

Supplementary Material of

Atypical Lindenane-type Sesquiterpenes from *Lindera myrrha*

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Summary of the Supporting Material content
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S1 HRESIMS of **1**

S2 ¹H-NMR spectrum of **1** (500 MHz, Acetone-*d*₆)

S3 ¹³C-NMR spectrum of **1** (125 MHz, Acetone-*d*₆)

S4 COSY spectrum of **1** (500 MHz, Acetone-*d*₆)

S5 HSQC spectrum of **1** (500/125 MHz, Acetone-*d*₆)

S6 HMBC spectrum of **1** (500/125 MHz, Acetone-*d*₆)

S7 NOESY spectrum of **1** (500 MHz, Acetone-*d*₆)

S8 HRESIMS of **2**

S9 ¹H-NMR spectrum of **2** (500 MHz, Acetone-*d*₆)

S10 ¹³C-NMR spectrum of **2** (125 MHz, Acetone-*d*₆)

S11 COSY spectrum of **2** (500/125 MHz, Acetone-*d*₆)

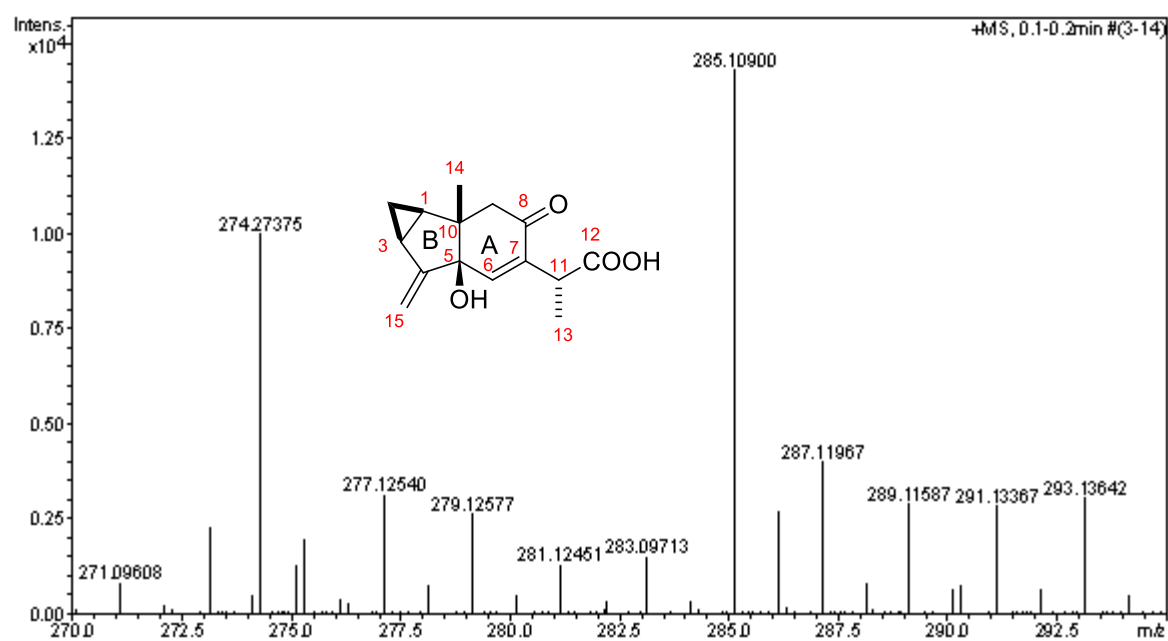
S12 HSQC spectrum of **2** (500/125 MHz, Acetone-*d*₆)

S13 HMBC spectrum of **2** (500/125 MHz, Acetone-*d*₆)

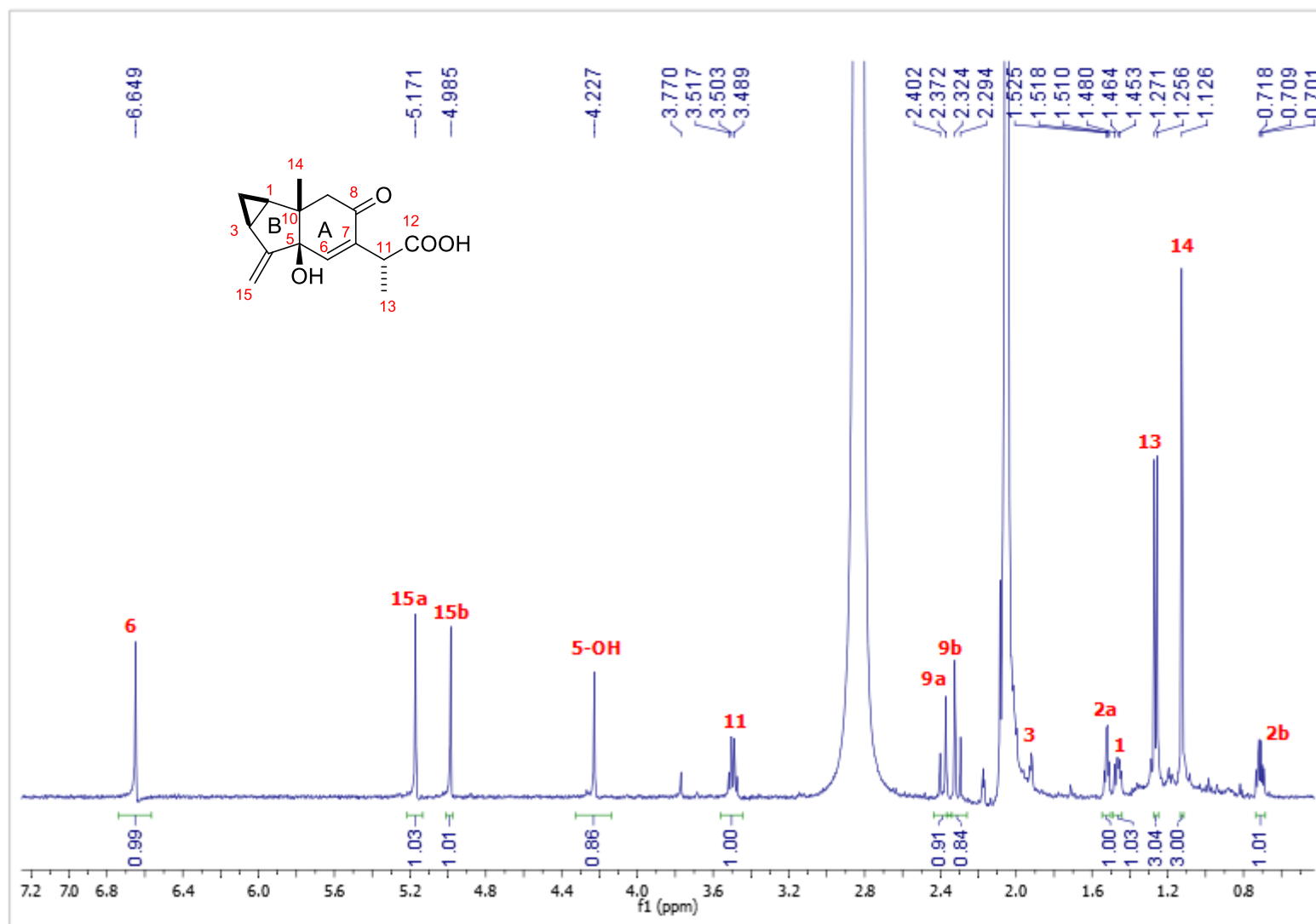
S14 Atomic coordinates (Ångstroms) of the lowest-energy conformers of candidate structures of myrrhalindenane A (**1A-1D**).

S15 Atomic coordinates (Ångstroms) of the lowest-energy conformers of candidate structures of myrrhalindenane B (**2A-2D**).

