

SUPPLEMENTARY MATERIAL

Two new chromone derivatives from the rhizosphere soil fungus

Ilyonectria robusta

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Abstract

Two new chromone derivatives (**1** and **2**), and two known compounds (**3** and **4**) were isolated from the rhizosphere soil fungus *Ilyonectria robusta*. Their planar structures and absolute configurations were determined by extensive spectroscopic analysis and electronic circular dichroism (ECD) calculations. Additionally, all the isolated compounds were evaluated for their antibacterial activity against *Staphylococcus aureus*, *Enterococcus faecalis*, *Pseudomonas aeruginosa* and *Escherichia coli*, but no obvious activity was observed at a concentration of 128 µg/mL.

Keywords: Rhizosphere soil fungi; *Ilyonectria robusta*; chromone derivatives; antibacterial activity

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Table S5. Geometry data of conformers of compound **2**

Table S1. ^1H and ^{13}C NMR data for compounds **1** and **2** in CD_3OD

no.	1		2	
	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)	δ_{C}
1				
2		167.2		167.1
3	6.05 (1H, s)	112.6	6.12 (1H, s)	112.9
4		182.2		181.7
5		163.4		160.2
6	6.65 (1H, d, $J = 2.4$ Hz)	102.6	6.74 (1H, s)	118.1
7		143.8		141.2
8	6.62 (1H, d, $J = 2.4$ Hz)	118.3		107.1
9		161.7		156.8
10		115.9		116.3
1'	2.65 (1H, dd, $J = 14.4$ Hz, 8.4 Hz) 2.69 (1H, dd, $J = 14.4$ Hz, 4.8 Hz)	44.4	2.74 (1H, dd, $J = 14.4$ Hz, 7.8 Hz) 2.78 (1H, dd, $J = 14.4$ Hz, 5.4 Hz)	44.3
2'	4.18 (1H, m)	66.5	4.27 (1H, m)	66.4
3'	1.27 (3H, d, $J = 6.0$ Hz)	23.7	1.32 (3H, d, $J = 6.0$ Hz)	23.7
7- CH_3	2.70 (3H, s)	23.3	2.70 (3H, s)	23.1

Recorded in CD_3OD , 600 MHz for ^1H and 150 MHz for ^{13}C , δ in ppm.

Table S2. ^1H and ^{13}C NMR data for compounds **3** and **4** in $\text{DMSO}-d_6$

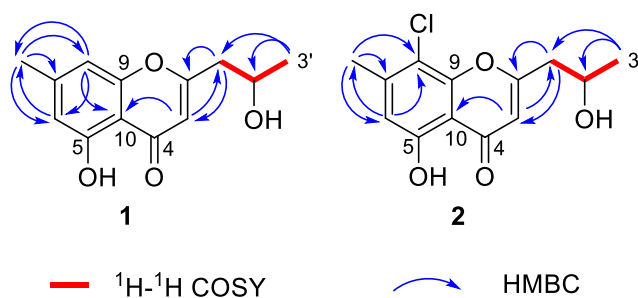
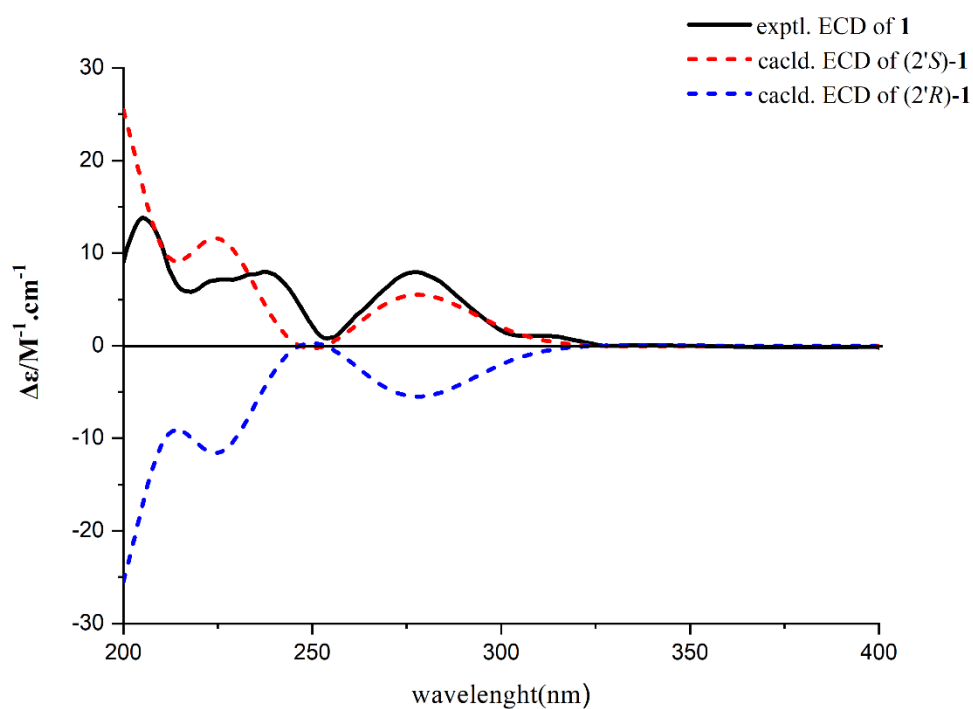
no.	3		4	
	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)	δ_{C}
1				164.5
2		163.7	6.55 (1H, d, $J = 2.4$ Hz)	107.7
3	5.95 (1H, s)	116.6		164.7
4		178.2	7.07 (1H, d, $J = 2.4$ Hz)	108.1
5		141.4	7.48 (1H, s)	112.2
6	6.61 (1H, d, $J = 2.4$ Hz)	110.7		159.3
7		161.2		140.9
8	6.59 (1H, d, $J = 2.4$ Hz)	100.5	8.26 (1H, s)	125.2
9		159.2		185.8
10		114.1		181.9
1'	2.64 (3H, s)	19.3	5.02 (1H, q, $J = 6.0$ Hz)	62.9
2'	2.26 (3H, s)	22.4	1.33 (3H, d, $J = 6.0$ Hz)	23.8
1a				109.1
4a				135.1
5a				133.3
8a				124.7

Recorded in $\text{DMSO}-d_6$, 600 MHz for ^1H and 150 MHz for ^{13}C , δ in ppm.

Table S3. Antibacterial activity of compounds **1-4**

Compounds	MIC ($\mu\text{g/mL}$)			
	<i>S. aureus</i>	<i>E. faecalis</i>	<i>P. Aeruginosa</i>	<i>E. coli</i>
1	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$
2	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$
3	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$
4	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$	> 128 $\mu\text{g/mL}$
vancomycin ^a	1 $\mu\text{g/mL}$	1 $\mu\text{g/mL}$	/	/
amikacin ^b	/	/	4 $\mu\text{g/mL}$	8 $\mu\text{g/mL}$

^a positive control of vancomycin; ^b positive control of amikacin.

**Figure S1.** Key ¹H-¹H COSY and HMBC correlations of compounds **1** and **2****Figure S2.** Experimental and calculated ECD spectra of compound **1** (in MeOH)

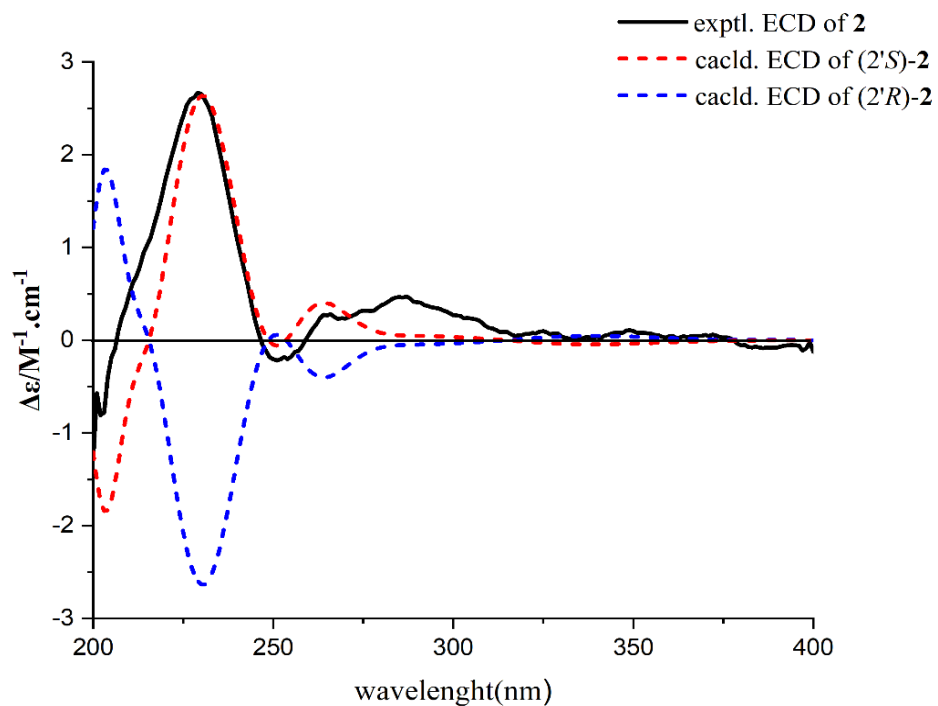


Figure S3. Experimental and calculated ECD spectra of compound **2** (in MeOH)

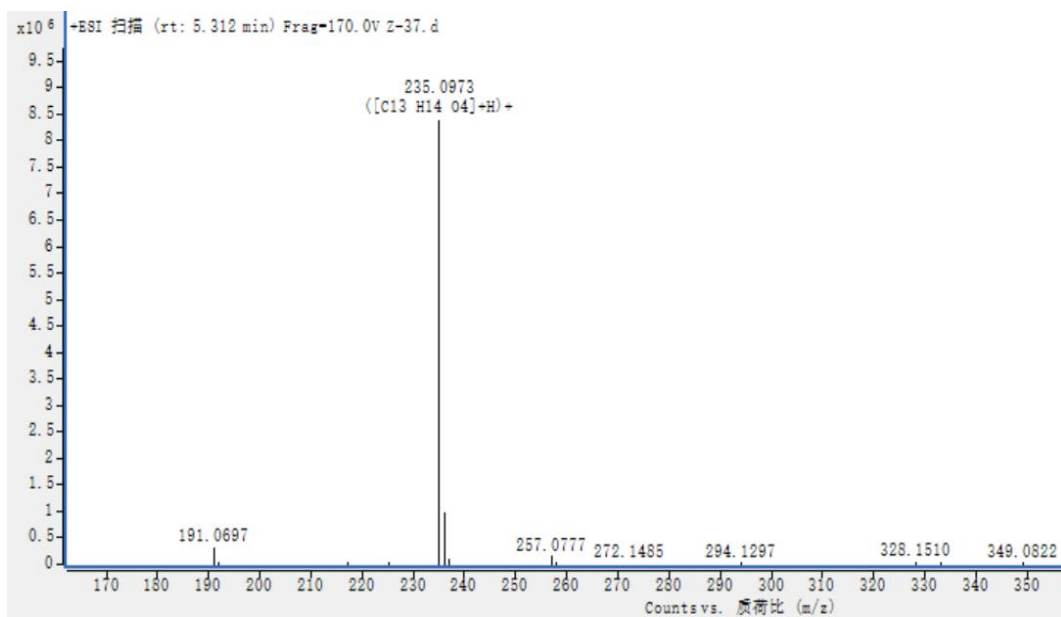


Figure S4. HRESIMS spectrum of compound **1**

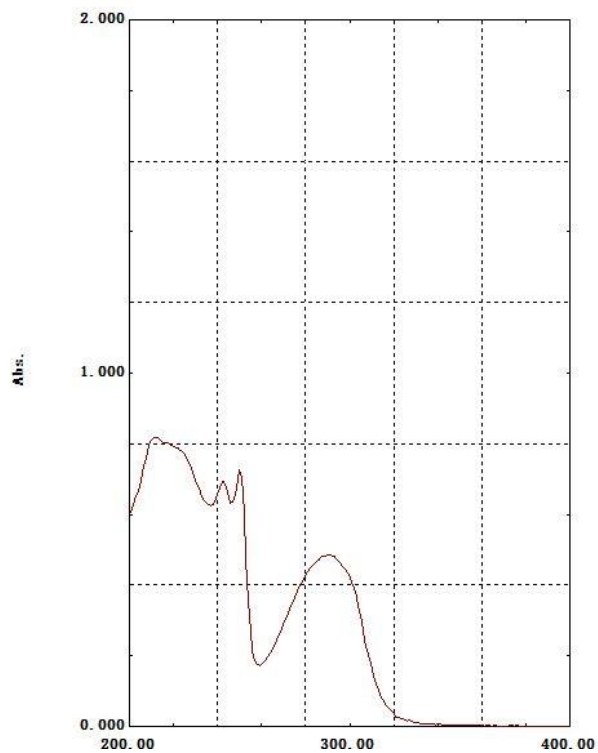


Figure S5. UV spectrum of compound **1** (in MeOH)

