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Chromolactol, an Oxygenated Diterpene from the Indo-Pacific Nudibranch *Goniobranchus coi*: Spectroscopic and Computational Studies

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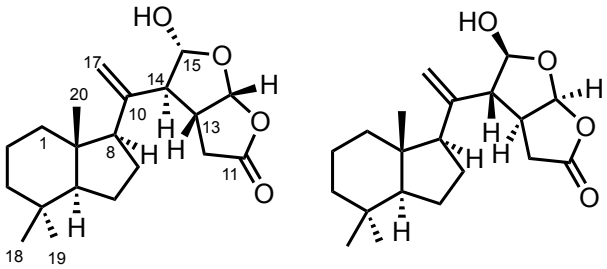


Figure S1. Structures of candidate diastereomers of chromolactol

Figure S2. Image of *Goniobranchus coi*

Figure S3. ^{1}H NMR spectrum of **1** (500 MHz, $CDCl_3$).

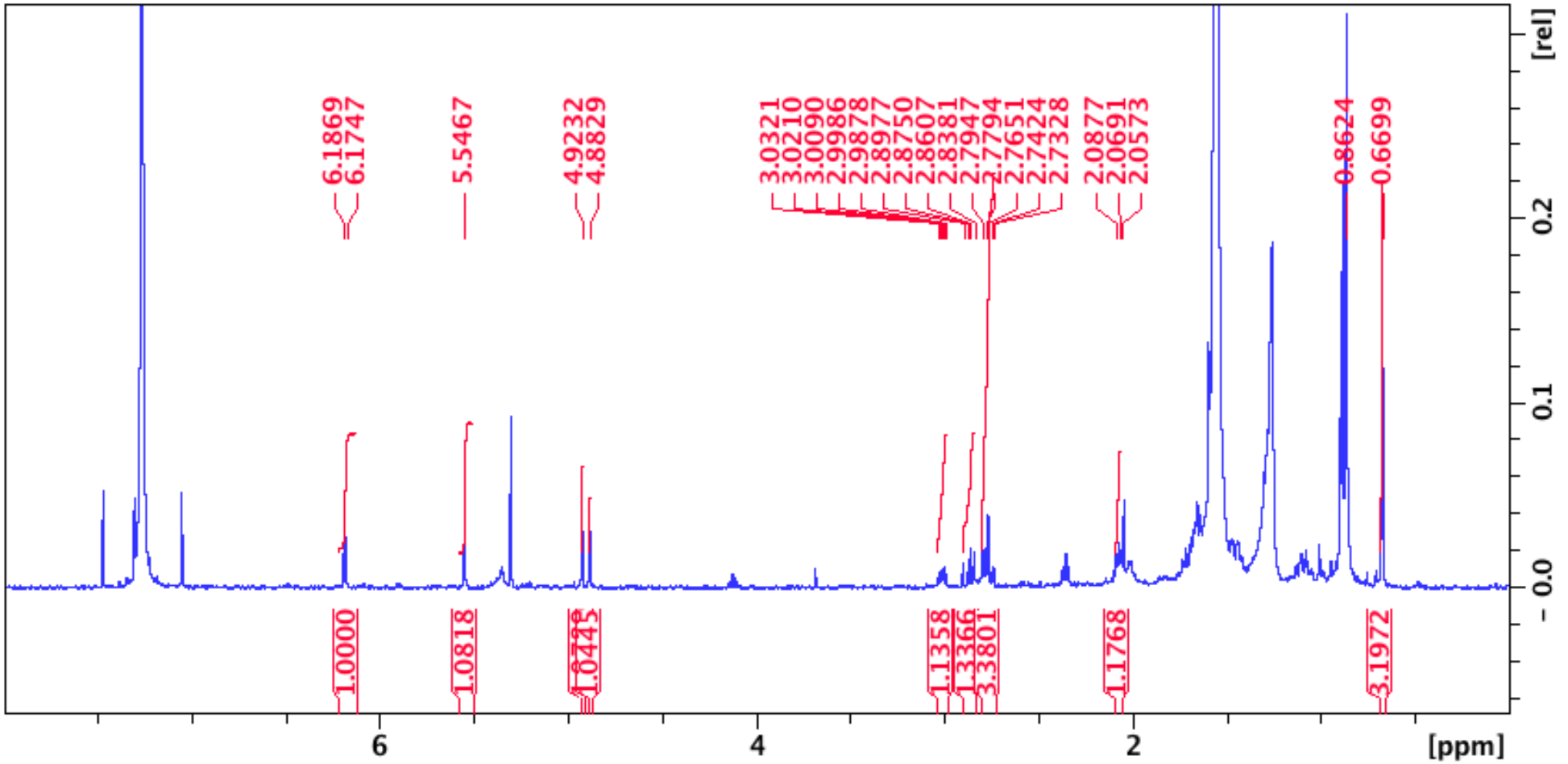


Figure S4. ^{1}H NMR spectrum of **1** (500 MHz, $CDCl_3$) down field region (2.5 – 6.5 ppm).