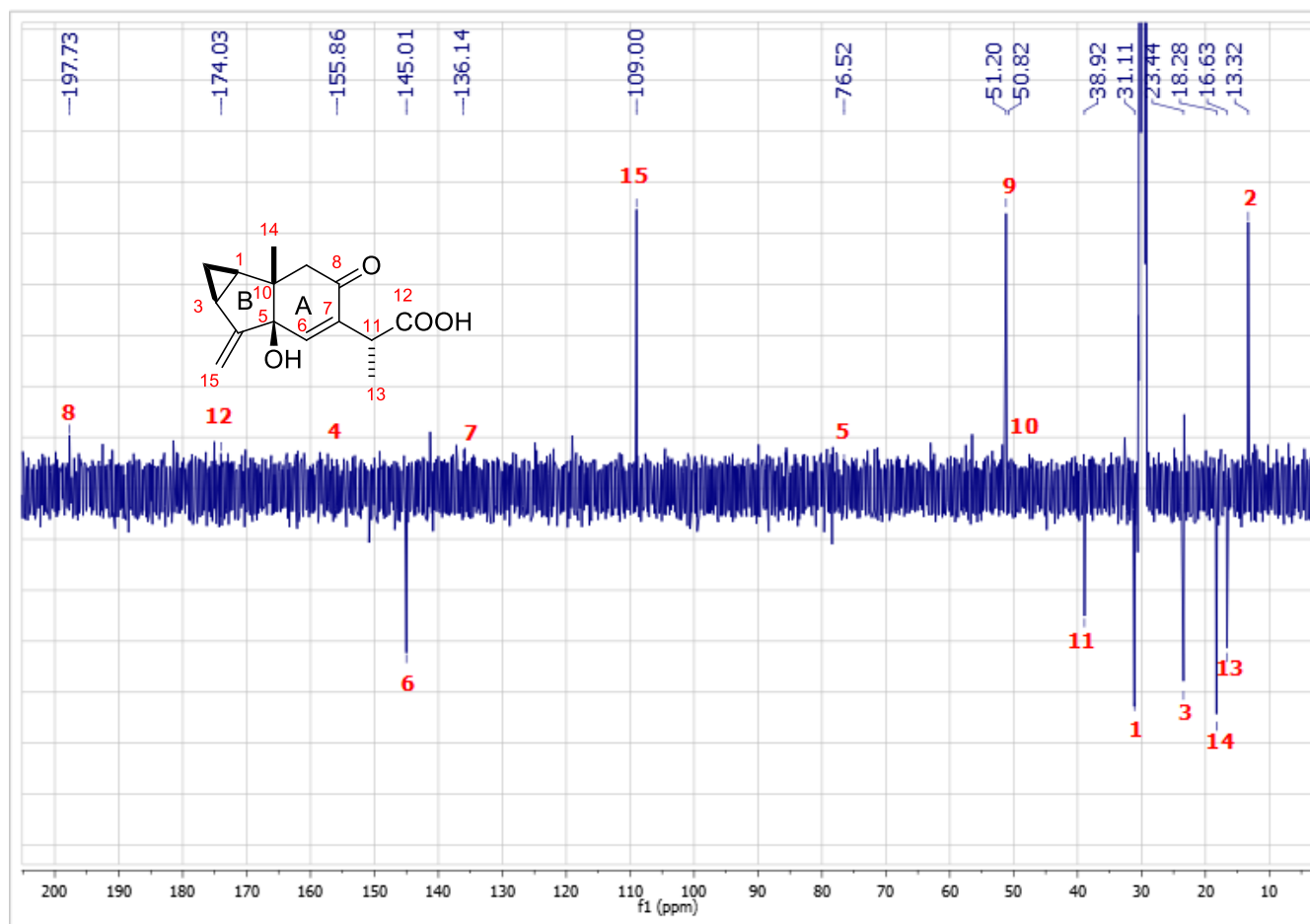
S1. HRESIMS of **1**



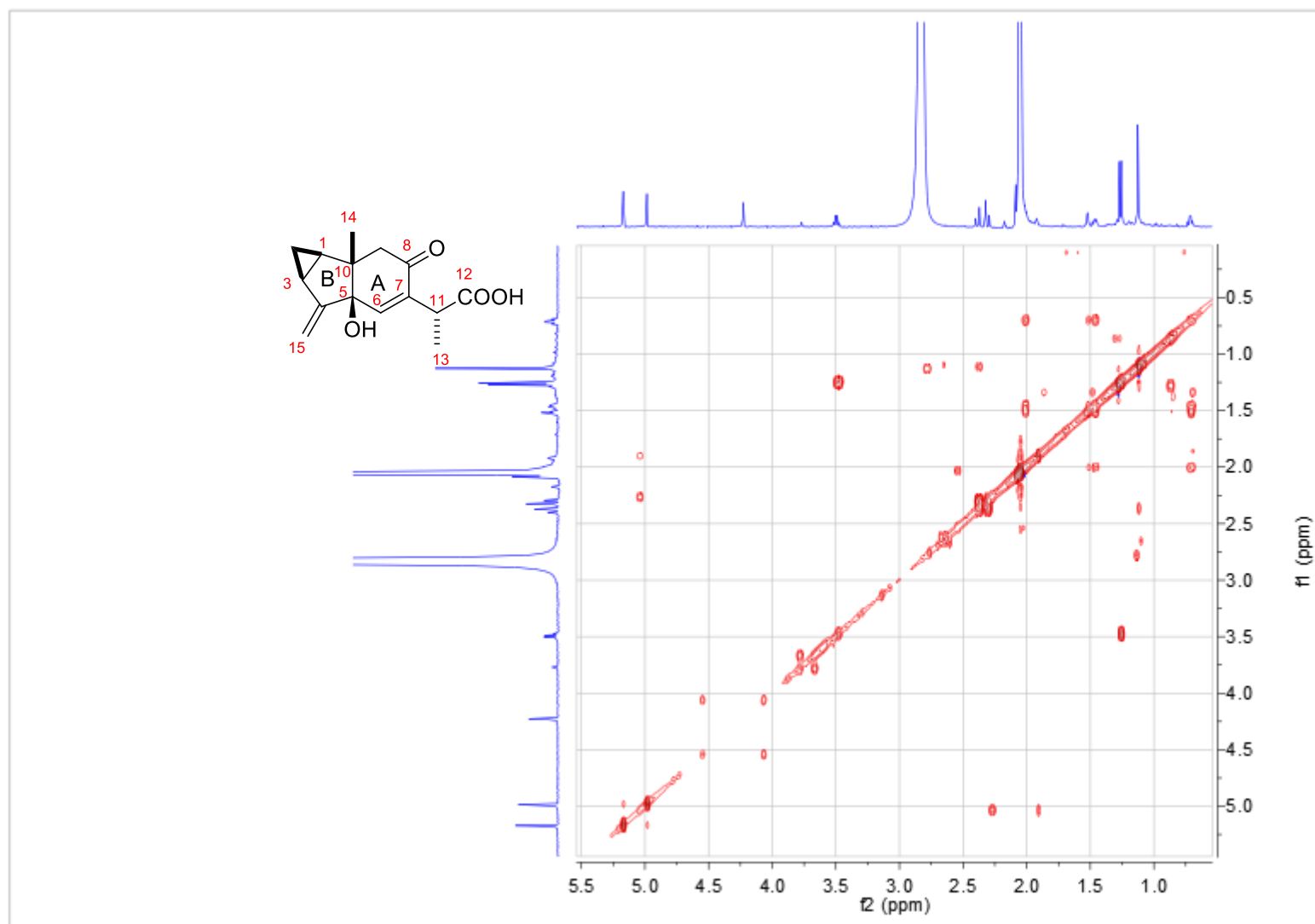
S2. ^1H -NMR spectrum of **1** (500 MHz, Acetone- d_6)