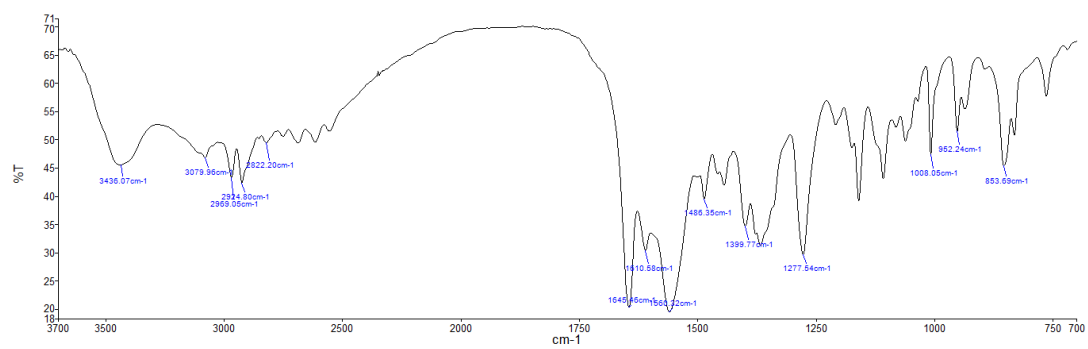
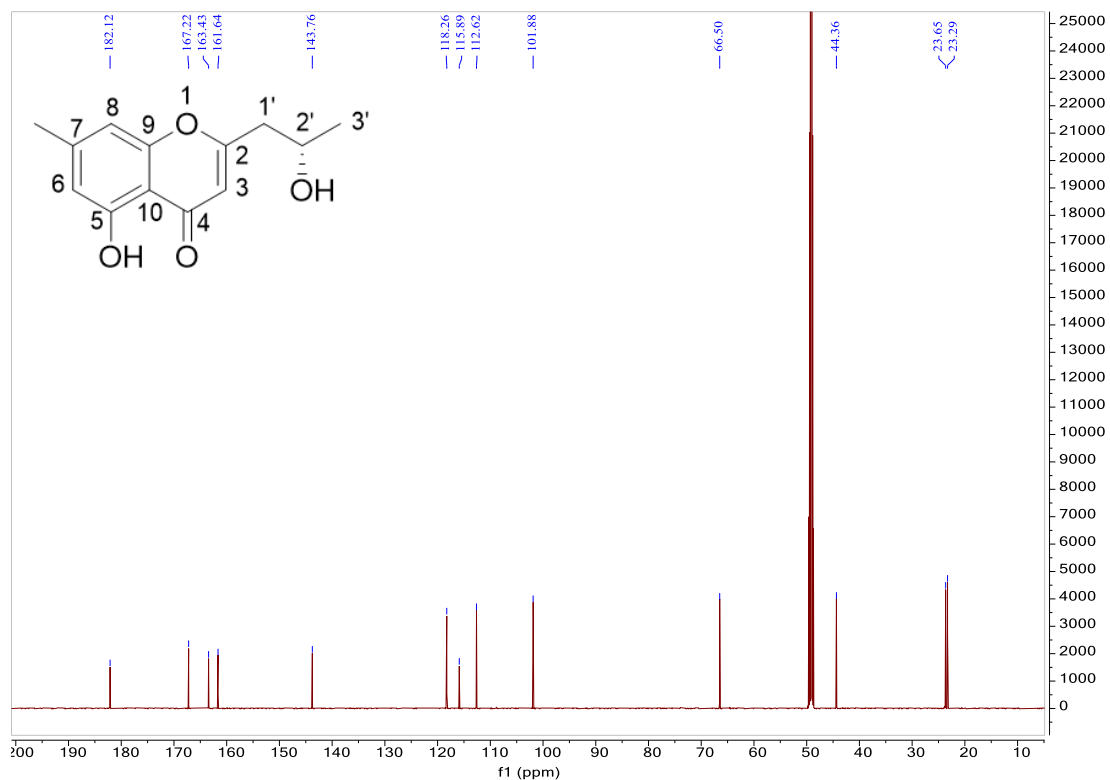
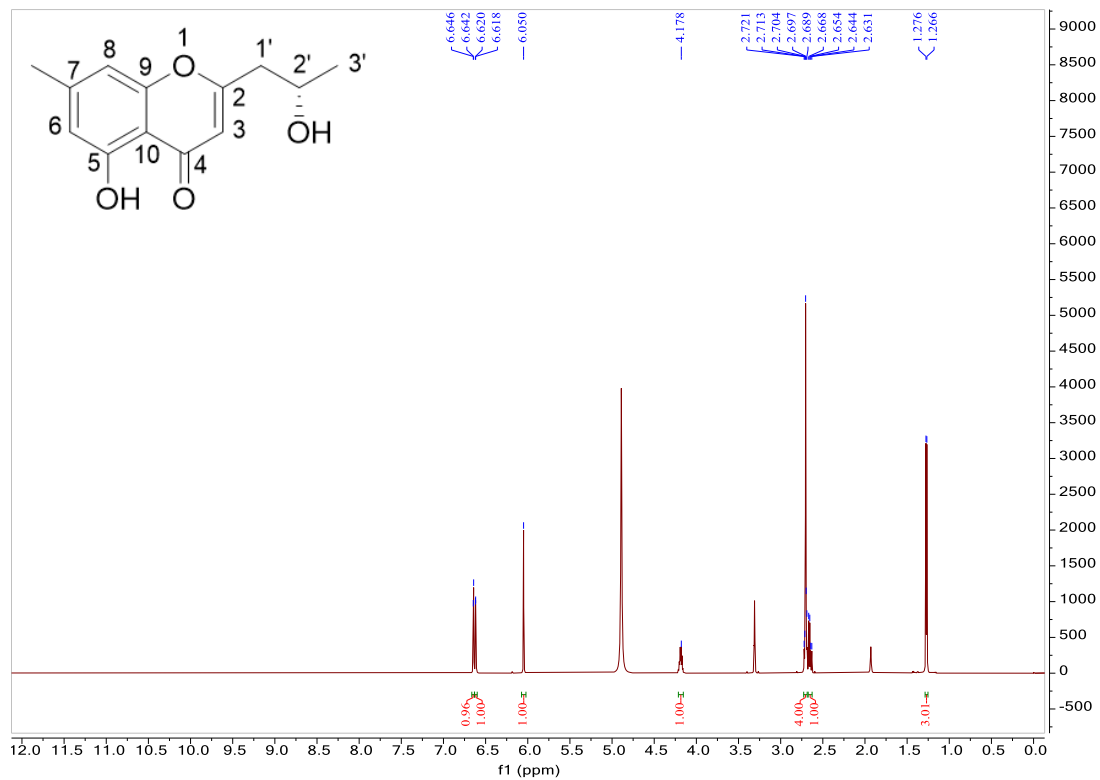


