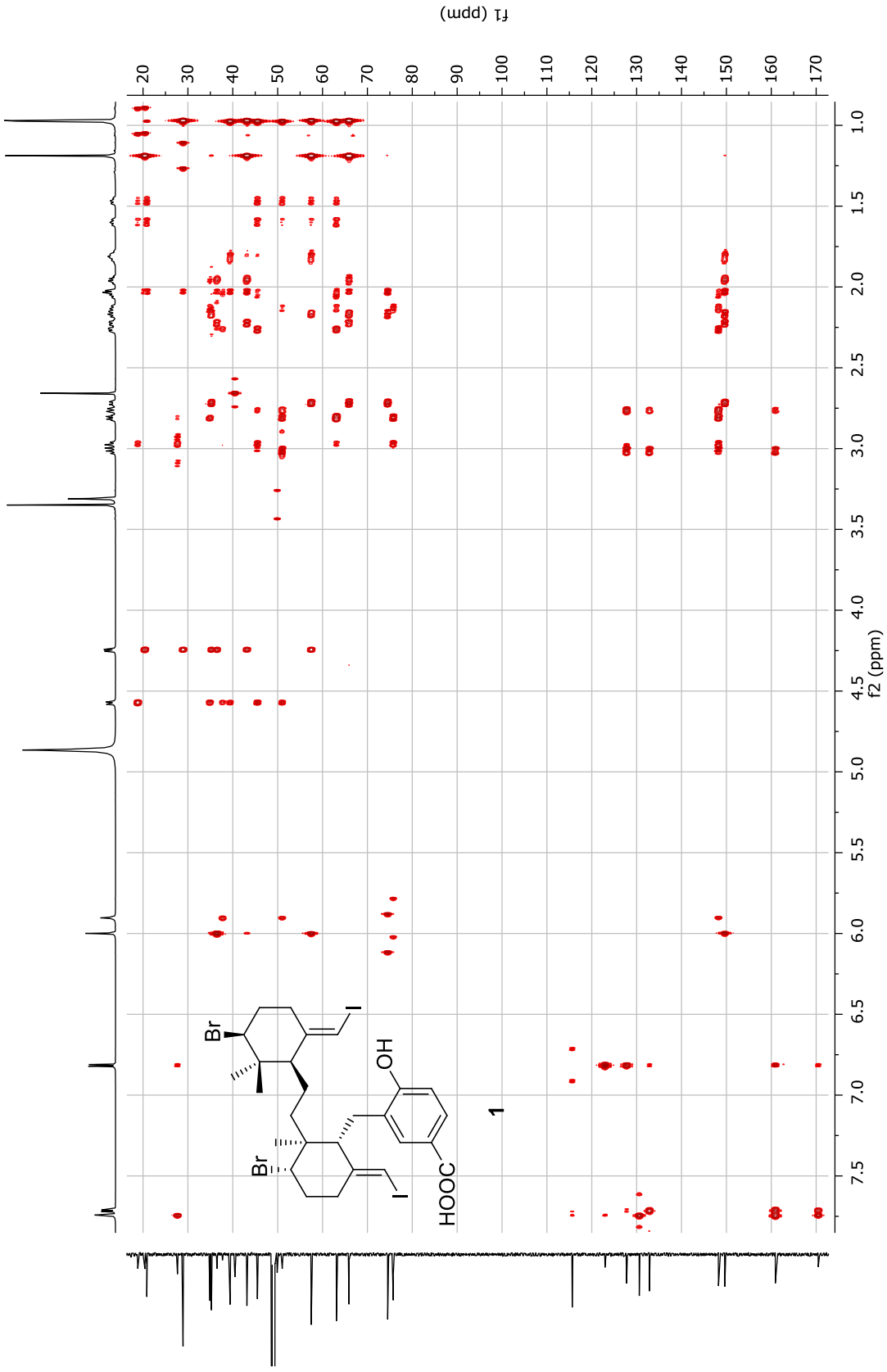


Figure S12. ^{1}H-^{13}C HMBC spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD.

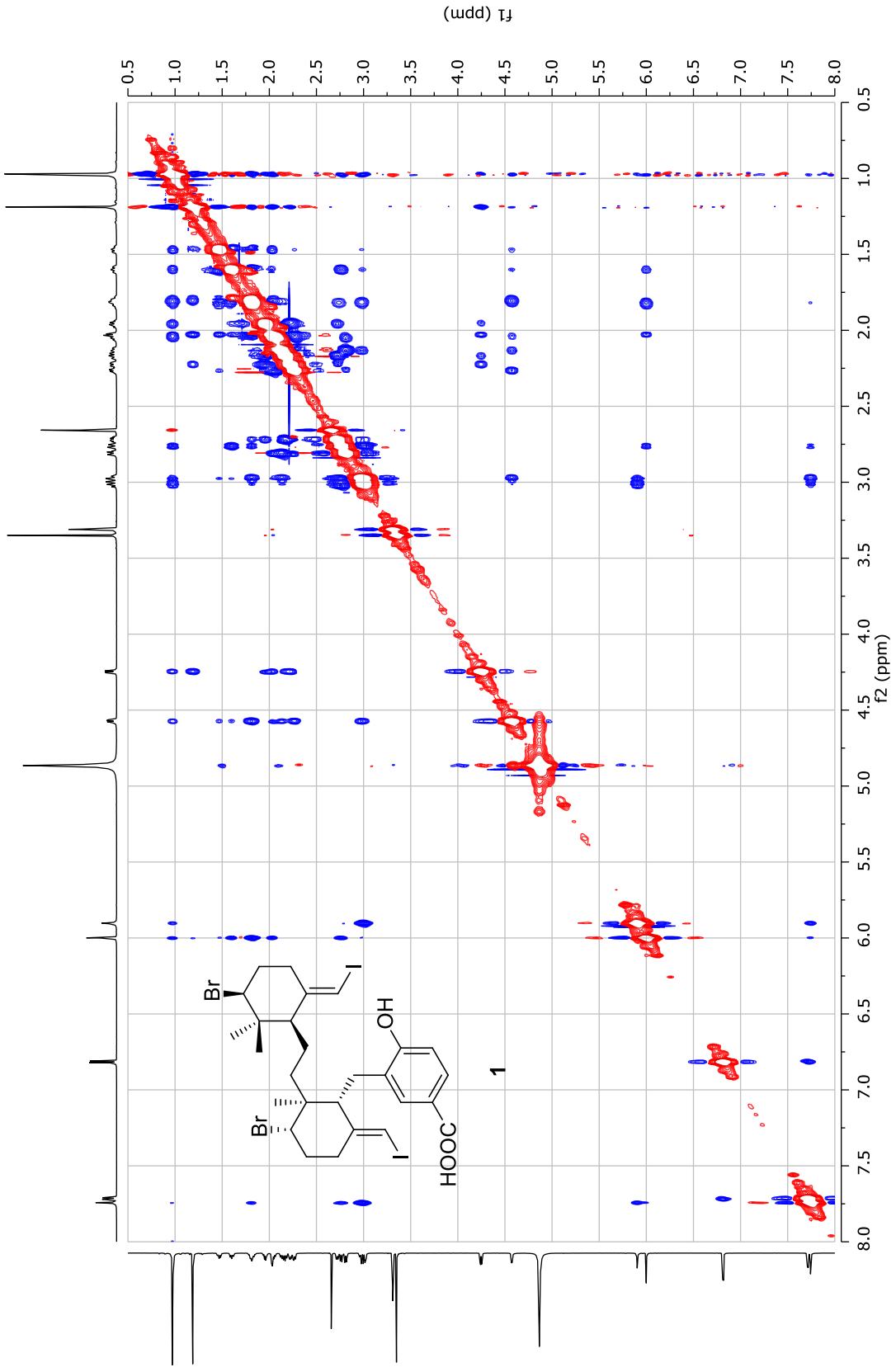
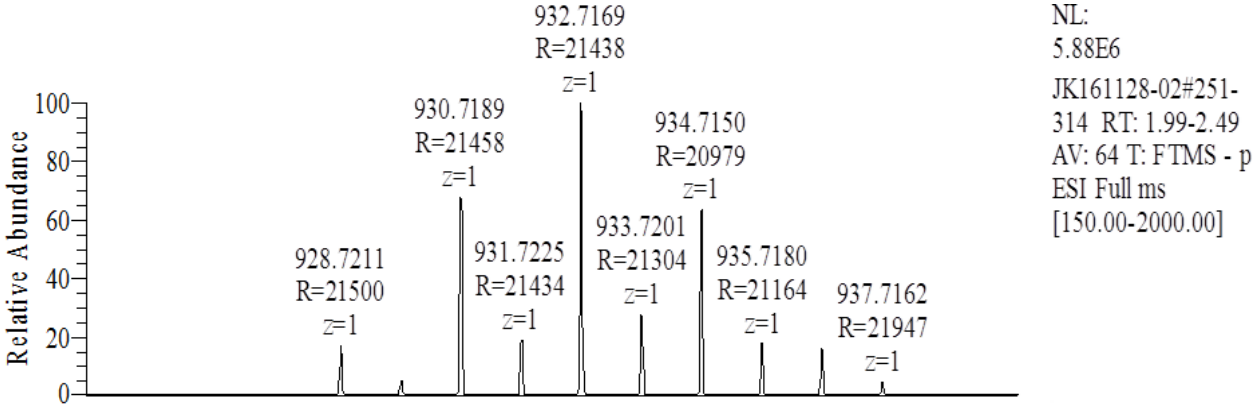
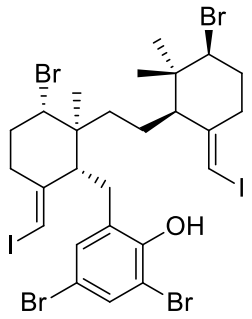


Figure S13. ^{1}H-^{1}H NOESY spectrum of iodocallophycoic acid A (**1**) at 800 MHz in CD_3OD.

SPECTRA OF IODOCALLOPHYCOL A (2)

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





2

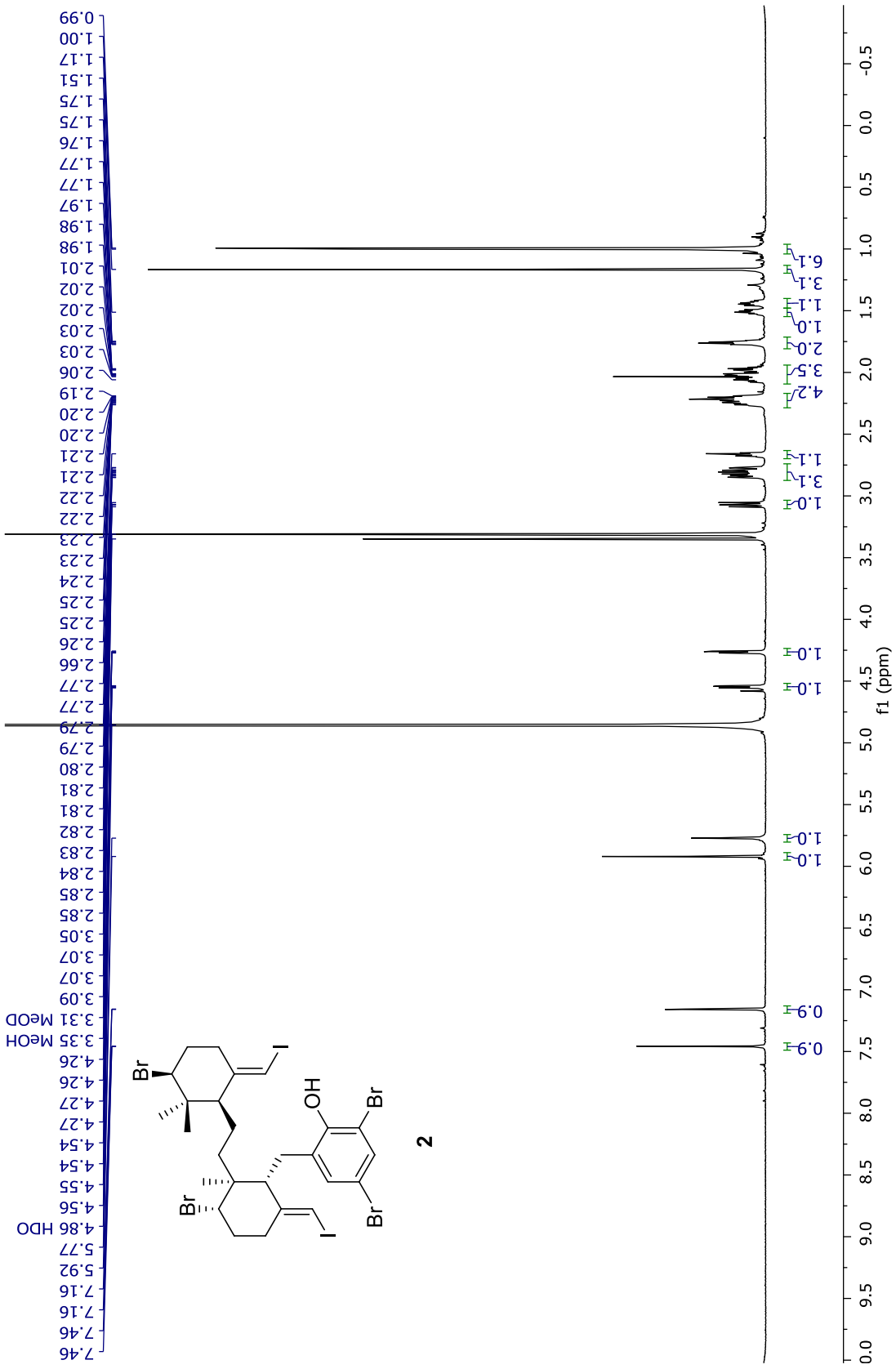


Figure S15. ^{1}H NMR spectrum of iodocallophycol A (**2**) at 800 MHz in CD_3OD.

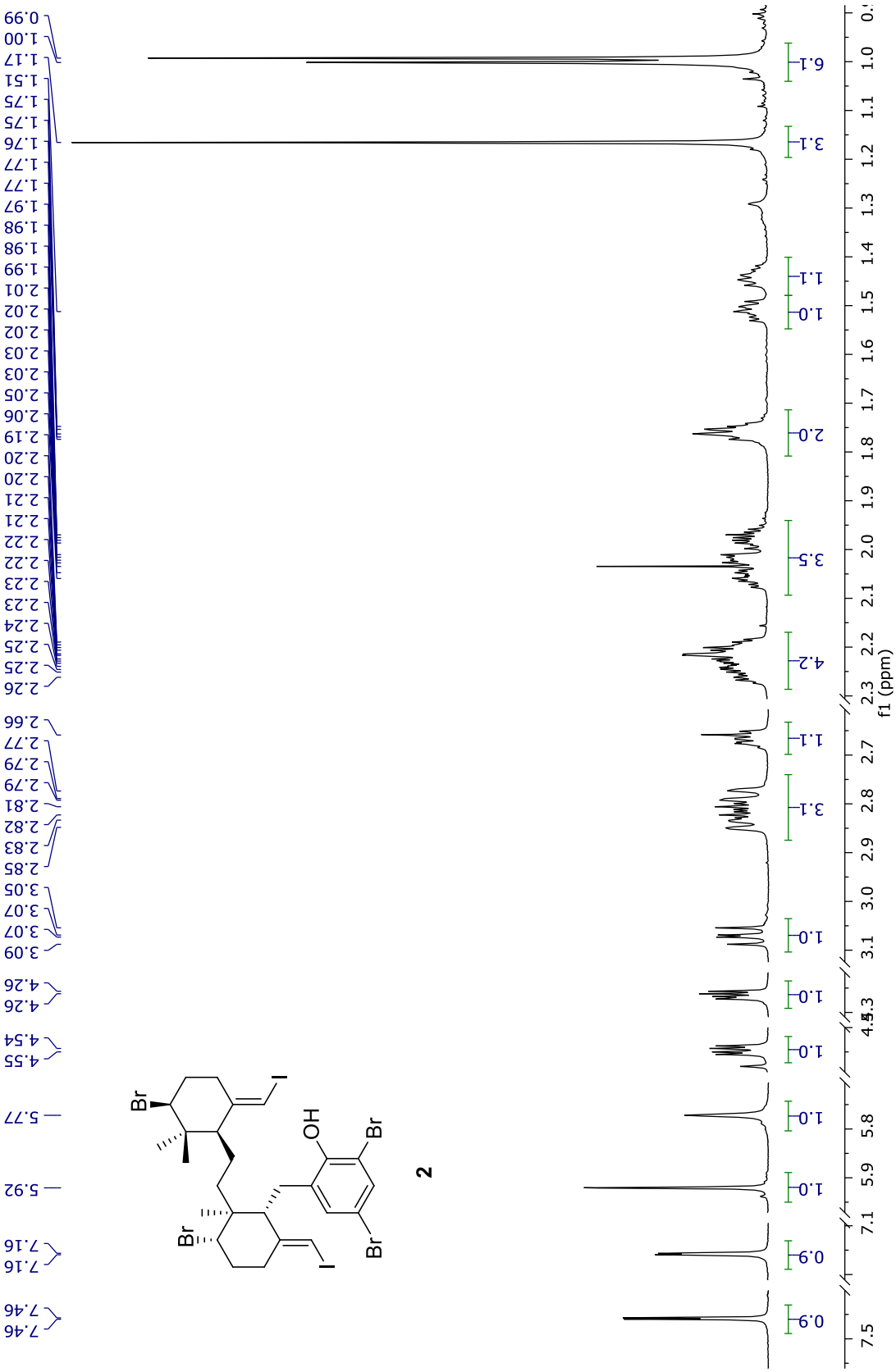


Figure S16. Enlarged ^{1}H NMR spectrum of iodocallophycol A (**2**) at 800 MHz in CD_3OD.

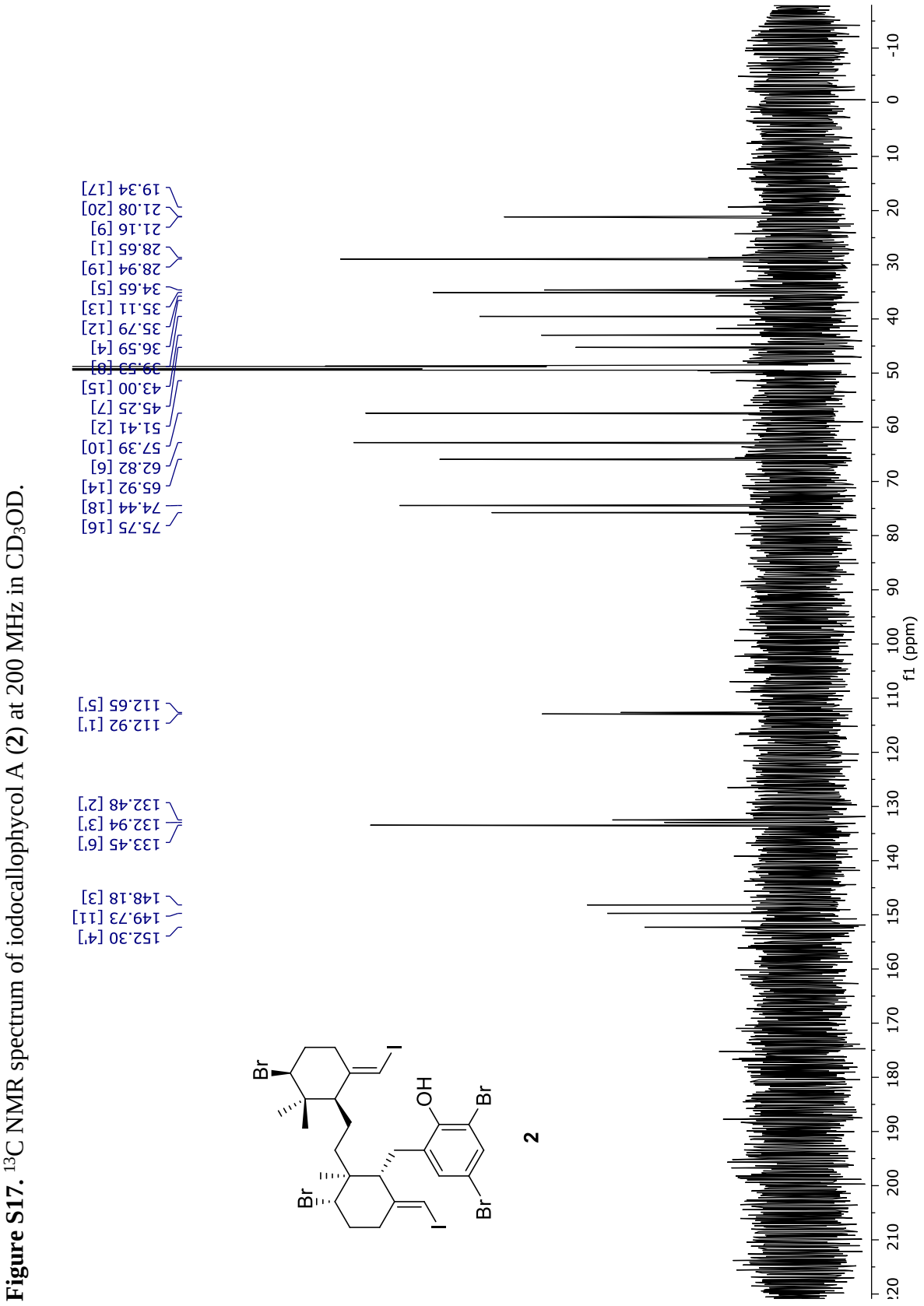


Figure S17. ^{13}C NMR spectrum of iodocallophycol A (**2**) at 200 MHz in CD_3OD.

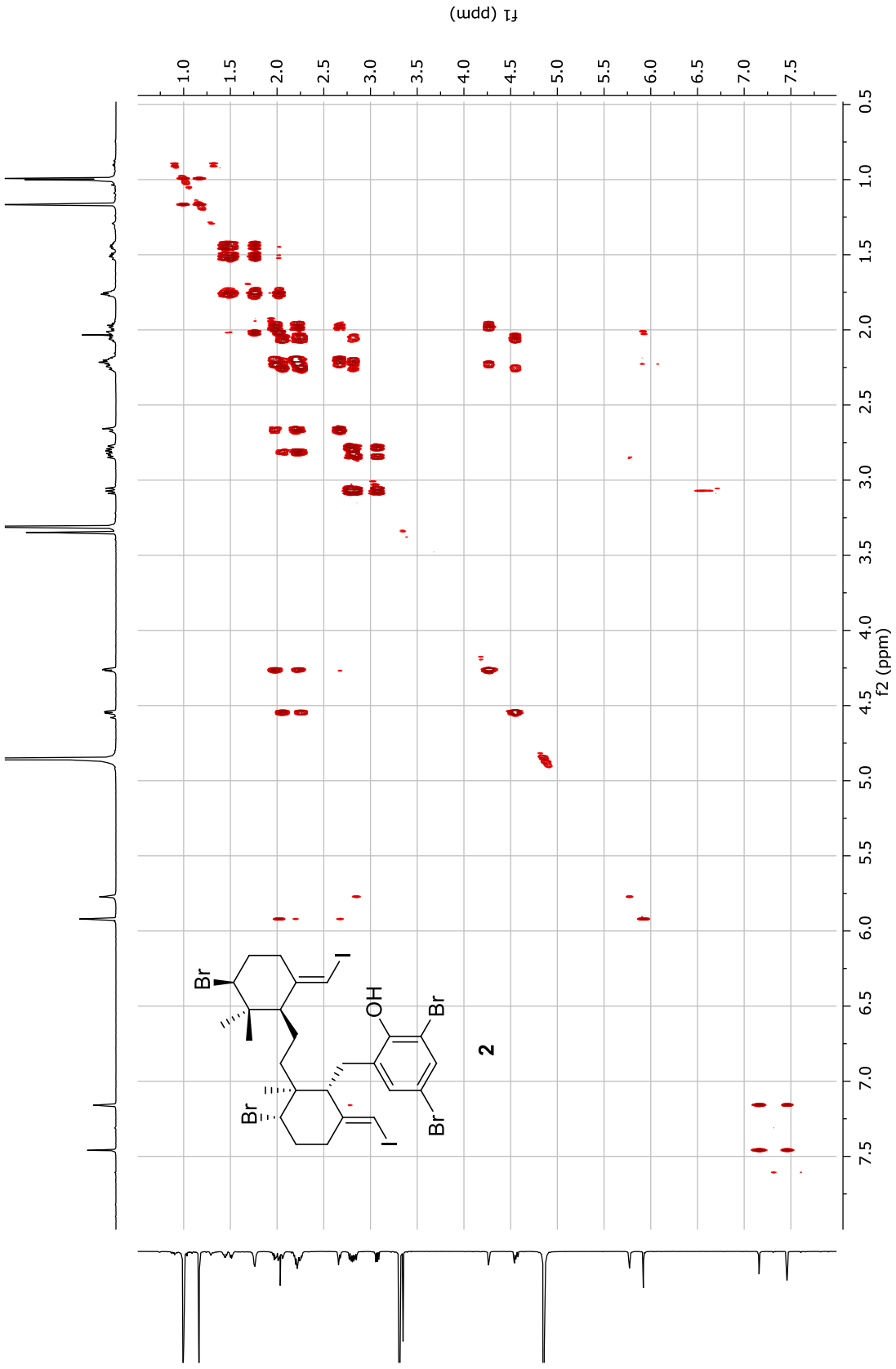


Figure S18. ^{1}H-^{1}H DQF-COSY spectrum of iodocallophycol A (**2**) at 800 MHz in CD_3OD.

