Supplementary Materials

Bioactive Polyphenols from *Isodon serra* with Antioxidant and Hepatoprotective Activities *in vitro* and *in vivo*

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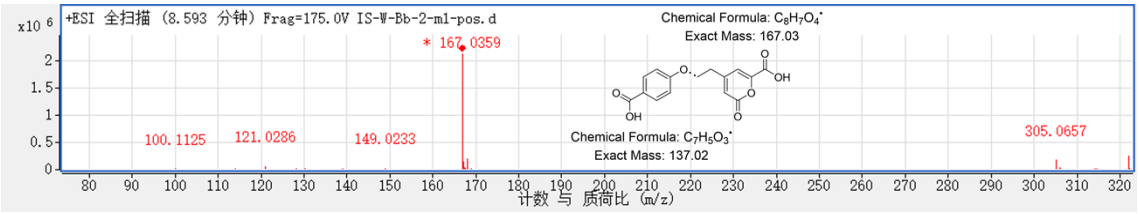


Formula (M)	Score (MFG)	Mass	Mass (MFG)	*m/z* (Calc)	Diff (ppm)	*m/z*
$C_{15}H_{12}O_7$	99.95	304.0584	304.0583	305.0656	-0.4	305.0657

Fig. S1. HR-ESI-MS spectrum of compound **1**

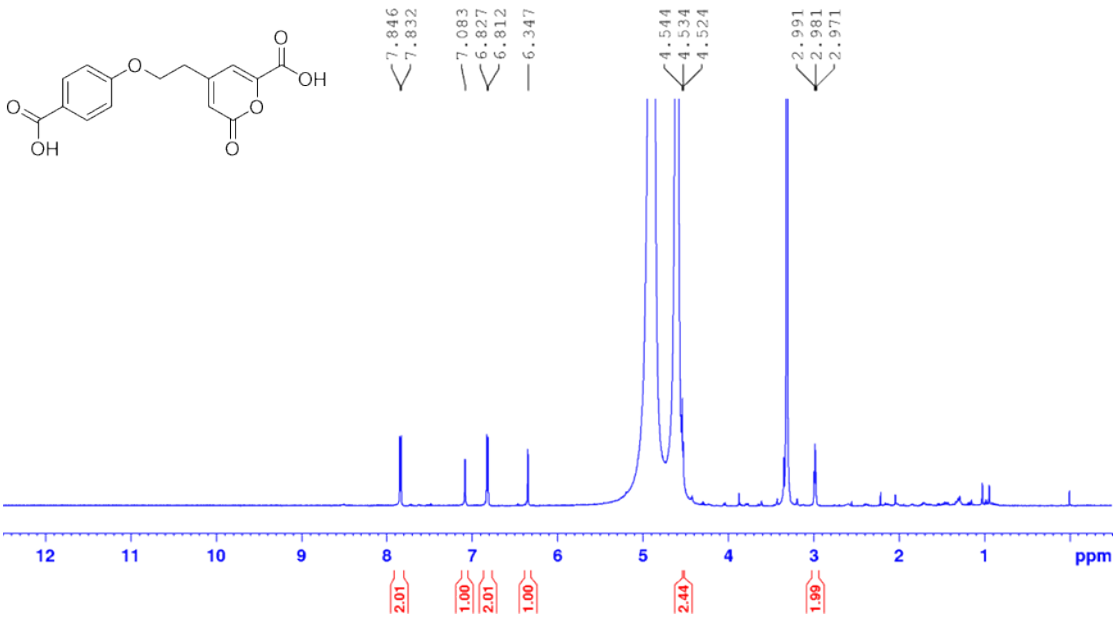


Fig. S2. ^{1}H NMR spectrum for compound **1**

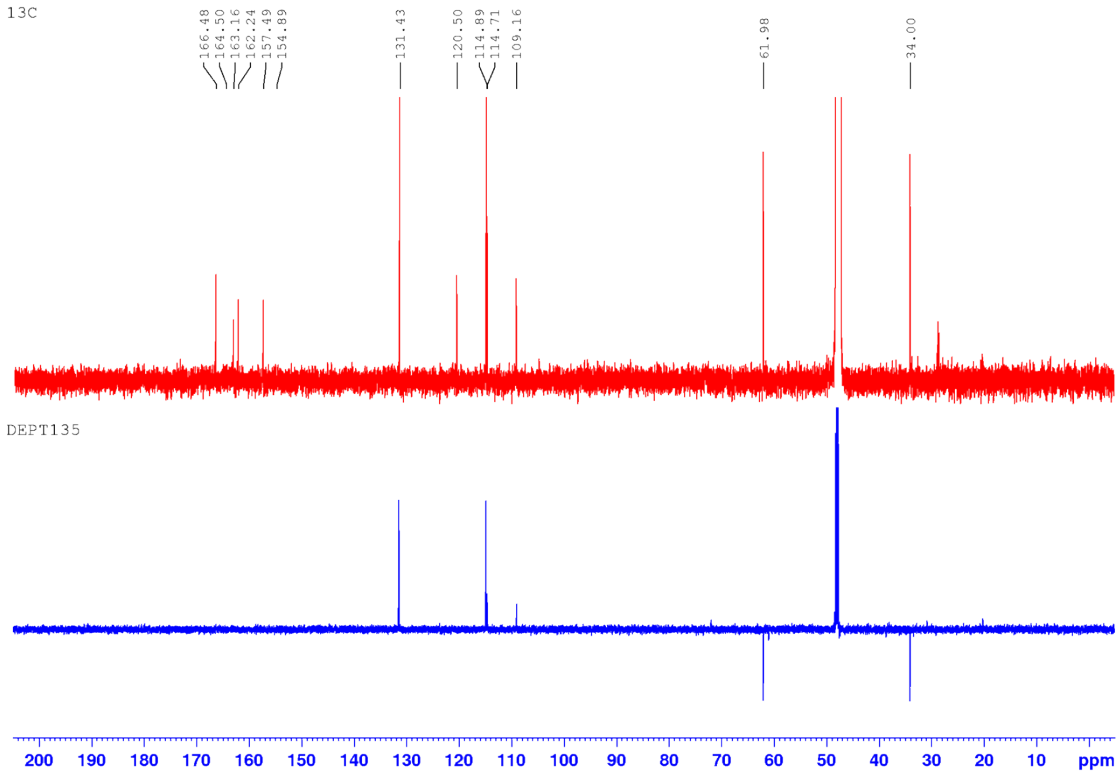


Fig. S3. ^{13}C and DEPT135 NMR spectra for compound **1**

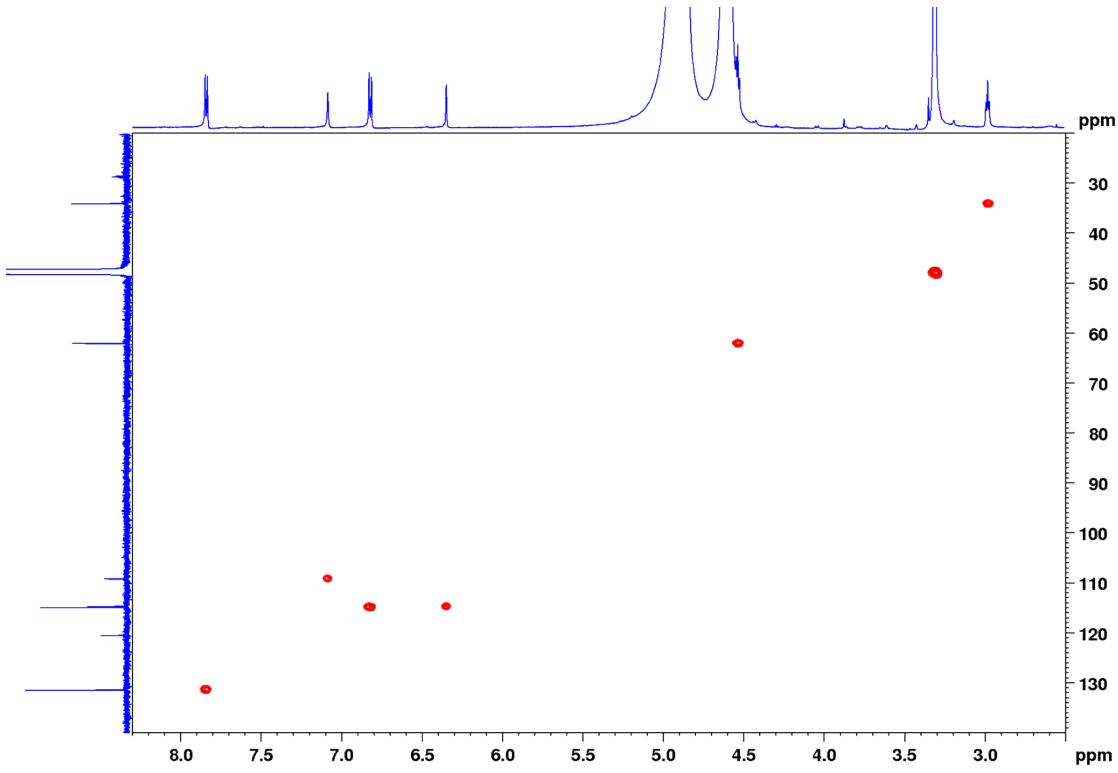


Fig. S4. HSQC NMR spectrum for compound **1**

