Supporting Information

Neocucurbins A-G, novel macrocyclic diterpenes and their derivatives from *Neocucurbitaria unguis-hominis* FS685

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List of Supporting Information

Table S1. X-ray crystallographic data for compound **1.**

Identification code	53p-3-8_collect
Empirical formula	$C_{20}H_{30}O_5$
Formula weight	350.44
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.17520(10)
b/Å	10.18530(10)
c/Å	22.0750(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1838.12(3)
Z	4
ρ_{calc}g/cm^3	1.266
μ/mm^{-1}	0.726
F(000)	760.0
Crystal size/mm^3	0.1 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.01 to 148.774
Index ranges	$-10 \leq h \leq 9$, $-12 \leq k \leq 12$, $-27 \leq l \leq 27$
Reflections collected	17927
Independent reflections	3702 [R_{int} = 0.0221, R_{sigma} = 0.0134]
Data/restraints/parameters	3702/4/243
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0287, wR_2 = 0.0714
Final R indexes [all data]	R_1 = 0.0289, wR_2 = 0.0716
Largest diff. peak/hole / e Å^{-3}	0.28/-0.25
Flack parameter	0.04(4)

Table S2. X-ray crystallographic data for compound **2.**

Identification code	hujinhua_53p-3-34_collect
Empirical formula	$C_{20}H_{30}O_5$
Formula weight	350.44
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	13.9823(4)
b/Å	7.7311(2)
c/Å	17.3343(5)
α/°	90
β/°	92.675(3)
γ/°	90
Volume/Å^3	1871.77(9)
Z	4
ρ_{calc}g/cm^3	1.244
μ/mm^{-1}	0.713
F(000)	760.0
Crystal size/mm^3	0.3 × 0.02 × 0.02
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.328 to 149.906
Index ranges	$-17 \leq h \leq 17$, $-9 \leq k \leq 9$, $-21 \leq l \leq 20$
Reflections collected	19209
Independent reflections	7440 [R_{int} = 0.0861, R_{sigma} = 0.0832]
Data/restraints/parameters	7440/1/463
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0811, wR_2 = 0.2020
Final R indexes [all data]	R_1 = 0.0894, wR_2 = 0.2126
Largest diff. peak/hole / e Å^{-3}	0.52/-0.44
Flack parameter	-0.1(2)

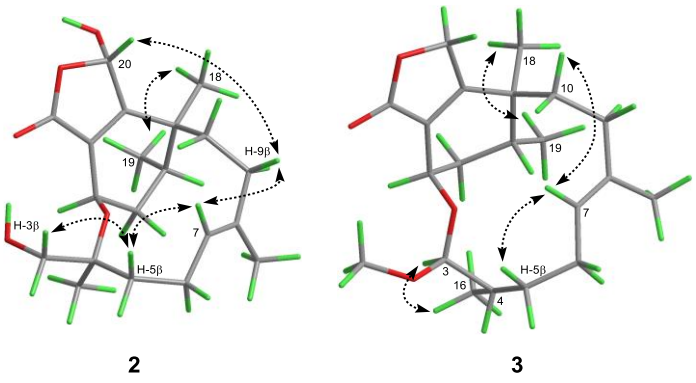


Figure S1. Key NOE correlations of compound **2** and **3**.

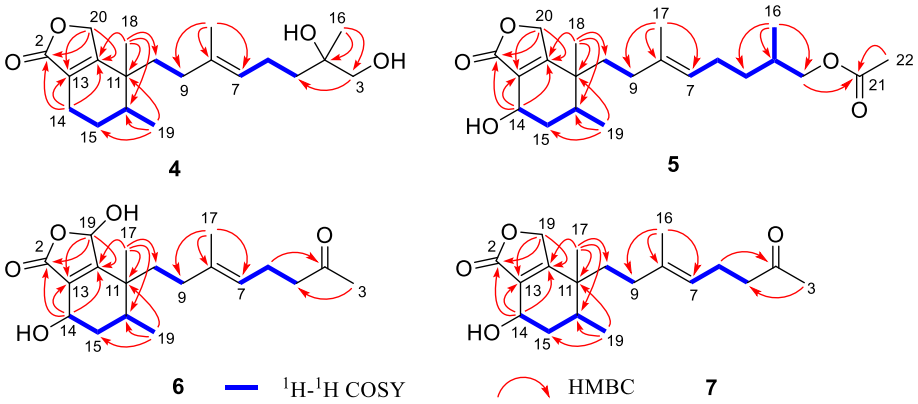


Figure S2. Key COSY and HMBC correlations of compounds **4-7**.

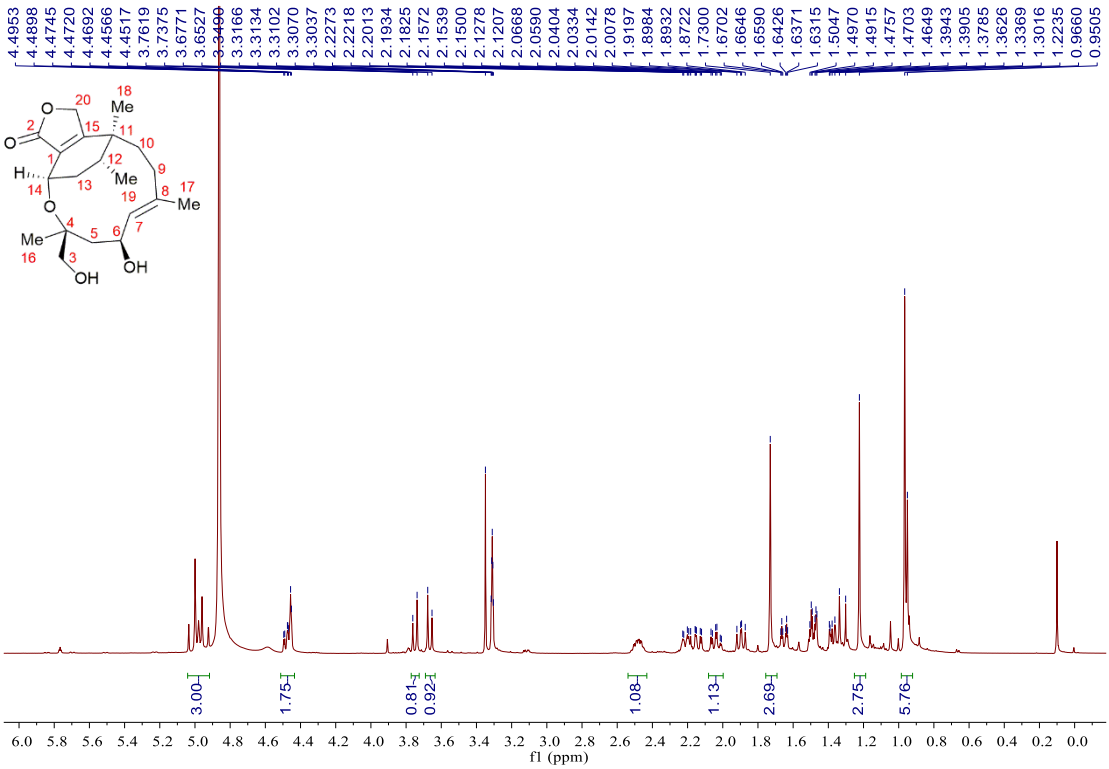


Figure S3. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **1**.

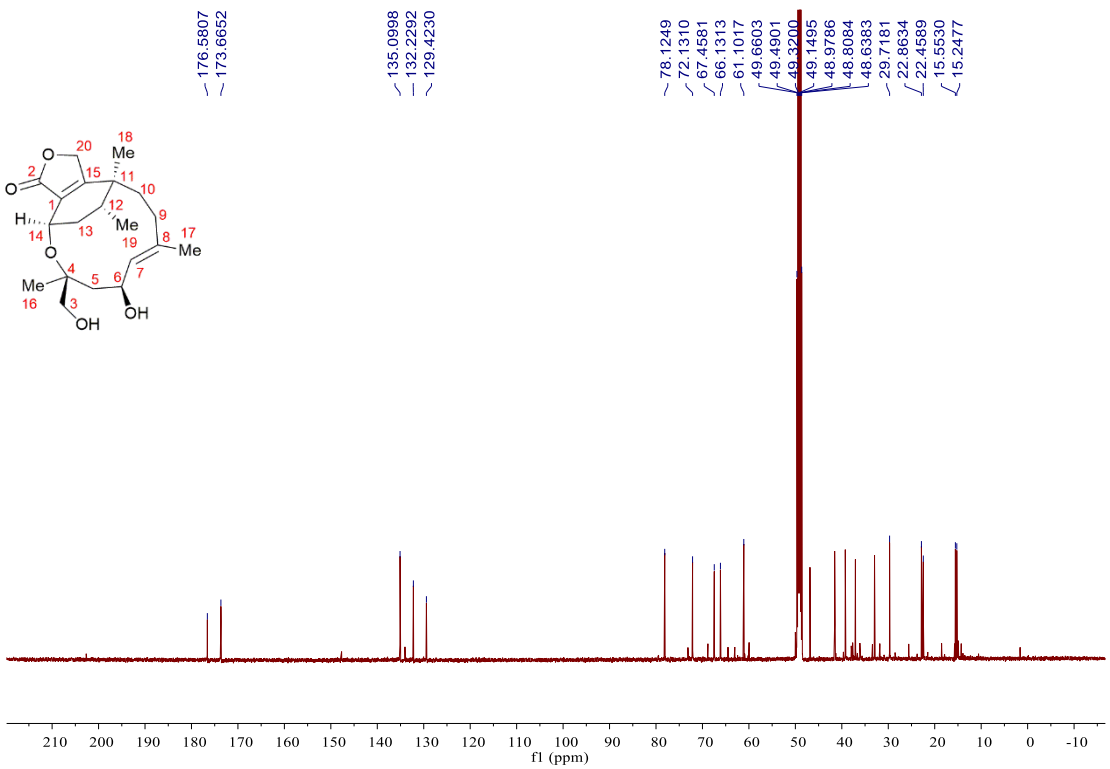


Figure S4. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **1**.

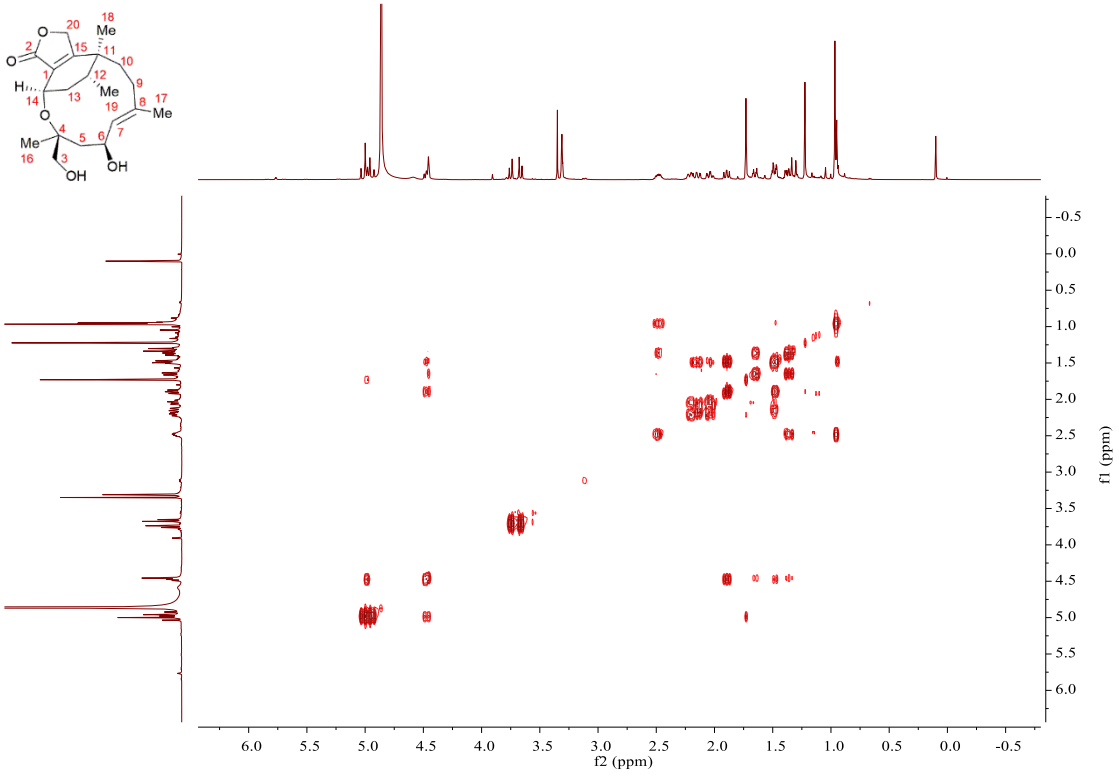


Figure S5. ^{1}H-^{1}H COSY spectrum (500 MHz, CD_3OD) of **1**.

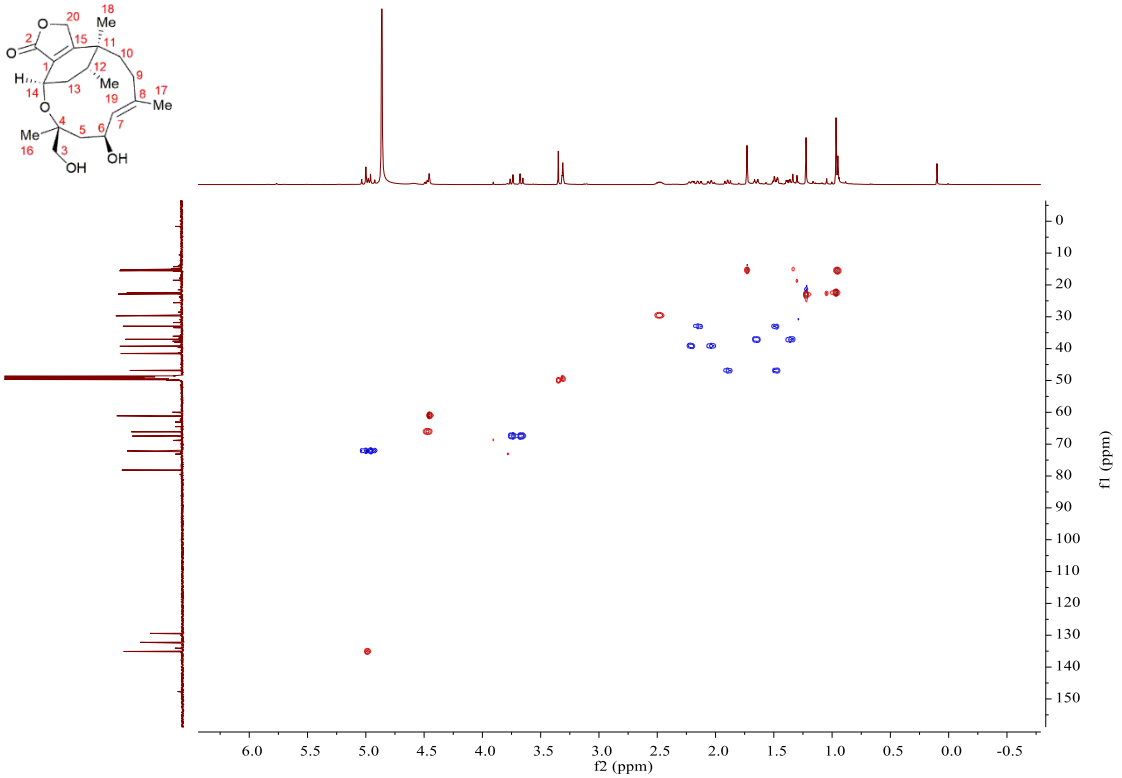


Figure S6. HSQC spectrum of **1**.

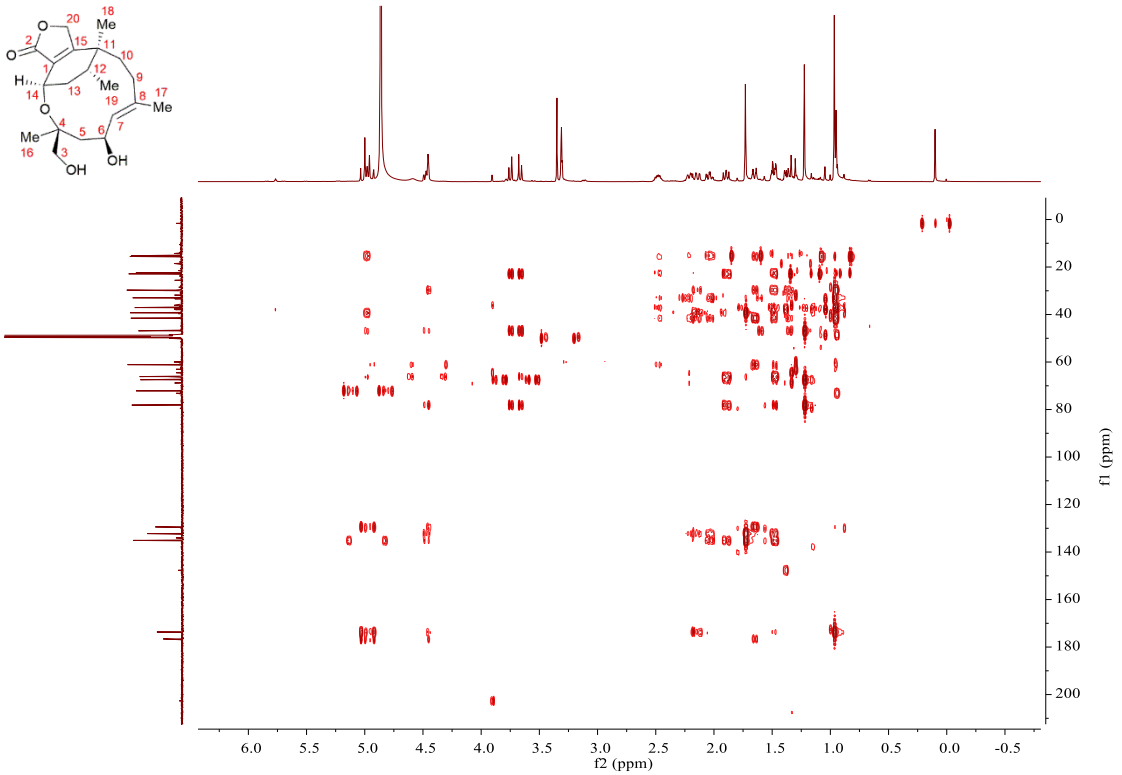


Figure S7. HMBC spectrum of **1**.

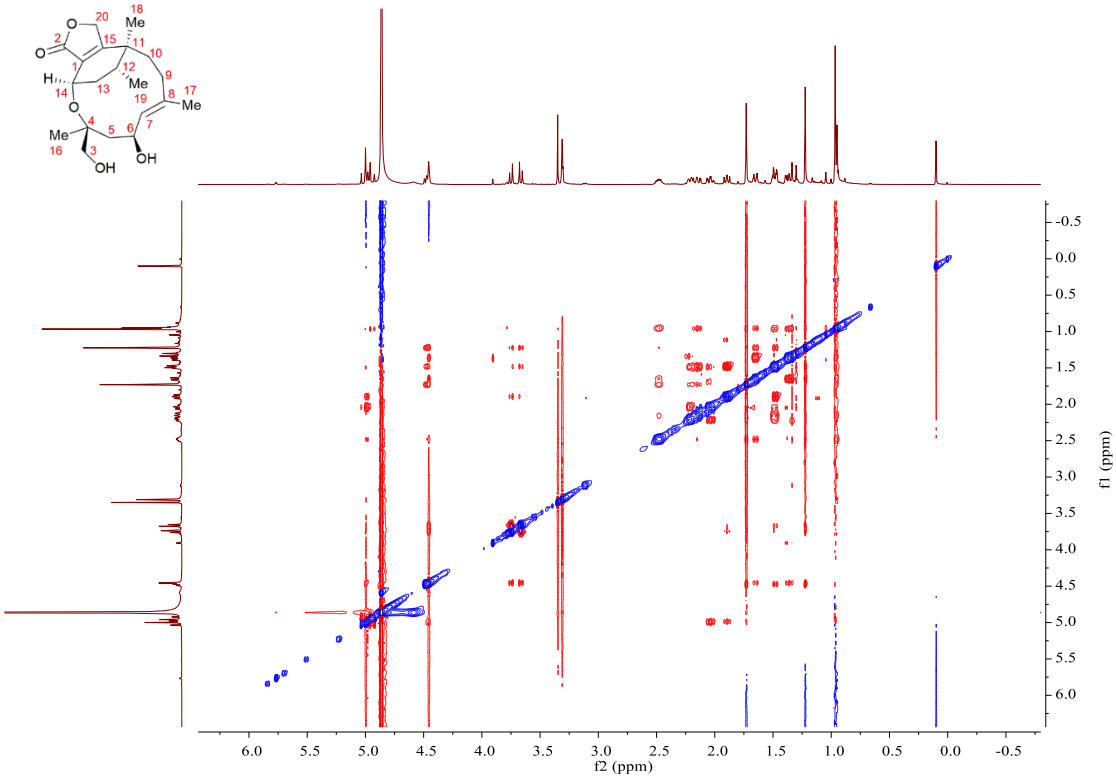


Figure S8. NOESY spectrum of **1**.

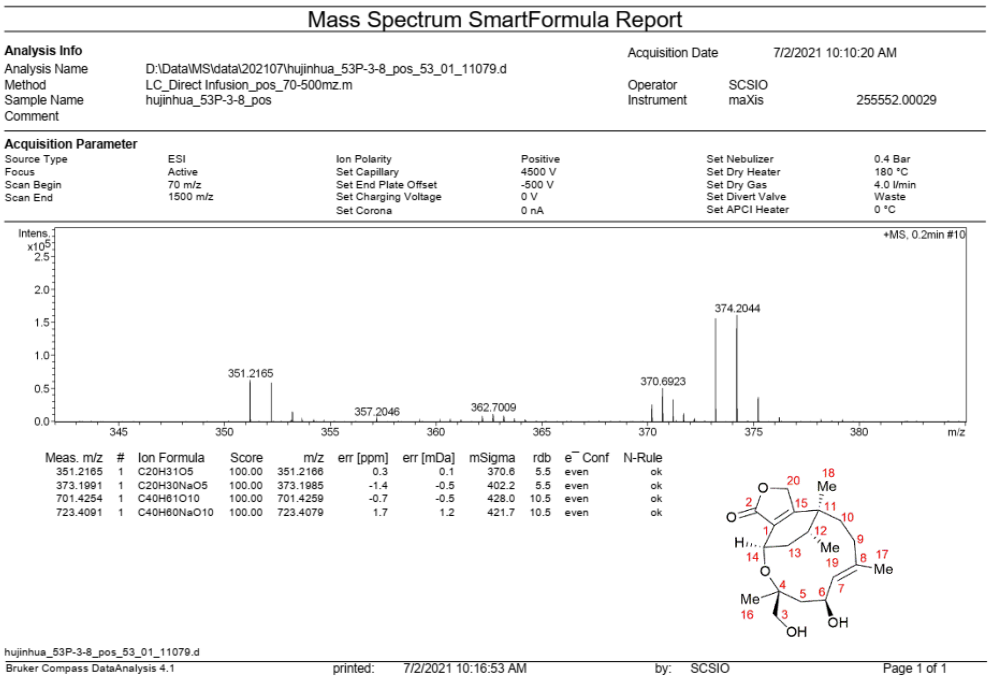


Figure S9. HRESIMS spectrum of **1**.

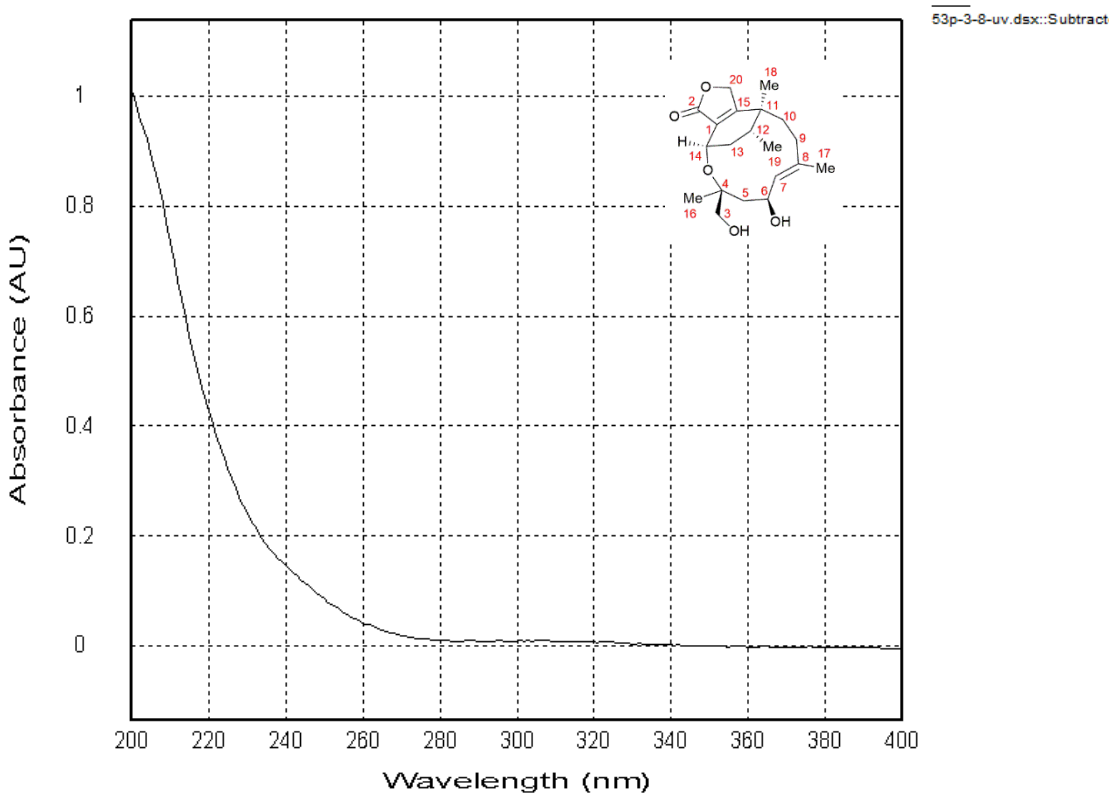


Figure S10. UV spectrum of **1**.