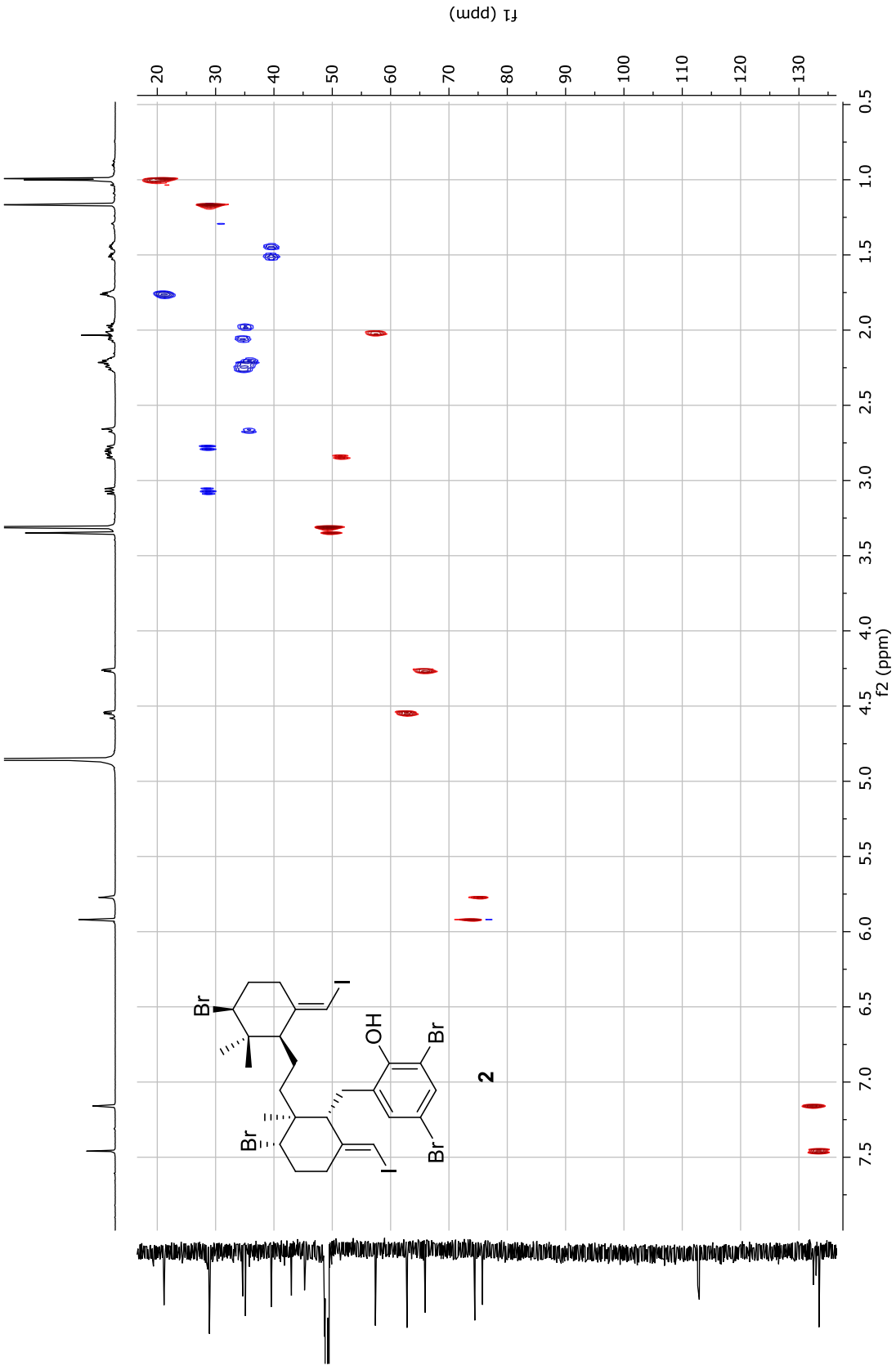


Figure S19. ^{1}H-^{13}C edited-HSQC spectrum of iodocallophycol A (**2**) at 800 MHz in CD_3OD.

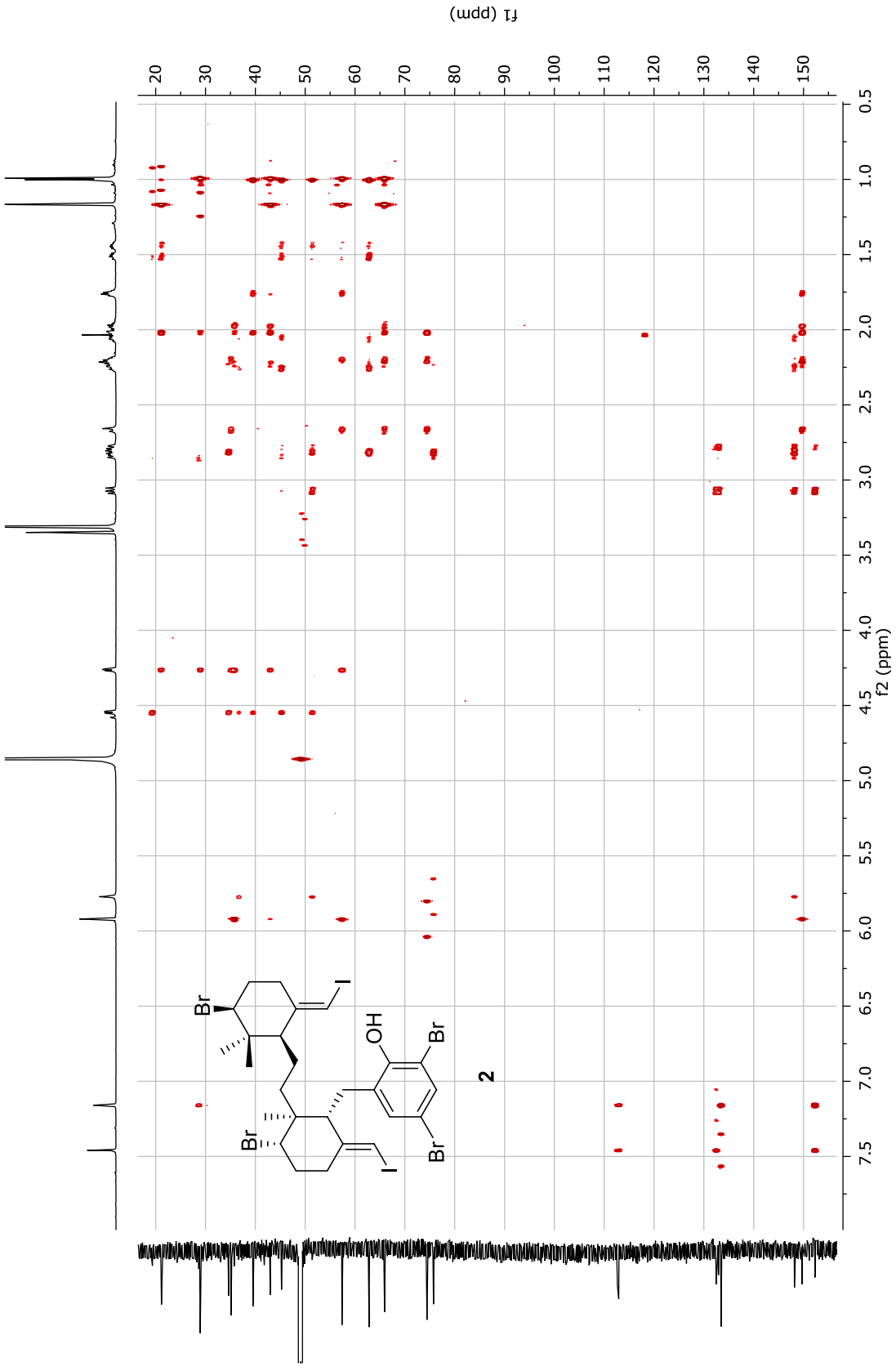


Figure S20. ^{1}H-^{13}C HMBC spectrum of iodocallophycol A (**2**) at 800 MHz in CD_3OD.

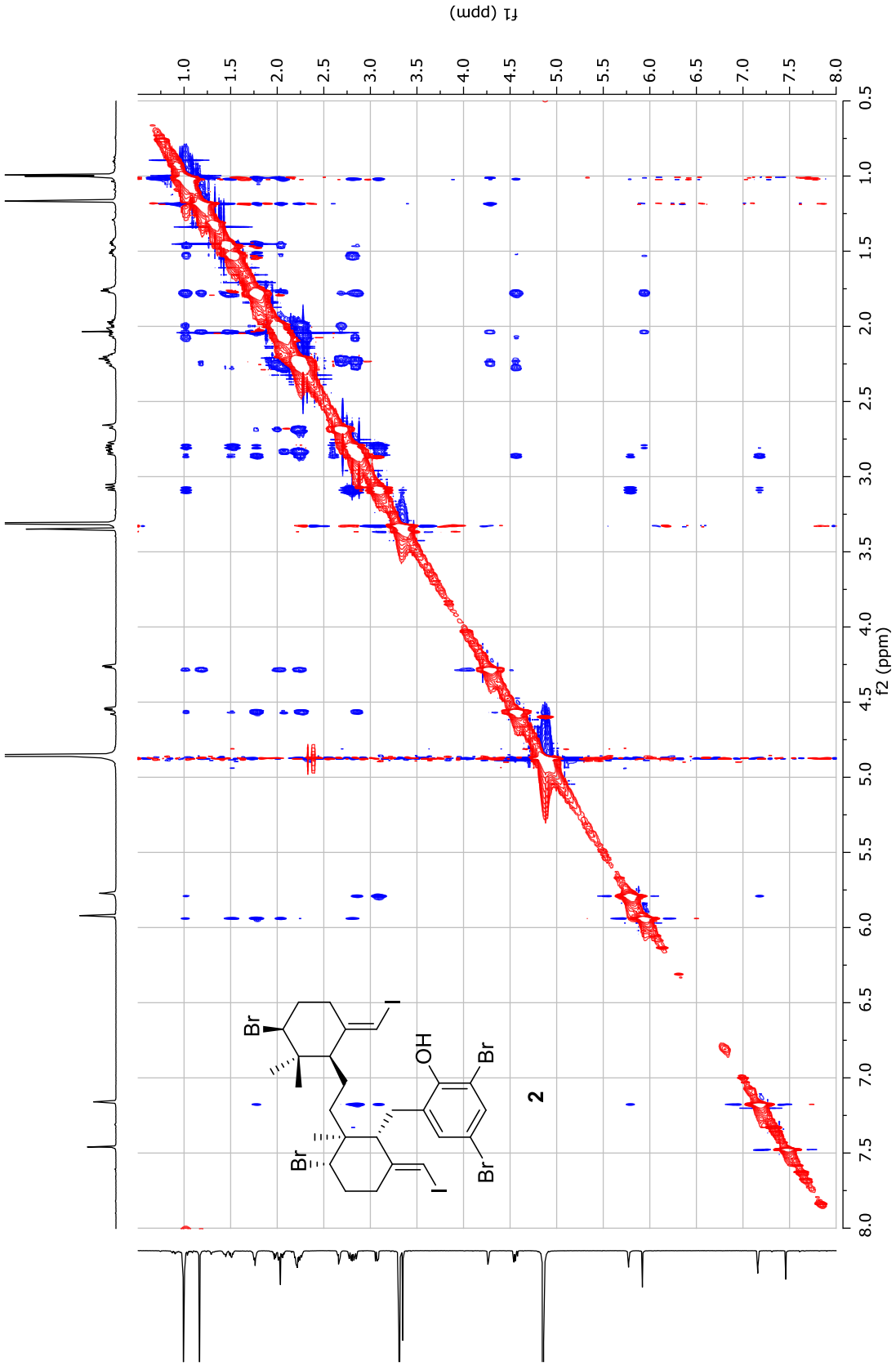
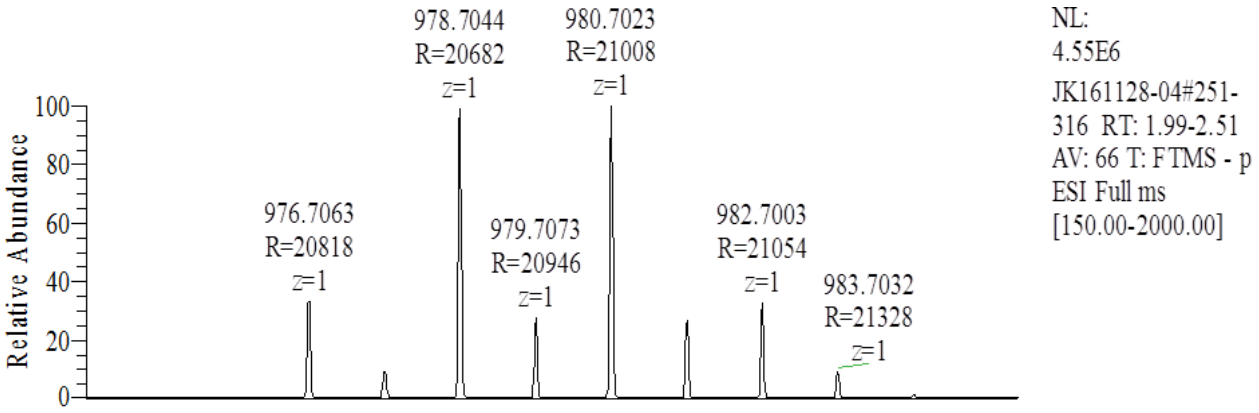
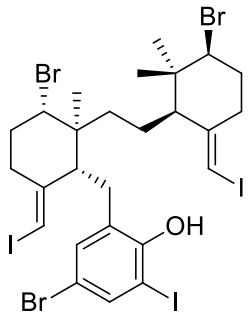


Figure S21. ^{1}H-^{1}H NOESY spectrum of iodocallophycol A (**2**) at 800 MHz in CD_3OD.

SPECTRA OF IODOCALLOPHYCOL B (3)

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





3

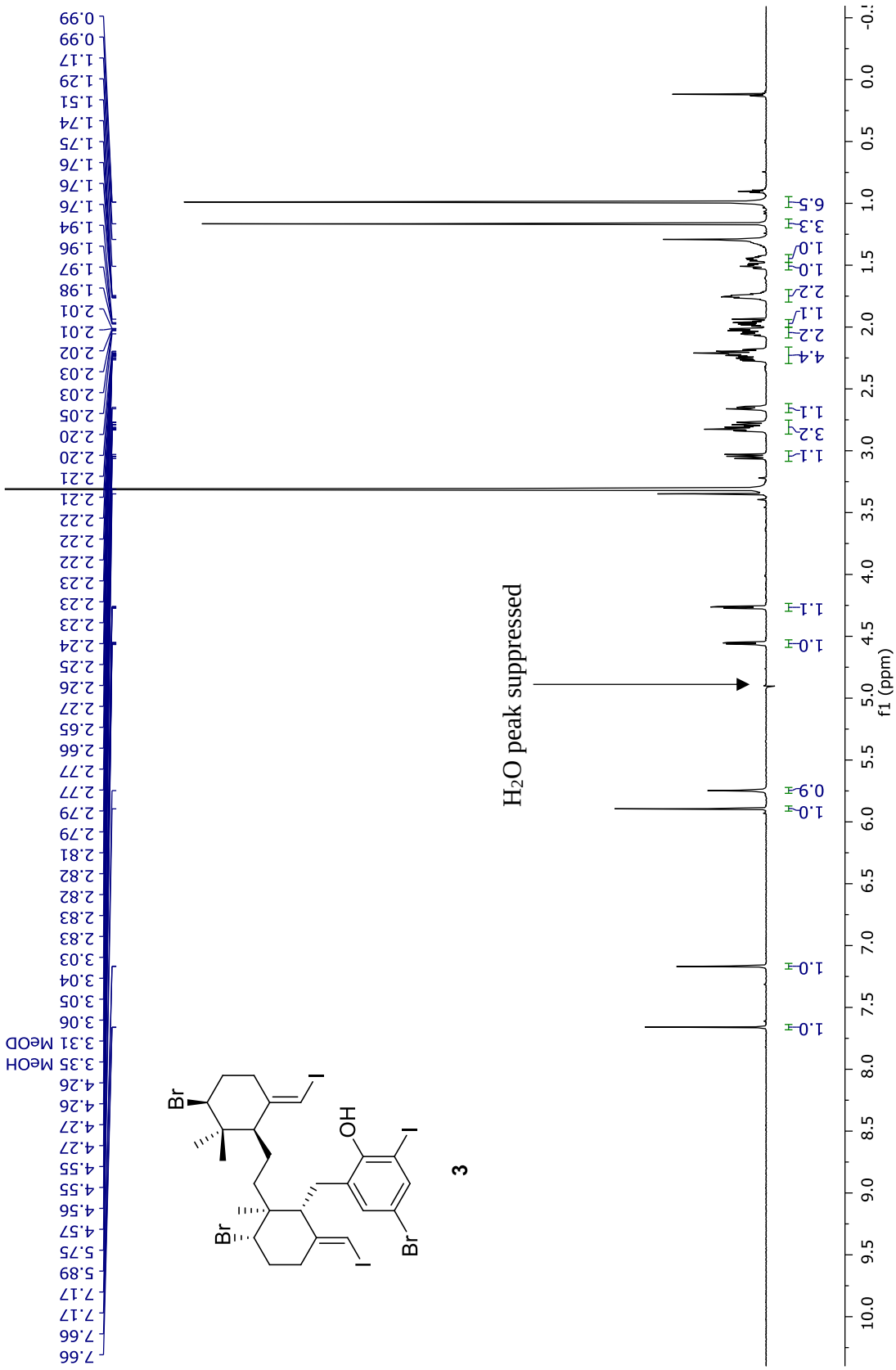


Figure S23. ^{1}H NMR spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD.

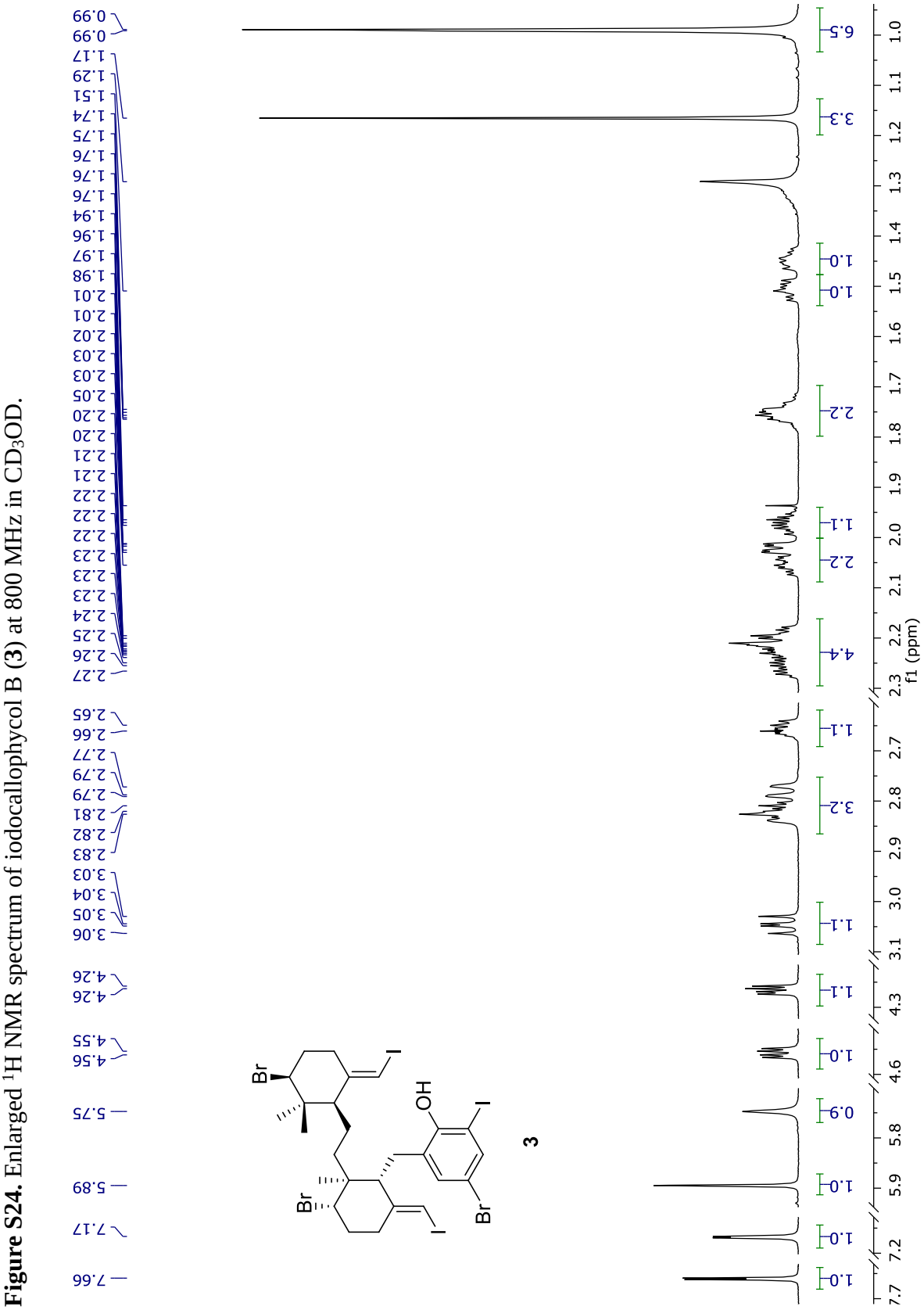


Figure S24. Enlarged ^{1}H NMR spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD.