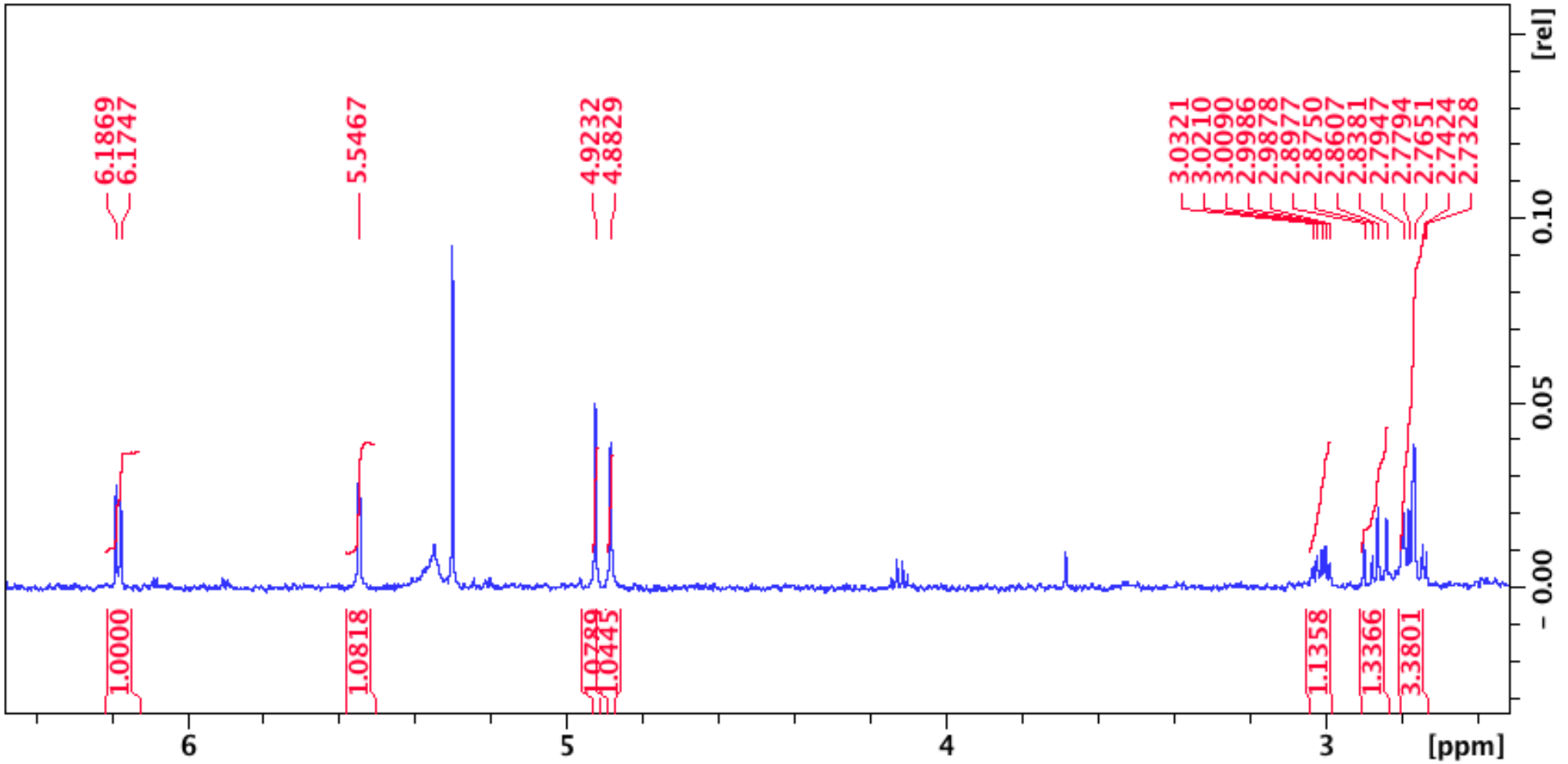


Figure S5. ^{1}H NMR spectrum of **1** (500 MHz, $CDCl_3$) up field region (0 - 2.5 ppm).

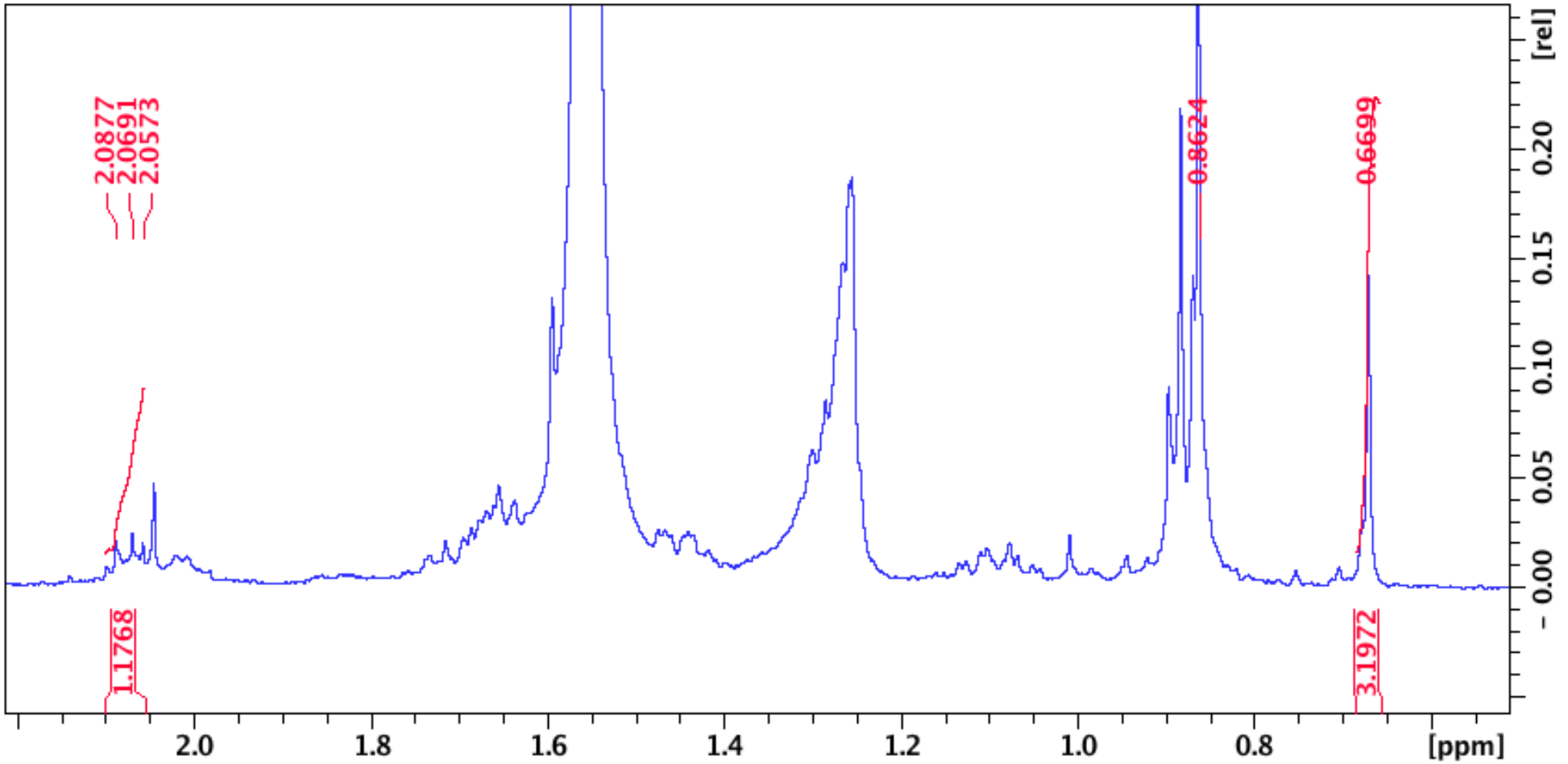


Figure S6. HSQC spectrum of **1** (700 MHz, $CDCl_3$).