Figure S6. IR spectrum of compound **1**



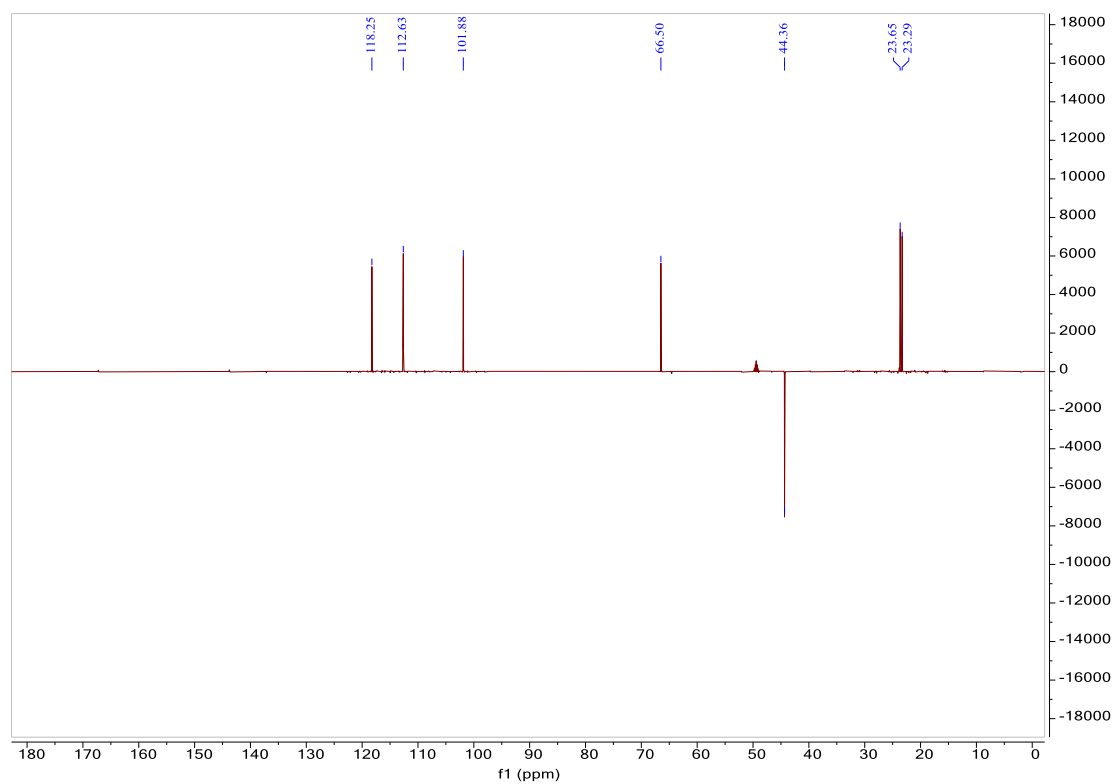


Figure S9. DEPT135 spectrum of compound **1** recorded in CD₃OD

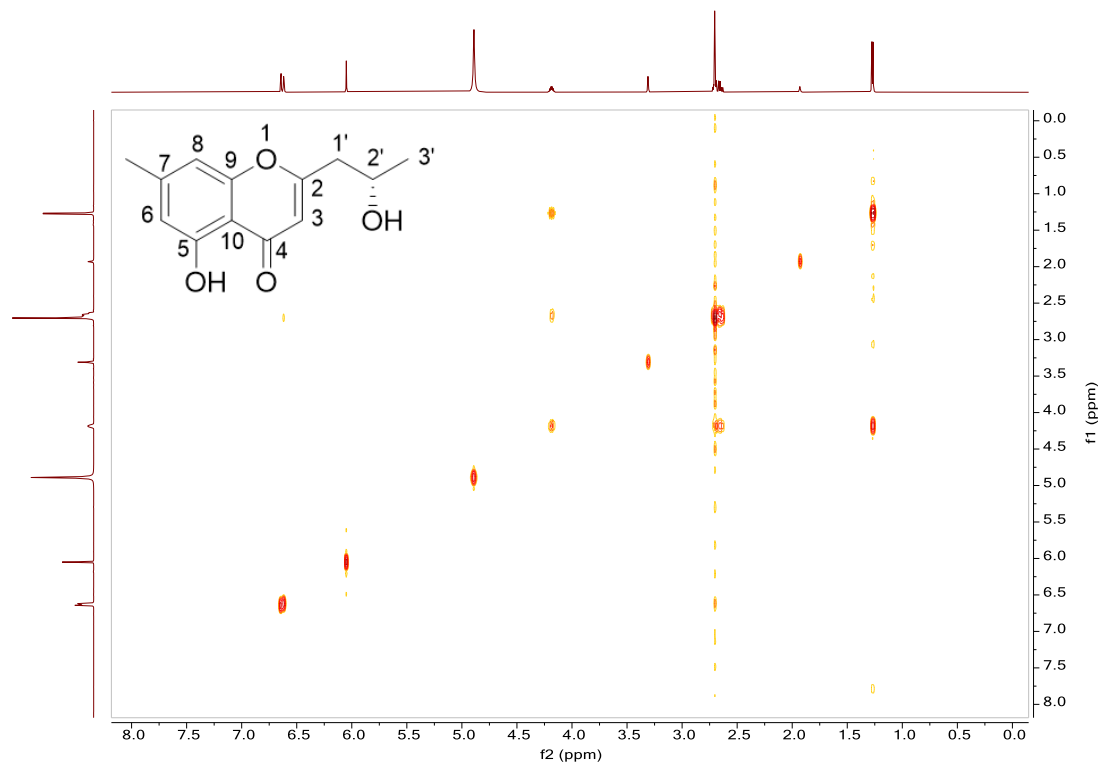


Figure S10. ¹H-¹H COSY spectrum of compound **1** recorded in CD₃OD

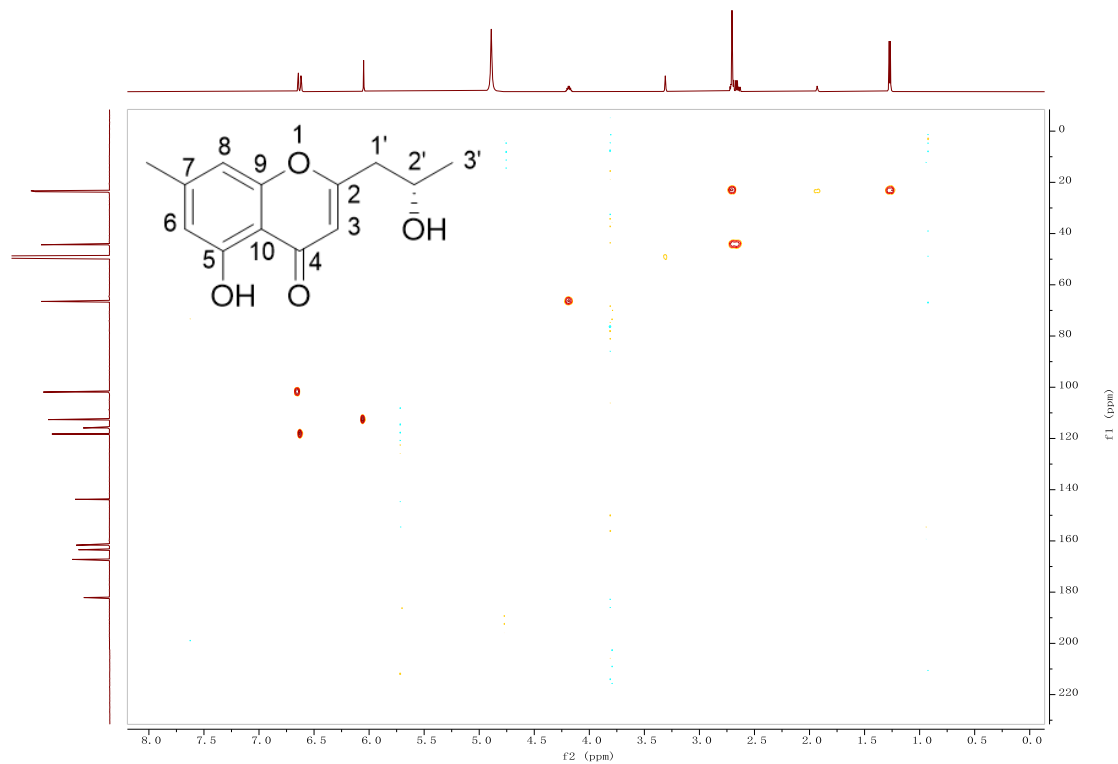


Figure S11. HSQC spectrum of compound **1** recorded in CD₃OD

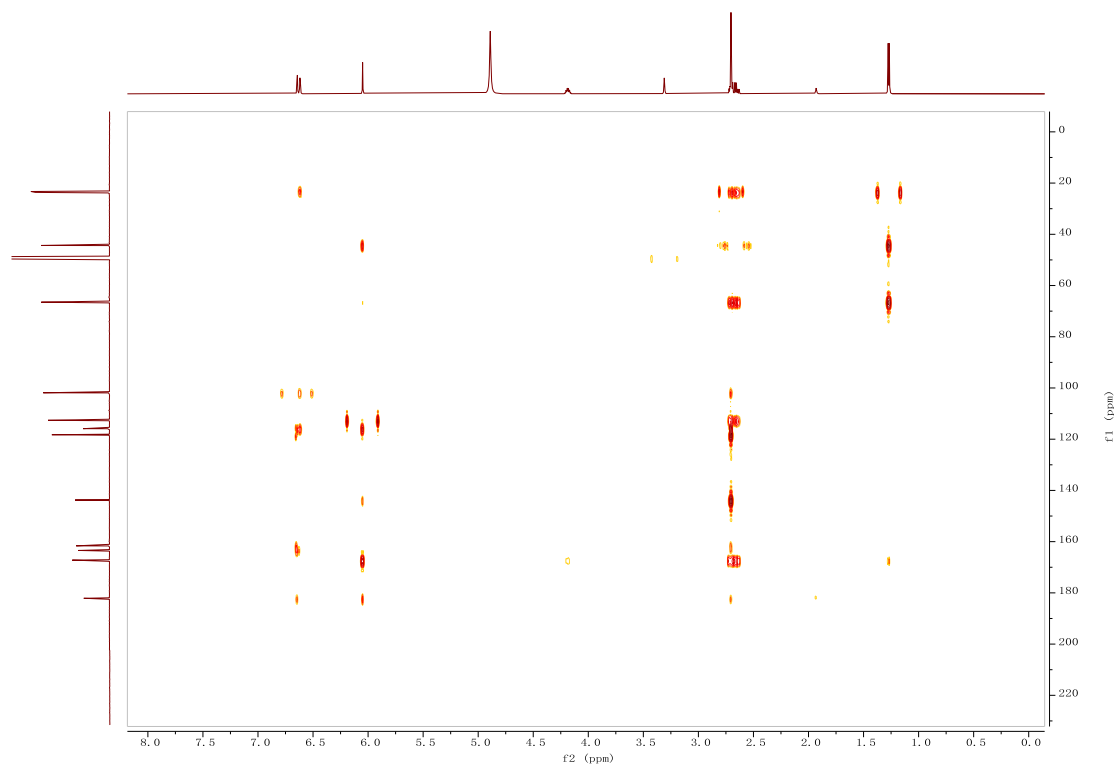


Figure S12. HMBC spectrum of compound **1** recorded in CD₃OD

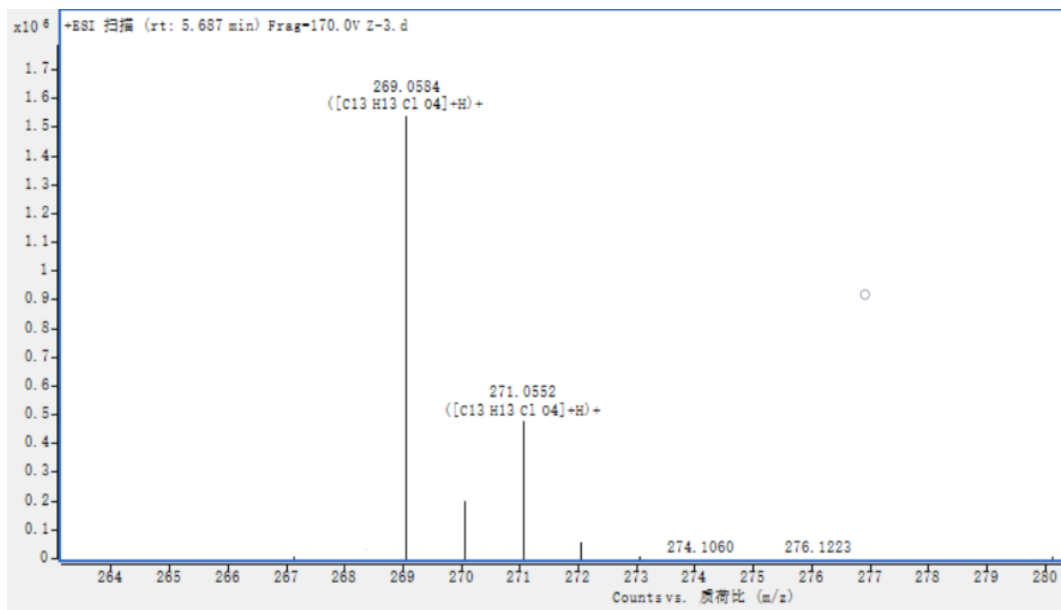


Figure S13. HRESIMS spectrum of compound **2**

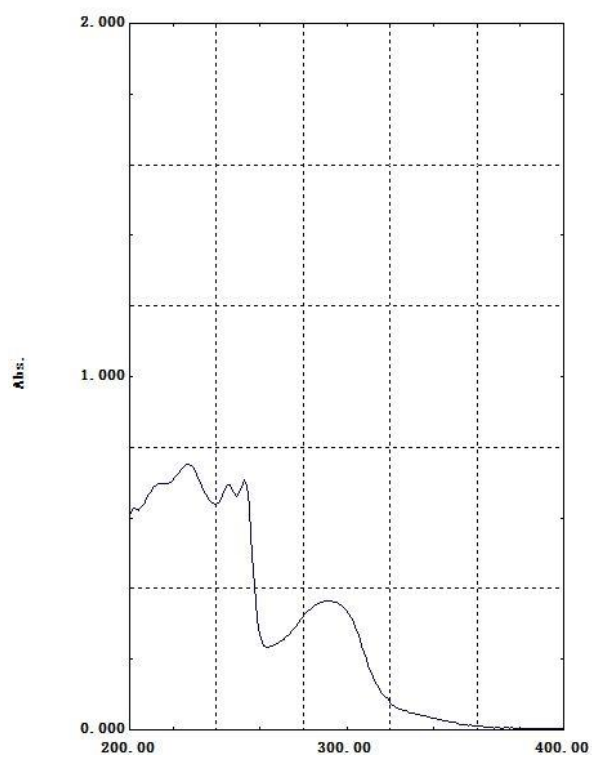


Figure S14. UV spectrum of compound **2** (in MeOH)