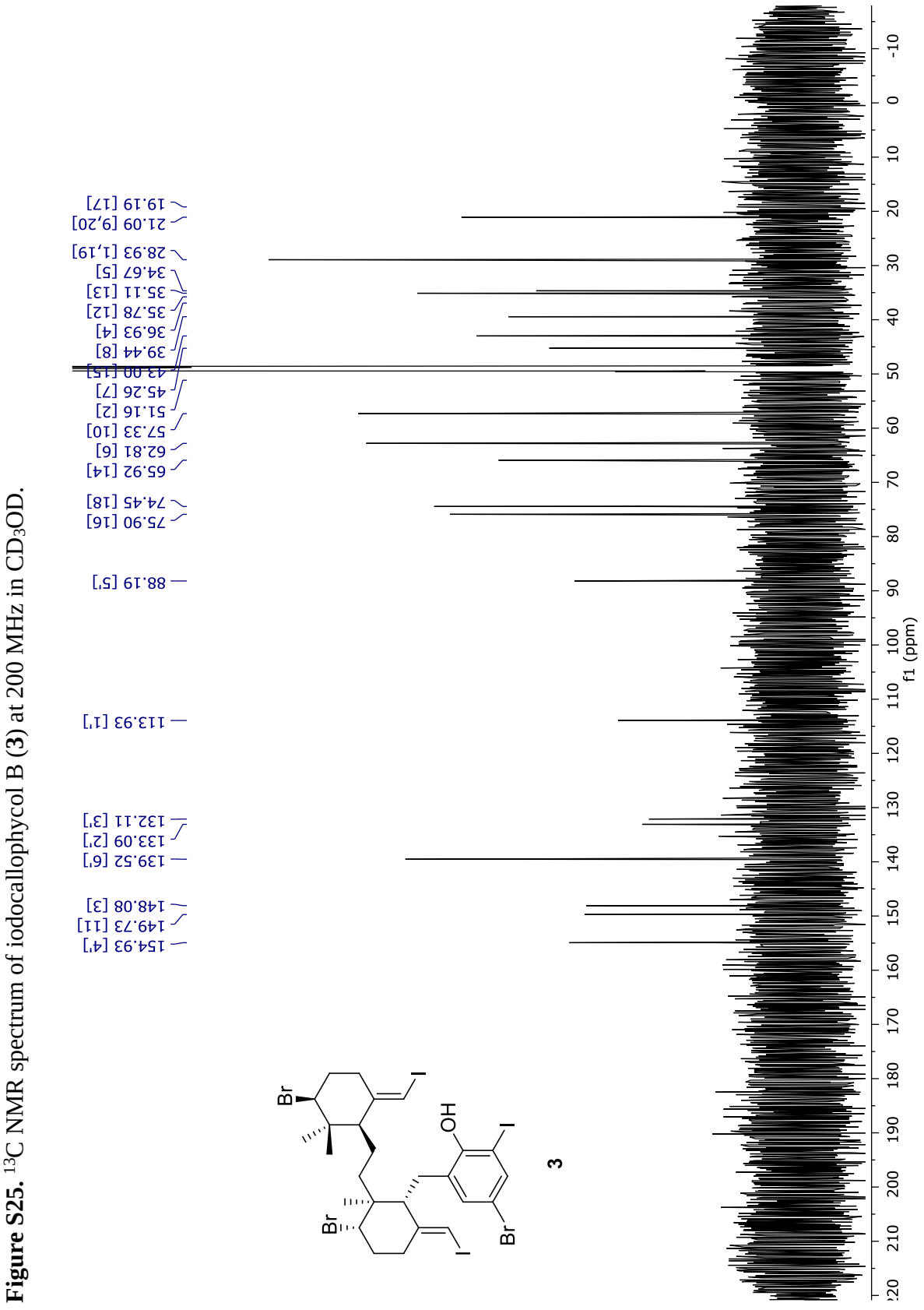


Figure S25. ^{13}C NMR spectrum of iodocallophycol B (**3**) at 200 MHz in CD_3OD.

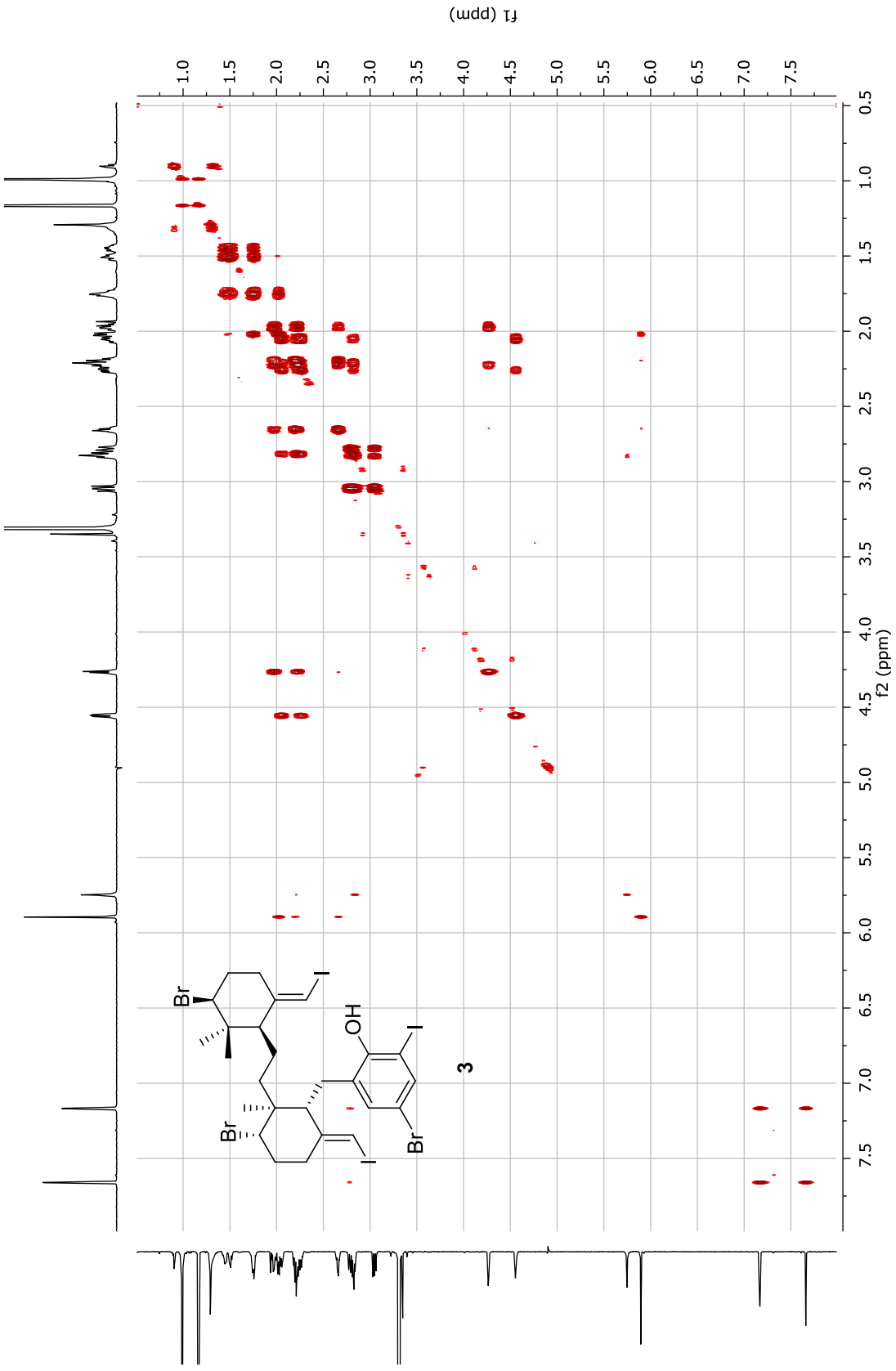


Figure S26. ^{1}H-^{1}H DQF-COSY spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD.

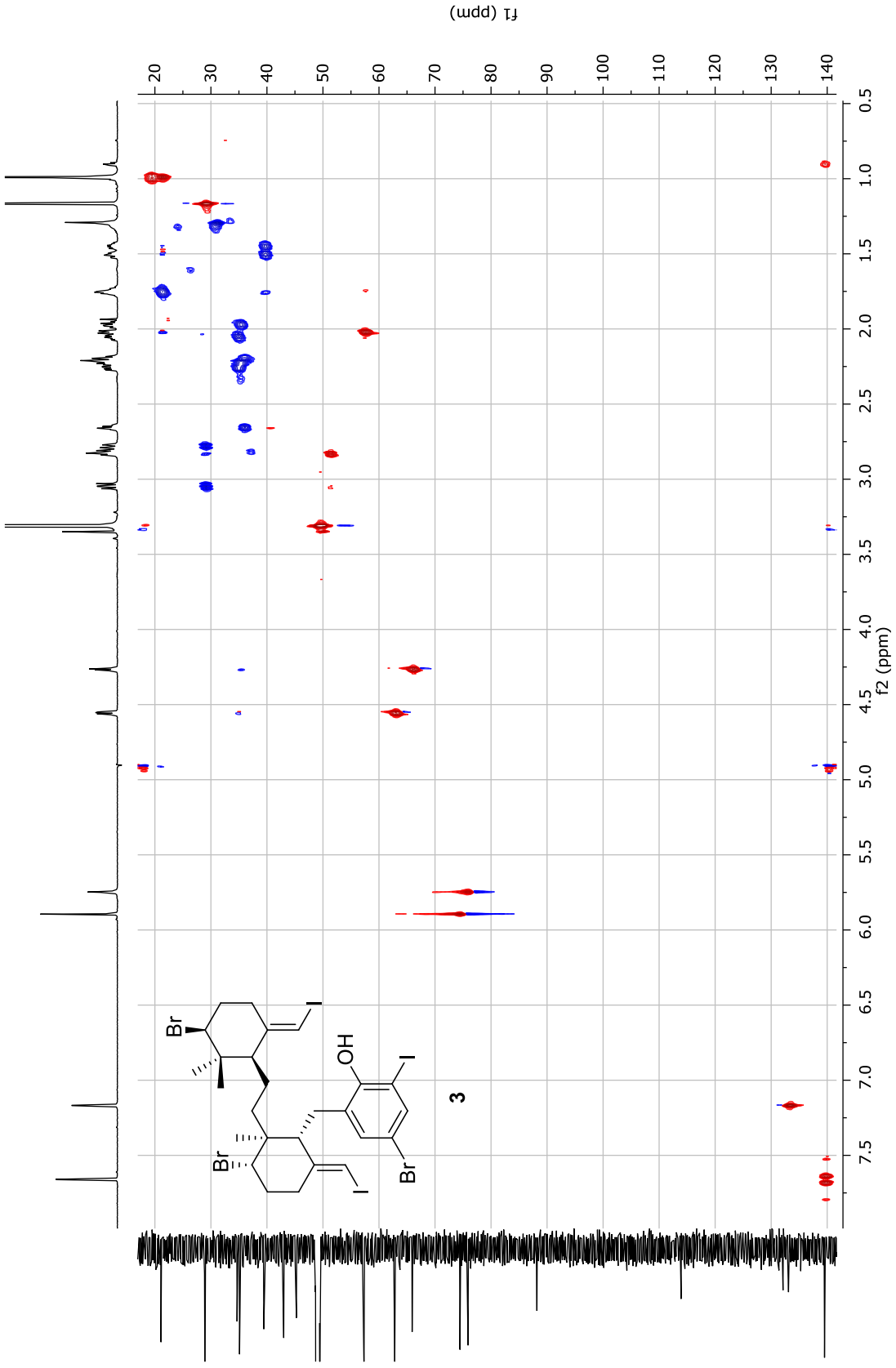


Figure S27. ^{1}H-^{13}C edited-HSQC spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD.

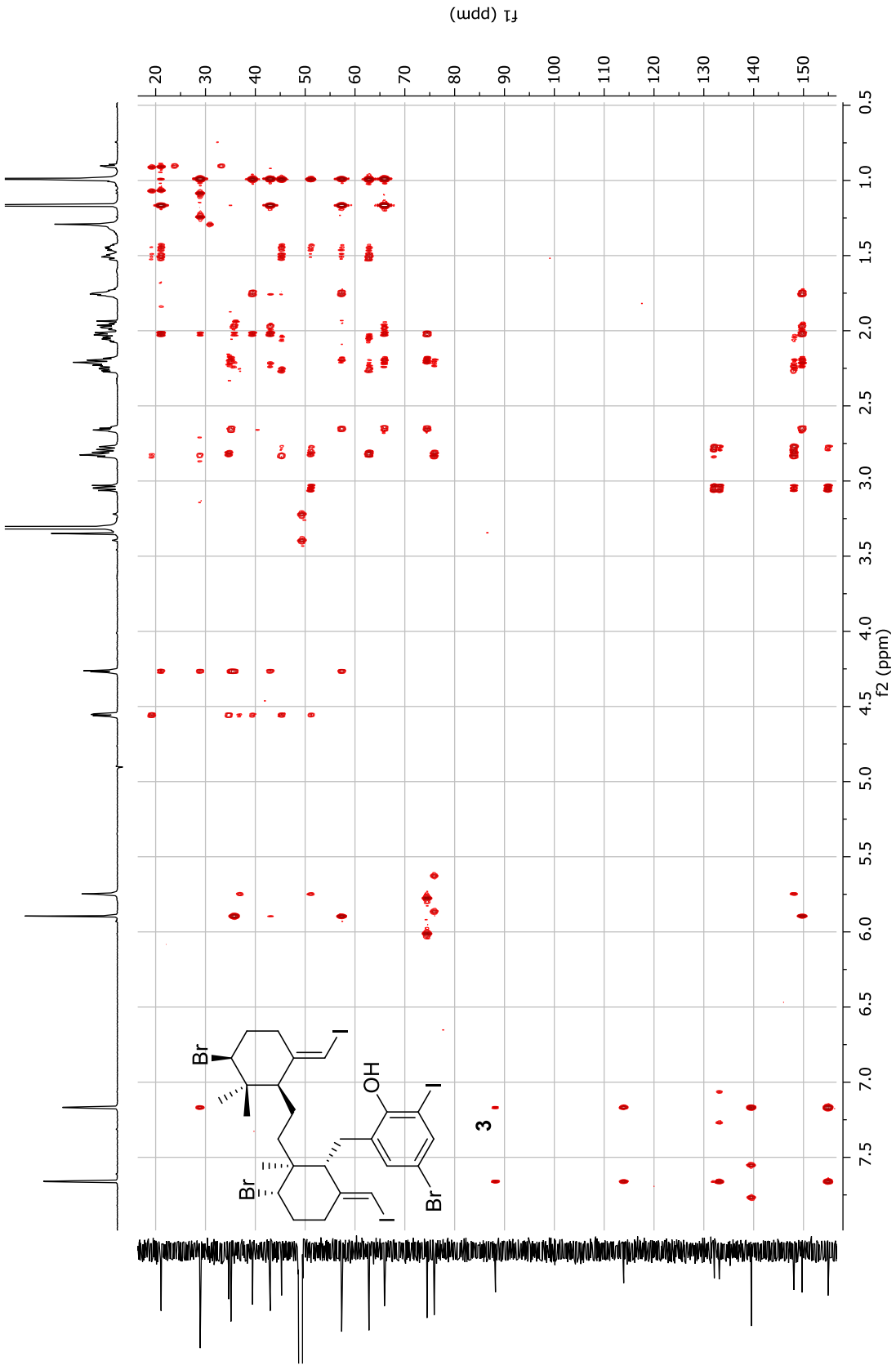


Figure S28. ^{1}H-^{13}C HMBC spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD.

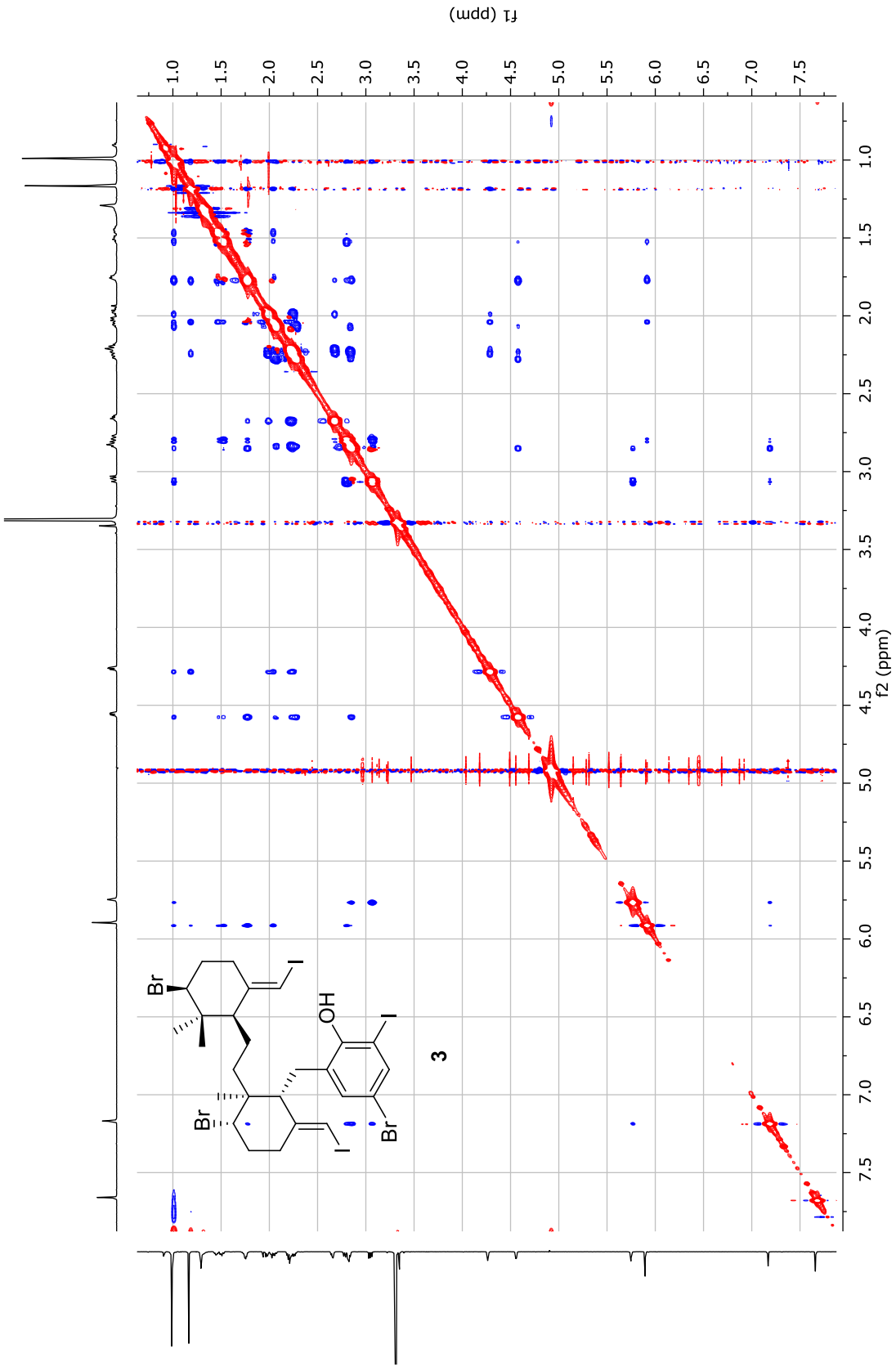
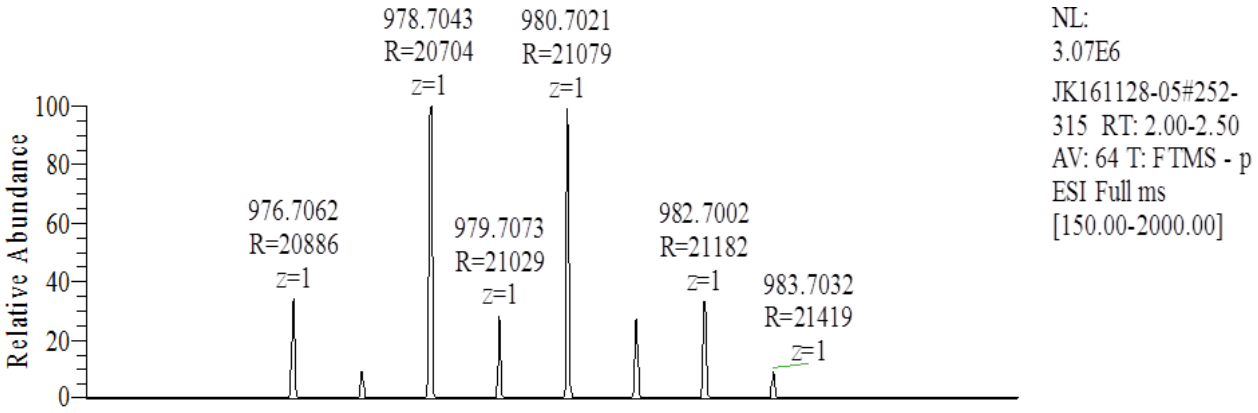
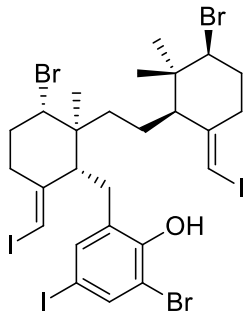


Figure S29. ^{1}H-^{1}H NOESY spectrum of iodocallophycol B (**3**) at 800 MHz in CD_3OD.

SPECTRA OF IODOCALLOPHYCOL C (4)

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





4

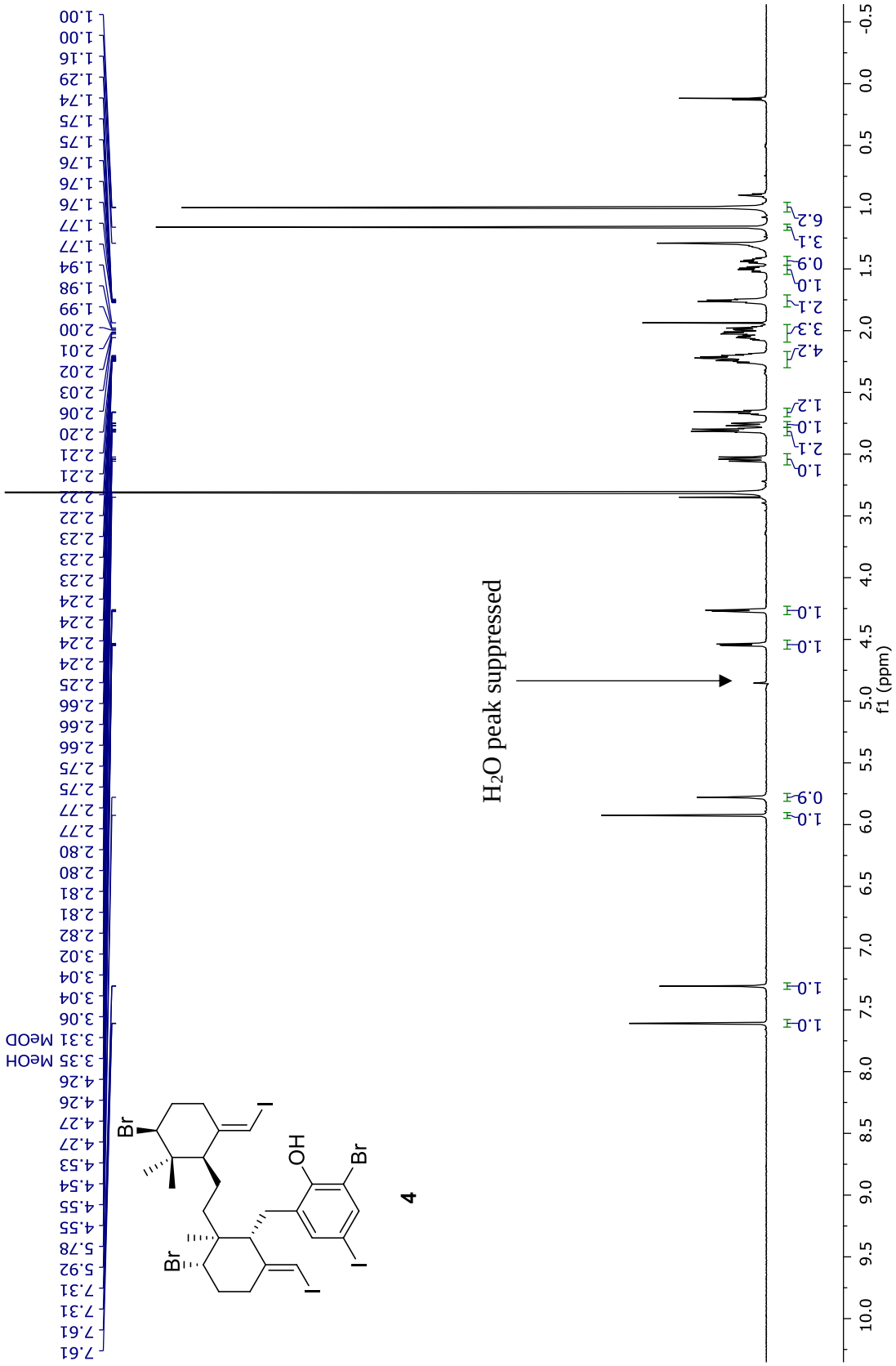


Figure S31. ^{1}H NMR spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD.