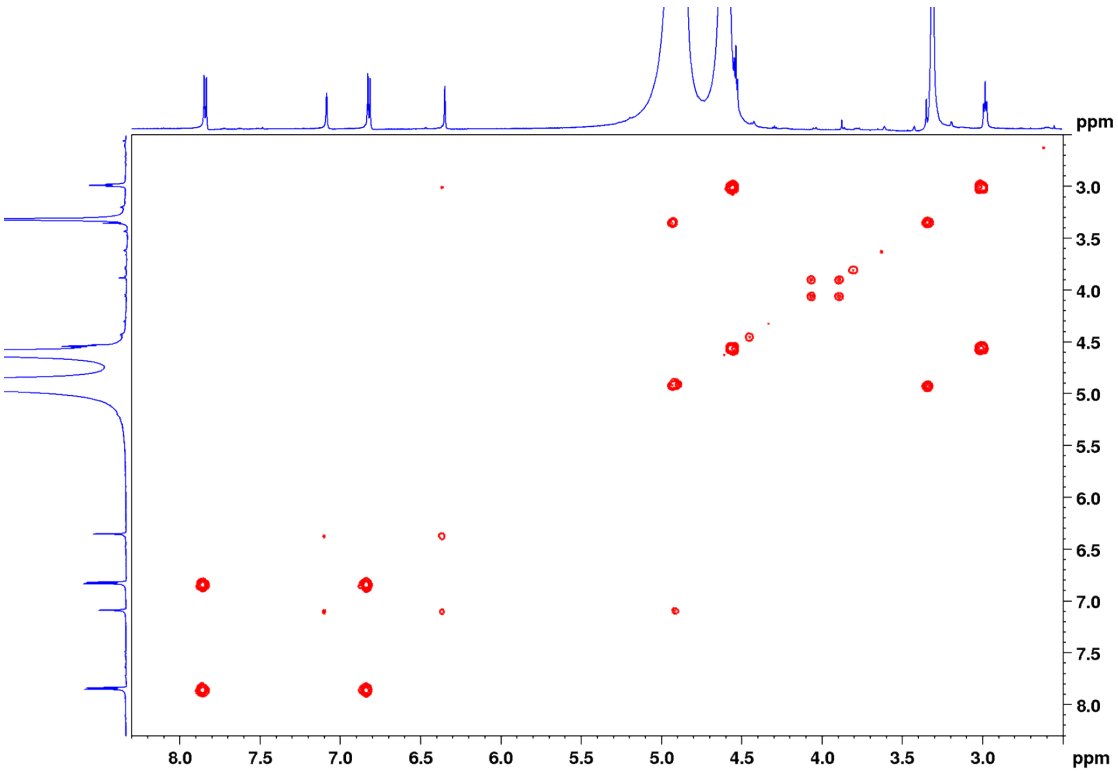


Fig. S5. ^{1}H–^{1}H COSY NMR spectrum for compound **1**

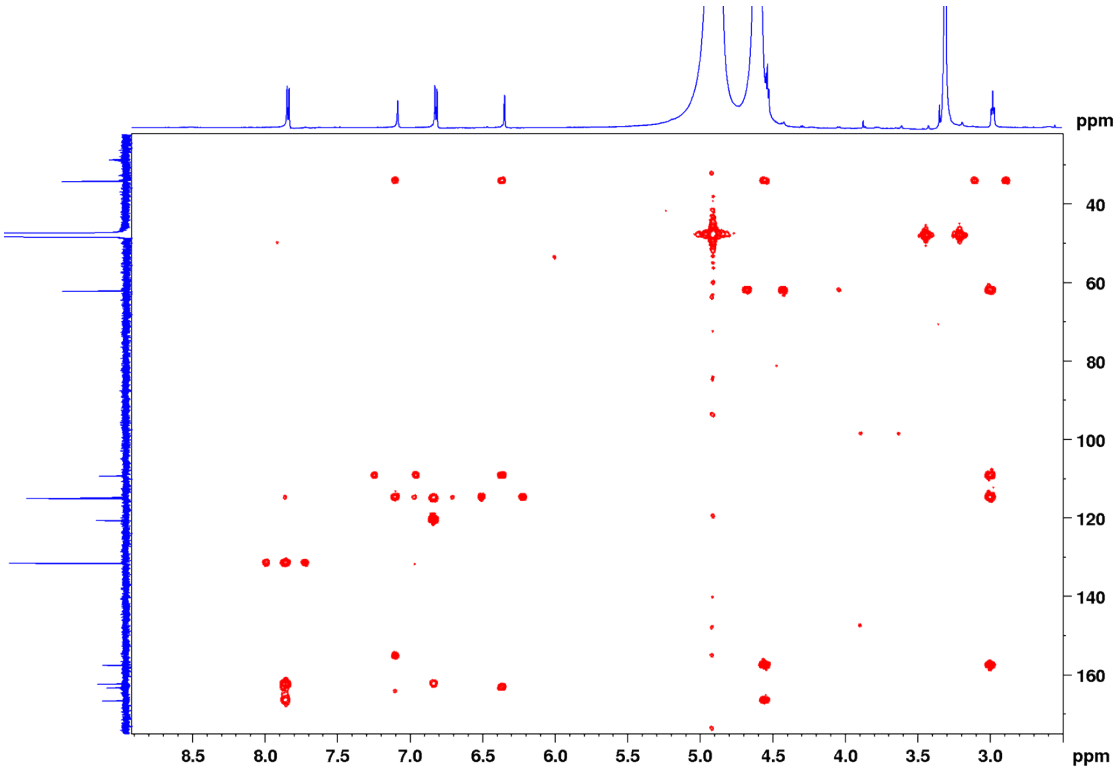


Fig. S6. HMBC NMR spectrum for compound **1**

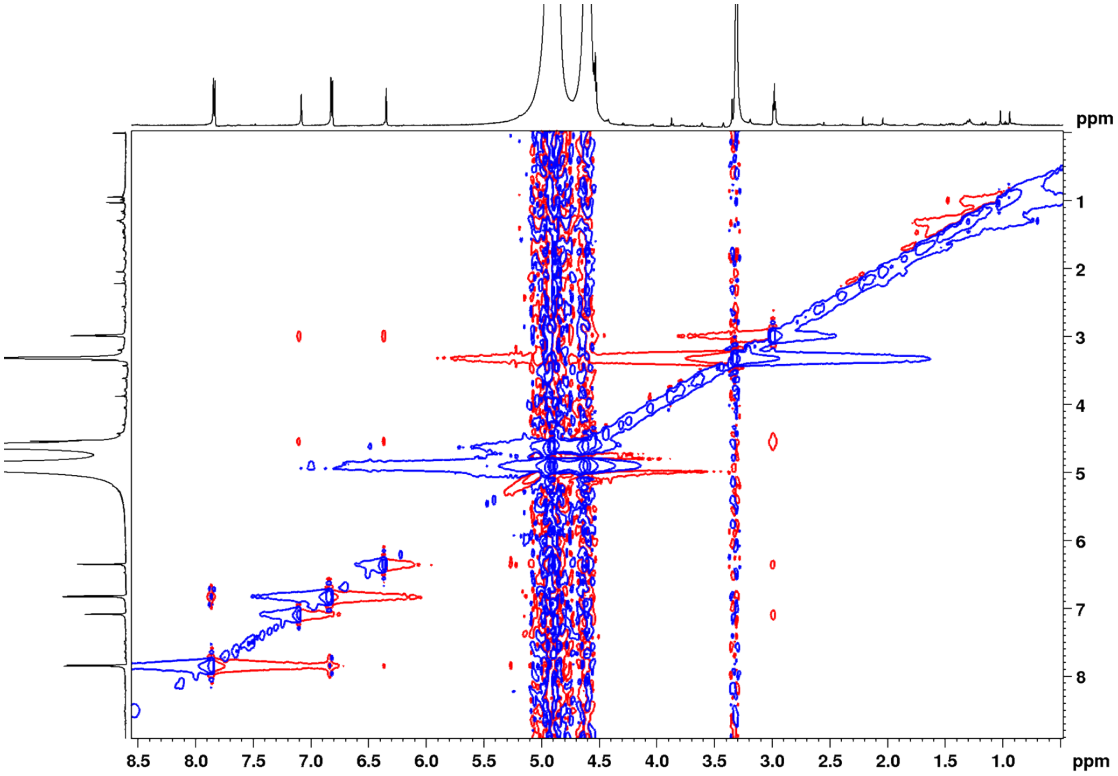


Fig. S7. NOESY NMR spectrum for compound **1**

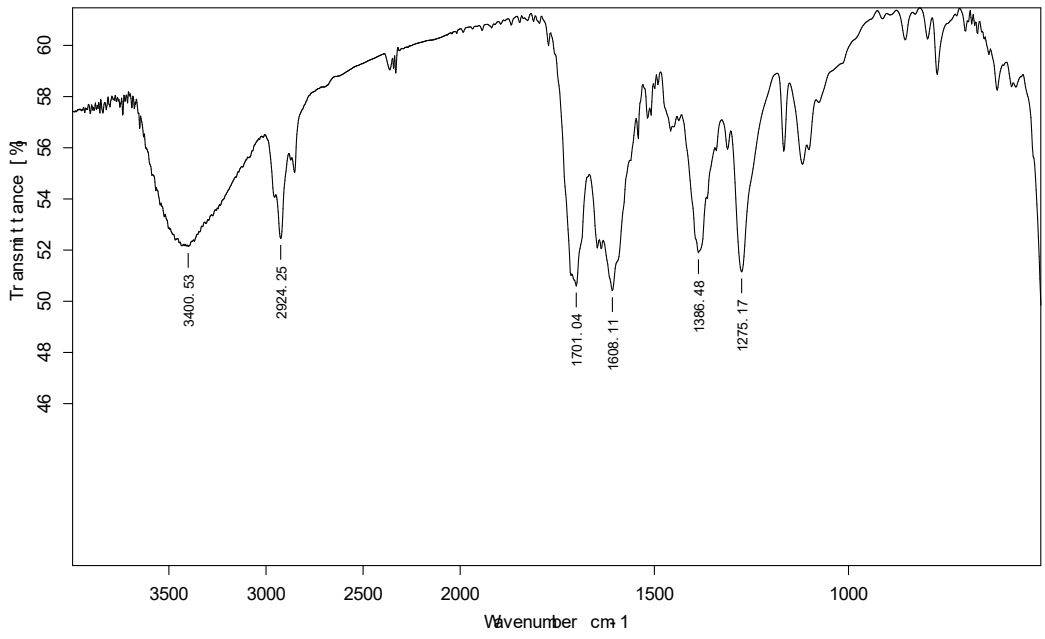


Fig. S8. IR spectrum of compound **1** (KBr)

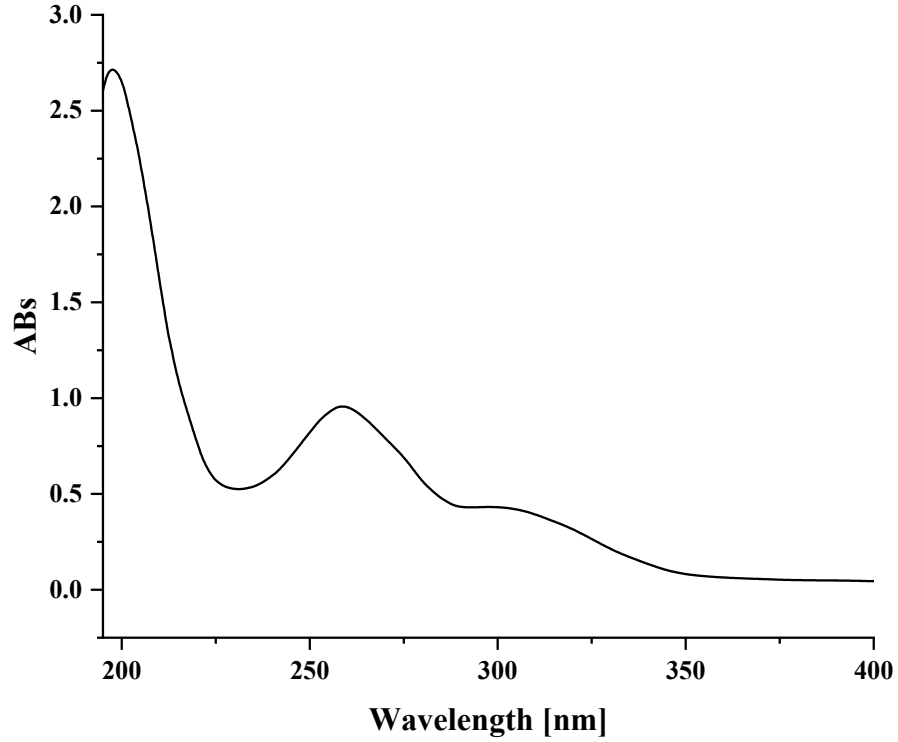


Fig. S9. UV spectrum of compound **1** in MeOH

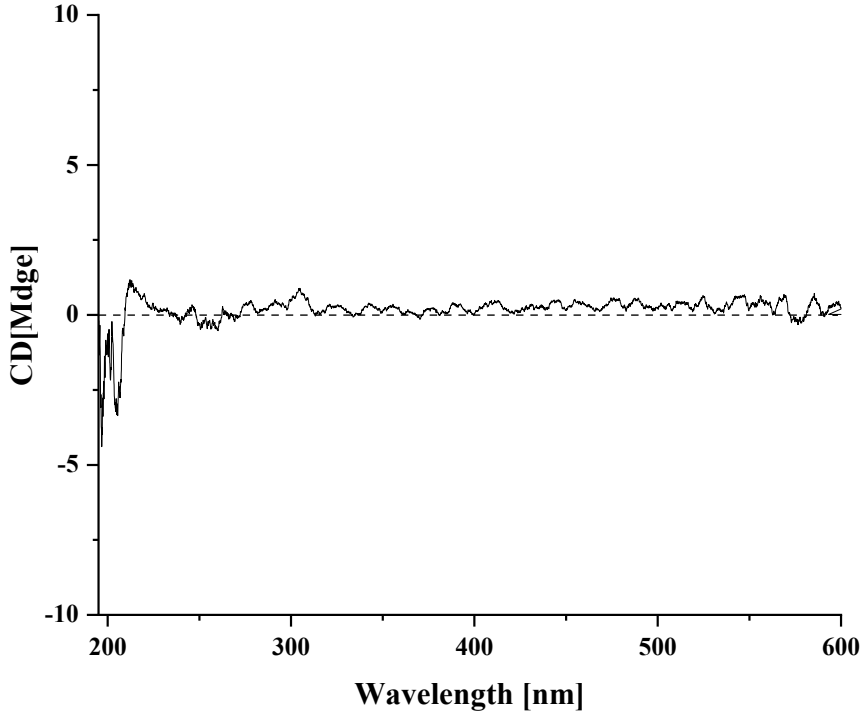
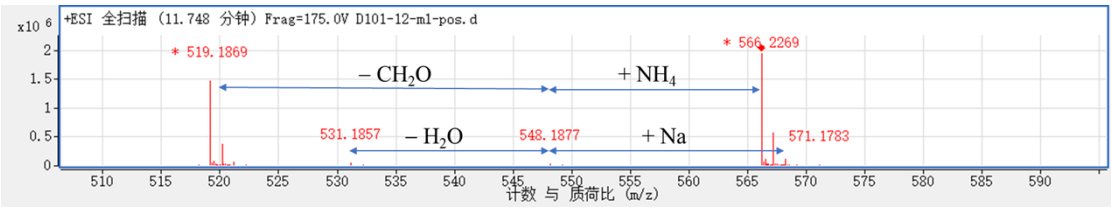


Fig. S10. CD spectrum of compound **1** in MeOH



Formula (M)	Score (MFG)	Mass	Mass (MFG)	*m/z* (Calc)	Diff (ppm)	*m/z*
$C_{27}H_{32}O_{12}$	99.84	548.1891	548.1894	571.1786	0.54	571.1783