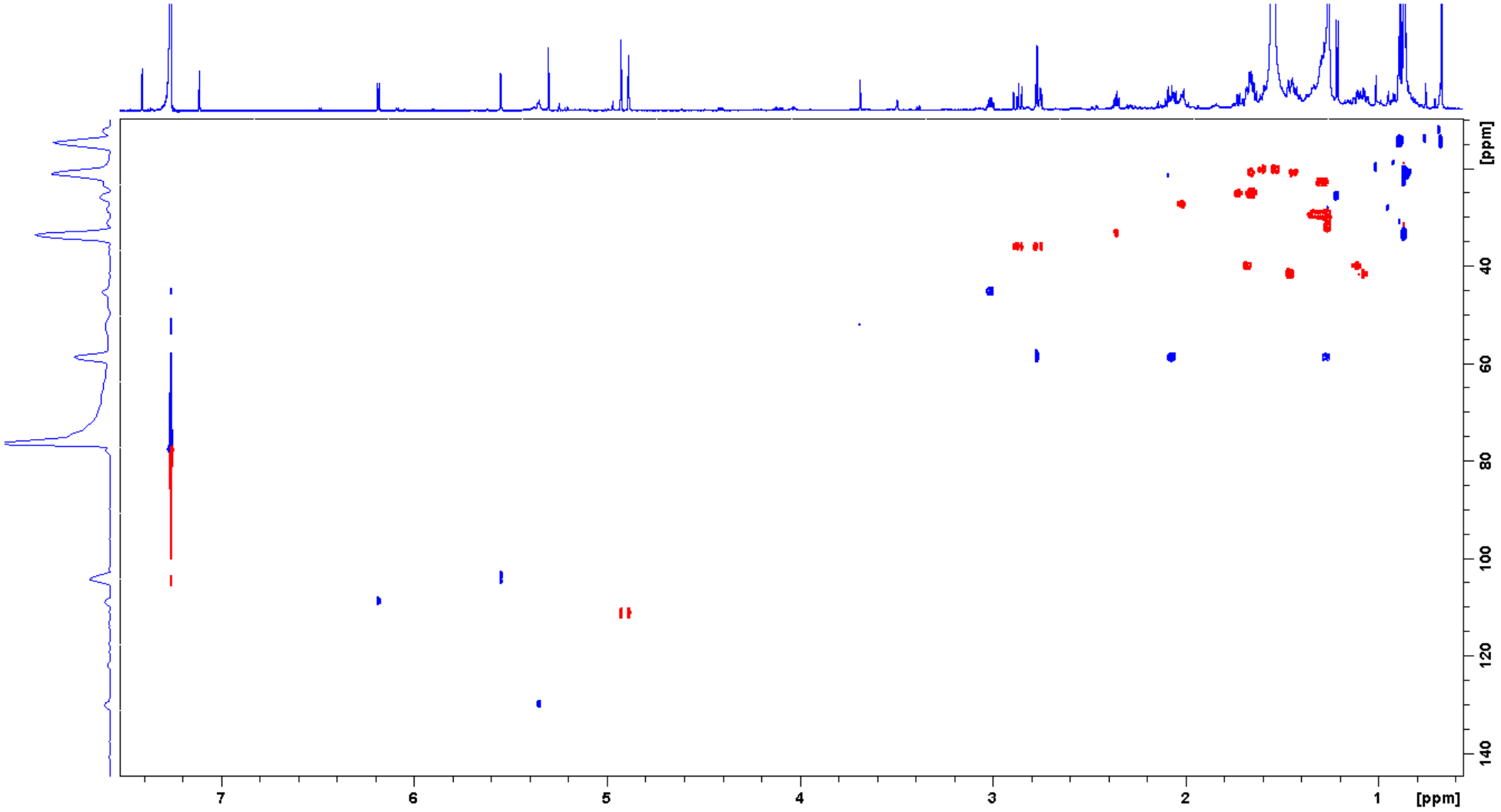


Figure S7. HMBC spectrum of **1** (700 MHz, $CDCl_3$).

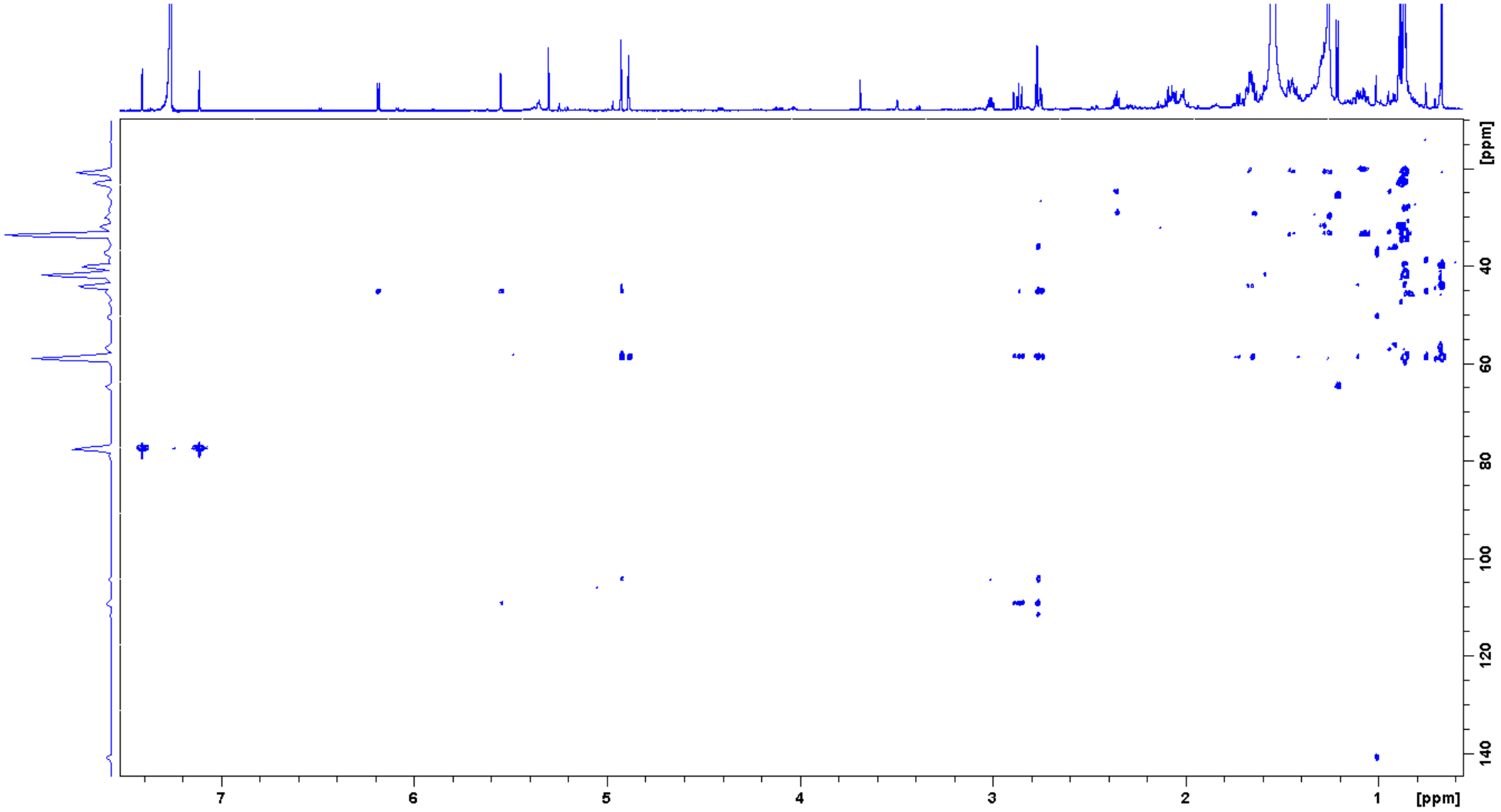


Figure S8. gCOSY spectrum of **1** (700 MHz, $CDCl_3$).

