Tsavoenones A–C: Unprecedented Polyketides with a 1,7-dioxadispiro[4.0.4.4]tetradecane core from the Lichen *Parmotrema tsavoense*

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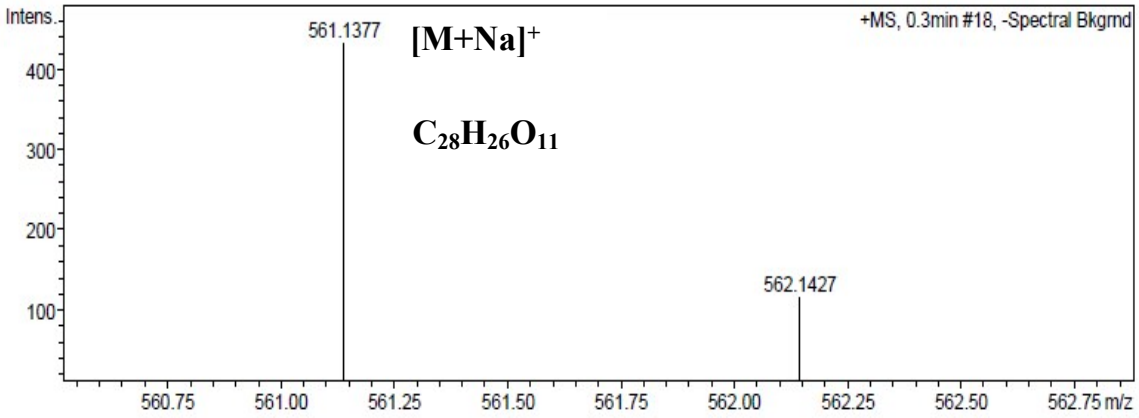
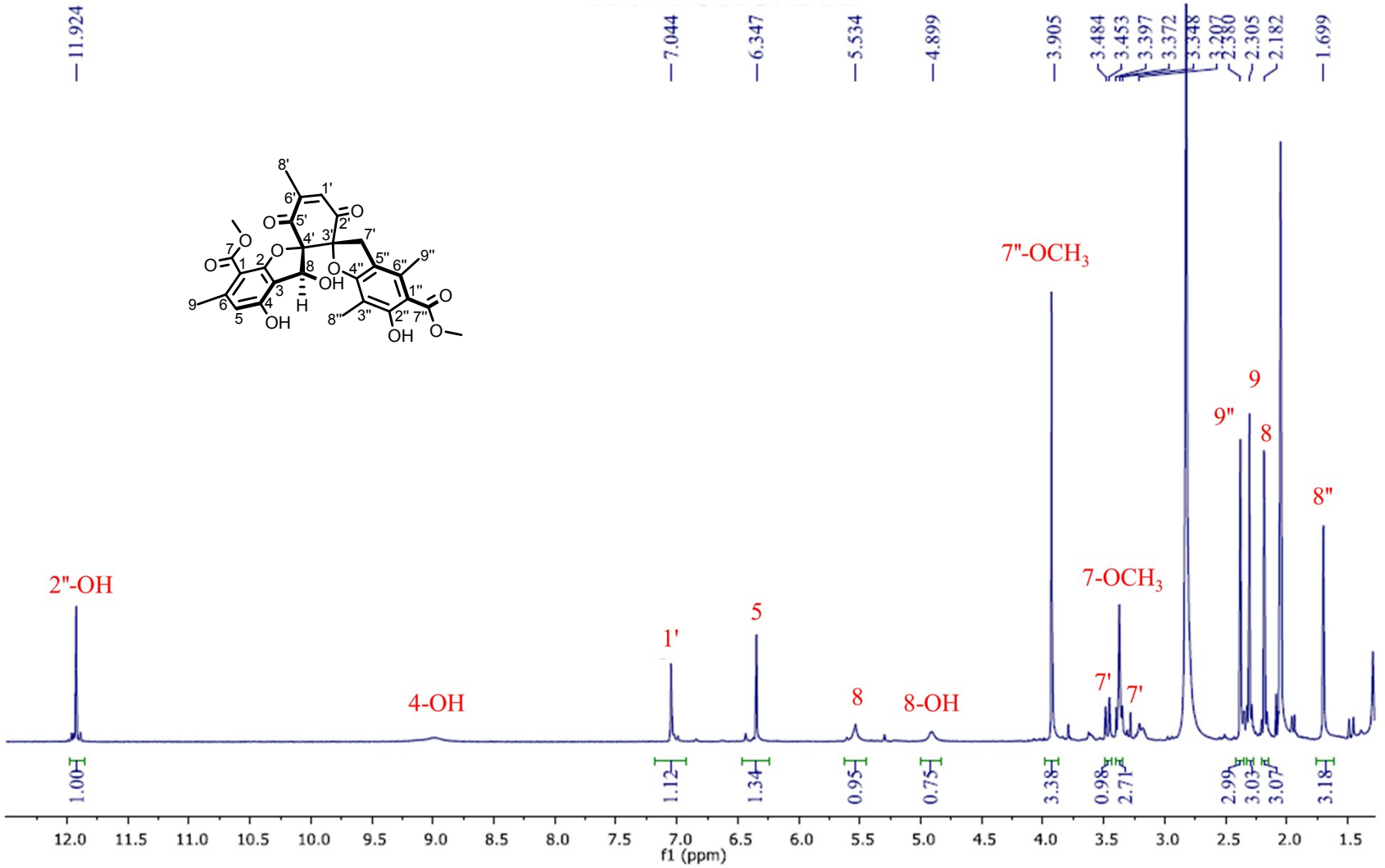
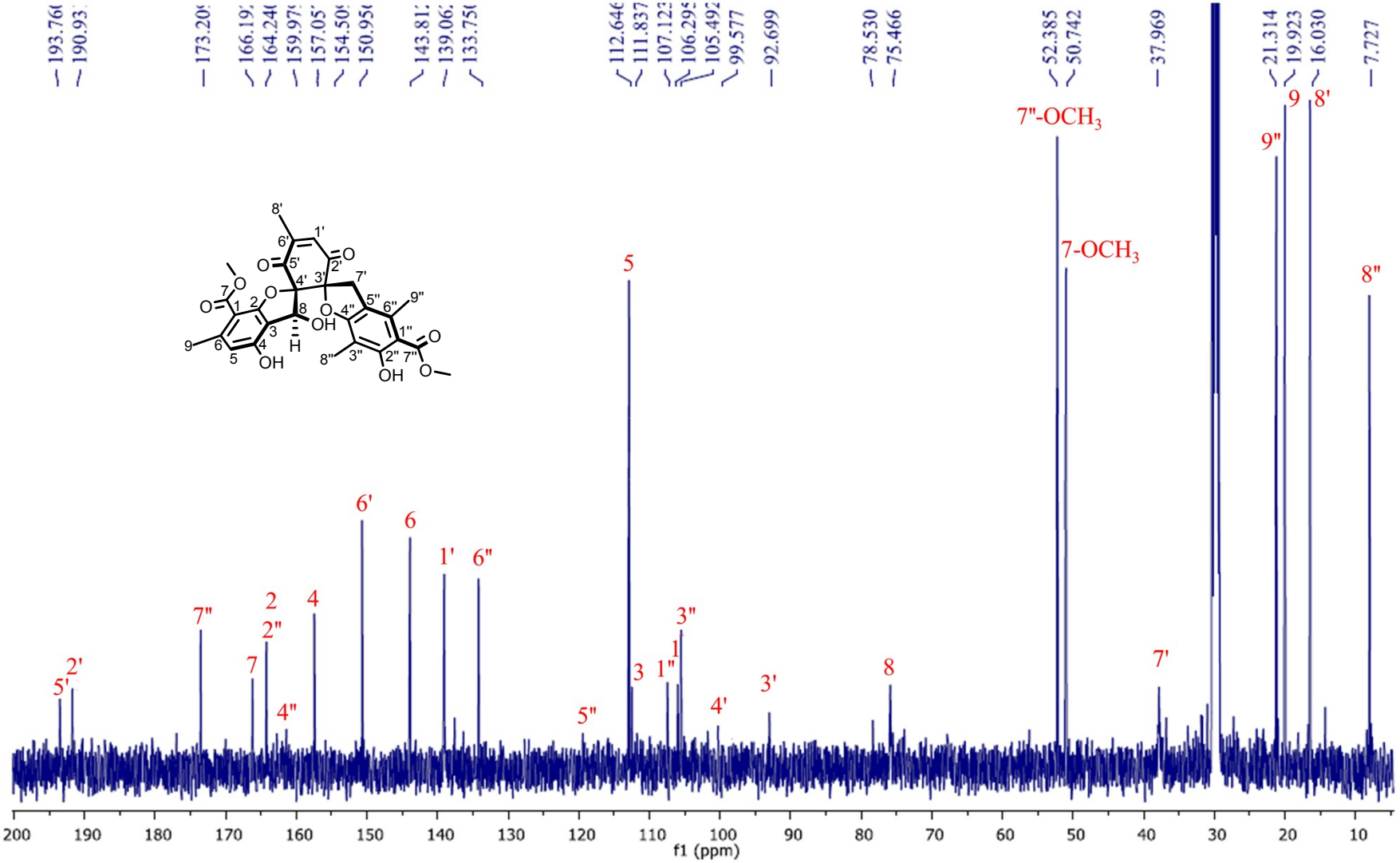
S1. HRESIMS spectrum of **1**



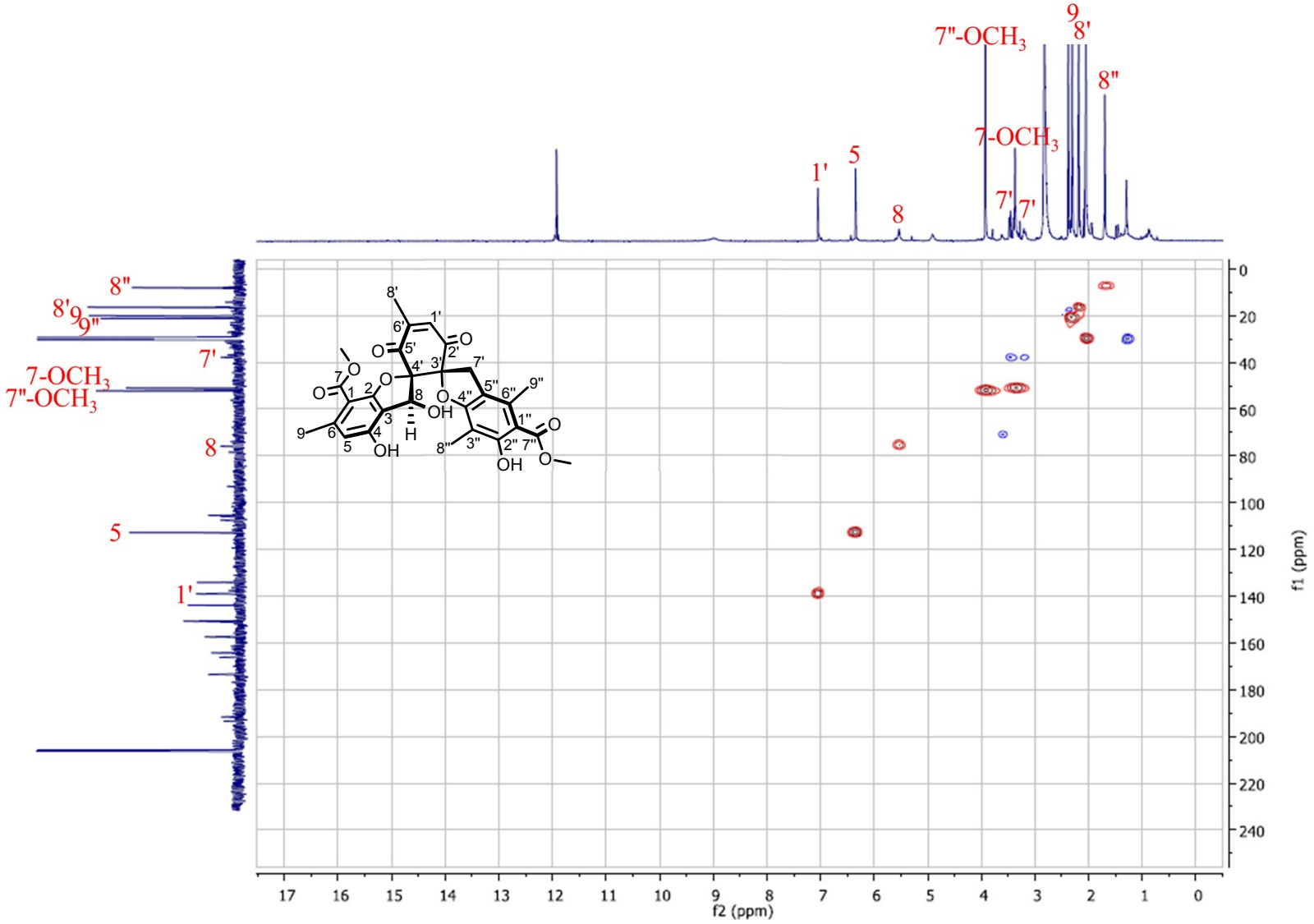
S2. ^{1}H NMR (acetone-d_6, 500 MHz) spectrum of **1**



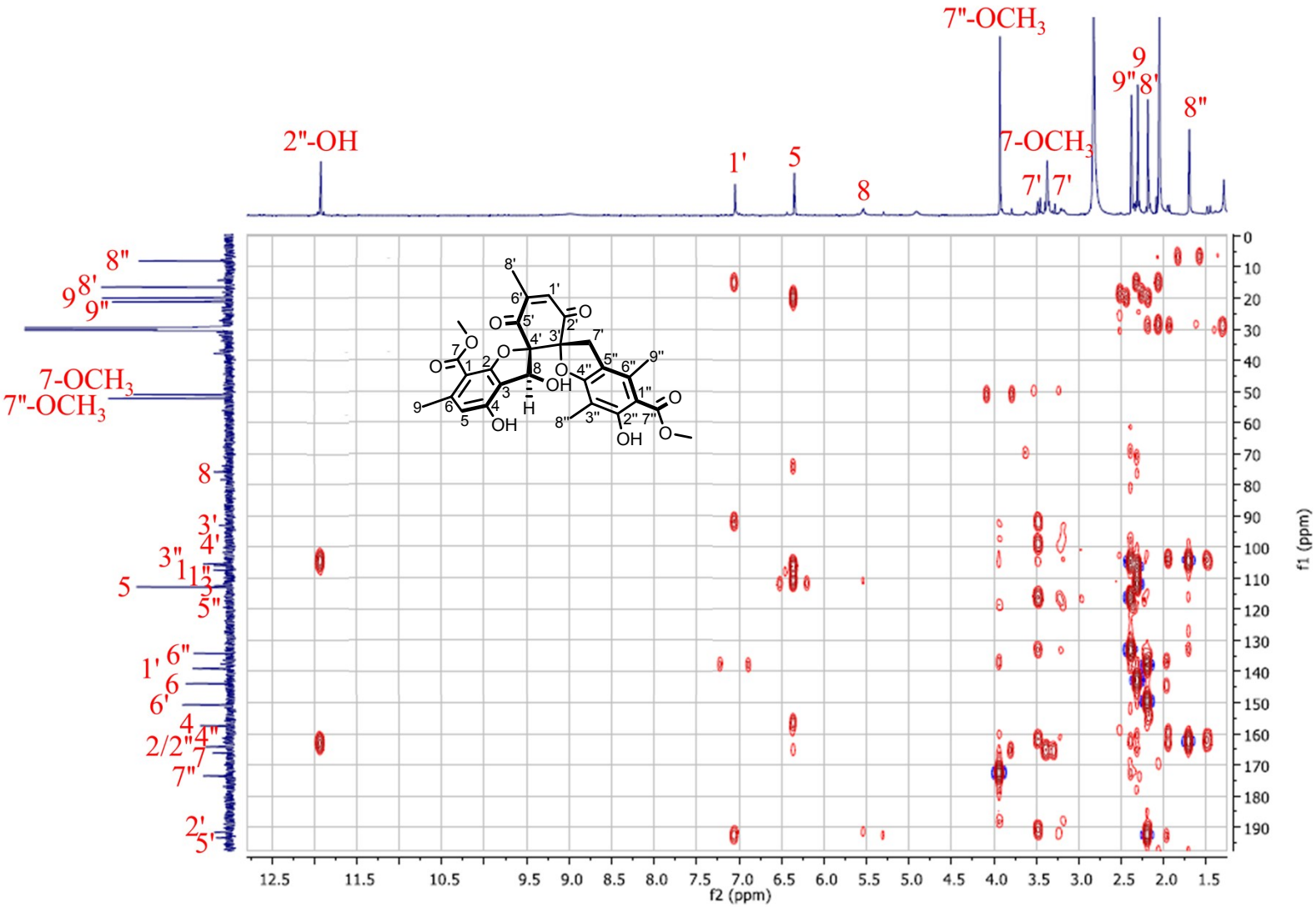
S3. ^{13}C NMR (acetone-d_6, 500 MHz) spectrum of **1**