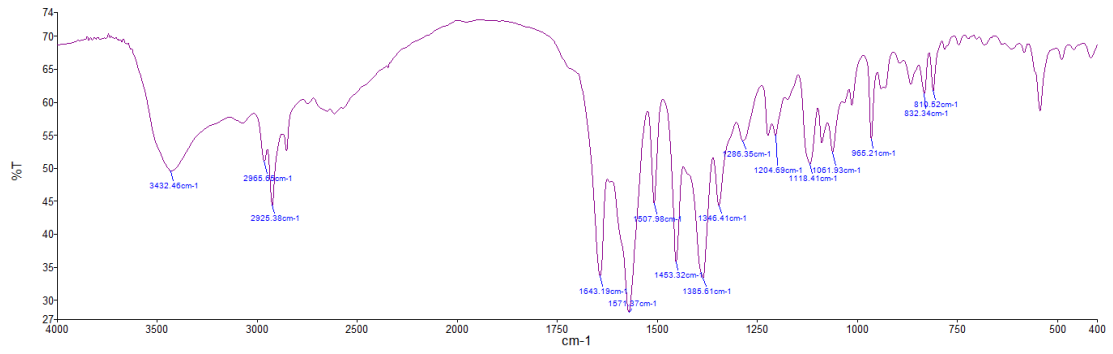


Figure S15. IR spectrum of compound **2**

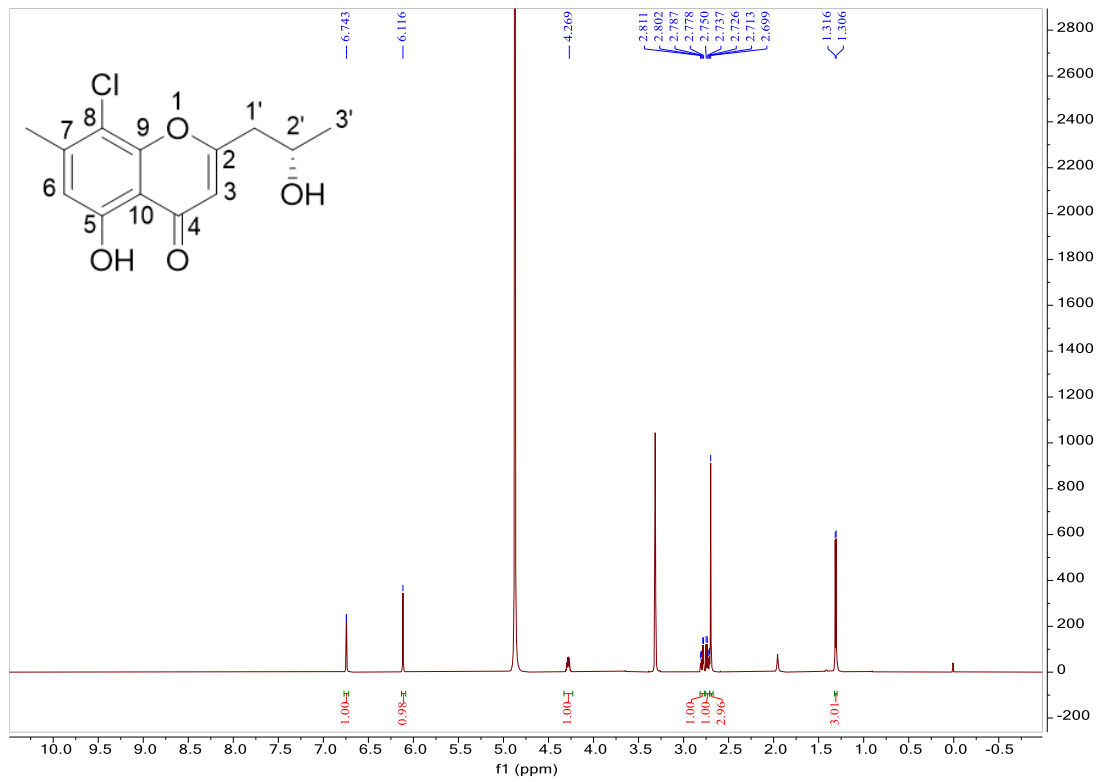


Figure S16. ¹H NMR spectrum of compound **2** recorded in CD₃OD at 600 MHz

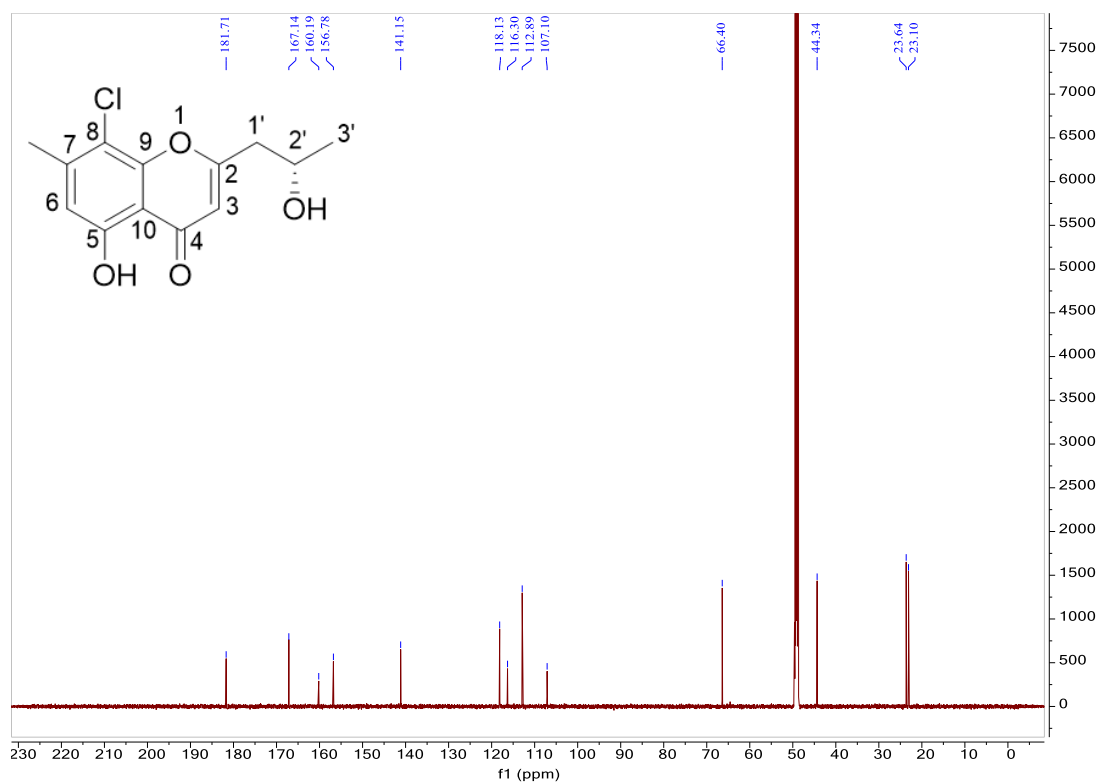


Figure S17. ¹³C NMR spectrum of compound 2 recorded in CD₃OD at 150 MHz

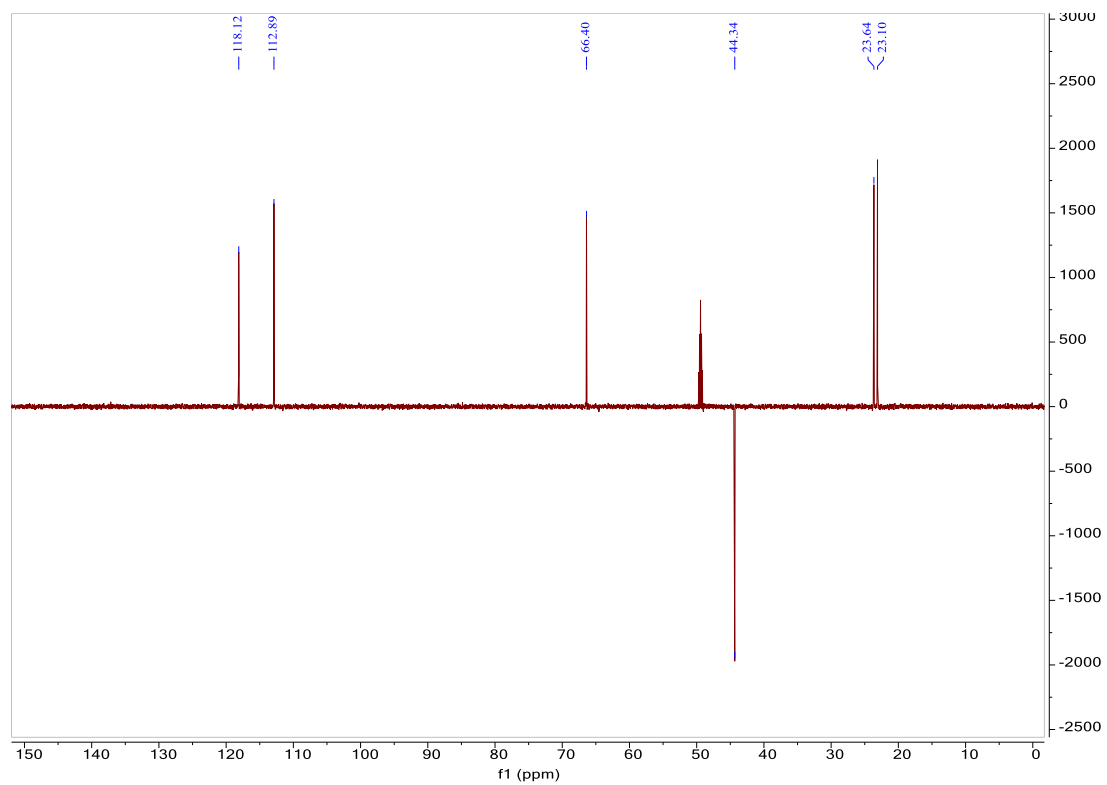


Figure S18. DEPT135 spectrum of compound 2 recorded in CD₃OD

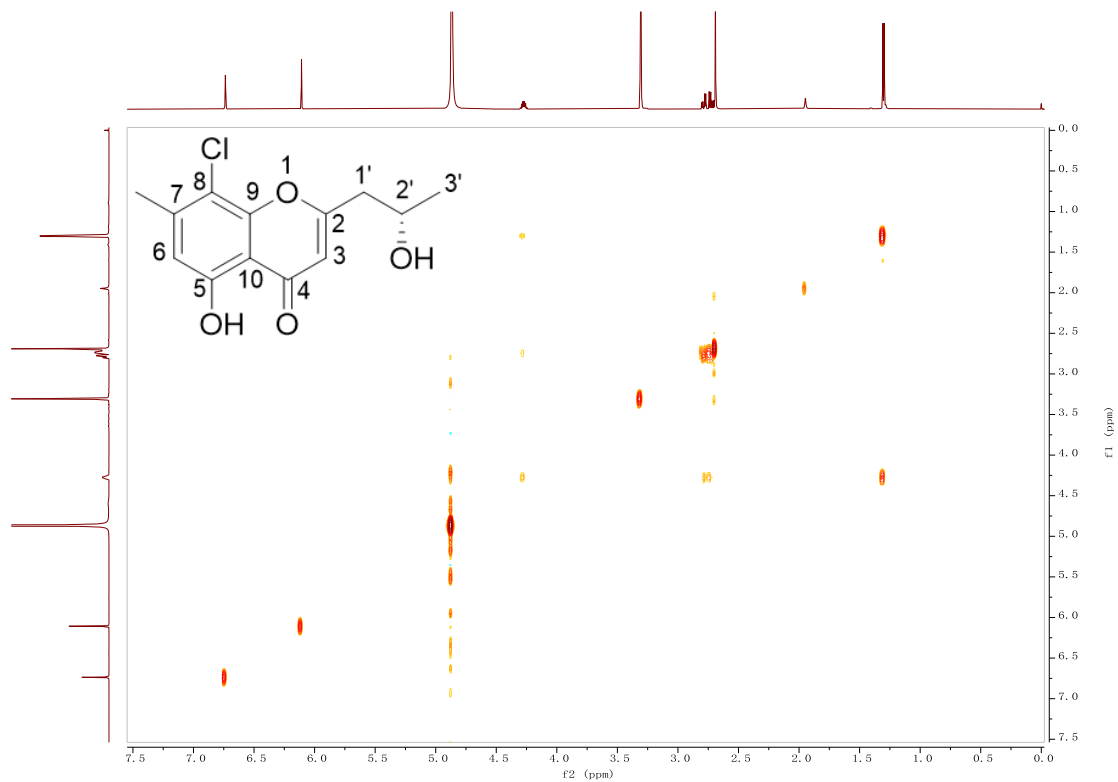


Figure S19. ^1H - ^1H COSY spectrum of compound **2** recorded in CD_3OD

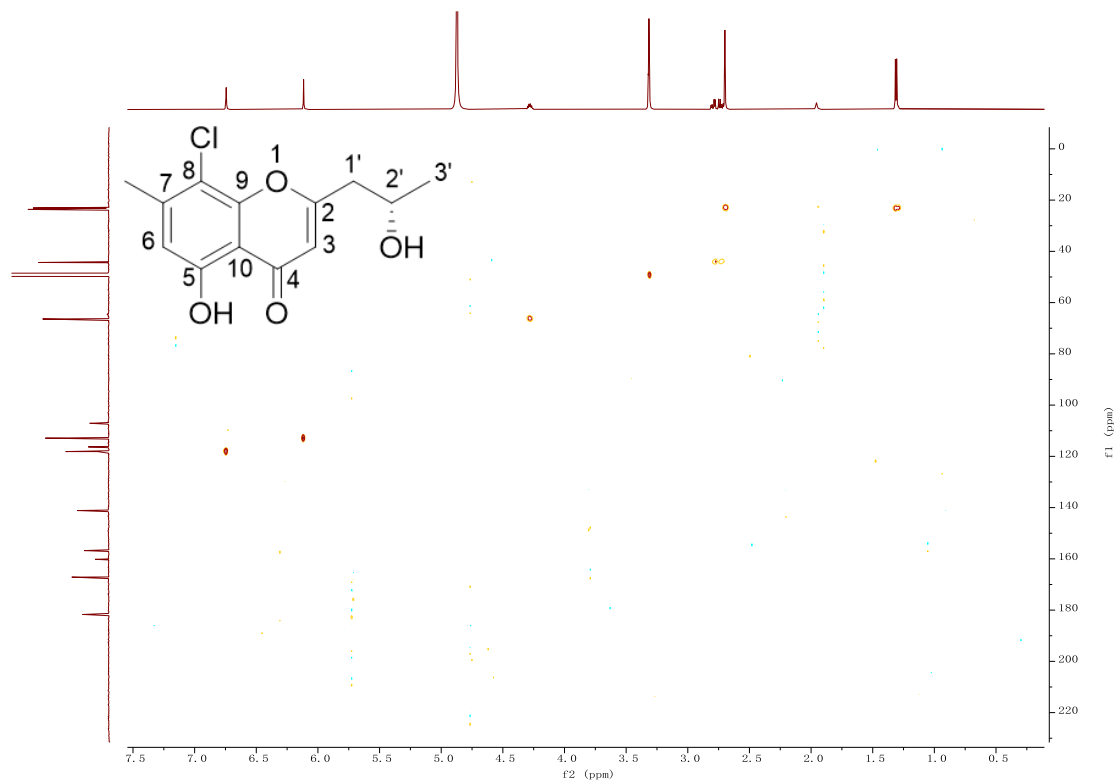


Figure S20. HSQC spectrum of compound **2** recorded in CD_3OD

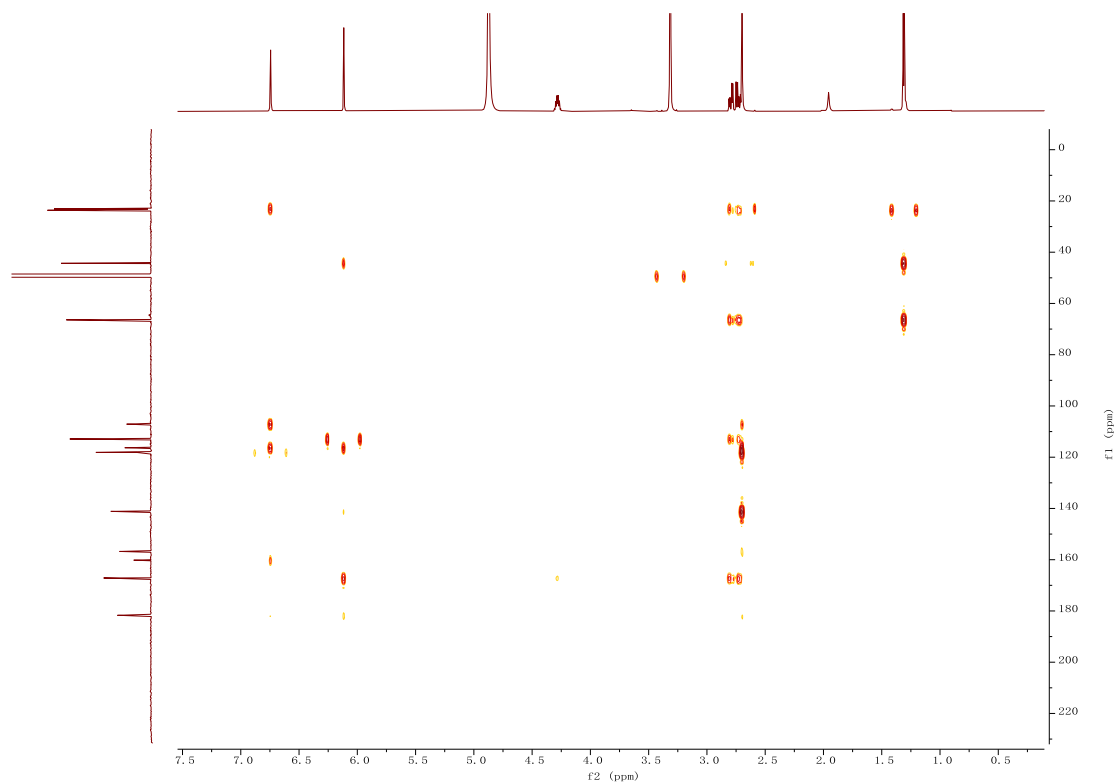


Figure S21. HMBC spectrum of compound **2** recorded in CD₃OD

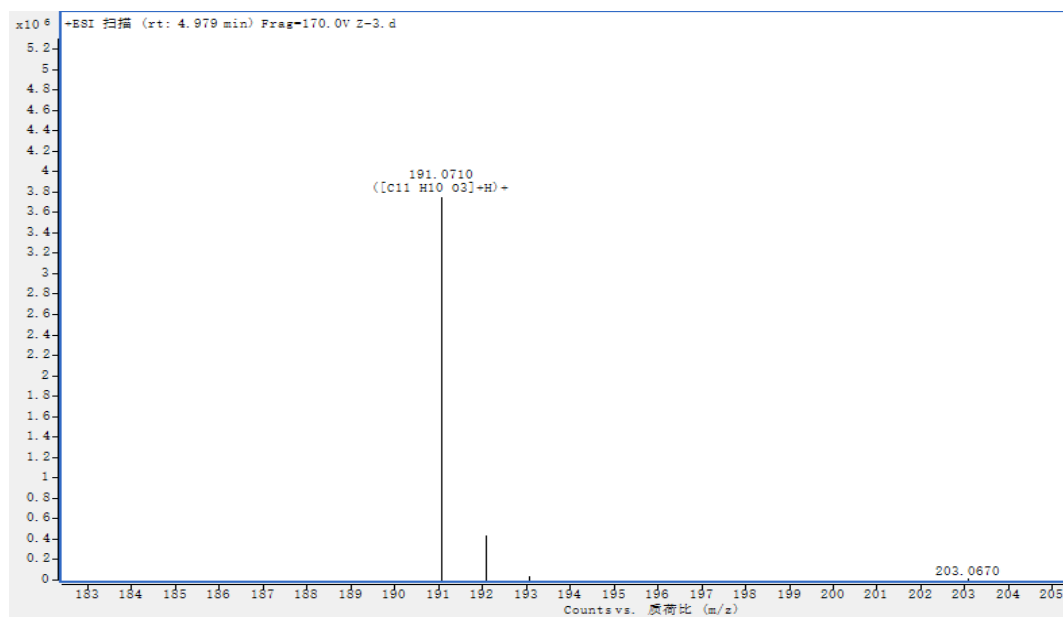


Figure S22. HRESIMS spectrum of compound **3**

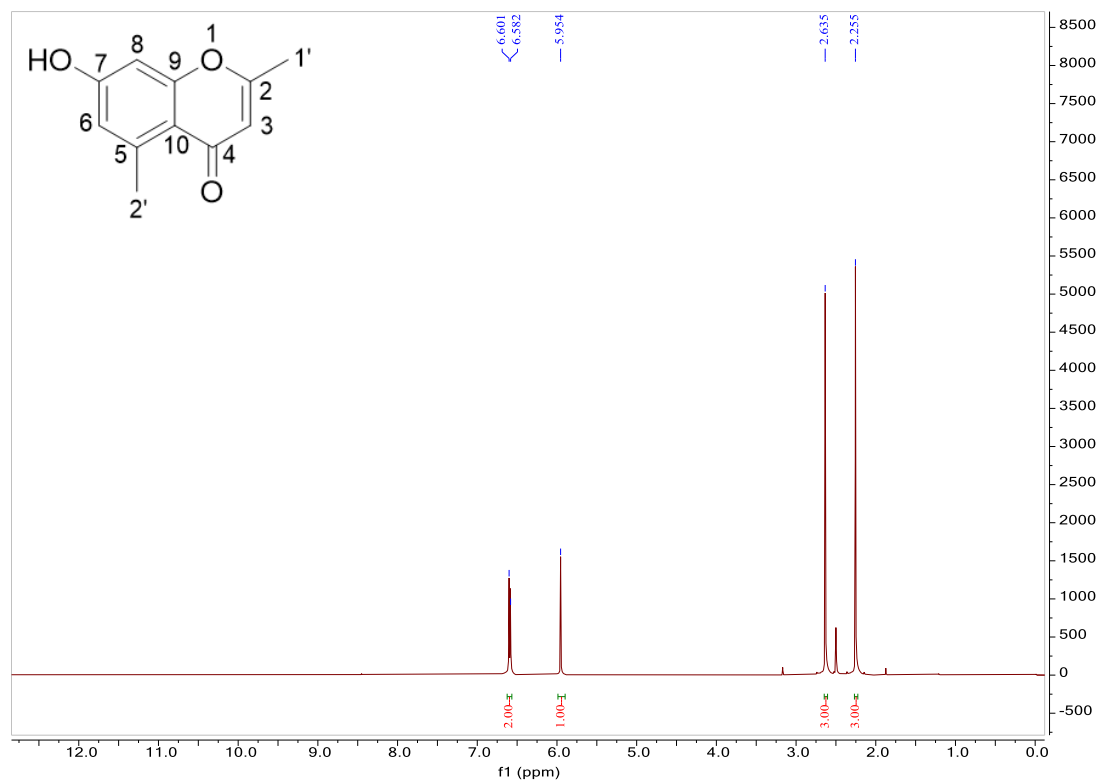


Figure S23. ¹H NMR spectrum of compound **3** recorded in DMSO-*d*₆ at 600 MHz

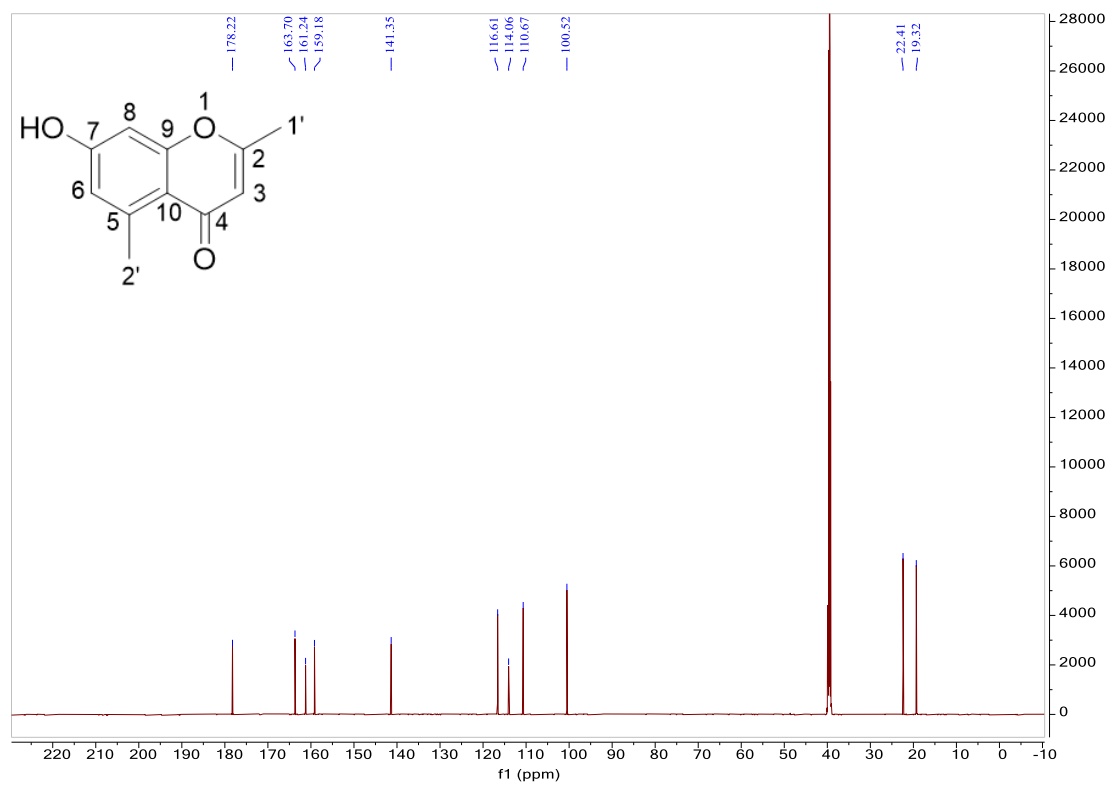


Figure S24. ¹³C NMR spectrum of compound **3** recorded in DMSO-*d*₆ at 150 MHz

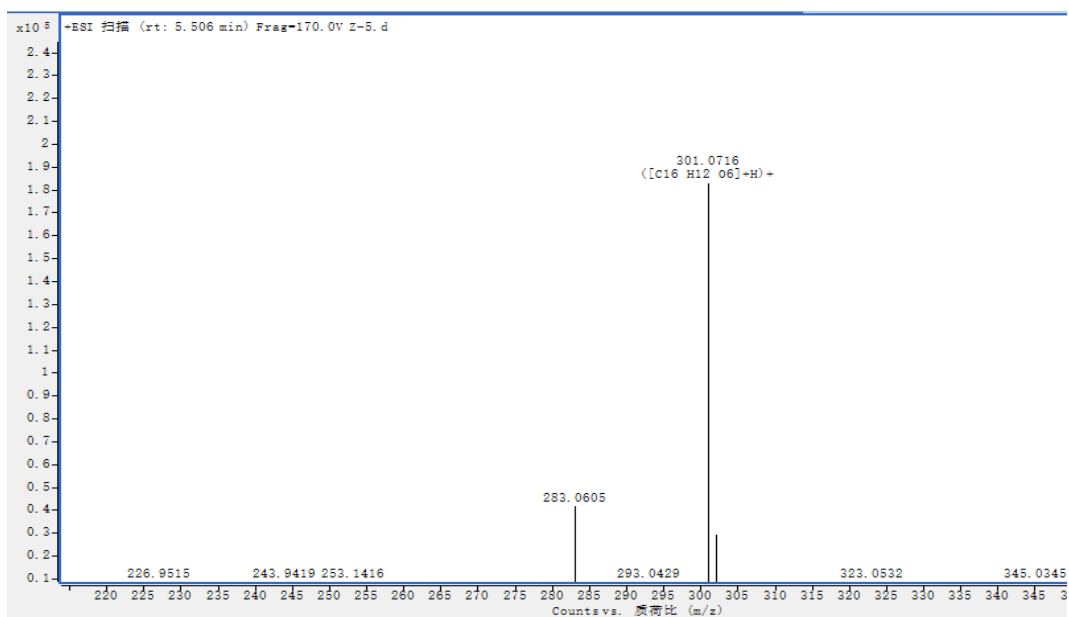


Figure S25. HRESIMS spectrum of compound 4

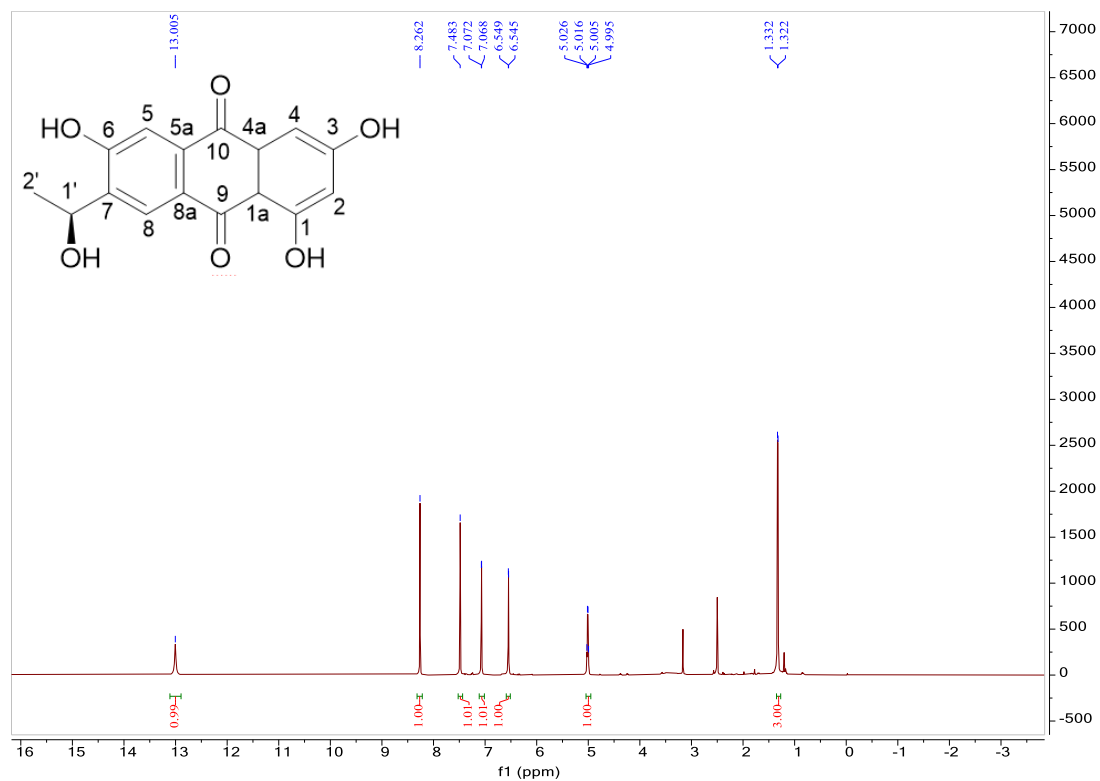


Figure S26. ¹H NMR spectrum of compound 4 recorded in DMSO-*d*₆ at 600 MHz

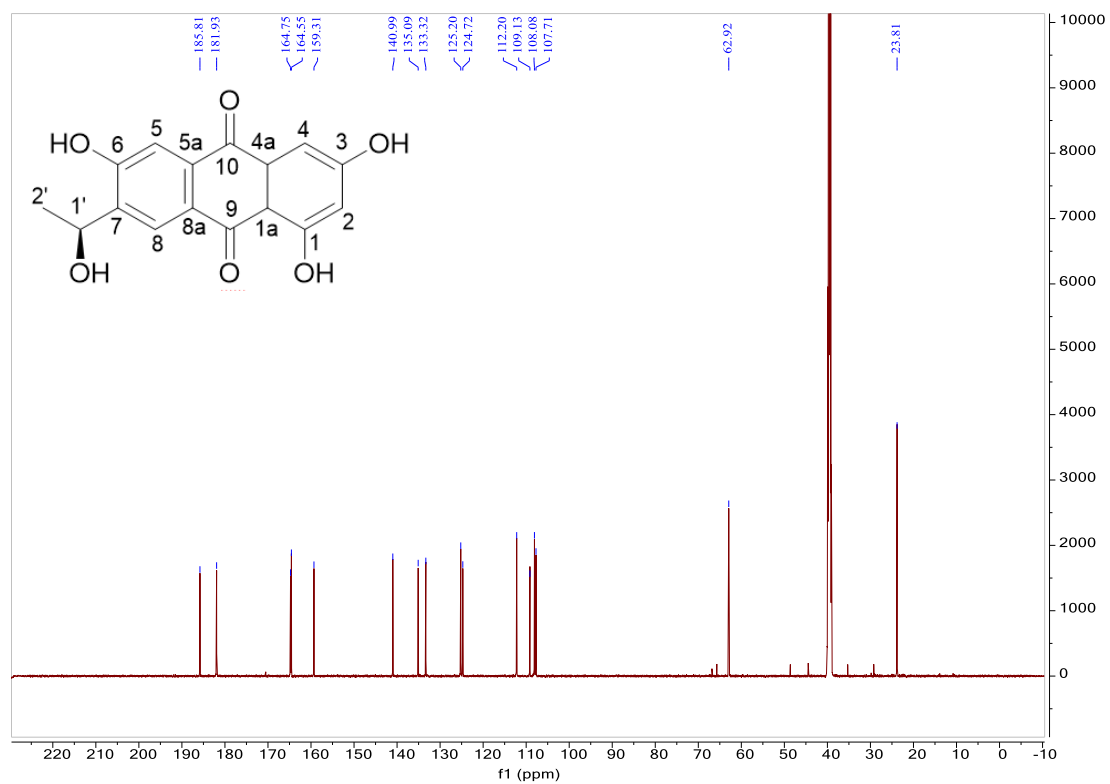
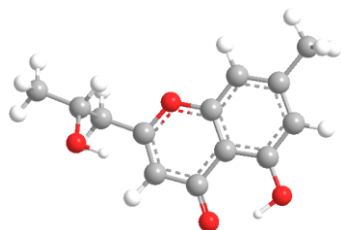


Figure S27. ^{13}C NMR spectrum of compound **4** recorded in $\text{DMSO-}d_6$ at 150 MHz

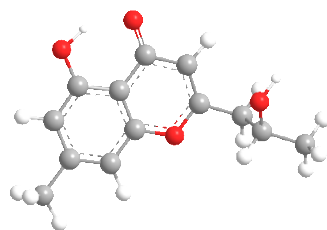
Table S4. Geometry data of conformers of compound **1**

3-new-C8, $\Delta G = 0.0000$ kcal/mol, population = 19.01 %



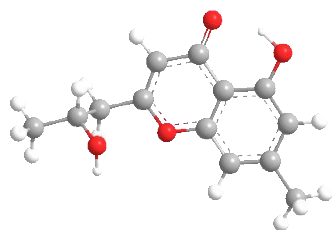
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C	1.138160	-0.639856	-0.123366
C	0.220443	-1.759744	-0.287308
C	-1.148650	-1.387322	-0.579258
C	-1.514552	-0.081026	-0.692902
C	-2.908160	0.407495	-0.900575
C	-3.597609	0.754549	0.441075
C	-4.995497	1.304372	0.214412
H	-5.468902	1.538325	1.179413
H	-4.963686	2.220579	-0.393252
H	-5.618142	0.558749	-0.305216
H	-2.982671	1.524568	0.947345
O	-3.720218	-0.394230	1.261484
H	-2.833612	-0.721350	1.470475
H	-3.497763	-0.368995	-1.408202
H	-2.880991	1.304465	-1.537540
O	-0.634895	0.930462	-0.531277
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H	4.417835	0.062856	0.543584
O	2.982613	-2.098852	0.296571
H	2.198395	-2.703327	0.148487
H	1.122088	2.786366	-0.209776
C	3.823971	2.718948	0.356335
H	4.287335	2.701480	1.356048
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1-C4, $\Delta G = 0.3476$ kcal/mol, population = 10.57 %



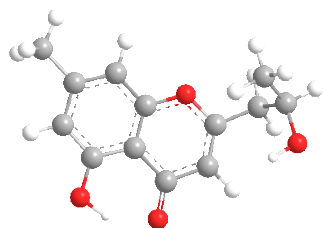
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C -1.160659 0.667197 -0.139038
C -0.320782 1.848055 -0.294520
C 1.076278 1.572556 -0.551927
C 1.538118 0.296508 -0.638501
C 2.956830 -0.103457 -0.871951
C 3.561223 -0.853897 0.332545
C 5.016554 -1.230912 0.083473
H 5.422629 -1.762004 0.957031
H 5.114809 -1.881163 -0.799433
H 5.628389 -0.329270 -0.088966
H 2.970482 -1.770672 0.490715
O 3.402544 -0.107124 1.527940
H 3.923262 0.705886 1.446200
H 3.550811 0.797427 -1.087865
H 3.003328 -0.754754 -1.760577
O 0.728121 -0.773665 -0.491276
H 1.765116 2.408079 -0.673124
O -0.788537 3.004630 -0.206594
C -2.556744 0.784440 0.121273
C -3.327922 -0.370203 0.266266
H -4.395897 -0.262097 0.466072