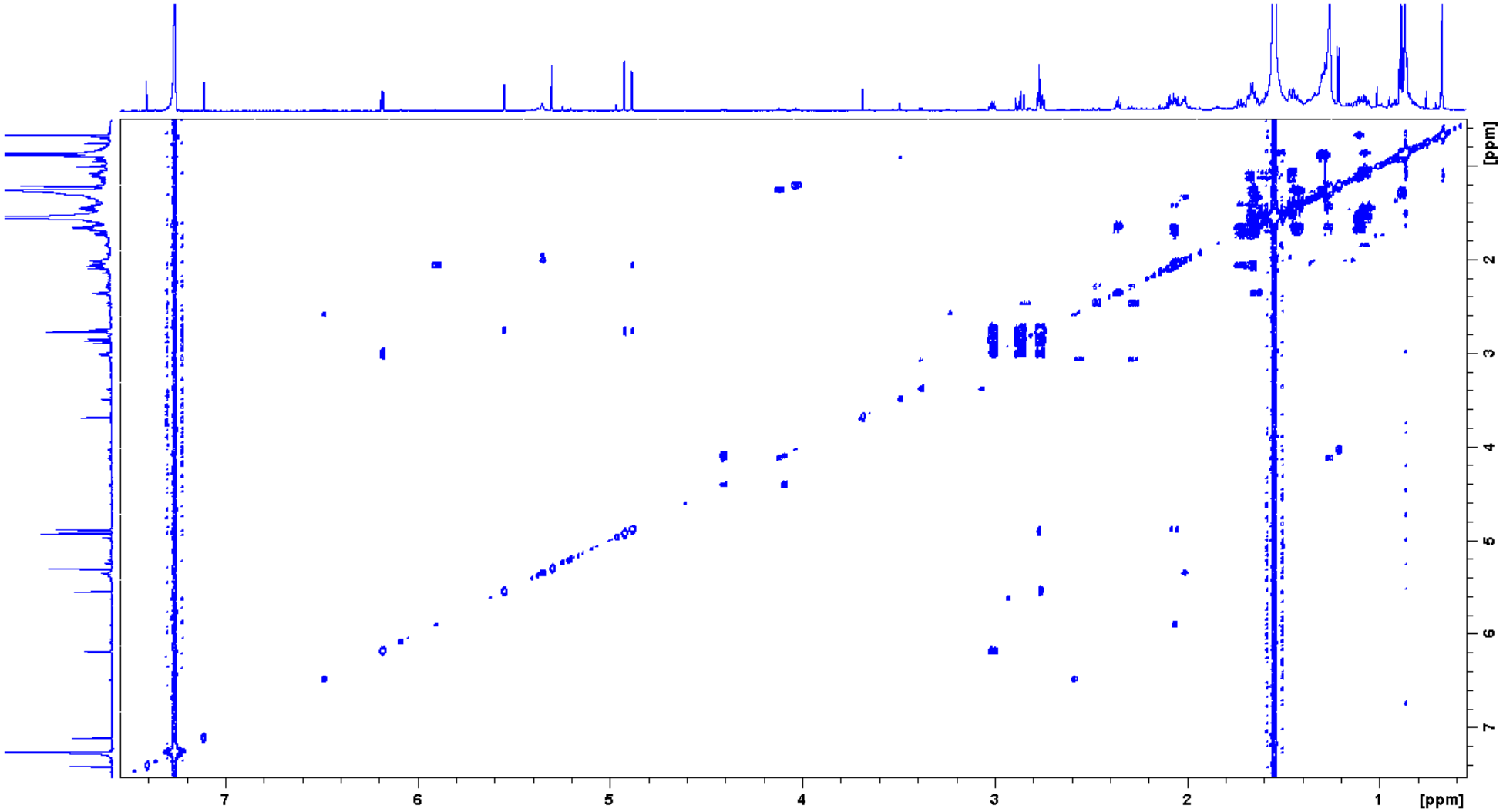


Figure S9. NOESY spectrum of **1** (700 MHz, $CDCl_3$).