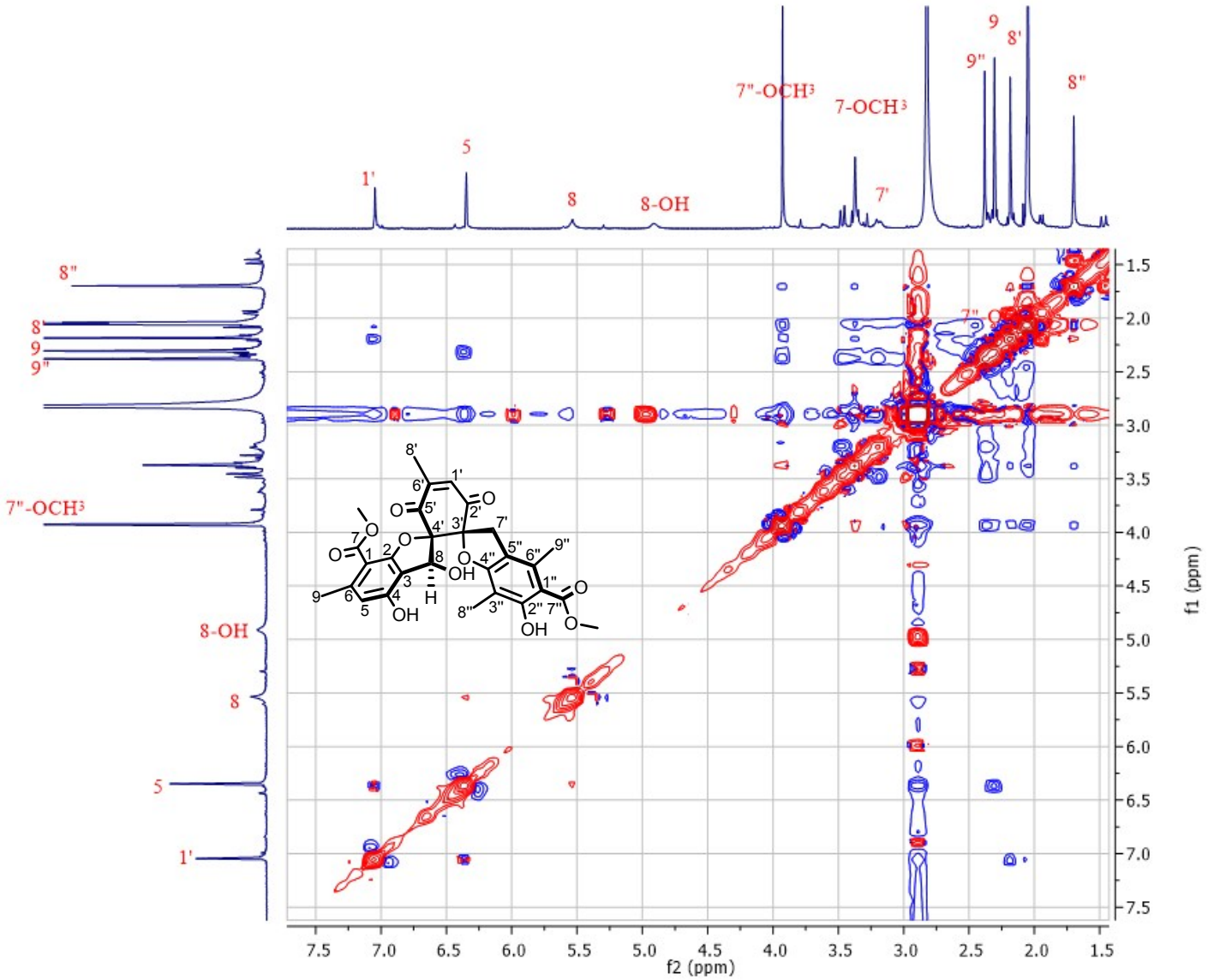
S4. HSQC (acetone-d_6, 500 MHz, 125 MHz) spectrum of **1**



S5. HMBC (acetone-d_6, 500 MHz, 125 MHz) spectrum of **1**



S6. NOESY (acetone-d_6, 500 MHz) spectrum of 1.

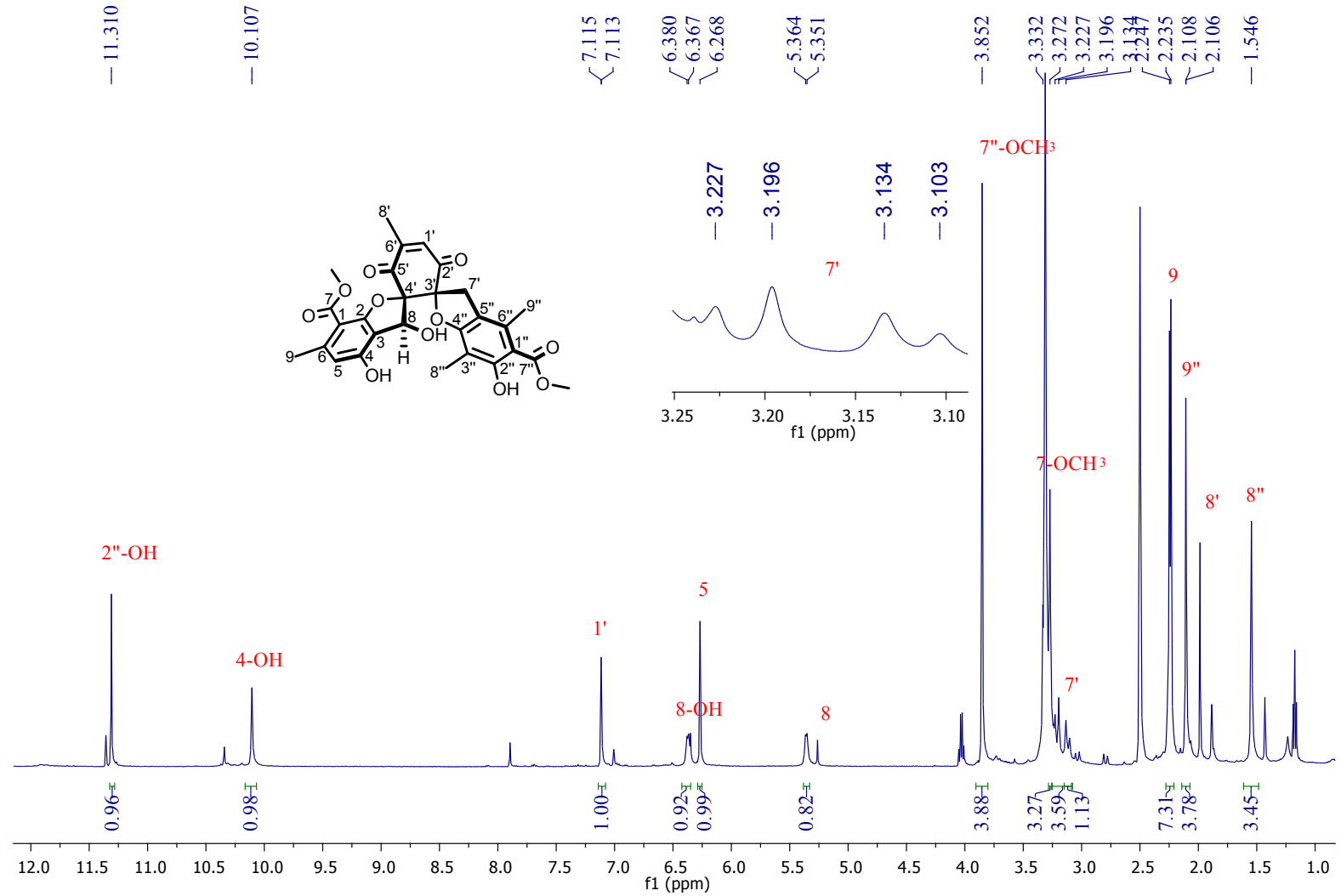


S7. ^{1}H and ^{13}C NMR (DMSO-d_6) Spectroscopic Data For Tsavoenones A (**1**)

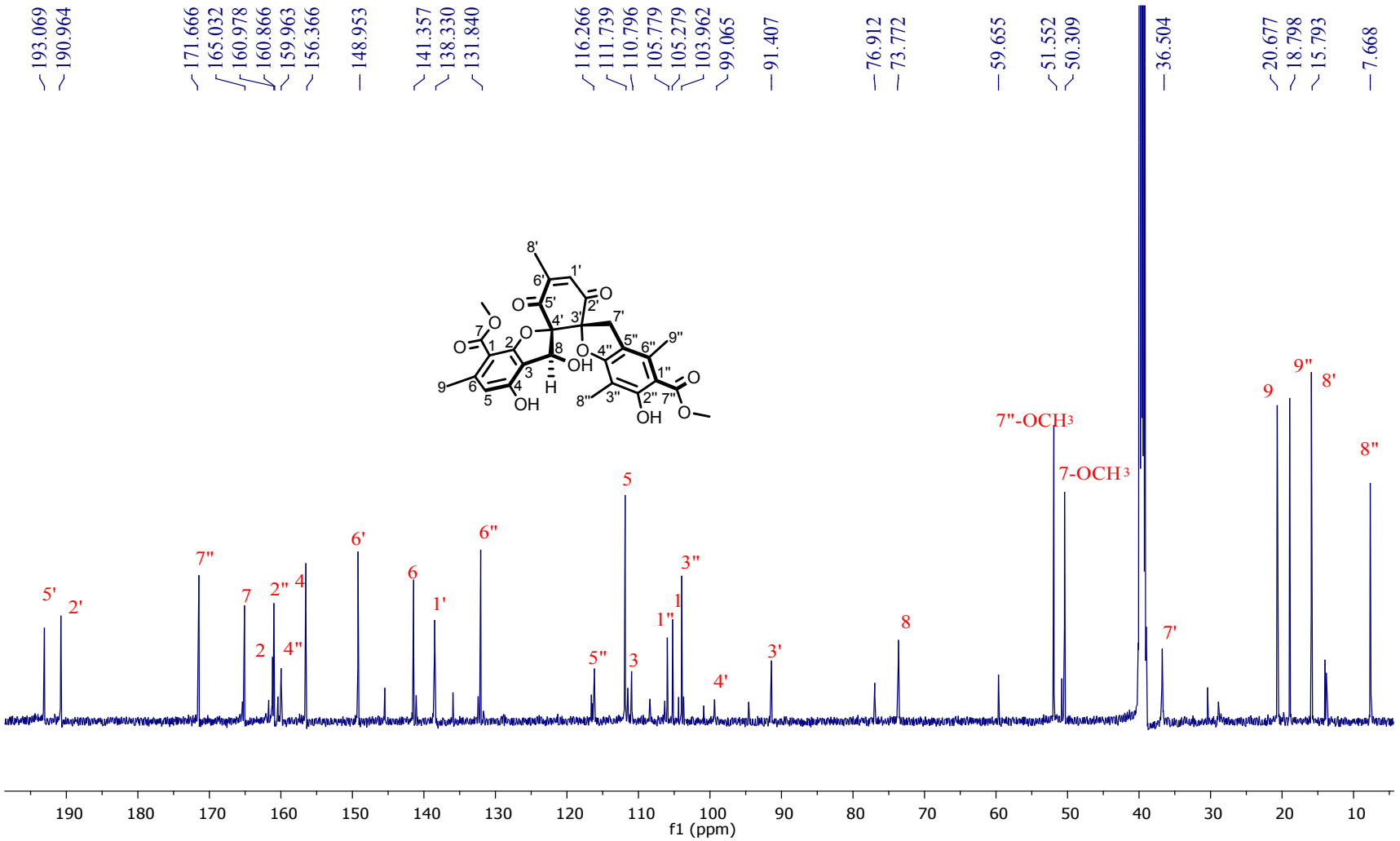
	1	
position	δ_H, mult (*J*, Hz)	δ_c
1		105.3
2		160.9
3		110.8
4		156.4
5	6.27, s	111.7
6		141.4
7		165.0
8	5.35, d (6.5)	73.8
9	2.24, s	20.7
7-OCH_3	3.27, s	50.3
1'	7.11, d (1.0)	138.3
2'		191.0
3'		91.4
4'		99.1
5'		193.1
6'		149.0
7'	3.20, d (15.5)	36.5
	3.11, d (15.5)	
8'	2.11, d (1.0)	15.8
1''		105.8
2''		161.0
3''		104.0
4''		160.0
5''		116.3
6''		131.8
7''		171.7
8''	1.55, s	7.7
9''	2.25, s	18.8
7''-OCH_3	3.85, s	51.6
4-OH	10.11, s	
8-OH	6.38, d (6.5)	
2''-OH	11.31, s	

Regarding spectra obtained in DMSO-d_6, unlabeled (1D NMR) and strikethrough signals (2D NMR) refer to peaks that appeared upon long storage of **1**, thus not belonging to the native molecule. This can be ascertained by comparison to the spectra recorded in acetone-d_6.