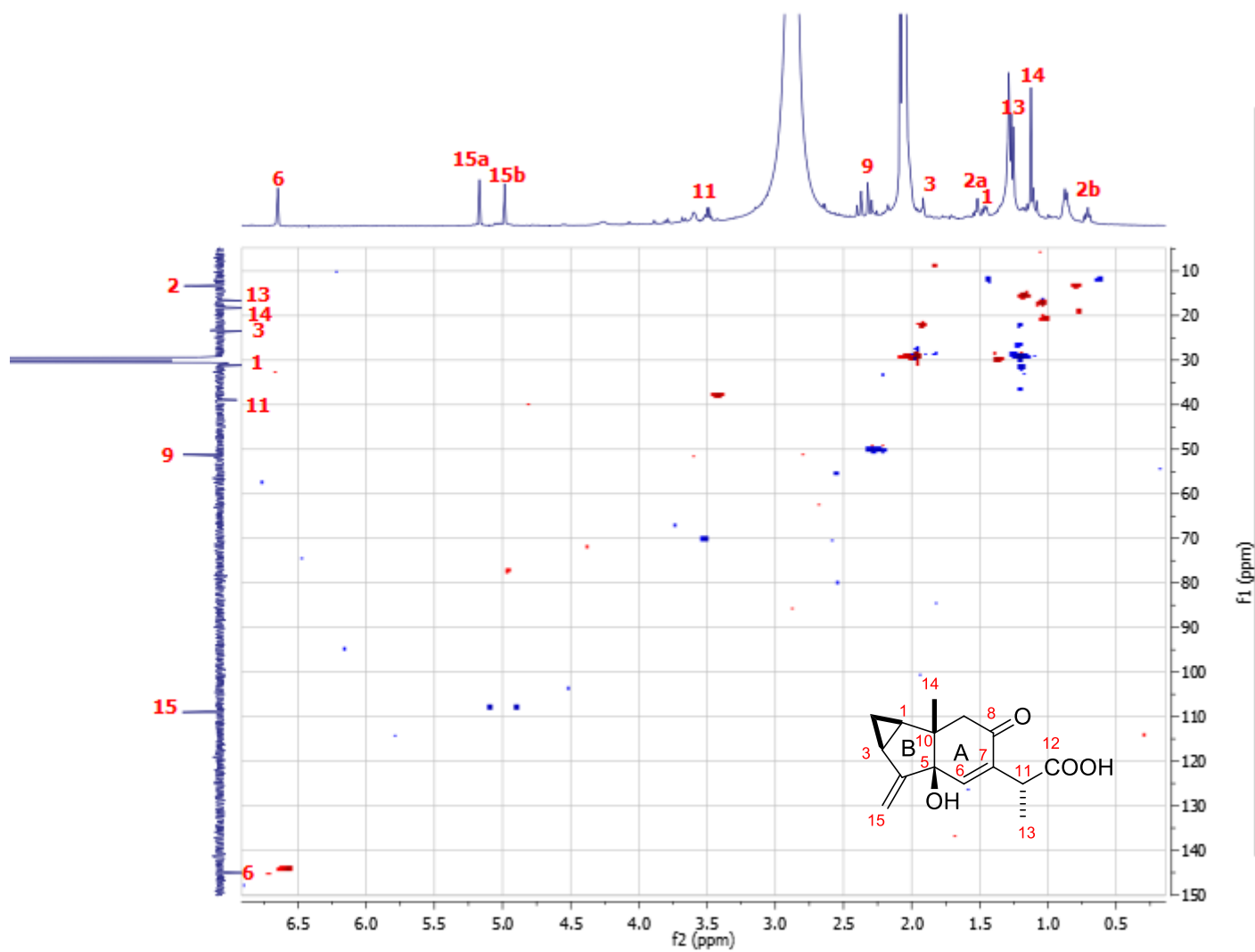
S3. ^{13}C -NMR spectrum of **1** (125 MHz, Acetone- d_6)



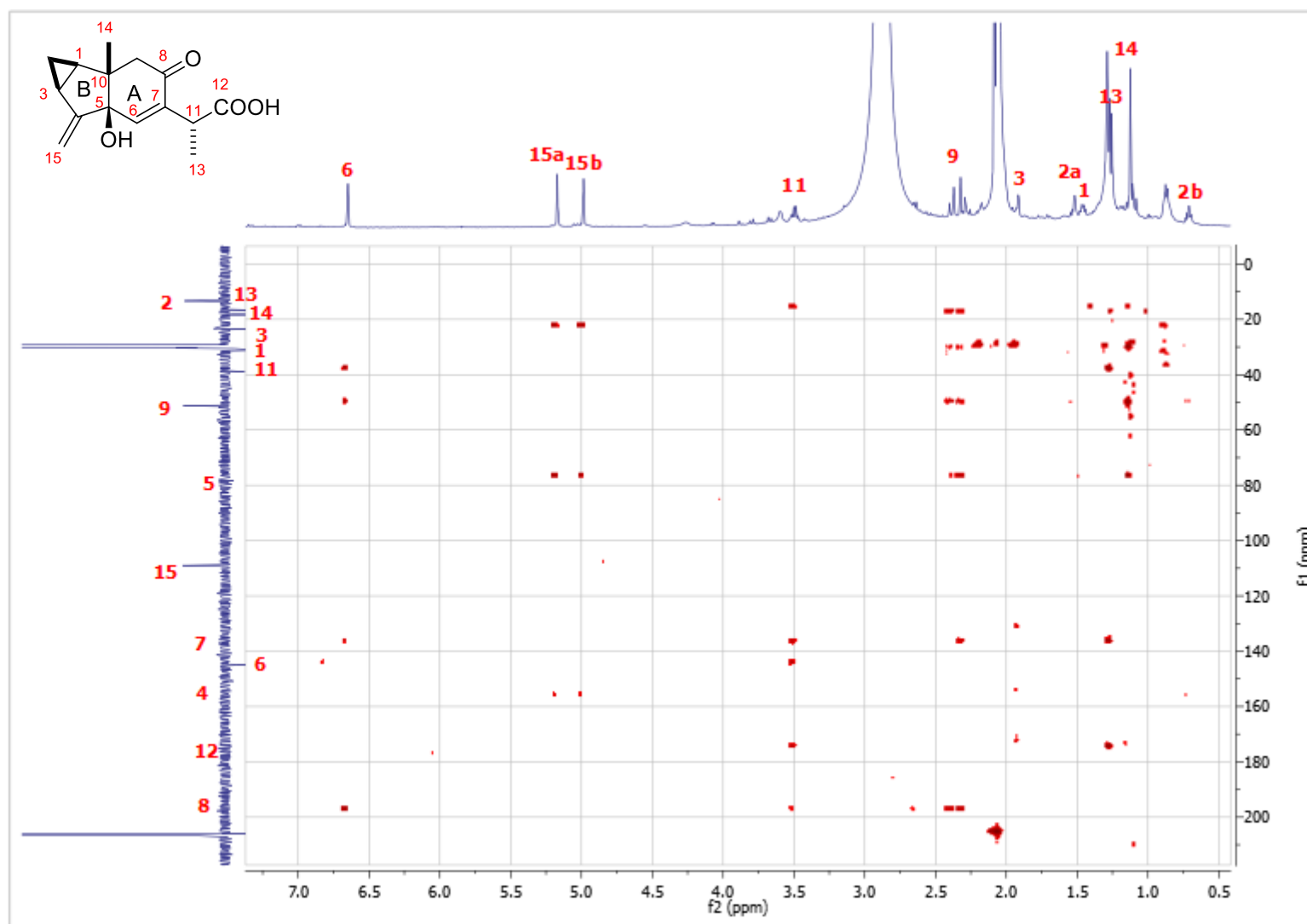
S4. COSY spectrum of **1** (500/125 MHz, Acetone-d₆)