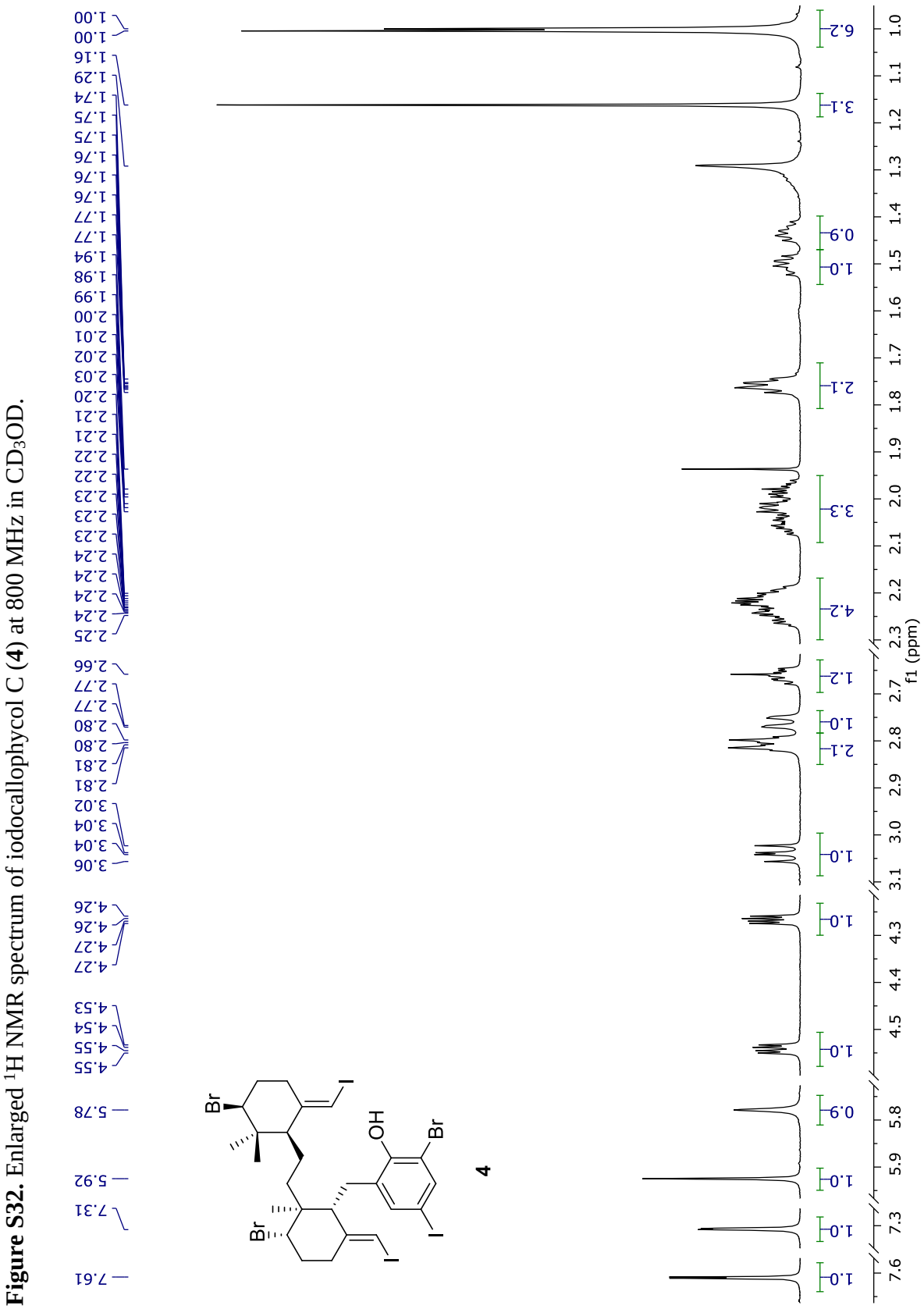


Figure S32. Enlarged ^{1}H NMR spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD.

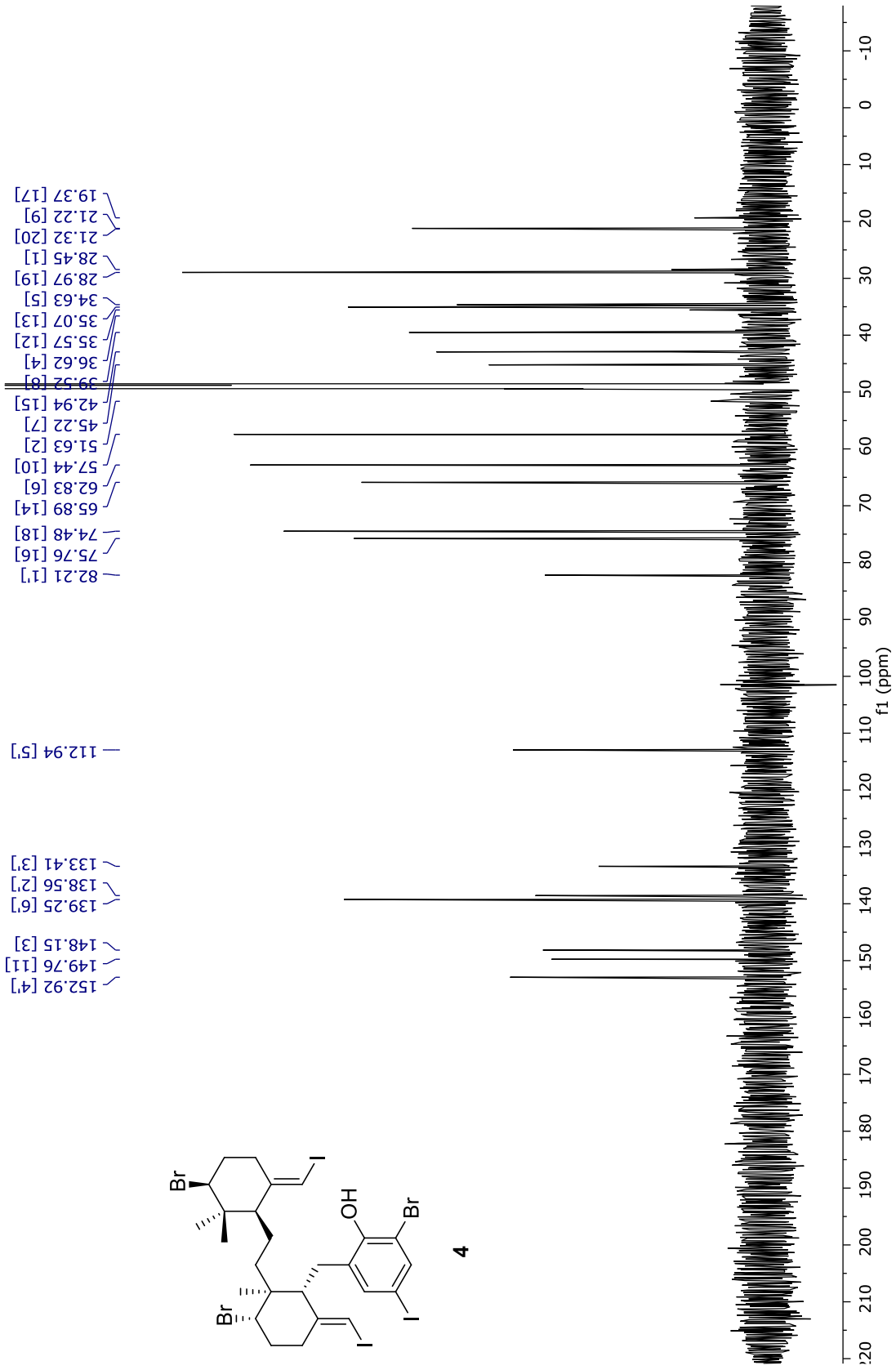


Figure S33. ^{13}C NMR spectrum of iodocallophycol C (**4**) at 200 MHz in CD_3OD.

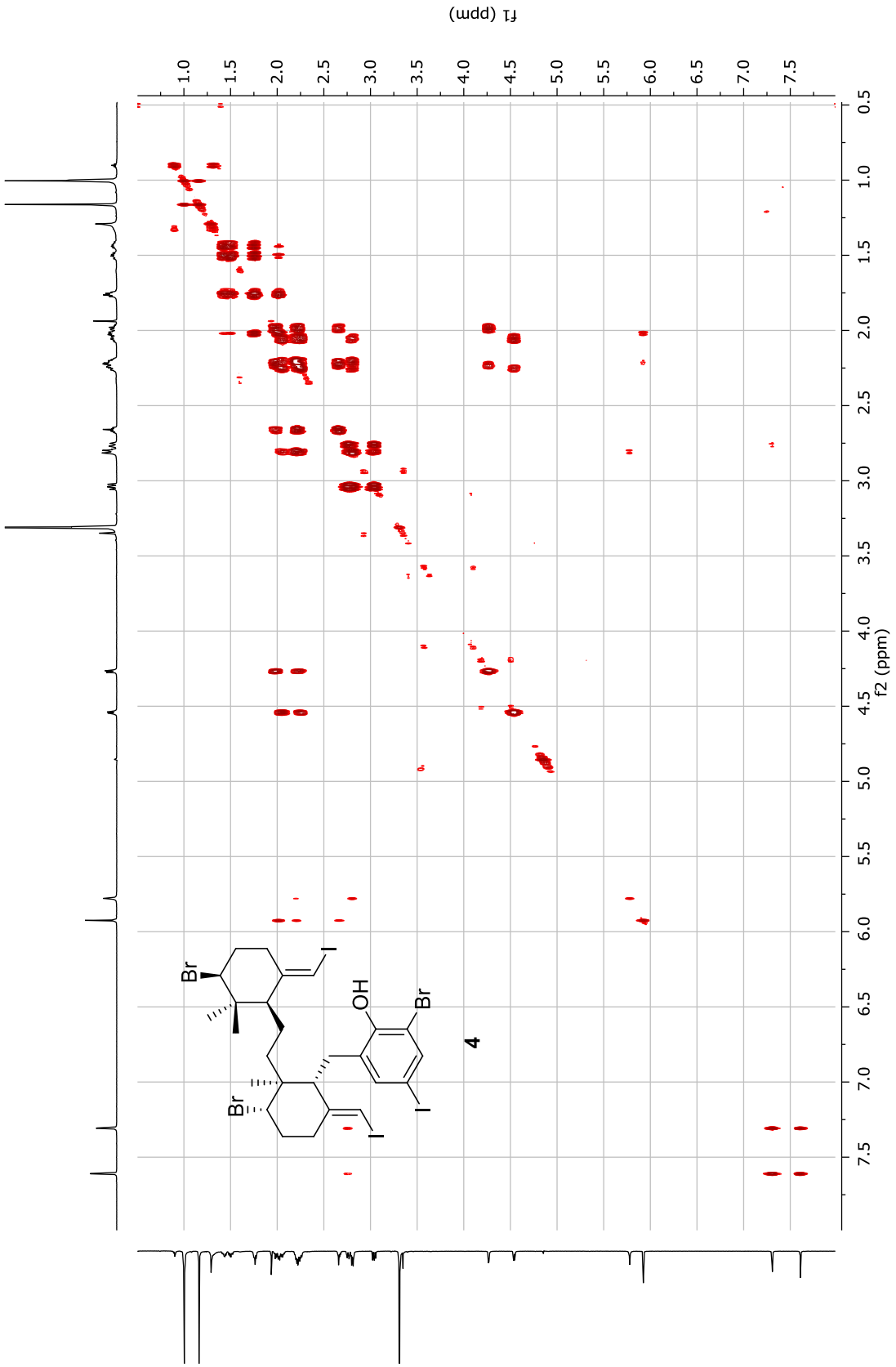


Figure S34. ^{1}H-^{1}H DQF-COSY spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD.

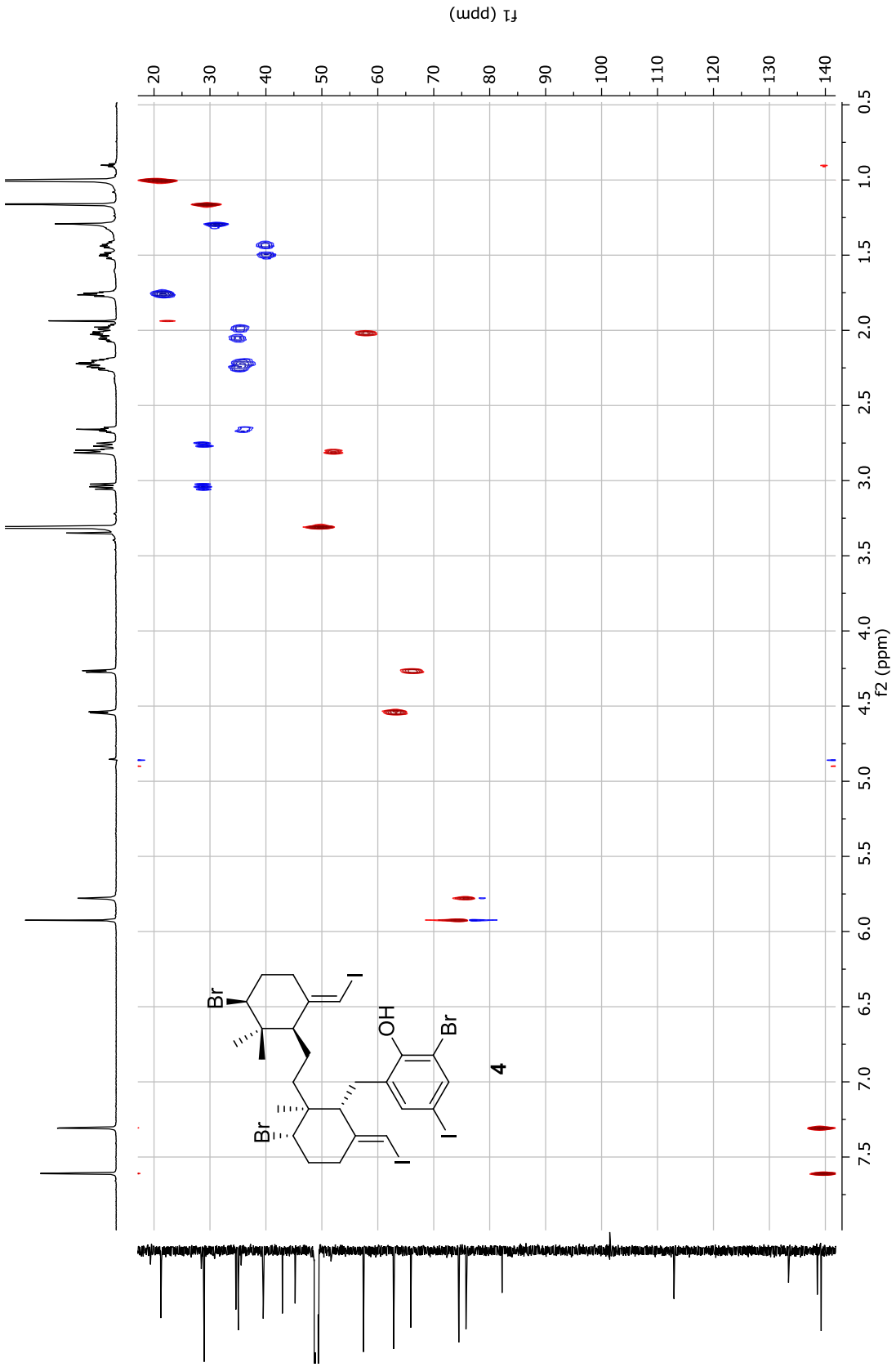


Figure S35. ^{1}H-^{13}C edited-HSQC spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD.

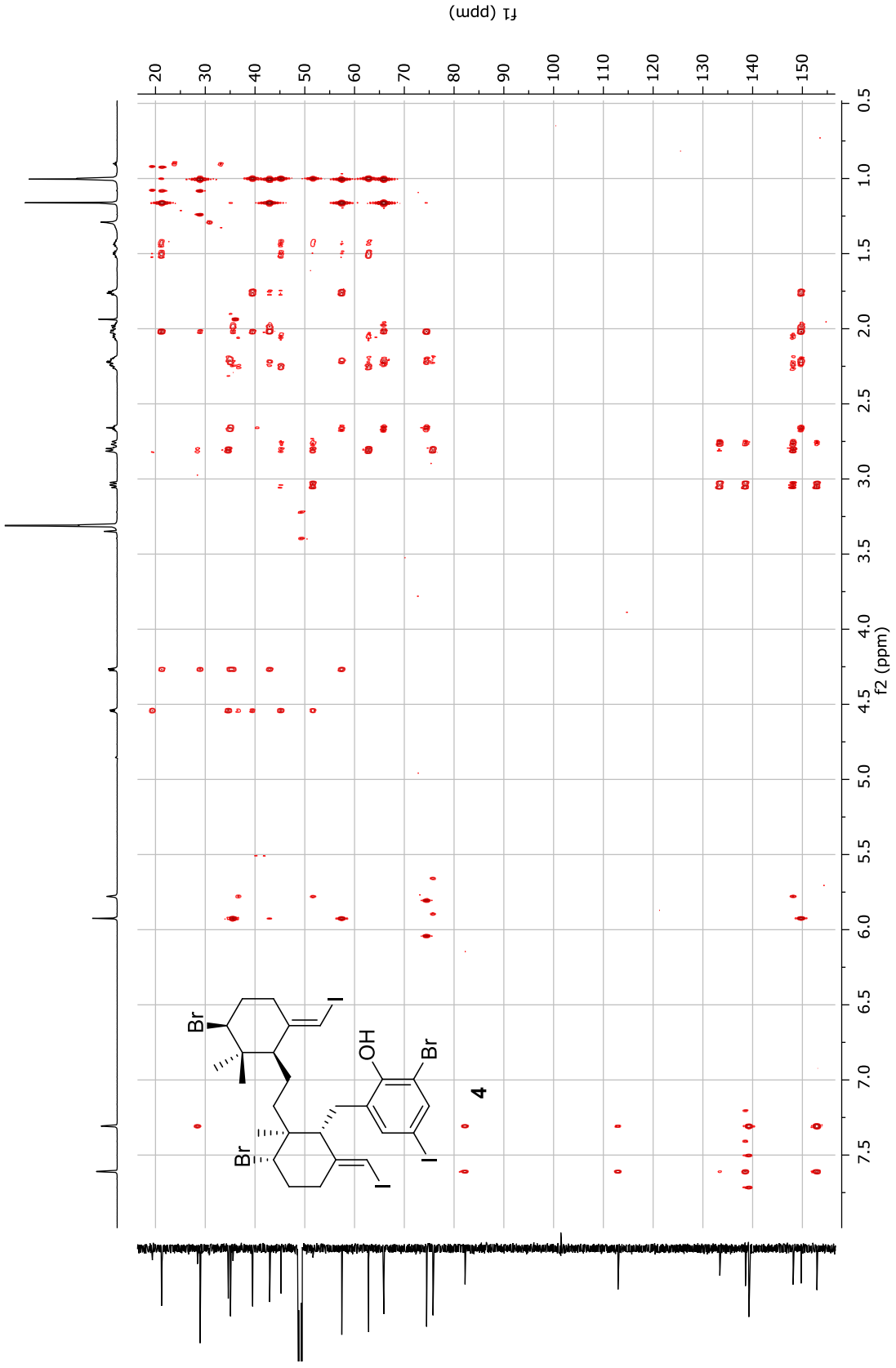


Figure S36. ^{1}H-^{13}C HMBC spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD.

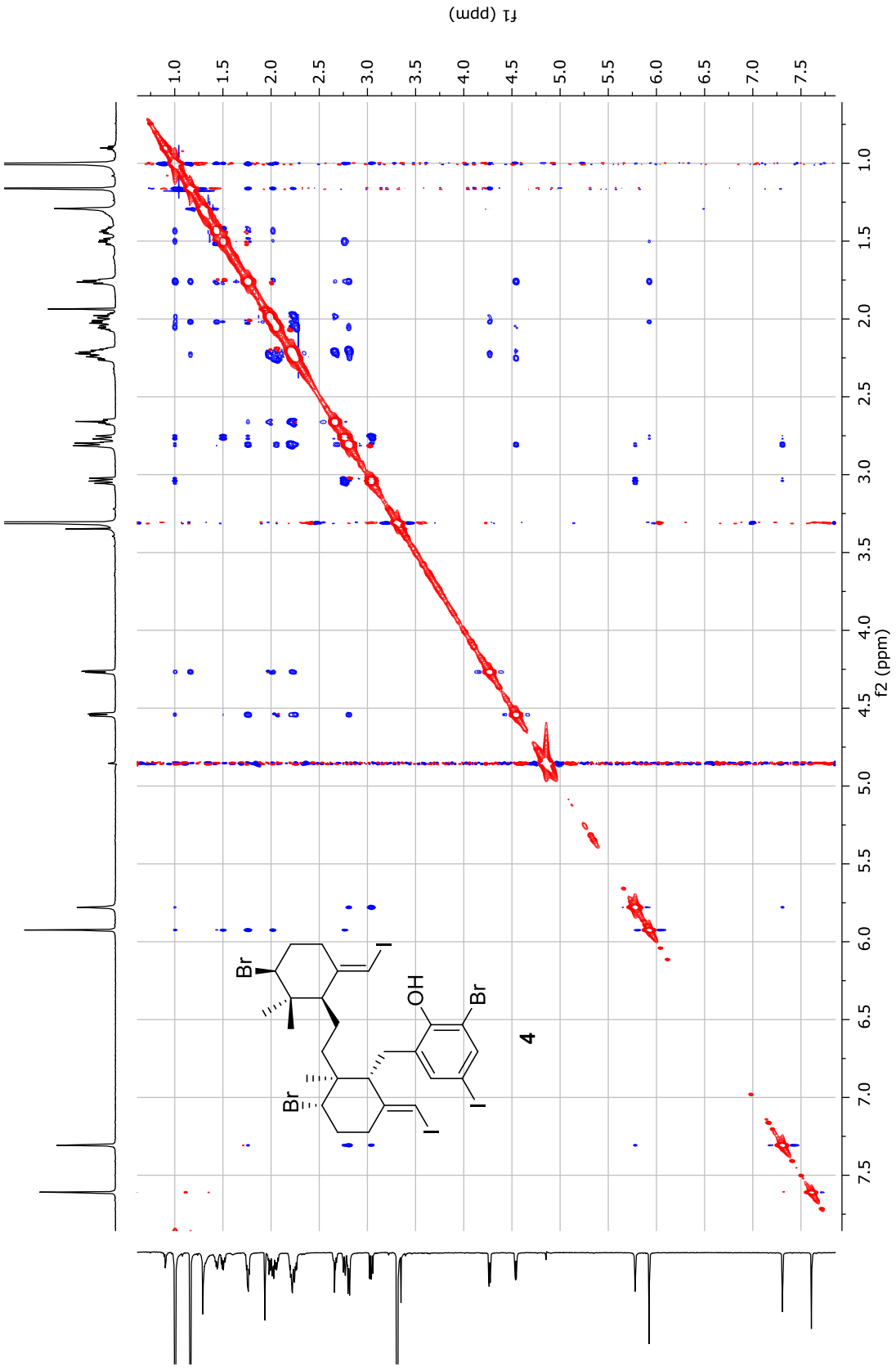
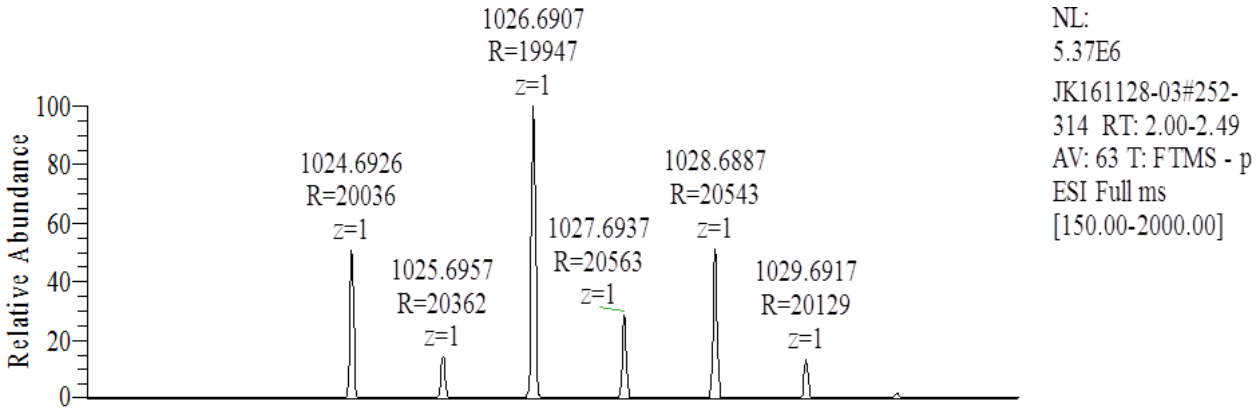
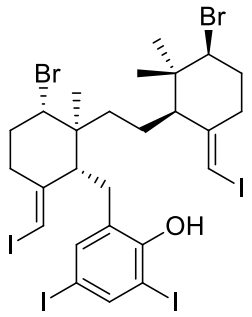


Figure S37. ^{1}H-^{1}H NOESY spectrum of iodocallophycol C (**4**) at 800 MHz in CD_3OD.