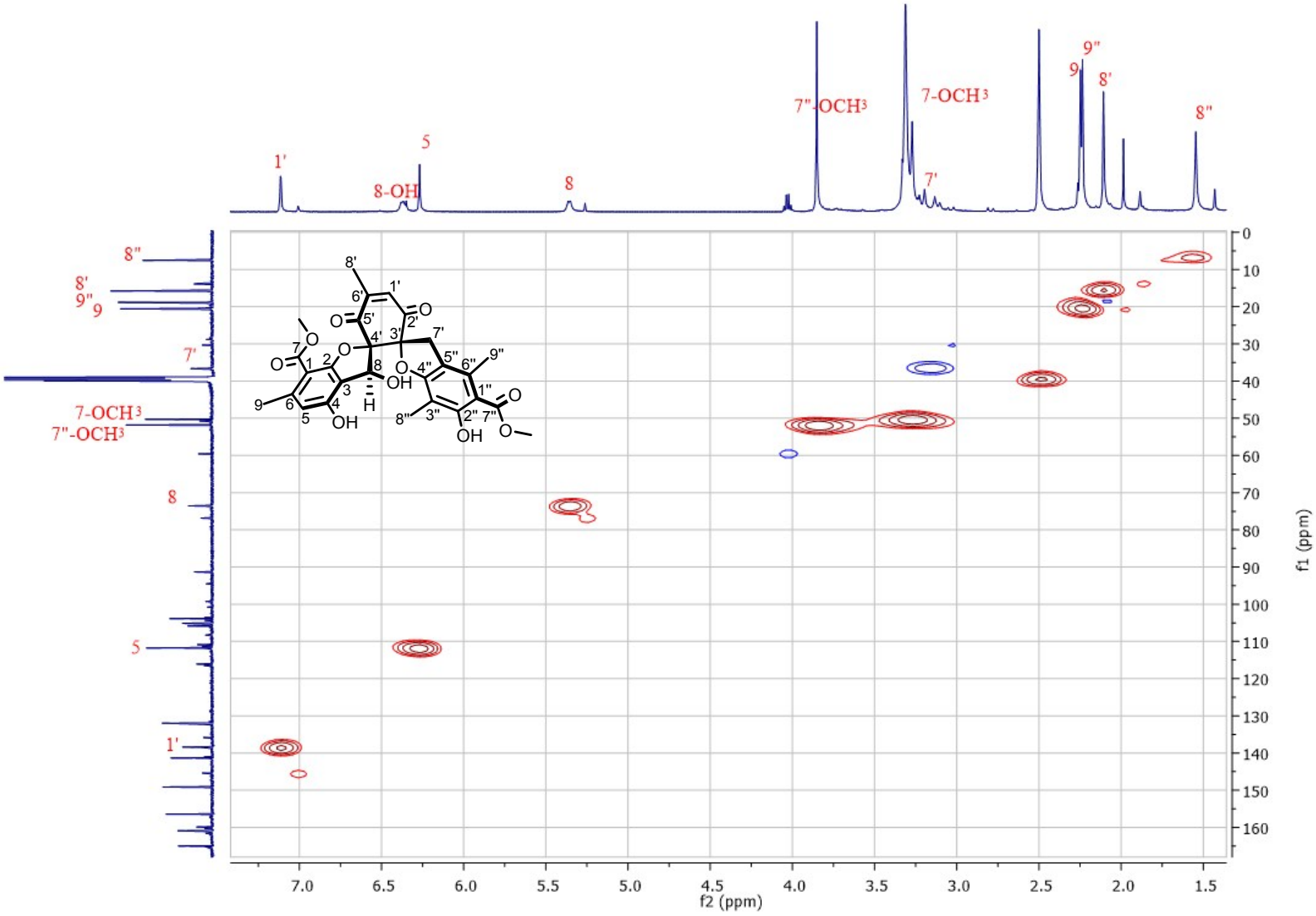
S8. ^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of **1**



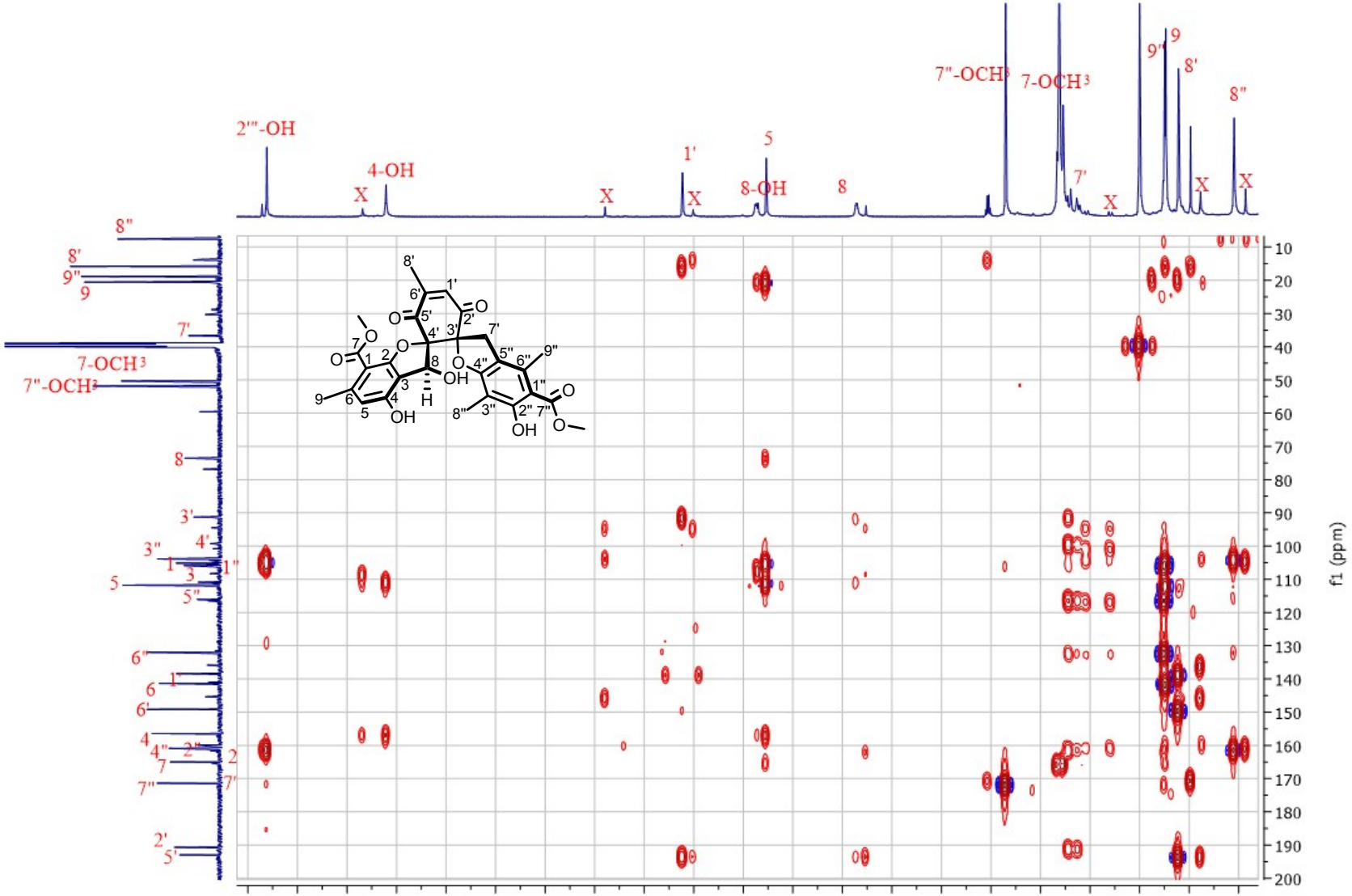
S9. ^{13}C NMR (DMSO-d_6, 125 MHz) spectrum of **1**



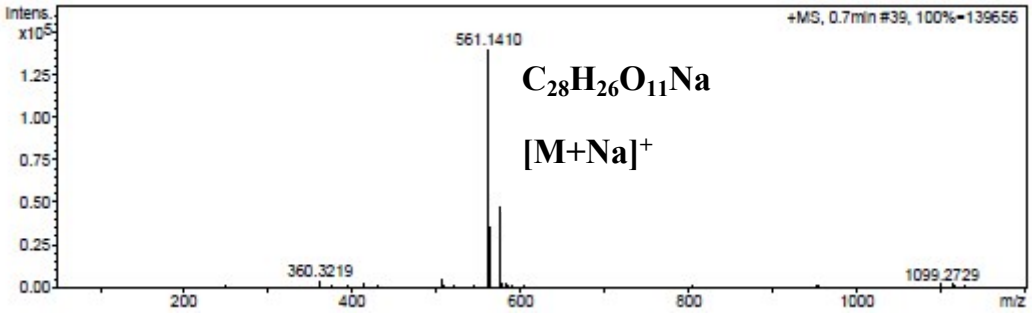
S10. HSQC (DMSO-d_6, 500 MHz, 125 MHz) spectrum of **1**



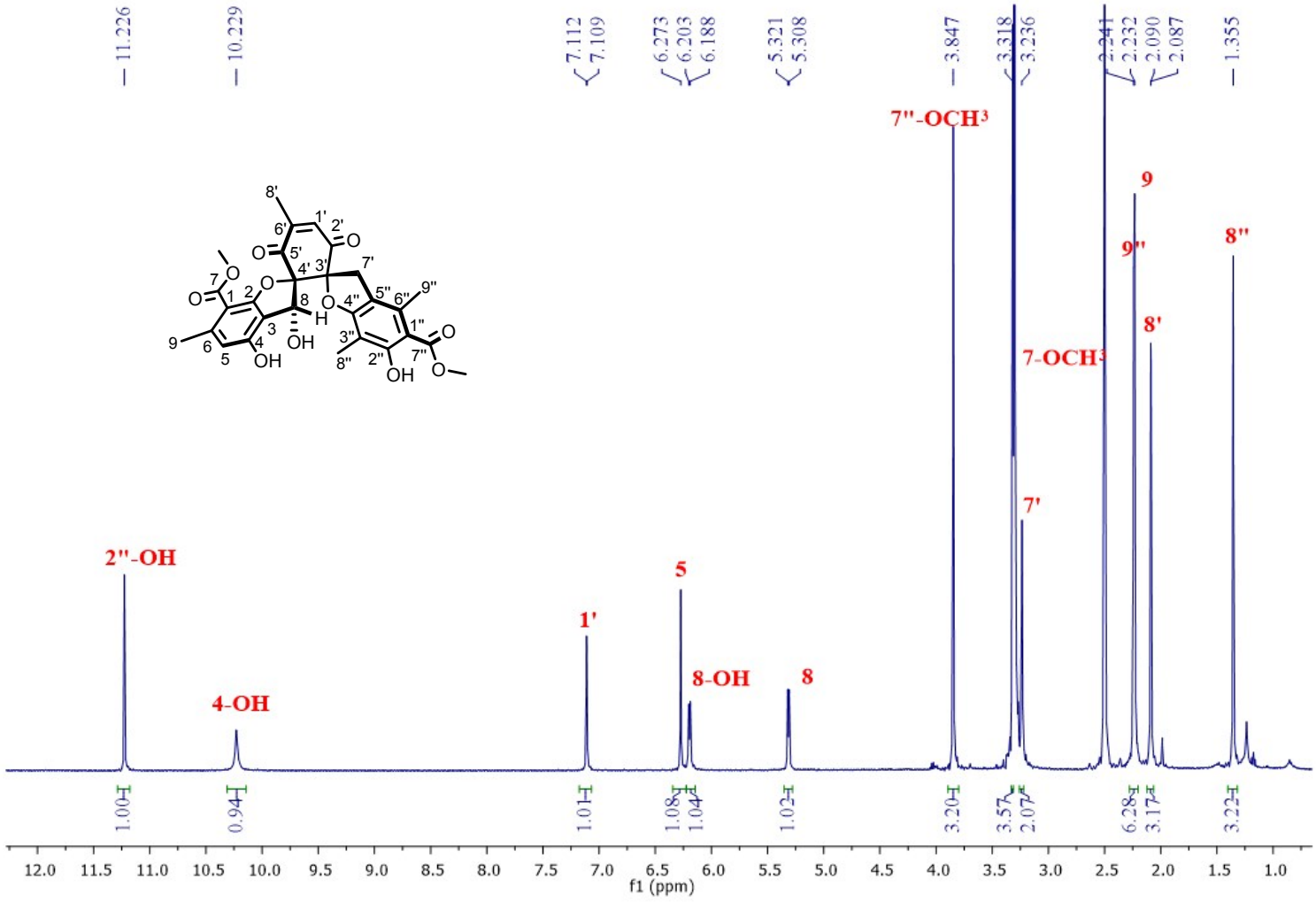
S11. HMBC (DMSO-d_6, 500 MHz, 125 MHz) spectrum of **1**



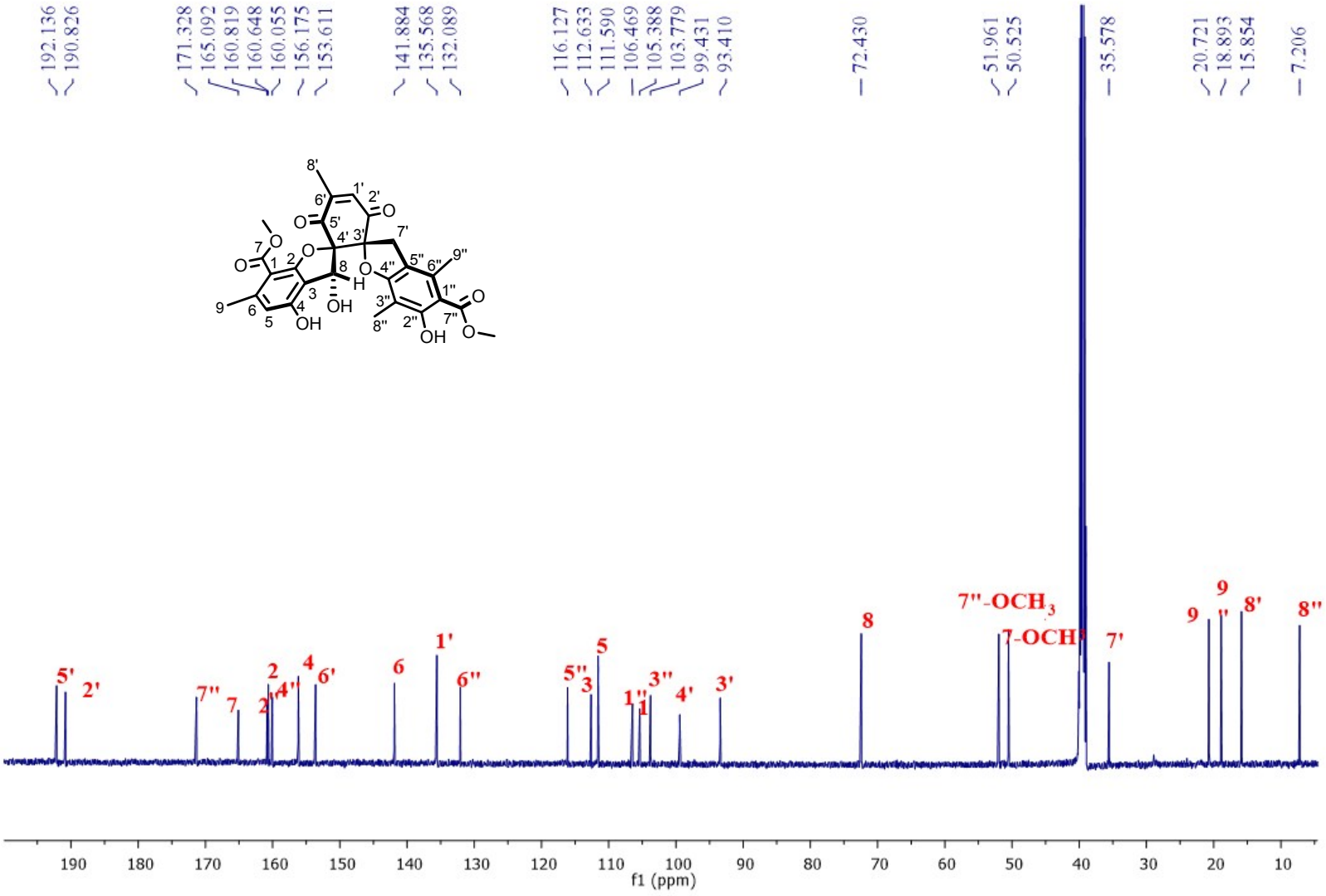
S12. HRESIMS spectrum of **2**.