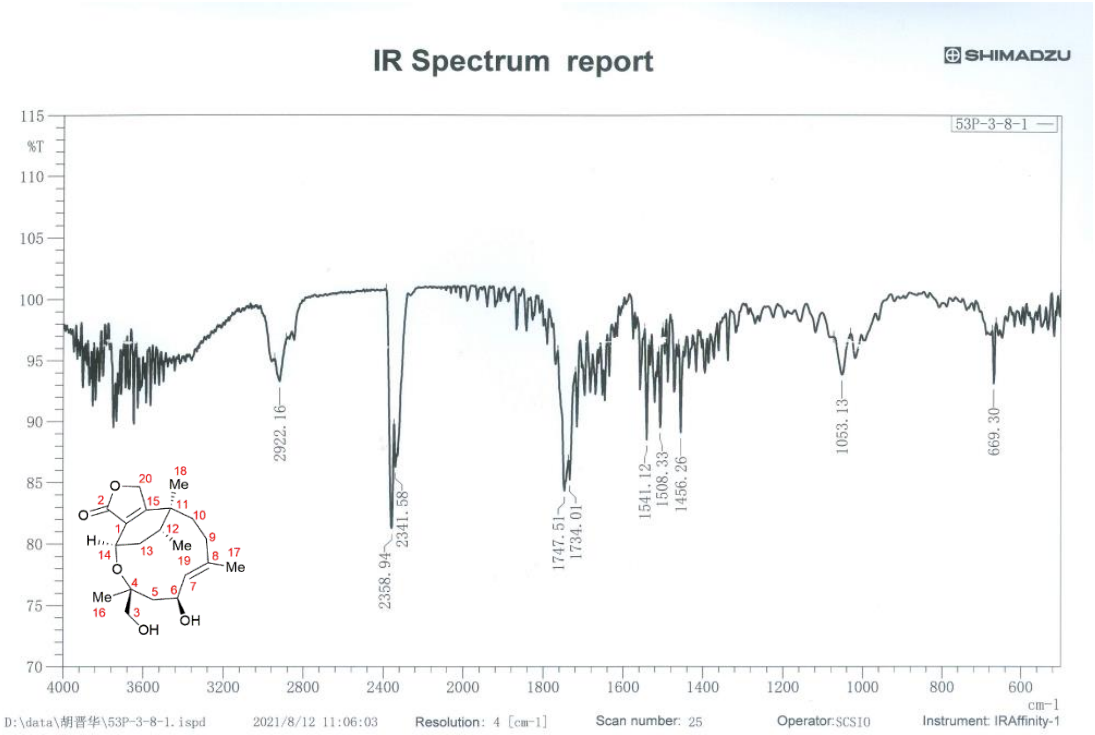


Figure S11. IR spectrum of **1**.

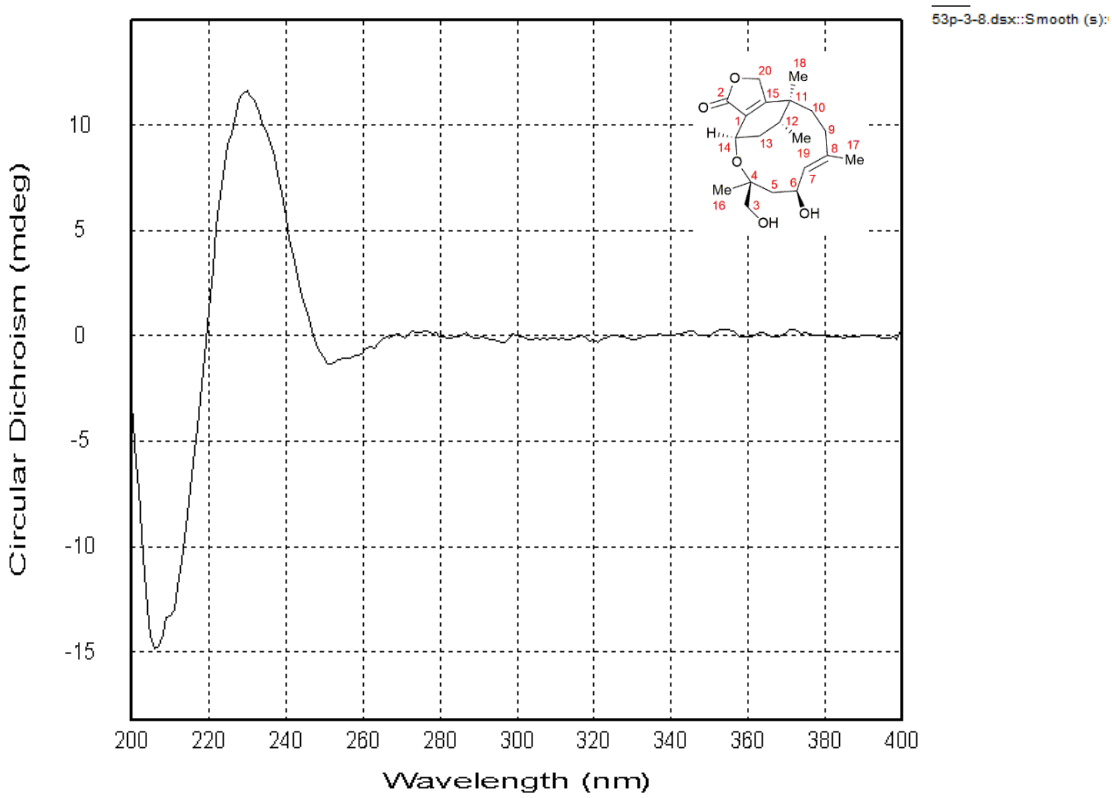


Figure S12. CD spectrum of **1**.

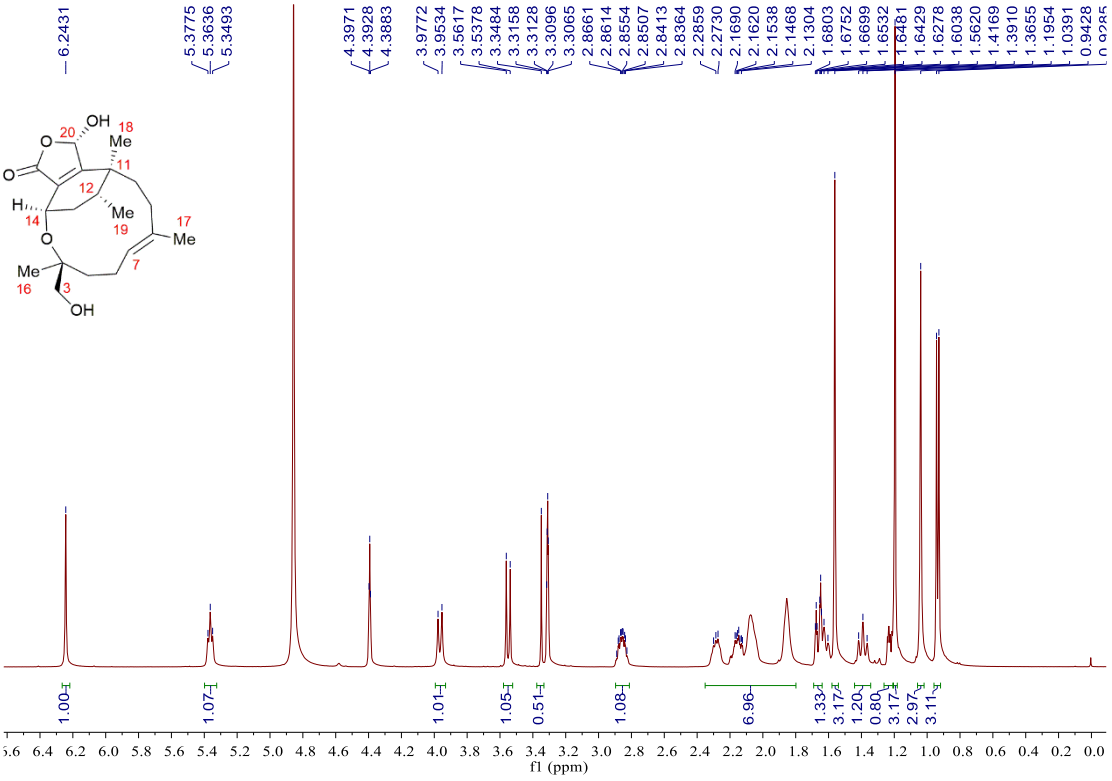


Figure S13. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **2**.

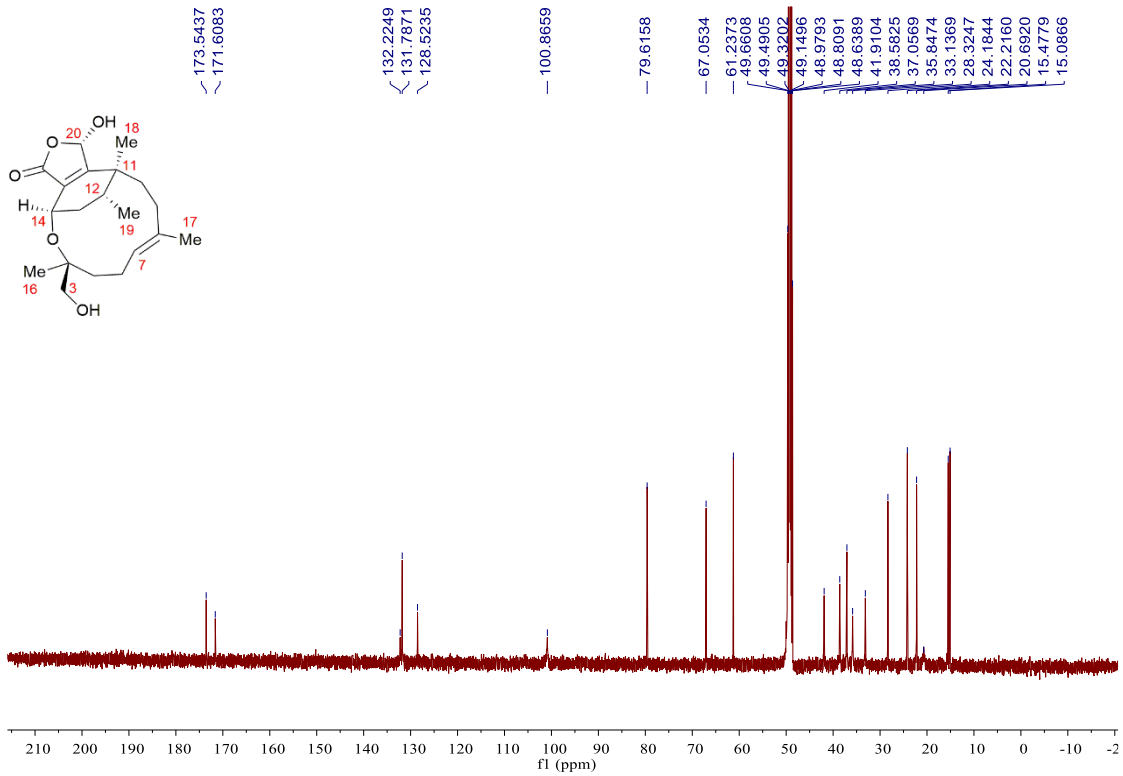


Figure S14. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **2**.

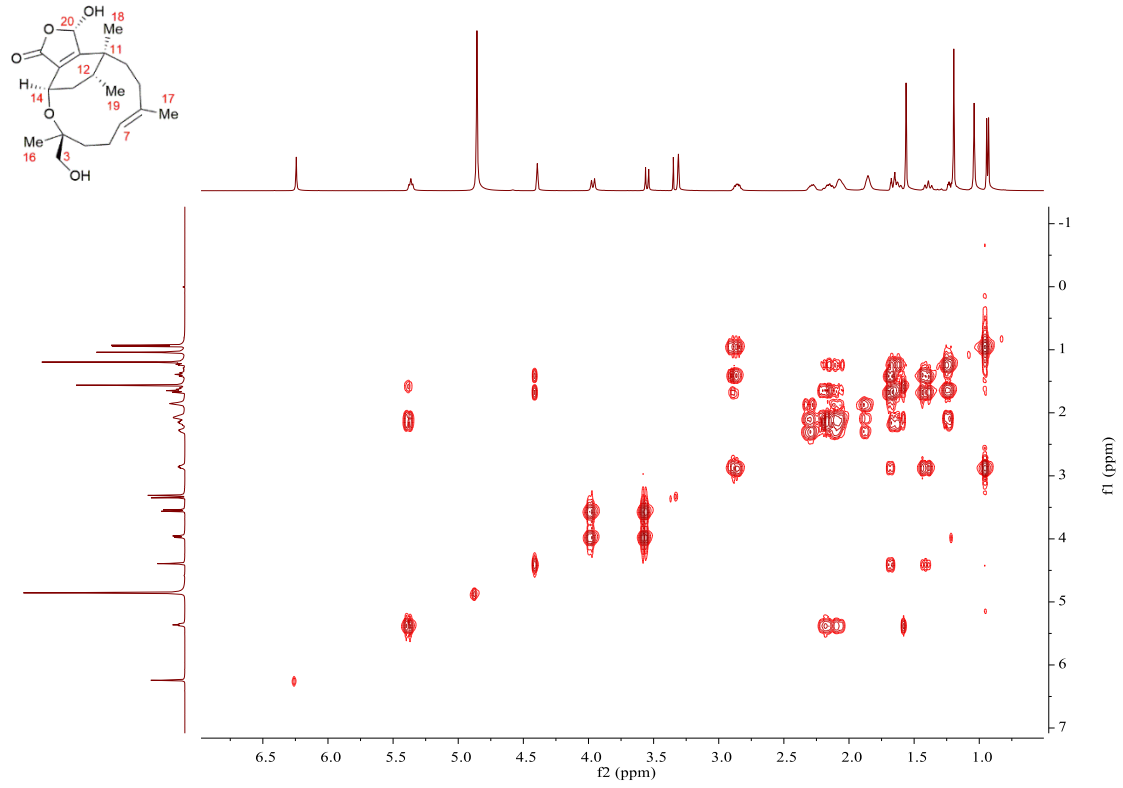


Figure S15. ^{1}H-^{1}H COSY spectrum of **2**.

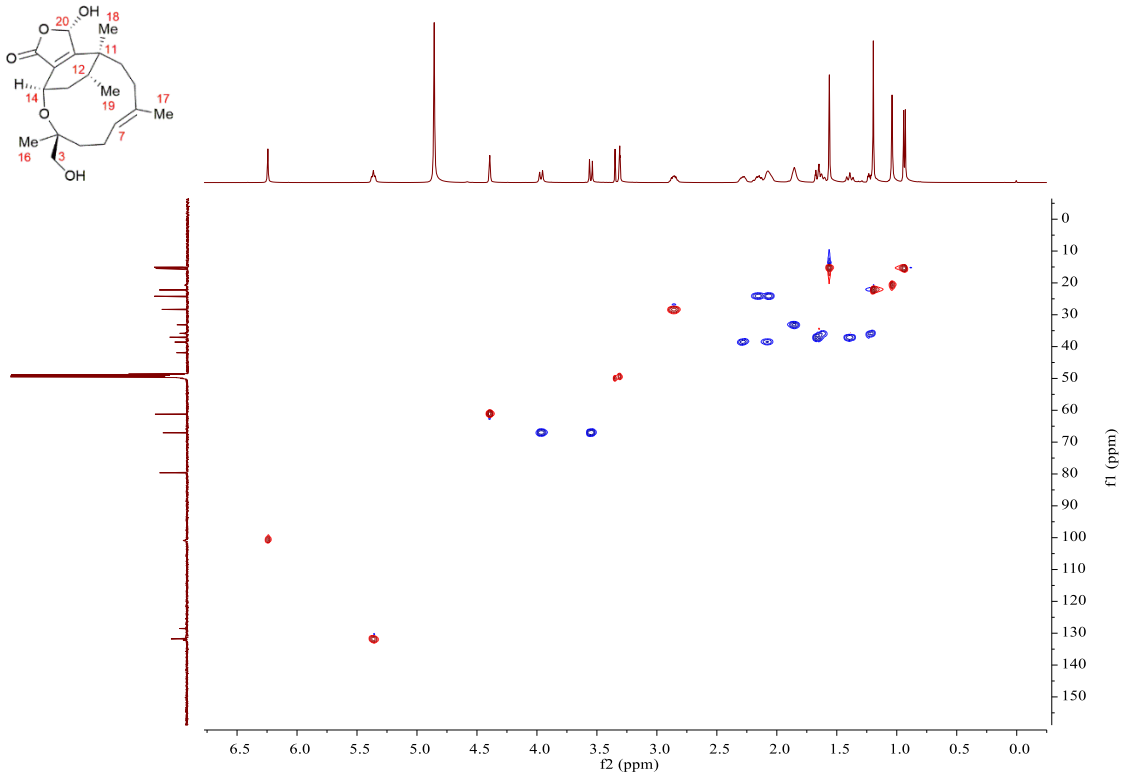


Figure S16. HSQC spectrum of **2**.

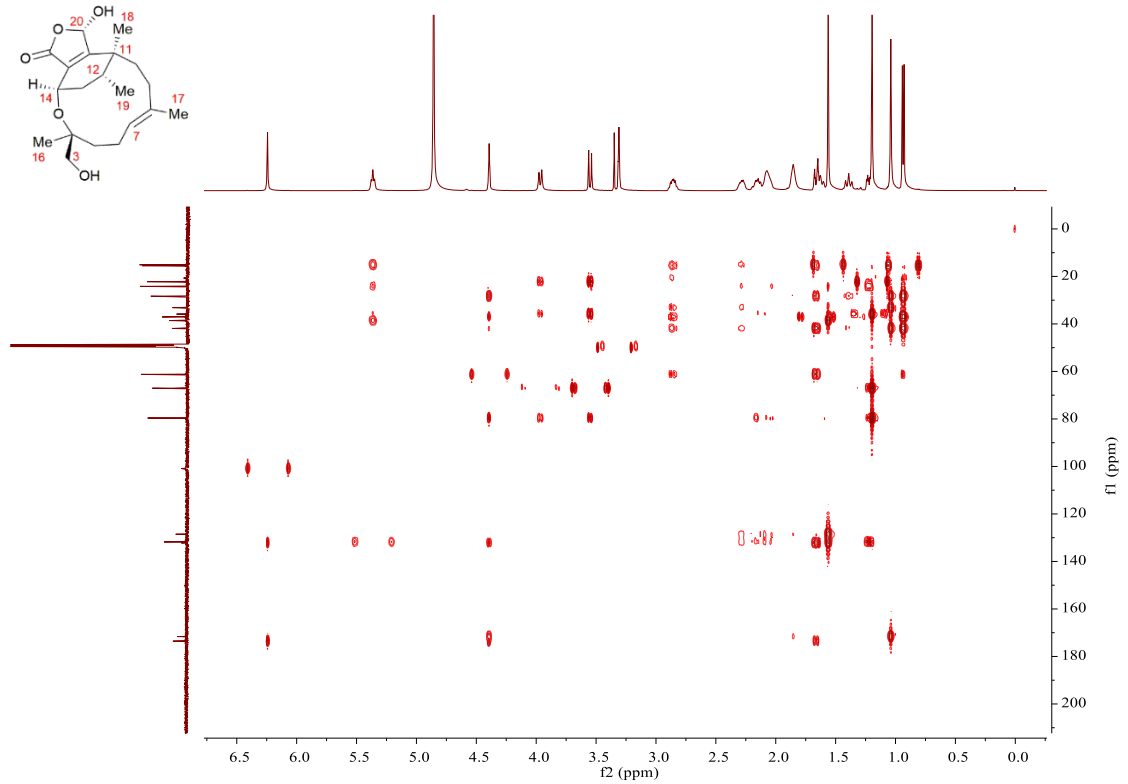


Figure S17. HMBC spectrum of **2**.

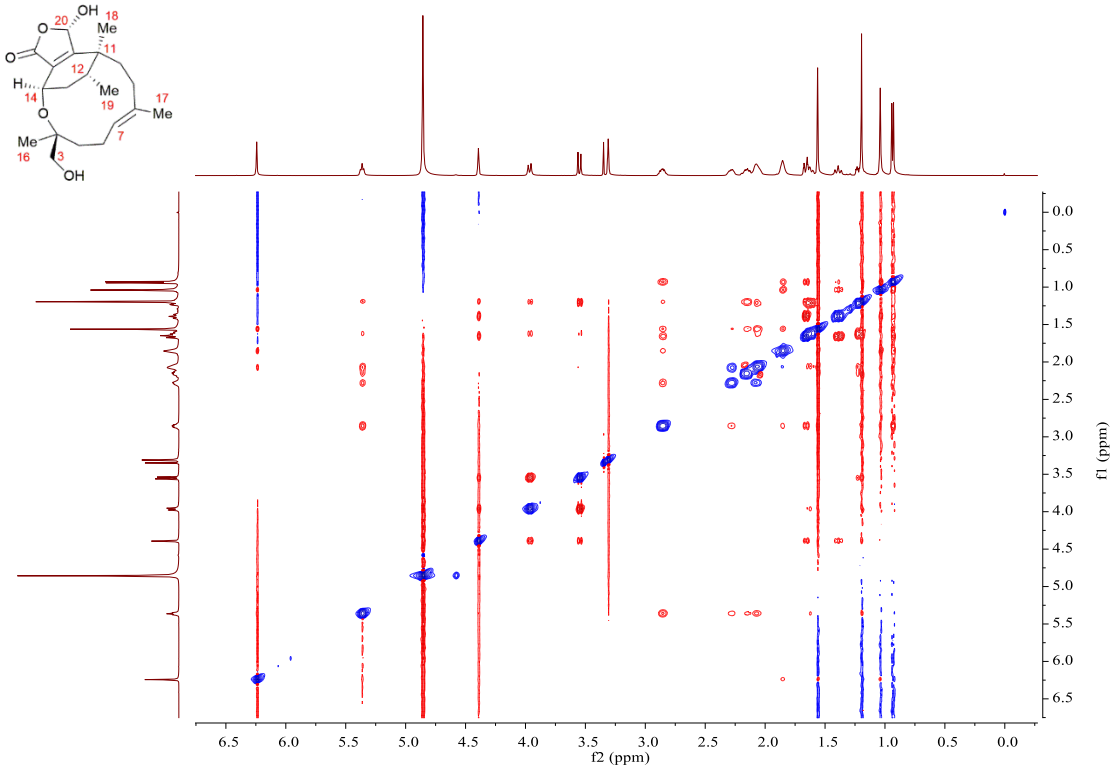


Figure S18. NOESY spectrum of **2**.

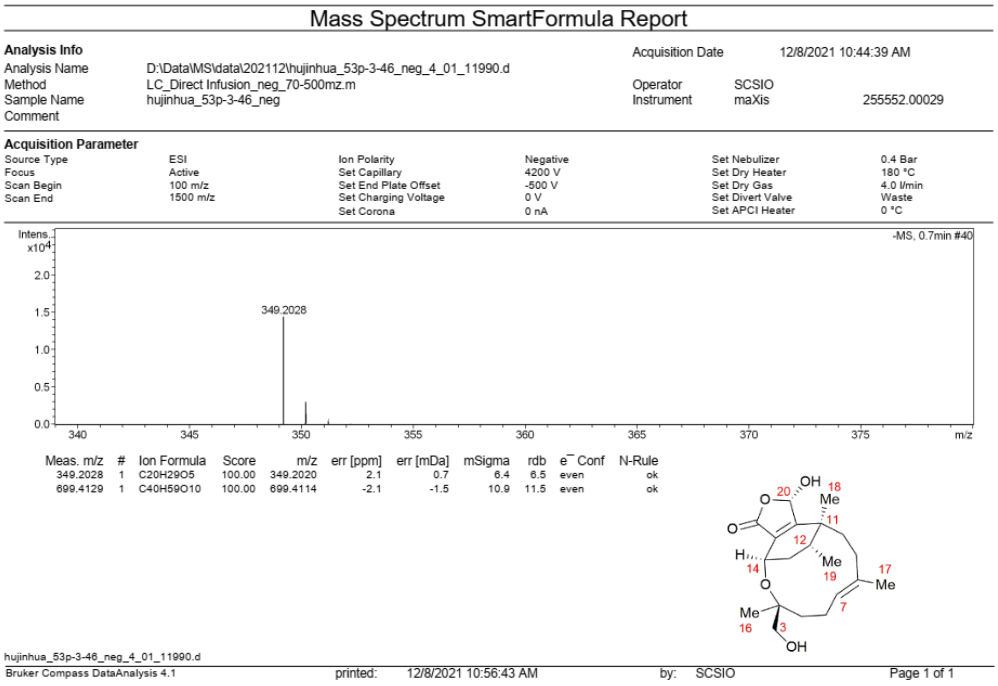


Figure S19. HRESIMS spectrum of **2**.

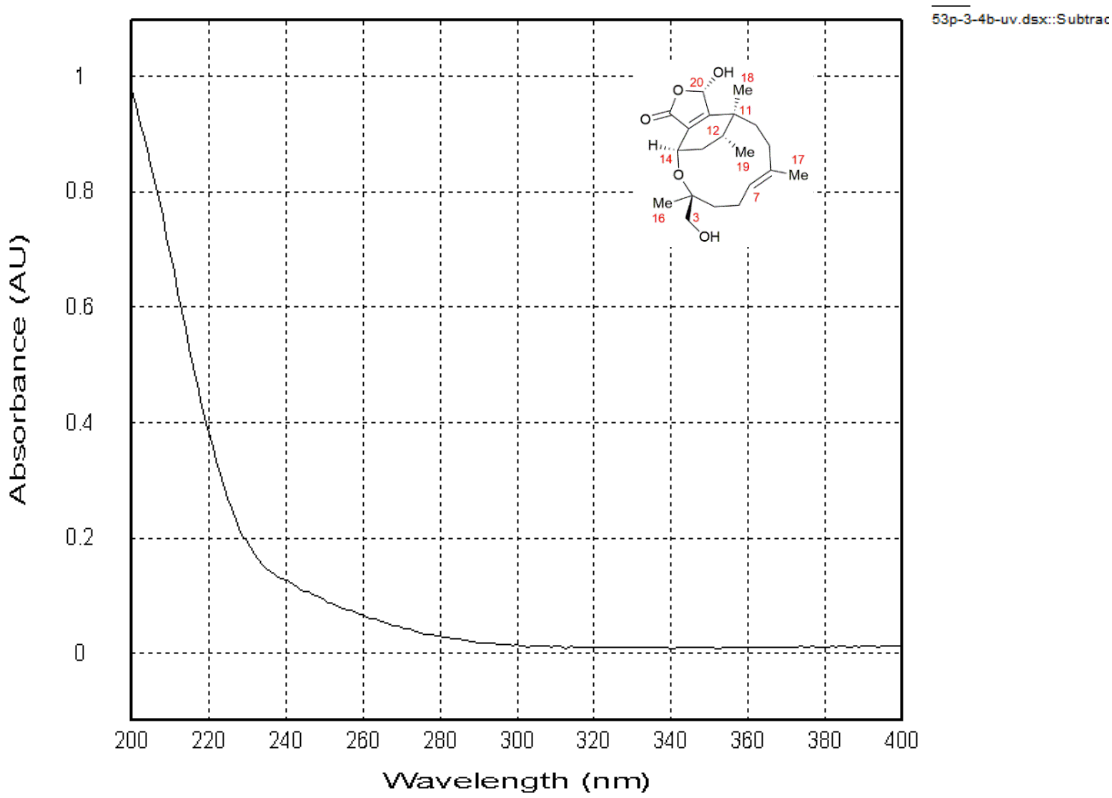


Figure S20. UV spectrum of **2**.