SPECTRA OF IODOCALLOPHYCOL D (5)

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





5

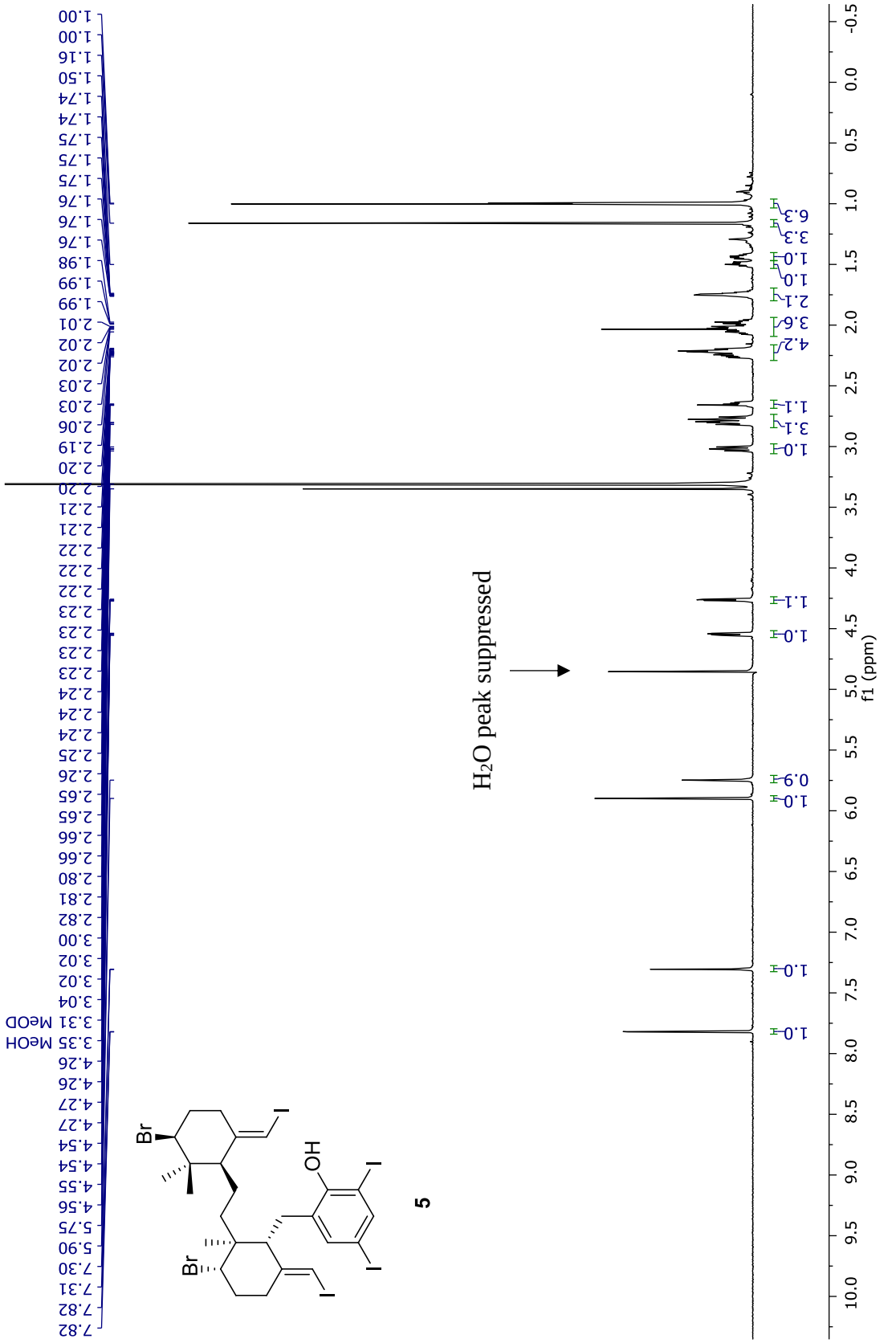


Figure S39. ^{1}H NMR spectrum of iodocallophycol D (**5**) at 800 MHz in CD_3OD.

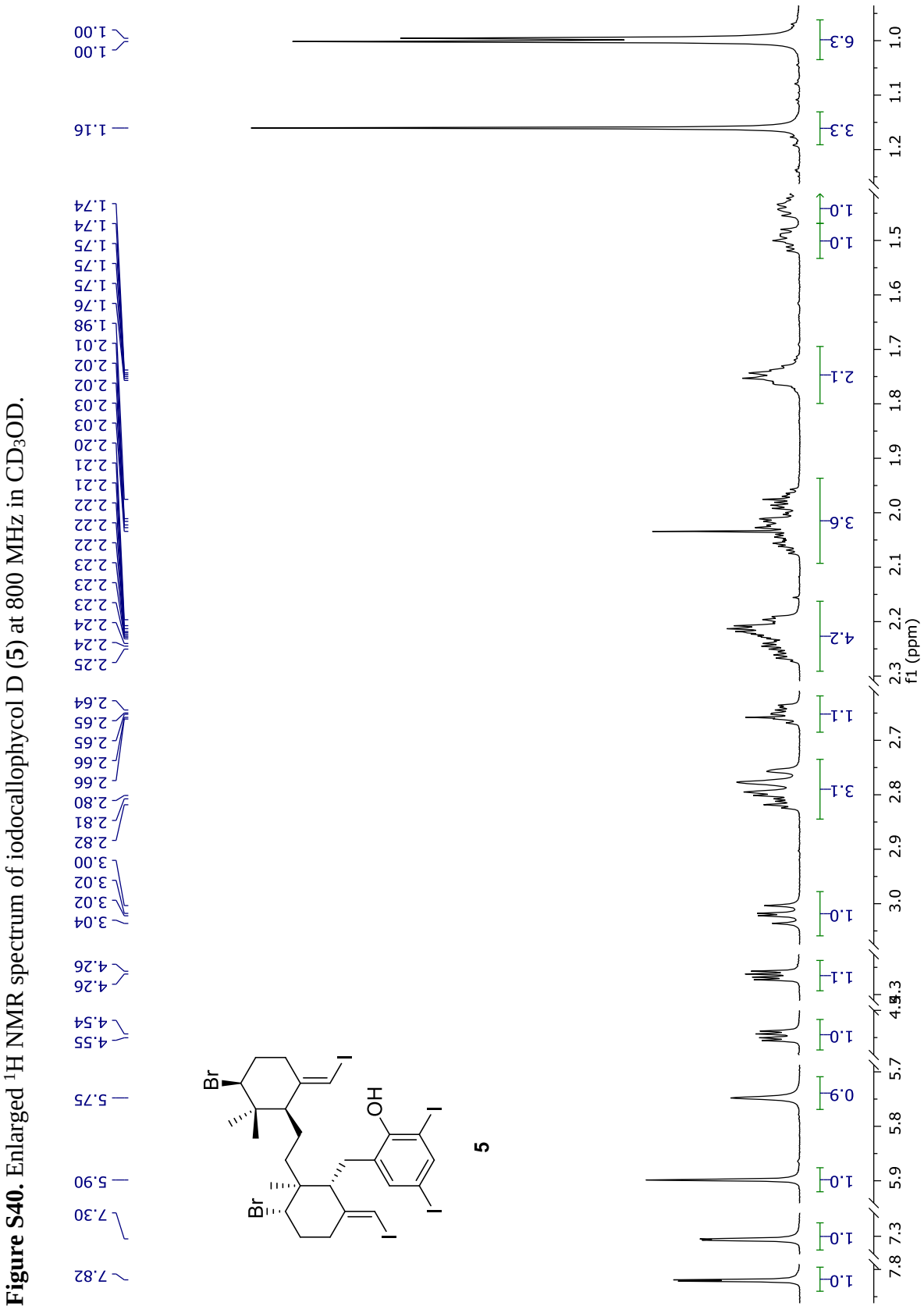


Figure S40. Enlarged ^{1}H NMR spectrum of iodocallophycol D (**5**) at 800 MHz in CD_3OD.

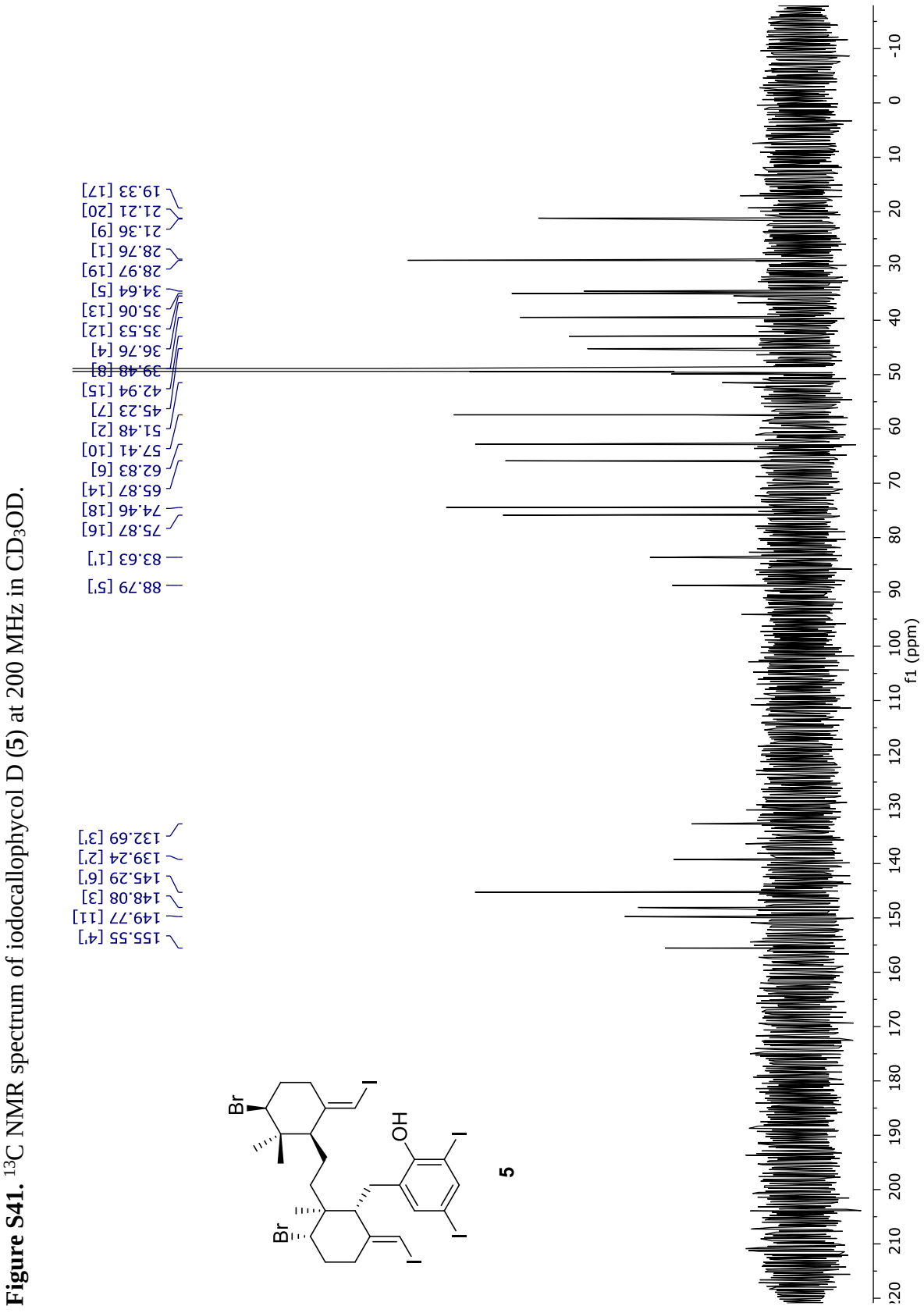


Figure S41. ^{13}C NMR spectrum of iodocallophycol D (**5**) at 200 MHz in CD_3OD.

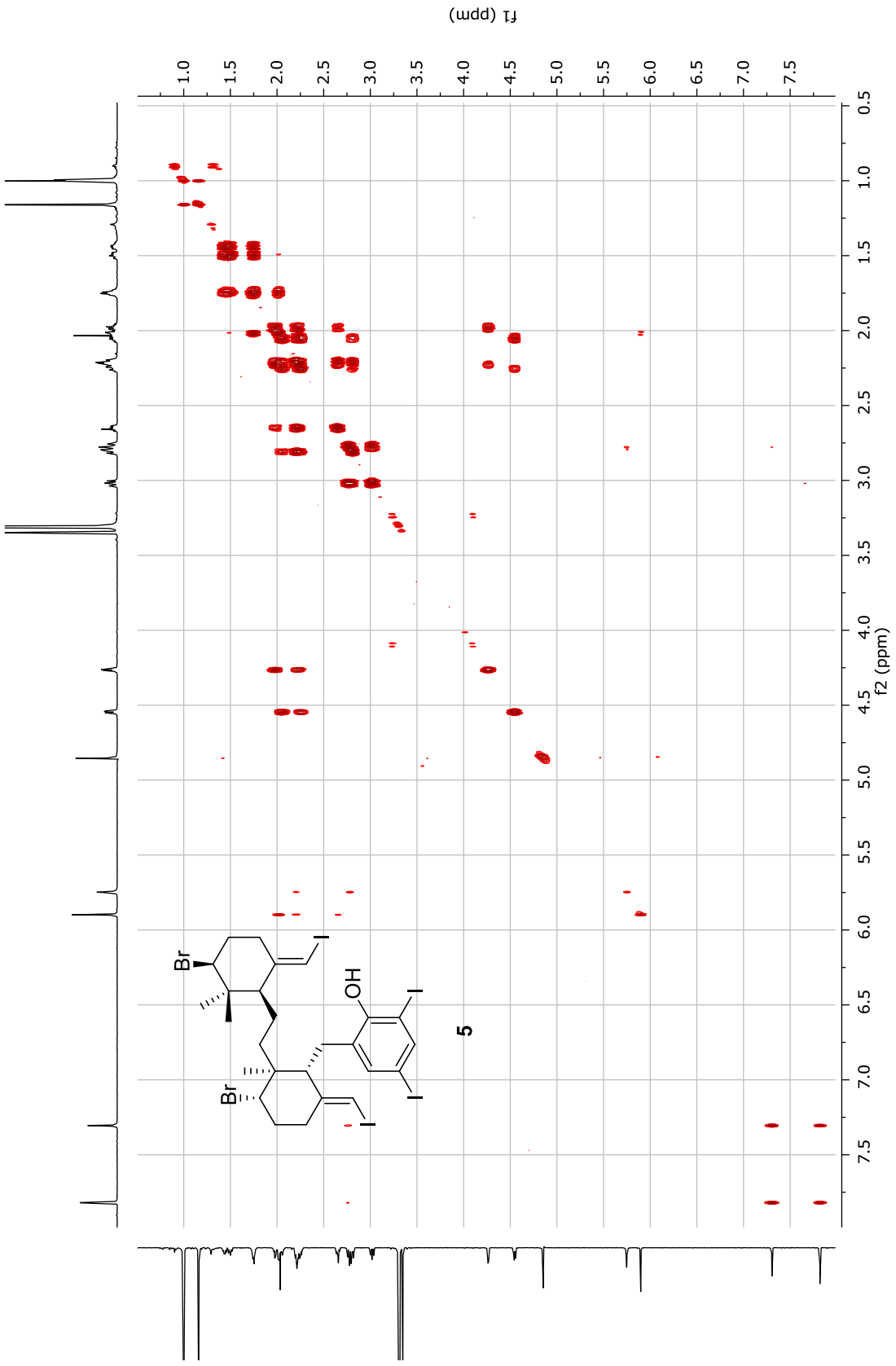


Figure S42. ^{1}H-^{1}H DQF-COSY spectrum of iodocallophycol D (**5**) at 800 MHz in CD_3OD.

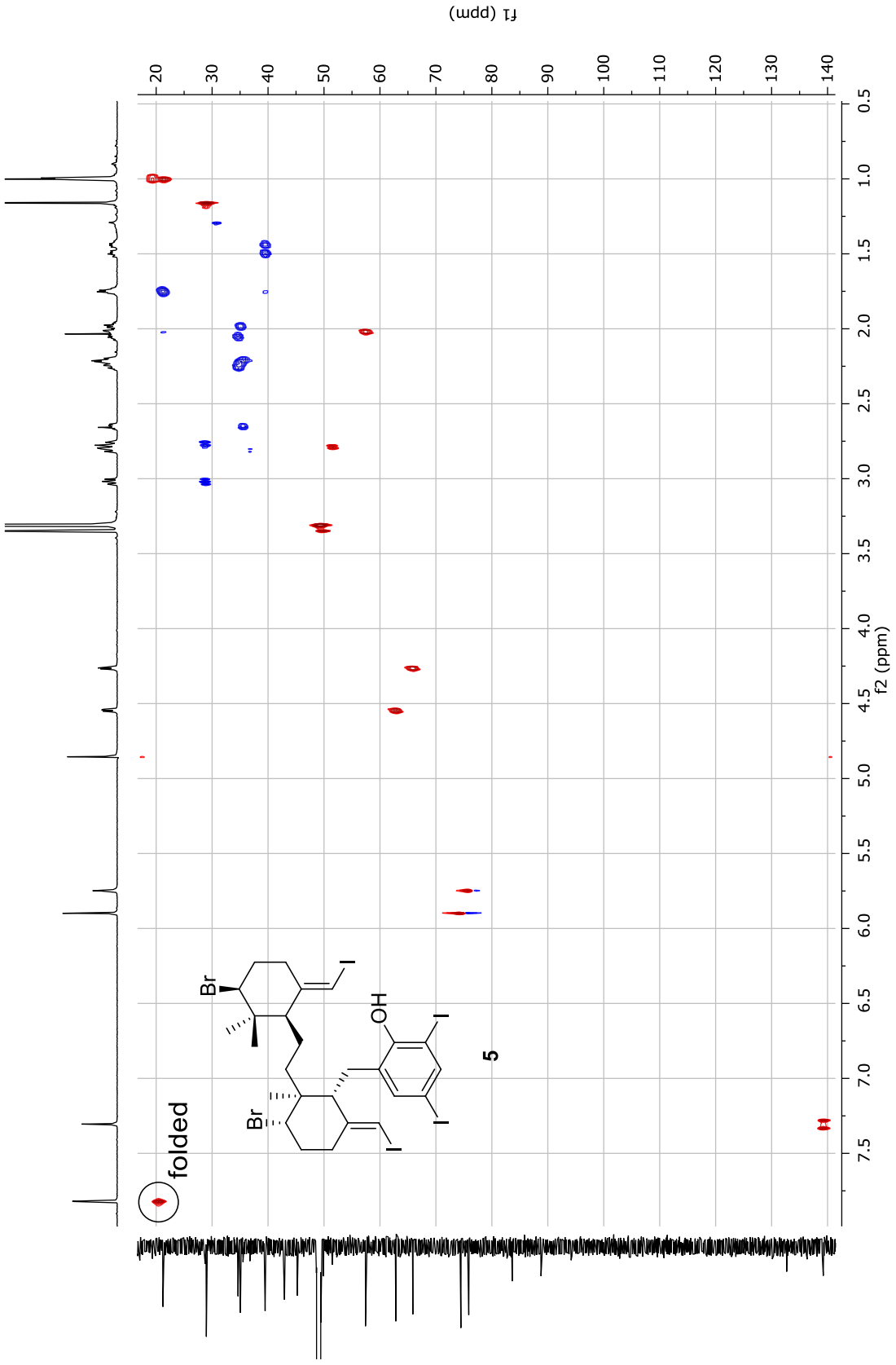


Figure S43. ^{1}H-^{13}C edited-HSQC spectrum of iodocallophycol D (**5**) at 800 MHz in CD_3OD.