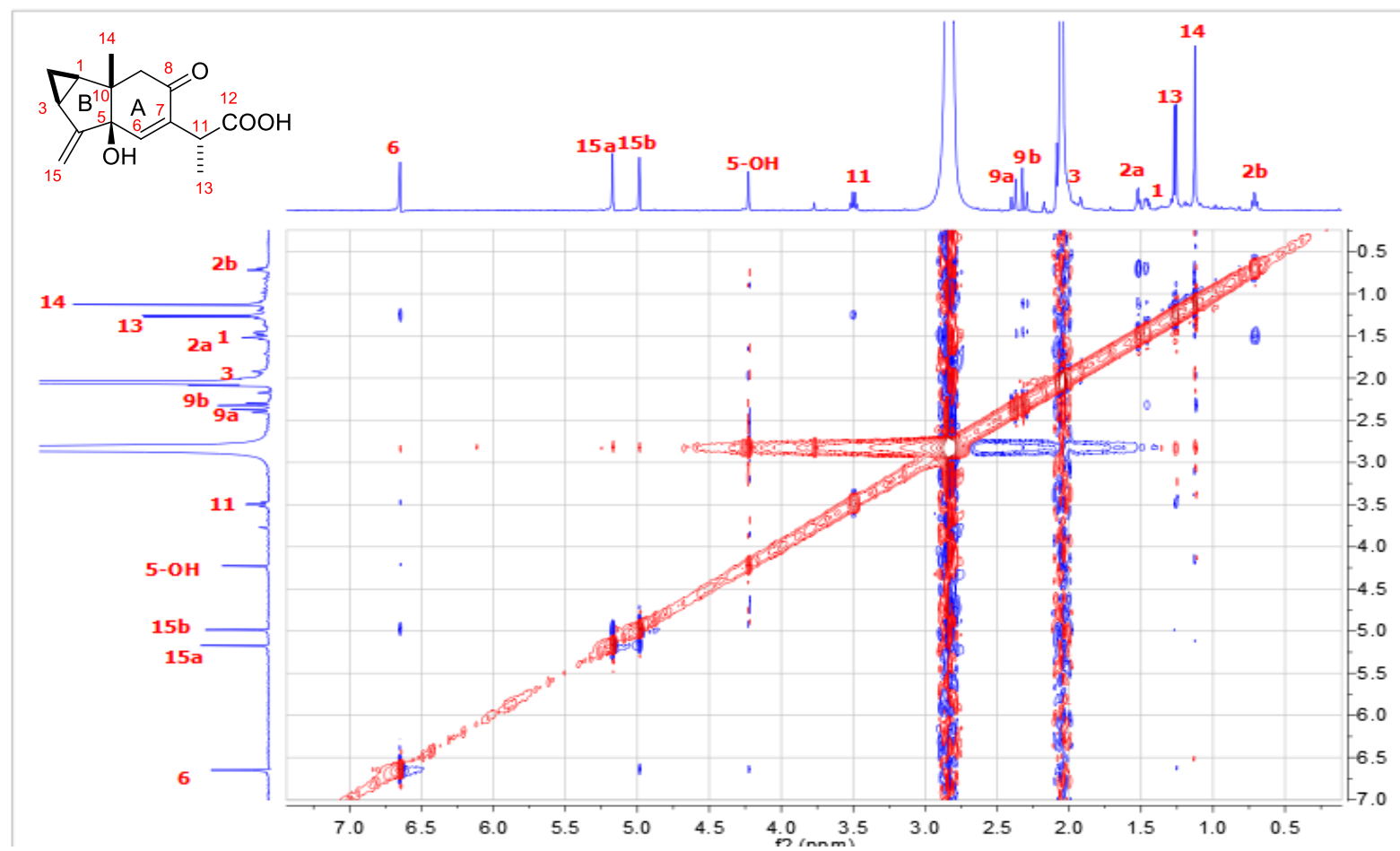
S5. HSQC spectrum of **1** (500/125 MHz, Acetone-d₆)



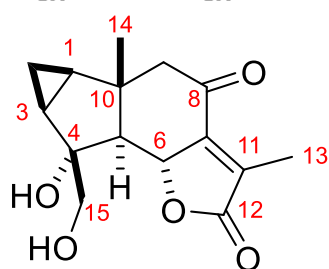
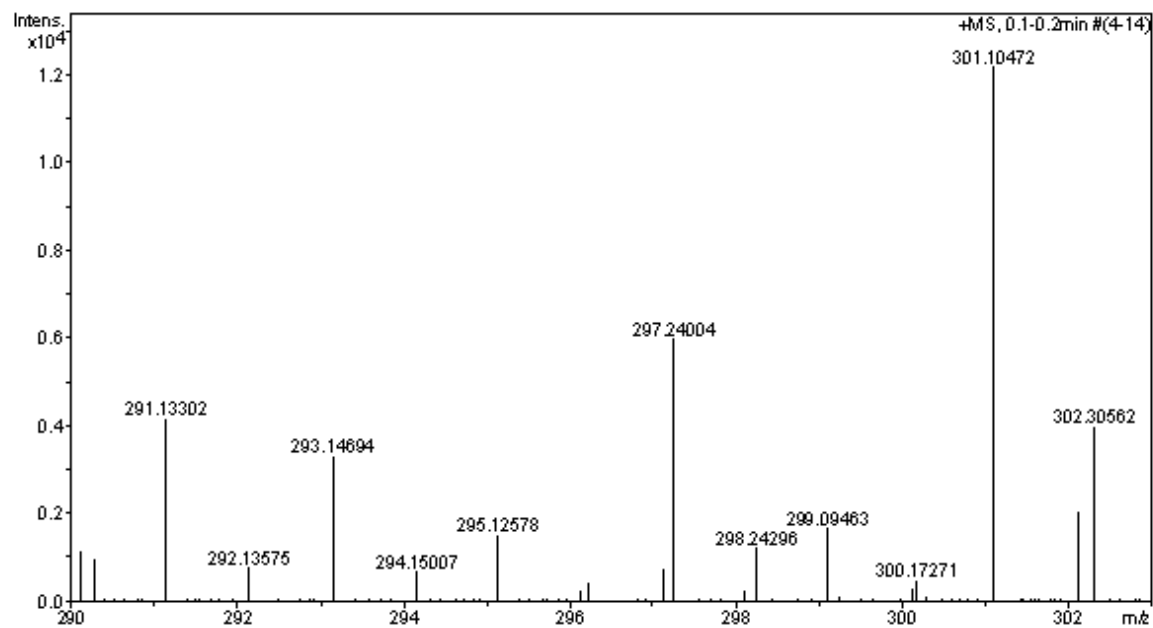
S6. HMBC spectrum of **1** (500/125 MHz, Acetone-d₆)



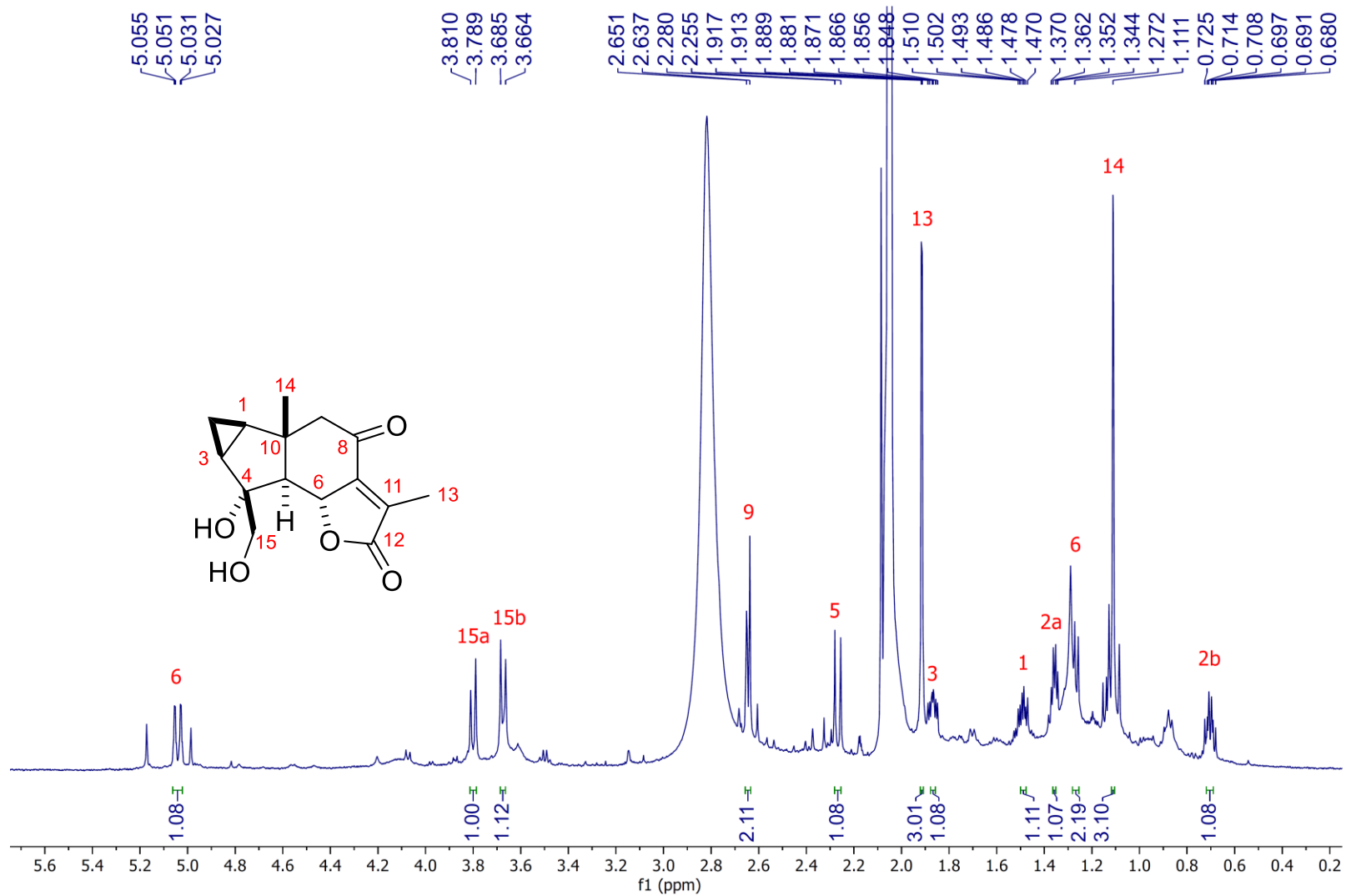
S7. NOESY spectrum of **1** (125 MHz, Acetone-d₆)