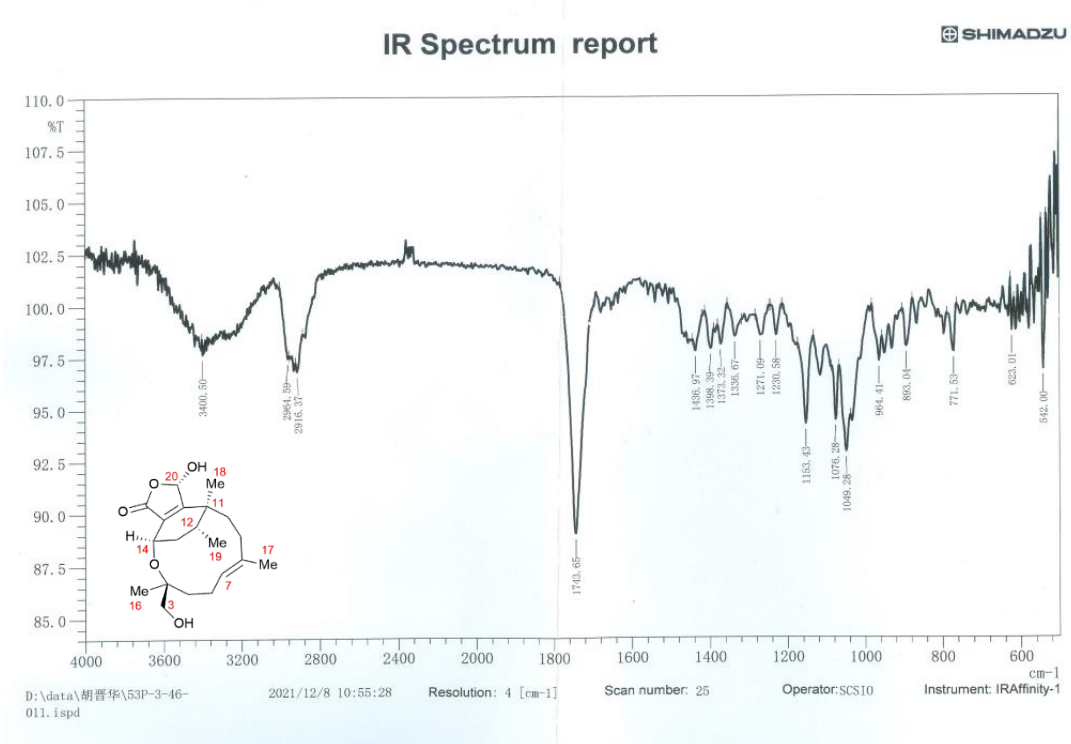


Figure S21. IR spectrum of **2**.

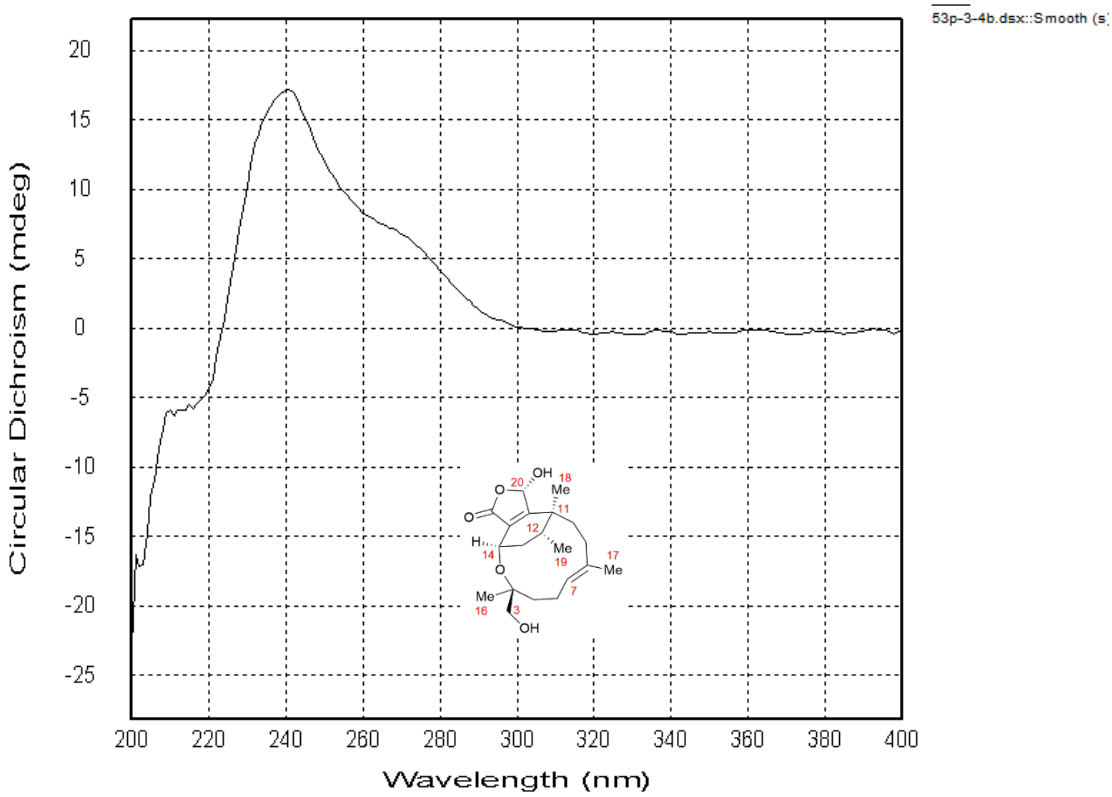


Figure S22. CD spectrum of **2**.

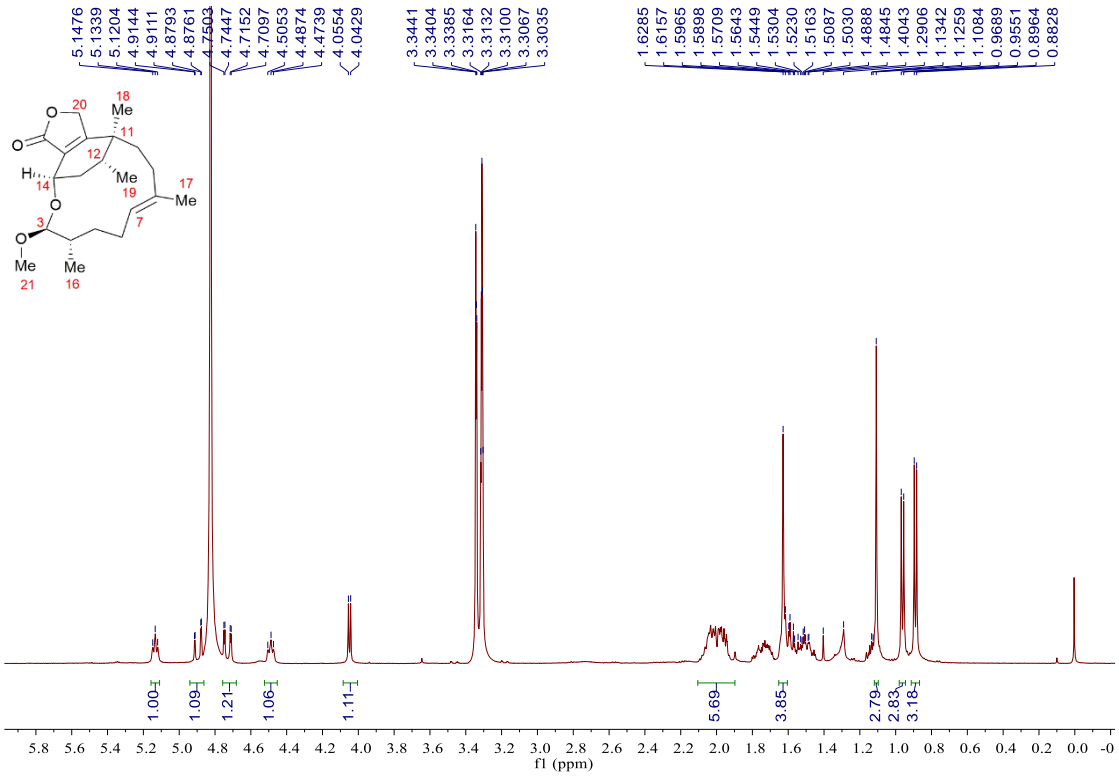


Figure S23. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **3**.

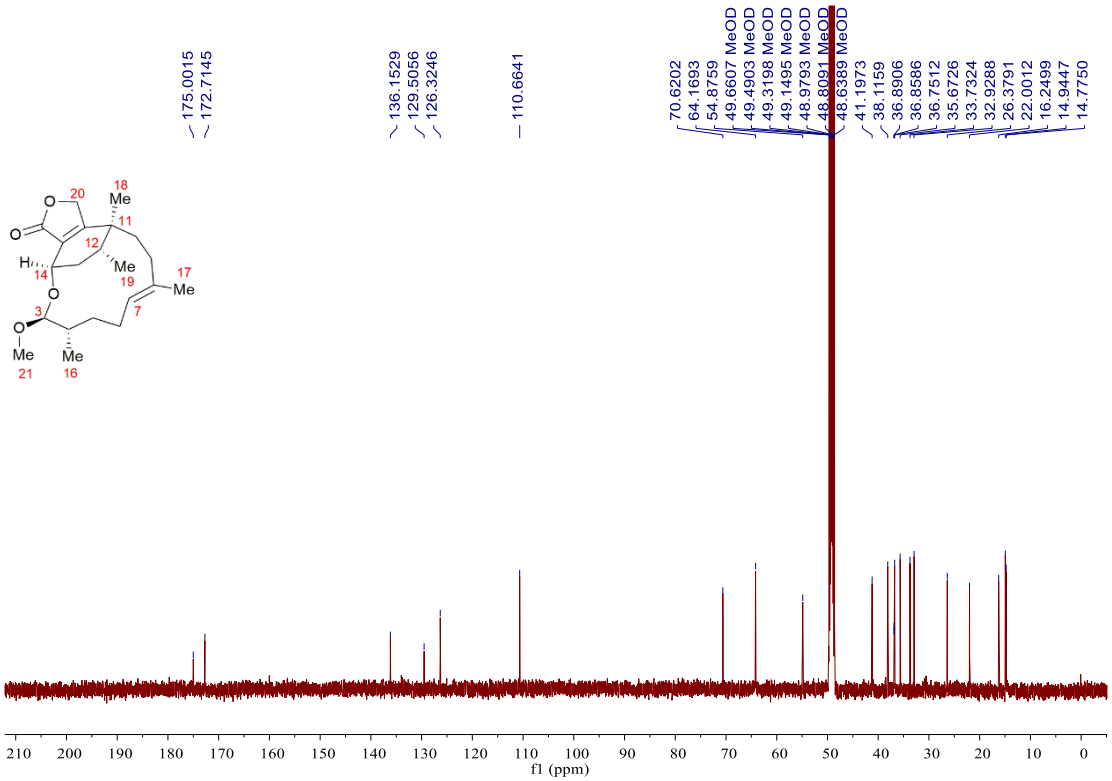


Figure S24. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **3**.

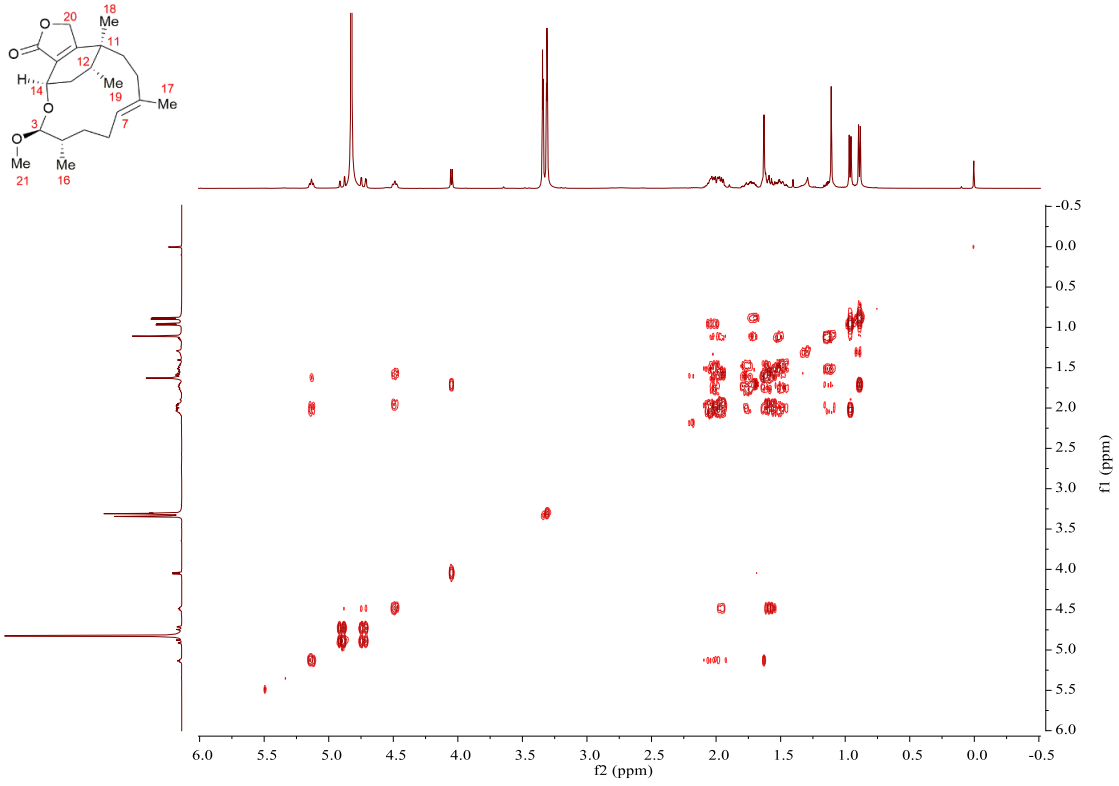


Figure S25. ^{1}H-^{1}H COSY spectrum of **3**.

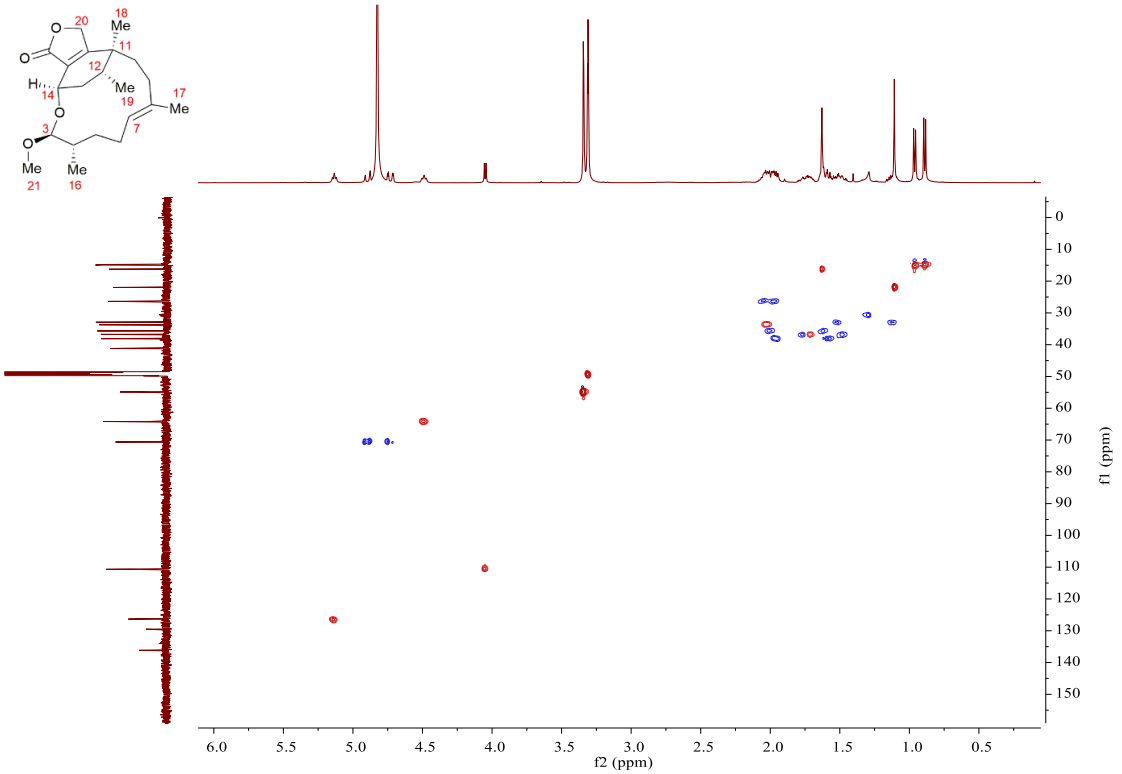


Figure S26. HSQC spectrum of **3**.

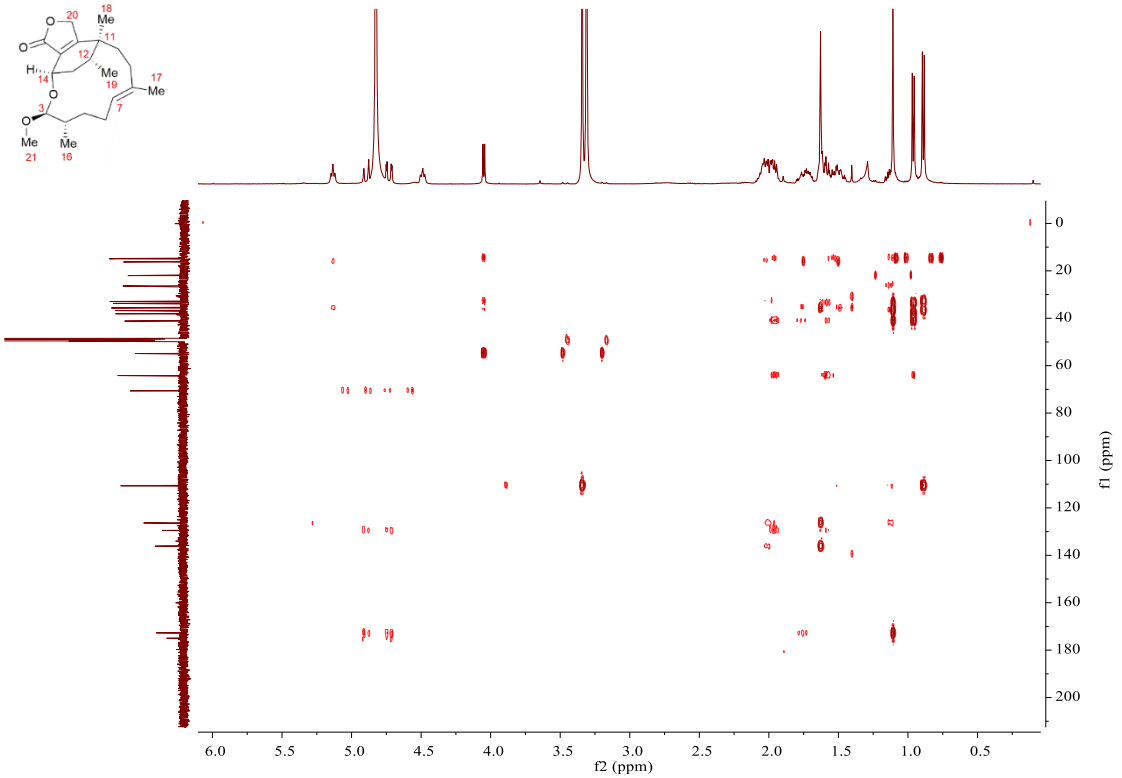


Figure S27. HMBC spectrum of **3**.

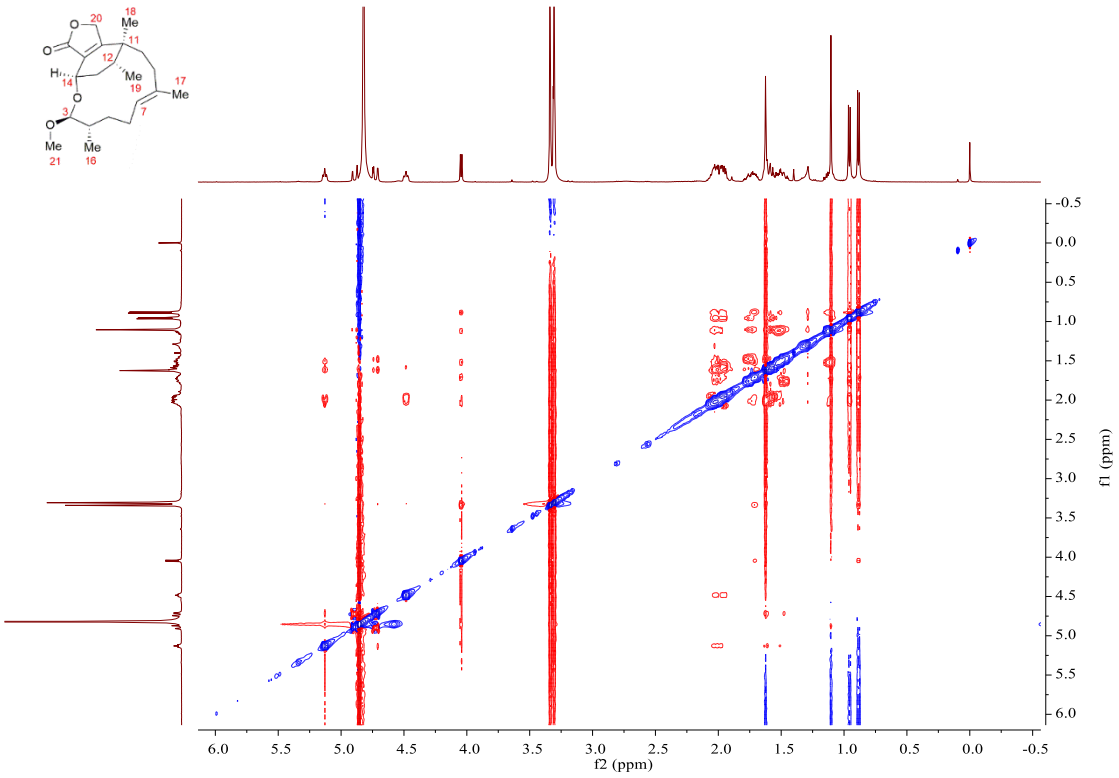


Figure S28. NOESY spectrum of **3**.

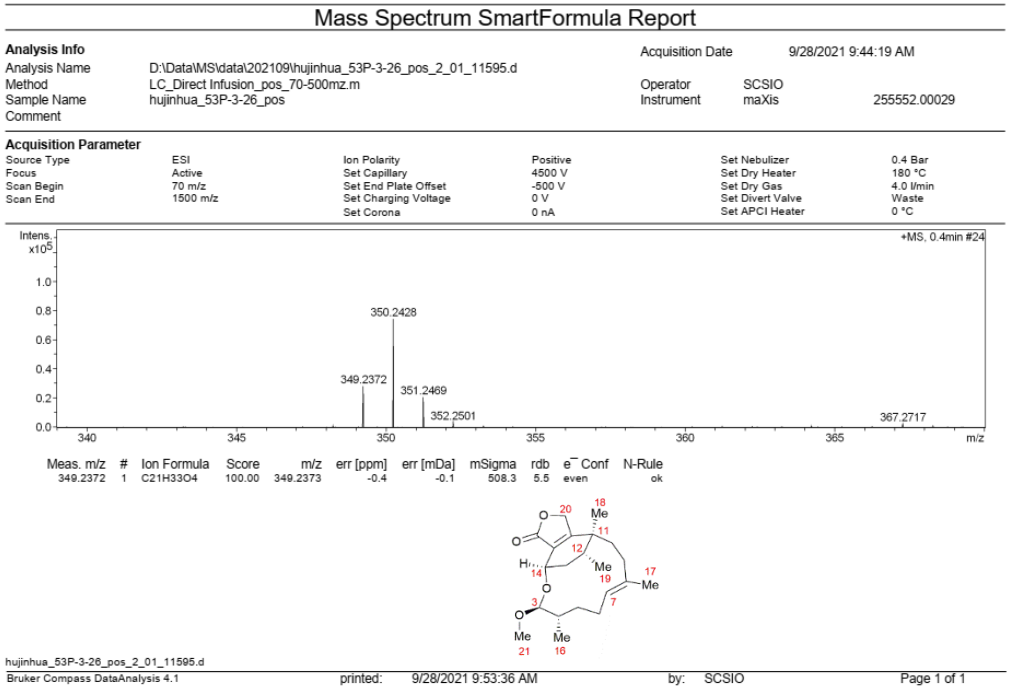


Figure S29. HRESIMS spectrum of **3**.