Fig. S11. HR-ESI-MS spectrum of compound **2**

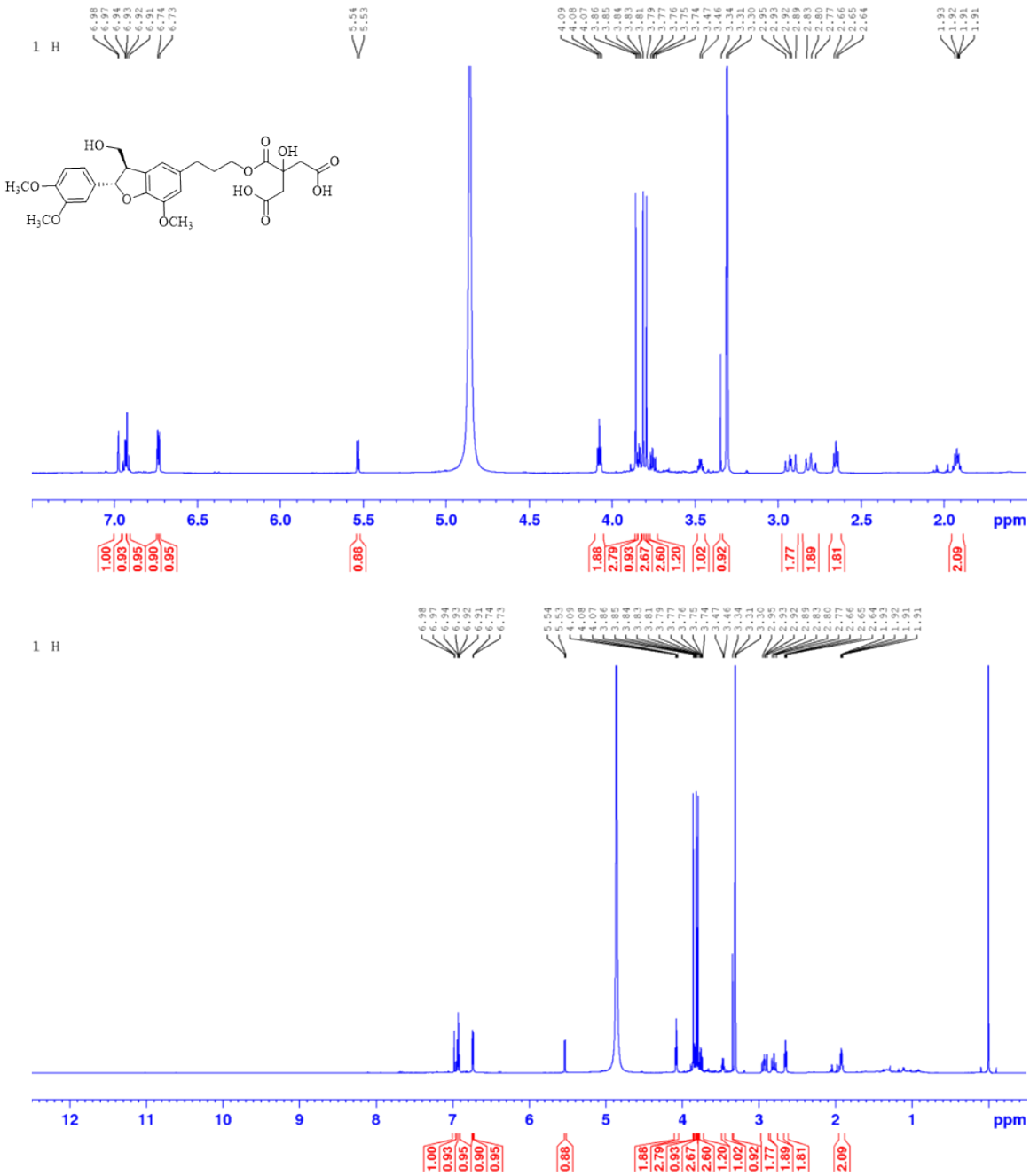


Fig. S12. ^{1}H NMR spectrum for compound **2**

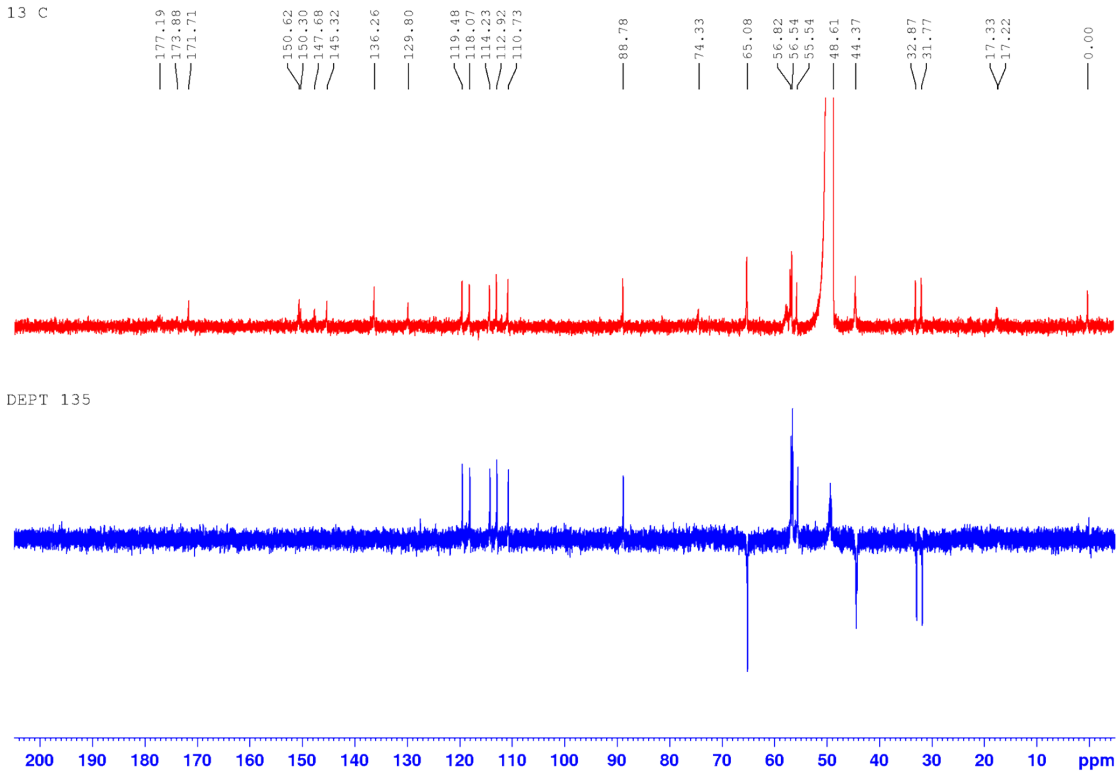


Fig. S13. ^{13}C and DEPT135 NMR spectra for compound **2**

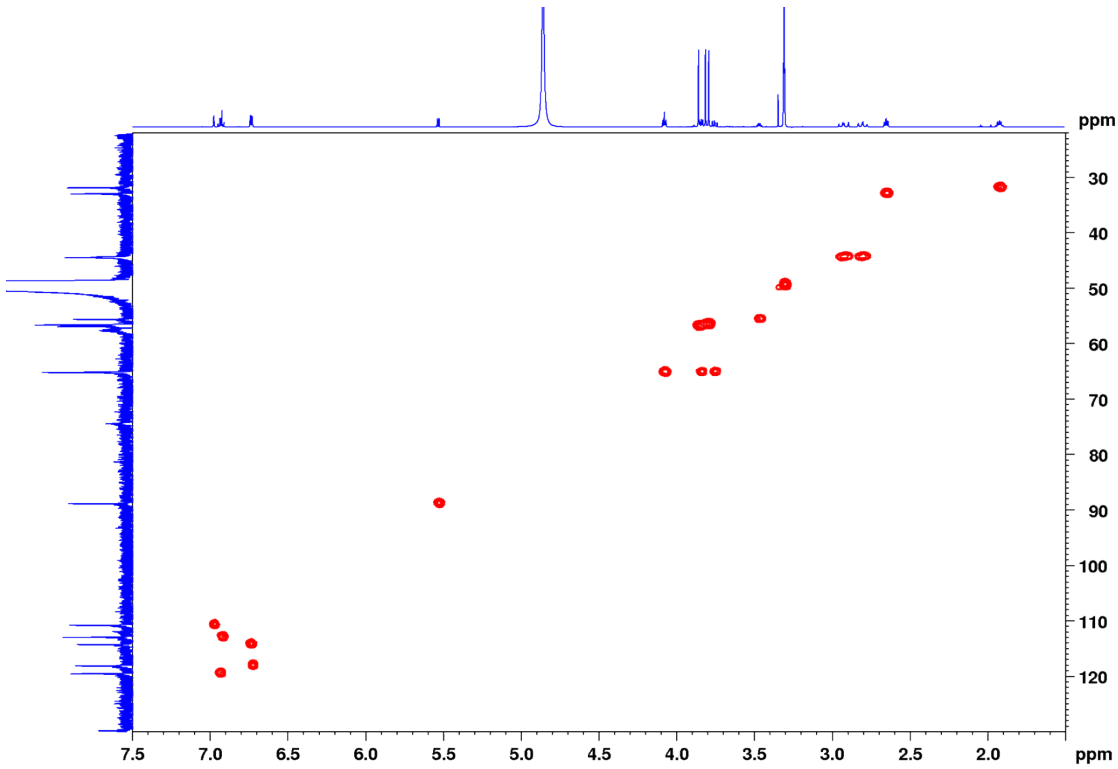


Fig. S14. HSQC NMR spectrum for compound **2**

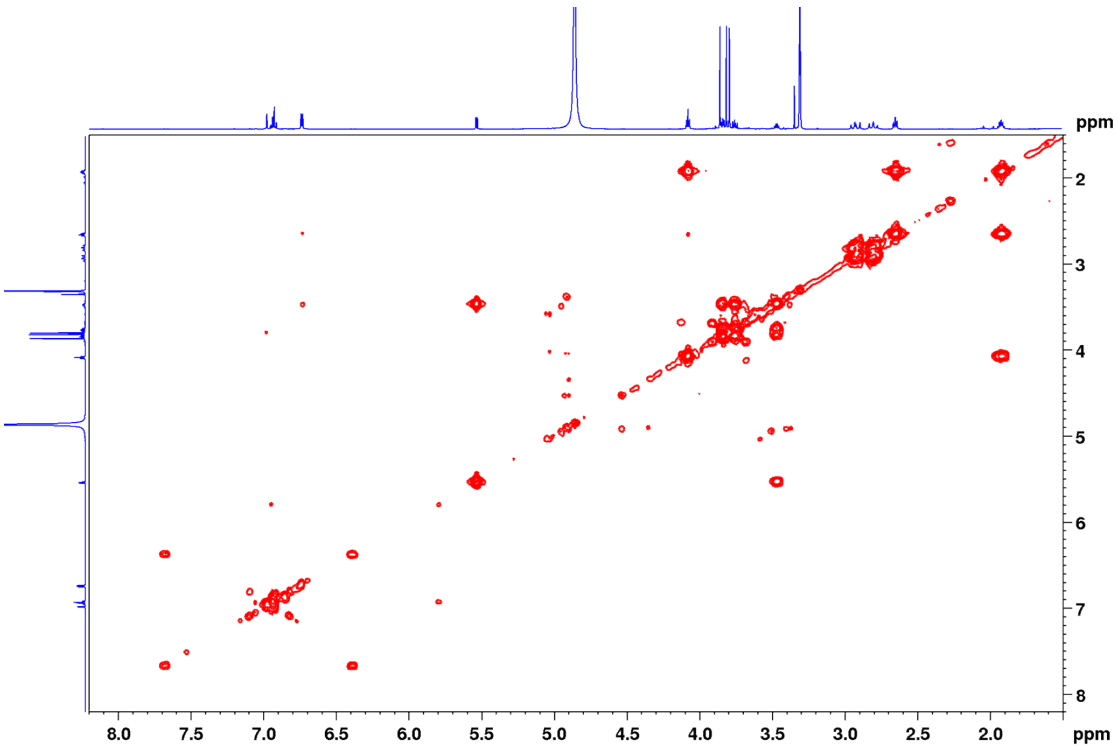


Fig. S15. ^{1}H–^{1}H COSY NMR spectrum for compound **2**

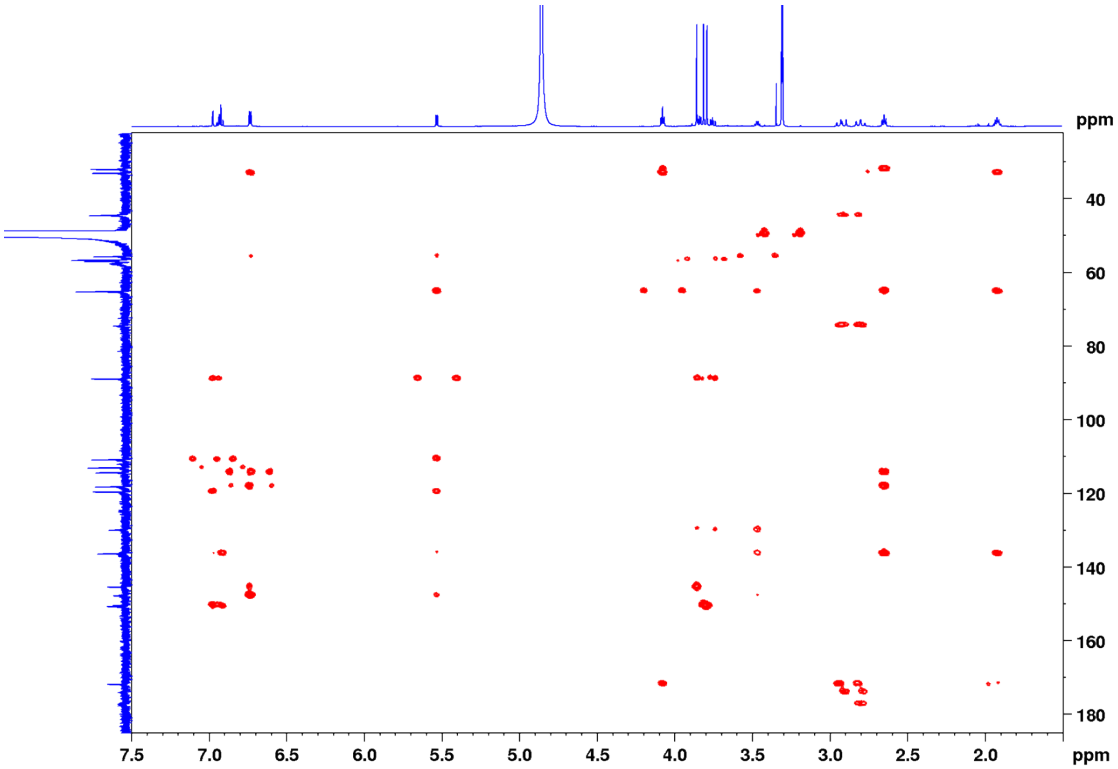


Fig. S16. HMBC NMR spectrum for compound **2**

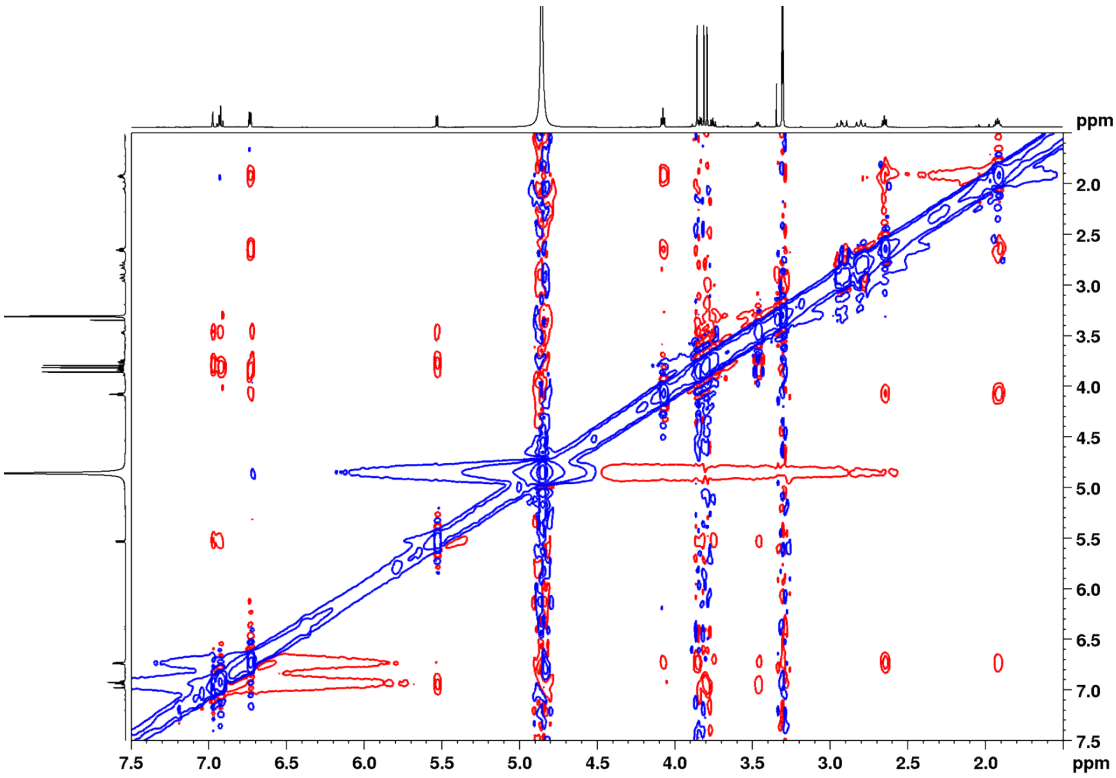


Fig. S17. NOESY NMR spectrum for compound **2**

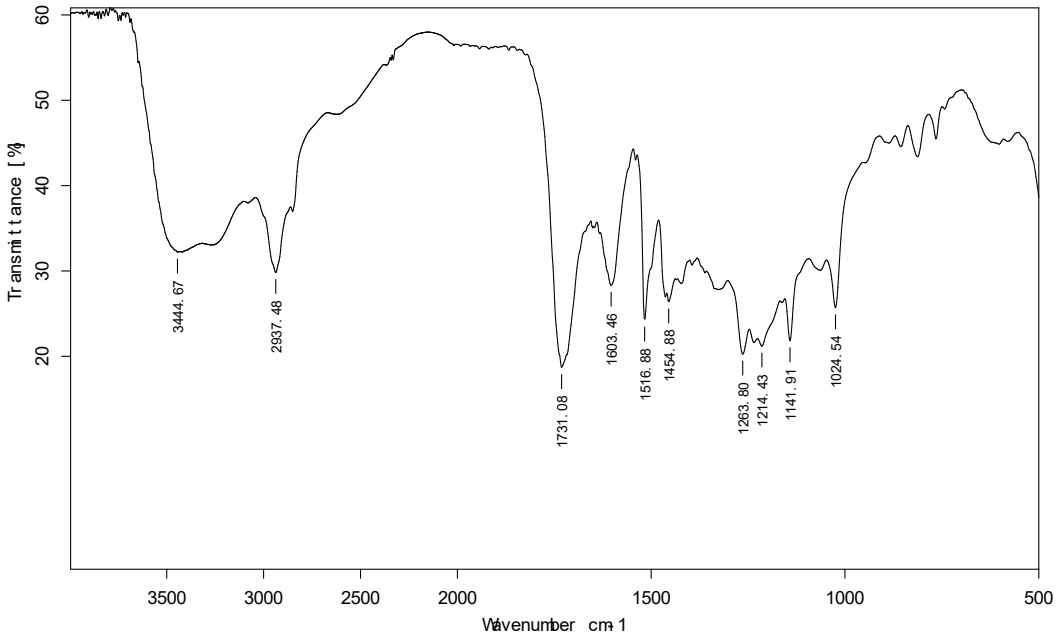


Fig. S18. IR spectrum of compound **2** (KBr)