O -3.112540 1.995096 0.224642
H -2.368337 2.651442 0.086685
H -0.898012 -2.749712 -0.182931
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1-C5, $\Delta G = 0.4512$ kcal/mol, population = 8.87 %



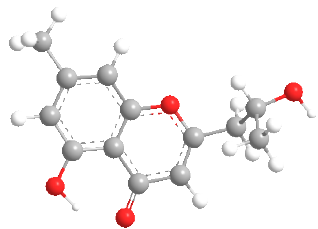
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C -3.742176 -0.220989 0.442146
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O -3.034528 -1.149812 1.245081
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C 2.549055 0.722924 0.236548
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O 3.130461 1.899650 0.486917
H 2.402921 2.585194 0.416841
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C 3.515663 -2.954789 0.015709
H 3.999497 -3.082488 0.997502
H 2.910473 -3.848234 -0.190416
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1-C2, $\Delta G = 0.6168$ kcal/mol, population = 6.71 %



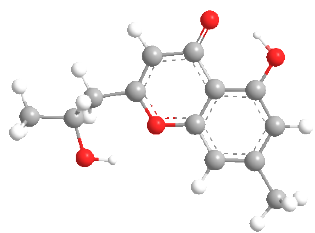
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H 3.769575 1.877797 2.125183
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H -1.912188 -2.806137 0.226000
H -1.217396 2.723165 -0.374273
C -3.896755 2.499506 0.253053
H -4.323929 2.504938 1.269000
H -3.456863 3.487179 0.058461
H -4.735825 2.349695 -0.445395

1-C3, $\Delta G = 0.6507$ kcal/mol, population = 6.33 %



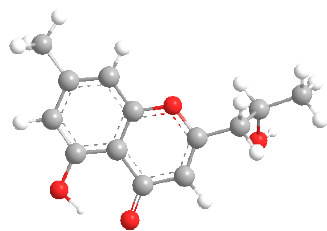
C -2.708764 1.693320 0.144731
C -1.333883 1.779140 -0.111393
C -0.597138 0.603443 -0.246690
C -1.188241 -0.666334 -0.134354
C -0.381800 -1.871393 -0.279046
C 1.023396 -1.637285 -0.536441
C 1.521091 -0.375335 -0.636373
C 2.948930 -0.014309 -0.872800
C 3.599322 0.744885 0.307219
C 3.658238 -0.089628 1.581231
H 2.651886 -0.382889 1.917379
H 4.240287 -1.012234 1.414378
H 4.140994 0.484600 2.385725
H 2.998760 1.649488 0.495175
O 4.878054 1.220132 -0.073952
H 5.464674 0.455545 -0.170886
H 3.011407 0.636901 -1.759560
H 3.520030 -0.930925 -1.082879
O 0.740347 0.718771 -0.497461
H 1.688173 -2.493104 -0.650087
O -0.880891 -3.013731 -0.182605
C -2.587158 -0.742321 0.126183
C -3.325655 0.434655 0.261519
H -4.396265 0.358081 0.461725
O -3.176936 -1.935802 0.239280
H -2.452329 -2.614376 0.106766
H -0.830088 2.741479 -0.206674
C -3.536889 2.942459 0.294385
H -2.923520 3.849813 0.208028
H -4.323597 2.982404 -0.476500
H -4.045944 2.958964 1.271501

1-C7, $\Delta G = 0.6683$ kcal/mol, population = 6.15 %



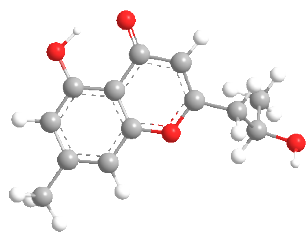
C 2.541157 -1.799088 0.006751
C 1.154300 -1.755251 -0.192929
C 0.516417 -0.517044 -0.216867
C 1.214518 0.690075 -0.049467
C 0.507250 1.963922 -0.079452
C -0.922882 1.865171 -0.288193
C -1.532655 0.661427 -0.448786
C -2.996562 0.444475 -0.647265
C -3.651856 -0.413520 0.459381
C -5.168168 -0.372672 0.356727
H -5.610683 -1.026418 1.123072
H -5.547445 0.648960 0.505741
H -5.494378 -0.730360 -0.632883
H -3.348978 0.009542 1.439008
O -3.257970 -1.771710 0.366822
H -2.291168 -1.800208 0.336730
H -3.161220 -0.067022 -1.611375
H -3.484664 1.427026 -0.696239
O -0.838618 -0.503595 -0.412654
H -1.513994 2.779983 -0.317970
O 1.103724 3.051932 0.067687
C 2.623967 0.633980 0.152231
C 3.265255 -0.606064 0.177918
H 4.345576 -0.630371 0.334130
O 3.316830 1.764004 0.315730
H 2.649048 2.507729 0.260353
H 0.570028 -2.665636 -0.330591
C 3.266656 -3.118523 0.037039
H 2.577747 -3.964861 -0.089001
H 4.022469 -3.165156 -0.763707
H 3.803318 -3.246719 0.990826