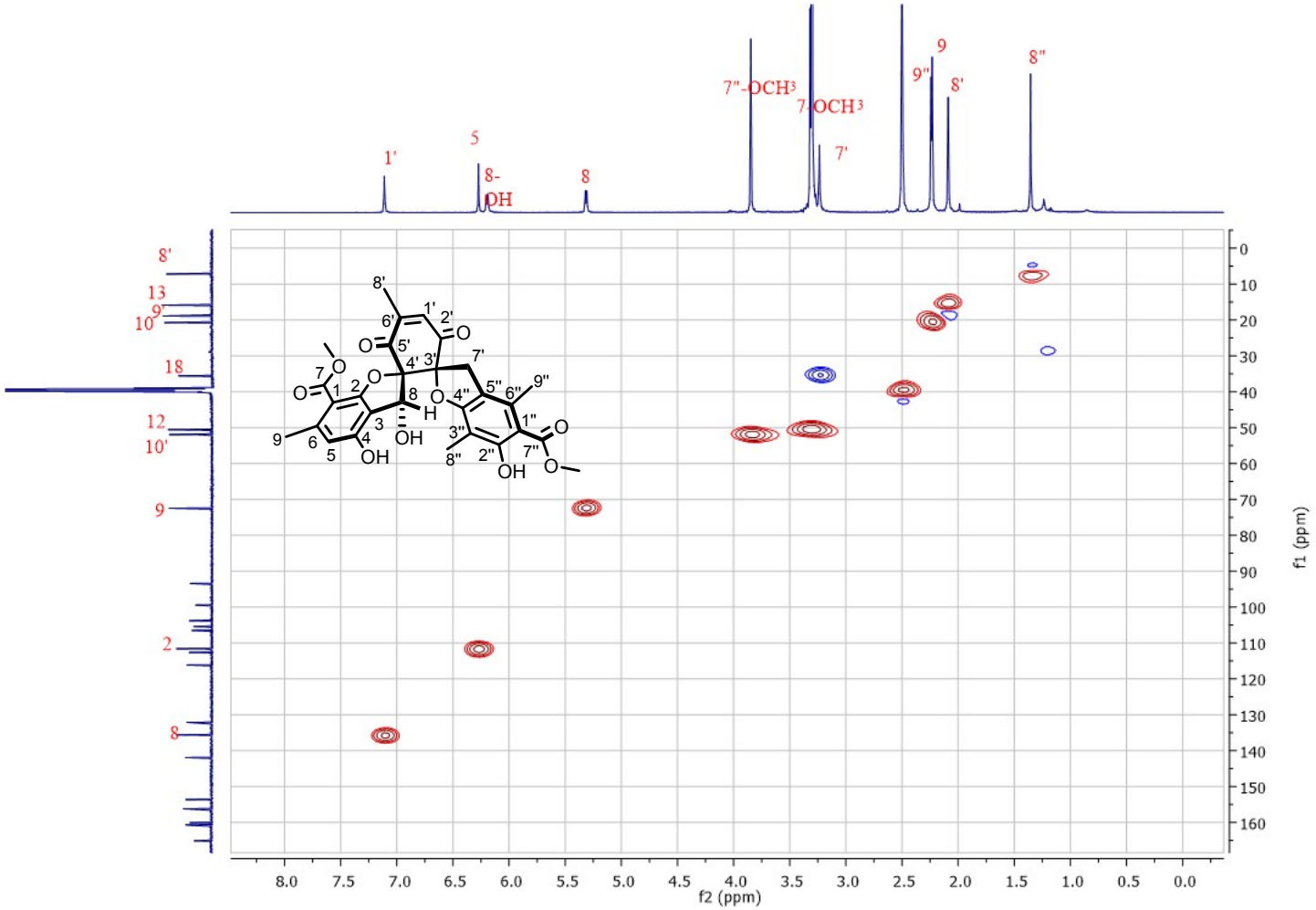
S13. ^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of **2**



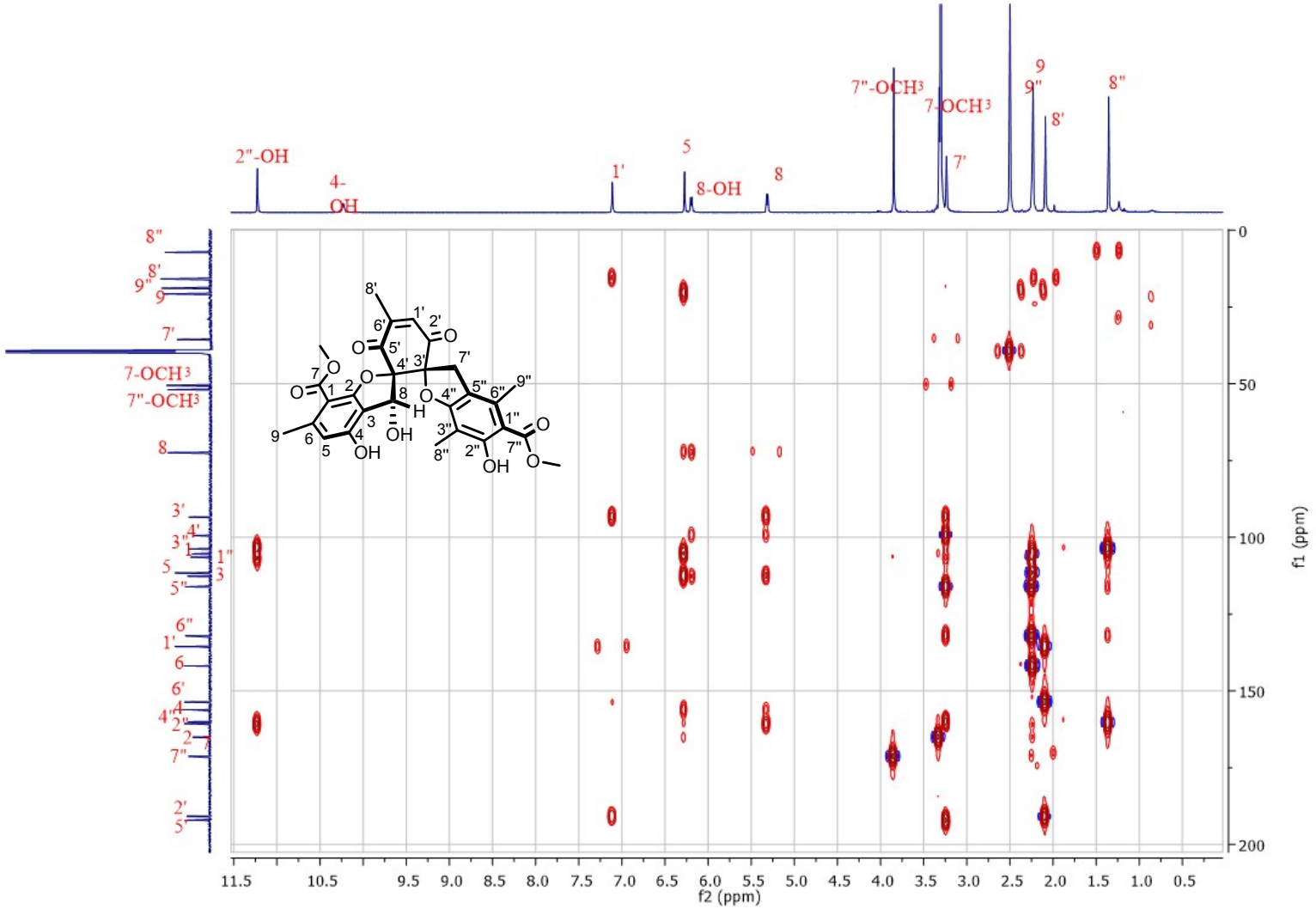
S14. ^{13}C NMR (DMSO-d_6, 125 MHz) spectrum of **2**



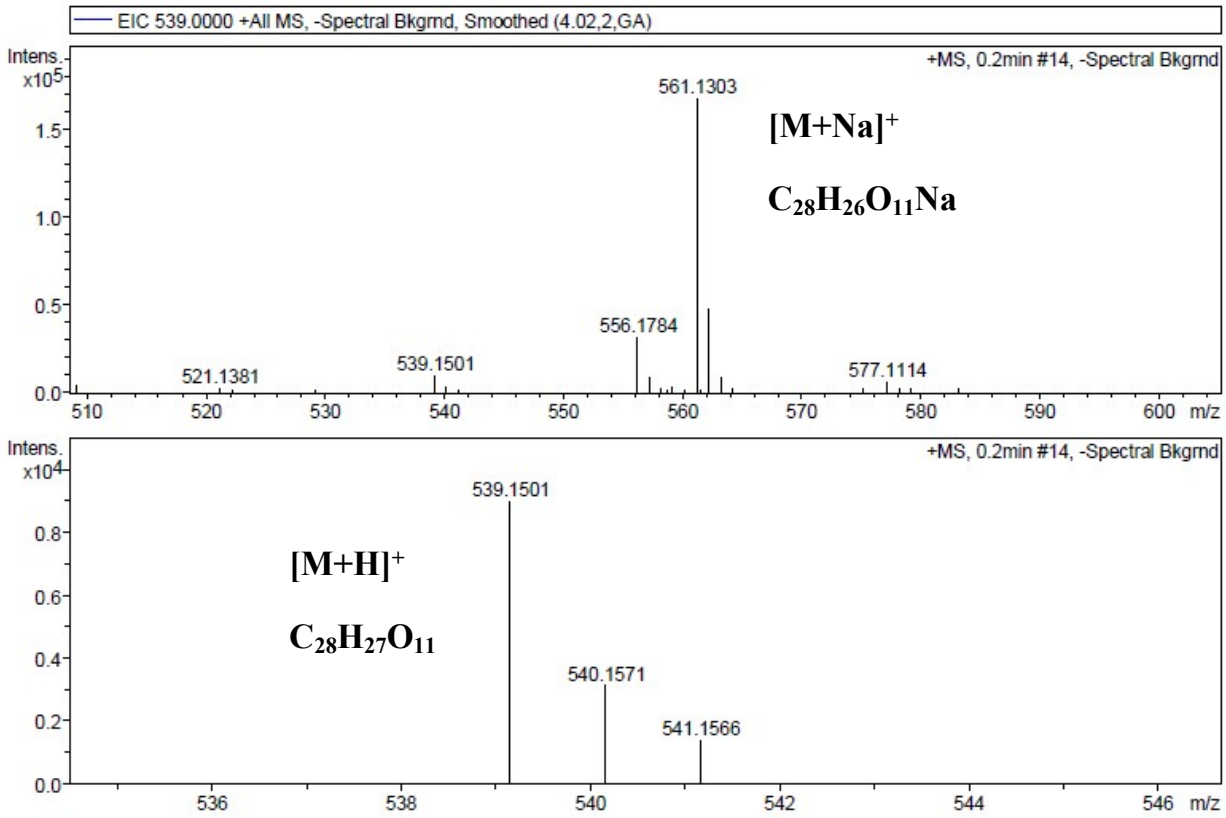
S15. HSQC (DMSO-d_6, 500 MHz, 125 MHz) spectrum of **2**



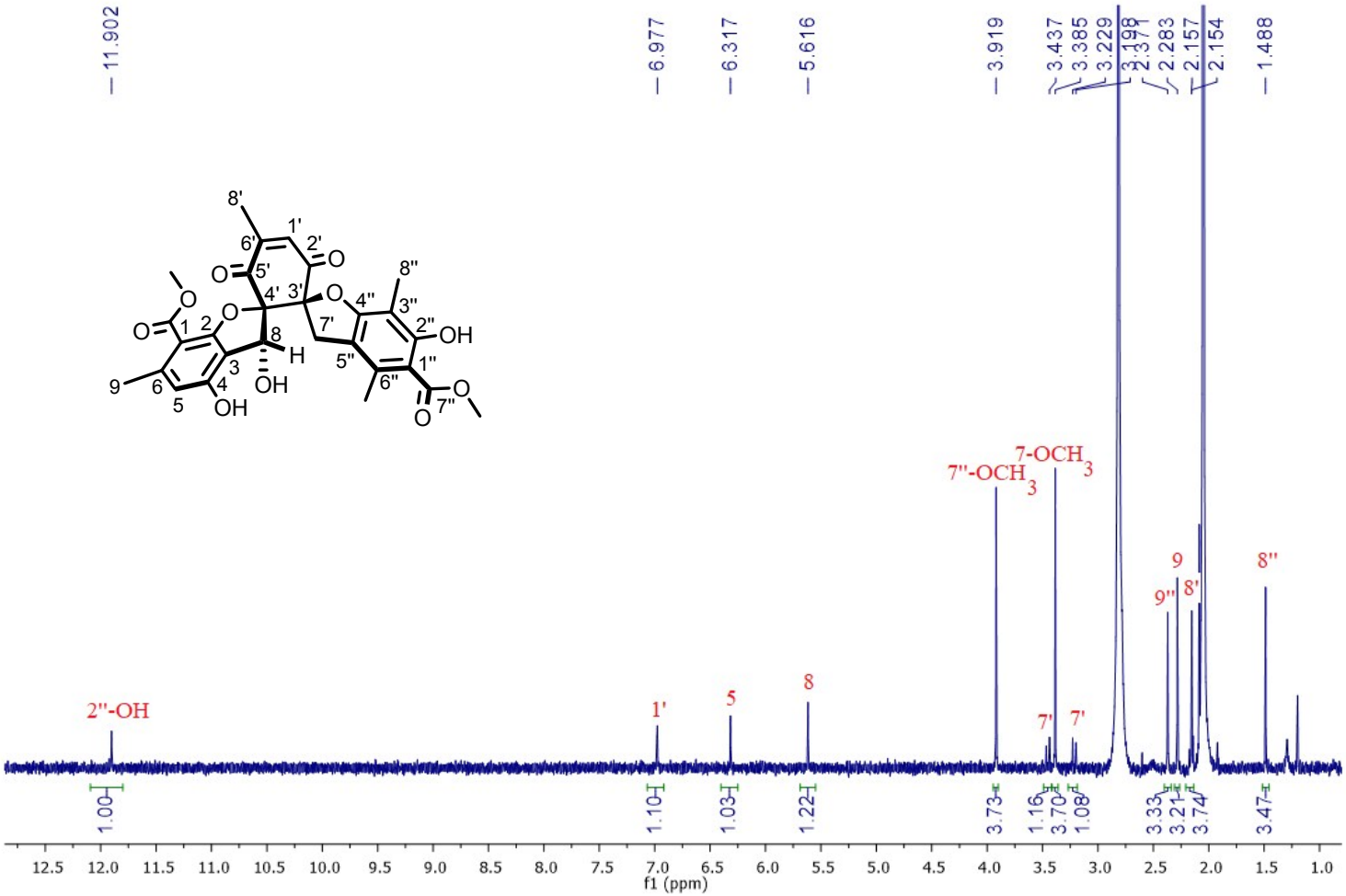
S16. HMBC (DMSO-d_6, 500 MHz, 125 MHz) spectrum of **2**