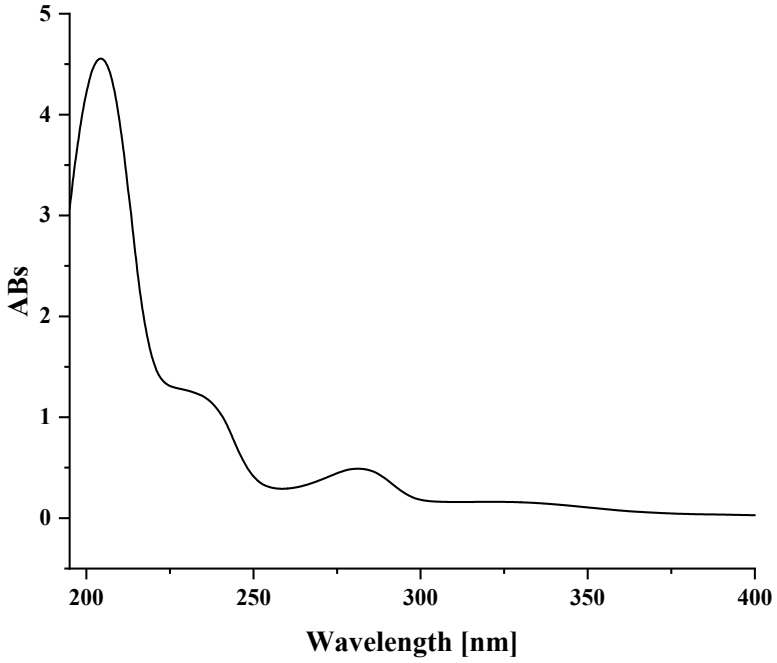


Fig. S19. UV spectrum of compound **2** in MeOH

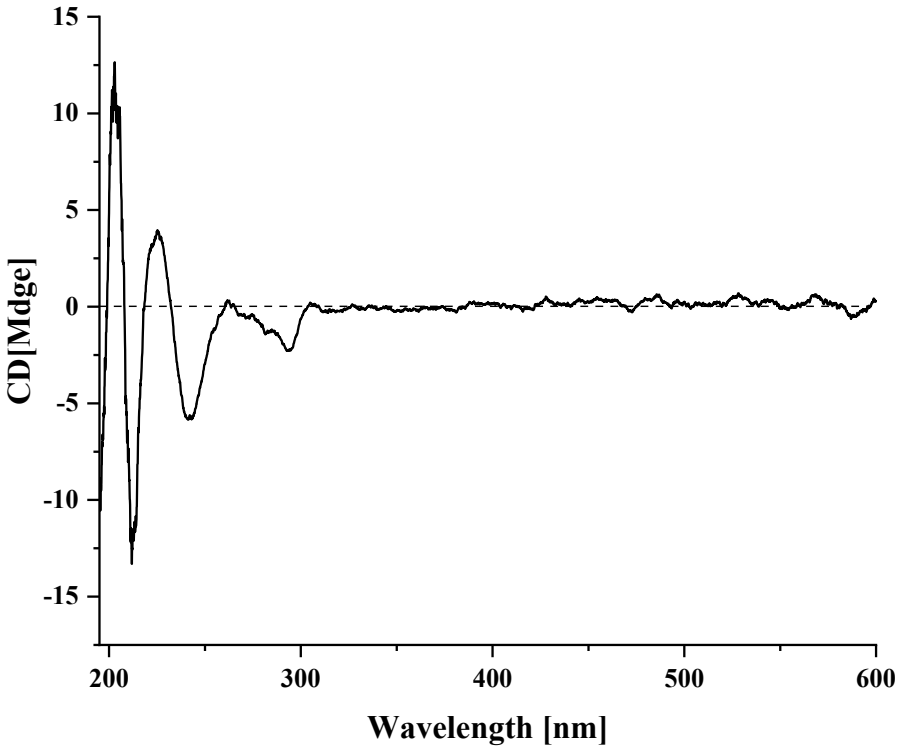
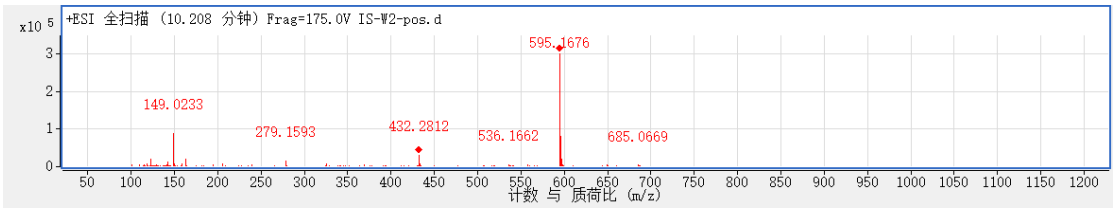


Fig. S20. CD spectrum of compound **2** in MeOH



Formula (M)	Score (MFG)	Mass	Mass (MFG)	*m/z* (Calc)	Diff (ppm)	*m/z*
$C_{27}H_{30}O_{15}$	94.57	594.1603	594.1585	595.1657	-3.12	571.1676