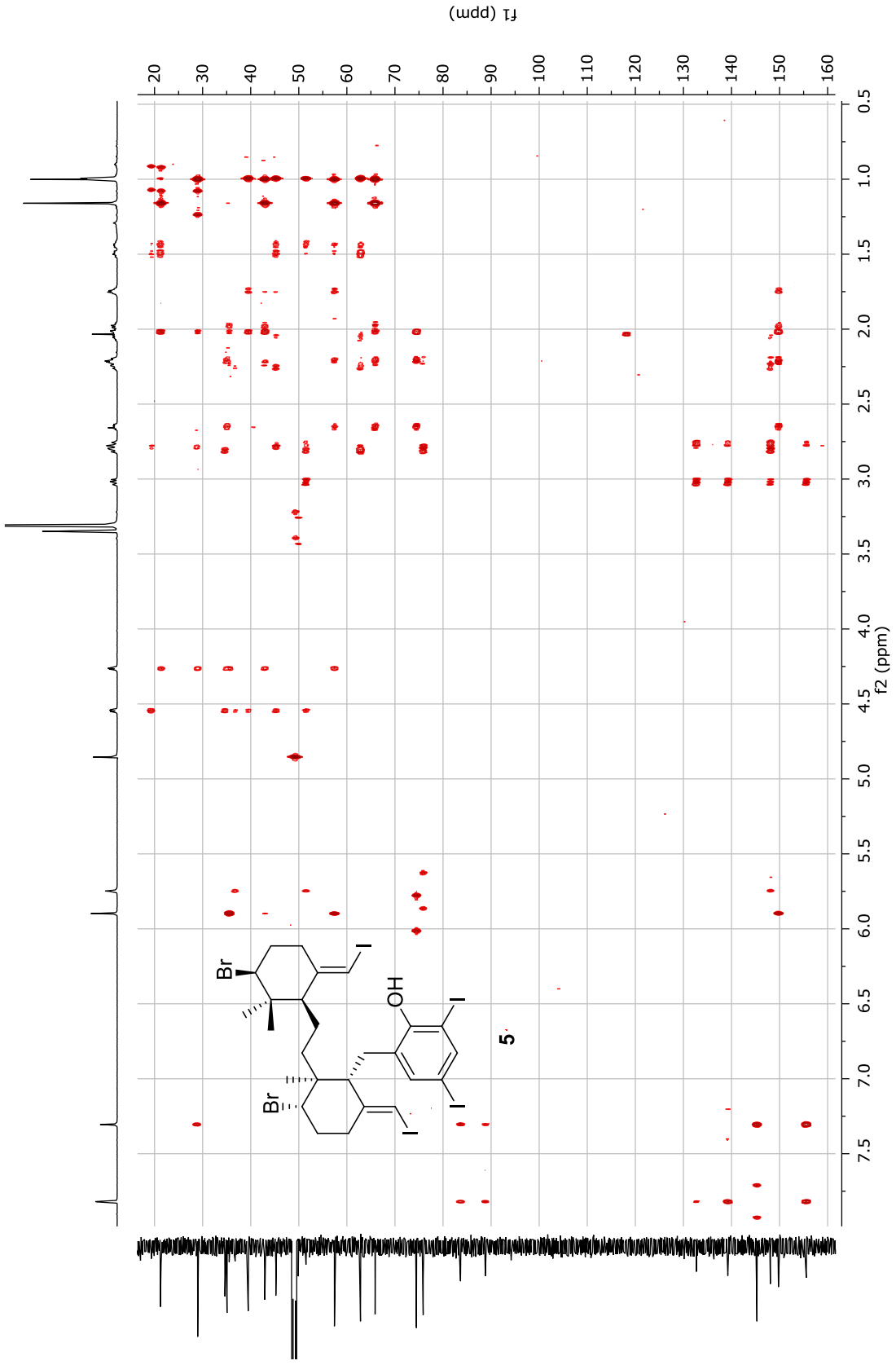


Figure S44. ^{1}H-^{13}C HMBC spectrum of iodocallophycol D (**5**) at 800 MHz in CD_3OD.

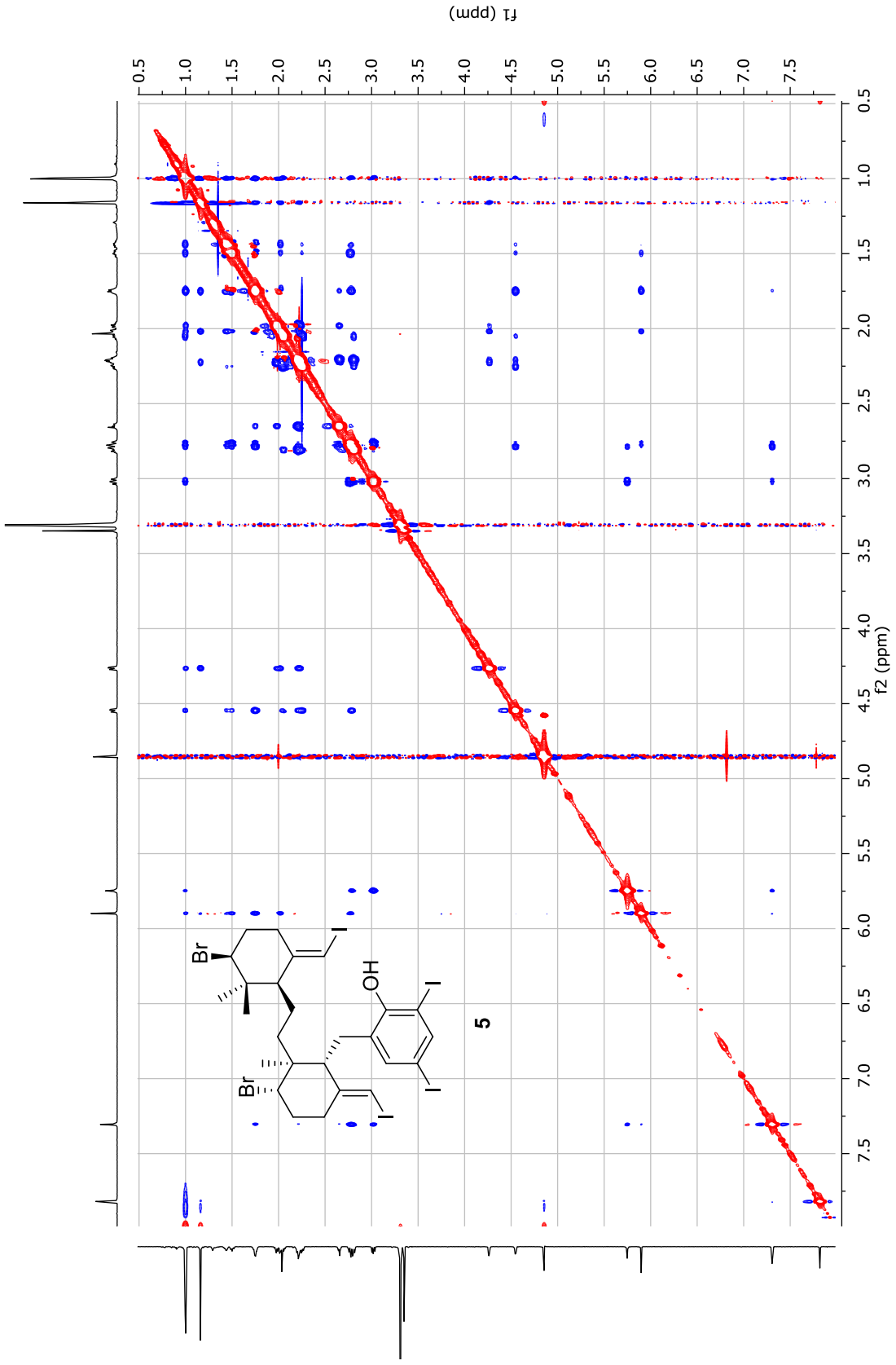
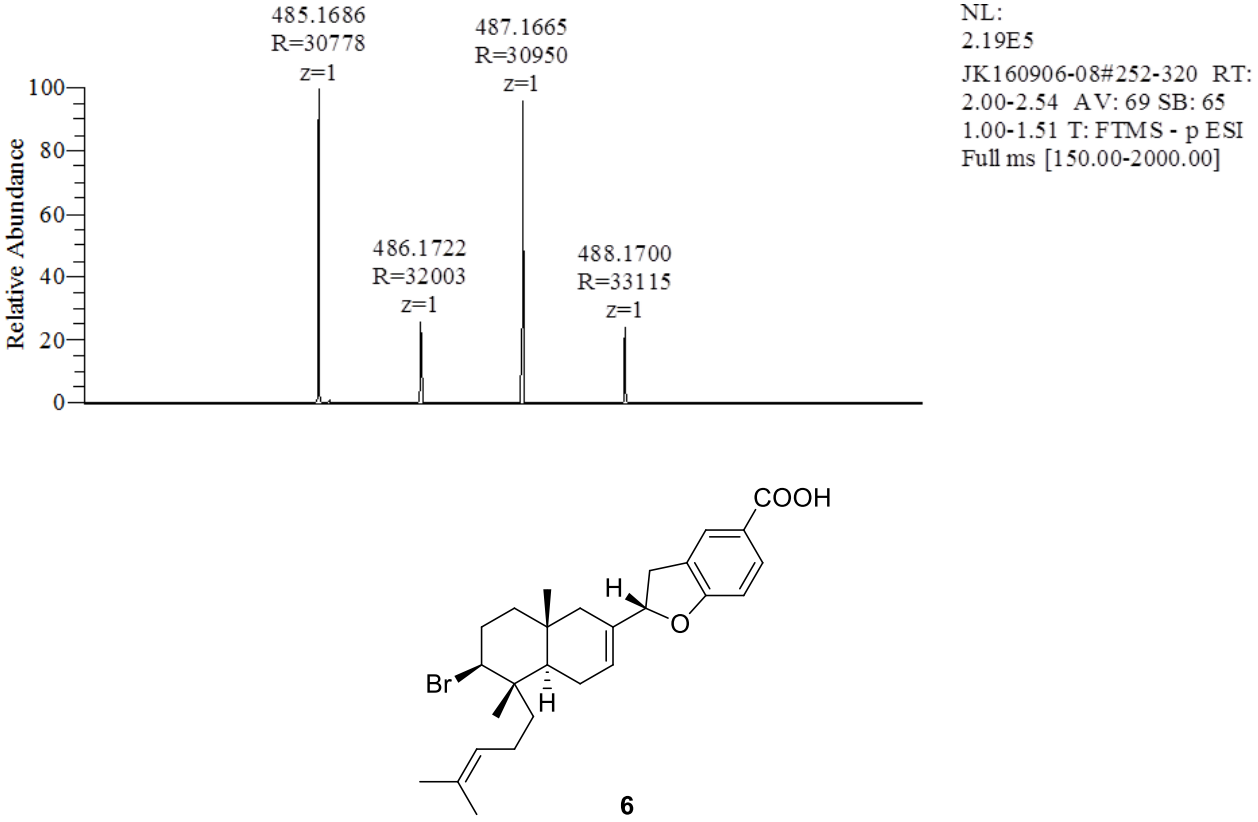


Figure S45. ^{1}H-^{1}H NOESY spectrum of iodocallophycol D (**5**) at 800 MHz in CD_3OD.

SPECTRA OF BROMOPHYCOIC ACID F (6)

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



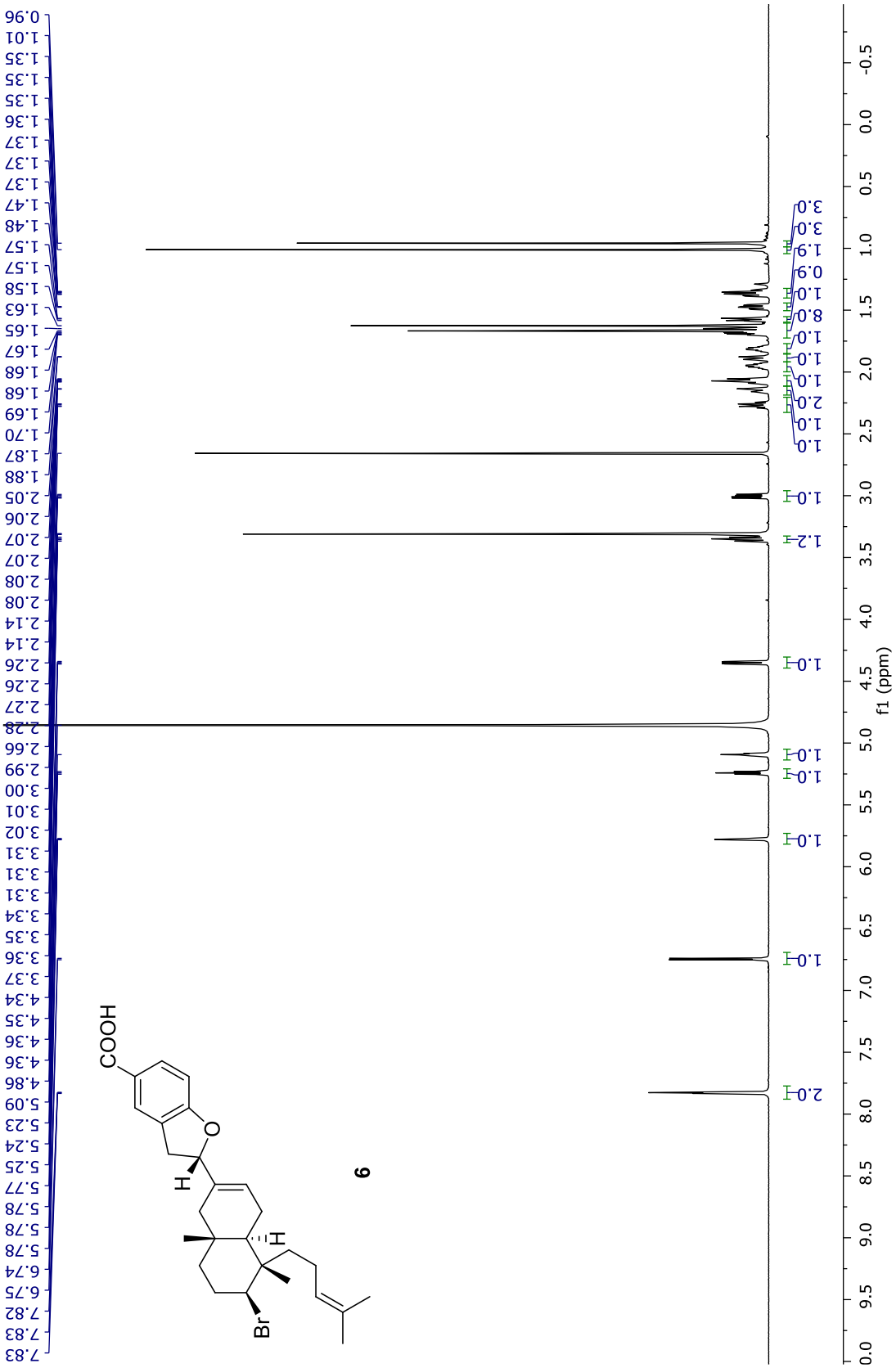


Figure S47. ^{1}H NMR spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD.

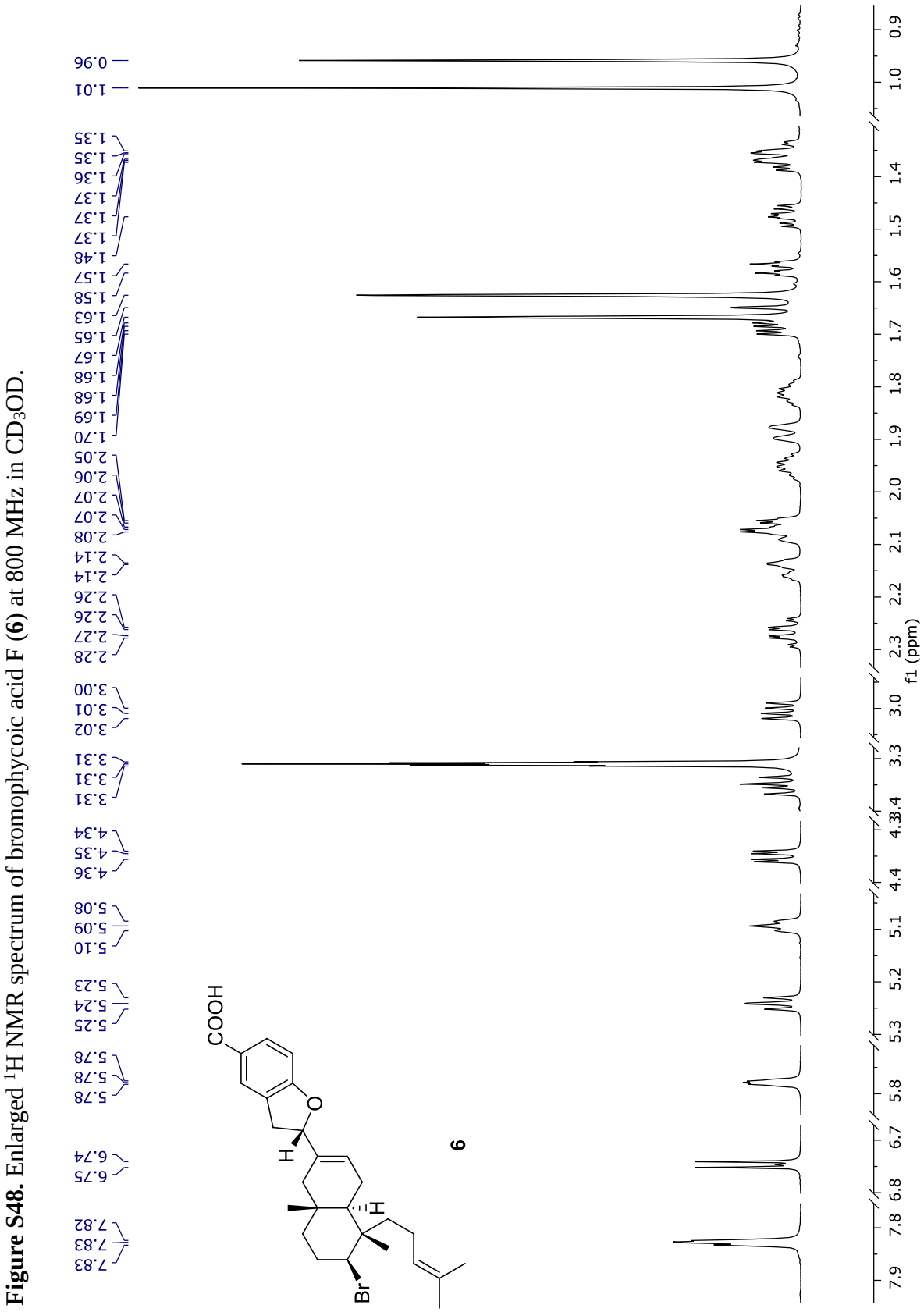


Figure S48. Enlarged ^{1}H NMR spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD.

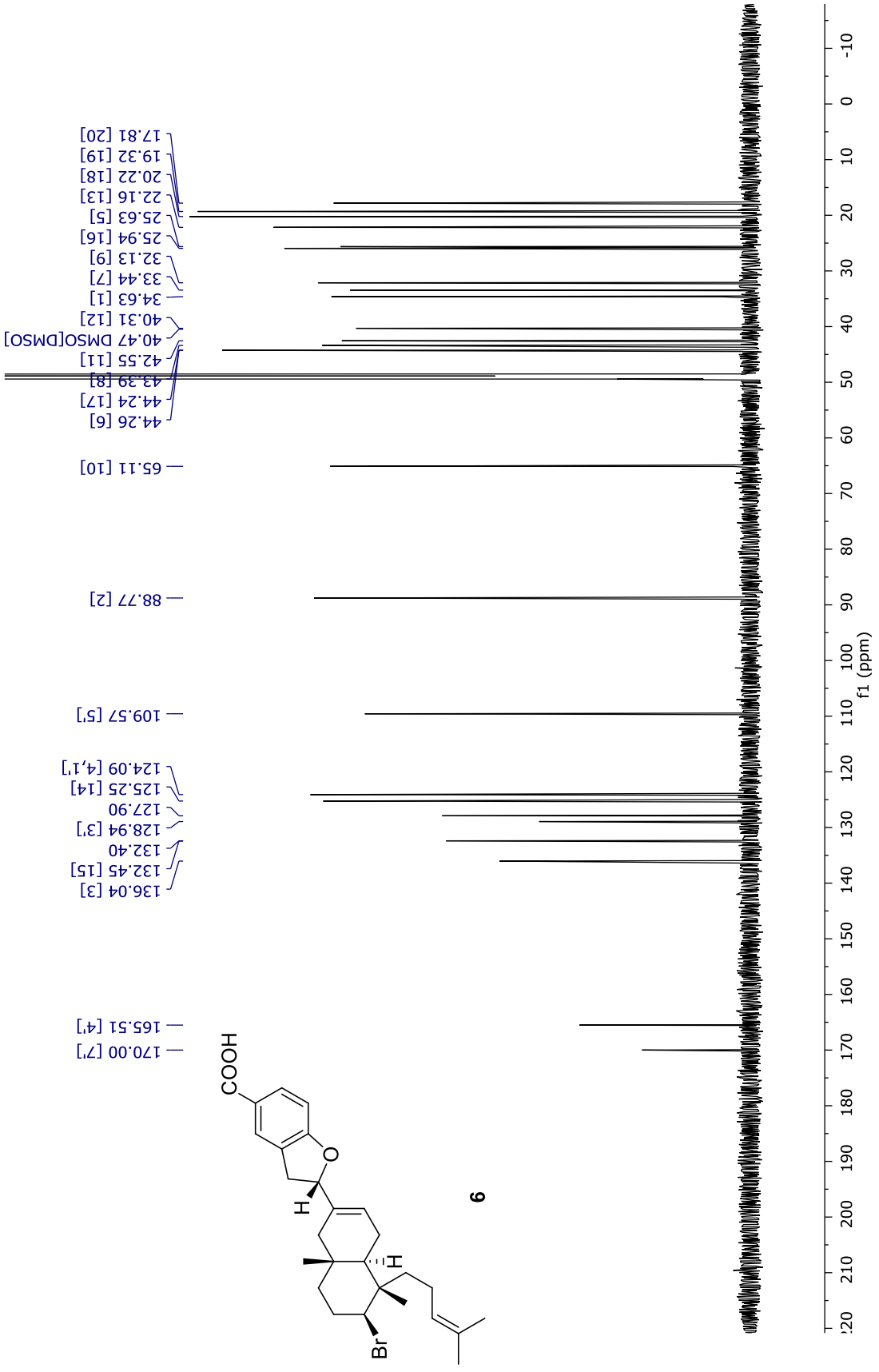


Figure S49. ^{13}C NMR spectrum of bromophycoic acid F (**6**) at 200 MHz in CD_3OD.

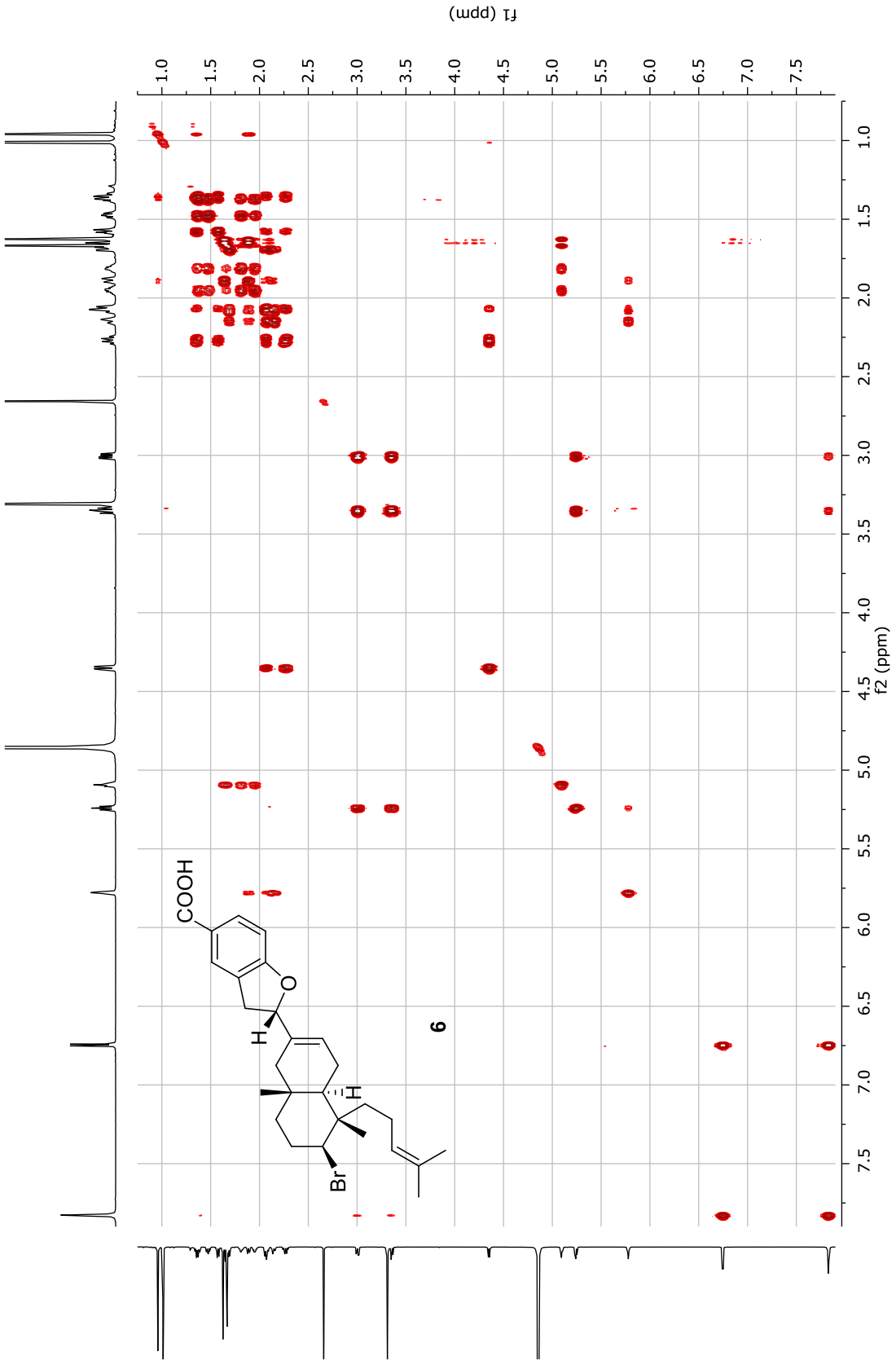


Figure S50. ^{1}H-^{1}H DQF-COSY spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD.