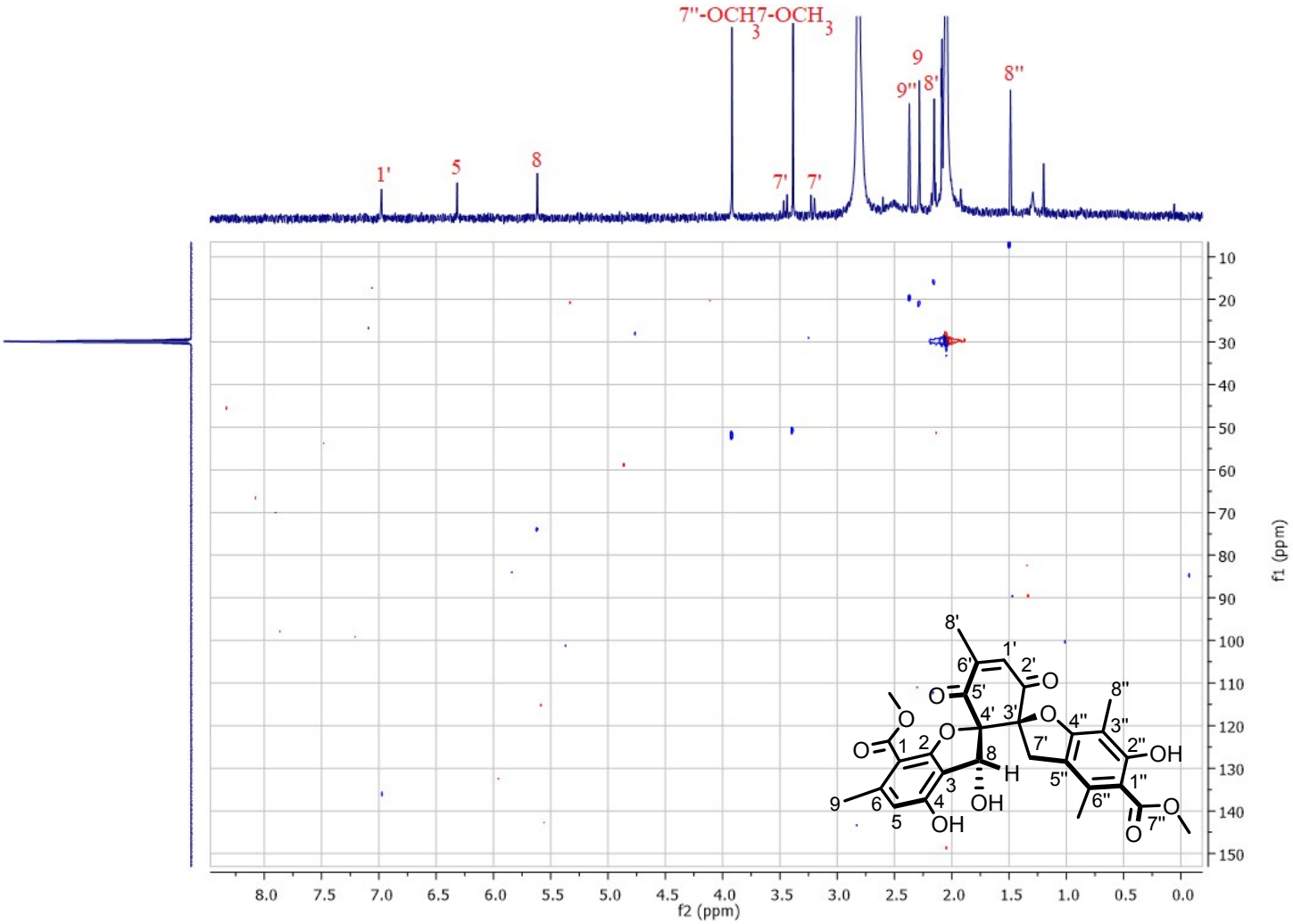
S17. HRESIMS spectrum of **3**.



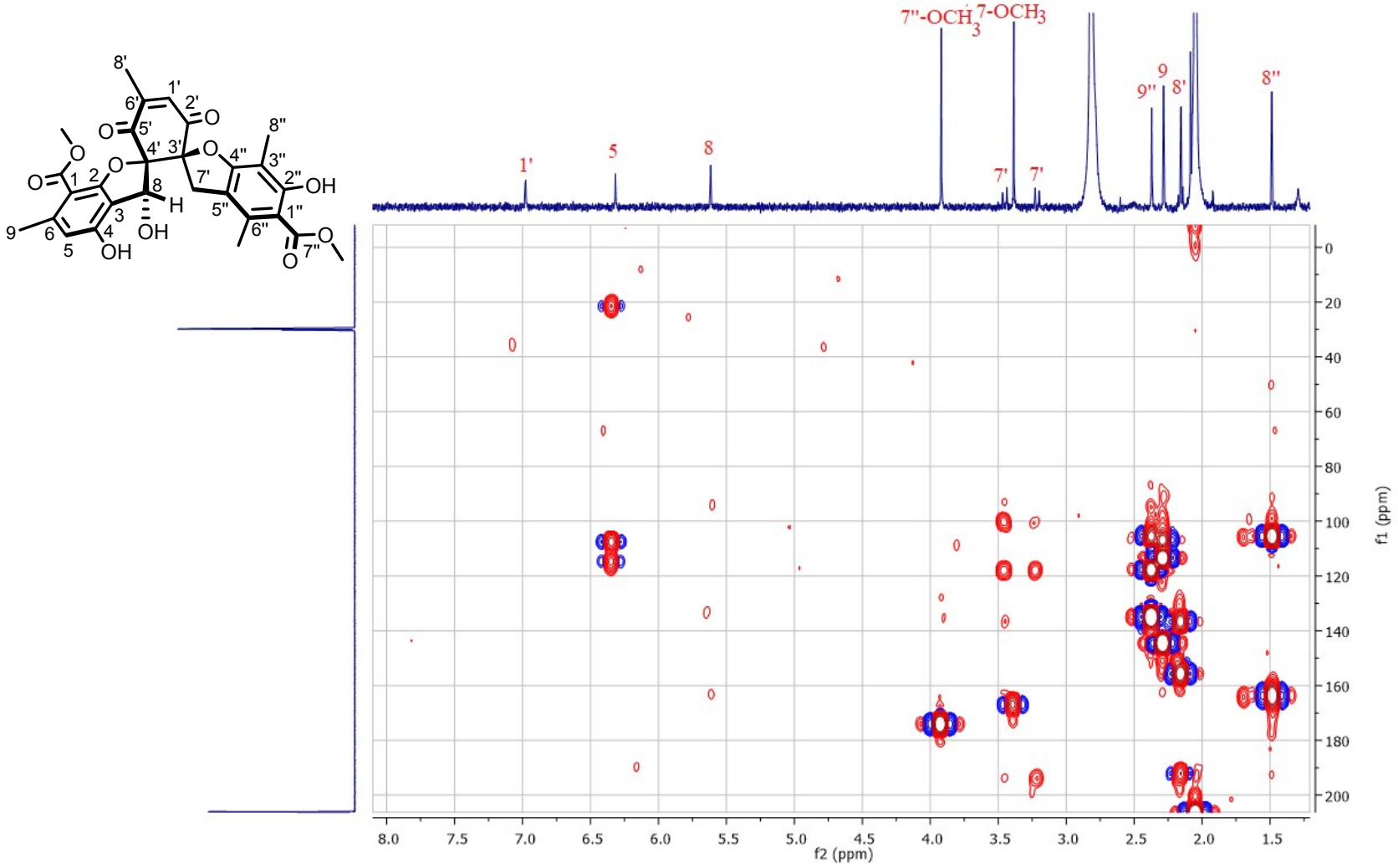
S18. ^{1}H NMR (acetone-d_6, 500 MHz) spectrum of **3**



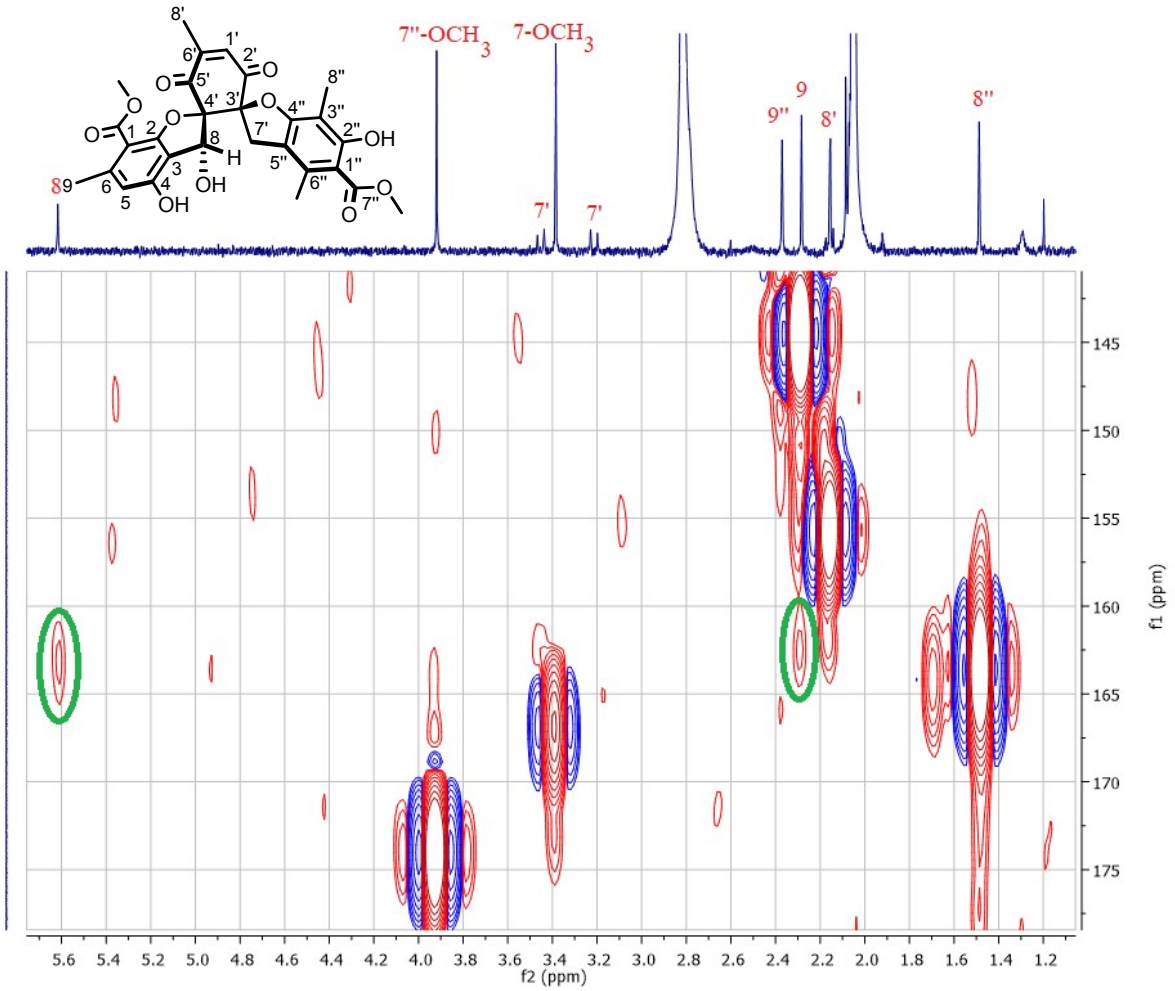
S19. HSQC (acetone-d_6, 500 MHz, 125 MHz) spectrum of **3**



S20. HMBC (acetone-d_6, 500 MHz, 125 MHz) spectrum of **3**



S21. HMBC (acetone-d_6, 500 MHz, 125 MHz) spectrum of **3** (closer view)



The two correlations circled in green can be associated to C-2 and C-4 even though these carbons could not be distinguished one from another.

Computational details

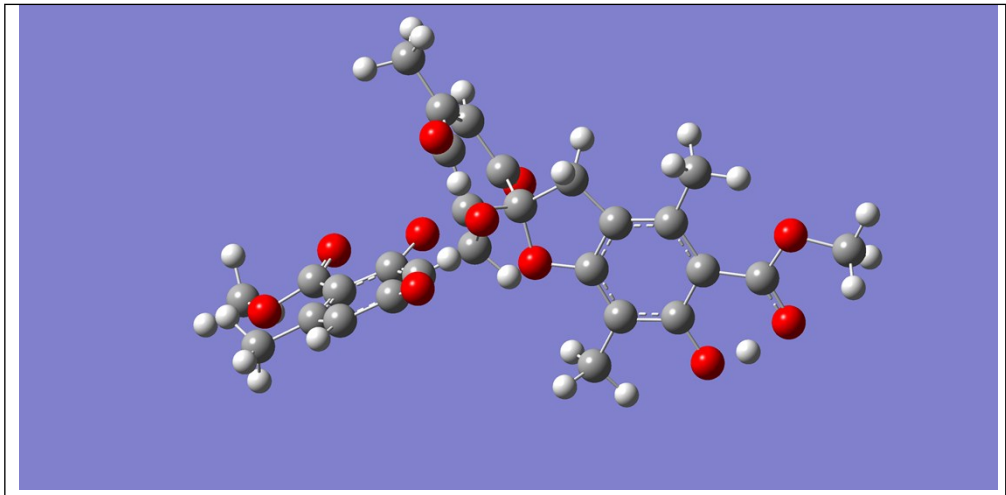
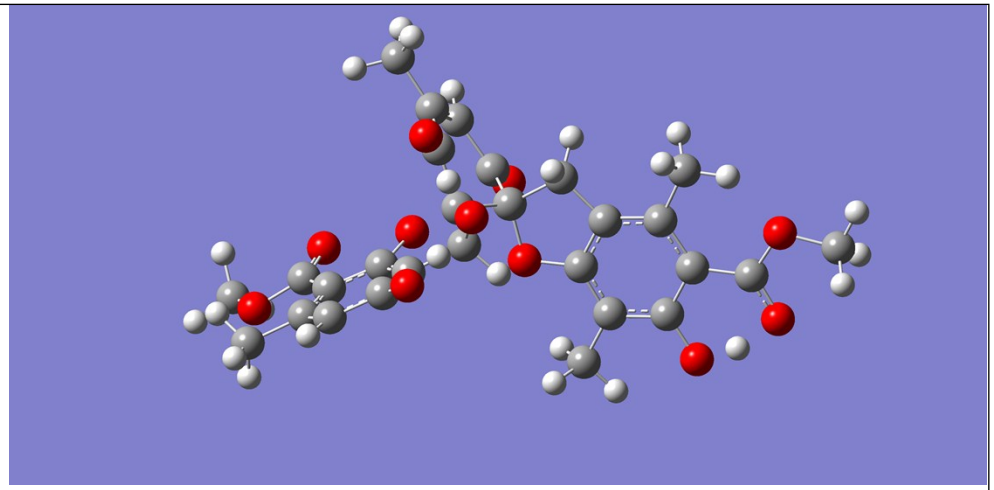
All DFT calculations have been performed using Gaussian16[1]. After a conformational analysis with GMMX package using the MMFF94 force field with a 1 kcal/mol threshold. 6, 2, 6 and 3 conformers were obtained for the 8S,3'R,4'S**,** 8R,3'R,4'S, 8R,3'S,4'R, 8R,3'S,4'S diastereoisomers respectively (As compound **2** and **3** are diastereoisomers, the calculation have been performed once). After geometry optimization using DFT at the STO-3G followed by a frequency calculation in order to confirm the presence of a minimum, NMR prediction was performed using the MPW1PW91/6-311+g(2d,p) method as recommended by the Tantillo's group (http://cheshirenmr.info). After Boltzmann weighing of the predicted chemical shift of each diastereoisomers, the DP4 parameters were calculated suing the Smith and Goodman Java source code[2]. The molecules visualization is performed using GaussView 6.