Fig. S21. HR-ESI-MS spectrum of compound **3**

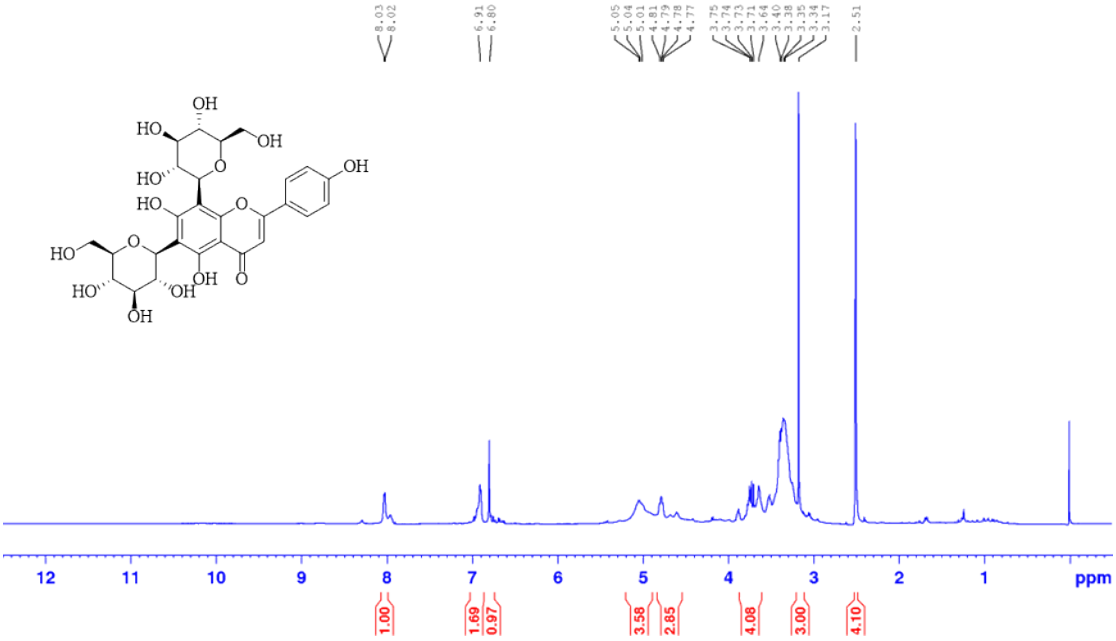


Fig. S22. ^{1}H NMR spectrum for compound **3**

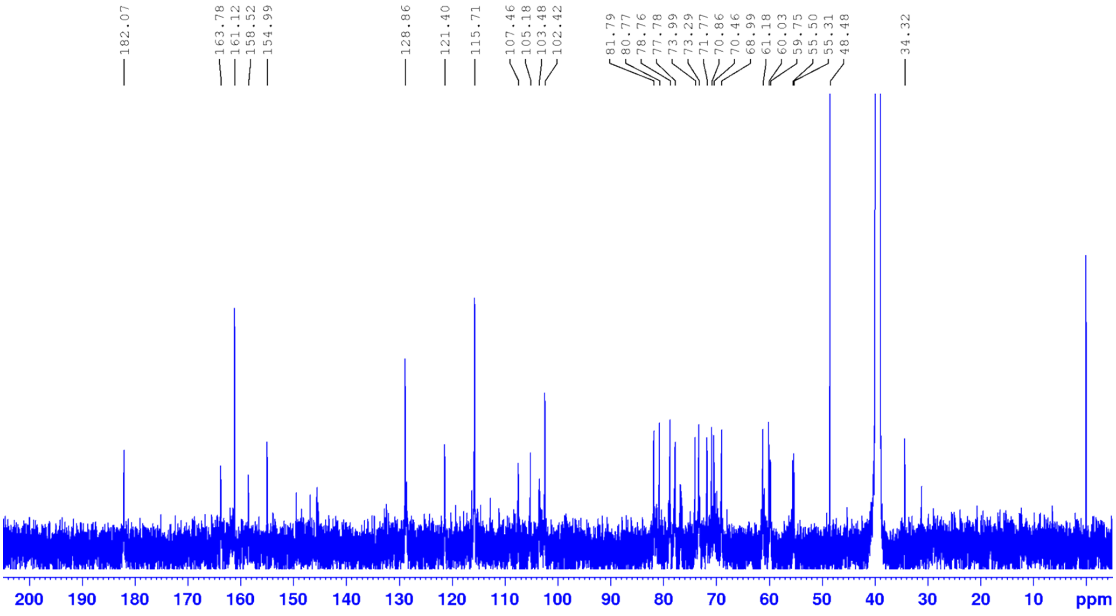


Fig. S23. ^{13}C NMR spectrum for compound **3**

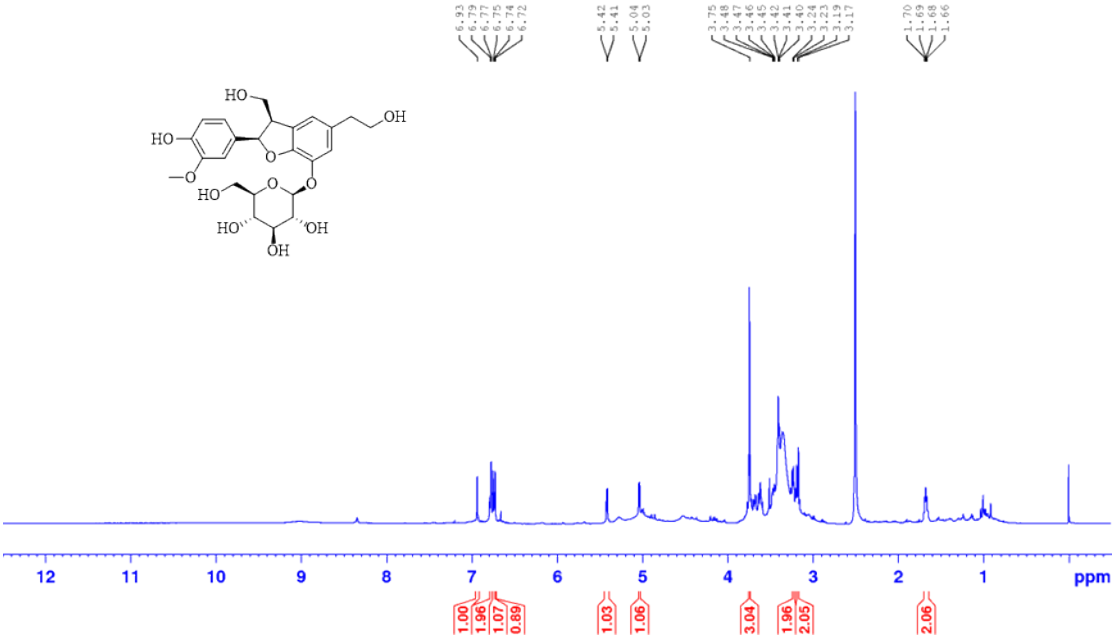


Fig. S24. ^{1}H NMR spectrum for compound **4**

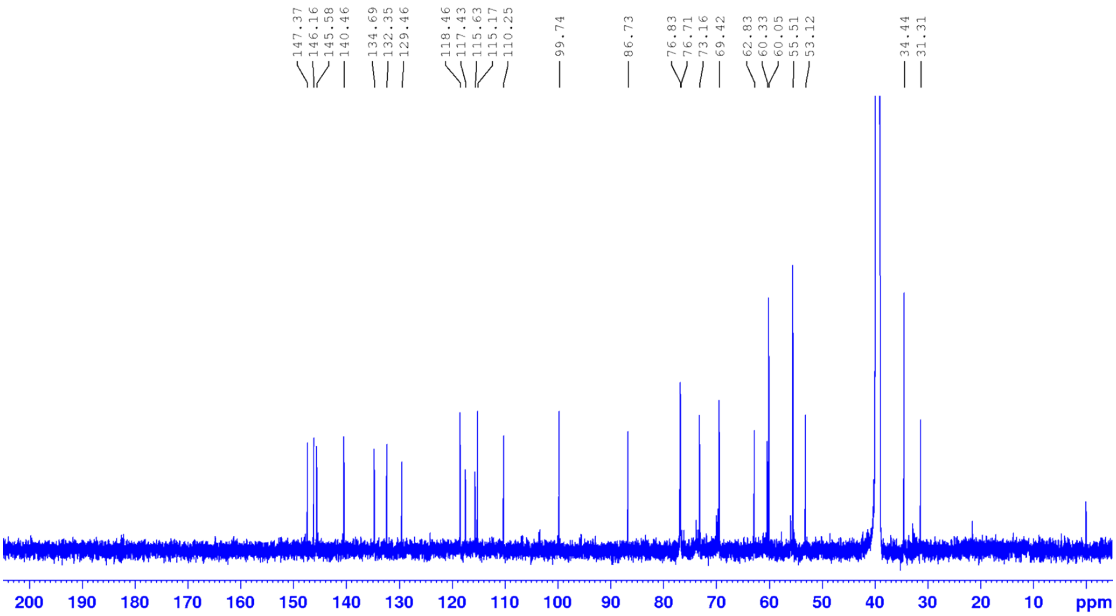


Fig. S25. ^{13}C NMR spectrum for compound **4**

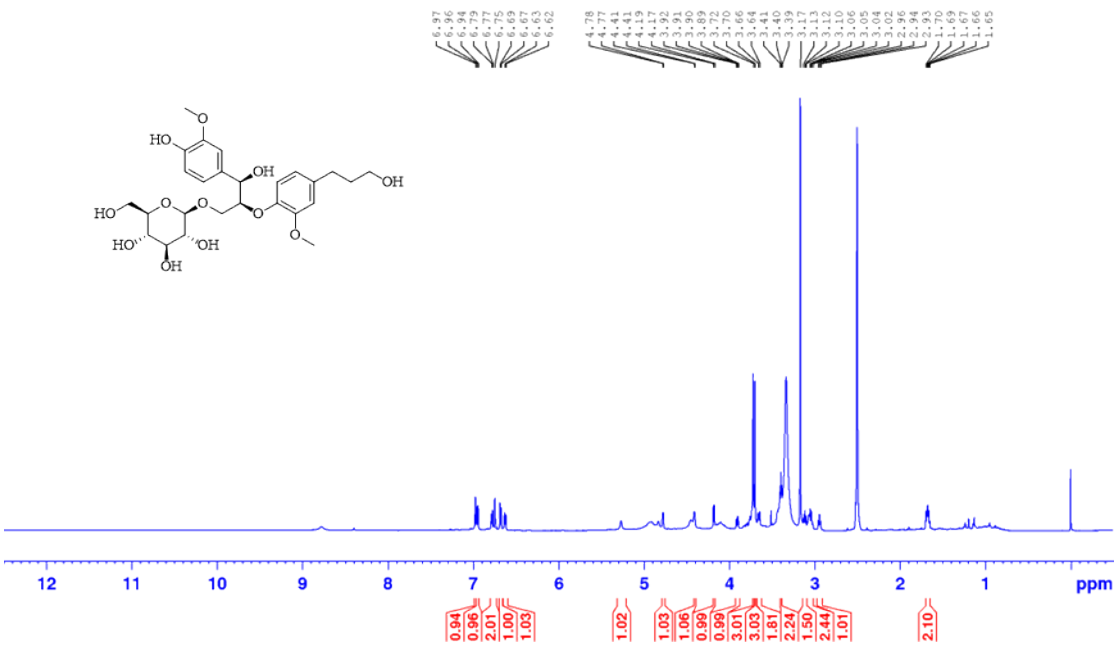


Fig. S26. ^{1}H NMR spectrum for compound **5**

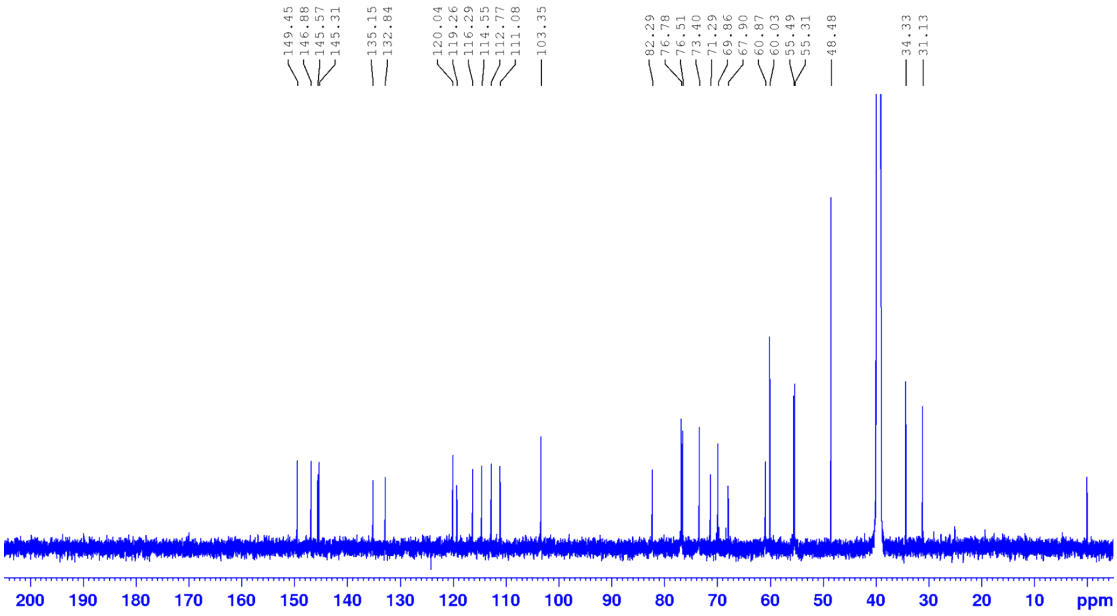


Fig. S27. ^{13}C NMR spectrum for compound **5**

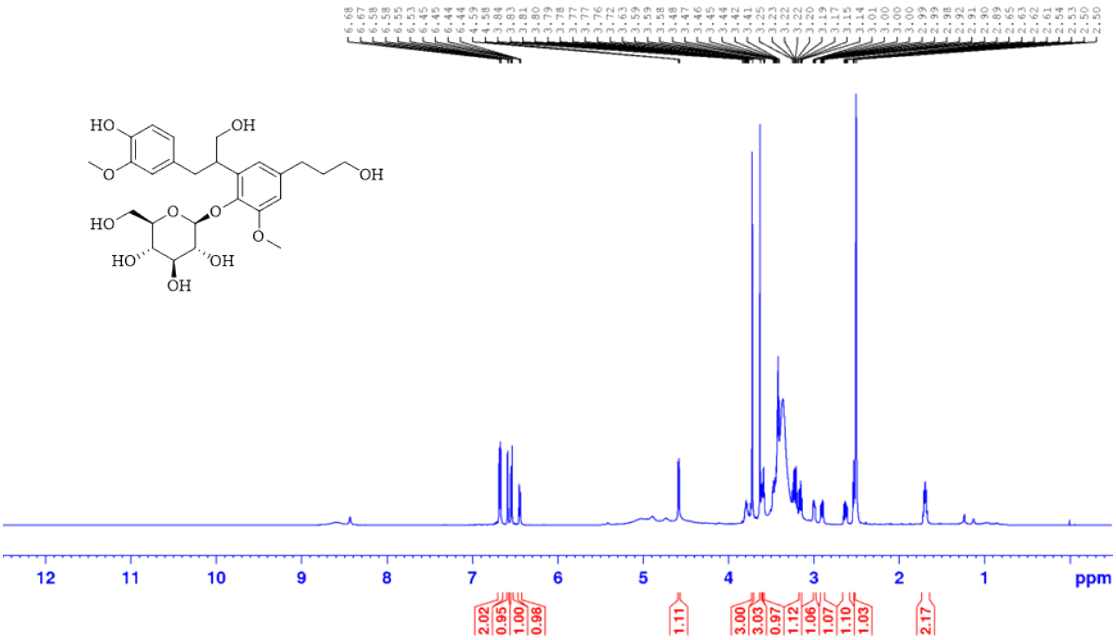


Fig. S28. [1]H NMR spectrum for compound **6**

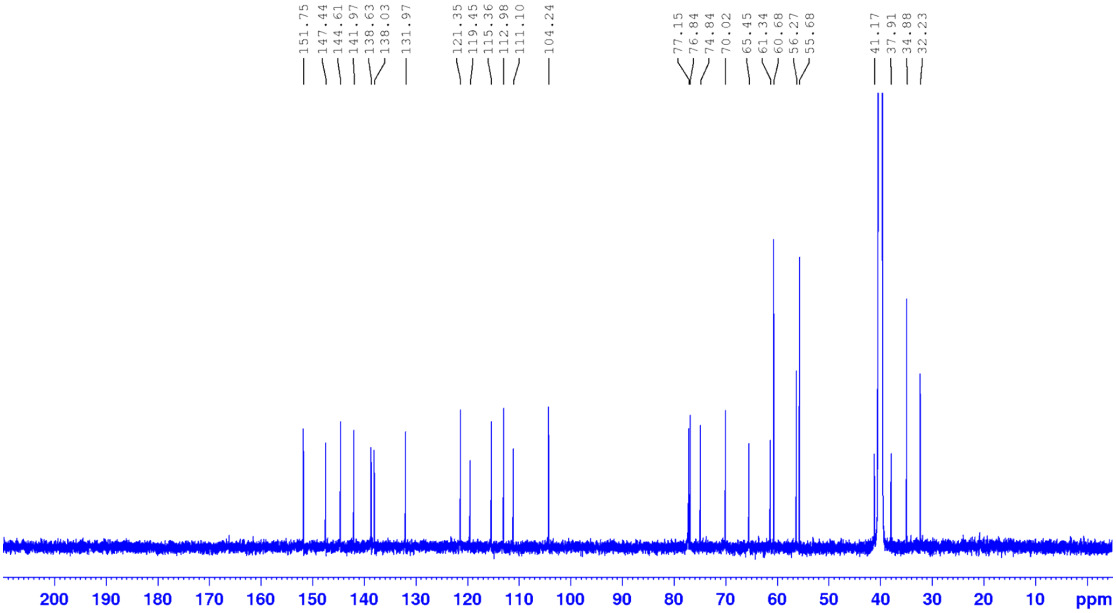


Fig. S29. [13]C NMR spectrum for compound **6**