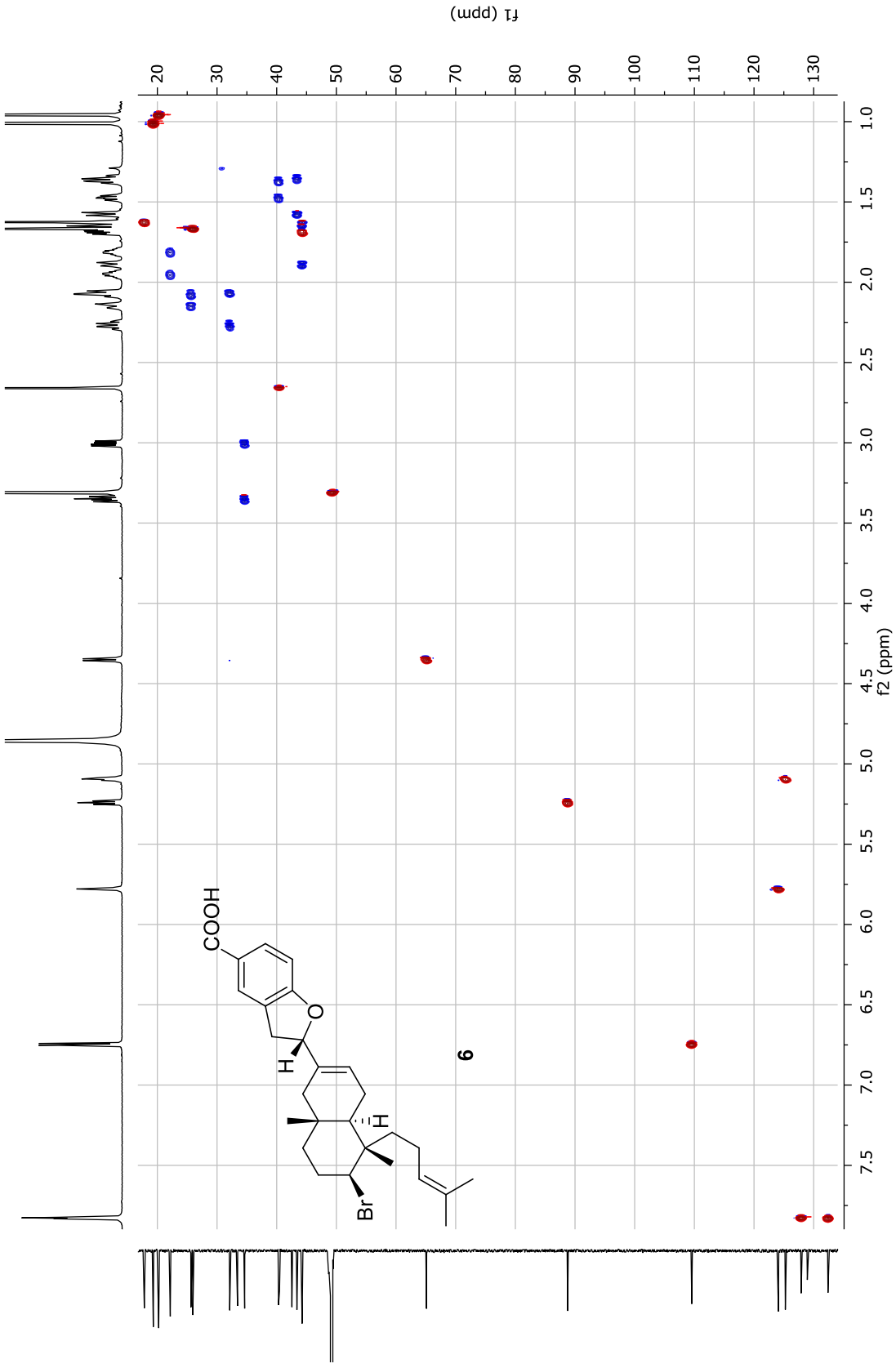


Figure S51. ^{1}H-^{13}C edited-HSQC spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD.

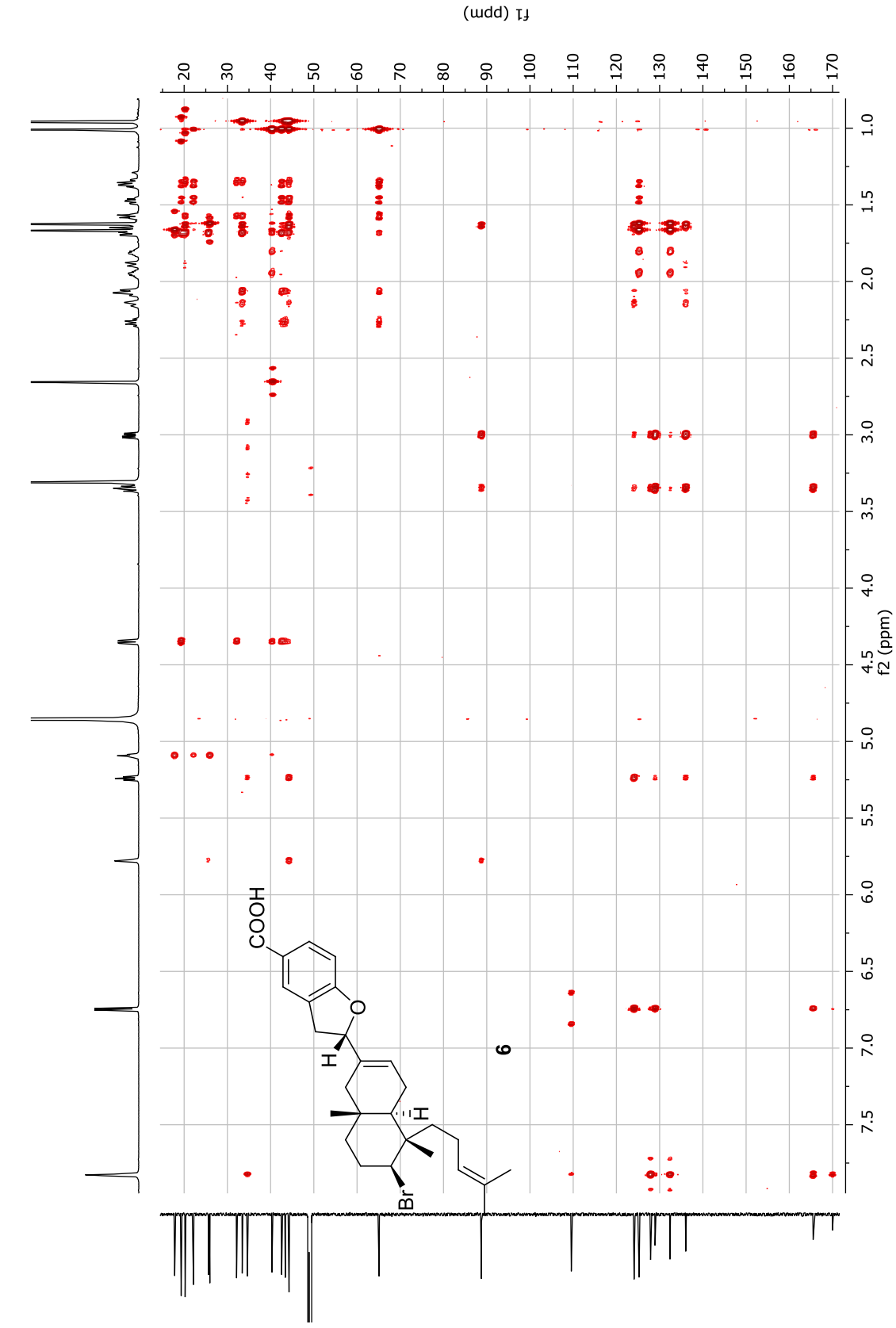


Figure S52. ^{1}H-^{13}C HMBC spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD.

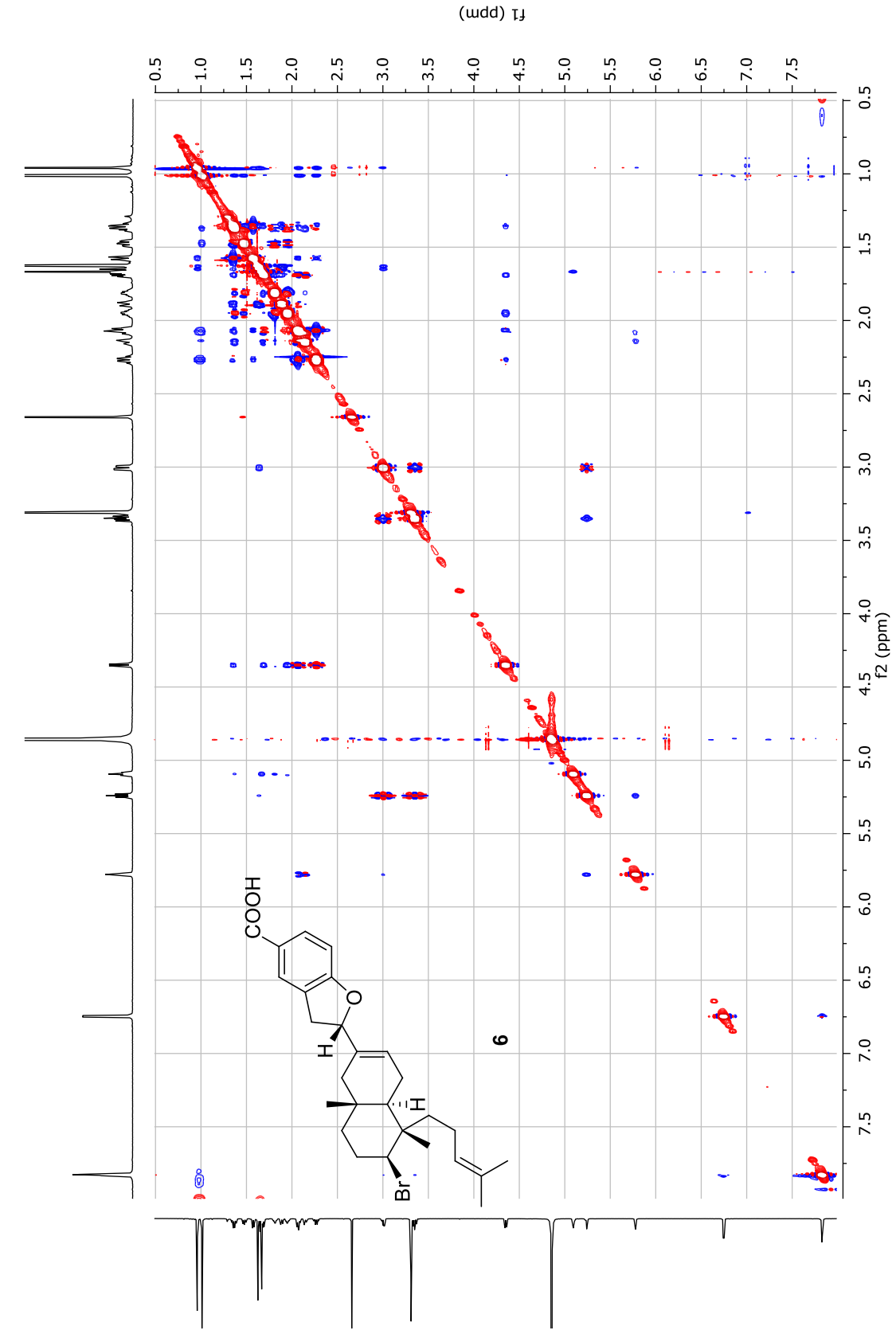
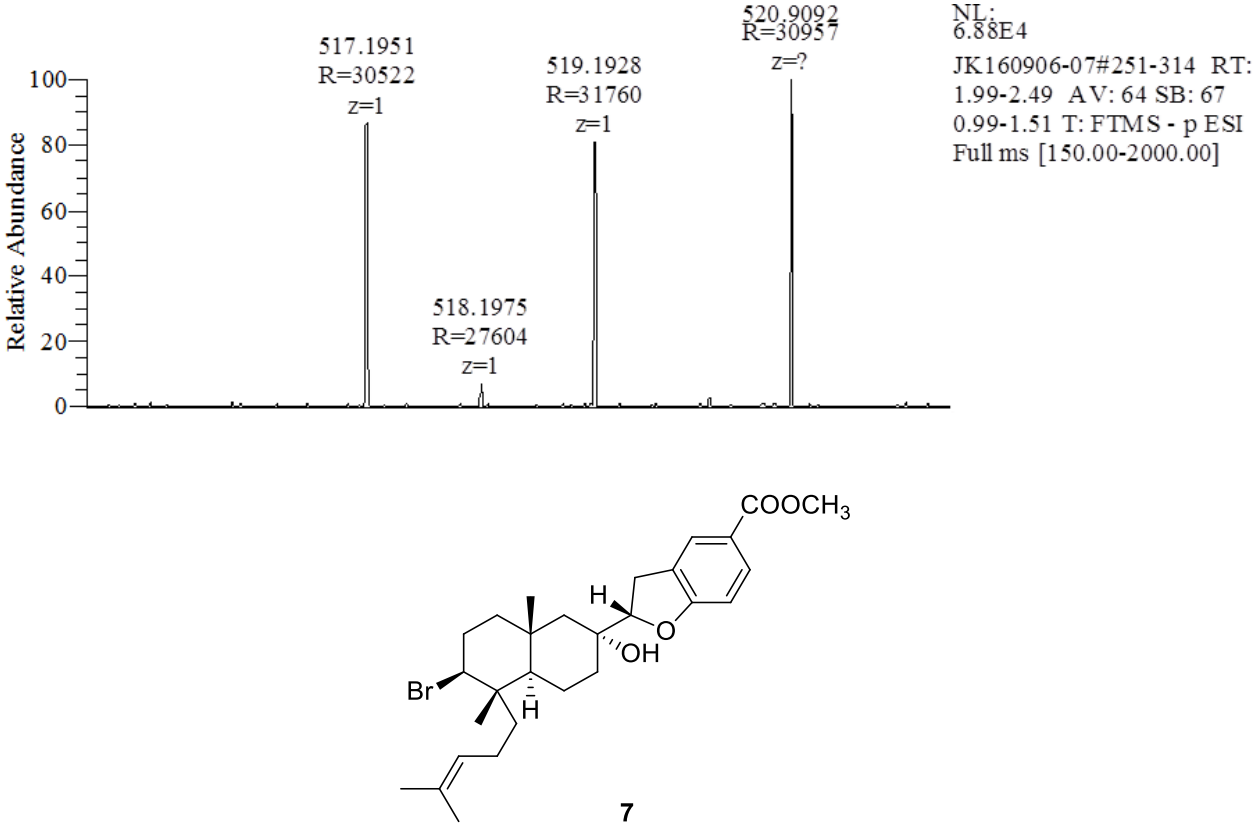


Figure S53. ^{1}H-^{1}H NOESY spectrum of bromophycoic acid F (**6**) at 800 MHz in CD_3OD.

SPECTRA OF BROMOPHYCOIC ACID A METHYL ESTER (7)

Figure S54. Negative-mode HRESIMS spectrum of bromophycoic Acid A methyl ester (**7**).



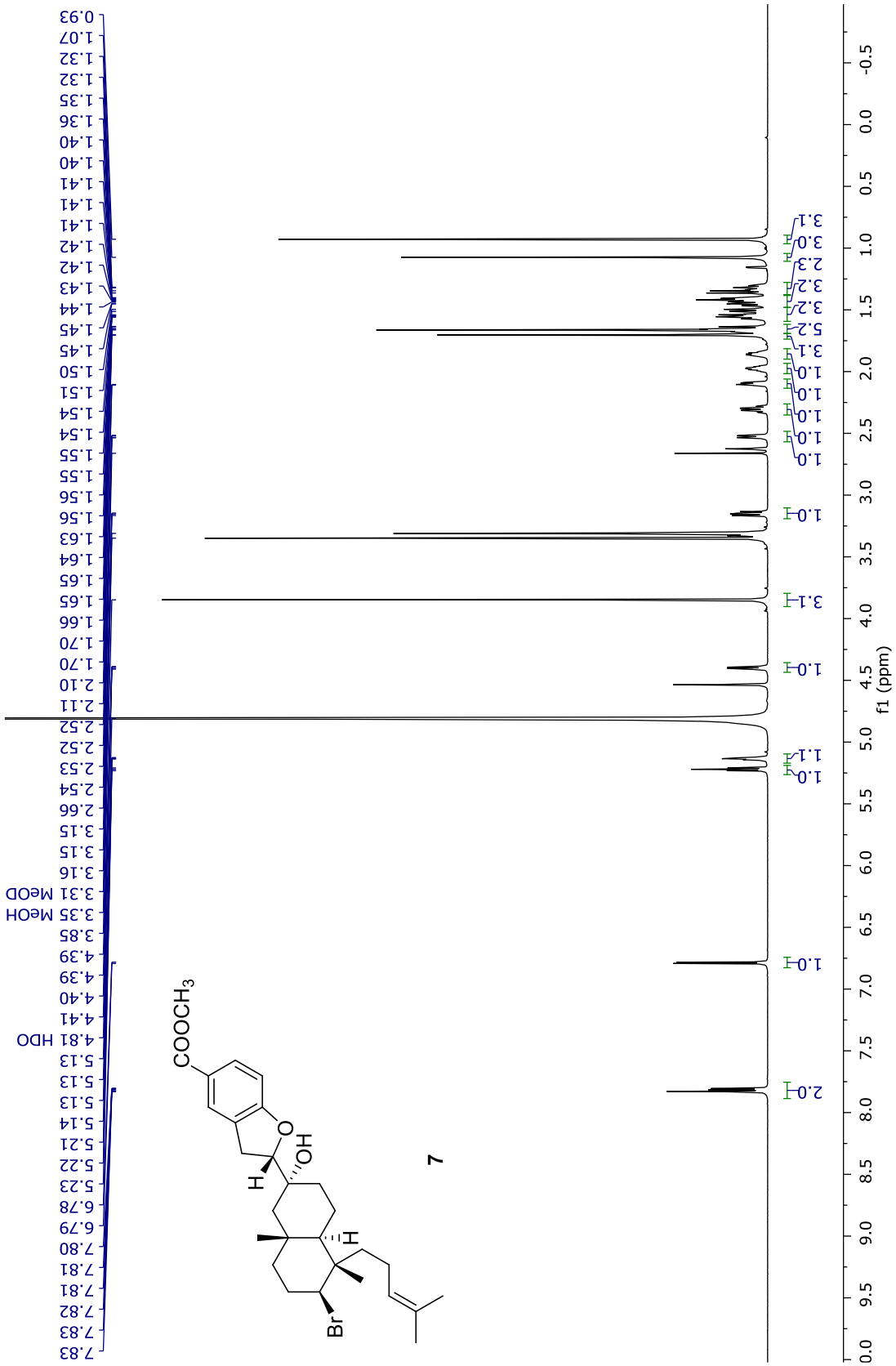


Figure S55. ^{1}H NMR spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD.

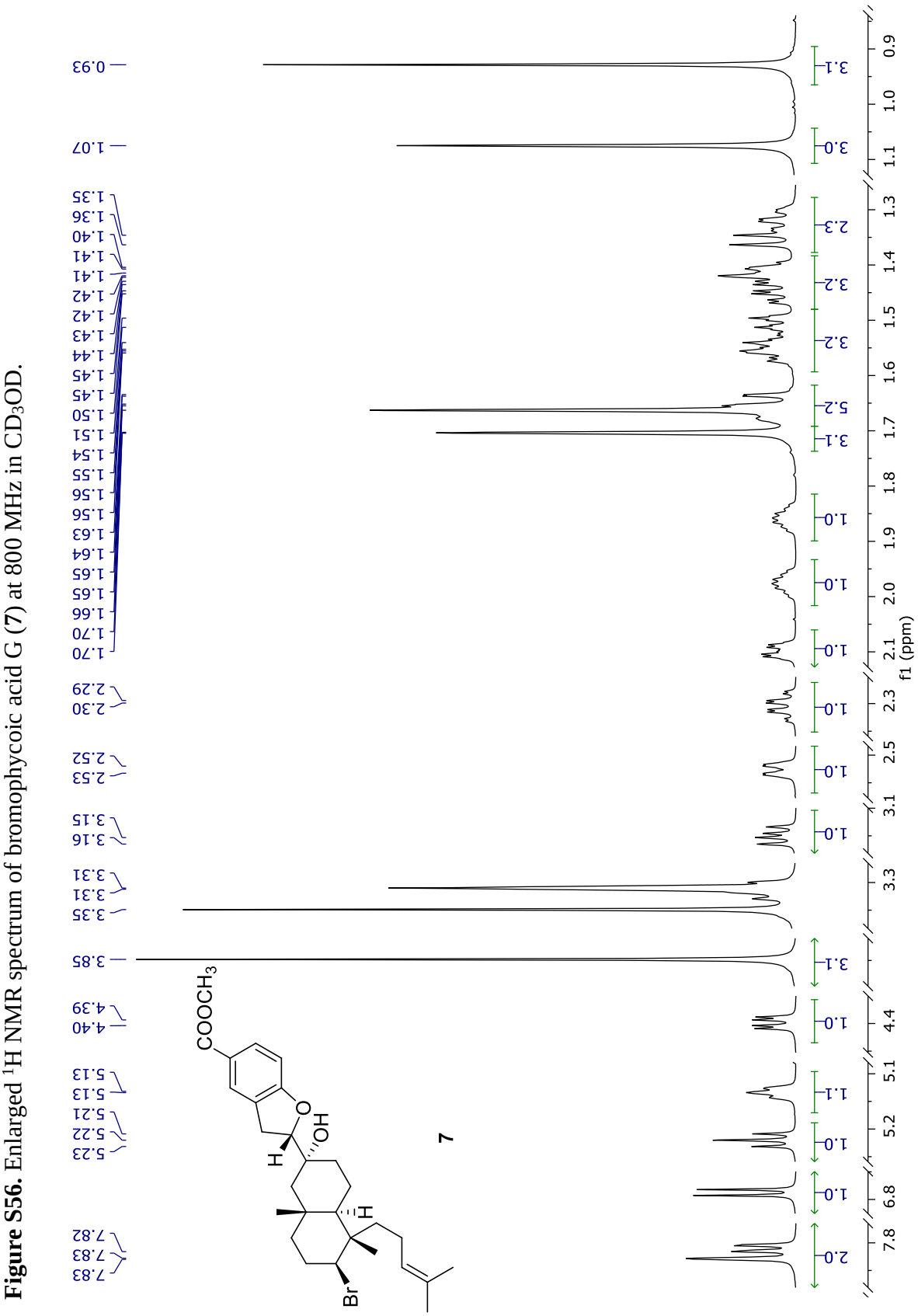


Figure S56. Enlarged ^{1}H NMR spectrum of bromophycoic acid G (**7**) at 800 MHz in CD_3OD.