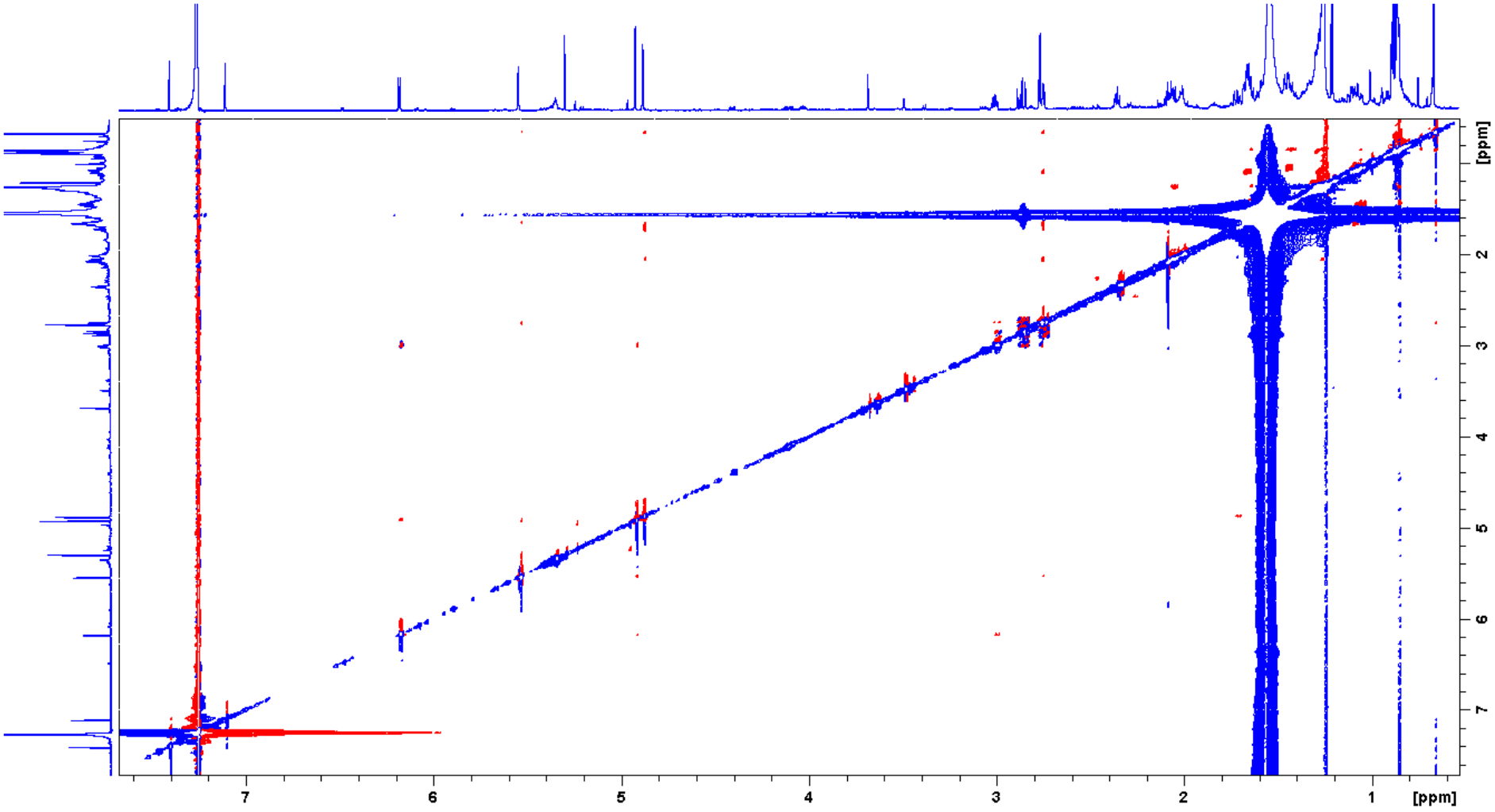
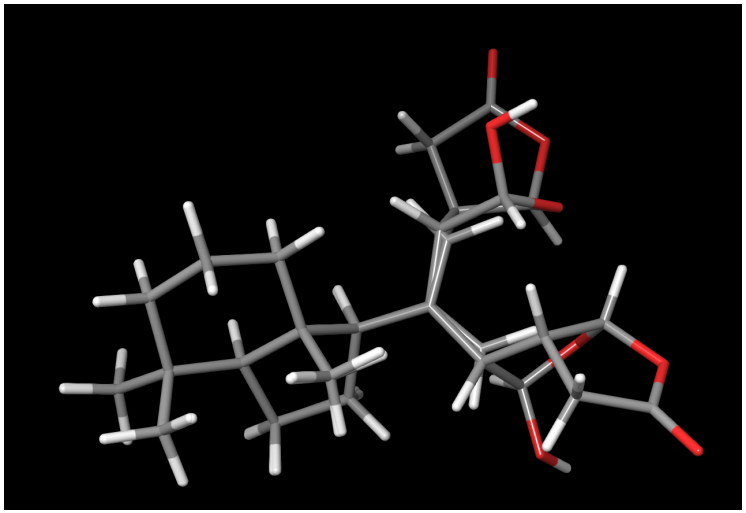
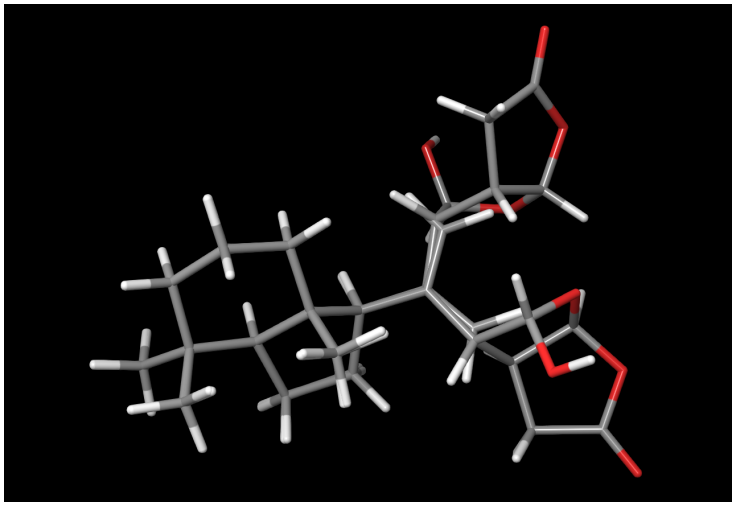


Figure S10. Overlay of lowest energy conformers of stereoisomers **1a** and **1b** of chromolactol



1a



1b

Table S1. ^{1}H NMR experimental and calculated chemical shifts

#	expt	1a	1b
1a	1.67	1.62	1.60
1b	1.1	1.11	1.13
2a	1.59	1.68	1.66
2b	1.52	1.53	1.52
3a	1.45	1.48	1.47
3b	1.07	1.17	1.18
5	1.26	1.35	1.35
6a	1.65	1.68	1.69
6b	1.43	1.60	1.58
7a	1.72	1.86	1.78
7b	1.65	1.71	1.72
8	2.06	2.24	2.26
12a	2.86	2.86	2.86
12b	2.75	2.65	2.66
13	3.01	3.04	2.98
14	2.76	2.82	2.81
15	5.54	5.30	5.38
16	6.18	6.02	6.01
17a	4.92	4.99	5.10
17b	4.88	5.00	4.98
18	0.86	0.90	0.91
19	0.86	0.91	0.91
20	0.67	0.75	0.75

Table S2. ^{13}C NMR experimental and calculated chemical shifts

#	expt	1a	1b
1	39.9	38.9	38.8
2	19.9	21.7	21.6
3	41.6	40.9	40.9
4	33.5	37.0	36.7
5	58.7	58.4	58.1
6	20.8	22.3	22.3
7	24.8	26.3	26.5
8	58.8	60.4	60.4
9	44	48.3	48.7
10	148.2	153.8	154.1
11	175.4	178.1	178.0
12	35.8	37.4	37.0
13	45.2	46.9	46.7
14	58.5	59.3	59.2

15	104.1	105.3	105.6
16	108.9	110.3	110.2
17	111.5	113.3	113.3
18	33.4	31.4	31.4
19	20.7	19.4	19.3
20	14.2	13.7	13.6

Table S3. Computed DP4 probabilities for compounds **1a** and **1b**

	1a	**1b**
DP4 (H data)	45.8%	54.2%
DP4 (C data)	68.1%	31.9%
DP4 (all data)	64.3%	35.7%