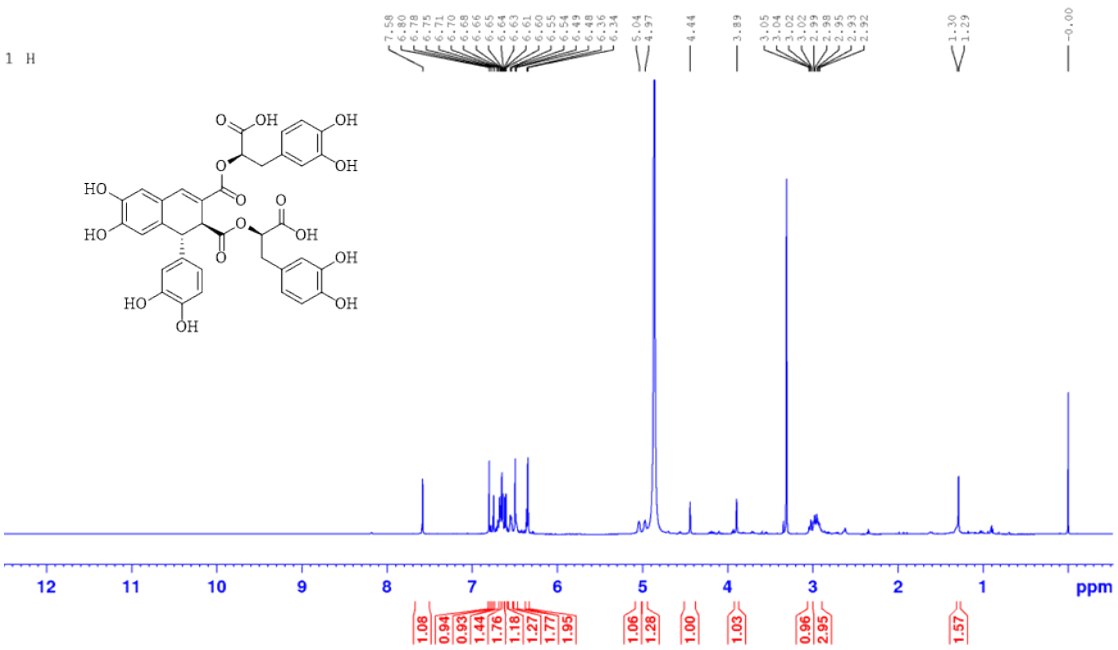


Fig. S30. ^{1}H NMR spectrum for compound **7**

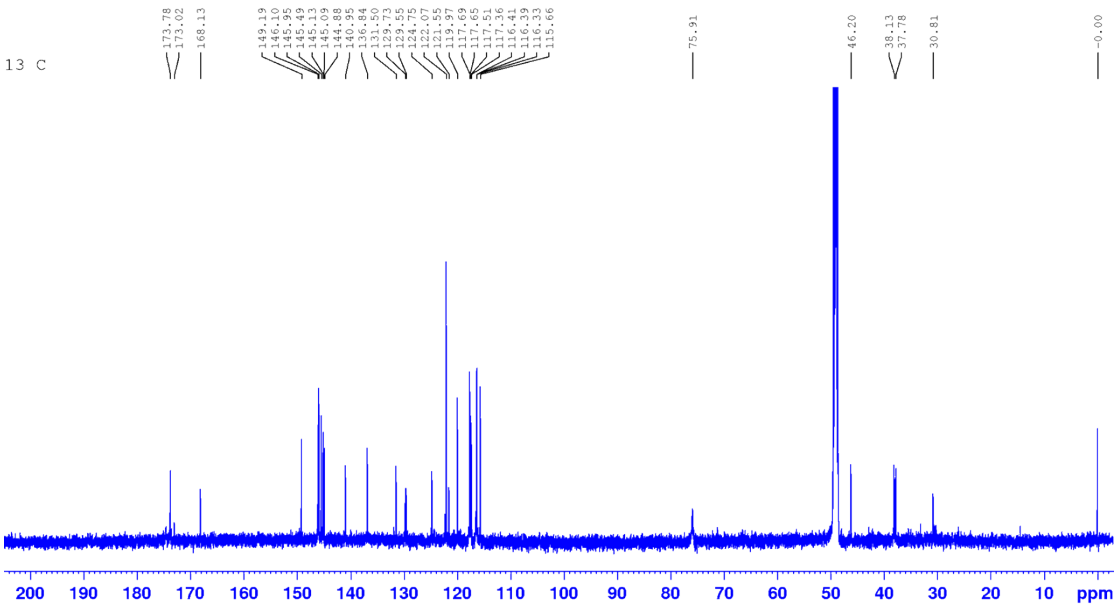


Fig. S31. ^{13}C NMR spectrum for compound **7**

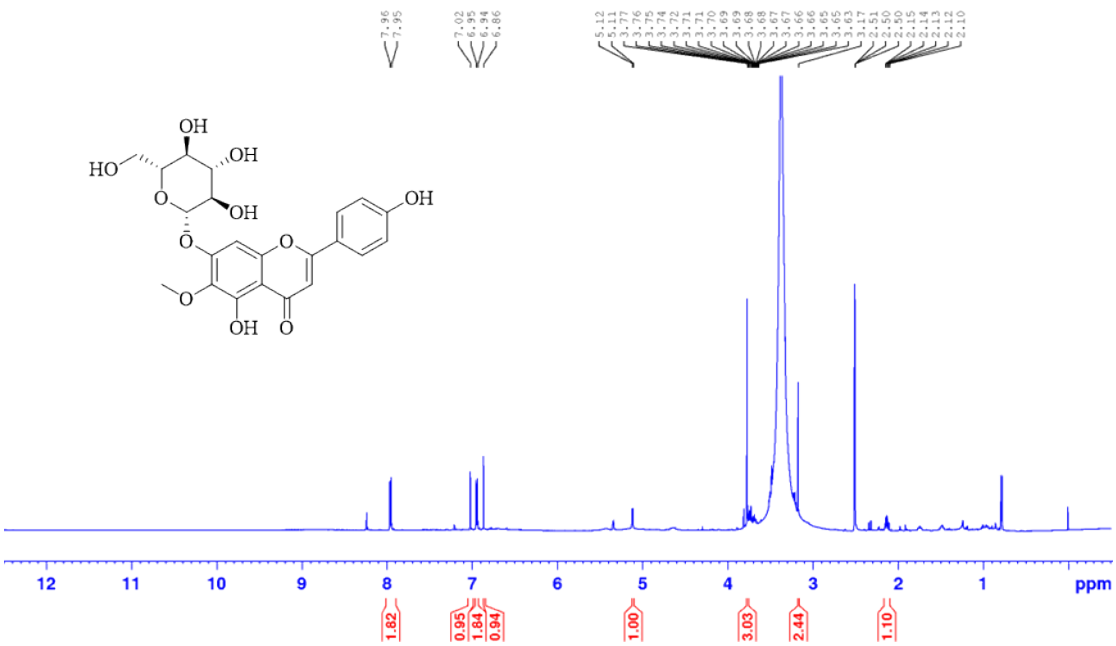


Fig. S32. [1]H NMR spectrum for compound **8**

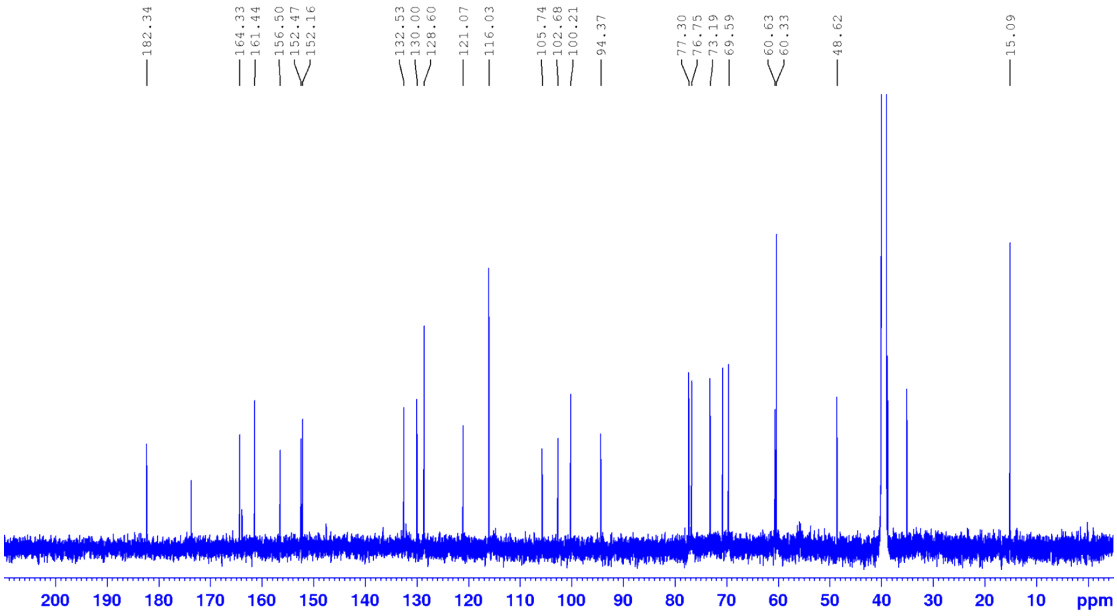


Fig. S33. [13]C NMR spectrum for compound **8**

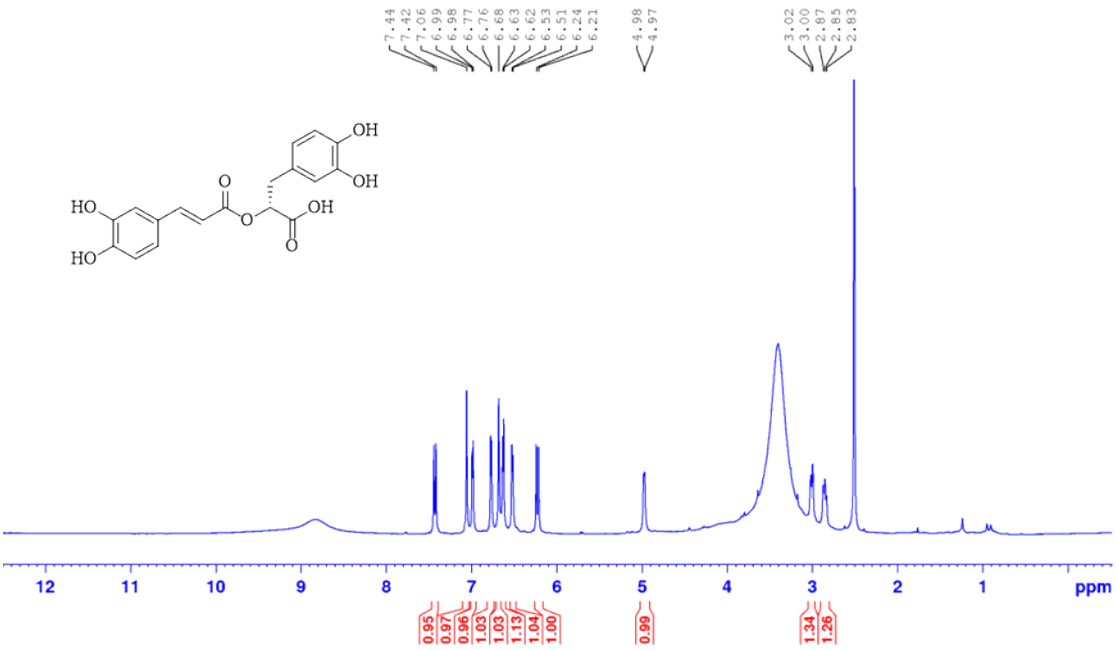


Fig. S34. ^{1}H NMR spectrum for compound **9**

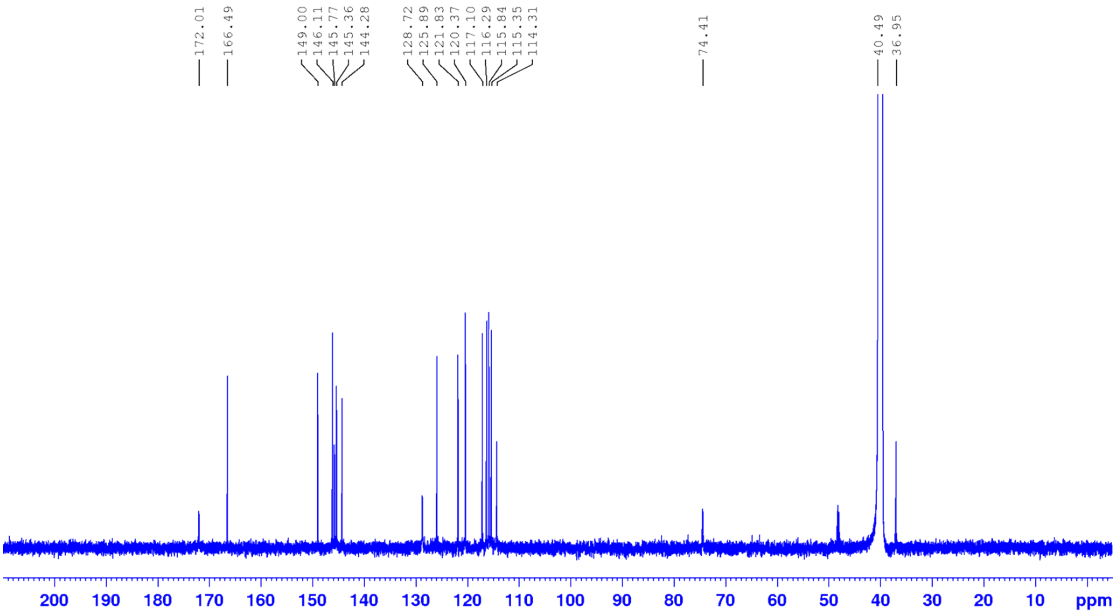


Fig. S35. ^{13}C NMR spectrum for compound **9**

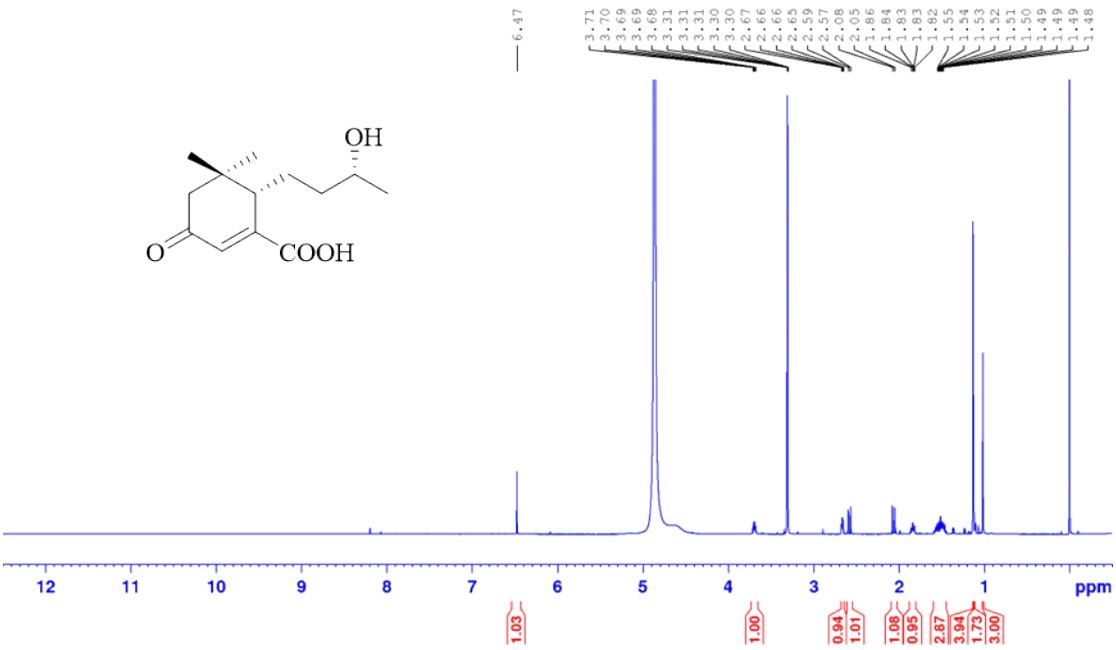


Fig. S36. [1]H NMR spectrum for compound **10**

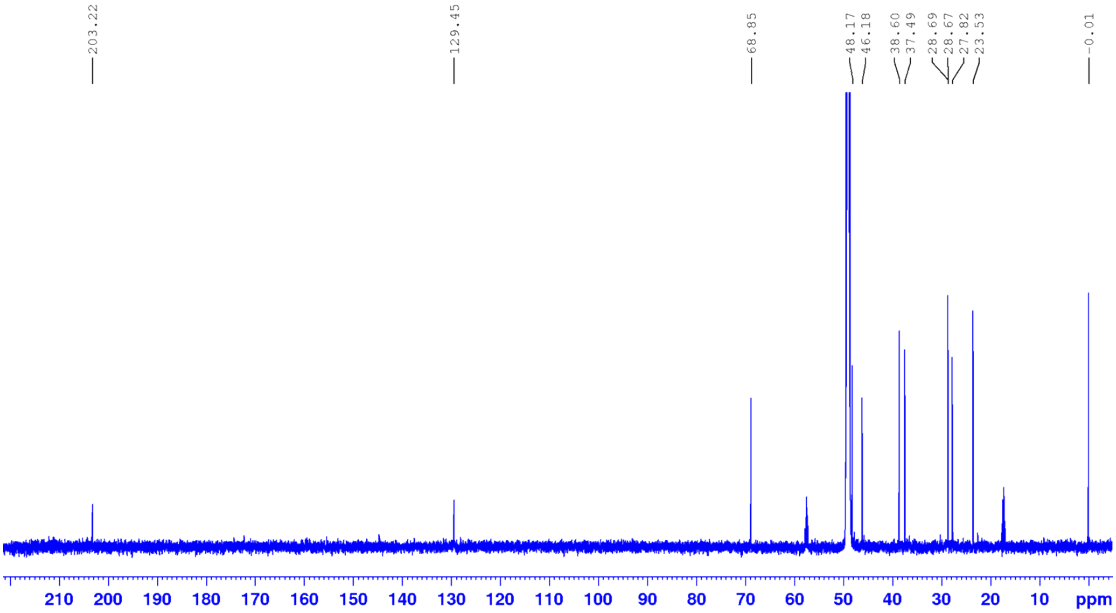
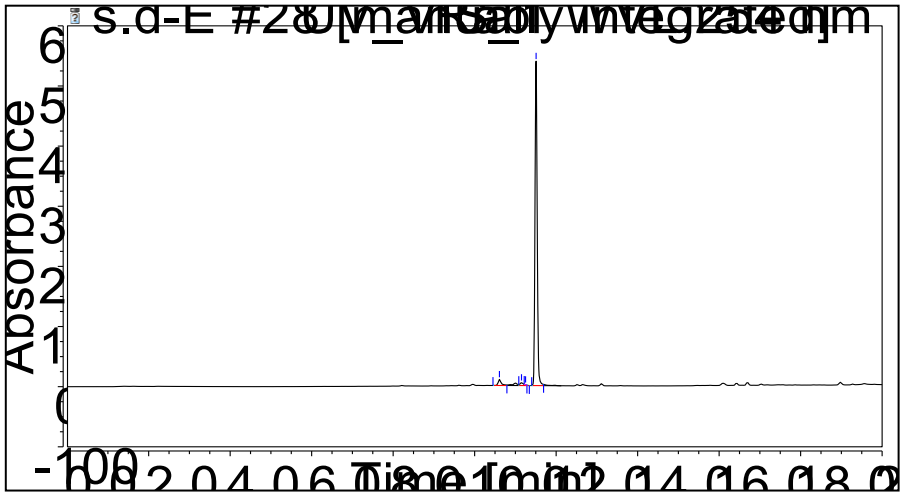
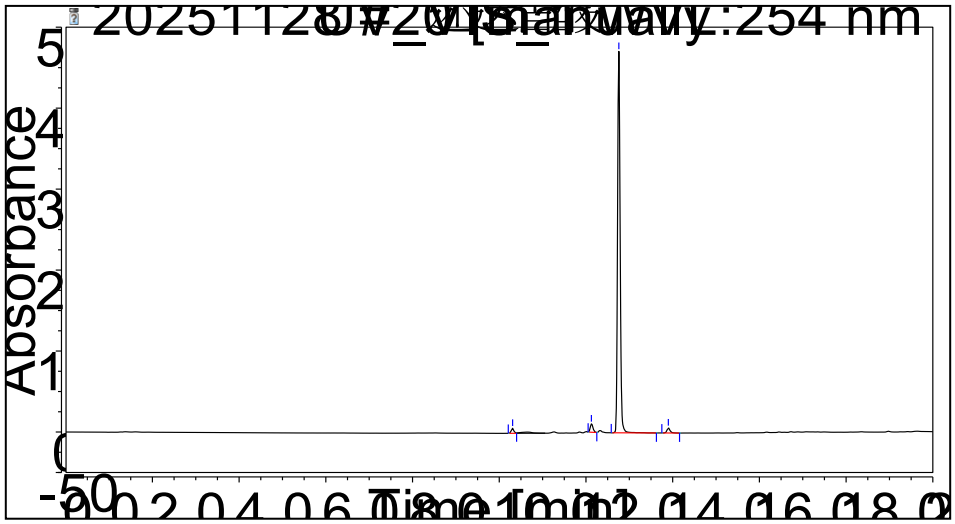