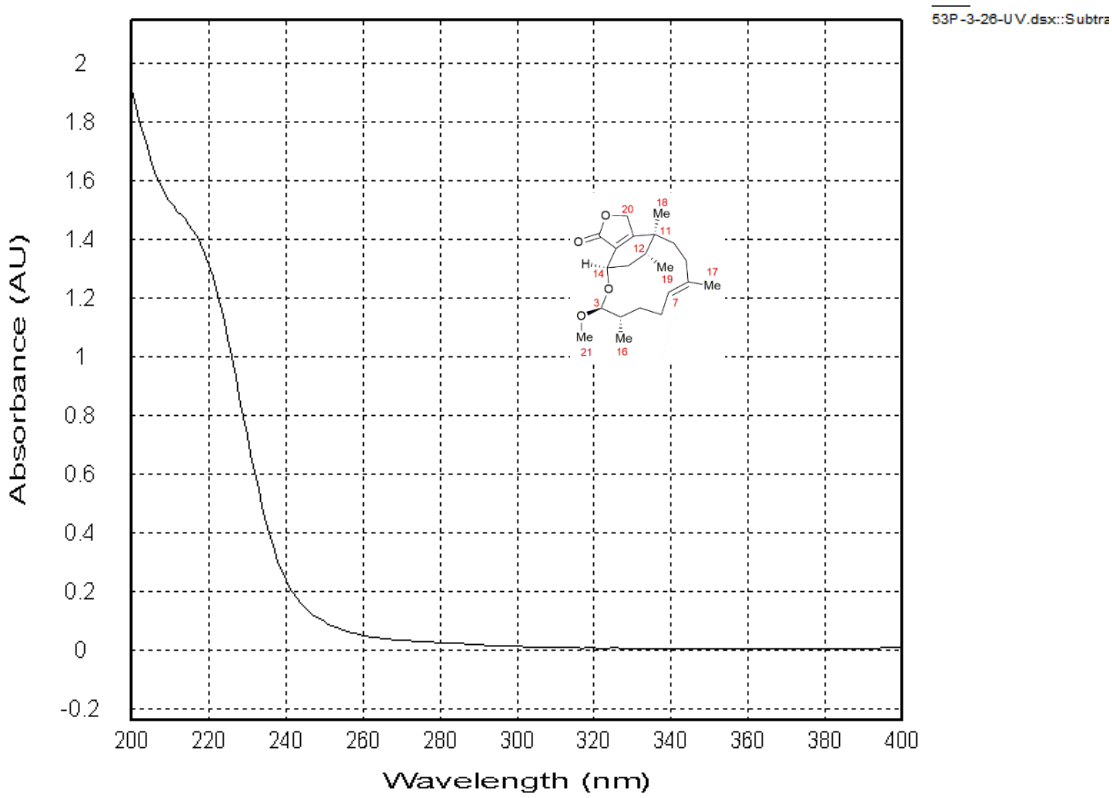


Figure S30. UV spectrum of **3**.

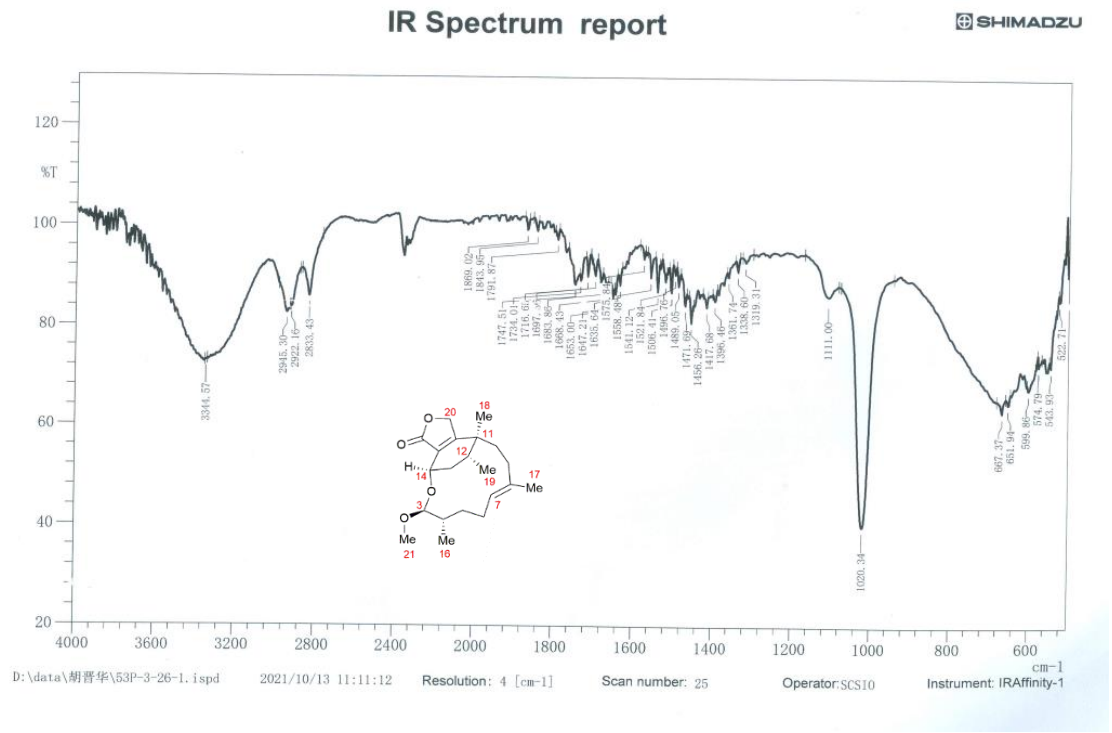


Figure S31. IR spectrum of **3**.

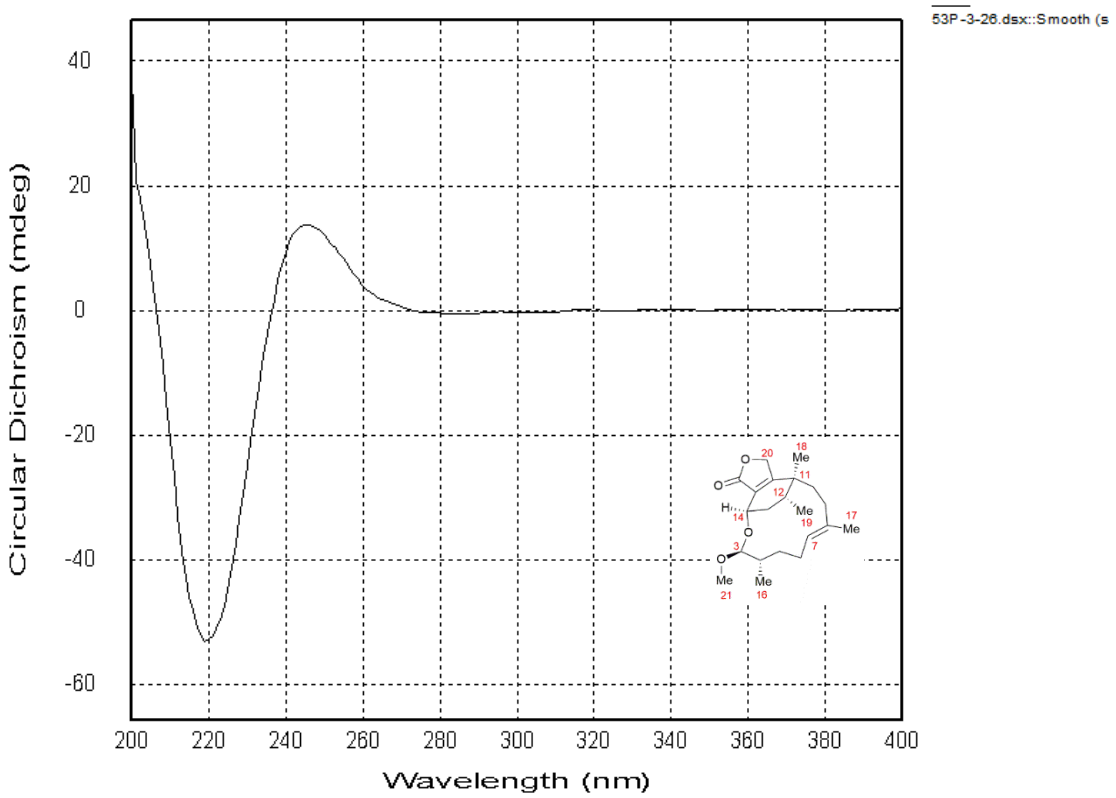


Figure S32. CD spectrum of **3**.

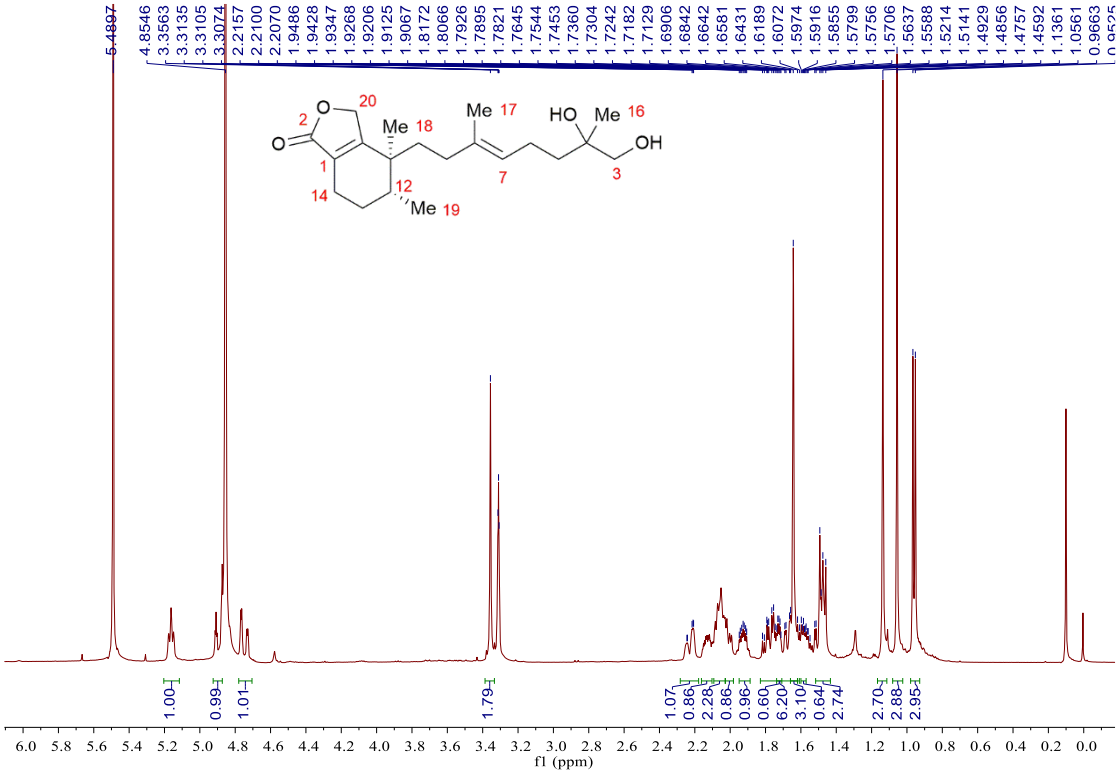


Figure S33. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **4**.

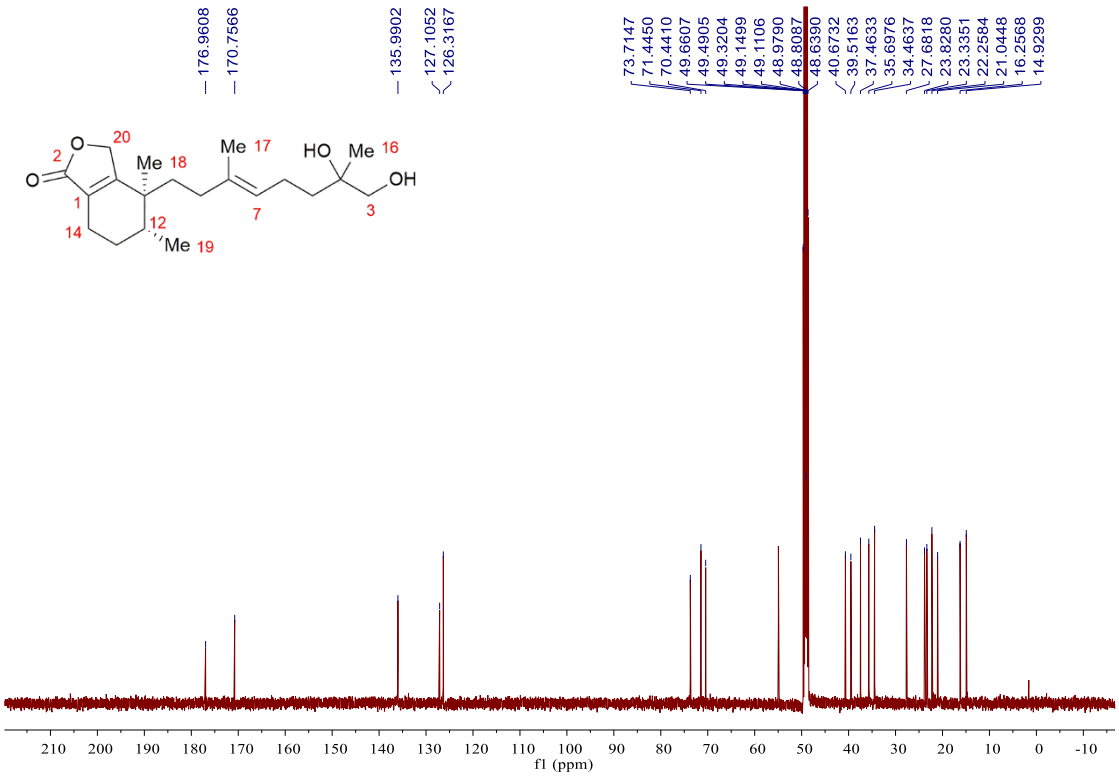


Figure S34. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **4**.

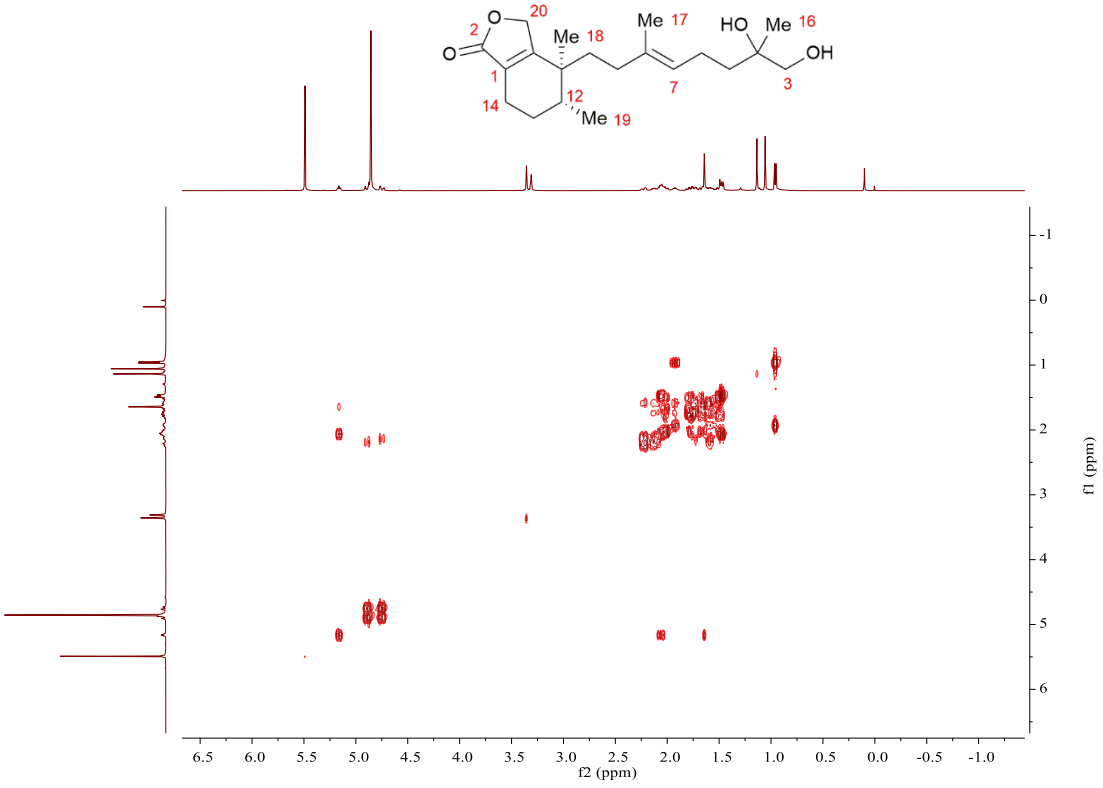


Figure S35. ^{1}H-^{1}H COSY spectrum of **4**.

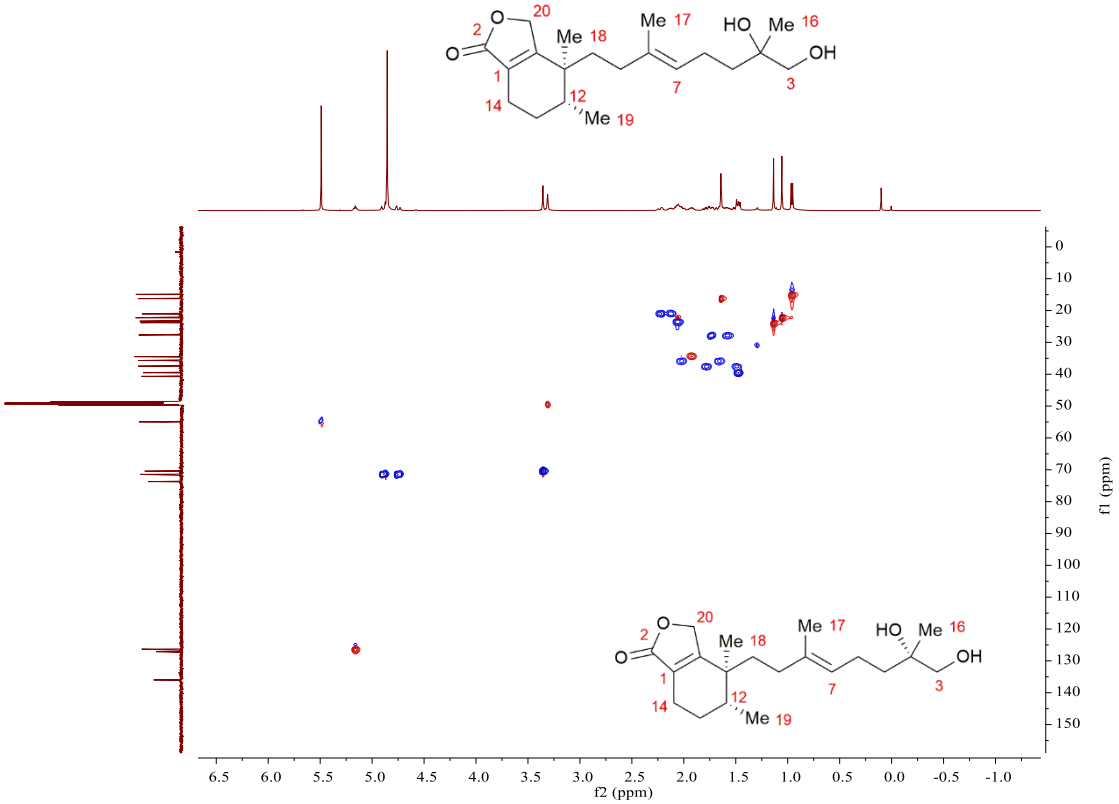


Figure S36. HSQC spectrum of **4**.

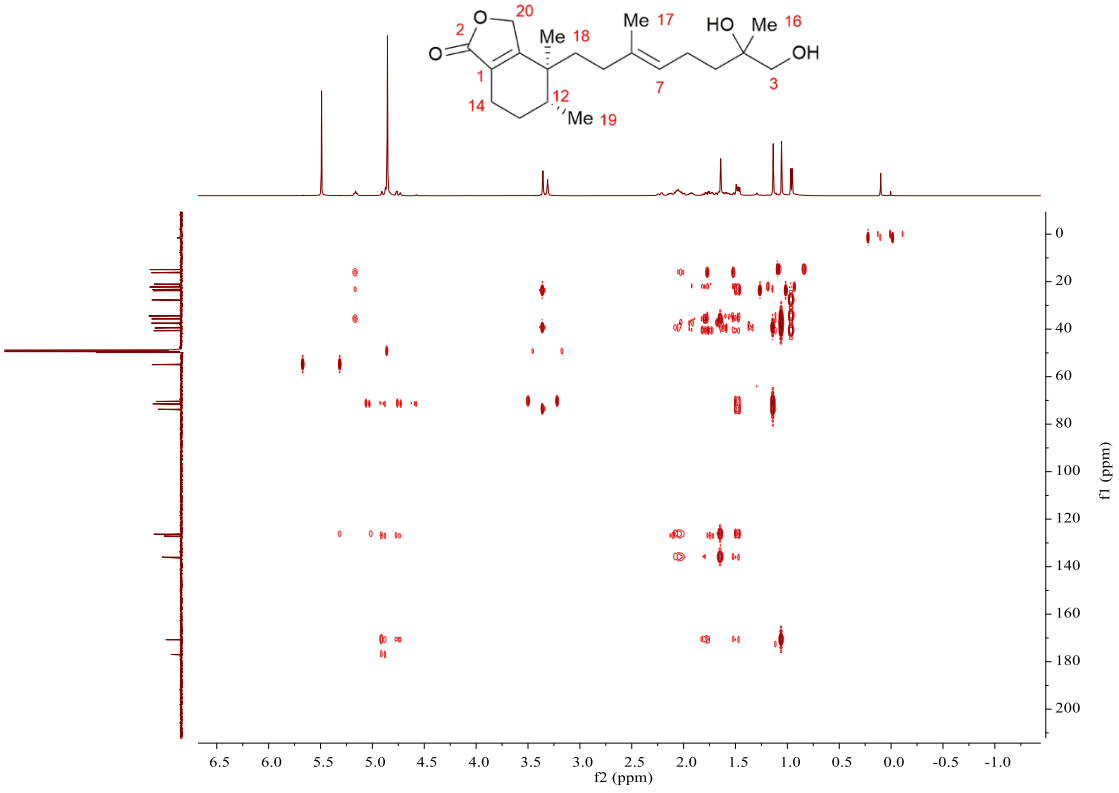


Figure S37. HMBC spectrum of **4**.

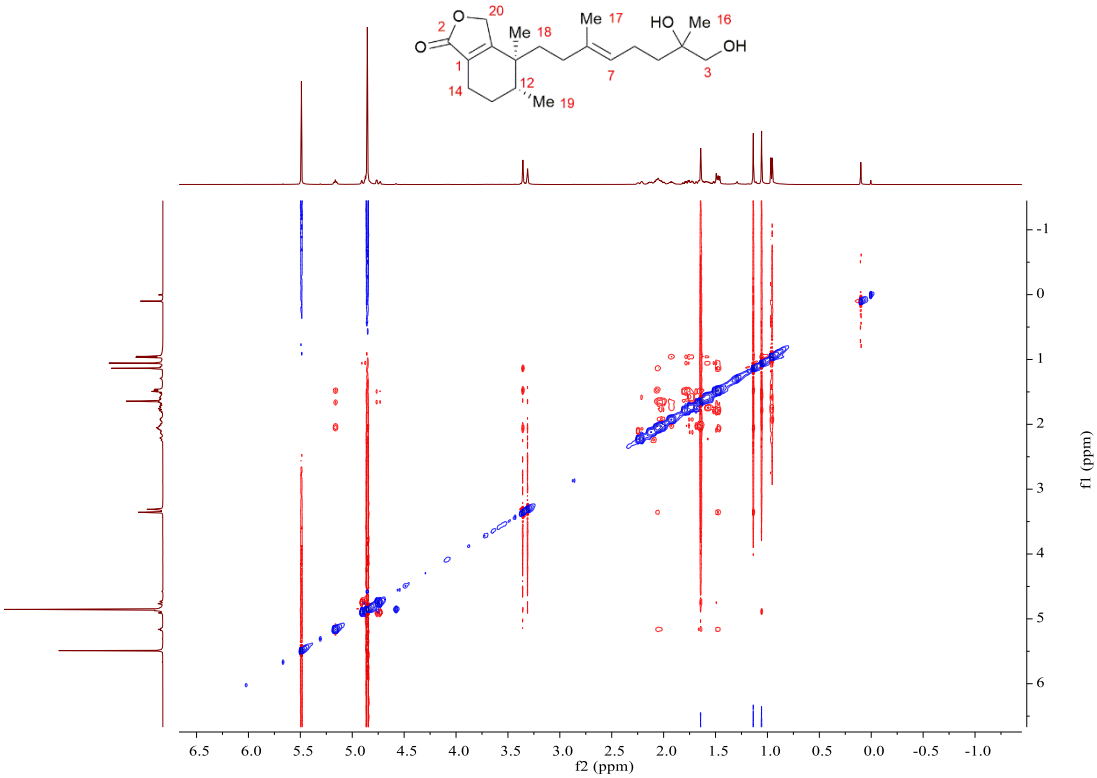


Figure S38. NOESY spectrum of **4**.

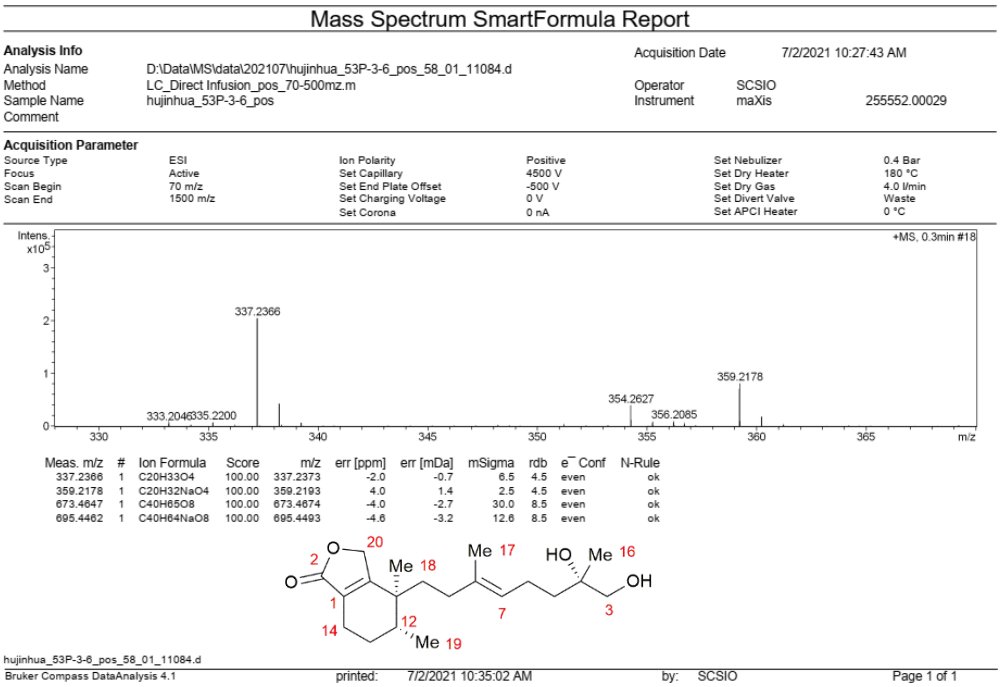


Figure S39. HRESIMS spectrum of **4**.