1-C11, $\Delta G = 0.6696$ kcal/mol, population = 6.13 %



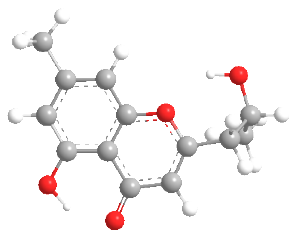
C -2.723401 1.661713 -0.165509
C -1.347766 1.771412 0.076427
C -0.592534 0.608657 0.224104
C -1.166430 -0.670828 0.138316
C -0.340840 -1.861708 0.294799
C 1.062527 -1.603244 0.533485
C 1.542570 -0.333035 0.605307
C 2.968296 0.048057 0.838361
C 3.563625 0.855111 -0.321109
C 5.019380 1.223719 -0.060739
H 5.628905 0.314864 0.065607
H 5.427161 1.798141 -0.907750
H 5.116896 1.842393 0.844954
H 2.969815 1.783295 -0.428017
O 3.423048 0.050779 -1.484007
H 3.717707 0.570295 -2.244496
H 3.559418 -0.865854 0.992149
H 3.028858 0.652664 1.758117
O 0.744772 0.746734 0.461158
H 1.741850 -2.446935 0.651211
O -0.825712 -3.012456 0.221899
C -2.566392 -0.771270 -0.107840
C -3.323189 0.392510 -0.255722
H -4.394371 0.297289 -0.444684
O -3.139239 -1.975176 -0.195465
H -2.402223 -2.640111 -0.058493
H -0.857294 2.742450 0.150988
C -3.570619 2.896309 -0.329164
H -2.970511 3.813710 -0.256697
H -4.082187 2.892430 -1.305162
H -4.356047 2.934974 0.443066

1-C12, $\Delta G = 0.7756$ kcal/mol, population = 5.13 %



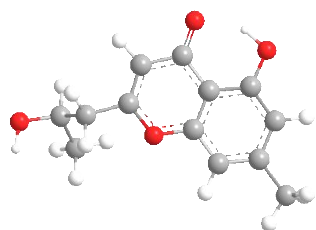
C -2.719664 -1.694201 -0.139338
C -1.345344 -1.786167 0.117646
C -0.601999 -0.613827 0.246086
C -1.185953 0.658531 0.126050
C -0.373016 1.860017 0.264391
C 1.030547 1.619802 0.524467
C 1.521359 0.355677 0.631112
C 2.947791 -0.010286 0.866117
C 3.602973 -0.747793 -0.325856
C 3.653505 0.106460 -1.581193
H 4.147649 -0.447930 -2.392638
H 2.642468 0.384167 -1.913374
H 4.224726 1.029718 -1.392666
H 3.005613 -1.656143 -0.533072
O 4.936088 -1.096796 0.004133
H 4.913219 -1.730985 0.734152
H 2.995132 -0.670867 1.748894
H 3.528014 0.895753 1.089138
O 0.734810 -0.735219 0.498086
H 1.700188 2.472312 0.634062
O -0.865936 3.004454 0.161052
C -2.584338 0.740789 -0.135477
C -3.329405 -0.432819 -0.263922
H -4.399514 -0.351407 -0.464894
O -3.167382 1.936827 -0.255956
H -2.438996 2.612136 -0.127159
H -0.846980 -2.750733 0.218816
C -3.554840 -2.939493 -0.281737
H -4.343325 -2.969292 0.487771
H -4.062032 -2.959966 -1.259754
H -2.947051 -3.849839 -0.187739

1-C1, $\Delta G = 0.7863$ kcal/mol, population = 5.04 %



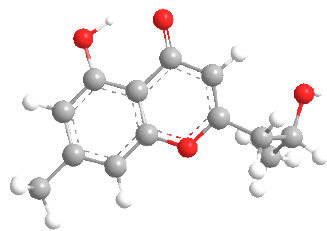
C -2.477286 1.749093 -0.057391
C -1.099262 1.747164 0.199552
C -0.430485 0.527679 0.279052
C -1.089131 -0.701283 0.110296
C -0.350023 -1.954322 0.196275
C 1.067173 -1.811820 0.460176
C 1.636857 -0.588850 0.621154
C 3.083656 -0.323515 0.880974
C 3.762515 0.563547 -0.190761
C 3.566871 0.032967 -1.608857
H 4.110297 0.668397 -2.323473
H 3.937934 -0.999574 -1.703597
H 2.501156 0.037603 -1.891142
H 4.839293 0.558461 0.043852
O 3.364371 1.919176 -0.074586
H 2.400575 1.948957 -0.163567
H 3.605586 -1.287270 0.953361
H 3.183926 0.190559 1.851280
O 0.914434 0.555768 0.531879
H 1.681845 -2.708723 0.530405
O -0.910768 -3.061070 0.047810
C -2.490033 -0.687878 -0.150022
C -3.162221 0.533351 -0.230225
H -4.235289 0.524840 -0.431576
O -3.145338 -1.839760 -0.316355
H -2.460715 -2.563482 -0.217609
H -0.545298 2.675955 0.339276
C -3.234912 3.047666 -0.145856
H -2.570032 3.914904 -0.033257
H -3.755170 3.131433 -1.113457
H -4.007680 3.100743 0.638299

1-C6, $\Delta G = 0.8101$ kcal/mol, population = 4.84 %



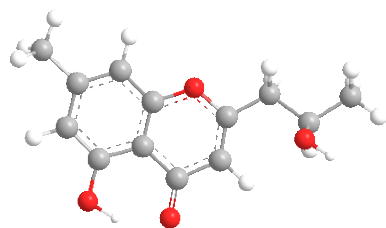
C 2.760917 -1.618321 -0.051453
C 1.387854 -1.734879 0.201558
C 0.614159 -0.577532 0.277456
C 1.166262 0.703305 0.107562
C 0.322170 1.888241 0.192450
C -1.075454 1.622065 0.456959
C -1.535640 0.350659 0.609556
C -2.963584 -0.027229 0.825156
C -3.747084 -0.300113 -0.483328
C -3.182104 -1.456363 -1.300593
H -2.154037 -1.254355 -1.635282
H -3.166189 -2.384667 -0.704593
H -3.810416 -1.623485 -2.188084
H -3.711081 0.620208 -1.089819
O -5.117452 -0.491445 -0.180105
H -5.207868 -1.344080 0.270550
H -3.477781 0.785816 1.355109
H -2.999830 -0.929044 1.457707
O -0.720109 -0.723271 0.528779
H -1.767366 2.460723 0.533492
O 0.786618 3.039833 0.044837
C 2.563866 0.810659 -0.148856
C 3.339292 -0.347741 -0.224386
H 4.408338 -0.247225 -0.422435
O 3.116911 2.015506 -0.314855
H 2.370303 2.676213 -0.217677
H 0.913221 -2.706797 0.339486
C 3.628319 -2.846597 -0.137746
H 4.146287 -2.891779 -1.109230
H 4.409002 -2.827090 0.640058
H 3.042236 -3.767602 -0.014460

1-C10, $\Delta G = 0.9206$ kcal/mol, population = 4.01 %



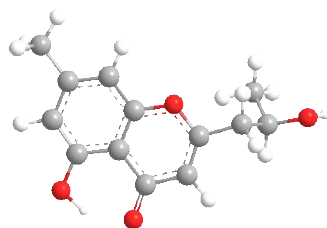
C -2.918074 -1.342205 -0.141388
C -1.590531 -1.676036 0.155739
C -0.654237 -0.653775 0.308807
C -0.999606 0.701704 0.176893
C 0.008910 1.740384 0.345938
C 1.337704 1.255601 0.645833
C 1.594882 -0.075447 0.753827
C 2.942065 -0.678904 0.991667
C 3.778358 -0.832073 -0.292321
C 3.071862 -1.616299 -1.393192
H 3.740161 -1.741345 -2.260381
H 2.780423 -2.618783 -1.044283
H 2.168360 -1.086340 -1.732826
H 4.694484 -1.381188 0.001800
O 4.113057 0.480670 -0.716126
H 4.575774 0.416344 -1.562666
H 2.811855 -1.665659 1.458045
H 3.507493 -0.040351 1.684949
O 0.631341 -1.010327 0.597847
H 2.151112 1.969176 0.766367
O -0.272297 2.954363 0.232904
C -2.353025 1.030342 -0.124446
C -3.290352 0.007521 -0.279152
H -4.322823 0.277414 -0.510332
O -2.710281 2.311131 -0.255489
H -1.876046 2.845125 -0.101720
H -1.273899 -2.713395 0.268206
C -3.955455 -2.419830 -0.318239
H -4.787338 -2.281658 0.391112
H -4.389289 -2.380666 -1.330677
H -3.531644 -3.421511 -0.163404

1-C18, $\Delta G = 0.9494$ kcal/mol, population = 3.82 %



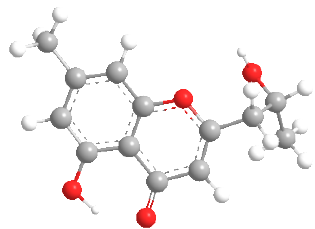
C -3.187645 1.371702 -0.040877
C -1.844457 1.769179 -0.030418
C -0.850176 0.792093 0.017645
C -1.153259 -0.579276 0.054437
C -0.083866 -1.567236 0.108372
C 1.255213 -1.020737 0.128671
C 1.467912 0.321741 0.083536
C 2.791174 1.025321 0.097891
C 4.007772 0.179970 -0.268832
C 5.249760 1.046405 -0.452086
H 6.122071 0.418541 -0.693311
H 5.114584 1.767644 -1.272969
H 5.469542 1.602169 0.473224
H 3.791789 -0.343783 -1.220797
O 4.195434 -0.768678 0.776514
H 4.920282 -1.356082 0.521920
H 2.947259 1.452936 1.105161
H 2.715770 1.880837 -0.590715
O 0.448911 1.209327 0.024789
H 2.109071 -1.689748 0.209498
O -0.324380 -2.794880 0.141194
C -2.522549 -0.972999 0.042678
C -3.517896 0.004562 -0.004476
H -4.562183 -0.314353 -0.012214
O -2.838668 -2.270828 0.077803
H -1.966611 -2.764054 0.108829
H -1.560434 2.821634 -0.057764
C -4.288053 2.399159 -0.090230
H -3.888448 3.422309 -0.110853
H -4.916969 2.254841 -0.983654
H -4.950333 2.303431 0.785362

1-C9, $\Delta G = 0.9984$ kcal/mol, population = 3.52 %



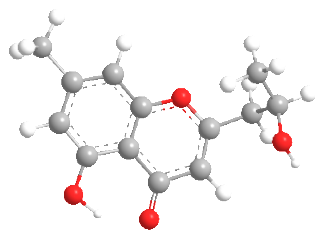
C -2.761351 1.615425 -0.062178
C -1.388133 1.734010 0.188803
C -0.613421 0.577554 0.267907
C -1.164736 -0.704337 0.103099
C -0.320121 -1.888239 0.193334
C 1.076982 -1.619858 0.459826
C 1.536403 -0.347773 0.604997
C 2.962840 0.031525 0.831002
C 3.749733 0.287449 -0.466921
C 3.197139 1.438226 -1.300609
H 3.828080 1.597528 -2.189983
H 2.174789 1.231221 -1.650414
H 3.184607 2.369447 -0.712459
H 3.710929 -0.641485 -1.070432
O 5.080121 0.542448 -0.043343
H 5.619544 0.699178 -0.830504
H 3.470069 -0.776616 1.375610
H 3.002464 0.940911 1.450461
O 0.720955 0.725283 0.517459
H 1.769190 -2.457706 0.542070
O -0.783032 -3.040760 0.049143
C -2.562453 -0.813670 -0.152186
C -3.338849 0.343783 -0.230611
H -4.408043 0.241784 -0.427062
O -3.114630 -2.019516 -0.313897
H -2.367640 -2.679382 -0.215032
H -0.914169 2.706716 0.323307
C -3.629902 2.842601 -0.151986
H -3.046580 3.764076 -0.019583
H -4.138132 2.890731 -1.128529
H -4.418357 2.818683 0.617723

1-C13, $\Delta G = 1.0147$ kcal/mol, population = 3.42 %



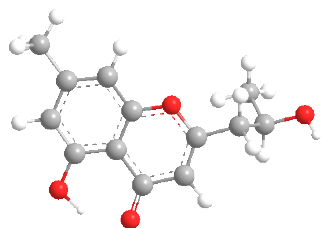
C -2.757313 1.535188 -0.062709
C -1.410213 1.725544 0.271053
C -0.568605 0.616066 0.345052
C -1.028484 -0.688264 0.096739
C -0.117218 -1.821704 0.187203
C 1.245189 -1.480459 0.534333
C 1.615724 -0.189582 0.754184
C 3.000505 0.278872 1.056799
C 3.771618 0.760972 -0.199630
C 4.099451 -0.363606 -1.168170
H 4.656750 0.038440 -2.027219
H 4.714988 -1.134281 -0.681145
H 3.179450 -0.835458 -1.546217
H 4.721099 1.193809 0.172204
O 3.033329 1.731083 -0.921882
H 2.796655 2.451625 -0.321356
H 3.567475 -0.530945 1.536990
H 2.933646 1.111858 1.774752
O 0.737513 0.832923 0.674754
H 1.984216 -2.277093 0.614725
O -0.500154 -2.993478 -0.024748
C -2.401130 -0.871122 -0.239354
C -3.243630 0.239345 -0.314586
H -4.292347 0.081232 -0.574136
O -2.867023 -2.100341 -0.478424
H -2.085985 -2.717121 -0.362688
H -1.006126 2.718204 0.471888
C -3.694367 2.710613 -0.158159
H -4.550262 2.584406 0.524258
H -3.189740 3.654382 0.090105
H -4.107587 2.797262 -1.176293

1-C16, $\Delta G = 1.0887$ kcal/mol, population = 3.02 %



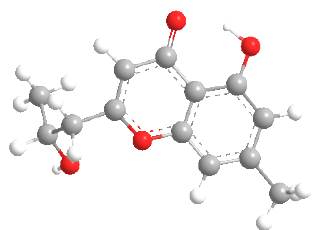
C -2.843086 1.483160 0.048973
C -1.507806 1.731626 -0.293878
C -0.616822 0.660941 -0.362223
C -1.015149 -0.660612 -0.099819
C -0.052604 -1.752024 -0.182194
C 1.290281 -1.353466 -0.540878
C 1.599701 -0.050135 -0.777724
C 2.967688 0.469609 -1.071627
C 3.802974 0.742714 0.205948
C 3.135208 1.713224 1.167277
H 3.805036 1.917043 2.015606
H 2.897634 2.663989 0.668241
H 2.202323 1.284715 1.565509
H 4.756314 1.185059 -0.141257
O 4.049630 -0.455061 0.922483
H 4.605185 -1.029600 0.377601
H 2.881892 1.399238 -1.653499
H 3.508005 -0.264124 -1.688333
O 0.677505 0.934594 -0.698843
H 2.068097 -2.112646 -0.607365
O -0.381214 -2.937401 0.046407
C -2.376153 -0.902563 0.245986
C -3.268254 0.168906 0.315715
H -4.307177 -0.034570 0.583100
O -2.783767 -2.149444 0.499644
H -1.974801 -2.730314 0.387182
H -1.150640 2.739816 -0.505995
C -3.832362 2.615495 0.137632
H -4.678017 2.450247 -0.549321
H -4.254825 2.685160 1.153211
H -3.369161 3.580425 -0.109980