XYZ coordinates for isomer **1a**

chromolactol**1a**-01 44.979%

C	-1.631188	0.246598	0.380638
C	-2.653159	0.626798	1.459249
H	-1.130660	-0.674983	0.685833
H	-2.288092	1.320993	2.220871
O	-3.126992	-0.565234	2.046859
H	-3.812482	-0.342788	2.700744
O	-3.695678	1.322546	0.762975
C	-3.820701	0.814209	-0.540443
C	-2.551505	-0.029593	-0.847173
C	-3.080463	-1.466205	-0.992264
C	-4.585688	-1.366996	-0.844309
H	-4.032583	1.647112	-1.211889
H	-2.082024	0.310626	-1.772302
H	-2.853834	-1.910655	-1.966124
H	-2.705859	-2.147490	-0.223683
O	-4.956472	-0.075640	-0.637709
O	-5.401925	-2.258583	-0.907032
C	-0.574563	1.304499	0.067023
C	-0.779779	2.607642	0.307750
H	-1.695874	2.974694	0.759327
H	-0.039530	3.359426	0.056243
C	0.684248	0.746151	-0.579557
C	1.414878	1.664761	-1.601853
C	2.889567	1.166468	-1.660572
H	0.372598	-0.156826	-1.125211
H	1.378902	2.711536	-1.290226
H	0.921542	1.615285	-2.578220
H	3.194758	0.909431	-2.679481
H	3.575280	1.947074	-1.313294
C	2.911738	-0.061425	-0.729337
C	1.851412	0.263746	0.369770
C	1.572488	-1.025216	1.167966
C	2.875977	-1.652784	1.704693
C	3.906783	-1.920647	0.593600
C	4.261784	-0.683781	-0.280486
H	2.440193	-0.874293	-1.306397
H	1.077885	-1.755192	0.510117
H	0.885900	-0.831937	2.002503
H	3.312843	-1.004464	2.474268
H	2.640279	-2.597304	2.210605
H	4.826467	-2.332626	1.030418
H	3.504493	-2.700759	-0.069325
C	2.236184	1.407010	1.333149
H	1.356464	1.724544	1.901090
H	2.993236	1.099687	2.055084

H	2.622495	2.286977	0.810182
C	5.020800	-1.175781	-1.533265
H	5.908511	-1.750641	-1.243344
H	4.390523	-1.823904	-2.153882
H	5.357629	-0.337968	-2.154022
C	5.206579	0.271165	0.481339
H	6.182781	-0.209685	0.615750
H	5.374321	1.199621	-0.075146
H	4.840014	0.540090	1.473258

chromolactol**1a**-02 53.677%

C	-1.627279	0.172895	-0.214928
C	-2.469218	1.417250	-0.580388
H	-1.170769	0.349727	0.758956
H	-1.959214	2.150347	-1.211601
O	-2.926366	2.002119	0.618679
H	-3.507824	2.752190	0.402887
O	-3.550576	0.916012	-1.372098
C	-3.901341	-0.372596	-0.941247
C	-2.721487	-0.922152	-0.092725
C	-3.323493	-1.101900	1.311641
C	-4.776640	-0.687277	1.195503
H	-4.193563	-0.954299	-1.816922
H	-2.369832	-1.875177	-0.490048
H	-3.285435	-2.137787	1.662544
H	-2.848661	-0.480247	2.075423
O	-5.065654	-0.331903	-0.083989
O	-5.618454	-0.668788	2.065035
C	-0.537962	-0.086926	-1.252167
C	-0.791606	-0.769909	-2.379226
H	-1.757116	-1.216267	-2.597511
H	-0.024014	-0.905338	-3.136038
C	0.855958	0.486674	-1.022319
C	0.947492	1.879921	-0.321933
C	2.342218	1.926758	0.372560
H	1.295915	0.598654	-2.020708
H	0.152780	2.021591	0.415564
H	0.833079	2.682846	-1.057950
H	2.903946	2.825196	0.099902
H	2.230406	1.941866	1.462474
C	3.039577	0.639990	-0.104595
C	1.884589	-0.401482	-0.227511
C	2.413902	-1.620119	-1.006224
C	3.700938	-2.180030	-0.365695
C	4.802987	-1.114068	-0.222840
C	4.376336	0.176294	0.535805
H	3.318749	0.833787	-1.153669
H	2.637873	-1.313848	-2.038471
H	1.650131	-2.405631	-1.070542
H	3.472406	-2.618274	0.613799

H	4.081018	-3.006740	-0.978808
H	5.681823	-1.550584	0.270656
H	5.130126	-0.821172	-1.231280
C	1.268267	-0.867548	1.109682
H	0.373078	-1.467263	0.912905
H	1.947018	-1.501209	1.680490
H	0.980978	-0.034301	1.758414
C	5.447267	1.261925	0.285894
H	6.437053	0.902557	0.592036
H	5.502733	1.532032	-0.775402
H	5.235773	2.173677	0.855686
C	4.326968	-0.073852	2.059096
H	5.344101	-0.229038	2.437986
H	3.906914	0.784669	2.594296
H	3.744100	-0.954551	2.333620

chromolactol**1a**-03 0.617%

C	1.839258	-0.344209	0.491786
C	2.854624	-1.381036	0.999361
H	1.585844	0.311914	1.328318
H	2.419935	-2.329667	1.325946
O	3.604635	-0.780364	2.032587
H	4.291640	-1.404070	2.326082
O	3.676581	-1.696099	-0.131889
C	3.793717	-0.572030	-0.964448
C	2.679763	0.436188	-0.564422
C	3.450801	1.660989	-0.044625
C	4.919408	1.322203	-0.203354
H	3.797470	-0.915480	-1.999753
H	2.072839	0.692491	-1.433642
H	3.241008	2.572040	-0.613382
H	3.261101	1.881495	1.009285
O	5.063041	0.090343	-0.759534
O	5.877288	2.004951	0.082004
C	0.546543	-0.938142	-0.077535
C	0.562444	-2.099227	-0.748269
H	1.486393	-2.644547	-0.915989
H	-0.335116	-2.553035	-1.147227
C	-0.695857	-0.130071	0.270019
C	-0.600613	1.398984	-0.047863
C	-2.061042	1.934494	0.034400
H	-0.764109	-0.209055	1.368661
H	-0.189133	1.551100	-1.051429
H	0.062058	1.919473	0.649723
H	-2.165262	2.714754	0.794415
H	-2.363270	2.381701	-0.918616
C	-2.906123	0.689552	0.378295
C	-2.119229	-0.501259	-0.263454
C	-2.712672	-1.814915	0.288108
C	-4.243923	-1.872612	0.108739