[1] Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[2] Assigning Stereochemistry to Single Diastereoisomers by GIAO NMR Calculation: The DP4 Probability S. G. Smith and J. M. Goodman J. Am. Chem. Soc. 2010, 132, 12946-12959

DOI: 10.1021/ja105035r

Cartesian coordinates of conformers 8S,3'R,4'S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C 0.28953 1.00829 -0.66583	C 0.28959 1.00797 -0.66587
C -0.12839 1.84611 -1.96207	C -0.12804 1.84539 -1.96245
C -1.00353 3.06886 -1.68911	C -1.00330 3.06818 -1.69009
C -0.82749 -0.00040 1.57487	C -0.82775 0.00012 1.57502
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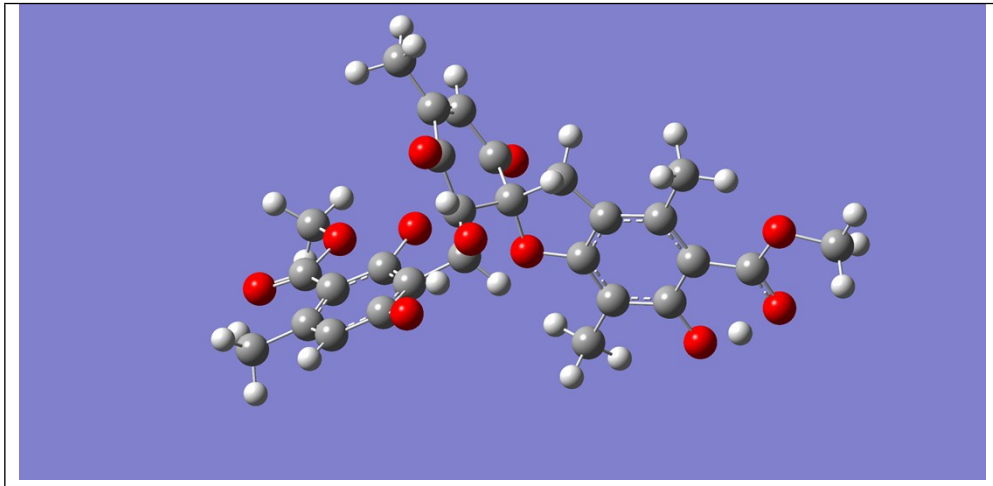

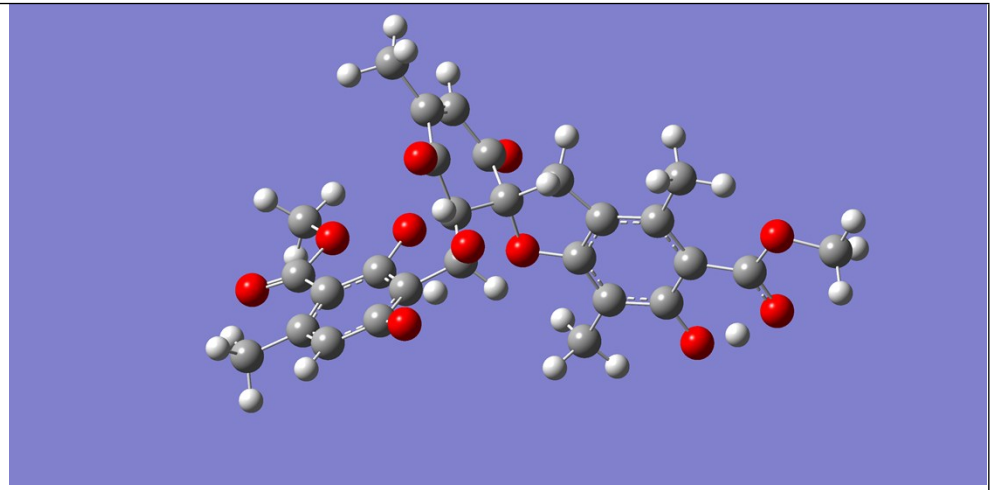

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C	-1.06401	3.24992	-1.08602	C	-1.10740	3.31104	-0.94676
C	-0.94160	-0.35968	1.57034	C	-0.90537	-0.41758	1.53509
C	-2.29846	-1.02970	1.40457	C	-2.25636	-1.09603	1.35568
C	-2.92214	-0.65022	0.21811	C	-2.90092	-0.66890	0.19683
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C	2.56259	0.59294	0.01816	C	2.55535	0.61887	0.01311
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O	0.61154	-0.23329	-1.09000	O	0.60661	-0.14600	-1.14205
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C	4.72993	-0.47583	-0.18376	C	4.71505	-0.45998	-0.21534
C	4.14412	-1.48392	-1.07244	C	4.12742	-1.42682	-1.14796
C	2.74202	-1.43999	-1.41312	C	2.72842	-1.35757	-1.49614
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O	4.90174	-2.48532	-1.60819
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O	6.86160	-1.63677	-0.48574
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H	-0.08899	-1.03865	1.33766

C	2.11687	-2.36683	-2.47173
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O	6.83731	-1.63232	-0.53976
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O	-6.02014	-1.11504	-1.86000
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C	-4.73221	0.55427	-3.41541
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H	-1.22189	4.18149	-1.61265
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H	-4.77666	-2.89330	2.84078	H	-4.69330	-3.05393	2.73584
H	-2.49944	5.31162	-0.14870	H	-2.51659	5.32546	0.13299
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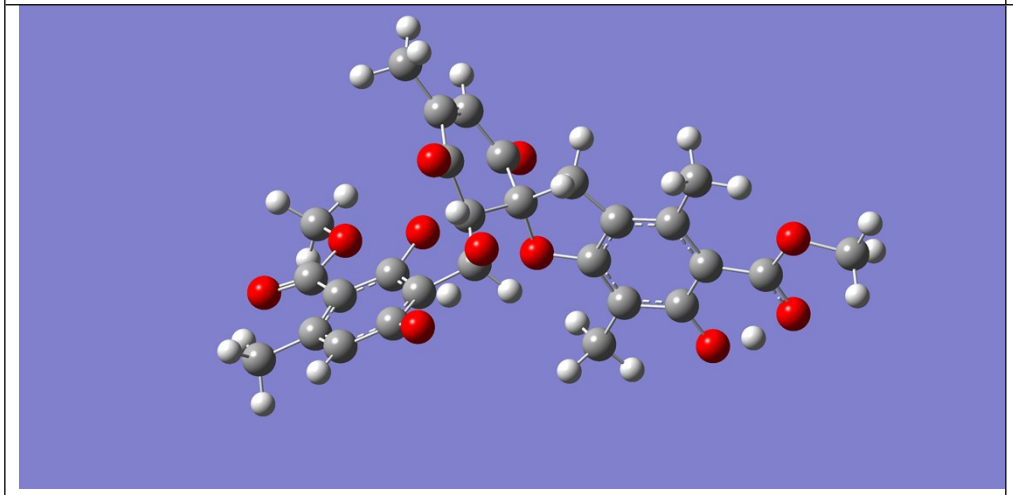

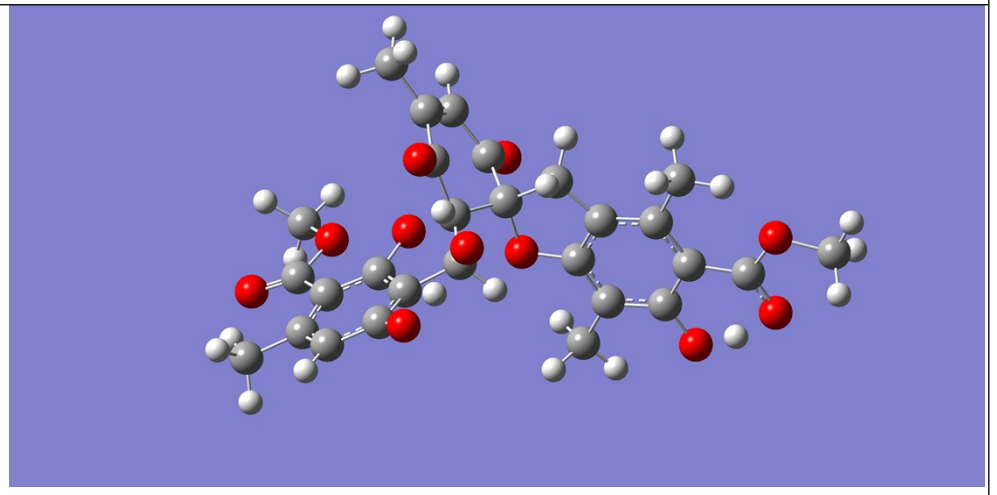

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C	1.99296	-0.32656	-0.89728	C	1.99302	-0.32712	-0.89691
O	0.60663	-0.14603	-1.14203	O	0.60666	-0.14675	-1.14165
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C	4.71507	-0.45999	-0.21529	C	4.71519	-0.46010	-0.21509
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C	6.16558	-0.67707	0.02574
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O	-6.02024	-1.11510	-1.85995
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C	8.27004	-0.16595	1.02840
H	-1.22136	4.18079	-1.61408
H	-0.04839	-1.07412	1.26049
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H	3.91783	1.54242	2.32740	H	4.30251	2.63461	0.97211
H	5.52545	1.44206	1.53132	H	3.91799	1.54324	2.32690
H	4.30246	2.63430	0.97306	H	5.52558	1.44262	1.53076
H	-1.53174	-1.17577	3.50756	H	-1.53225	-1.17474	3.50800
H	-4.03389	1.23686	-3.93392	H	-4.03327	1.23545	-3.93470
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H	-5.68639	1.08270	-3.21363	H	-4.94846	-0.31885	-4.06605
H	-6.85967	-2.54804	1.27550	H	-6.86017	-2.54695	1.27596
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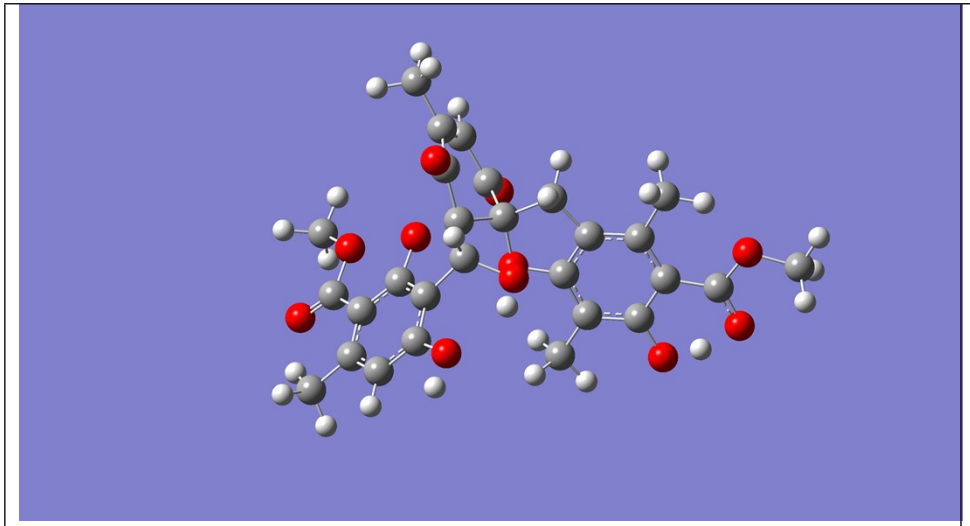
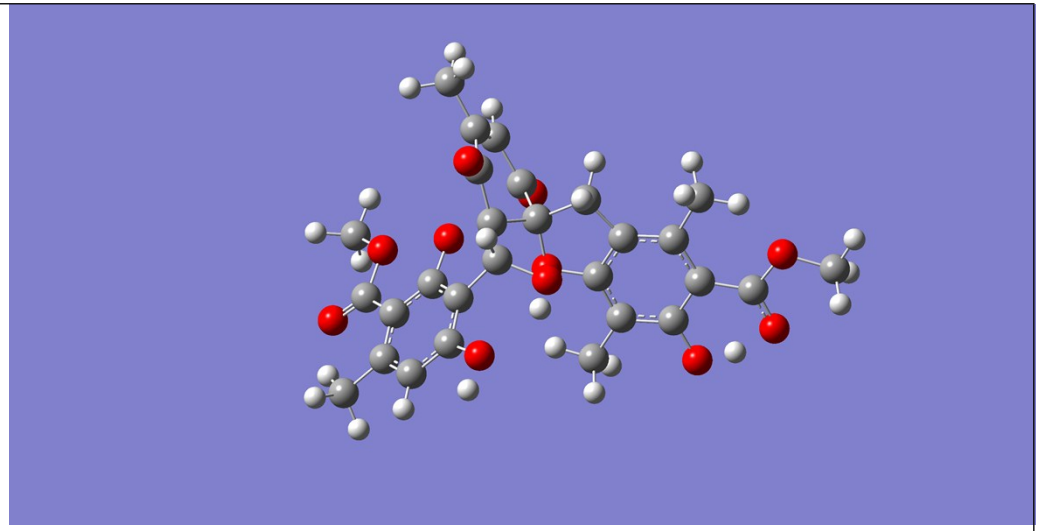
Cartesian coordinates of conformers 8R,3'R,4'S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C	-1.07834	0.11897	1.98590
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O	0.27158	-0.11214	-0.78543
C	3.74165	0.67777	0.21018
C	4.45352	-0.45723	-0.32303
C	3.73190	-1.51959	-1.03045
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C	-3.43322	-2.98254	1.71161
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O	0.26900	-0.11865	-0.77419
C	3.74155	0.67696	0.20978
C	4.45423	-0.45829	-0.32290
C	3.73226	-1.52134	-1.02642
C	2.30326	-1.44887	-1.20585
C	-2.40484	-2.15397	2.24603
C	-3.43312	-2.97886	1.71417
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O	-0.13172	1.94027	-2.61255	O	-0.12677	1.92653	-2.61278
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C	-1.61121	2.59044	1.30720	C	-1.61240	2.59739	1.30075
O	-1.86647	2.80220	2.52047	O	-1.87384	2.81342	2.51201
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O	4.38856	-2.60466	-1.54078	O	4.38507	-2.60904	-1.53588
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H	1.23346	1.77473	1.57971	H	1.23222	1.76620	1.58479
H	1.57996	2.79303	0.14505	H	1.57905	2.78983	0.15367
H	-3.65036	-3.95080	2.18103	H	-3.64833	-3.94752	2.18369
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H	2.28466	-3.26960	-2.36034	H	2.02021	-2.76085	-2.92438
H	0.86528	-3.09212	-1.28249	H	0.50473	-2.26399	-2.10639
H	0.95607	-2.13917	-2.78502	H	1.56964	-3.49976	-1.36873
H	5.42567	-2.38573	-1.26138	H	5.42143	-2.39222	-1.25801
H	4.02293	1.89096	2.00111	H	4.24181	2.78484	0.47863
H	5.51417	1.63324	1.03241	H	4.03173	1.88633	2.00203