Fig. S37. [13]C NMR spectrum for compound **10**



No.	Retention Time (min)	Area (mAU*min)	Height (mAU)	Relative Area (%)	Relative Height (%)
1	10.608	0.897	10.204	2.54	1.84
2	11.150	0.528	4.928	1.50	0.89
3	11.250	0.007	0.179	0.02	0.03
4	11.508	33.860	539.439	**95.94**	97.24
Total:		35.292	554.749	100.00	100

Fig. S38. The UPLC chromatographic purity of compound **7**.



No.	Retention Time (min)	Area (mAU*min)	Height (mAU)	Relative Area (%)	Relative Height (%)
1	10.308	0.428	6.275	1.25	1.84
2	12.125	0.748	10.370	2.19	0.89
3	12.758	32.491	471.092	**95.06**	0.03
4	13.900	0.514	6.349	1.50	97.24
Total:		34.181	494.087	100.00	100

Fig. S39. The UPLC chromatographic purity of compound **9**.

Table S1. List of Primers for Real-time PCR.

Gene	Forward Sequence	Reverse Sequence
Nrf2	GGTTGGGGTCTTCTGTGGAG	GGTTCCAAGTCCAGAAGCCA
Keap1	ATCTTCGAGGAGCTCACCCT	CTGGGGTTGTAAGCCTCCAG
NF-κB	GACAGTGACAGTGTCTGCGA	AGTTAGCAGTGAGGCACCAC
IL-6	AGTGAGGAACAAGCCAGAGC	GGTCAGGGGTGGTTATTGCA
IL-1β	CCACCTCCAGGGACAGGATA	TCAACACGCAGGACAGGTAC
GAPDH	GAGAAGGCTGGGGCTCATTT	AGTGATGGCATGGACTGTGG

Table S2. Key conformers of compound **2**.

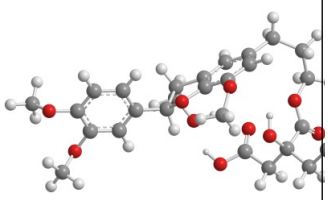
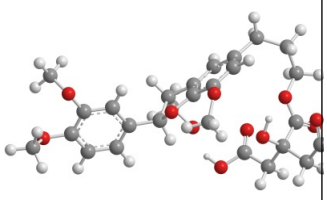
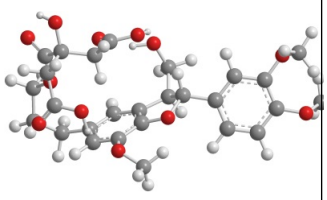
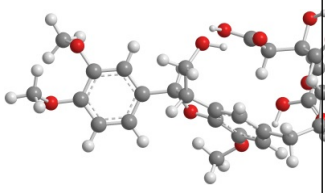
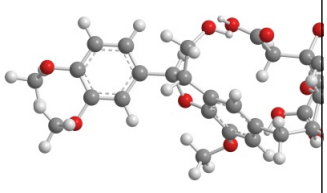
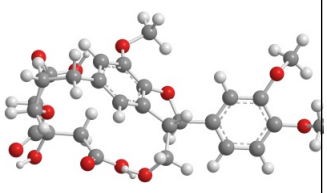
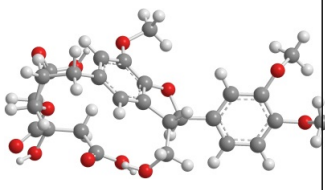
		
Conformer A 47.77%	**Conformer B 32.41%**	**Conformer C 6.09%**
		
Conformer D 6.07%	**Conformer E 3.34%**	**Conformer F 2.16%**
		
Conformer G 2.15%		

Table S3. Conformers and Bolzmann distributions of the optimized **2**.

species	*E'=E+ZPE*	*E*	*H*	*G*	*ΔG*	*ΔE(kcal/mol)*	*p%*
A	-1950.308519	-1950.26983	-1950.268886	-1950.382458	0	0	47.77%
B	-1950.307894	-1950.269272	-1950.268328	-1950.382092	0.000366	0.229668477	32.41%
C	-1950.307964	-1950.2696	-1950.268656	-1950.380514	0.001944	1.219878468	6.09%
D	-1950.307962	-1950.269599	-1950.268655	-1950.380512	0.001946	1.221133487	6.07%
E	-1950.307962	-1950.269701	-1950.268757	-1950.379949	0.002509	1.574421336	3.34%
F	-1950.307921	-1950.269712	-1950.268768	-1950.379538	0.00292	1.83232774	2.16%
G	-1950.30792	-1950.269712	-1950.268767	-1950.379534	0.002924	1.834837778	2.15%

E, *E'*, *H, G*: total energy, total energy with zero point energy (ZPE), enthalpy, and Gibbs free energy

Table S4. Optimized Z-matrixes of isomer **1** in the gas phase (Å) at B3LYP/6-31G(d,p) level.

A					**B**			
atom	X	Y	Z		atom	X	Y	Z
C	-5.59551	1.067078	1.346158		C	-5.57773	-1.75316	-0.85782
C	-6.38769	0.117401	0.698088		C	-6.37381	-0.91001	-0.08468
C	-5.77473	-0.84249	-0.12797		C	-5.77428	0.16009	0.610223
C	-4.39221	-0.80917	-0.31437		C	-4.39636	0.34847	0.537065
C	-3.60206	0.160164	0.31246		C	-3.59436	-0.50628	-0.22948
C	-4.2152	1.091827	1.158529		C	-4.19801	-1.55564	-0.92912
C	-2.12205	0.209928	0.035647		C	-2.11282	-0.26658	-0.35866
O	-1.39301	0.558133	1.246433		O	-1.54842	0.129165	0.921838
C	-0.28043	1.262706	0.854551		C	-0.49379	0.96997	0.65046
C	-0.33112	1.684013	-0.47175		C	-0.47661	1.425728	-0.66528
C	-1.67643	1.256825	-1.02852		C	-1.70175	0.857474	-1.35575
C	-1.70558	0.73584	-2.46986		C	-1.52994	0.374828	-2.80037
O	-0.82532	-0.35067	-2.73205		O	-0.51149	-0.60153	-2.98902
C	0.807236	1.581909	1.678513		C	0.475753	1.380051	1.573886
C	1.836241	2.343989	1.107613		C	1.447355	2.279894	1.118947
C	1.812543	2.765994	-0.22948		C	1.49122	2.741047	-0.20268
C	0.702942	2.434689	-1.02185		C	0.504781	2.308943	-1.10211
C	2.950916	3.587111	-0.80863		C	2.577159	3.699484	-0.65601
C	4.370018	2.990465	-0.69704		C	4.036153	3.251792	-0.42604
C	4.613333	1.680662	-1.43493		C	4.480987	1.992987	-1.15931
O	3.999877	0.608413	-0.68416		O	3.945672	0.83993	-0.46907
C	4.355625	-0.64268	-0.99522		C	4.464007	-0.34711	-0.79126
C	3.634454	-1.67464	-0.0997		C	3.837138	-1.50262	0.025556
O	5.1403	-0.95904	-1.86163		O	5.354838	-0.53198	-1.59413
O	2.807046	-1.07439	0.881725		O	2.862508	-1.06783	0.952178
C	2.763037	-2.59024	-0.99373		C	3.125089	-2.47486	-0.93641

C	1.631014	-1.81536	-1.63034		C	1.979363	-1.80466	-1.66512
O	0.445906	-2.4166	-1.52484		O	0.847019	-2.50808	-1.63067
O	5.988783	-2.47509	2.597841		O	6.552181	-2.14855	2.506792
C	5.562228	-1.73159	1.551637		C	5.659905	-1.42246	1.799291
C	4.692324	-2.53955	0.613308		C	4.980717	-2.25813	0.738817
O	5.883705	-0.57349	1.398792		O	5.46124	-0.24394	2.012604
O	1.801125	-0.74339	-2.19807		O	2.099626	-0.73643	-2.24984
O	-7.74566	0.111621	0.928393		O	-7.73453	-1.12036	-0.04873
C	-8.55021	0.464891	-0.20407		C	-8.24052	-1.56812	1.215901
O	-6.50871	-1.80086	-0.79137		O	-6.51886	1.004013	1.405214
C	-7.10446	-2.795	0.053299		C	-7.40341	1.876799	0.691524
O	0.91244	1.260247	3.001135		O	0.522269	1.012922	2.889243
C	0.567309	-0.07938	3.386444		C	0.243268	-0.35795	3.207465
H	-6.08668	1.783319	1.997241		H	-6.05756	-2.57013	-1.38711
H	-3.94766	-1.56763	-0.9526		H	-3.95466	1.162962	1.101076
H	-3.60744	1.8268	1.675122		H	-3.58816	-2.23441	-1.51918
H	-1.76662	-0.7801	-0.27956		H	-1.61059	-1.19612	-0.65785
H	-2.36947	2.111603	-0.99482		H	-2.49517	1.620485	-1.37669
H	-2.71428	0.380267	-2.70446		H	-2.46386	-0.08535	-3.13984
H	-1.48878	1.564661	-3.15755		H	-1.34183	1.239325	-3.45131
H	0.108435	-0.06008	-2.67516		H	0.375549	-0.20885	-2.85436
H	2.675149	2.589419	1.752073		H	2.19424	2.595899	1.841525
H	0.659406	2.765834	-2.05636		H	0.514171	2.666192	-2.12892
H	2.738043	3.784391	-1.86642		H	2.440058	3.905878	-1.72457
H	2.970992	4.570167	-0.3186		H	2.446925	4.663538	-0.1453
H	5.075176	3.7254	-1.1055		H	4.69298	4.066368	-0.75696
H	4.651702	2.848526	0.35241		H	4.236224	3.114429	0.642751
H	4.181569	1.681681	-2.44171		H	4.122814	1.965172	-2.19416
H	5.681205	1.464562	-1.52052		H	5.570704	1.90642	-1.17563
H	2.807624	-0.11546	0.730124		H	3.152939	-0.21048	1.298396
H	2.355359	-3.40599	-0.39352		H	2.750852	-3.33226	-0.37348
H	3.379324	-3.01259	-1.79465		H	3.840619	-2.82671	-1.68664
H	-0.23245	-1.83204	-1.95091		H	0.156022	-1.9958	-2.12497
H	6.564703	-1.89522	3.125228		H	6.948738	-1.54053	3.154109
H	5.349222	-3.00691	-0.12905		H	5.740337	-2.5709	0.014973
H	4.198232	-3.33512	1.175896		H	4.58746	-3.16242	1.21425
H	-8.3257	1.486563	-0.53471		H	-7.80393	-2.53769	1.485489
H	-8.39622	-0.22907	-1.03588		H	-8.03307	-0.84233	2.007694
H	-9.58765	0.415153	0.132114		H	-9.31903	-1.68088	1.089685
H	-6.33233	-3.35783	0.592023		H	-6.83746	2.549141	0.034693
H	-7.79558	-2.34507	0.772123		H	-8.12842	1.312053	0.097637
H	-7.64724	-3.47159	-0.60953		H	-7.92445	2.467292	1.44758
H	1.133425	-0.80681	2.794686		H	0.874299	-1.0279	2.613114

H	0.850497	-0.16165	4.437419		H	0.487875	-0.46636	4.265978
H	-0.50316	-0.2667	3.274785		H	-0.80795	-0.60473	3.042497
C					**D**			
atom	X	Y	Z		atom	X	Y	Z
C	5.395835	-1.63907	0.21375		C	-5.39544	-1.63934	-0.21343
C	6.209838	-0.50508	0.254012		C	-6.2096	-0.50547	-0.25376
C	5.61659	0.769993	0.207802		C	-5.61651	0.769675	-0.20767
C	4.230597	0.881413	0.08957		C	-4.23054	0.881326	-0.08956
C	3.417153	-0.25455	0.023389		C	-3.41693	-0.25453	-0.02333
C	4.012672	-1.51938	0.099849		C	-4.01228	-1.51944	-0.09962
C	1.931309	-0.09607	-0.16591		C	-1.93109	-0.09582	0.165846
O	1.209454	-1.06158	0.661083		O	-1.20917	-1.06151	-0.66086
C	0.075371	-1.41264	-0.02586		C	-0.07508	-1.41232	0.026199
C	0.074223	-0.98535	-1.3537		C	-0.07389	-0.98452	1.353863
C	1.414768	-0.32707	-1.61793		C	-1.41447	-0.32626	1.617915
C	1.441631	0.922536	-2.51147		C	-1.44156	0.923699	2.510989
O	0.671703	2.030373	-2.05779		O	-0.67192	2.031524	2.056834
C	-1.00254	-2.13845	0.494391		C	1.002735	-2.1385	-0.49379
C	-2.08162	-2.3988	-0.35377		C	2.081755	-2.39865	0.354488
C	-2.11504	-1.94989	-1.67957		C	2.1152	-1.94926	1.680137
C	-1.00968	-1.24773	-2.18385		C	1.009943	-1.24676	2.184155
C	-3.31833	-2.23862	-2.55447		C	3.318448	-2.23794	2.555099
C	-4.66683	-1.70023	-2.03576		C	4.666939	-1.6993	2.036581
C	-4.77716	-0.18642	-1.92268		C	4.776865	-0.1855	1.923142
O	-4.1231	0.250444	-0.70056		O	4.122804	0.250797	0.700817
C	-4.45746	1.46031	-0.26583		C	4.457199	1.460414	0.265391
C	-3.8684	1.821423	1.114941		C	3.867977	1.820784	-1.11549
O	-5.24373	2.209204	-0.81781		O	5.243529	2.209613	0.816864
O	-4.22317	3.164038	1.372855		O	4.222293	3.163407	-1.37394
C	-4.56377	0.924763	2.203781		C	4.563637	0.923858	-2.20398
C	-4.1663	-0.54114	2.211185		C	4.16616	-0.54202	-2.21097
O	-2.98627	-0.71833	2.845251		O	2.986281	-0.71941	-2.84528
O	-0.32627	2.630348	0.402357		O	0.32608	2.630457	-0.40356
C	-1.56002	2.249147	0.042592		C	1.559688	2.249204	-0.04352
C	-2.34082	1.714895	1.214064		C	2.340438	1.713701	-1.21446
O	-1.94404	2.238828	-1.11804		O	1.943726	2.239632	1.11714
O	-4.79816	-1.44643	1.709244		O	4.797865	-1.44716	-1.70854
O	7.569614	-0.66632	0.393992		O	-7.56933	-0.66693	-0.39381
C	8.34798	-0.25335	-0.73727		C	-8.34795	-0.25362	0.73715
O	6.372605	1.920268	0.242452		O	-6.37278	1.919801	-0.24242
C	7.005932	2.186654	1.50168		C	-7.00546	2.186217	-1.50195