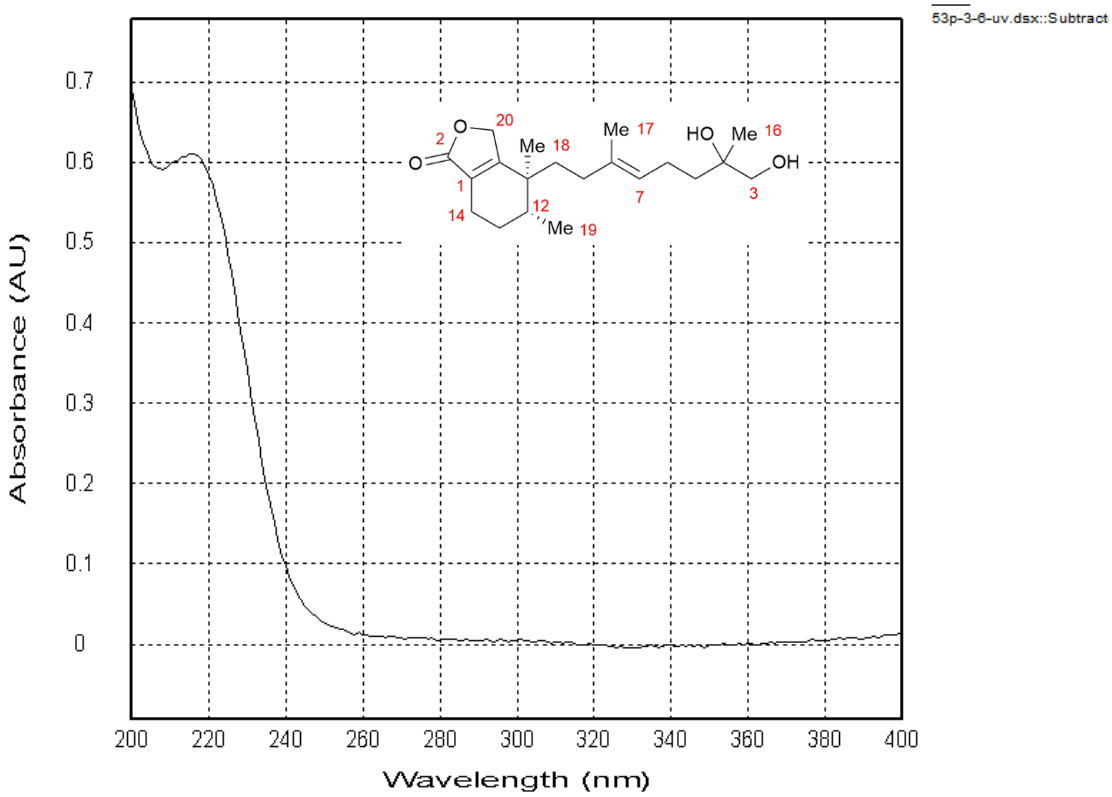


Figure S40. UV spectrum of **4**.

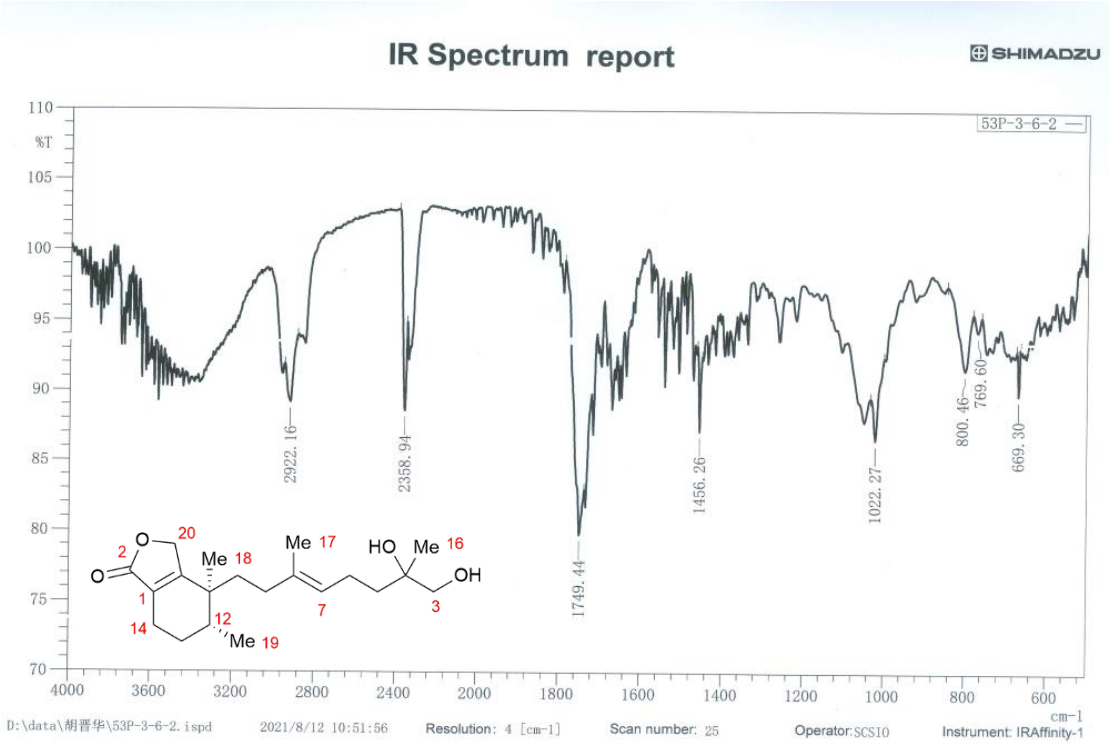


Figure S41. IR spectrum of **4**.

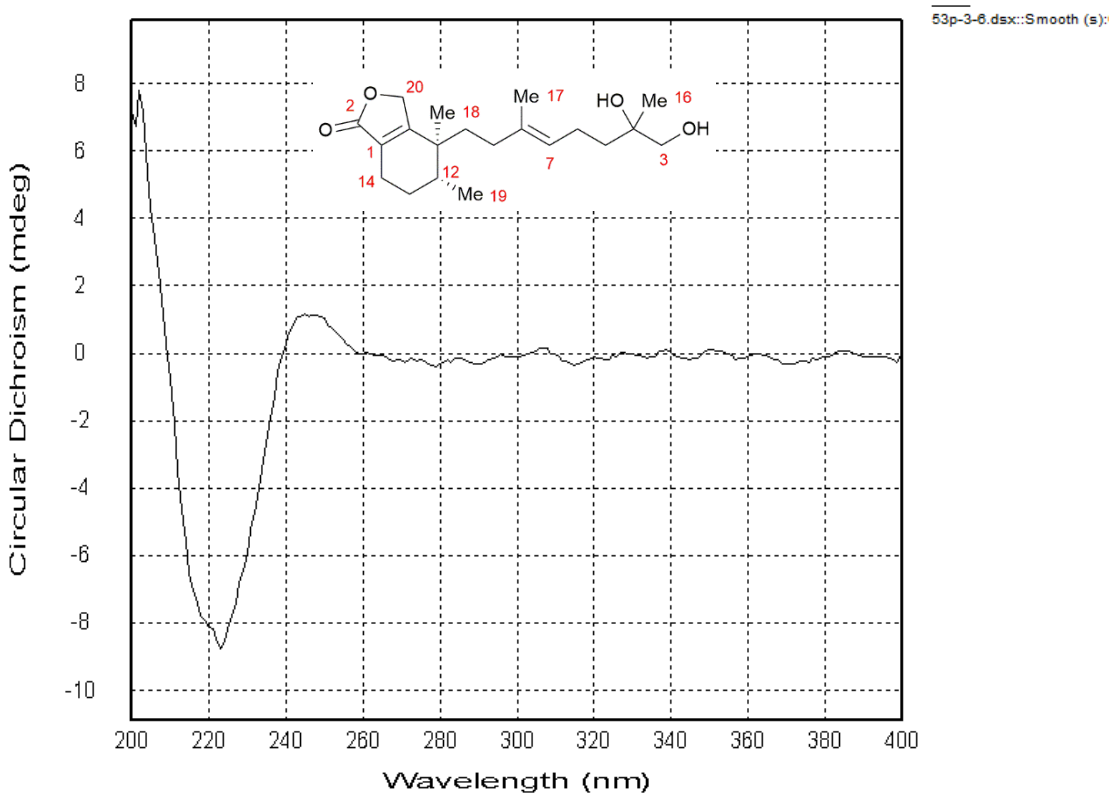


Figure S42. CD spectrum of **4**.

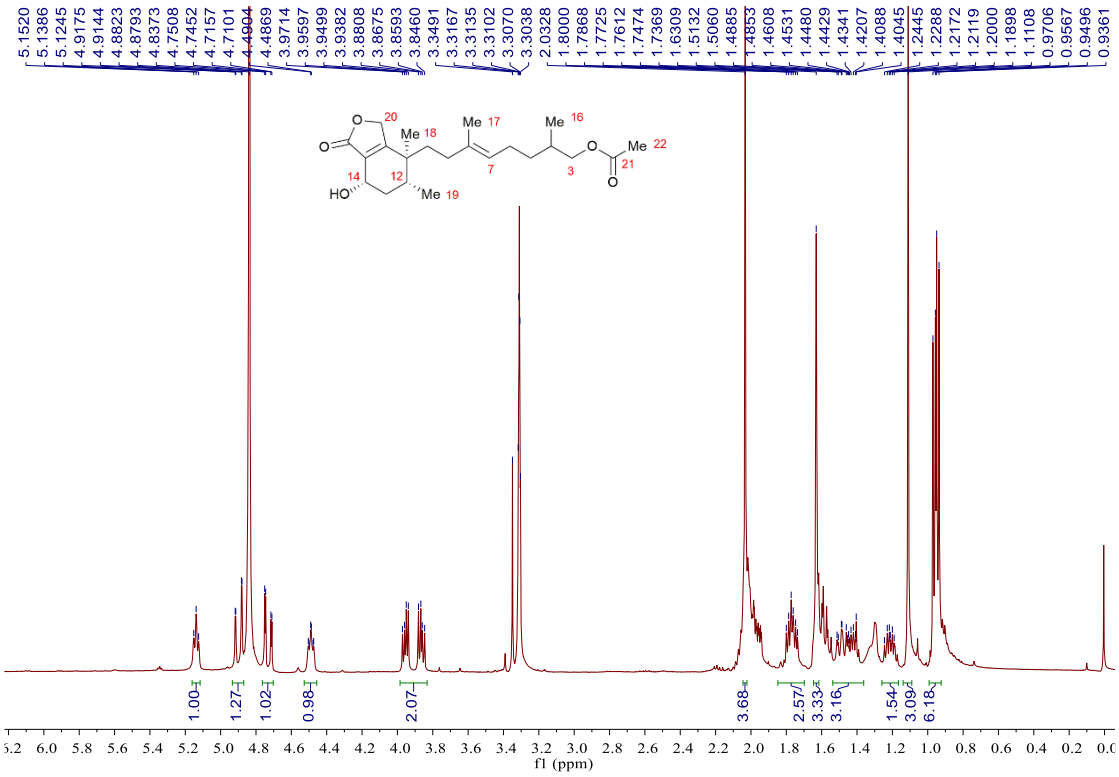


Figure S43. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **5**.

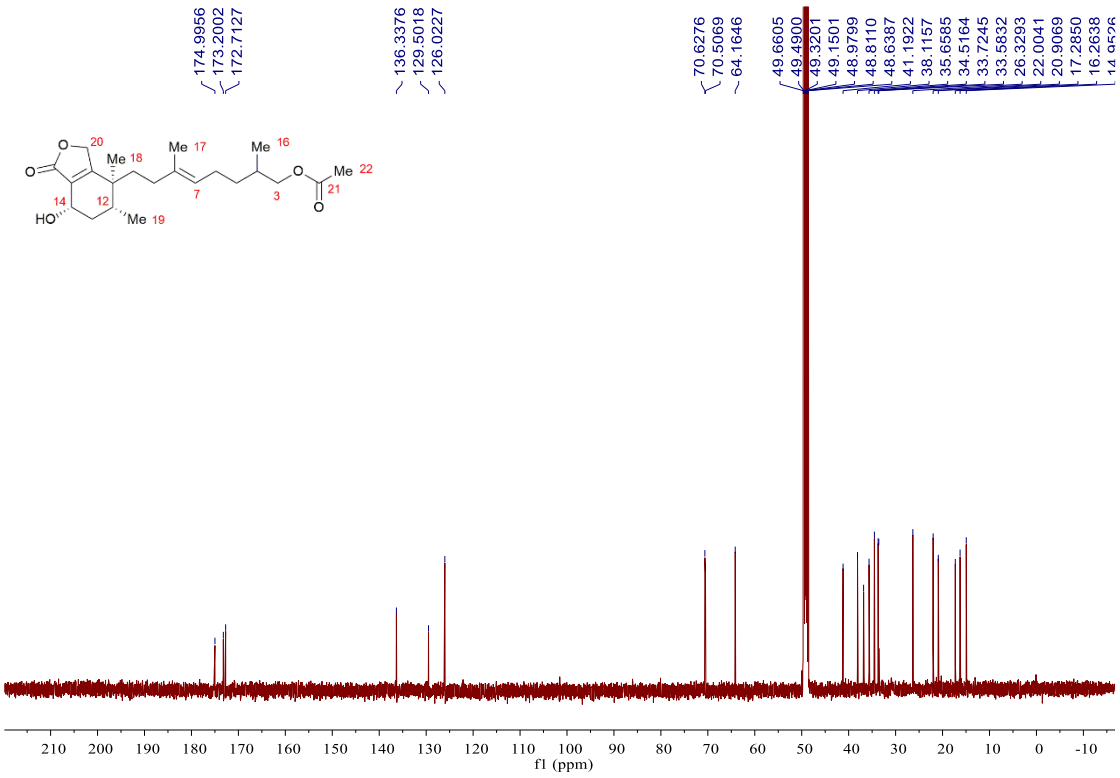


Figure S44. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **5**.

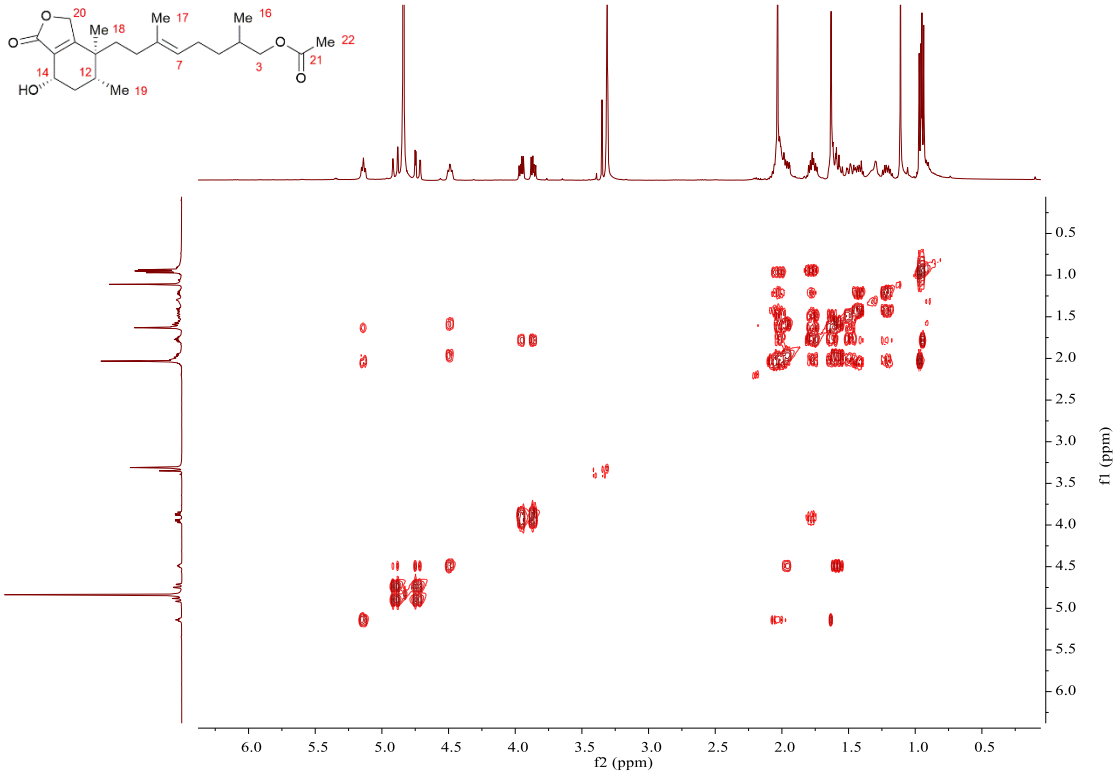


Figure S45. ^{1}H-^{1}H COSY spectrum of **5**.

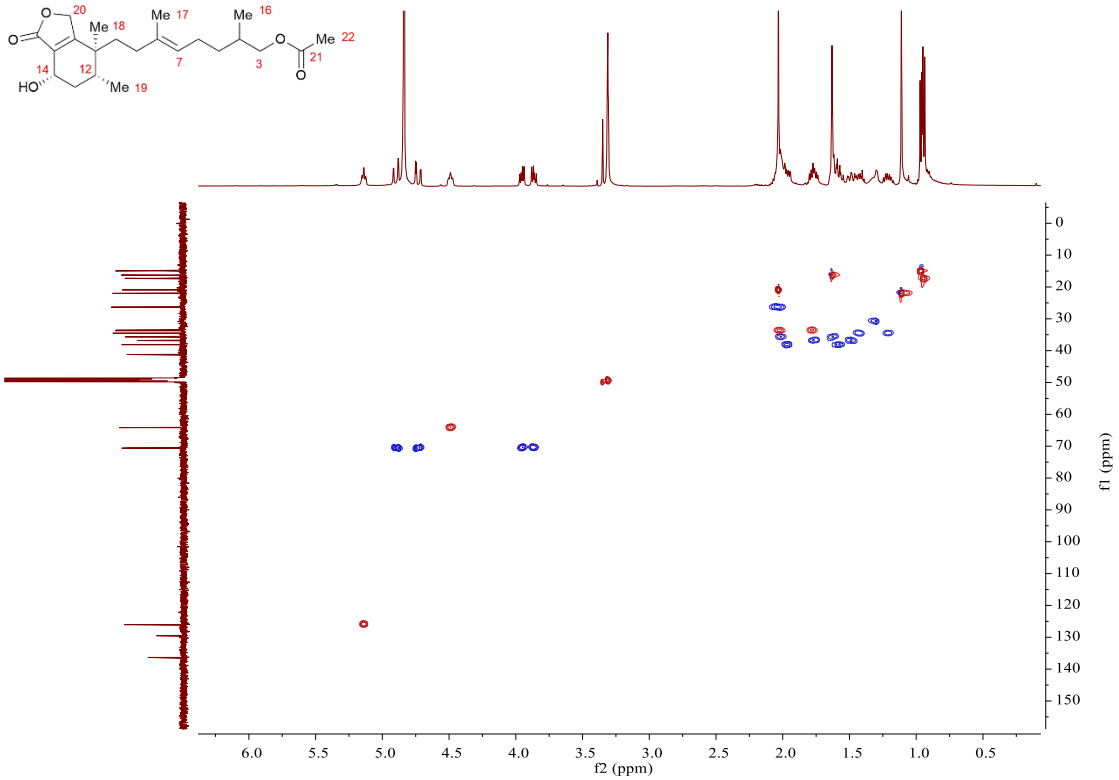


Figure S46. HSQC spectrum of **5**.

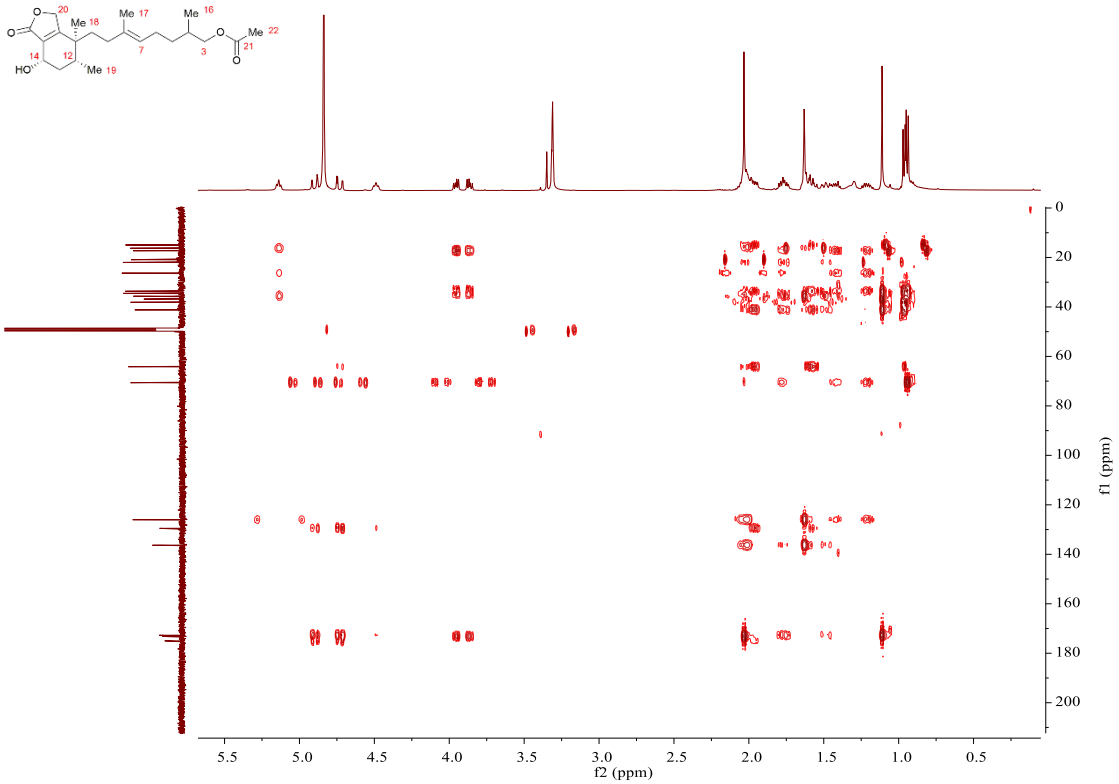


Figure S47. HMBC spectrum of **5**.

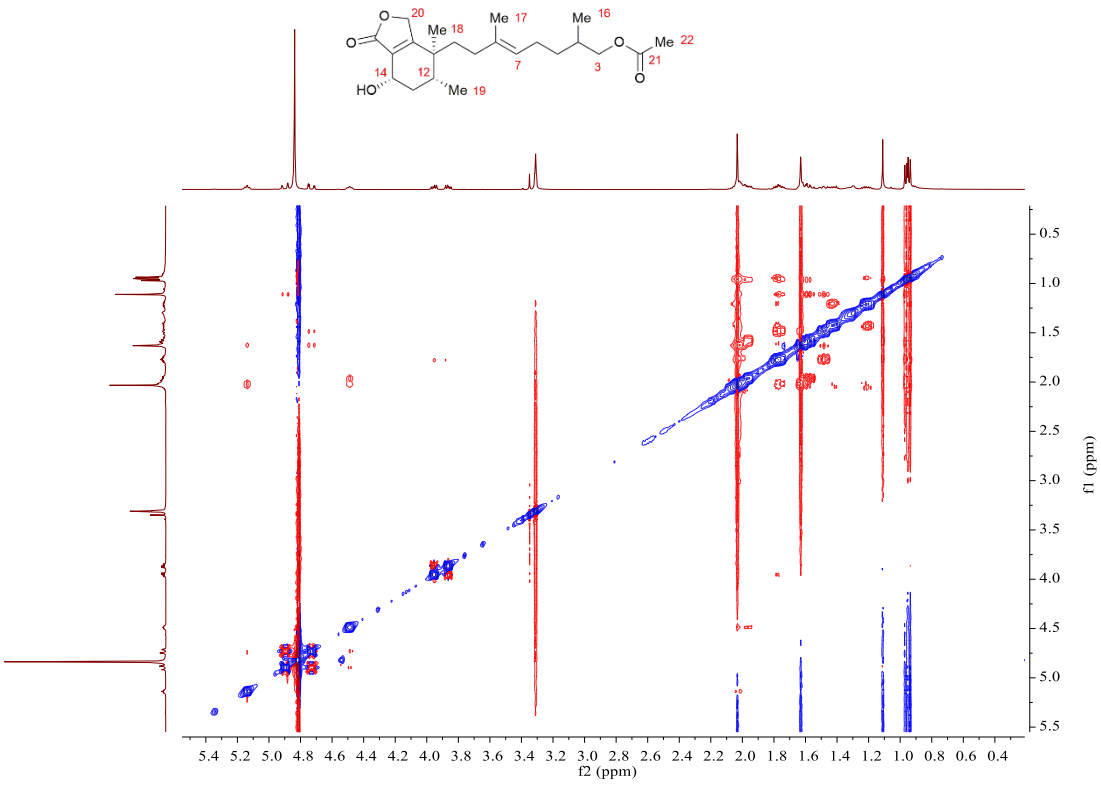


Figure S48. NOESY spectrum of **5**.