H	4.25080	2.78357	0.47677	H	5.51582	1.63970	1.01995
H	-1.88577	-3.43096	3.60705	H	-1.88215	-3.42189	3.61042
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H	8.67879	0.68100	0.94396	H	8.68214	0.68376	0.93283
H	8.29624	-1.09009	0.93751	H	8.52847	-0.22074	-0.62968
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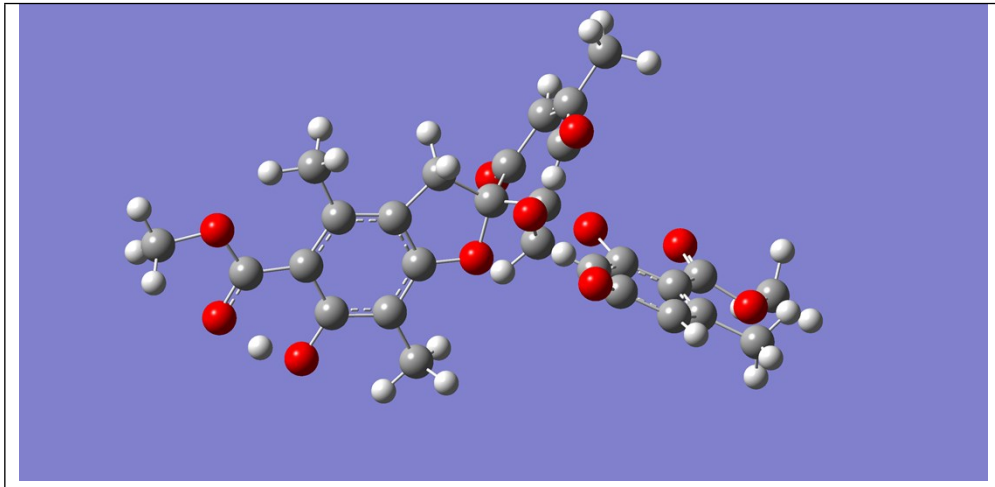
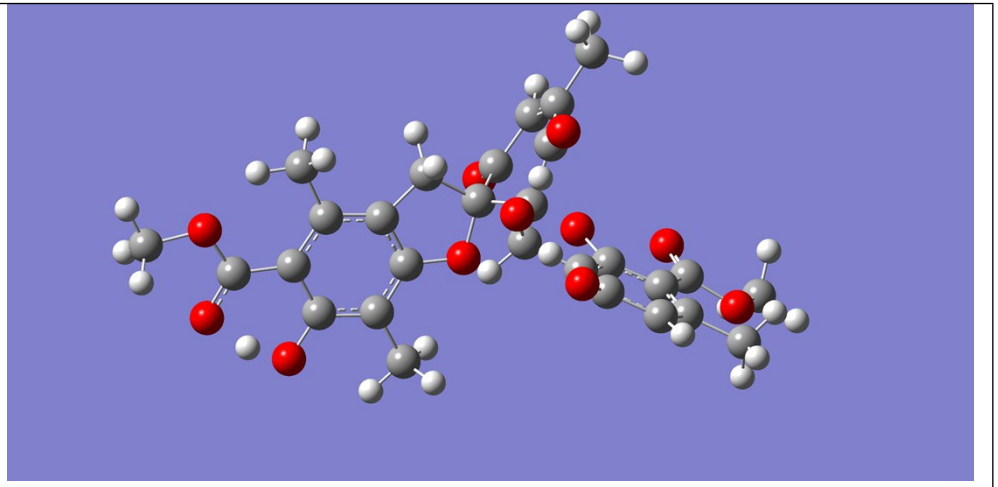
Cartesian coordinates of conformers of the 8R,3'S,4'R





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C	0.82788	0.00032	1.57511
C	2.18918	-0.67971	1.56240
C	2.84366	-0.50639	0.34578
O	2.10238	0.32043	-0.56680

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C	-0.28958	1.00799	-0.66590
C	0.12806	1.84544	-1.96246
C	1.00335	3.06820	-1.69010
C	0.82772	0.00013	1.57500
C	2.18901	-0.67994	1.56229
C	2.84359	-0.50644	0.34575
O	2.10239	0.32054	-0.56676

C	-1.54651	1.65164	0.06559	C	-1.54649	1.65175	0.06560
C	-2.62740	0.59181	-0.16670	C	-2.62736	0.59192	-0.16680
C	-2.03656	-0.52375	-0.83425	C	-2.03649	-0.52355	-0.83451
O	-0.65215	-0.37322	-1.10675	O	-0.65211	-0.37291	-1.10706
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C	4.73898	-1.74085	1.23483	C	4.73884	-1.74104	1.23474
C	4.13636	-1.05919	0.11112	C	4.13630	-1.05922	0.11109
O	-0.26558	1.53999	-3.11626	O	-0.26542	1.54065	-3.11618
C	2.44893	4.59797	-0.24483	C	2.44906	4.59802	-0.24408
C	1.46244	2.36460	0.65030	C	1.46240	2.36455	0.65063
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C	-4.55807	1.82844	0.91203
C	4.74536	-0.81887	-1.26163
O	4.26366	-0.07369	-2.15190
O	5.96568	-1.55898	-1.46177
O	2.22162	-0.99991	3.94757
C	6.48825	-1.28352	-2.81802
C	6.12635	-2.40281	1.10902
O	0.64448	0.67713	2.88423
C	-8.33465	-0.06778	0.97119
H	1.11584	3.76329	-2.53781
H	-0.01835	-0.71414	1.45091

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C	-4.55801	1.82833	0.91220
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H	3.51085	4.32937	-0.10845	H	3.51084	4.32931	-0.10685
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H	-1.56473	-2.54447	-2.80723	H	-1.56540	-2.54428	-2.80815
H	-5.86875	-2.53686	-0.79462	H	-5.86862	-2.53683	-0.79477
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H	5.76555	-1.57827	-3.60608	H	5.76559	-1.57821	-3.60623
H	6.73315	-0.21043	-2.95608	H	6.73308	-0.21040	-2.95599

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H	6.09376	-3.24288	0.39576	H	6.09334	-3.24368	0.39638
H	6.87514	-1.68654	0.73498	H	6.87479	-1.68704	0.73399
H	6.45178	-2.78371	2.08829	H	6.45201	-2.78314	2.08838
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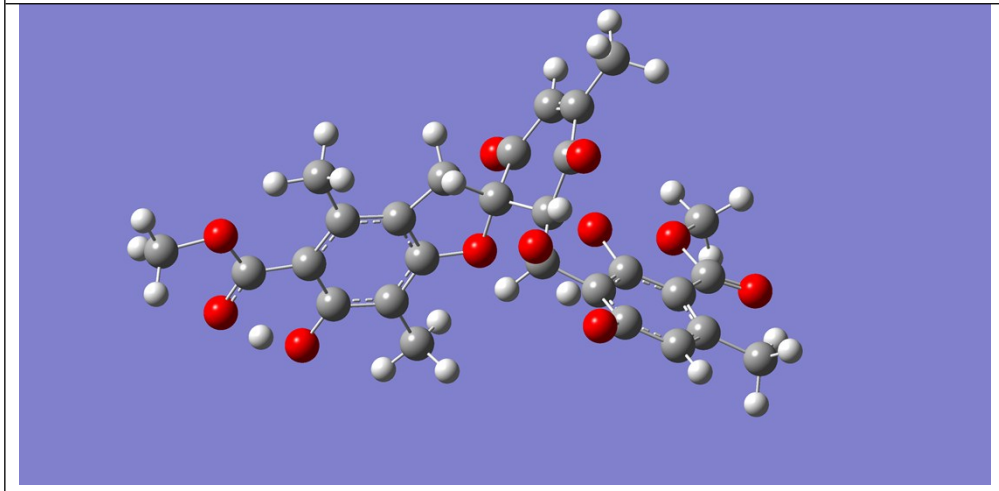				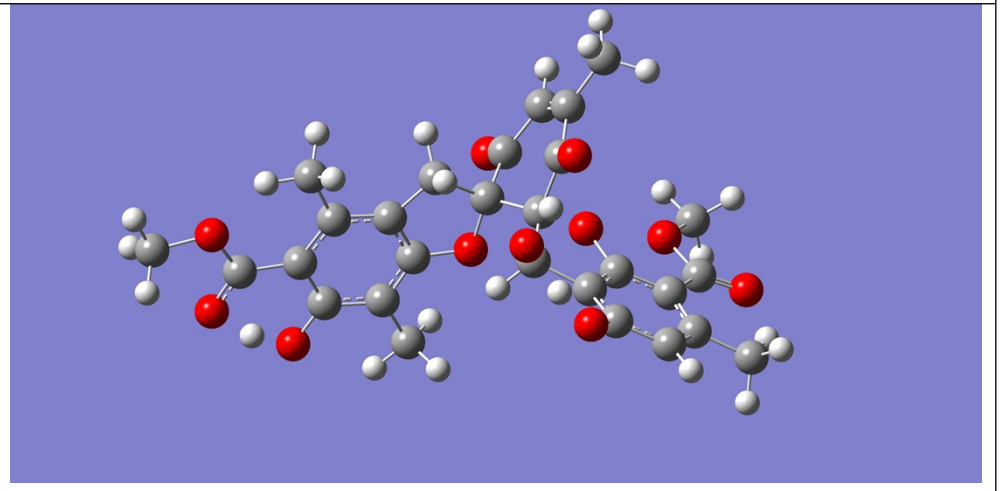			
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C	1.10715	3.31073	-0.94737
C	0.90559	-0.41741	1.53525
C	2.25662	-1.09579	1.35588
C	2.90106	-0.66885	0.19689
O	2.16488	0.35557	-0.49506
C	-1.44987	1.57468	0.47082
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C	-1.99302	-0.32688	-0.89706
O	-0.60667	-0.14645	-1.14179
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O	1.89293	2.10949	2.40068
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O	2.28824	-1.94735	3.60820
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O	0.73713	-0.05037	2.96414
C	-8.26994	-0.16624	1.02844
H	1.22155	4.18104	-1.61347
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H	4.94944	-0.31825	-4.06555	H	4.94897	-0.31904	-4.06576
H	4.03310	1.23544	-3.93480	H	4.03300	1.23487	-3.93505
H	5.68557	1.08348	-3.21401	H	5.68555	1.08261	-3.21448
H	6.86002	-2.54741	1.27564	H	6.04793	-3.82574	0.33654
H	6.04774	-3.82597	0.33592	H	6.51684	-2.28854	-0.48285
H	6.51677	-2.28860	-0.48306	H	6.86026	-2.54693	1.27589
H	1.32077	0.83111	2.98440	H	1.32103	0.83184	2.98429
H	-8.70416	0.56737	1.73234	H	-8.70419	0.56778	1.73230
H	-8.78559	-0.10053	0.04941	H	-8.78577	-0.10014	0.04939
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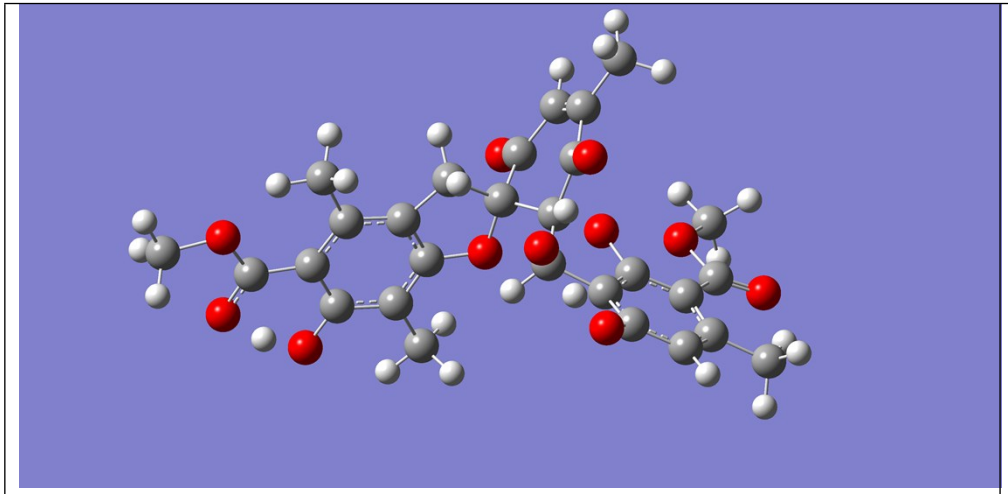	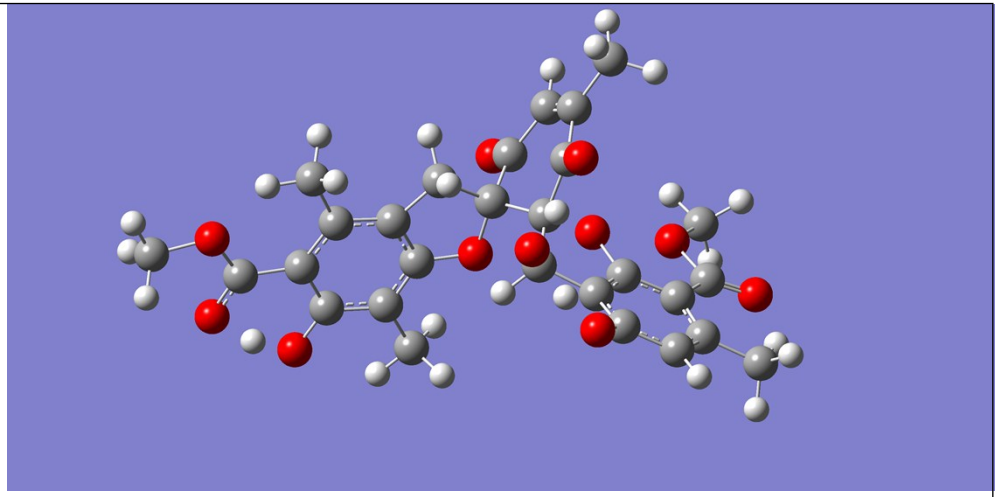
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C 0.21201 2.19296 -1.48147	C 0.21183 2.19240 -1.48183
C 1.10720 3.31075 -0.94742	C 1.10691 3.31044 -0.94805
C 0.90555 -0.41734 1.53525	C 0.90579 -0.41714 1.53544
C 2.25658 -1.09574 1.35591	C 2.25686 -1.09547 1.35613
C 2.90103 -0.66883 0.19692	C 2.90119 -0.66874 0.19700

O	2.16489	0.35559	-0.49505	O	2.16491	0.35549	-0.49512
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C	-2.55538	0.61872	0.01317	C	-2.55545	0.61862	0.01313
C	-1.99299	-0.32685	-0.89708	C	-1.99307	-0.32721	-0.89689
O	-0.60665	-0.14641	-1.14183	O	-0.60669	-0.14694	-1.14152
C	-3.90367	0.57461	0.37198	C	-3.90375	0.57466	0.37191
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C	-2.72849	-1.35795	-1.49577	C	-2.72862	-1.35837	-1.49539
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C	4.18102	-1.18656	-0.15834	C	4.18120	-1.18641	-0.15823
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O	6.02017	-1.11515	-1.86000	O	6.02025	-1.11511	-1.86001
O	4.05180	0.15038	-2.16526	O	4.05163	0.14999	-2.16548
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H	2.51636	5.32549	0.13180	H	2.51636	5.32536	0.13032
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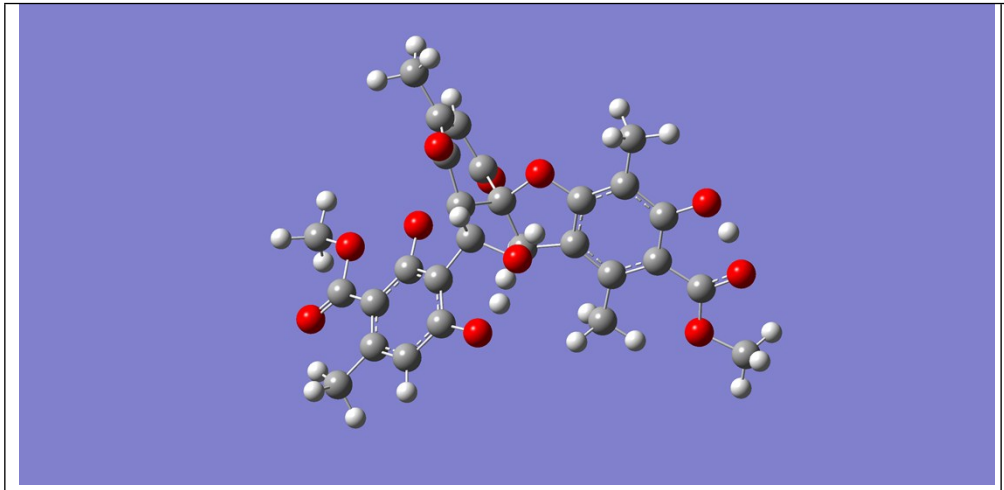
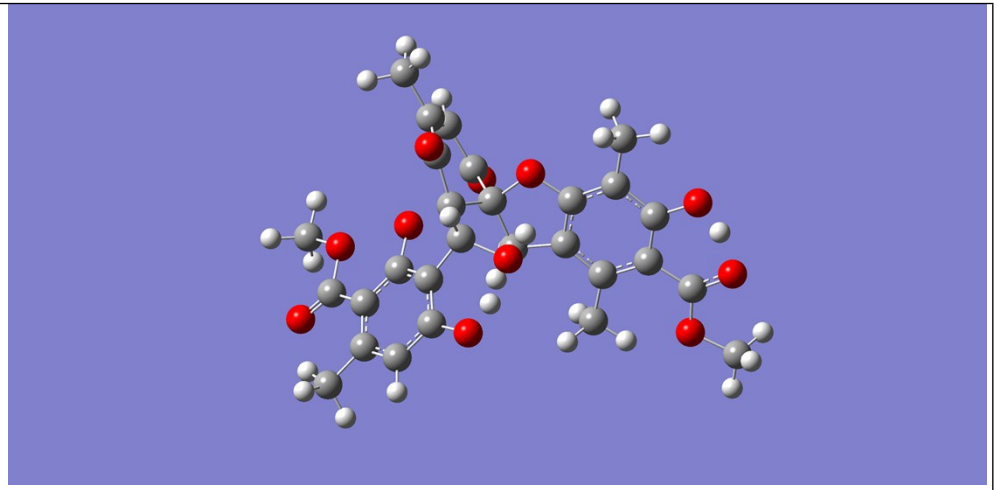
H	6.51673	-2.28867	-0.48296	H	6.04811	-3.82560	0.33655
H	6.85994	-2.54743	1.27575	H	6.51704	-2.28837	-0.48274
H	1.32074	0.83119	2.98438	H	1.32102	0.83173	2.98426
H	-8.78567	-0.10037	0.04957	H	-8.70414	0.56758	1.73259
H	-8.39228	-1.19233	1.42972	H	-8.78583	-0.10012	0.04960
H	-8.70405	0.56717	1.73263	H	-8.39241	-1.19196	1.42984