C	-4.966667	-0.657925	0.715953
C	-4.449286	0.720613	0.215664
H	-2.772332	0.534622	1.461231
H	-2.475935	-1.884744	1.359944
H	-2.259284	-2.692073	-0.187172
H	-4.490715	-1.959062	-0.957012
H	-4.626284	-2.788712	0.576022
H	-6.045840	-0.732577	0.525465
H	-4.843155	-0.691321	1.808402
C	-2.141462	-0.484209	-1.814921
H	-1.281377	-1.013995	-2.228265
H	-3.036430	-0.966519	-2.212176
H	-2.117441	0.531145	-2.219602
C	-5.022601	1.820233	1.137072
H	-6.118055	1.773028	1.155621
H	-4.665277	1.705029	2.167341
H	-4.740555	2.821300	0.791898
C	-4.958269	1.007670	-1.213777
H	-6.045649	1.147160	-1.193446
H	-4.520092	1.925714	-1.620268
H	-4.748218	0.199510	-1.916095

chromolactol**1a**-04 0.727%

C	-2.037429	1.090477	0.518584
C	-2.499848	1.383849	-0.924933
H	-2.716899	1.616622	1.192769
H	-1.939872	2.172699	-1.436910
O	-3.876197	1.683806	-0.881271
H	-4.199746	1.816441	-1.789668
O	-2.245016	0.184811	-1.668399
C	-2.382116	-0.933288	-0.834423
C	-2.272372	-0.444960	0.635701
C	-3.611667	-0.859332	1.269184
C	-4.426958	-1.471851	0.147036
H	-1.661786	-1.686117	-1.158384
H	-1.438088	-0.930747	1.139642
H	-3.493473	-1.612962	2.054562
H	-4.174947	-0.027392	1.700095
O	-3.688456	-1.537115	-0.991127
O	-5.562885	-1.887736	0.192356
C	-0.623613	1.587392	0.816976
C	-0.490855	2.536285	1.758057
H	-1.349026	2.899881	2.317282
H	0.463297	2.992672	1.997138
C	0.540860	1.069994	-0.025095
C	1.348678	2.200394	-0.744596
C	2.749095	1.603810	-1.066650
H	0.111631	0.442218	-0.813450
H	1.434771	3.078067	-0.098439
H	0.822029	2.528382	-1.647054

H	2.993282	1.680741	-2.130469
H	3.532962	2.141425	-0.521720
C	2.645285	0.137538	-0.606951
C	1.677913	0.180264	0.620708
C	1.273231	-1.268044	0.958690
C	2.505406	-2.177434	1.148446
C	3.444473	-2.160529	-0.070383
C	3.919664	-0.746063	-0.509239
H	2.049561	-0.369398	-1.383960
H	0.667504	-1.673804	0.135260
H	0.651271	-1.299029	1.863290
H	3.053573	-1.881325	2.051105
H	2.170017	-3.206411	1.328581
H	4.320363	-2.793554	0.125397
H	2.916149	-2.619833	-0.918773
C	2.254882	0.859543	1.878843
H	1.465445	0.988800	2.624730
H	3.037425	0.260507	2.344038
H	2.681310	1.845292	1.669739
C	4.547464	-0.861165	-1.916824
H	5.360741	-1.596740	-1.915086
H	3.807580	-1.181887	-2.659808
H	4.967095	0.094823	-2.249354
C	5.020086	-0.219821	0.438374
H	5.931463	-0.814937	0.306408
H	5.276222	0.822142	0.218240
H	4.747490	-0.279050	1.493293

XYZ coordinates for isomer **1b**

chromolactol**1b**-01 43.302%

C	-1.622085	-0.184638	0.023849
C	-2.298392	-0.811221	1.263865
H	-1.138778	0.745064	0.332681
H	-1.692870	-1.552666	1.794077
O	-2.696402	0.232552	2.125225
H	-3.185774	-0.147586	2.875764
O	-3.422177	-1.530544	0.746625
C	-3.929848	-0.874320	-0.386423
C	-2.842548	0.119676	-0.879343
C	-3.483798	1.504191	-0.679781
C	-4.882039	1.240185	-0.158100
H	-4.265380	-1.633063	-1.094980
H	-2.610372	-0.048042	-1.931769
H	-2.959341	2.128307	0.048683
H	-3.560777	2.077559	-1.608542
O	-5.102088	-0.096855	-0.050614
O	-5.737404	2.048482	0.125075
C	-0.559394	-1.122676	-0.545171
C	-0.828940	-1.991432	-1.529370
H	-1.804439	-2.054326	-2.001513
H	-0.082454	-2.681275	-1.907424
C	0.794533	-1.010584	0.140357
C	1.633034	-2.316570	0.260310
C	3.114787	-1.868053	0.434150
H	0.591858	-0.665178	1.164632
H	1.525855	-2.939636	-0.631109
H	1.280276	-2.919294	1.103591
H	3.563378	-2.280163	1.343165
H	3.725360	-2.217815	-0.405556
C	3.042382	-0.328869	0.479108
C	1.831666	0.031022	-0.438871
C	1.480179	1.515178	-0.215539
C	2.713425	2.423670	-0.401811
C	3.895119	2.009842	0.493293
C	4.333766	0.523977	0.351460
H	2.678097	-0.082873	1.490346
H	1.101027	1.644681	0.808828
H	0.679788	1.836545	-0.895157
H	3.021553	2.423568	-1.454624
H	2.436316	3.460307	-0.173188
H	4.756345	2.662987	0.298221
H	3.609951	2.181041	1.541697
C	2.047524	-0.238669	-1.943422
H	2.703042	0.500660	-2.404471
H	2.481114	-1.224323	-2.137075

H	1.088697	-0.194092	-2.468735
C	5.272283	0.180102	1.529769
H	6.127506	0.866152	1.552516
H	4.752430	0.261334	2.491825
H	5.667467	-0.838372	1.444617
C	5.137106	0.312459	-0.950347
H	6.096455	0.838484	-0.878223
H	5.358146	-0.747110	-1.118594
H	4.627522	0.690418	-1.838083

chromolactol**1b**-02 54.785%

C	-1.618436	-0.349641	0.078119
C	-2.487363	-1.392673	0.798683
H	-1.161199	0.289015	0.833923
H	-1.995221	-2.349401	0.993899
O	-2.958999	-0.808899	1.993267
H	-3.555423	-1.436804	2.437204
O	-3.561498	-1.683673	-0.104580
C	-3.868498	-0.543637	-0.864837
C	-2.688737	0.458576	-0.719603
C	-3.307401	1.664108	0.007862
C	-4.774646	1.329131	0.186502
H	-4.118139	-0.866866	-1.876184
H	-2.309248	0.743570	-1.702038
H	-2.875410	1.846745	0.995521
H	-3.230006	2.594807	-0.562381
O	-5.050871	0.112222	-0.352476
O	-5.635922	2.003447	0.704603
C	-0.536698	-0.933214	-0.828765
C	-0.723532	-2.086723	-1.490420
H	-1.625299	-2.682221	-1.386868
H	0.035382	-2.468512	-2.167828
C	0.764676	-0.161652	-1.016696
C	0.673041	1.397235	-1.028651
C	2.067110	1.919914	-0.566982
H	1.149513	-0.469466	-1.996548
H	-0.108661	1.765165	-0.358163
H	0.414907	1.756122	-2.030677
H	2.480829	2.651735	-1.267212
H	1.989728	2.420027	0.404891
C	2.930772	0.648542	-0.479427
C	1.938638	-0.460543	-0.011091
C	2.616842	-1.829112	-0.207812
C	3.992329	-1.879453	0.489259
C	4.928918	-0.745335	0.033202
C	4.340730	0.689011	0.170638
H	3.145110	0.371854	-1.525194
H	2.760151	-2.004691	-1.283985
H	1.975693	-2.640215	0.160119
H	3.862443	-1.844867	1.578103