O	-1.11629	-2.54731	1.808167		O	1.116409	-2.54789	-1.8074
C	0.023481	-3.18168	2.405905		C	-0.02338	-3.18251	-2.40482
H	5.873294	-2.6121	0.271849		H	-5.87276	-2.61244	-0.27143
H	3.80215	1.879233	0.062638		H	-3.80223	1.879209	-0.06276
H	3.390408	-2.40783	0.078474		H	-3.38989	-2.40779	-0.07819
H	1.61458	0.897825	0.16969		H	-1.61448	0.898002	-0.17008
H	2.075763	-1.05591	-2.11275		H	-2.07534	-1.05499	2.113067
H	2.473955	1.280821	-2.58037		H	-2.47398	1.281748	2.579782
H	1.131872	0.640309	-3.52682		H	-1.1317	0.641951	3.526436
H	-0.28289	1.86775	-2.17528		H	0.282723	1.869202	2.174408
H	-2.92503	-2.93434	0.070522		H	2.925161	-2.93439	-0.06957
H	-1.01031	-0.91114	-3.21763		H	1.010592	-0.9098	3.217804
H	-3.13616	-1.83004	-3.55598		H	3.136157	-1.82952	3.556645
H	-3.42071	-3.32421	-2.68521		H	3.420977	-3.32353	2.685695
H	-5.44995	-2.02911	-2.73049		H	5.449977	-2.02784	2.731572
H	-4.91408	-2.13202	-1.0603		H	4.914514	-2.13125	1.061269
H	-4.3042	0.333879	-2.76271		H	4.303619	0.334897	2.762955
H	-5.82128	0.130775	-1.87544		H	5.820886	0.13202	1.875943
H	-4.86538	3.398458	0.677441		H	4.864718	3.398222	-0.67886
H	-5.64426	0.992479	2.061493		H	5.644093	0.991658	-2.06152
H	-4.30881	1.372945	3.167678		H	4.308788	1.371769	-3.16803
H	-2.63778	-1.61481	2.659581		H	2.637732	-1.61579	-2.65926
H	0.210803	2.711631	-0.42106		H	-0.21106	2.71233	0.419759
H	-2.02381	0.673355	1.312435		H	2.023735	0.671925	-1.3113
H	-2.02351	2.221191	2.128578		H	2.022877	2.218639	-2.12963
H	8.092778	-0.85095	-1.62113		H	-9.39098	-0.4328	0.46974
H	8.198596	0.807377	-0.95894		H	-8.0933	-0.85131	1.621118
H	9.391049	-0.43292	-0.47024		H	-8.19824	0.807053	0.958844
H	6.255762	2.321731	2.290278		H	-6.25489	2.321917	-2.29006
H	7.689566	1.379957	1.782622		H	-7.6885	1.379224	-1.78353
H	7.563194	3.116078	1.370893		H	-7.56333	3.115293	-1.37126
H	0.865231	-2.49131	2.489611		H	-0.86538	-2.49239	-2.4881
H	-0.29818	-3.50239	3.397954		H	0.298008	-3.50295	-3.39704
H	0.322082	-4.05865	1.819968		H	-0.32149	-4.05967	-1.8189
E					**F**			
atom	X	Y	Z		atom	X	Y	Z
C	-5.39691	1.932769	-0.44056		C	5.396609	-1.77844	-0.86883
C	-6.18213	0.78575	-0.33941		C	6.184588	-0.68644	-0.50954
C	-5.56365	-0.45372	-0.07551		C	5.563119	0.487291	-0.03538
C	-4.17861	-0.52166	0.051974		C	4.17885	0.525718	0.111572
C	-3.38735	0.628003	-0.06692		C	3.387684	-0.57763	-0.23331

C	-4.00969	1.856311	-0.30813		C	4.007778	-1.72212	-0.74345
C	-1.89457	0.563363	0.120993		C	1.896509	-0.55789	-0.02504
O	-1.34544	-0.59749	-0.57771		O	1.338437	0.723587	-0.45623
C	-0.27841	-1.04342	0.158873		C	0.275392	0.996784	0.365773
C	-0.19616	-0.46751	1.426607		C	0.206373	0.164013	1.482654
C	-1.40933	0.427003	1.595582		C	1.425602	-0.73723	1.449143
C	-1.22505	1.763757	2.330466		C	1.254726	-2.19816	1.893044
O	-0.29015	2.669071	1.753656		O	0.312161	-2.96876	1.155276
C	0.660132	-1.99357	-0.25971		C	-0.67186	2.007624	0.165811
C	1.687749	-2.32728	0.625431		C	-1.69436	2.13737	1.108422
C	1.806083	-1.73544	1.889006		C	-1.79787	1.290735	2.218846
C	0.836637	-0.80543	2.294131		C	-0.82059	0.302231	2.40945
C	2.953904	-2.11185	2.803741		C	-2.93759	1.457651	3.20354
C	4.36615	-1.85625	2.240495		C	-4.35608	1.317997	2.615451
C	4.71048	-0.40253	1.949479		C	-4.69859	-0.04164	2.022747
O	4.12665	-0.0177	0.675036		O	-4.13084	-0.13989	0.688456
C	4.654657	1.056989	0.099123		C	-4.65432	-1.0765	-0.095
C	4.124595	1.341602	-1.32318		C	-4.13185	-1.05174	-1.54794
O	5.560262	1.725383	0.565031		O	-5.54899	-1.83771	0.227362
O	4.696748	2.565896	-1.7346		O	-4.70257	-2.1637	-2.2063
C	4.655723	0.218121	-2.28683		C	-4.67216	0.24772	-2.24952
C	4.026039	-1.15389	-2.12051		C	-4.04211	1.556574	-1.80572
O	2.827581	-1.21352	-2.74154		O	-2.84708	1.745284	-2.40732
O	0.761157	2.789555	-0.75358		O	-0.76251	-2.57572	-1.31047
C	1.924233	2.265937	-0.34048		C	-1.92153	-2.14996	-0.78823
C	2.600456	1.480918	-1.43329		C	-2.6075	-1.15847	-1.69059
O	2.313938	2.335592	0.816196		O	-2.29982	-2.45525	0.333628
O	4.507858	-2.08137	-1.50534		O	-4.52104	2.336412	-1.01001
O	-7.5487	0.897369	-0.46297		O	7.548555	-0.76217	-0.67864
C	-8.09759	0.292997	-1.64224		C	8.308825	-0.7616	0.53715
O	-6.29474	-1.61776	0.013667		O	6.299444	1.591909	0.331655
C	-7.14849	-1.70655	1.162125		C	6.938998	2.276426	-0.75429
O	0.690191	-2.56492	-1.51615		O	-0.71738	2.834462	-0.93926
C	-0.53868	-3.10629	-2.02302		C	0.506599	3.463604	-1.34552
H	-5.89174	2.877697	-0.64032		H	5.891406	-2.66468	-1.25273
H	-3.72562	-1.49098	0.231641		H	3.725906	1.440415	0.479091
H	-3.40961	2.756107	-0.41138		H	3.406503	-2.57665	-1.04109
H	-1.42405	1.44572	-0.32667		H	1.423494	-1.3261	-0.64662
H	-2.17504	-0.1197	2.168056		H	2.194935	-0.31636	2.115464
H	-2.18525	2.289886	2.343518		H	2.215331	-2.71211	1.783387
H	-0.95601	1.561214	3.375943		H	1.000985	-2.2174	2.961528
H	0.626408	2.367643	1.897326		H	-0.60256	-2.70302	1.36613
H	2.426771	-3.0425	0.278397		H	-2.44101	2.903703	0.925394

H	0.90182	-0.35342	3.28084		H	-0.87457	-0.34842	3.278764
H	2.847644	-1.56852	3.750702		H	-2.81687	0.728045	4.013665
H	2.88326	-3.17802	3.057228		H	-2.86852	2.446761	3.67563
H	5.093284	-2.21794	2.978494		H	-5.07467	1.507369	3.42283
H	4.536558	-2.43442	1.326136		H	-4.54092	2.07882	1.849801
H	4.328071	0.282151	2.714357		H	-4.30294	-0.87185	2.617903
H	5.790942	-0.25956	1.879454		H	-5.77943	-0.17363	1.937554
H	5.375912	2.770043	-1.06522		H	-5.37266	-2.51209	-1.58935
H	5.73405	0.127155	-2.14115		H	-5.7491	0.303527	-2.07832
H	4.469036	0.580806	-3.30105		H	-4.49516	0.106353	-3.31901
H	2.338298	-2.01103	-2.45133		H	-2.35701	2.467008	-1.96129
H	0.253901	3.054241	0.050043		H	-0.24687	-2.99712	-0.58229
H	2.112002	0.50293	-1.42459		H	-2.12322	-0.20159	-1.47914
H	2.370865	1.929635	-2.4026		H	-2.38079	-1.39376	-2.73302
H	-7.88889	-0.78048	-1.67402		H	8.13756	0.151801	1.11438
H	-9.17534	0.459892	-1.59601		H	8.056635	-1.63507	1.151
H	-7.69501	0.77059	-2.54383		H	9.35747	-0.82096	0.239925
H	-6.55762	-1.67968	2.086122		H	6.193694	2.657238	-1.46328
H	-7.88376	-0.89666	1.176135		H	7.476504	3.1163	-0.31004
H	-7.65829	-2.669	1.088707		H	7.640953	1.62226	-1.27973
H	-1.29072	-2.32635	-2.15882		H	1.242863	2.726951	-1.67348
H	-0.29278	-3.56012	-2.98426		H	0.243679	4.124406	-2.17302
H	-0.92321	-3.87695	-1.34497		H	0.920093	4.05861	-0.523
G								
atom	X	Y	Z					
C	5.396115	-1.77858	-0.86855					
C	6.184291	-0.68664	-0.50951					
C	5.563033	0.487267	-0.03551					
C	4.178774	0.525911	0.11154					
C	3.387418	-0.57737	-0.23309					
C	4.007305	-1.72204	-0.74308					
C	1.896267	-0.55737	-0.02471					
O	1.338391	0.724181	-0.45584					
C	0.275207	0.997347	0.366026					
C	0.206113	0.164553	1.482891					
C	1.425443	-0.73657	1.449509					
C	1.254794	-2.19742	1.893687					
O	0.312322	-2.96833	1.156105					
C	-0.67212	2.008094	0.165923					
C	-1.69479	2.137672	1.108384					
C	-1.7984	1.290983	2.218749					

C	-0.82103	0.302605	2.409511					
C	-2.93831	1.457761	3.203238					
C	-4.35668	1.318087	2.614876					
C	-4.69912	-0.04158	2.022211					
O	-4.13092	-0.14001	0.688137					
C	-4.65404	-1.07682	-0.09534					
C	-4.13116	-1.05217	-1.54811					
O	-5.54874	-1.83807	0.226854					
O	-4.70152	-2.16433	-2.20647					
C	-4.67147	0.247112	-2.24997					
C	-4.04169	1.556093	-1.80612					
O	-2.84647	1.744836	-2.40736					
O	-0.76197	-2.57621	-1.30987					
C	-1.92102	-2.15024	-0.78783					
C	-2.60674	-1.15871	-1.69031					
O	-2.2995	-2.4554	0.333997					
O	-4.52096	2.335996	-1.01069					
O	7.548237	-0.76261	-0.67868					
C	8.308569	-0.76196	0.53707					
O	6.299503	1.591838	0.331327					
C	6.939301	2.276015	-0.75468					
O	-0.71764	2.835001	-0.93906					
C	0.506342	3.463938	-1.34563					
H	5.890763	-2.66496	-1.25233					
H	3.725988	1.440739	0.478925					
H	3.405874	-2.57654	-1.04053					
H	1.423052	-1.32553	-0.64621					
H	2.194739	-0.31544	2.115714					
H	2.215465	-2.71125	1.784069					
H	1.001113	-2.21652	2.962191					
H	-0.60242	-2.70249	1.366717					
H	-2.4415	2.903932	0.925268					
H	-0.87509	-0.34808	3.278794					
H	-2.81772	0.728097	4.013334					
H	-2.86936	2.446833	3.675419					
H	-5.07543	1.507525	3.422096					
H	-4.54137	2.078867	1.849141					
H	-4.3038	-0.87178	2.617607					
H	-5.77995	-0.17344	1.936669					
H	-5.37175	-2.51272	-1.58967					
H	-5.74845	0.302819	-2.07903					
H	-4.4942	0.105691	-3.31941					
H	-2.35661	2.466641	-1.96123					

H	-0.24649	-2.99758	-0.58156					
H	-2.12264	-0.20181	-1.47858					
H	-2.3797	-1.39386	-2.73271					
H	8.136863	0.15121	1.114528					
H	8.056862	-1.63573	1.150692					
H	9.357233	-0.82068	0.23979					
H	7.641129	1.621596	-1.27997					
H	6.194128	2.65688	-1.46379					
H	7.476966	3.11584	-0.31054					
H	1.242354	2.72721	-1.67396					
H	0.243263	4.124957	-2.1729					
H	0.920237	4.058712	-0.52313					