Cartesian coordinates of conformers of the 8S,3'R,4'S-**3**

							
C	-1.91253	3.61310	-0.01272	C	-1.91270	3.61298	-0.01238
C	-1.31957	1.10386	0.57727	C	-1.31946	1.10372	0.57722
C	-0.14961	1.24082	-0.47777	C	-0.14961	1.24091	-0.47792
C	-0.68023	2.15082	-1.68282	C	-0.68035	2.15106	-1.68277
C	-1.43160	3.40185	-1.26484	C	-1.43193	3.40190	-1.26459
C	-1.04125	0.17446	1.84486	C	-1.04098	0.17420	1.84470
C	-1.96025	-0.99149	1.55195	C	-1.96015	-0.99164	1.55188
C	-2.80314	-0.71643	0.47082	C	-2.80311	-0.71650	0.47082
O	-2.53195	0.54417	-0.14483	O	-2.53185	0.54408	-0.14483

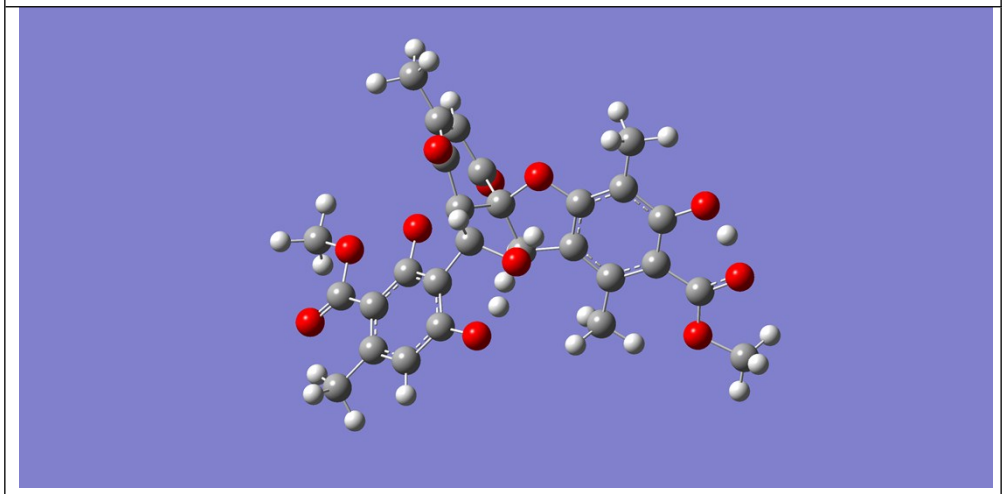
C	0.46032	-0.10034	-1.03314
C	1.93607	0.01927	-0.63955
C	2.12702	1.25615	0.04765
O	0.94292	2.02069	0.20981
C	2.99889	-0.85775	-0.86566
C	4.29938	-0.47104	-0.38069
C	4.48311	0.80133	0.32243
C	3.36592	1.68727	0.54185
C	-1.87701	-2.26237	2.16569
C	-2.85781	-3.22392	1.77044
C	-3.79456	-2.92483	0.75695
C	-3.77813	-1.66968	0.04755
O	-0.45122	1.85074	-2.88304
C	-2.65005	4.89466	0.39843
C	-1.73850	2.55796	1.08187
O	-1.94440	2.78761	2.30196

C	0.46038	-0.10013	-1.03350
C	1.93611	0.01944	-0.63981
C	2.12703	1.25625	0.04750
O	0.94293	2.02079	0.20968
C	2.99894	-0.85759	-0.86588
C	4.29938	-0.47095	-0.38077
C	4.48309	0.80139	0.32243
C	3.36591	1.68731	0.54183
C	-1.87691	-2.26258	2.16551
C	-2.85781	-3.22404	1.77030
C	-3.79465	-2.92485	0.75693
C	-3.77820	-1.66966	0.04759
O	-0.45127	1.85126	-2.88305
C	-2.65029	4.89443	0.39898
C	-1.73831	2.55779	1.08210
O	-1.94387	2.78731	2.30226

C	3.56489	3.01843	1.27260
O	5.70843	1.18618	0.78878
C	5.55467	-1.25494	-0.52068
O	5.49476	-2.50277	-1.18565
O	6.69622	-0.84327	-0.06028
C	2.73341	-2.17782	-1.61228
C	-4.72189	-1.38502	-1.10845
O	-5.60662	-2.13439	-1.60347
O	-4.47859	-0.06276	-1.61750
O	-0.83505	-2.52238	3.05396
C	-5.39349	0.21144	-2.74797
C	-4.83066	-3.99992	0.37041
O	0.30206	-0.41164	2.08001
C	6.83513	-3.13874	-1.23126
H	-1.58681	4.15412	-2.05391
H	-1.35202	0.78422	2.73226

C	3.56474	3.01843	1.27271
O	5.70838	1.18614	0.78898
C	5.55464	-1.25492	-0.52063
O	5.49476	-2.50270	-1.18569
O	6.69615	-0.84334	-0.06004
C	2.73348	-2.17761	-1.61260
C	-4.72201	-1.38489	-1.10833
O	-5.60681	-2.13419	-1.60334
O	-4.47865	-0.06263	-1.61736
O	-0.83484	-2.52272	3.05361
C	-5.39359	0.21163	-2.74778
C	-4.83087	-3.99983	0.37044
O	0.30231	-0.41206	2.07959
C	6.83509	-3.13876	-1.23124
H	-1.58739	4.15419	-2.05359
H	-1.35152	0.78396	2.73219

H	-0.03470	-0.98882	-0.60357	H	-0.03465	-0.98870	-0.60415
H	0.31558	-0.10372	-2.13206	H	0.31571	-0.10328	-2.13244
H	-2.86120	-4.21631	2.23664	H	-2.86120	-4.21646	2.23644
H	-2.59998	5.64995	-0.39942	H	-2.60191	5.64913	-0.39953
H	-3.70971	4.67300	0.61396	H	-3.70947	4.67234	0.61641
H	-2.20307	5.30560	1.31920	H	-2.20206	5.30637	1.31870
H	4.63719	3.14960	1.48344	H	4.63689	3.14904	1.48471
H	3.21316	3.86596	0.66077	H	3.21423	3.86616	0.66044
H	3.01301	3.04310	2.22796	H	3.01174	3.04340	2.22740
H	6.33660	0.34079	0.48039	H	6.33654	0.34070	0.48065
H	1.99284	-2.78235	-1.06292	H	2.32133	-1.97077	-2.61401
H	2.32140	-1.97103	-2.61377	H	3.66848	-2.74695	-1.71205
H	3.66837	-2.74723	-1.71158	H	1.99304	-2.78227	-1.06320
H	-0.20763	-1.69078	2.85411	H	-0.20739	-1.69117	2.85372
H	-5.24189	-0.50316	-3.58252	H	-5.15318	1.23495	-3.09037
H	-6.45718	0.16377	-2.43721	H	-5.24255	-0.50339	-3.58208

H	-5.15357	1.23502	-3.09013	H	-6.45726	0.16468	-2.43680
H	-4.32773	-4.94653	0.11766	H	-4.32804	-4.94649	0.11765
H	-5.51307	-4.19141	1.21449	H	-5.51325	-4.19127	1.21454
H	-5.40546	-3.62855	-0.49751	H	-5.40568	-3.62840	-0.49745
H	0.79593	0.30039	2.62580	H	0.79638	0.29989	2.62531
H	6.68730	-4.09652	-1.76323	H	6.68736	-4.09619	-1.76386
H	7.56239	-2.50945	-1.78242	H	7.56261	-2.50919	-1.78173
H	7.22653	-3.32995	-0.21199	H	7.22610	-3.33066	-0.21195
							
C	-1.91264	3.61300	-0.01243				

C	-1.31946	1.10373	0.57722
C	-0.14959	1.24090	-0.47789
C	-0.68033	2.15102	-1.68278
C	-1.43186	3.40190	-1.26463
C	-1.04102	0.17424	1.84473
C	-1.96018	-0.99160	1.55188
C	-2.80314	-0.71646	0.47082
O	-2.53185	0.54411	-0.14484
C	0.46039	-0.10016	-1.03344
C	1.93612	0.01941	-0.63978
C	2.12704	1.25623	0.04753
O	0.94294	2.02076	0.20971
C	2.99893	-0.85762	-0.86586
C	4.29940	-0.47098	-0.38078
C	4.48311	0.80136	0.32240
C	3.36593	1.68729	0.54182

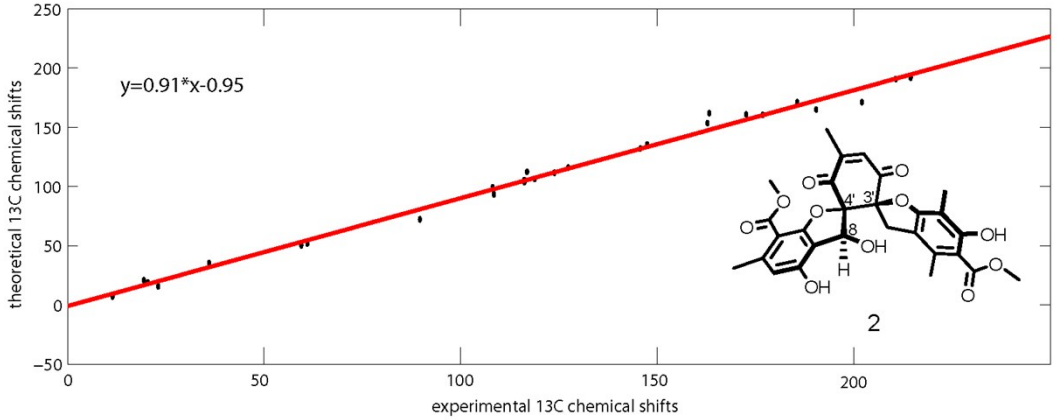
C	-1.87696	-2.26252	2.16553
C	-2.85786	-3.22399	1.77033
C	-3.79469	-2.92480	0.75696
C	-3.77823	-1.66962	0.04759
O	-0.45128	1.85116	-2.88306
C	-2.65025	4.89445	0.39890
C	-1.73828	2.55782	1.08207
O	-1.94380	2.78739	2.30223
C	3.56486	3.01840	1.27269
O	5.70839	1.18610	0.78896
C	5.55466	-1.25495	-0.52065
O	5.49477	-2.50273	-1.18571
O	6.69618	-0.84337	-0.06009
C	2.73346	-2.17766	-1.61255
C	-4.72207	-1.38487	-1.10832
O	-5.60693	-2.13414	-1.60326

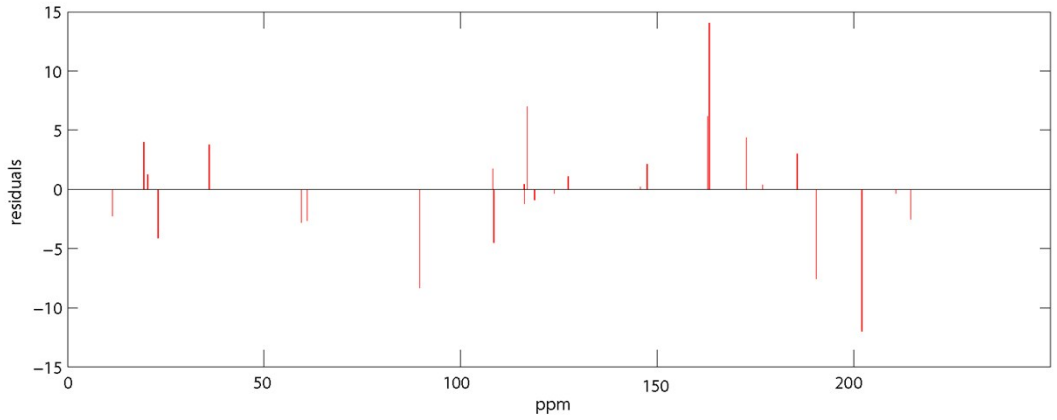
O	-4.47864	-0.06266	-1.61745
O	-0.83489	-2.52265	3.05364
C	-5.39360	0.21154	-2.74787
C	-4.83090	-3.99979	0.37047
O	0.30227	-0.41202	2.07967
C	6.83511	-3.13875	-1.23122
H	-1.58729	4.15418	-2.05364
H	-1.35158	0.78400	2.73220
H	-0.03464	-0.98872	-0.60406
H	0.31568	-0.10335	-2.13238
H	-2.86126	-4.21640	2.23649
H	-2.60117	5.64945	-0.39928
H	-3.70963	4.67250	0.61550
H	-2.20258	5.30592	1.31910
H	4.63700	3.14892	1.48477
H	3.21447	3.86612	0.66035

H	3.01180	3.04350	2.22735
H	6.33656	0.34069	0.48061
H	1.99309	-2.78234	-1.06309
H	2.32122	-1.97083	-2.61394
H	3.66848	-2.74696	-1.71207
H	-0.20745	-1.69108	2.85374
H	-6.45724	0.16540	-2.43669
H	-5.15264	1.23453	-3.09103
H	-5.24313	-0.50401	-3.58181
H	-4.32806	-4.94642	0.11759
H	-5.51322	-4.19130	1.21461
H	-5.40577	-3.62832	-0.49736
H	0.79632	0.29988	2.62546
H	6.68738	-4.09629	-1.76364
H	7.56257	-2.50926	-1.78188
H	7.22621	-3.33043	-0.21191

*Calculation results for compound **2***

	R2	RMSD	DP4
8S,3'R,4'S	0,9932	2,898645426	0%
8R,3'R,4'S	0,9957	**2,704296412**	1,2%
8R,3'S,4'R	0,9932	2,897847248	0%
8R,3'S,4'S	**0,9959**	2,717420034	**98,6%**





*Calculation results for compound **3***

	R2	RMSD	DP4
8S,3'R,4'S	0,9954	2,852029384	0%
8R,3'R,4'S	**0,9973**	**2,6351447**	**99,90%**
8R,3'S,4'R	0,9954	2,8514905	0%
8R,3'S,4'S	0,9970	2,681839412	0%