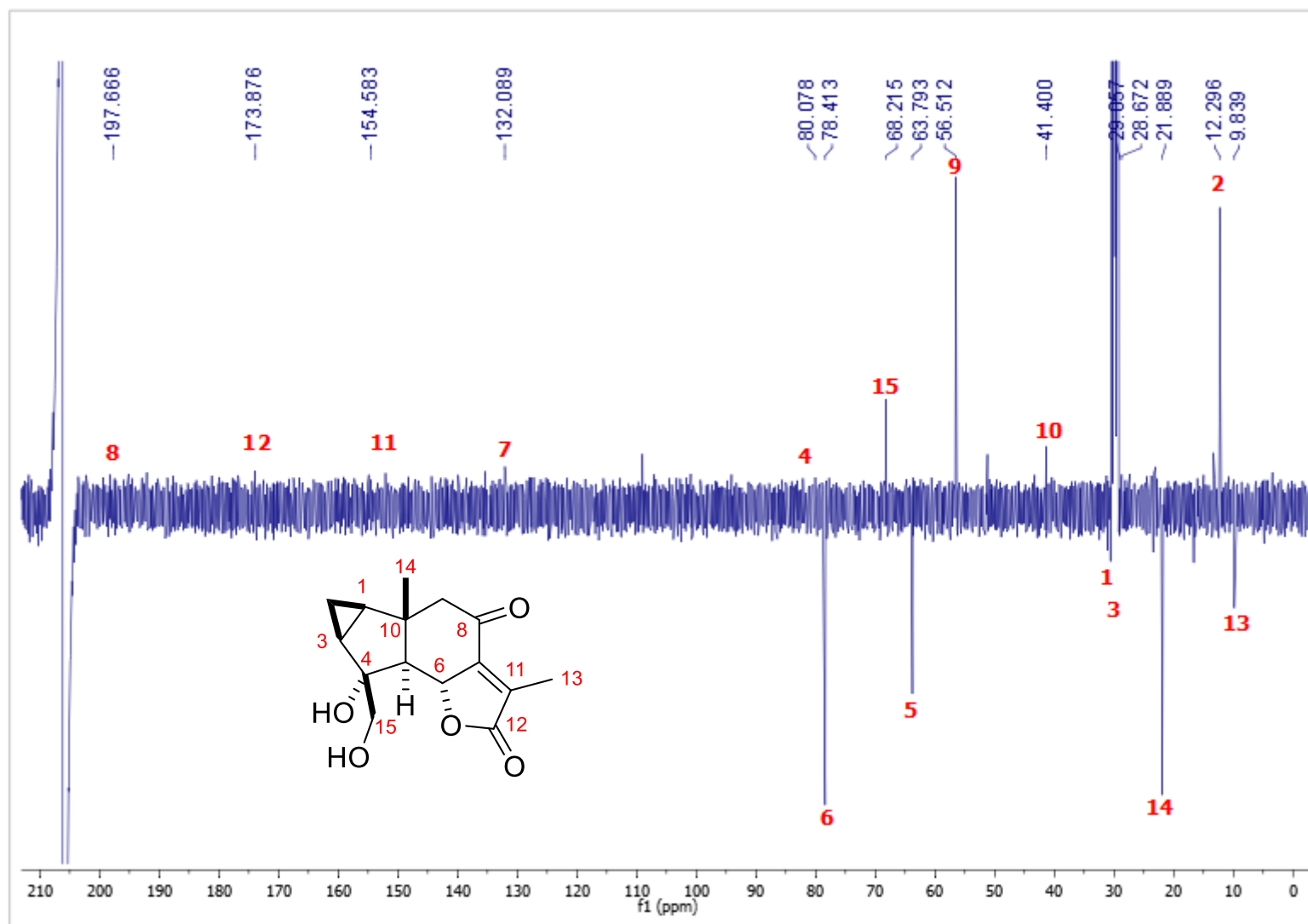
S8. HRESIMS of 2



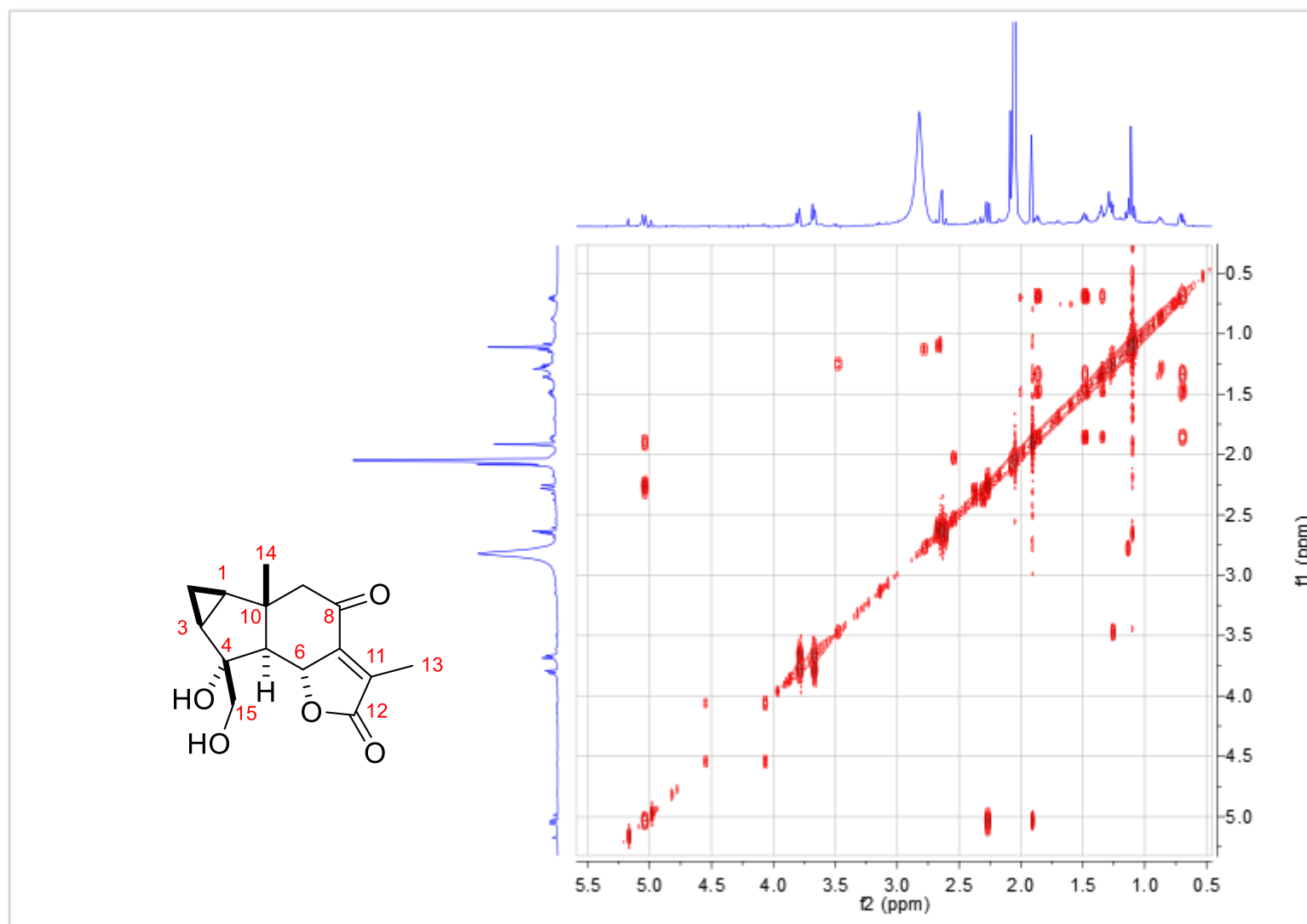
S9. ^1H -NMR spectrum of **2** (500 MHz, Acetone- d_6)