1-C14, $\Delta G = 1.2895$ kcal/mol, population = 2.15 %



C -2.766403 1.625554 -0.044184
C -1.395241 1.741901 0.219080
C -0.619389 0.585386 0.285119
C -1.167597 -0.694392 0.095261
C -0.321974 -1.878649 0.172584
C 1.072304 -1.612923 0.454135
C 1.529155 -0.342430 0.624152
C 2.955128 0.035329 0.852875
C 3.754451 0.276266 -0.452551
C 3.196237 1.409386 -1.297582
H 3.175842 2.346883 -0.719426
H 3.834834 1.559709 -2.180656
H 2.175328 1.188939 -1.640038
H 3.720768 -0.660227 -1.043389
O 5.093275 0.610263 -0.131919
H 5.500681 -0.148860 0.307888
H 3.447104 -0.772712 1.414347
H 2.997480 0.951947 1.460519
O 0.712928 0.730915 0.547024
H 1.764741 -2.451434 0.528224
O -0.782493 -3.029258 0.006039
C -2.563105 -0.801484 -0.172450
C -3.340615 0.356104 -0.238116
H -4.408041 0.255869 -0.444901
O -3.112198 -2.005270 -0.358110
H -2.364793 -2.665562 -0.264268
H -0.923659 2.712948 0.372744
C -3.636848 2.852629 -0.116191
H -4.172252 2.897014 -1.078053
H -4.403419 2.831972 0.675721
H -3.050194 3.774513 -0.002409

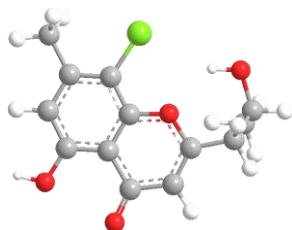
1-C17, $\Delta G = 1.5983$ kcal/mol, population = 1.28 %



C 2.796094 -1.495943 -0.091772
C 1.450518 -1.719396 0.226310
C 0.590034 -0.626814 0.333865
C 1.030806 0.692466 0.134302
C 0.100654 1.806772 0.259635
C -1.256927 1.430336 0.587282
C -1.608420 0.125936 0.756254
C -2.990872 -0.364858 1.047491
C -3.799459 -0.741570 -0.209190
C -4.071061 0.437240 -1.137520
H -4.615688 1.238967 -0.614907
H -3.131485 0.851297 -1.534012
H -4.689590 0.111289 -1.989321
H -4.770730 -1.126436 0.160509
O -3.082798 -1.771783 -0.871210
H -3.560518 -1.993004 -1.682412
H -3.540658 0.409309 1.600038
H -2.912757 -1.256341 1.687339
O -0.713589 -0.877040 0.646437
H -2.008820 2.211676 0.693936
O 0.465305 2.991726 0.091830
C 2.402235 0.909086 -0.186283
C 3.263030 -0.184275 -0.295048
H 4.310606 -0.000525 -0.542092
O 2.849069 2.153655 -0.378792
H 2.057039 2.752843 -0.245895
H 1.060871 -2.724694 0.389134
C 3.752776 -2.652087 -0.221979
H 3.260923 -3.612334 -0.014696
H 4.177468 -2.693574 -1.238226
H 4.599811 -2.538539 0.473642

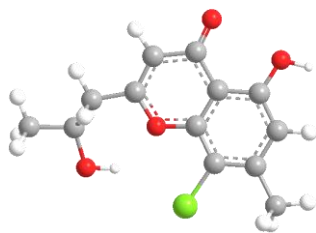
Table S5. Geometry data of conformers of compound **2**

2-C1, $\Delta G = 0.0000$ kcal/mol, population = 35.75 %



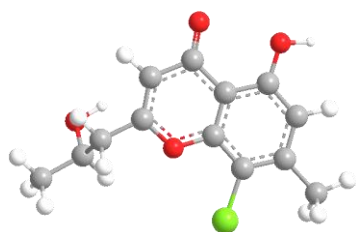
C -2.388379 1.376002 -0.176563
C -3.104951 0.175439 -0.272017
C -2.494162 -1.075240 -0.139637
C -1.096820 -1.161379 0.105450
C -0.354300 -2.440802 0.237778
C 1.083944 -2.278271 0.450339
C 1.673980 -1.067698 0.558121
O 0.949070 0.077736 0.453842
C -0.387174 0.052959 0.211039
C -1.012525 1.298983 0.066842
Cl -0.044972 2.752610 0.185763
C 3.124584 -0.785380 0.773993
C 3.742532 0.178945 -0.267302
C 3.470882 -0.249618 -1.707724
H 3.823516 -1.276361 -1.892388
H 2.392989 -0.213775 -1.935372
H 3.986166 0.429340 -2.403035
H 4.830680 0.159168 -0.092985
O 3.356832 1.522797 -0.034446
H 2.390491 1.573040 -0.094862
H 3.256215 -0.325805 1.768171
H 3.666430 -1.741123 0.772898
H 1.686354 -3.183116 0.529340
O -0.874411 -3.551044 0.168959
O -3.210490 -2.208216 -0.243572
H -4.137201 -1.983694 -0.416233
H -4.180755 0.216848 -0.460406
C -3.076869 2.701666 -0.332801
H -4.151346 2.570444 -0.515220
H -2.642548 3.270060 -1.170450
H -2.943992 3.319045 0.569704

2-C5, $\Delta G = 0.1939$ kcal/mol, population = 25.76 %



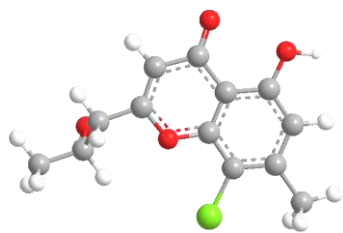
C 2.479003 -1.387196 0.153069
C 3.211183 -0.195268 0.236837
C 2.609099 1.063199 0.144127
C 1.204247 1.166598 -0.045970
C 0.471239 2.455067 -0.141581
C -0.975032 2.309703 -0.307214
C -1.582925 1.106320 -0.398541
O -0.867756 -0.047281 -0.322980
C 0.478152 -0.039243 -0.136225
C 1.095582 -1.293486 -0.034806
Cl 0.109789 -2.735582 -0.139493
C -3.044024 0.846901 -0.563854
C -3.637831 -0.090354 0.512783
C -5.158013 -0.061598 0.479892
H -5.559926 -0.769208 1.220371
H -5.541299 0.943398 0.710144
H -5.523617 -0.359748 -0.515809
H -3.296492 0.271879 1.504318
O -3.240282 -1.435580 0.315087
H -2.272931 -1.467843 0.276444
H -3.564722 1.813986 -0.553808
H -3.221845 0.377983 -1.547750
H -1.568374 3.222160 -0.365182
O 1.005053 3.559300 -0.083234
O 3.341146 2.187220 0.234911
H 4.271352 1.951079 0.368969
H 4.293129 -0.250332 0.381790
C 3.159624 -2.721517 0.263480
H 2.987256 -3.323954 -0.642527
H 2.751345 -3.298469 1.108357
H 4.241383 -2.602913 0.407318

2-C6, $\Delta G = 1.0348$ kcal/mol, population = 6.22 %



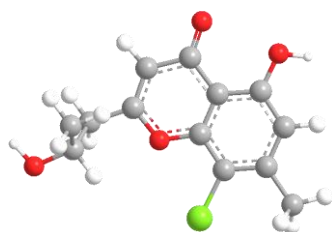
```
C 2.813607 -0.853390 -0.294047
C 3.192182 0.495777 -0.330730
C 2.284266 1.534755 -0.107637
C 0.921911 1.240052 0.171074
C -0.115579 2.274437 0.411336
C -1.451088 1.731348 0.660561
C -1.701592 0.402254 0.693443
O -0.722537 -0.507971 0.475660
C 0.551652 -0.121949 0.211346
C 1.474636 -1.152681 -0.019106
Cl 0.923440 -2.810273 0.035381
C -3.032965 -0.247596 0.863818
C -3.599270 -0.741723 -0.486788
C -4.920823 -1.467499 -0.302728
H -4.797496 -2.347700 0.345296
H -5.664731 -0.795379 0.153966
H -5.307571 -1.800237 -1.277426
H -2.858921 -1.441192 -0.923529
O -3.829328 0.345471 -1.367098
H -2.994807 0.818190 -1.498552
H -2.926035 -1.105487 1.546035
H -3.737873 0.469649 1.307440
H -2.261099 2.439529 0.835100
O 0.096680 3.483935 0.401717
O 2.678242 2.820228 -0.153029
H 3.625765 2.856304 -0.352382
H 4.234892 0.744825 -0.543779
C 3.817205 -1.942677 -0.543658
H 3.517634 -2.559030 -1.406155
H 3.879342 -2.621927 0.321325
H 4.814042 -1.525570 -0.737379
```

2-C13, $\Delta G = 1.0925$ kcal/mol, population = 5.64 %



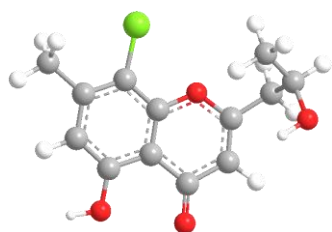
```
C 2.657709 -1.127216 -0.266690
C 3.214039 0.158986 -0.305743
C 2.447570 1.312737 -0.119716
C 1.050960 1.207012 0.122001
C 0.152259 2.373352 0.316929
C -1.248562 2.016532 0.529707
C -1.675700 0.734501 0.567012
O -0.817805 -0.299698 0.400985
C 0.501381 -0.092230 0.166791
C 1.283957 -1.240501 -0.027046
Cl 0.513756 -2.809345 0.030328
C -3.075791 0.261248 0.787245
C -3.577676 -0.648780 -0.338577
C -5.002638 -1.126566 -0.085725
H -5.342873 -1.773009 -0.910429
H -5.067554 -1.707765 0.847367
H -5.688901 -0.267714 -0.014330
H -2.904216 -1.525626 -0.388476
O -3.481097 0.106245 -1.539252
H -3.705947 -0.476593 -2.277263
H -3.115897 -0.298456 1.736679
H -3.735881 1.135342 0.881866
H -1.961832 2.829842 0.662790
O 0.526617 3.543680 0.299364
O 3.013850 2.532525 -0.166542
H 3.961728 2.434741 -0.342415
H 4.286133 0.265372 -0.490274
C 3.512811 -2.344288 -0.476887
H 3.154154 -2.929004 -1.338828
H 3.463565 -3.011772 0.398001
H 4.560672 -2.066665 -0.650544
```


2-C4, $\Delta G = 1.1270$ kcal/mol, population = 5.32 %



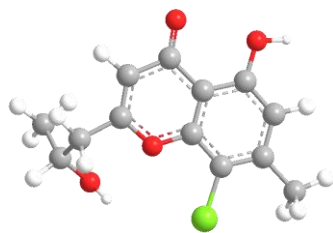
C 2.653242 -1.136074 0.257602
C 3.222278 0.144409 0.300128
C 2.468980 1.305745 0.107079
C 1.073203 1.213918 -0.144875
C 0.186987 2.389377 -0.339331
C -1.215916 2.046607 -0.566645
C -1.654404 0.768549 -0.617084
O -0.807522 -0.275007 -0.443680
C 0.511835 -0.080057 -0.196708
C 1.280570 -1.235941 0.005060
Cl 0.493959 -2.796001 -0.056769
C -3.056191 0.305377 -0.831787
C -3.598526 -0.566978 0.322542
C -3.664676 0.186623 1.645811
H -4.067920 -0.467468 2.432988
H -2.669415 0.537085 1.959660
H -4.320148 1.070084 1.557366
H -2.923360 -1.430722 0.432119
O -4.854023 -1.117636 -0.036002
H -5.498694 -0.395491 -0.067164
H -3.704757 1.182277 -0.976938
H -3.096919 -0.301340 -1.751564
H -1.920069 2.867406 -0.702157
O 0.569697 3.556406 -0.308948
O 3.046483 2.519877 0.156376
H 3.992179 2.413785 0.338810
H 4.293906 0.240146 0.493525
C 3.493776 -2.361487 0.477449
H 3.119344 -2.942594 1.335096
H 4.542208 -2.094153 0.663178
H 3.448057 -3.028441 -0.398064

2-C2, $\Delta G = 1.2582$ kcal/mol, population = 4.27 %



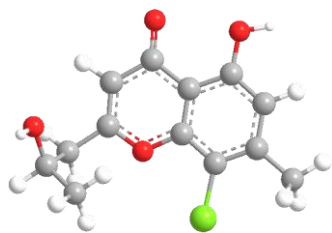
C -2.792065 0.569174 0.305300
C -3.019356 -0.813010 0.360461
C -2.009916 -1.748706 0.117724
C -0.695907 -1.309799 -0.200489
C 0.445225 -2.225777 -0.452853
C 1.708085 -1.541225 -0.727772
C 1.809514 -0.192575 -0.781949
O 0.735812 0.604691 -0.568464
C -0.479880 0.083899 -0.263803
C -1.502593 1.010157 -0.011615
Cl -1.135920 2.717752 -0.085857
C 3.065728 0.589383 -0.973349
C 3.750783 0.948410 0.371278
C 2.894045 1.824383 1.280937
H 2.578747 2.746843 0.769974
H 1.981935 1.295616 1.601187
H 3.466112 2.096039 2.180452
H 4.669663 1.497936 0.110150
O 4.194777 -0.221116 1.037461
H 3.413263 -0.712075 1.332957
H 3.772787 -0.005754 -1.566867
H 2.834765 1.512807 -1.525681
H 2.589503 -2.157303 -0.905283
O 0.367573 -3.451311 -0.429636
O -2.260785 -3.068846 0.182120
H -3.193209 -3.204452 0.408030
H -4.022148 -1.172831 0.604793
C -3.900742 1.544374 0.581228
H -4.839544 1.022426 0.808002
H -4.063158 2.205899 -0.284438
H -3.643915 2.196263 1.431279

2-C7, $\Delta G = 1.4132$ kcal/mol, population = 3.28 %



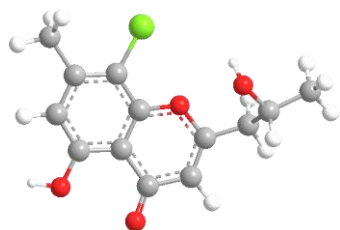
```
C 2.713827 -0.814037 -0.255433
C 3.068027 0.535783 -0.391280
C 2.151009 1.574213 -0.204829
C 0.804367 1.279450 0.141783
C -0.244621 2.309992 0.351298
C -1.570401 1.761477 0.635585
C -1.798292 0.433844 0.752028
O -0.795272 -0.467159 0.614896
C 0.459973 -0.081909 0.281694
C 1.390355 -1.112785 0.084385
Cl 0.861746 -2.771593 0.254517
C -3.104527 -0.247650 0.988054
C -3.717327 -0.846528 -0.304856
C -4.254873 0.219009 -1.247058
H -3.454709 0.915346 -1.543062
H -4.652778 -0.255002 -2.156774
H -5.063100 0.792770 -0.769783
H -4.560054 -1.487229 0.022930
O -2.771875 -1.610724 -1.035038
H -2.248807 -2.144838 -0.420585
H -2.937332 -1.060595 1.713582
H -3.818916 0.456927 1.435128
H -2.392656 2.465996 0.760091
O -0.046692 3.520777 0.287079
O 2.521277 2.859046 -0.352547
H 3.459117 2.894314 -0.593448
H 4.098638 0.785212 -0.656630
C 3.725821 -1.902671 -0.472098
H 4.707888 -1.484339 -0.728327
H 3.406070 -2.576936 -1.282404
H 3.830432 -2.523959 0.431501
```