H	4.470572	-2.844112	0.278303
H	5.877912	-0.801836	0.583325
H	5.176767	-0.909428	-1.025779
C	1.441097	-0.331439	1.445075
H	2.223568	-0.550692	2.171392
H	1.056746	0.666897	1.675867
H	0.636674	-1.052090	1.626186
C	5.231176	1.658186	-0.639145
H	6.272395	1.596531	-0.300638
H	5.212357	1.419211	-1.709143
H	4.905814	2.697714	-0.519612
C	4.376910	1.157922	1.641829
H	5.417186	1.315231	1.950502
H	3.850147	2.109240	1.774093
H	3.941464	0.437347	2.335975

chromolactol**1b**-03 1.412%

C	-2.002891	0.933980	0.648797
C	-2.011145	-0.415632	1.391714
H	-2.659112	1.611754	1.199285
H	-1.167154	-0.580583	2.065003
O	-3.237147	-0.509201	2.084291
H	-3.292072	-1.382725	2.510024
O	-1.902958	-1.422109	0.377581
C	-2.530541	-0.984487	-0.796507
C	-2.657075	0.561367	-0.718471
C	-4.169434	0.820396	-0.822239
C	-4.819896	-0.549032	-0.861863
H	-1.979371	-1.390994	-1.646040
H	-2.122610	1.031686	-1.546034
H	-4.582111	1.382862	0.019291
H	-4.445609	1.354604	-1.737176
O	-3.871777	-1.520912	-0.895959
O	-6.001128	-0.812286	-0.888883
C	-0.643566	1.618439	0.517368
C	-0.526872	2.859335	1.017445
H	-1.351639	3.336686	1.540224
H	0.379682	3.446173	0.918133
C	0.471656	0.916666	-0.253262
C	1.058324	1.756924	-1.433942
C	2.470528	1.173501	-1.729002
H	0.038462	0.010666	-0.691244
H	1.119457	2.812843	-1.157200
H	0.398013	1.703117	-2.306347
H	2.578700	0.868042	-2.774218
H	3.246015	1.923087	-1.536441
C	2.588929	-0.023653	-0.766276
C	1.768854	0.405358	0.493669
C	1.572999	-0.836836	1.385224
C	2.914746	-1.531513	1.698519

C	3.699124	-1.905476	0.428554
C	3.958449	-0.724372	-0.549555
H	1.971226	-0.819808	-1.213719
H	0.916686	-1.551116	0.869761
H	1.074909	-0.564779	2.325365
H	3.527955	-0.890407	2.343780
H	2.721837	-2.441180	2.280828
H	4.657568	-2.365759	0.704146
H	3.131364	-2.676440	-0.112742
C	2.401854	1.540680	1.323629
H	3.293505	1.208528	1.855090
H	2.689178	2.403129	0.714497
H	1.690760	1.887663	2.078769
C	4.431606	-1.307653	-1.900168
H	5.319132	-1.935608	-1.757098
H	3.654180	-1.927511	-2.362528
H	4.697762	-0.515480	-2.608910
C	5.091681	0.183738	-0.023595
H	6.044089	-0.357827	-0.066723
H	5.201460	1.085764	-0.635273
H	4.947842	0.499298	1.011002

chromolactol**1b**-04 0.500%

C	-1.837245	0.083654	-0.103584
C	-2.466765	0.808013	1.106485
H	-1.582584	0.833226	-0.856922
H	-1.773106	1.042032	1.918348
O	-3.113117	1.968500	0.632837
H	-3.570612	2.400581	1.375363
O	-3.398380	-0.128949	1.658085
C	-3.949886	-0.912934	0.633515
C	-3.026152	-0.779888	-0.608388
C	-3.921069	-0.118546	-1.670753
C	-5.272307	0.074737	-1.011789
H	-4.109494	-1.918623	1.025659
H	-2.681966	-1.759478	-0.942591
H	-3.557808	0.856725	-2.005589
H	-4.056043	-0.740926	-2.560821
O	-5.256528	-0.422174	0.252837
O	-6.269478	0.570283	-1.486602
C	-0.566034	-0.686374	0.267950
C	-0.637829	-1.909785	0.810350
H	-1.589706	-2.392123	1.012589
H	0.239253	-2.486926	1.071494
C	0.716767	0.040620	-0.111351
C	0.822235	1.513578	0.403928
C	2.314384	1.916150	0.207454
H	0.666313	0.105675	-1.211894
H	0.546078	1.561527	1.462792
H	0.144063	2.184321	-0.131064

H	2.418560	2.772355	-0.465893
H	2.764632	2.210263	1.161551
C	2.979379	0.650910	-0.376371
C	2.137307	-0.532208	0.206592
C	2.522659	-1.814038	-0.561473
C	4.048670	-2.041430	-0.568549
C	4.834085	-0.833032	-1.106699
C	4.525111	0.512050	-0.389975
H	2.719781	0.650820	-1.447434
H	2.170978	-1.720826	-1.599534
H	2.026334	-2.697582	-0.144170
H	4.392511	-2.288732	0.443762
H	4.278352	-2.921511	-1.182179
H	5.912370	-1.035088	-1.052254
H	4.596306	-0.712134	-2.173793
C	2.322638	-0.717358	1.736605
H	3.185974	-1.344760	1.966306
H	2.470170	0.233597	2.255214
H	1.450509	-1.194374	2.187123
C	5.118315	1.661889	-1.234244
H	6.194434	1.512877	-1.383892
H	4.647337	1.716114	-2.223021
H	4.983928	2.632050	-0.742756
C	5.206141	0.560184	0.995099
H	6.294541	0.593152	0.866327
H	4.917472	1.456633	1.554628
H	4.979020	-0.307313	1.616590

Table S4. Computed DP4 probabilities for cheloviolenes A and B

	Cheloviolene A	Cheloviolene B
DP4 (H data)	83.1%	16.9%
DP4 (C data)	44.3%	55.7%
DP4 (all data)	79.6%	20.4%