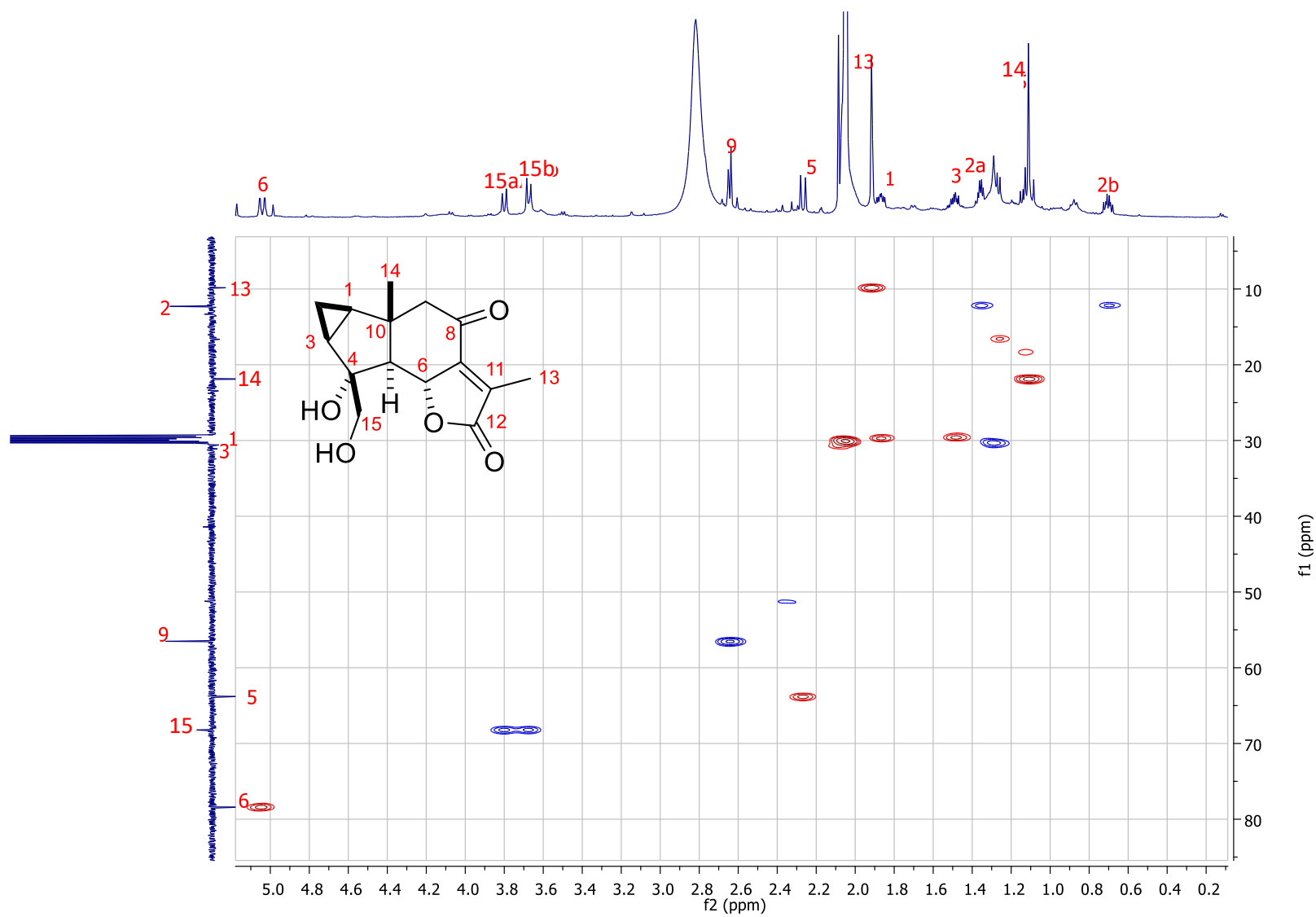
S10. ^{13}C -NMR spectrum of **2** (125 MHz, Acetone- d_6)



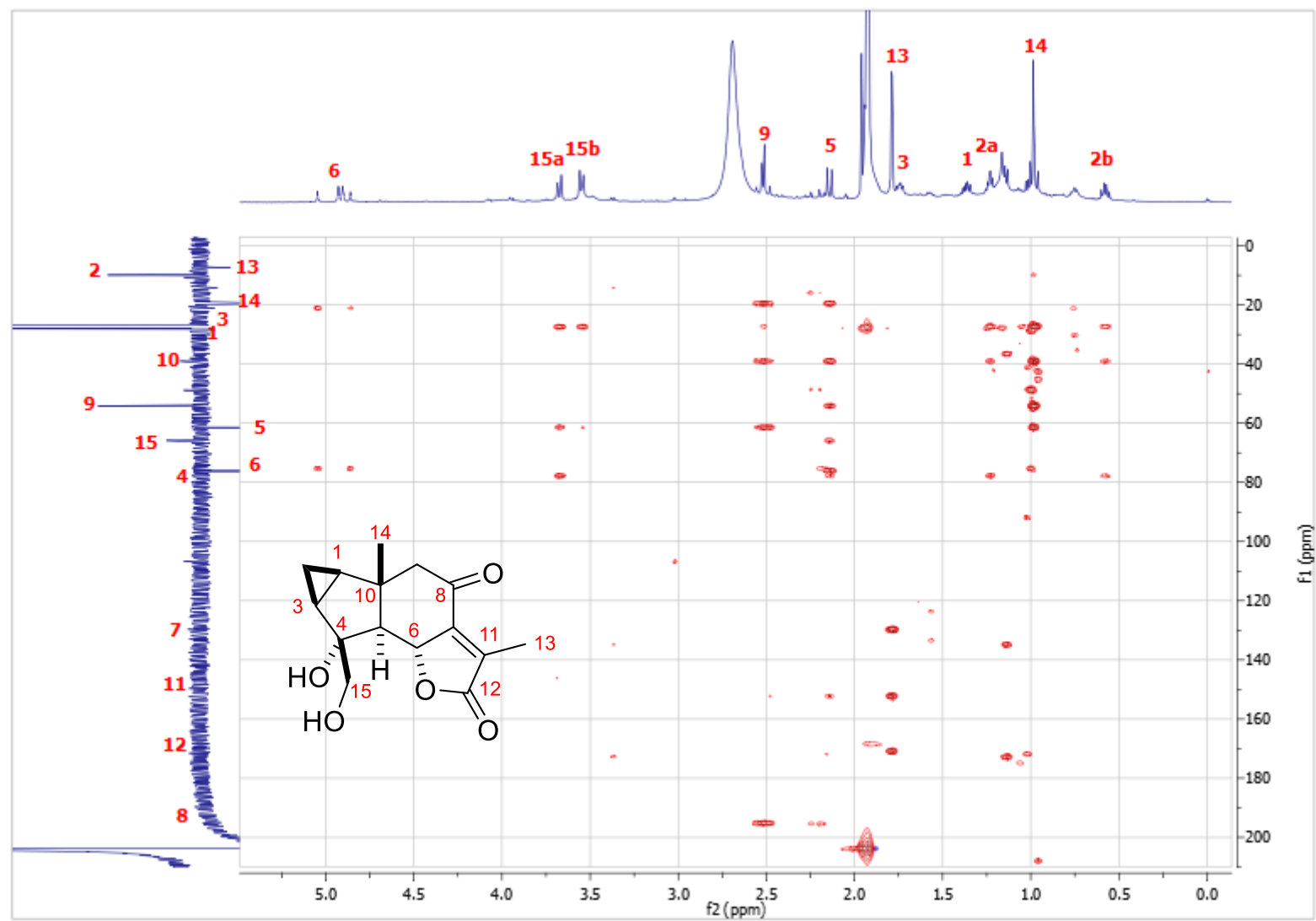
S11. COSY spectrum of **2** (500/125 MHz, Acetone-d₆)