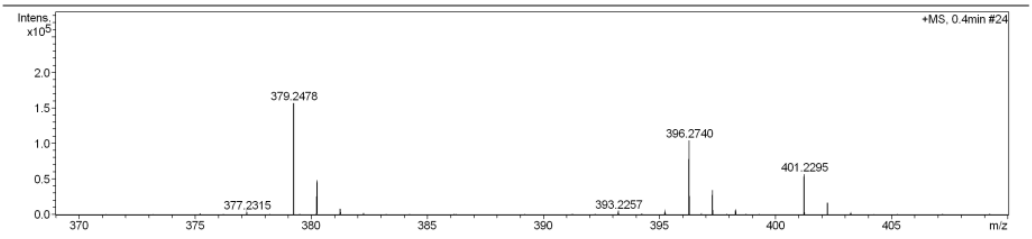
Mass Spectrum SmartFormula Report

Analysis Info

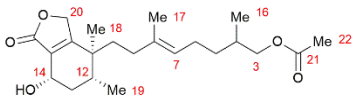
Analysis Name	D:\Data\MS\data\202109\hujinhua_53P-3-23_pos_1_01_11594.d	Acquisition Date	9/28/2021 9:40:56 AM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	hujinhua_53P-3-23_pos	Instrument	maXis 255552.00029
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
379.2478	1	C22H35O5	100.00	379.2479	0.4	0.1	34.1	5.5	even	ok
401.2295	1	C22H34NaO5	100.00	401.2298	0.9	0.3	26.6	5.5	even	ok



hujinhua_53P-3-23_pos_1_01_11594.d

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Figure S49. HRESIMS spectrum of **5**.

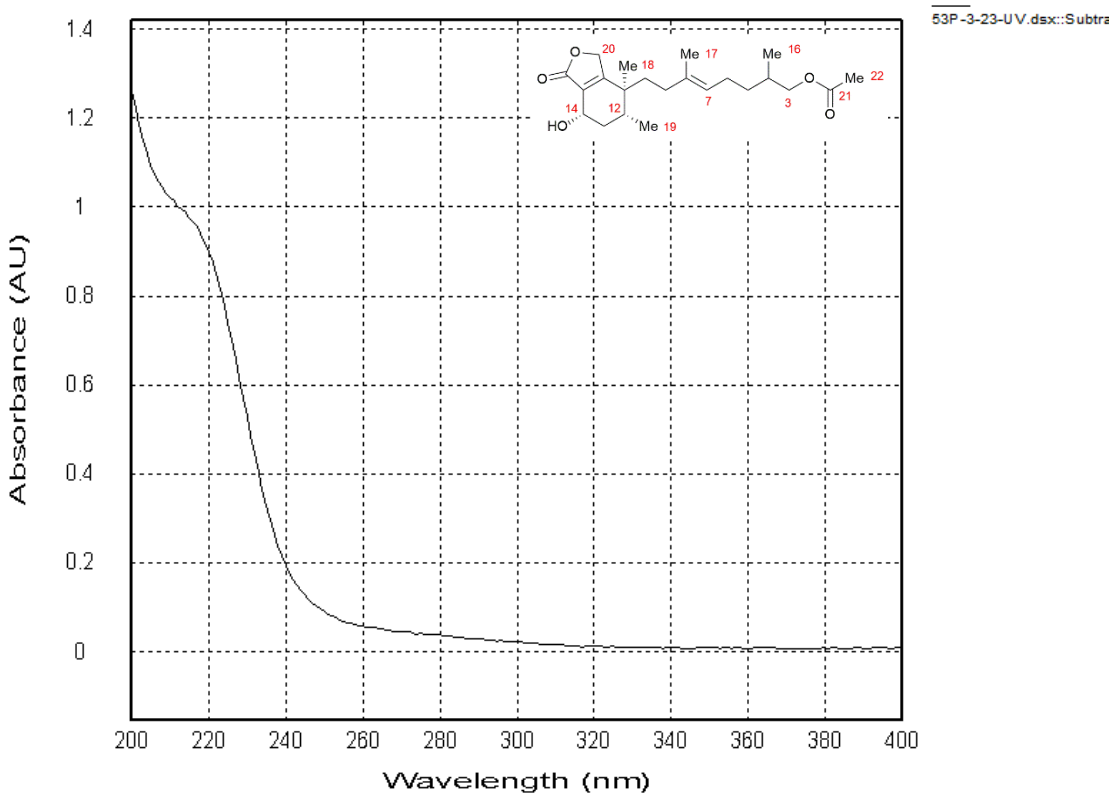


Figure S50. UV spectrum of **5**.

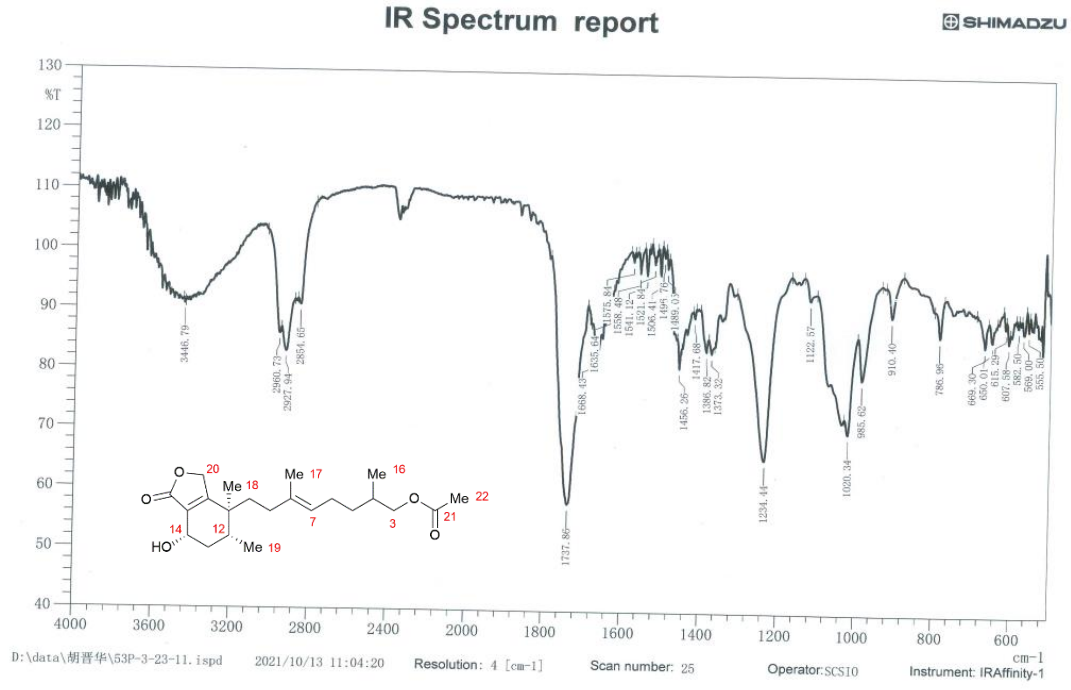


Figure S51. IR spectrum of **5**.

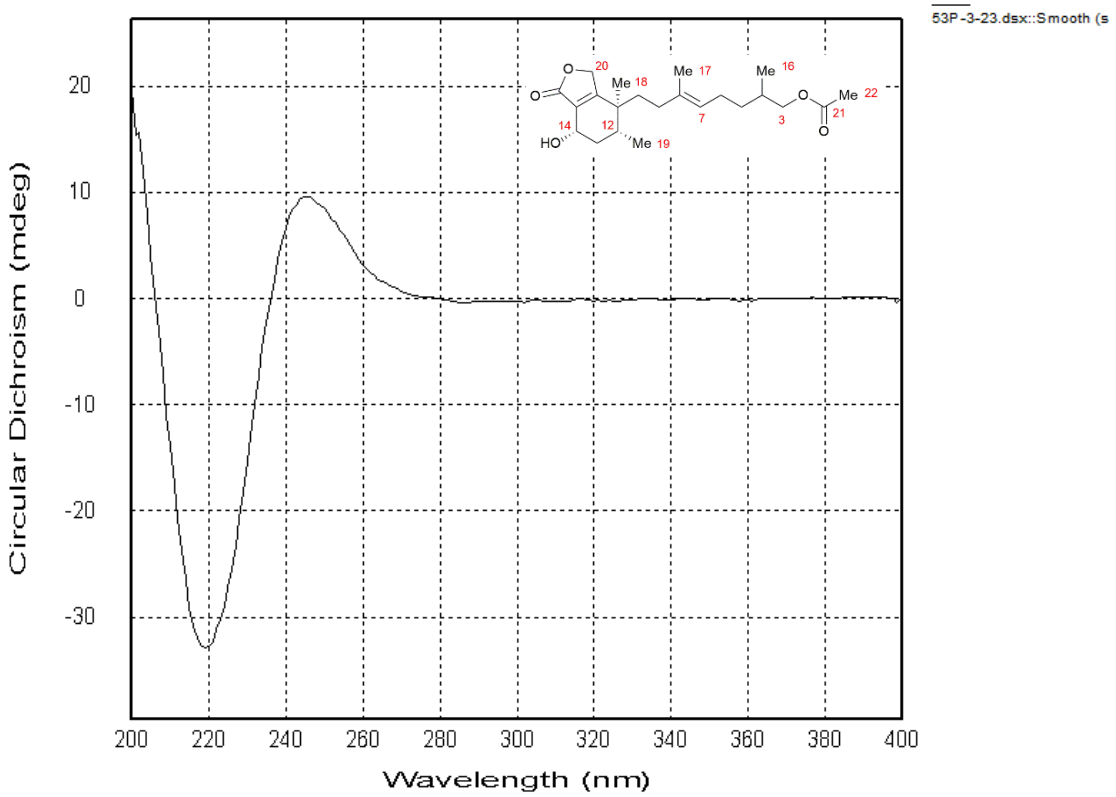


Figure S52. CD spectrum of **5**.

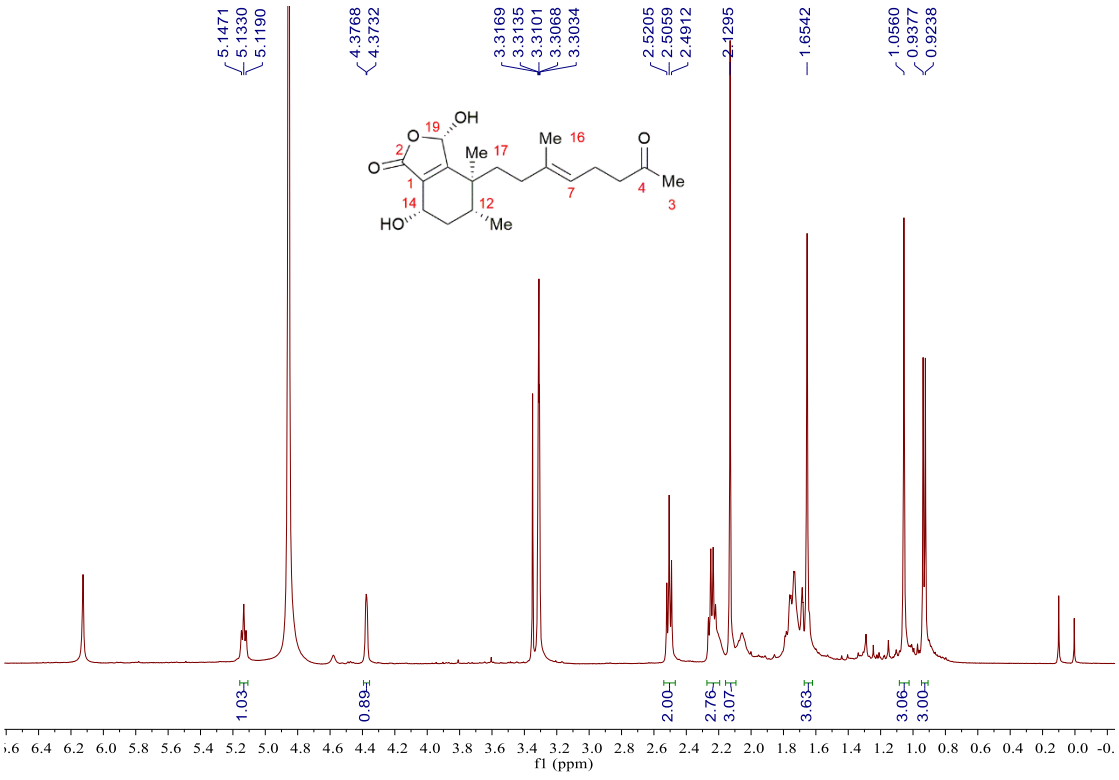


Figure S53. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **6**.

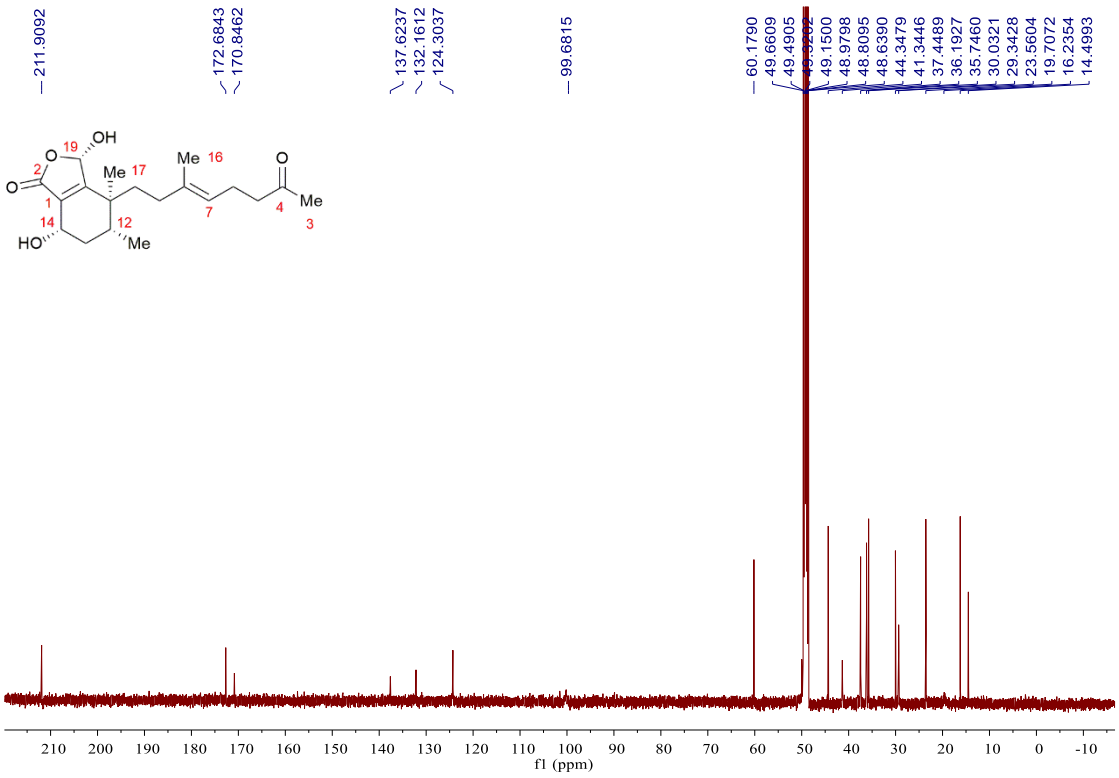


Figure S54. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **6**.

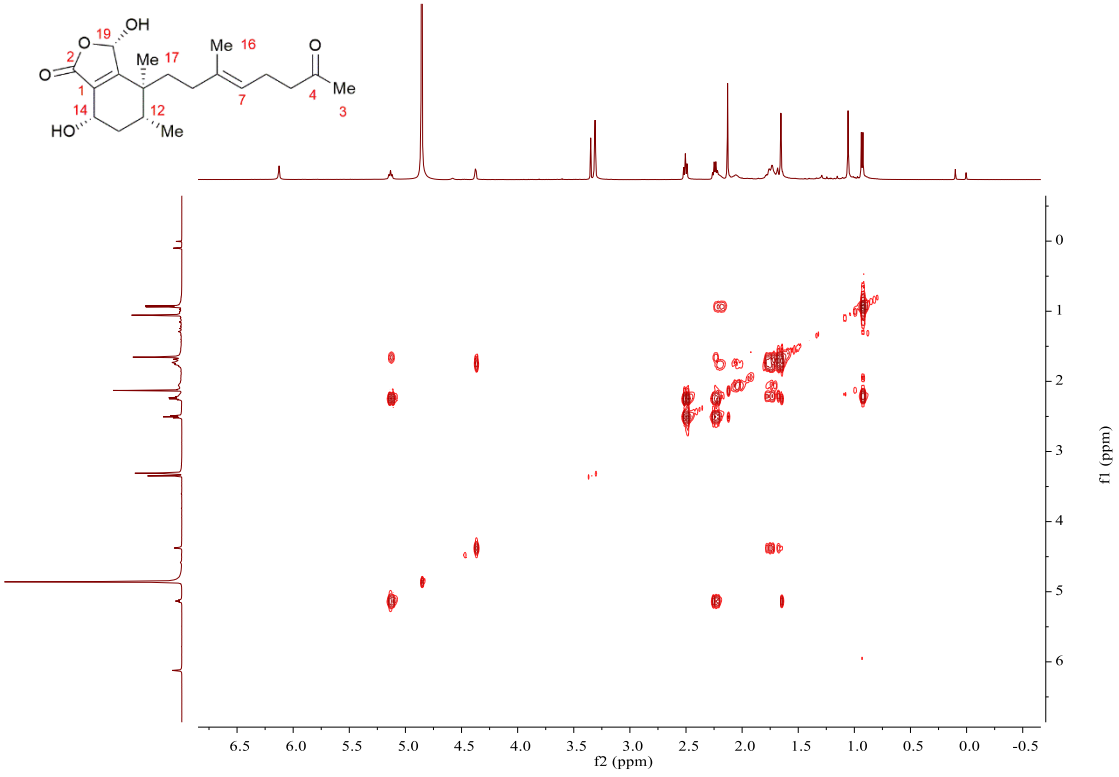


Figure S55. ^{1}H-^{1}H COSY spectrum of **6**.

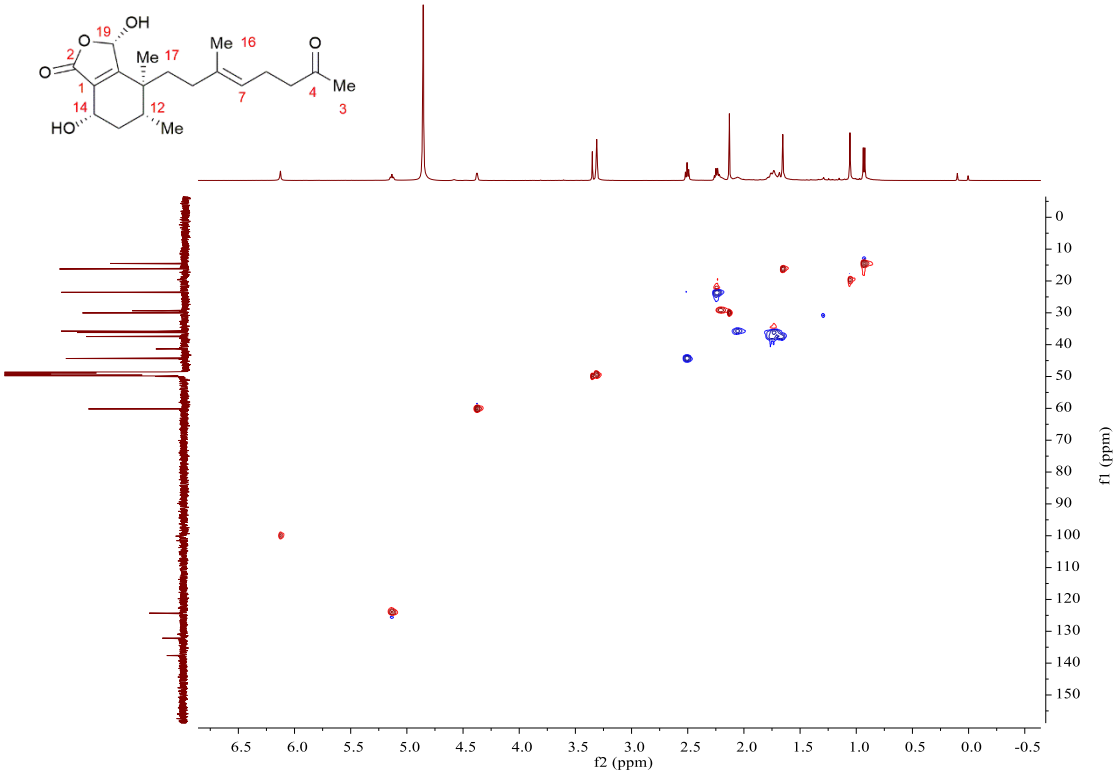


Figure S56. HSQC spectrum of **6**.

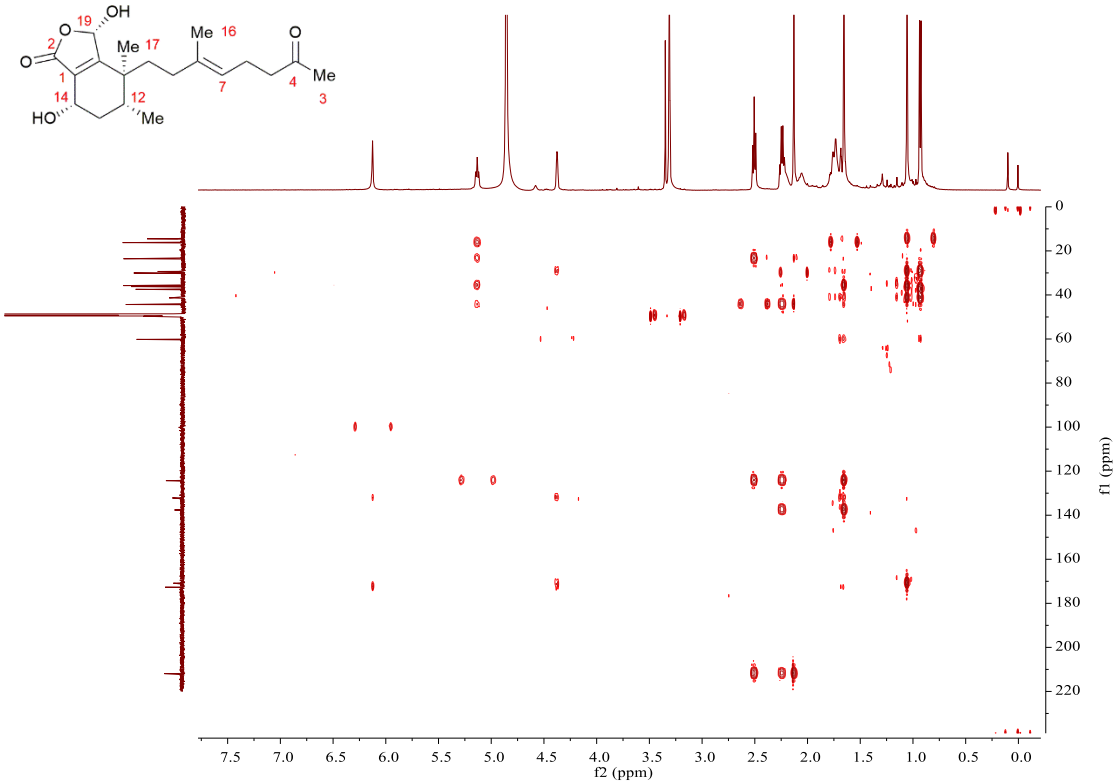


Figure S57. HMBC spectrum of **6**.

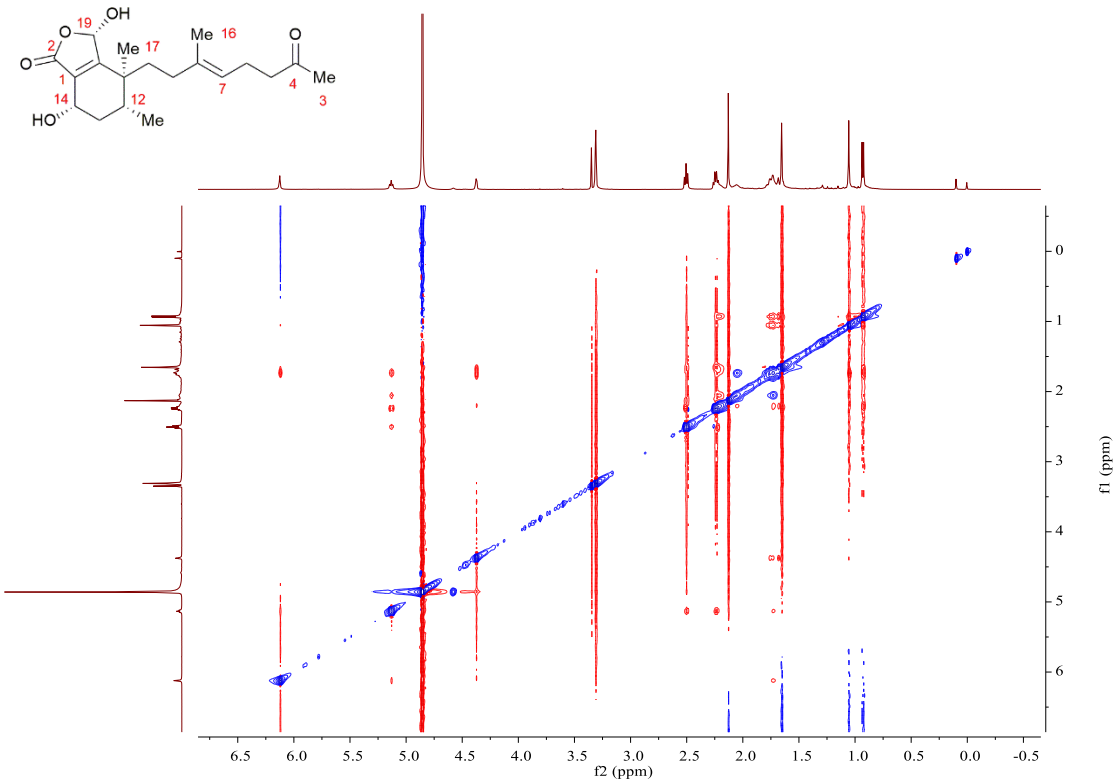


Figure S58. NOESY spectrum of **6**.