2-C10, $\Delta G = 1.4138$ kcal/mol, population = 3.28 %



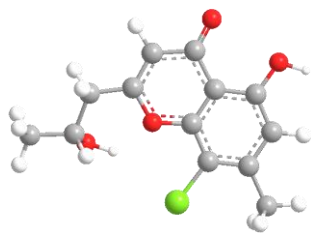
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C 2.778643 -0.491409 0.368073
C 3.005982 0.891631 0.335100
C 1.995654 1.809894 0.036327
C 0.681511 1.351755 -0.252953
C -0.458579 2.249207 -0.570887
C -1.721278 1.549753 -0.796248
C -1.827021 0.202975 -0.749145
O -0.752314 -0.580197 -0.487595
C 0.463858 -0.042698 -0.222300
C 1.488113 -0.951043 0.085394
Cl 1.122894 -2.660658 0.119790
C -3.075606 -0.598548 -0.923089
C -3.738118 -1.019030 0.401847
C -2.855612 -1.878806 1.302342
H -3.427494 -2.206629 2.185529
H -2.500394 -2.777348 0.775337
H -1.977411 -1.315695 1.650207
H -4.629955 -1.612839 0.118652
O -4.136401 0.179172 1.051369
H -4.530603 -0.057617 1.902046
H -3.801790 -0.001575 -1.491521
H -2.840865 -1.502285 -1.505871
H -2.604078 2.153164 -1.005328
O -0.376070 3.473652 -0.637489
O 2.245775 3.131969 0.019974
H 3.177658 3.281733 0.238947
H 4.009518 1.265587 0.553865
C 3.889090 -1.447112 0.699759
H 4.828620 -0.911458 0.888290
H 4.047937 -2.162017 -0.123077
H 3.637198 -2.044087 1.590633
```

2-C3, $\Delta G = 1.4370$ kcal/mol, population = 3.15 %



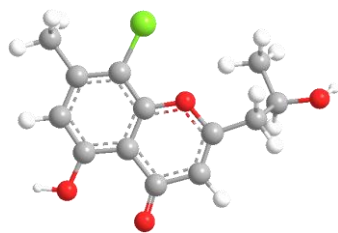
C -2.591860 1.194651 0.177018
C -3.183742 -0.069071 0.313820
C -2.453778 -1.255467 0.198522
C -1.059108 -1.208632 -0.071905
C -0.195677 -2.411044 -0.193803
C 1.214246 -2.109446 -0.435401
C 1.674960 -0.845185 -0.568579
O 0.842743 0.220499 -0.491337
C -0.475338 0.067783 -0.218788
C -1.220313 1.249585 -0.091995
Cl -0.400483 2.785252 -0.261717
C 3.089898 -0.415846 -0.767052
C 3.766421 0.034044 0.549591
C 5.120444 0.680483 0.276305
H 5.596206 0.973770 1.223827
H 5.793554 -0.010213 -0.255311
H 4.997068 1.583772 -0.344348
H 3.911693 -0.862675 1.175000
O 2.924746 0.877788 1.317908
H 2.611706 1.601404 0.754764
H 3.669761 -1.237319 -1.209702
H 3.097092 0.425162 -1.481112
H 1.905299 -2.949260 -0.509940
O -0.602357 -3.566329 -0.095448
O -3.052591 -2.451709 0.342572
H -3.993168 -2.314706 0.530945
H -4.254859 -0.130019 0.522858
C -3.407125 2.448389 0.318239
H -4.459591 2.215059 0.525763
H -3.353115 3.054682 -0.599842
H -3.016787 3.077415 1.134002

2-C16, $\Delta G = 1.4740$ kcal/mol, population = 2.96 %



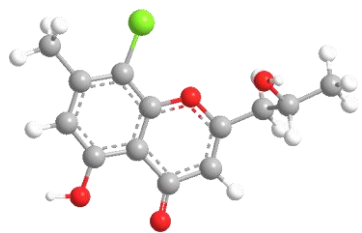
```
C 2.398131 -1.477275 -0.129580
C 3.187197 -0.318968 -0.166148
C 2.641458 0.964952 -0.072417
C 1.237568 1.131155 0.073988
C 0.556177 2.449539 0.142562
C -0.899383 2.363878 0.247549
C -1.558572 1.186435 0.328819
O -0.891096 0.007913 0.282766
C 0.456603 -0.041156 0.129987
C 1.015892 -1.321563 0.017990
Cl -0.048585 -2.709918 0.042941
C -3.037851 0.998737 0.498933
C -3.558795 -0.380714 0.058398
C -5.077357 -0.429116 0.111364
H -5.445693 -0.191708 1.120676
H -5.505921 0.299601 -0.595486
H -5.434624 -1.431443 -0.166964
H -3.150481 -1.137974 0.752204
O -3.157460 -0.688999 -1.270145
H -2.235202 -0.977691 -1.228037
H -3.288697 1.150616 1.563663
H -3.551436 1.794519 -0.062620
H -1.458287 3.299508 0.279278
O 1.140167 3.529693 0.106372
O 3.426807 2.055529 -0.122680
H 4.348983 1.778447 -0.231363
H 4.269547 -0.422141 -0.278580
C 3.018723 -2.839786 -0.249909
H 2.613395 -3.376689 -1.122217
H 2.786508 -3.454450 0.634226
H 4.109247 -2.769966 -0.354361
```

2-C9, $\Delta G = 1.8066$ kcal/mol, population = 1.69 %



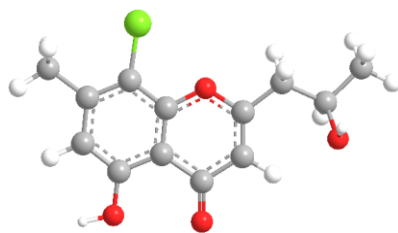
C -2.678223 1.056722 -0.237243
C -3.224114 -0.233754 -0.280784
C -2.445557 -1.382227 -0.114026
C -1.047287 -1.265963 0.113598
C -0.137298 -2.425678 0.287695
C 1.263749 -2.058254 0.485281
C 1.682740 -0.772992 0.527074
O 0.812426 0.255390 0.384952
C -0.508326 0.037651 0.164761
C -1.302640 1.180273 -0.013075
Cl -0.545527 2.755083 0.041051
C 3.089733 -0.309089 0.708717
C 3.766028 0.205373 -0.574852
C 3.192804 1.517792 -1.098515
H 3.278367 2.304036 -0.331612
H 3.750544 1.842087 -1.992321
H 2.133722 1.422600 -1.374206
H 3.646900 -0.575732 -1.352631
O 5.137325 0.346481 -0.229216
H 5.606188 0.687730 -1.003097
H 3.113948 0.492104 1.465898
H 3.690261 -1.148170 1.084204
H 1.984071 -2.867149 0.607378
O -0.500244 -3.599217 0.267163
O -3.000209 -2.606842 -0.167813
H -3.950662 -2.517306 -0.333908
H -4.297228 -0.347388 -0.454460
C -3.545841 2.267960 -0.428591
H -3.202985 2.861043 -1.291244
H -3.490686 2.930151 0.449923
H -4.593498 1.982835 -0.590634

2-C14, $\Delta G = 2.2201$ kcal/mol, population = 0.84 %



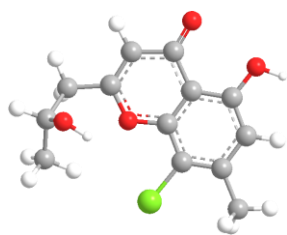
C -2.772188 0.927895 0.241814
C -3.200307 -0.404267 0.329240
C -2.328239 -1.482958 0.160328
C -0.952363 -1.249732 -0.109579
C 0.048249 -2.330568 -0.299803
C 1.397517 -1.845420 -0.575054
C 1.702716 -0.528657 -0.635495
O 0.758791 0.423488 -0.460433
C -0.530515 0.094991 -0.198845
C -1.420433 1.166947 -0.027196
Cl -0.812905 2.801099 -0.151643
C 3.064914 0.048651 -0.856312
C 3.876862 0.165630 0.441685
C 5.242737 0.795730 0.193531
H 5.126198 1.812821 -0.213076
H 5.811813 0.862682 1.134568
H 5.834391 0.197504 -0.516806
H 4.019425 -0.858492 0.840811
O 3.099955 0.935422 1.346697
H 3.562849 0.955625 2.195471
H 3.618474 -0.585012 -1.563174
H 2.953530 1.049638 -1.300870
H 2.179754 -2.589431 -0.728415
O -0.208911 -3.530909 -0.235558
O -2.771383 -2.750661 0.247998
H -3.722504 -2.742640 0.432255
H -4.254048 -0.606824 0.537815
C -3.739247 2.061727 0.431517
H -4.752193 1.688525 0.631534
H -3.768786 2.703927 -0.462996
H -3.427301 2.704876 1.269708

2-C8, $\Delta G = 2.4335$ kcal/mol, population = 0.59 %



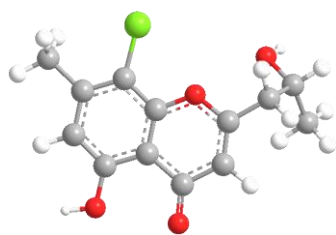
C -3.140836 0.549662 -0.011150
C -3.278558 -0.843073 -0.093526
C -2.177019 -1.702238 -0.130039
C -0.859162 -1.171754 -0.083481
C 0.370465 -2.002981 -0.116930
C 1.612420 -1.238329 -0.037191
C 1.632040 0.111449 0.035504
O 0.483889 0.835164 0.049725
C -0.729824 0.231528 0.001621
C -1.847199 1.080352 0.035974
Cl -1.596604 2.807636 0.137974
C 2.827390 1.011180 0.120360
C 4.163582 0.406885 -0.326751
C 5.262573 1.464405 -0.364083
H 5.401724 1.914671 0.633282
H 6.213456 1.004849 -0.670989
H 5.018441 2.272469 -1.070666
H 4.031918 -0.011634 -1.338330
O 4.548320 -0.702405 0.476396
H 4.663616 -0.389798 1.386217
H 2.607046 1.905709 -0.484109
H 2.918265 1.374289 1.161819
H 2.554742 -1.781715 -0.016076
O 0.372730 -3.229496 -0.199199
O -2.342770 -3.035537 -0.208296
H -3.290283 -3.236166 -0.230761
H -4.283090 -1.272817 -0.130316
C -4.348513 1.442533 0.025532
H -4.336890 2.150162 -0.818641
H -4.357243 2.050211 0.944291
H -5.275682 0.856328 -0.018475

2-C12, $\Delta G = 2.5941$ kcal/mol, population = 0.45 %



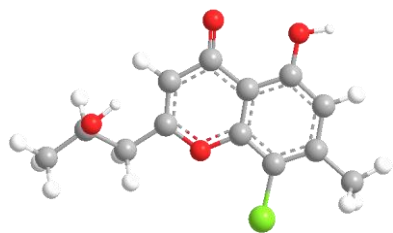
C 2.257545 -1.584058 0.107705
C 3.096959 -0.464385 0.178866
C 2.608878 0.842978 0.101720
C 1.215709 1.073044 -0.059294
C 0.602226 2.423539 -0.121697
C -0.851064 2.410615 -0.271153
C -1.567367 1.269283 -0.376764
O -0.964221 0.054658 -0.314904
C 0.379677 -0.060720 -0.144862
C 0.884567 -1.365989 -0.054667
Cl -0.222264 -2.717659 -0.131648
C -3.047342 1.180239 -0.581827
C -3.761419 0.107286 0.283896
C -3.840992 -1.259485 -0.390804
H -4.369497 -1.967976 0.265240
H -4.389689 -1.193848 -1.343042
H -2.837746 -1.658340 -0.599715
H -4.789068 0.471390 0.443170
O -3.192879 0.024032 1.583422
H -2.371630 -0.483345 1.507213
H -3.459454 2.175392 -0.366592
H -3.246634 0.977114 -1.648517
H -1.359701 3.373867 -0.309768
O 1.234611 3.474176 -0.049107
O 3.441449 1.896375 0.179304
H 4.348829 1.575765 0.292472
H 4.172155 -0.617293 0.302874
C 2.817834 -2.974453 0.204212
H 3.908882 -2.953284 0.323486
H 2.571562 -3.558476 -0.696715
H 2.378813 -3.513496 1.058675

2-C17, $\Delta G = 2.5941$ kcal/mol, population = 0.45 %



C -2.792481 0.683051 -0.281539
C -3.070011 -0.687893 -0.376664
C -2.092680 -1.665067 -0.171478
C -0.760636 -1.282951 0.145073
C 0.343071 -2.247353 0.380788
C 1.624568 -1.617588 0.687001
C 1.785038 -0.275164 0.745708
O 0.746792 0.567372 0.539354
C -0.489720 0.100026 0.238915
C -1.484567 1.068381 0.030809
Cl -1.062699 2.759370 0.163539
C 3.067460 0.449235 1.004313
C 3.822975 0.870229 -0.270455
C 4.262084 -0.306854 -1.134767
H 4.912132 -0.994265 -0.571298
H 3.391477 -0.870538 -1.503139
H 4.831587 0.055110 -2.005942
H 4.728743 1.406169 0.077026
O 2.974889 1.754684 -0.986358
H 3.426329 2.001945 -1.805002
H 2.841894 1.355846 1.585765
H 3.726016 -0.191188 1.606836
H 2.477208 -2.272582 0.865965
O 0.219243 -3.469069 0.326572
O -2.393141 -2.973437 -0.268142
H -3.332913 -3.067402 -0.484311
H -4.087710 -1.004439 -0.619341
C -3.870274 1.704514 -0.508849
H -4.829126 1.222977 -0.741161
H -3.601744 2.377364 -1.338625
H -3.999643 2.339987 0.381568

2-C15, $\Delta G = 2.7297$ kcal/mol, population = 0.35 %



```
C 3.032887 -0.722417 0.125461
C 3.268474 0.656057 0.219489
C 2.239019 1.598044 0.142623
C 0.896177 1.169478 -0.038385
C -0.260784 2.093123 -0.135393
C -1.546279 1.419990 -0.315297
C -1.663097 0.073804 -0.389476
O -0.579500 -0.730697 -0.297392
C 0.668314 -0.220614 -0.131220
C 1.713175 -1.153405 -0.051473
Cl 1.342096 -2.856637 -0.174597
C -2.924012 -0.715490 -0.576294
C -4.165670 -0.081185 0.065558
C -5.392878 -0.956601 -0.130030
H -5.236393 -1.941599 0.337835
H -6.270487 -0.486571 0.337487
H -5.602073 -1.106113 -1.199609
H -4.355009 0.896939 -0.419136
O -3.986381 0.091586 1.463098
H -3.243027 0.695708 1.601335
H -3.095157 -0.857424 -1.657864
H -2.759393 -1.715133 -0.144860
H -2.427198 2.055641 -0.403284
O -0.177847 3.317133 -0.075746
O 2.497200 2.914680 0.238481
H 3.449565 3.043725 0.361601
H 4.293923 1.008115 0.358444
C 4.165058 -1.705709 0.213204
H 4.013140 -2.401591 1.053490
H 5.125737 -1.192242 0.349491
H 4.218678 -2.321241 -0.698707
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