S12. HSQC spectrum of **2** (500/125 MHz, Acetone-d₆)



S13. HMBC spectrum of **2** (500/125 MHz, Acetone-d₆)



S14. Atomic coordinates (Ångstroms) of the lowest-energy conformers of candidate structures of myrrhalindenane A (**1A-1D**).

1A

C	1.18951200	0.48189900	-0.07867600
C	0.41226700	-0.45490100	0.47647700
C	-1.74854100	-1.53047800	-0.38434400
H	0.87891800	-1.26471100	1.02749600
C	2.70663200	0.52007100	0.05869700
H	3.08186500	1.11545600	-0.77070500
C	0.56108000	1.59187600	-0.84181300
O	1.20857600	2.53617900	-1.25400300
C	-1.75199000	0.87704600	0.04000100
C	-1.09406700	-0.46457800	0.50578400
C	-1.86529600	1.92215900	1.15450100
H	-0.88733700	2.19348800	1.55350800
H	-2.32729800	2.82827700	0.76002700
H	-2.47152400	1.55600700	1.97812100
O	-1.47626100	-0.69725900	1.88351500
H	-1.34334100	-1.63286100	2.06913100
C	-3.10985100	0.45956100	-0.53279400
H	-3.56933500	1.13751000	-1.23970300
C	-3.07594000	-1.03238100	-0.81499300
H	-3.52434800	-1.46092500	-1.69928600
C	-3.99850500	-0.45296400	0.25036400
H	-5.04862300	-0.44065900	-0.00511600
H	-3.77973200	-0.64858300	1.28760700
C	-0.91573200	1.44245500	-1.13145100
H	-0.99204300	0.76752800	-1.99030200
H	-1.30170700	2.41082200	-1.44625100
C	3.27604500	-0.87790300	-0.07124900
O	3.67213000	-1.15182100	-1.33706700
H	3.99618200	-2.06444600	-1.33944600
O	3.36591200	-1.68897500	0.81791300
C	3.13819600	1.17141500	1.38252200
H	4.22342000	1.25964800	1.43344700
H	2.71161800	2.17017800	1.45534100
H	2.80156100	0.57910700	2.23097900
C	-1.17936700	-2.67914500	-0.74342000
H	-1.70574000	-3.39759900	-1.35726700
H	-0.17204800	-2.93802200	-0.44808000

1B

C	1.21640700	0.42543600	-0.04321500
C	0.41380200	-0.64362100	0.04085500
C	-2.08593300	-1.52238600	0.04541900
H	0.80592100	-1.61148900	0.32583400
C	2.70379200	0.40748600	0.27979800
C	0.66530200	1.76637100	-0.45346400
O	1.41047800	2.70984400	-0.63125000
C	-1.63317400	0.83968900	0.08405700
C	-1.49230100	1.06706300	1.60627300
H	-0.47880800	1.35085000	1.87850600
H	-2.15762400	1.87318300	1.91586400
H	-1.74086900	0.18161200	2.18889500
C	-3.11362300	0.65269700	-0.32903400
H	-3.51247000	1.28065300	-1.11334700
C	-3.38869800	-0.85224800	-0.31824300
H	-4.01184800	-1.32201300	-1.06802200
C	-4.07460900	0.06355100	0.66712900
H	-5.12689900	0.23866700	0.49004500
H	-3.80781300	0.00971500	1.71049900
C	-0.84657200	1.93693600	-0.63693300
H	-1.03119200	1.91473400	-1.71125100
H	-1.10263300	2.93462500	-0.28028800
C	-1.02011000	-0.52420200	-0.37337800
O	-0.94640000	-0.57257100	-1.82737700
H	-1.83136500	-0.73362000	-2.17166900
C	3.30743600	-0.93556000	-0.07701000
O	3.84479700	-0.93889300	-1.31862000
H	4.17336900	-1.83507000	-1.48187800
O	3.31554800	-1.91404800	0.62963500
C	2.96779700	0.75319600	1.75471600
H	2.54469600	-0.00624400	2.40931900
H	4.03814400	0.81570400	1.95002700
H	2.52452700	1.71849100	1.99303100
H	3.16764500	1.16287900	-0.35119600
C	-1.91348300	-2.72756400	0.57117300
H	-0.92881600	-3.12677700	0.77293400
H	-2.75554700	-3.36163100	0.81473700

1C

C	-1.18918000	0.40777200	0.24715800
C	-0.41296400	-0.63173500	-0.07964600
C	1.90758800	-1.29964800	0.77255900
H	-0.87388800	-1.59588600	-0.26575700
C	-2.70235600	0.34241600	0.39830100
C	-0.55927700	1.72400300	0.53648600
O	-1.22224000	2.72652300	0.72669400
C	1.68075900	0.84333300	-0.38194300
C	1.07554600	-0.59857600	-0.31054200
C	1.58521300	1.47936600	-1.77244200
H	0.55049900	1.57152000	-2.10421700
H	2.01759200	2.48061300	-1.74598100
H	2.12161700	0.89172000	-2.51203200
O	1.31031500	-1.24857600	-1.58380500
H	1.23822100	-2.19853500	-1.44319300
C	3.12361700	0.67849800	0.10580500
H	3.60942500	1.56300300	0.49583400
C	3.23464300	-0.64418400	0.84360400
H	3.81318300	-0.75142200	1.74942100
C	3.98165000	-0.40568400	-0.46310400
H	5.05038300	-0.27606900	-0.36740200
H	3.65916300	-0.92942800	-1.34826800
C	0.94769500	1.72443100	0.65532500
H	1.17452200	1.36085900	1.66303600
H	1.29452400	2.75504900	0.59768000
C	-3.10997300	0.04325400	1.85019600
H	-2.66879900	0.78273800	2.51602500
H	-4.19295400	0.08752200	1.96380300
H	-2.77490200	-0.94848200	2.14739700
C	1.47307400	-2.29104700	1.54758500
H	2.12079800	-2.75462600	2.27951200
H	0.46082600	-2.66626900	1.48833500
C	-3.29057700	-0.67829400	-0.55329000
O	-3.38633000	-1.86305300	-0.34334600
O	-3.69730800	-0.11777200	-1.71604000
H	-4.02684800	-0.83601800	-2.27586400
H	-3.08160700	1.32331400	0.11733000

1D

C	-1.23612800	0.43470100	0.20790500
C	-0.40352800	-0.59008300	0.43167300
C	2.11631500	-1.41063400	0.44067500
H	-0.78572300	-1.59117400	0.58915800
C	-2.75267600	0.29721900	0.17834700
C	-0.70344900	1.83185100	0.03343100
O	-1.46571200	2.77567900	-0.03873300
C	1.55173300	0.76600600	-0.41820100
C	1.21759500	0.41110500	-1.88489500
H	0.16647100	0.57358200	-2.10965000
H	1.80280600	1.04319600	-2.55295000
H	1.43650500	-0.62775900	-2.12621200
C	3.07842700	0.74361900	-0.16049600
H	3.54025600	1.61984700	0.27246300
C	3.41997700	-0.65535900	0.35713900
H	4.14998600	-0.80986000	1.14093800
C	3.93798500	-0.18009500	-0.97923700
H	4.99462000	0.04640800	-1.01894900
H	3.54943600	-0.62366700	-1.88206600
C	0.80970500	2.05537200	-0.05713400
H	1.12576300	2.43511600	0.91458600
H	0.97329300	2.84771600	-0.78778100
C	1.06218100	-0.32700200	0.58792600
O	1.16207900	0.17369300	1.95252700
H	2.08754300	0.15101000	2.21833500
C	-3.35042600	0.34245600	1.59256400
H	-3.01308900	-0.50856500	2.18036600
H	-3.04355800	1.26015100	2.09047800
H	-4.43929200	0.32161200	1.55097700
C	1.93943600	-2.72490100	0.43611400
H	0.95795800	-3.16922800	0.53069100
H	2.77528500	-3.40561100	0.34414900
C	-3.13840400	-0.97750600	-0.54386500
O	-3.30516600	-2.05826800	-0.03525900
O	-3.26103300	-0.78541100	-1.88090000
H	-3.47690200	-1.64581000	-2.26900300
H	-3.13515800	1.13699700	-0.39830100

S15 Atomic coordinates (Ångstroms) of the lowest-energy conformers of candidate structures of myrrhalindenane B (**2A-2D**).