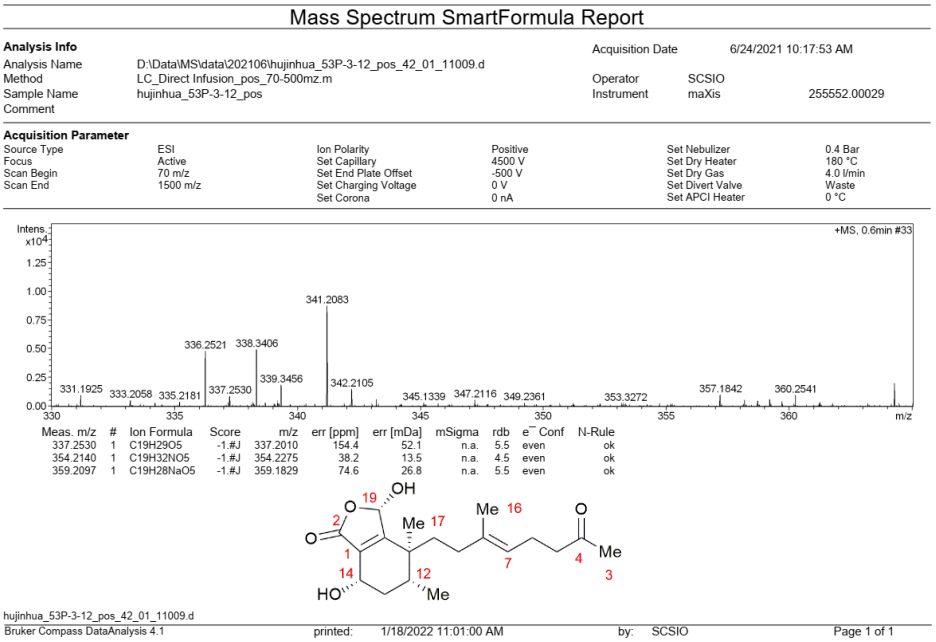


Figure S59. HRESIMS spectrum of **6**.

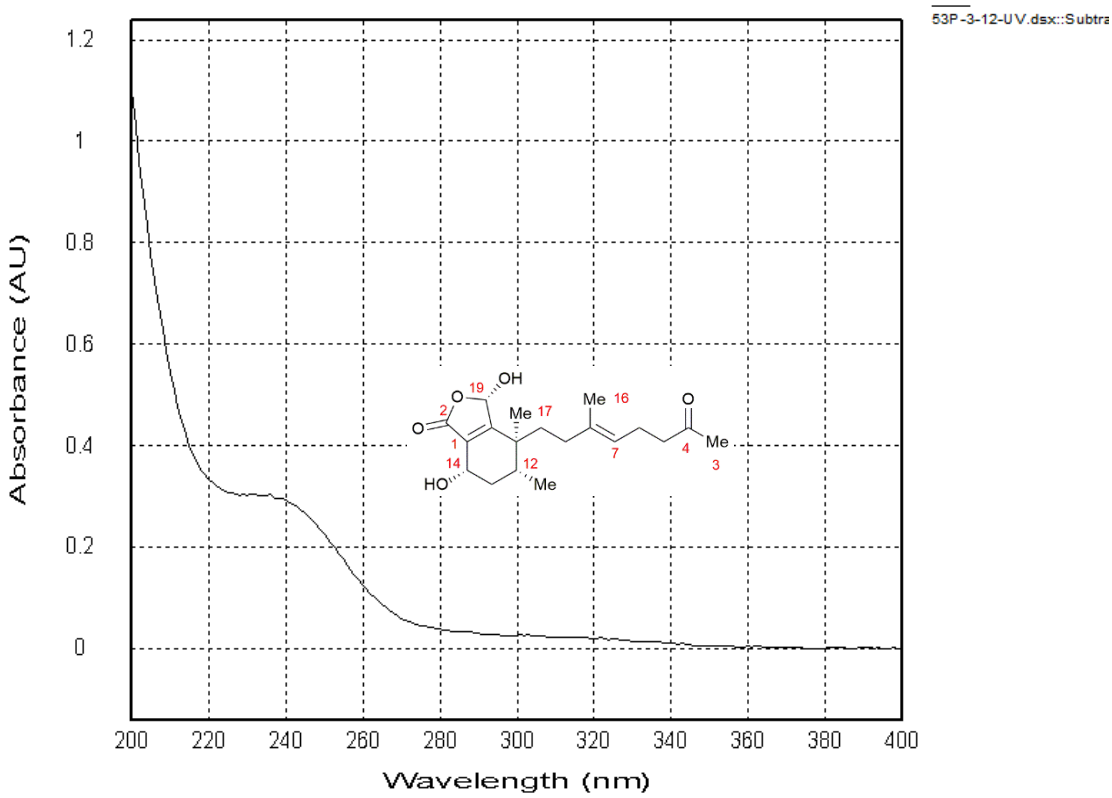


Figure S60. UV spectrum of **6**.

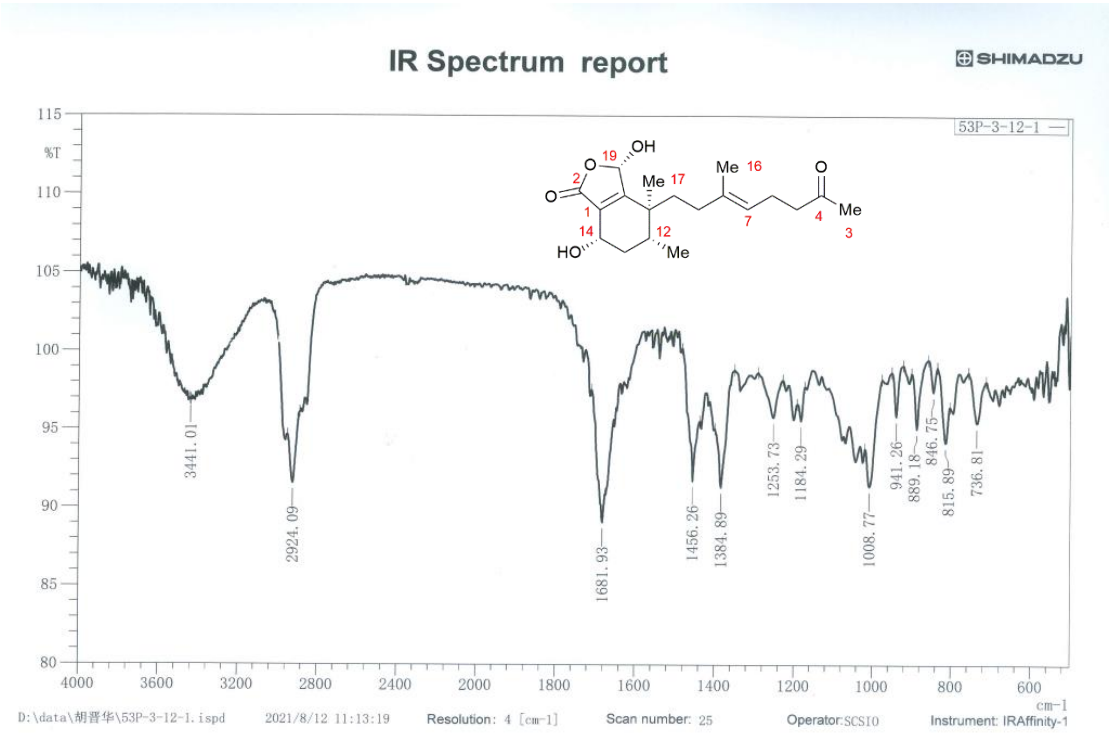


Figure S61. IR spectrum of **6**.

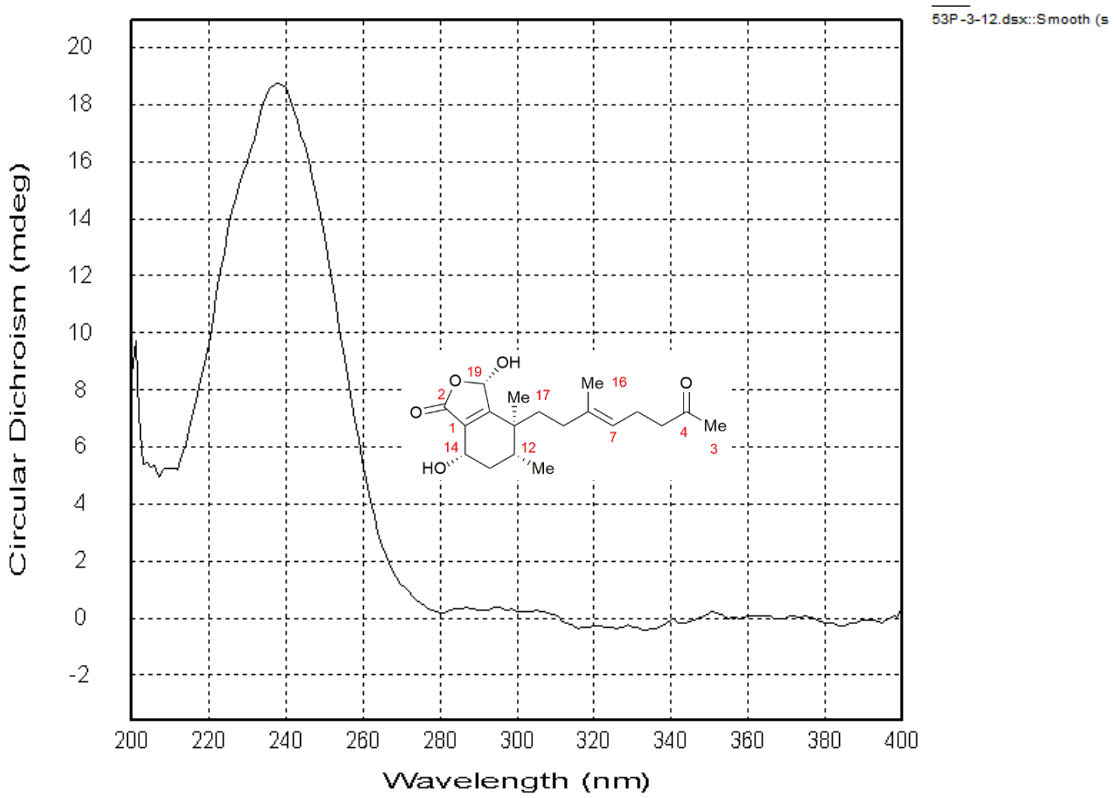


Figure S62. CD spectrum of **6**.

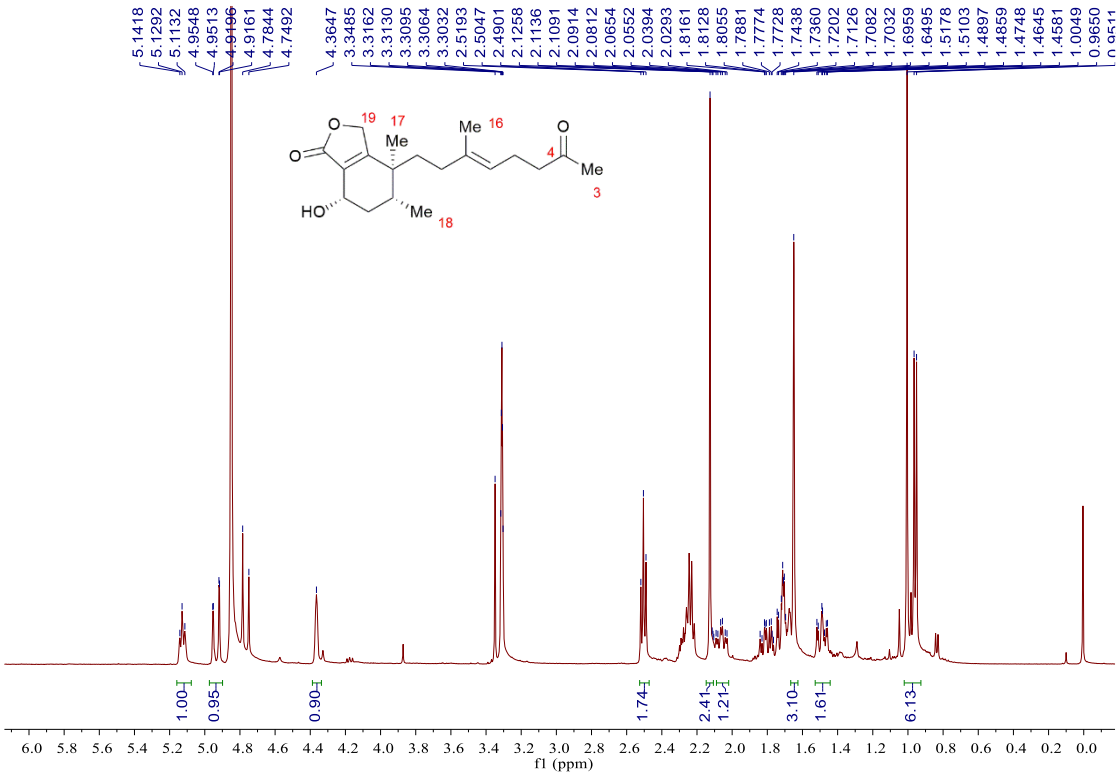


Figure S63. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **7**.

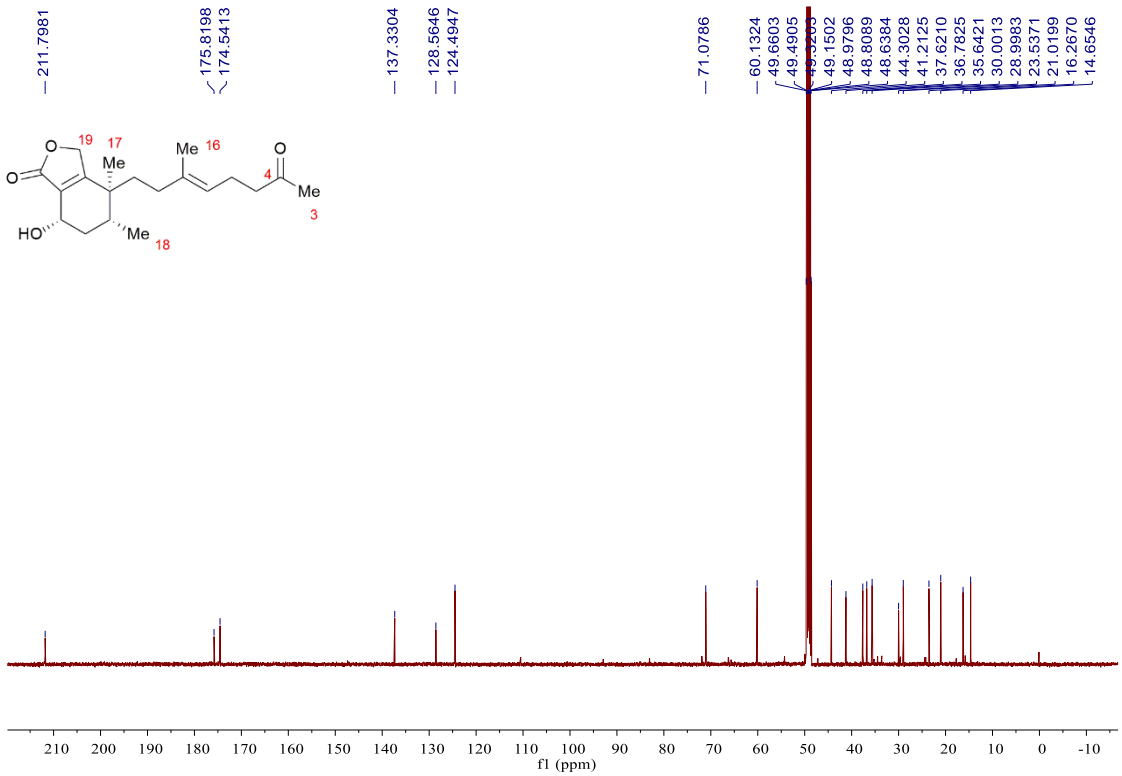


Figure S64. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **7**.

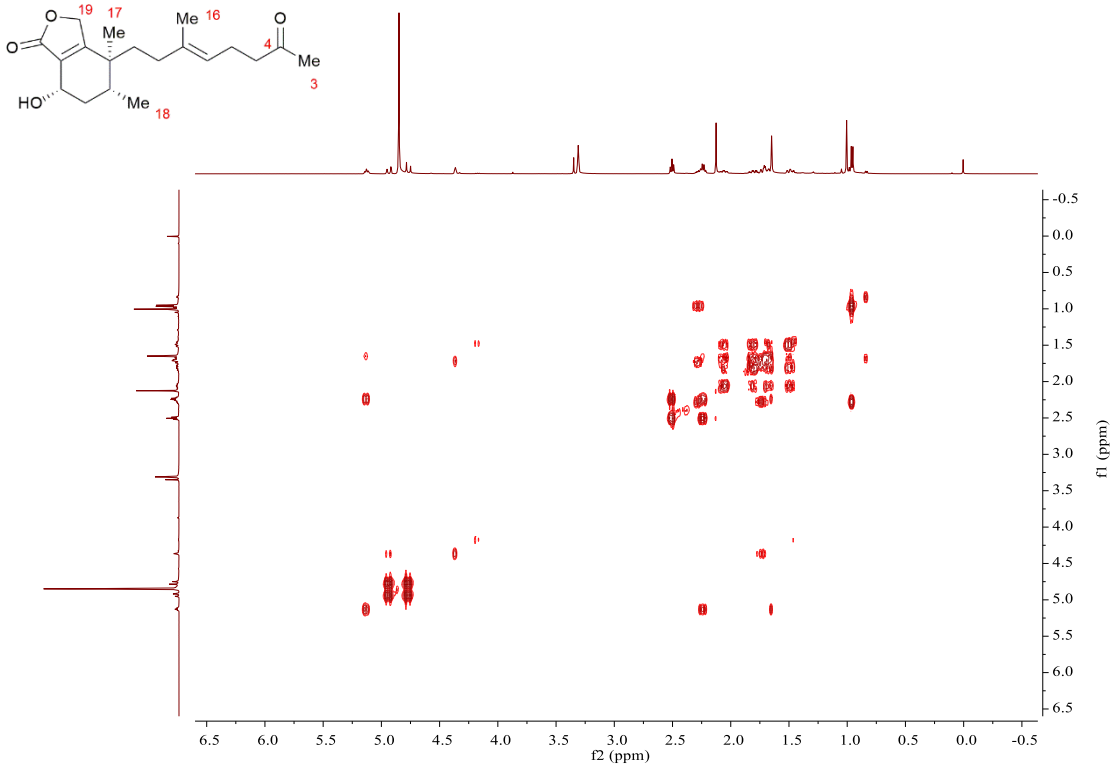


Figure S65. ^{1}H-^{1}H COSY spectrum of **7**.

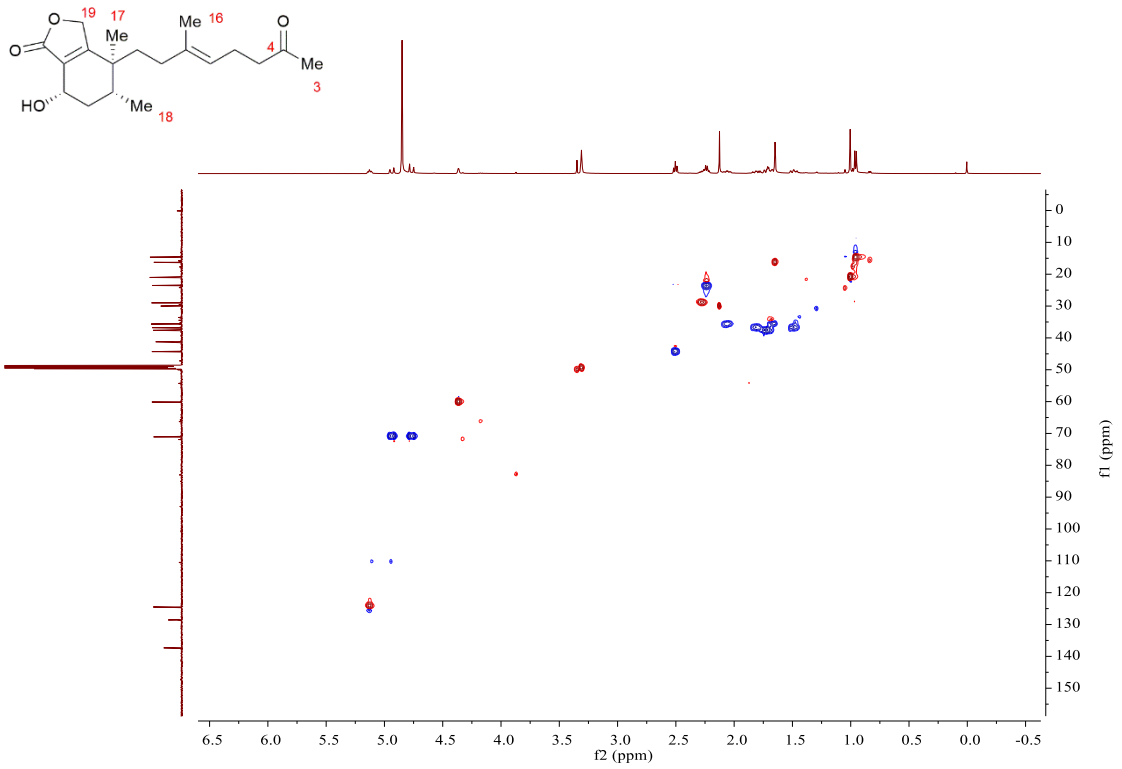


Figure S66. HSQC spectrum of **7**.

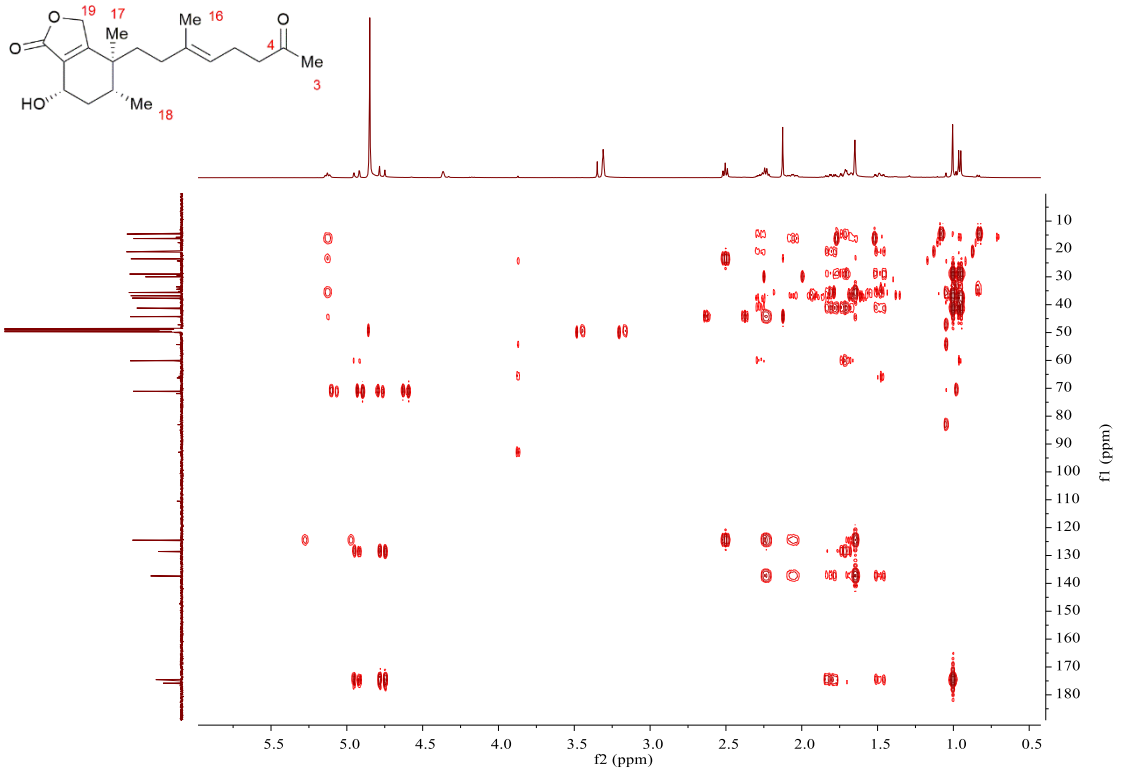


Figure S67. HMBC spectrum of **7**.

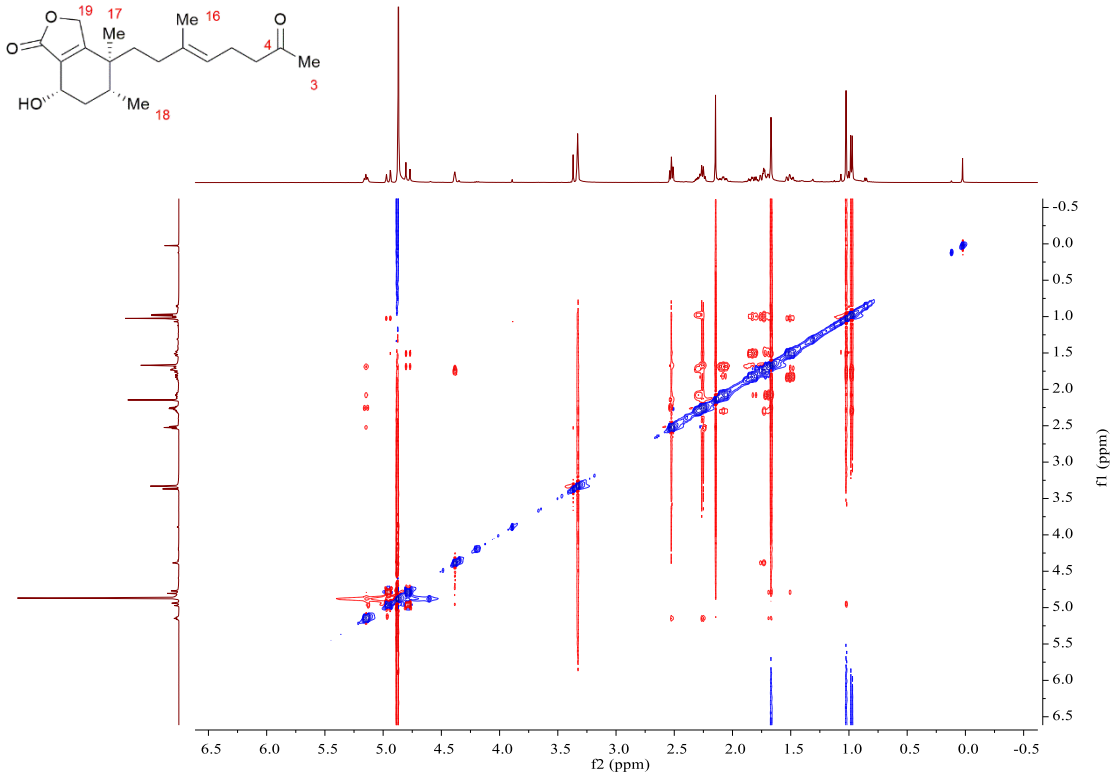


Figure S68. NOESY spectrum of **7**.