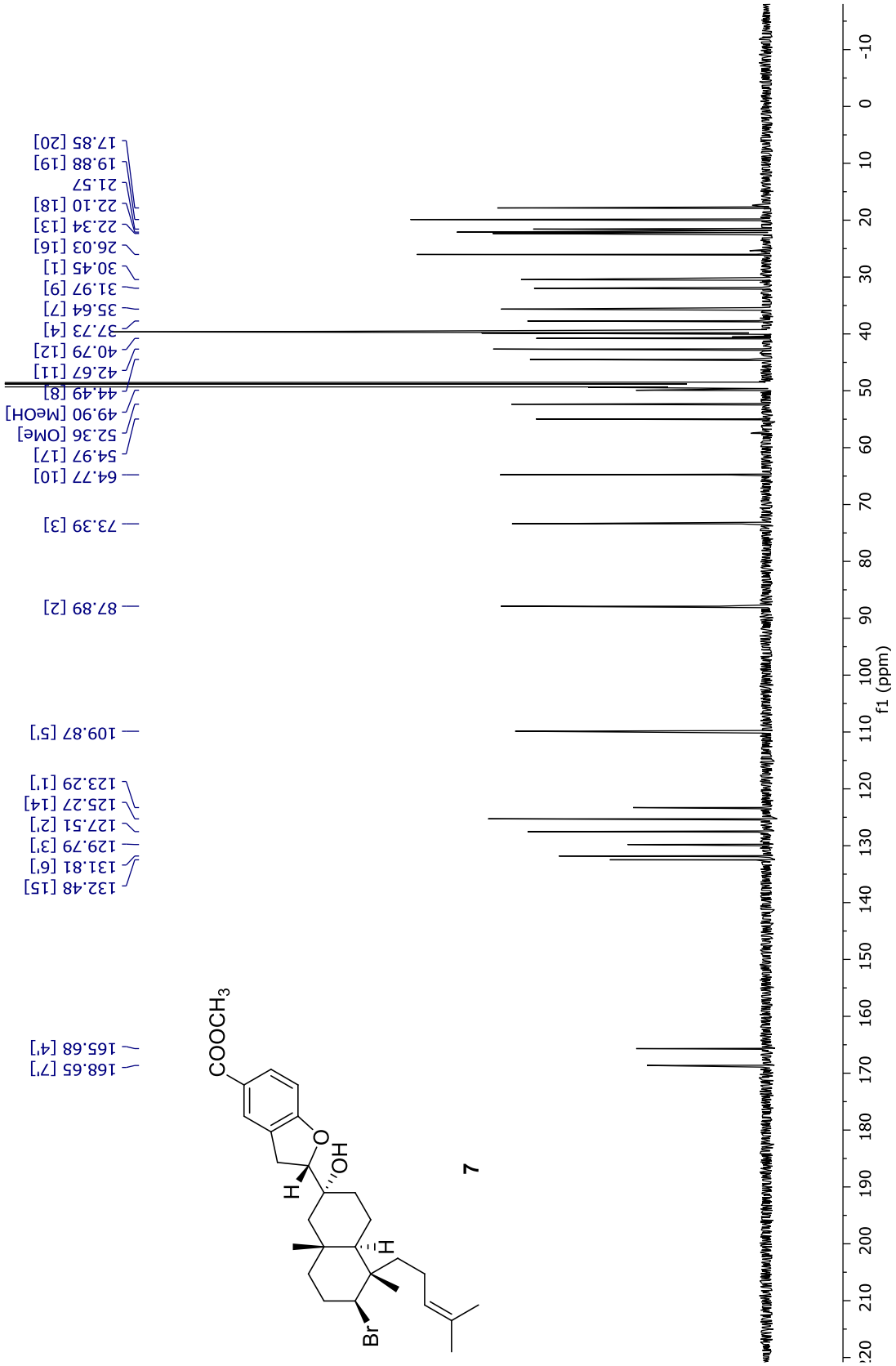


Figure S57. ^{13}C NMR spectrum of bromophycoic acid A methyl ester (**7**) at 200 MHz in CD_3OD.

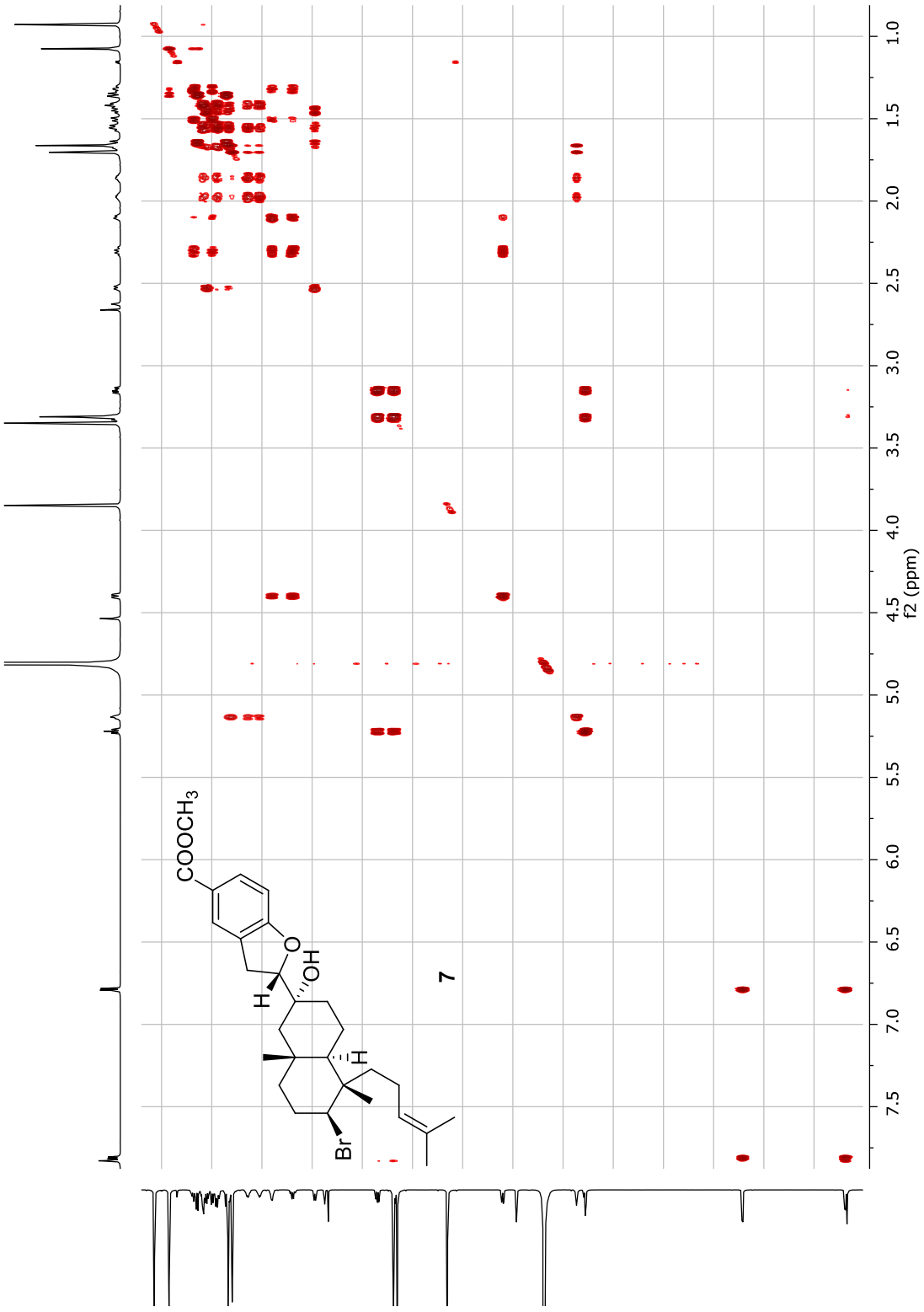


Figure S58. ^{1}H-^{1}H DQF-COSY spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD.

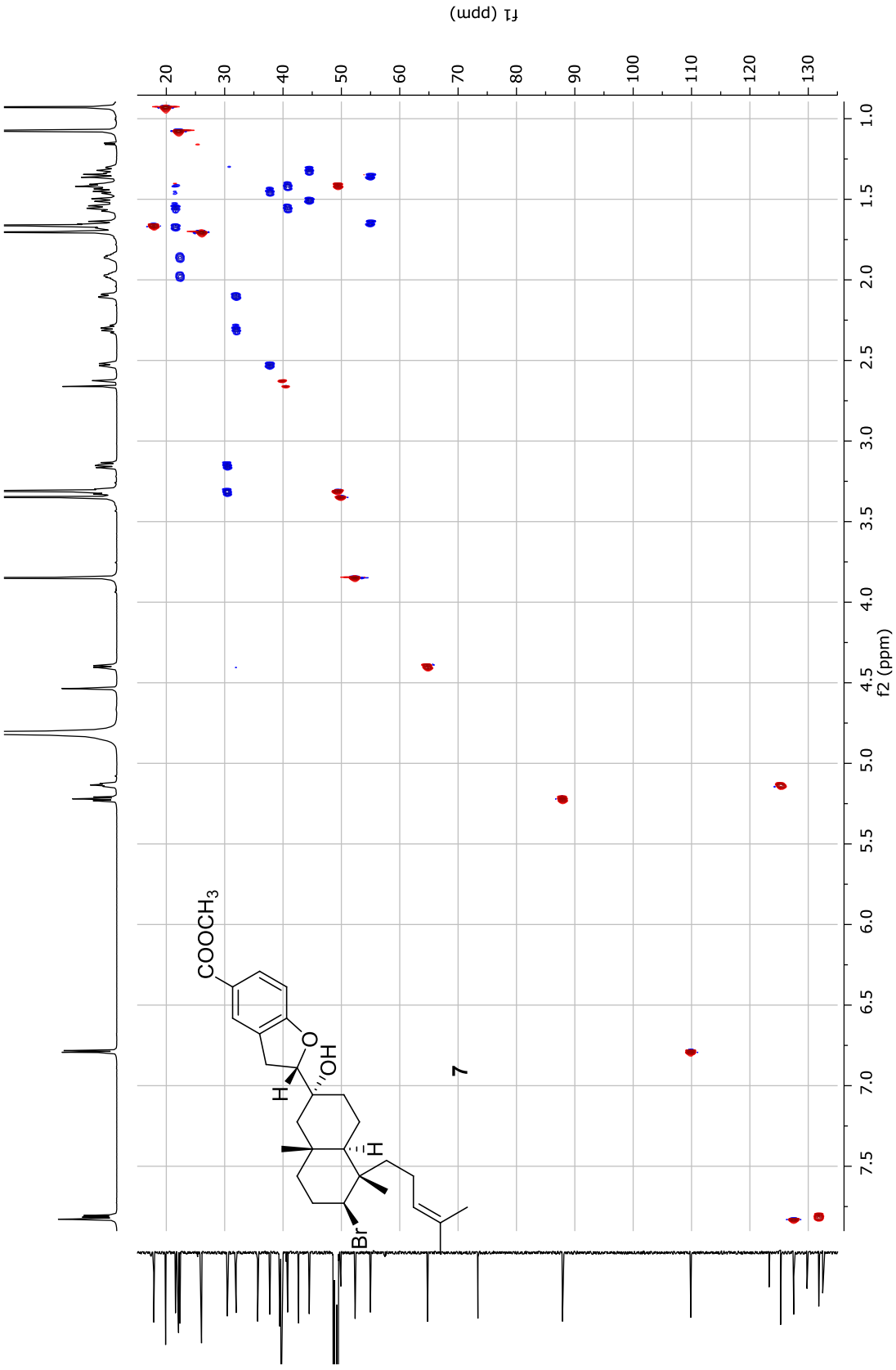


Figure S59. ^{1}H-^{13}C edited-HSQC spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD.

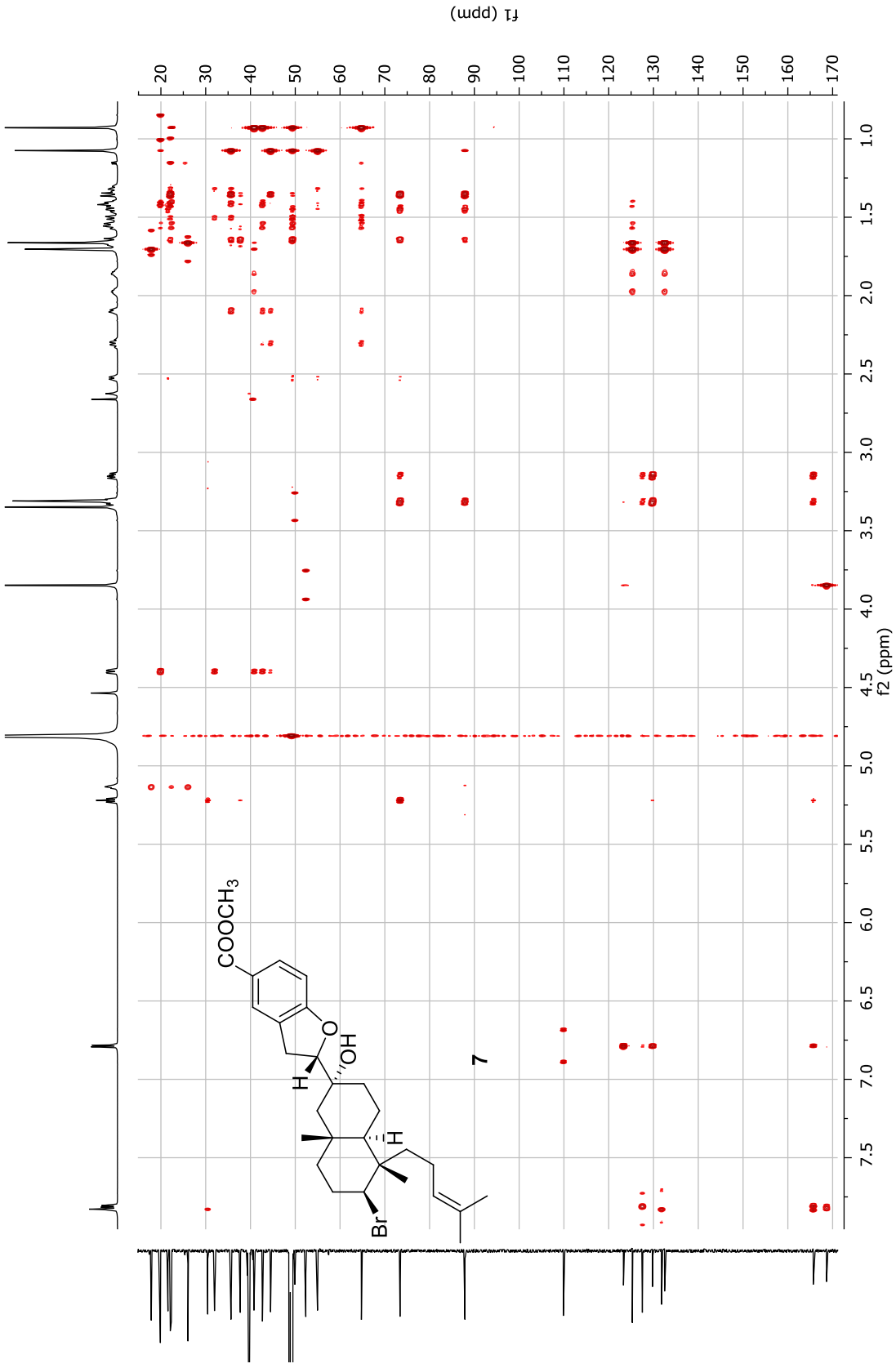


Figure S60. ^{1}H-^{13}C HMBC spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD.

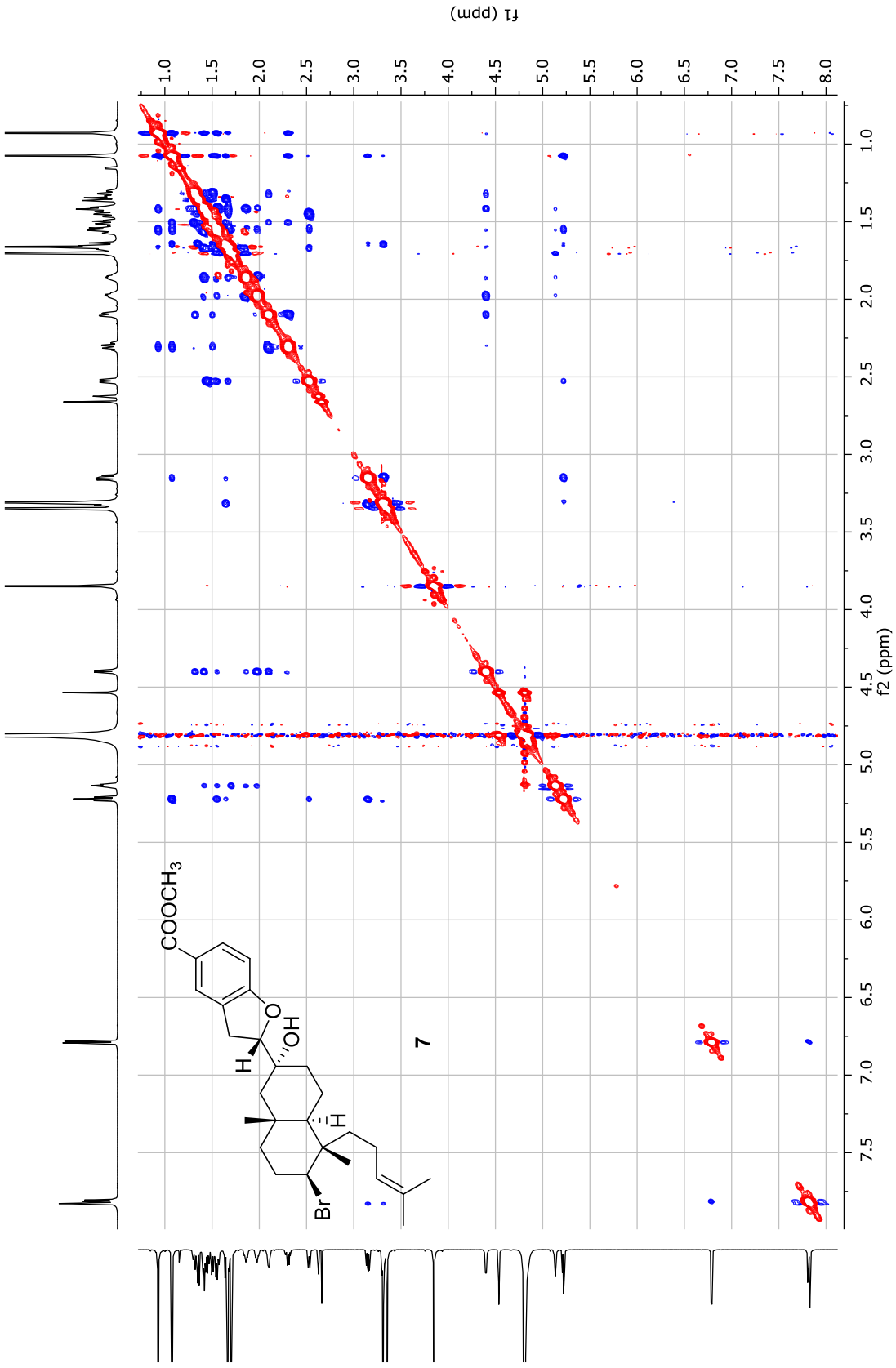


Figure S61. ^{1}H-^{1}H NOESY spectrum of bromophycoic acid A methyl ester (**7**) at 800 MHz in CD_3OD.

SPECTRA OF 3-GERANYLGERANYL-4-HYDROXYBENZOIC ACID (8)

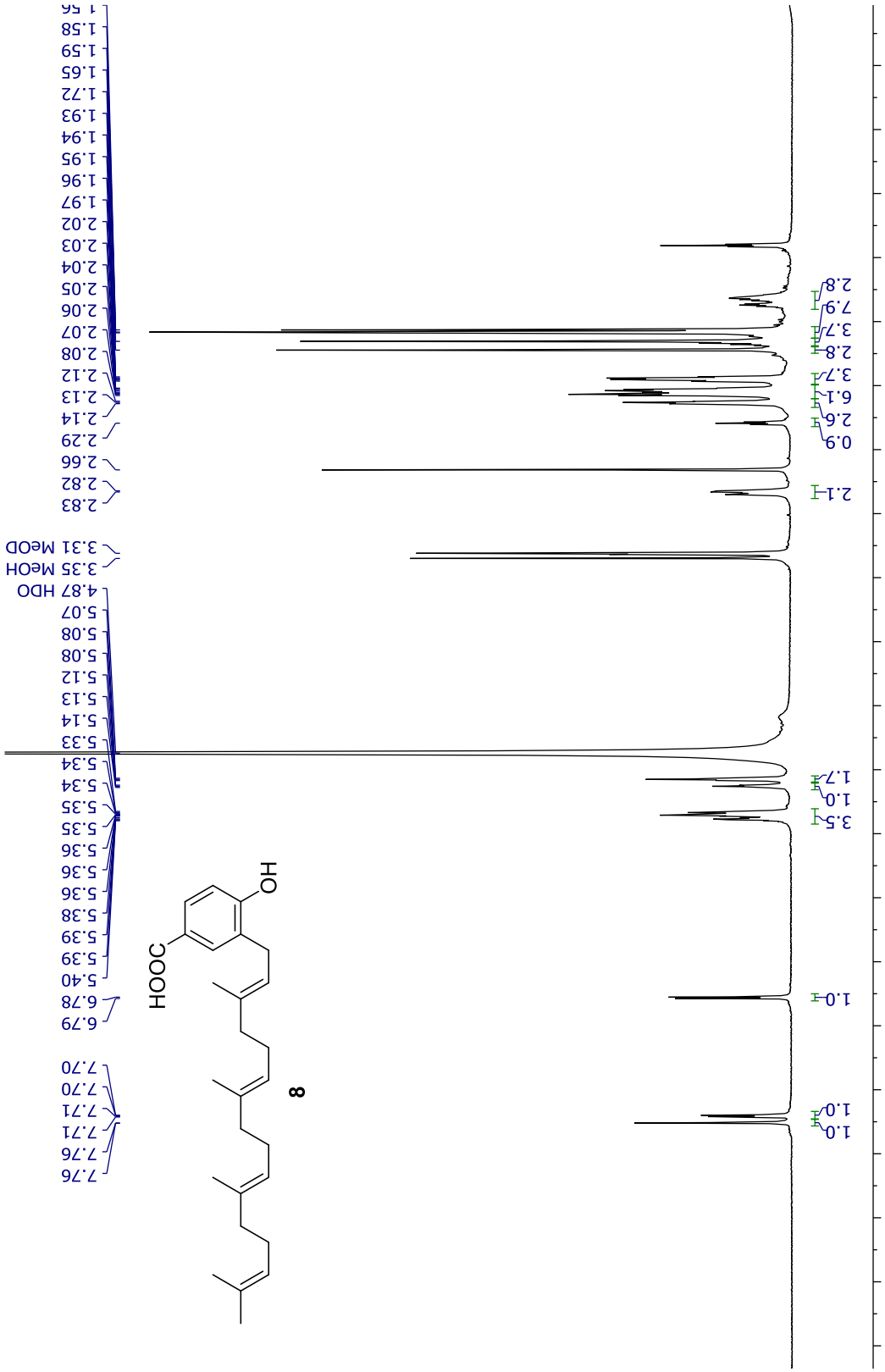


Figure S62. ^{1}H NMR spectrum of 3-geranylgeranyl-4-hydroxybenzoic acid (**8**) at 500 MHz in CD_3OD.