2A

C	1.743484	1.858031	0.016413
O	2.678695	2.618113	0.154998
C	-0.790076	1.504597	0.033040
C	-0.925346	1.862364	1.531369
H	0.036918	1.861755	2.044674
H	-1.336012	2.867731	1.623589
H	-1.581507	1.188604	2.077511
C	-2.110810	1.712263	-0.737354
H	-2.124512	2.461455	-1.517090
C	-2.765581	0.359405	-0.944663
H	-3.254578	0.114160	-1.875189
C	-3.410125	1.376975	-0.050042
H	-4.302564	1.853492	-0.430843
H	-3.428837	1.223952	1.017962
C	0.387171	2.330904	-0.518622
H	0.434674	2.235665	-1.608332
H	0.293942	3.392678	-0.291514
C	-0.489854	0.001446	-0.266758
C	2.435773	-1.816818	0.098136
O	1.104852	-1.808257	0.420822
O	3.060866	-2.825623	-0.070919
H	-0.127948	-0.030588	-1.297820
C	-1.837329	-0.748866	-0.392111
O	-1.648566	-1.750568	-1.391788
H	-2.402878	-2.349633	-1.333936
C	-2.322856	-1.442488	0.879196
H	-1.551894	-2.141552	1.208894
C	0.662939	-0.456561	0.612585
H	0.407135	-0.372376	1.670565
C	1.864106	0.392267	0.267924
C	2.904891	-0.402683	-0.018664
H	-2.520383	-0.726213	1.679091
O	-3.523405	-2.146126	0.539225
H	-3.687630	-2.826999	1.195636
C	4.288726	-0.091394	-0.460793
H	4.553218	-0.697076	-1.327821
H	4.408142	0.965131	-0.681584
H	4.994500	-0.357133	0.329572

2B

C	-1.433613	-2.051944	-0.043449
O	-2.280208	-2.908724	0.091897
C	1.046783	-1.448942	-0.020424
C	1.234649	-1.871662	1.453769
H	0.280008	-1.969312	1.973411
H	1.715967	-2.849330	1.487958
H	1.842082	-1.166156	2.011956
C	2.370829	-1.467967	-0.814567
H	2.429987	-2.122796	-1.673464
C	2.894144	-0.044132	-0.896335
H	3.325405	0.340248	-1.810782
C	3.655406	-1.085245	-0.128120
H	4.571850	-1.443216	-0.575838
H	3.689226	-1.001000	0.945930
C	-0.048096	-2.349909	-0.620922
H	-0.122584	-2.187244	-1.701804
H	0.155433	-3.409242	-0.467014
C	0.618054	0.041952	-0.215725
C	-2.499761	1.526453	0.083552
O	-1.173799	1.647833	0.439667
O	-3.202358	2.476087	-0.112154
H	0.301362	0.121942	-1.261336
C	1.926026	0.878907	-0.133918
C	-0.598761	0.336544	0.637551
H	-0.351387	0.269554	1.697656
C	-1.704403	-0.611204	0.247814
C	-2.818553	0.076671	-0.043174
O	2.345238	1.078530	1.215036
H	2.062830	1.973342	1.454128
C	1.836118	2.257588	-0.810707
H	1.328692	2.179767	-1.776029
O	1.217451	3.223051	0.030122
H	0.273405	3.025222	0.097861
H	2.846285	2.626287	-0.984554
C	-4.156926	-0.371885	-0.510089
H	-4.470033	0.207370	-1.378901
H	-4.162075	-1.433684	-0.737717
H	-4.898403	-0.187304	0.270451

2C

C	1.465259	1.960007	0.224773
O	2.338479	2.766988	0.464360
C	-1.029693	1.427695	0.232059
C	-1.180401	1.633670	1.756650
H	-0.241906	1.504282	2.295276
H	-1.514814	2.654811	1.944860
H	-1.914133	0.964590	2.198318
C	0.075603	2.380501	-0.259267
H	0.112348	2.378983	-1.353308
H	-0.091725	3.409557	0.056823
C	-0.661157	-0.026203	-0.199354
C	2.404466	-1.626270	-0.213682
O	1.094795	-1.759791	0.158014
O	3.083833	-2.552185	-0.559148
H	-0.347469	0.020441	-1.244135
C	-1.983023	-0.834112	-0.258120
O	-1.783814	-1.829431	-1.281241
H	-2.637518	-2.209674	-1.512539
C	-2.425383	-1.568984	1.013670
C	0.570158	-0.485296	0.566694
H	0.361682	-0.574039	1.632253
C	1.692651	0.487940	0.286467
C	2.773272	-0.180819	-0.140051
H	-2.622631	-0.872561	1.826021
C	4.113514	0.291261	-0.574757
H	4.385396	-0.165683	-1.526392
H	4.150888	1.374379	-0.645954
H	4.866634	-0.028659	0.148978
C	-2.675483	1.133543	-1.797958
H	-1.859069	0.858778	-2.450051
H	-3.508506	1.592110	-2.310660
C	-2.410607	1.609140	-0.397370
H	-3.026827	2.411554	-0.014605
C	-3.009901	0.235157	-0.633910
H	-4.051068	0.034467	-0.416984
O	-1.472620	-2.494745	1.494508
H	-1.085118	-2.953075	0.738965
H	-3.377195	-2.070332	0.786127

2D

C	-1.504867	-1.988449	0.035993
O	-2.403833	-2.790406	0.169639
C	0.997186	-1.519537	0.155316
C	1.110198	-1.881379	1.654748
H	0.151087	-1.833843	2.172566
H	1.462797	-2.909883	1.744652
H	1.808086	-1.228356	2.170468
C	-0.114767	-2.383413	-0.466198
H	-0.128836	-2.257318	-1.554150
H	0.021976	-3.445662	-0.266301
C	0.673589	-0.013638	-0.112909
C	-2.363916	1.647639	-0.023056
O	-1.049986	1.707842	0.388550
O	-3.000718	2.626867	-0.286401
H	0.403817	0.075696	-1.168294
C	2.019061	0.746206	0.064604
C	-0.564207	0.375216	0.666202
H	-0.372193	0.338767	1.738663
C	-1.703850	-0.523649	0.258381
C	-2.761558	0.214256	-0.109484
C	-4.102359	-0.176762	-0.619089
H	-4.343153	0.381701	-1.523836
H	-4.159762	-1.245283	-0.804100
H	-4.865030	0.082505	0.118607
C	2.715854	-0.988970	-1.760832
H	1.926207	-0.634636	-2.407783
H	3.565366	-1.384076	-2.298663
C	2.393283	-1.651055	-0.449431
H	2.978772	-2.513608	-0.162721
C	3.023309	-0.272692	-0.465269
H	4.054696	-0.115782	-0.185532
O	2.318178	0.980587	1.441132
H	2.081362	1.903931	1.612648
C	2.090197	2.094566	-0.673155
H	3.135100	2.386895	-0.768529
H	1.667207	2.011141	-1.677114
O	1.468640	3.139217	0.069431
H	0.511338	3.004915	0.065682