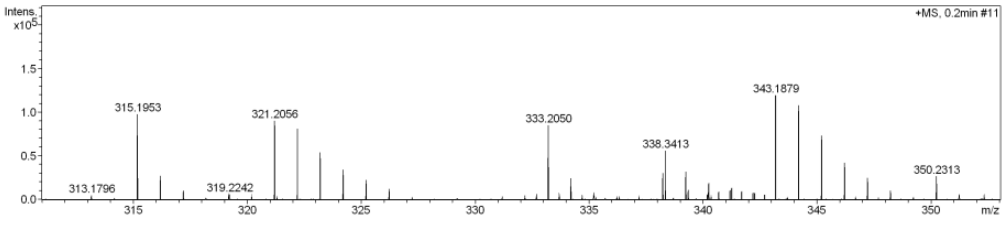
Mass Spectrum SmartFormula Report

Analysis Info

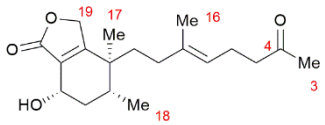
Analysis Name	D:\Data\MS\data\202106\hujinhua_53P-3-13_pos_43_01_11010.d	Acquisition Date	6/24/2021 10:21:18 AM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	hujinhua_53P-3-13_pos	Instrument	maXis 255552.00029
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
321.2056	1	C19H29O4	100.00	321.2060	-1.2	-0.4	517.1	5.5	even	ok
343.1879	1	C19H28NaO4	100.00	343.1880	0.2	0.1	524.5	5.5	even	ok



hujinhua_53P-3-13_pos_43_01_11010.d

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Figure S69. HRESIMS spectrum of **7**.

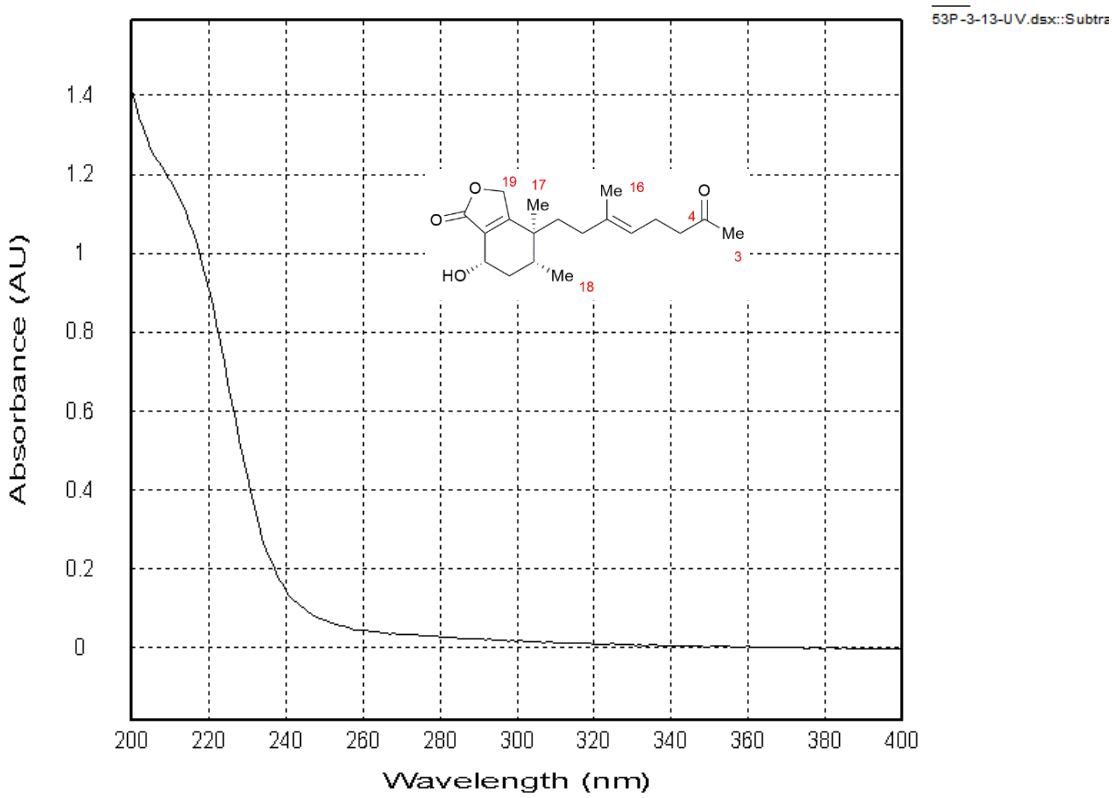

Figure S70. UV spectrum of **7**.

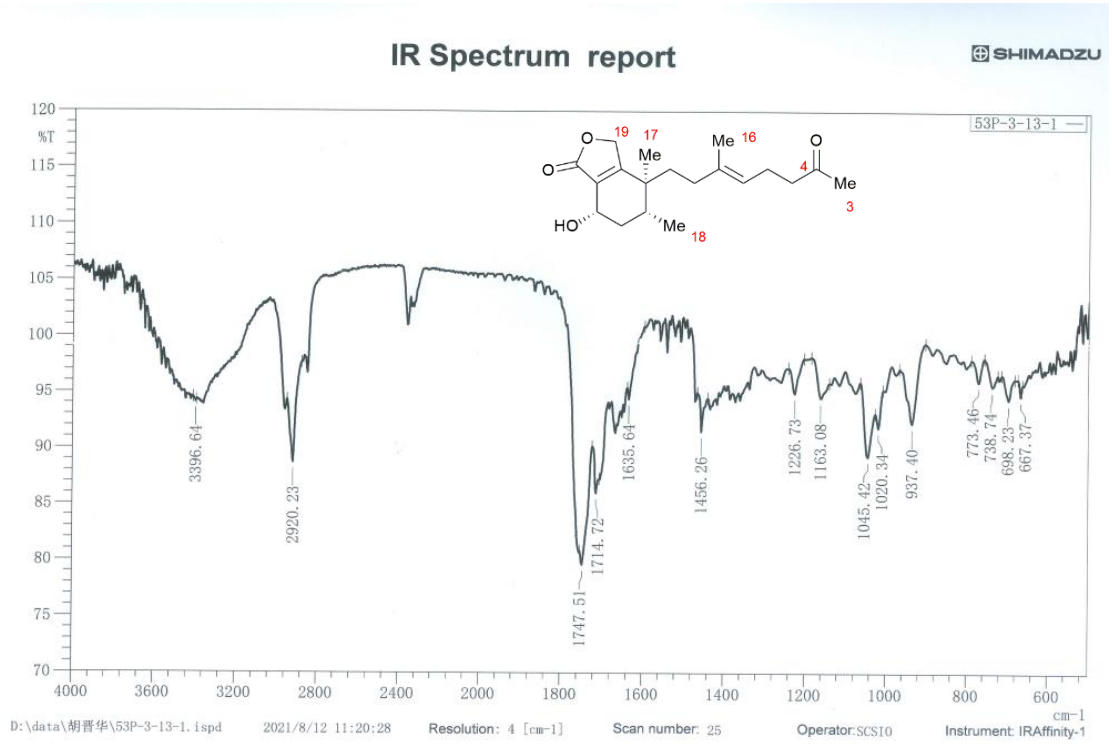

Figure S71. IR spectrum of **7**.

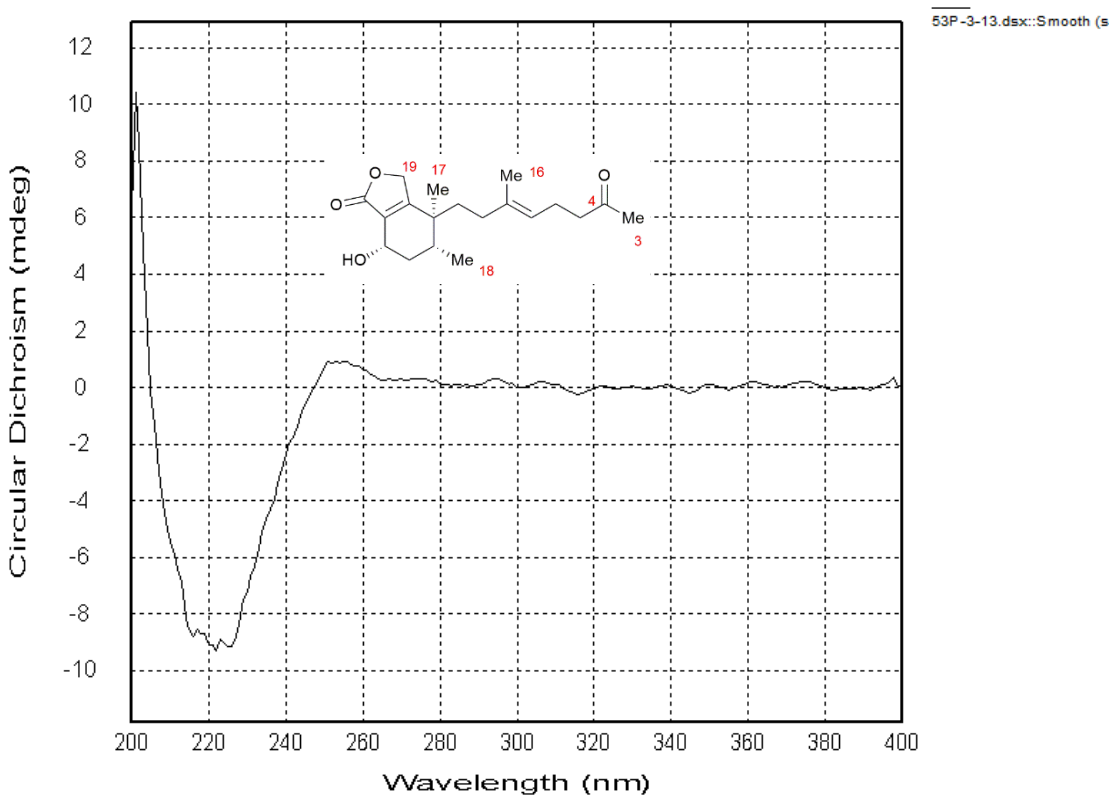

Figure S72. CD spectrum of **7**.

The details of the ECD calculations of compounds 1-7.

The conformers of compounds **1-7** was generated by Confab with 50kcal/mol cutoff energy.[1] Gaussian09 software package was used to perform DFT calculations.[2] The optimization and frequency calculation of conformers were performed on B3LYP/SVP level of theory with IEF-PCM solvent model (MeOH). The population of each conformer was calculated by Boltzmann distribution based on Gibbs free energy. Theoretical ECD (TDDFT) of compounds **1-7** were calculated on mPW1PW91/SVP level with IEF-PCM solvent model (MeOH) as well. SpecDis v1.71 was used to simulate the ECD curve with sigma/gamma value 0.3 eV.[3] The calculated ECD curve of each conformer was Boltzmann averaged based on their Gibbs free energy. The averaged calculated ECD curves of **1-7** were adjusted by blue or red shifting for 0 ~ 15 nm.

[1] N. M. O'Boyle, T. Vandermeersch, C. J. Flynn, A. R. Maguire, G. R. Hutchison, *J. Cheminform.* **2011**, *3*, 8.

[2] Gaussian 09, Revision A.02, 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. 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. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. 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.

[3]. Bruhn, T.; Schaumlöffel, A.; Hemberger, Y.; Bringmann, G. Chirality **2013**, *25*, 243–249.

Coordinates of the dominating conformers of **1**

1-c1, ΔG = 0.0000 kcal/mol, population = 87.09 %

O -0.928178 0.013382 -0.818941
C 0.057206 0.785016 -1.480395
H -0.389446 1.546137 -2.142052
C 0.836355 1.435878 -0.380223
C 1.929978 0.899873 0.191977
C 2.402988 1.851232 1.255662
H 2.487296 1.399099 2.254762
H 3.372238 2.311714 1.005334
O 1.398824 2.878199 1.306256
C 0.439449 2.618894 0.385875
O -0.578364 3.284218 0.310858
C 2.537300 -0.434995 -0.154313
C 3.985110 -0.199280 -0.639331
H 4.003395 0.349794 -1.592891
H 4.509503 -1.154662 -0.780704
H 4.557762 0.382641 0.098358
C 2.585732 -1.327207 1.127675
H 3.459216 -1.013608 1.723303
H 2.810228 -2.355971 0.803780
C 1.377193 -1.332704 2.093611
H 1.218510 -0.317062 2.484819
H 1.699032 -1.939224 2.960997
C 0.038986 -1.866795 1.619900
C -1.020152 -1.042839 1.563471
H -0.860556 0.006981 1.827506
C -2.453695 -1.337501 1.160626
H -2.711542 -2.354761 1.503436
C -2.731121 -1.352391 -0.362747
H -3.814238 -1.507417 -0.497513
H -2.224504 -2.237168 -0.780953
C -2.280658 -0.148031 -1.219630
C -2.420805 -0.503030 -2.703440
H -1.867895 -1.425334 -2.932286
H -3.479043 -0.665473 -2.958814
H -2.040916 0.302757 -3.349556
C -3.064965 1.156620 -0.957271
H -2.777831 1.901161 -1.720570
H -4.140063 0.956156 -1.091289
O -2.879497 1.702732 0.333454
H -2.063497 2.244406 0.334173
O -3.341956 -0.470532 1.848731
H -3.186674 0.423452 1.475594
C -0.011289 -3.327636 1.253499
H -1.038911 -3.692462 1.114632
H 0.470791 -3.945773 2.030698
H 0.534955 -3.528138 0.315196
C 1.660734 -1.131858 -1.254851
H 0.815535 -1.582488 -0.719262
C 2.389991 -2.248933 -2.002271
H 2.872356 -2.961795 -1.315982
H 1.673261 -2.817199 -2.615261
H 3.164630 -1.856586 -2.679186
C 1.020062 -0.136666 -2.236063
H 1.783877 0.470168 -2.751252
H 0.468729 -0.689465 -3.010241

1-c7, ΔG = 1.6780 kcal/mol, population = 5.11 %

O -1.017005 -0.436660 -0.785320
C -0.151734 0.342790 -1.598892
H -0.712275 0.921462 -2.350892
C 0.577269 1.261846 -0.667591
C 1.740196 0.949533 -0.065785
C 2.146587 2.118890 0.786183
H 2.279443 1.869363 1.848839
H 3.068400 2.602926 0.426702
O 1.062445 3.052864 0.674217
C 0.118742 2.556466 -0.159121
O -0.922400 3.155180 -0.370580
C 2.527825 -0.319977 -0.259690
C 3.884777 0.094788 -0.879463
H 4.427358 0.781437 -0.212395
H 3.746033 0.600655 -1.847122
H 4.525539 -0.783224 -1.035829
C 2.819732 -0.978834 1.128638
H 3.144206 -0.186862 1.822736
H 3.704728 -1.623667 1.005664
C 1.733705 -1.849255 1.802504
H 2.159143 -2.141197 2.781430
H 1.625019 -2.785321 1.234126
C 0.355574 -1.250982 2.031669
C -0.707918 -1.834491 1.454122
H -0.506892 -2.730630 0.854633

C -2.186435 -1.496484 1.475485
H -2.661370 -2.311138 2.061340
C -2.835913 -1.629536 0.073461
H -3.928754 -1.560278 0.194266
H -2.627355 -2.653242 -0.276067
C -2.396358 -0.651205 -1.050181
C -2.616189 -1.309676 -2.416955
H -2.305147 -0.647273 -3.239243
H -2.037507 -2.242429 -2.483057
H -3.679855 -1.552215 -2.564393
C -3.174599 0.680973 -1.027312
H -2.899643 1.275008 -1.915085
H -4.249686 0.452530 -1.116073
O -2.967181 1.448807 0.141715
H -2.275923 2.117992 -0.048345
O -2.532450 -0.300114 2.134216
H -2.576011 0.417905 1.465492
C 0.291209 -0.019145 2.906763
H 1.172296 0.041312 3.565987
H -0.618426 -0.004160 3.517094
H 0.266405 0.904464 2.306821
C 1.728047 -1.291288 -1.194283
H 0.984738 -1.779230 -0.555361
C 2.590231 -2.392103 -1.812109
H 3.275953 -2.001809 -2.580233
H 3.195204 -2.912429 -1.053196
H 1.947824 -3.144581 -2.295652
C 0.895241 -0.560204 -2.261894
H 1.533164 0.048299 -2.925630
H 0.384799 -1.302592 -2.893520

1-c2, ΔG = 1.8957 kcal/mol, population = 3.54 %

O -1.034096 -0.464947 0.509946
C -0.004810 -1.118865 1.237291
H -0.388043 -2.008183 1.766081
C 0.959966 -1.517665 0.168133
C 2.003244 -0.771825 -0.235001
C 2.652831 -1.483650 -1.389938
H 2.698196 -0.878882 -2.308407
H 3.672352 -1.830738 -1.157844
O 1.818828 -2.626769 -1.640155
C 0.787494 -2.639039 -0.758864
O -0.103280 -3.464584 -0.816323
C 2.432706 0.541422 0.368410
C 3.829700 0.334417 0.998796
H 4.243162 1.289806 1.350641
H 4.536947 -0.078925 0.264356
H 3.783303 -0.357999 1.852739
C 2.562212 1.621949 -0.749607
H 3.469177 1.396447 -1.335170
H 2.772589 2.583125 -0.254588
C 1.406537 1.800604 -1.762980
H 1.260745 0.864738 -2.323762
H 1.762396 2.546167 -2.497763
C 0.066138 2.249875 -1.218050
C -0.999879 1.435775 -1.309501
H -0.862067 0.475262 -1.814568
C -2.369224 1.655119 -0.710721
H -2.283972 2.305999 0.172612
C -3.055663 0.338909 -0.299743
H -3.073603 -0.332607 -1.173629
H -4.100377 0.573201 -0.043855
C -2.416829 -0.441422 0.864888
C -2.649602 0.239774 2.214657
H -2.202959 -0.340811 3.036128
H -2.207464 1.246260 2.226344
H -3.727275 0.332521 2.417601
C -2.977515 -1.879776 0.905098
H -2.548397 -2.405340 1.780945
H -4.064108 -1.817119 1.081297
O -2.779105 -2.603028 -0.281941
H -1.833754 -2.830296 -0.372404
O -3.229462 2.380220 -1.602095
H -3.230573 1.904001 -2.445173
C 0.028497 3.619113 -0.590212
H -0.979423 3.907825 -0.265722
H 0.375003 4.374449 -1.316948
H 0.704010 3.695111 0.277809
C 1.376642 0.989593 1.441466
H 0.554061 1.441239 0.876729
C 1.907266 2.037670 2.421178
H 1.074234 2.457629 3.006000
H 2.627340 1.607400 3.134585
H 2.404012 2.875735 1.908949
C 0.734505 -0.183197 2.198821
H 1.493465 -0.770351 2.744324
H 0.038952 0.211175 2.952200

1-c3, ΔG = 2.0055 kcal/mol, population = 2.94 %

O -0.934848 -0.061958 -0.926782
C -0.067005 0.991864 -1.313284
H -0.613977 1.807197 -1.807383
C 0.652472 1.496188 -0.091532
C 1.799894 0.960366 0.370862
C 2.227002 1.743360 1.579133
H 2.328634 1.135825 2.491084
H 3.175965 2.279590 1.419178
O 1.184673 2.706286 1.783613
C 0.244906 2.575446 0.817920
O -0.742665 3.288231 0.802906
C 2.544600 -0.200282 -0.237978
C 3.946891 0.301434 -0.654028
H 4.570318 -0.534660 -0.999971
H 4.468087 0.768324 0.194656
H 3.883712 1.043621 -1.464159
C 2.727453 -1.330907 0.824057
H 3.587145 -1.063144 1.460693
H 3.036645 -2.242117 0.287871
C 1.560418 -1.654406 1.783489
H 1.321798 -0.761972 2.380054
H 1.961762 -2.393967 2.501212
C 0.266170 -2.209977 1.224130
C -0.863378 -1.490329 1.329885
H -0.787390 -0.491161 1.770384
C -2.271637 -1.858133 0.924454
H -2.380843 -2.958905 0.970178
C -2.711889 -1.460608 -0.495833
H -3.801780 -1.612148 -0.551433
H -2.251504 -2.173725 -1.197167
C -2.358804 -0.052570 -1.009628
C -2.810407 0.093098 -2.465958
H -2.333220 -0.677462 -3.089751
H -3.902993 -0.018467 -2.544956
H -2.547792 1.085673 -2.855240
C -2.988129 1.056914 -0.144733
H -4.069795 0.847050 -0.067651
H -2.581320 0.991807 0.876144
O -2.814042 2.348184 -0.690190
H -2.084816 2.780580 -0.202485
O -3.201189 -1.261324 1.834232
H -2.892439 -1.448382 2.731698
C 0.343487 -3.572404 0.587861
H 0.874142 -4.284399 1.243236
H 0.912917 -3.535977 -0.357017
H -0.646489 -3.987966 0.353994
C 1.741999 -0.740445 -1.472572
H 0.953734 -1.382972 -1.060608
C 2.581880 -1.587636 -2.429580
H 3.145998 -2.373156 -1.903589
H 1.925110 -2.086801 -3.158907
H 3.302324 -0.978791 -2.997471
C 0.993306 0.370754 -2.227749
H 1.685584 1.150383 -2.588224
H 0.492193 -0.058480 -3.108674

1-c19, ΔG = 2.9022 kcal/mol, population = 0.65 %

O -1.034296 0.449443 -0.506717
C -0.013192 1.118910 -1.231717
H -0.407287 2.005762 -1.756513
C 0.947413 1.524984 -0.161807
C 1.999167 0.789466 0.237909
C 2.641803 1.504593 1.394672
H 2.693846 0.897407 2.311204
H 3.657504 1.863153 1.163282
O 1.795851 2.638156 1.648720
C 0.763706 2.641854 0.768315
O -0.135734 3.457759 0.828227
C 2.441208 -0.517776 -0.369346
C 3.836985 -0.296748 -0.997383
H 3.785325 0.396660 -1.850224
H 4.259906 -1.247647 -1.350137
H 4.539369 0.121963 -0.261318
C 2.577938 -1.599751 0.746082
H 3.481679 -1.367557 1.334058
H 2.797777 -2.557978 0.249383
C 1.421731 -1.789631 1.756526
H 1.267676 -0.856293 2.319310
H 1.782294 -2.533737 2.490507
C 0.084466 -2.249180 1.211294
C -0.989436 -1.448911 1.318381
H -0.864025 -0.495589 1.838876
C -2.357353 -1.678440 0.726898
H -2.263700 -2.335283 -0.157493

C -3.048890 -0.367741 0.304604
H -3.076789 0.300485 1.178550
H -4.094146 -0.597715 0.036682
C -2.415434 0.411440 -0.863440
C -2.639727 -0.276593 -2.211547
H -3.716103 -0.383052 -2.414931
H -2.200205 0.307348 -3.034458
H -2.185346 -1.277588 -2.219687
C -2.990700 1.844115 -0.909559
H -2.565618 2.369963 -1.787198
H -4.076332 1.770164 -1.087336
O -2.801761 2.573925 0.274746
H -1.858323 2.807236 0.369678
O -3.155246 -2.333606 1.721707
H -4.042190 -2.450924 1.351990
C 0.062433 -3.613774 0.571852
H 0.425347 -4.369761 1.289819
H 0.732196 -3.672864 -0.301812
H -0.943282 -3.914948 0.251433
C 1.390187 -0.972689 -1.444236
H 0.571946 -1.433913 -0.880975
C 1.931541 -2.012007 -2.427391
H 2.646949 -1.571758 -3.139414
H 2.437202 -2.846569 -1.918156
H 1.102908 -2.438705 -3.013593
C 0.736533 0.196114 -2.197456
H 1.489484 0.793912 -2.739722
H 0.045769 -0.202296 -2.953096

1-c15, ΔG = 3.2392 kcal/mol, population = 0.37 %

O -0.820734 -0.137048 -1.238301
C 0.131558 0.867960 -1.557435
H -0.312283 1.662549 -2.180196
C 0.761681 1.463383 -0.326026
C 1.821278 0.918086 0.303590
C 2.199712 1.819001 1.445777
H 2.121646 1.331712 2.430642
H 3.220908 2.220062 1.346991
O 1.272133 2.905890 1.389042
C 0.428767 2.743621 0.326855
O -0.397836 3.577857 0.040202
C 2.569445 -0.321807 -0.125662
C 4.012968 0.108807 -0.482461
H 4.028923 0.777089 -1.356504
H 4.631486 -0.770567 -0.709273
H 4.490371 0.635283 0.356648
C 2.653759 -1.353067 1.039865
H 3.477581 -1.045389 1.704745
H 2.972765 -2.316288 0.611471
C 1.422769 -1.560484 1.945643
H 1.189408 -0.617496 2.460985
H 1.744579 -2.262857 2.736662
C 0.143602 -2.101503 1.342482
C -0.956682 -1.331021 1.339976
H -0.855823 -0.311559 1.724812
C -2.349603 -1.670226 0.874432
H -2.508487 -2.760002 0.959097
C -2.707400 -1.293484 -0.572515
H -3.801817 -1.365977 -0.664797
H -2.276275 -2.054207 -1.240230
C -2.227549 0.069459 -1.107621
C -2.861465 0.337666 -2.474551
H -2.731615 -0.525272 -3.145259
H -3.935970 0.537978 -2.352752
H -2.405910 1.220448 -2.949498
C -2.559646 1.227781 -0.140405
H -1.889619 1.168961 0.732718
H -2.350368 2.188927 -0.631905
O -3.913544 1.222080 0.253913
H -3.980789 0.490855 0.898533
O -3.314018 -1.011723 1.719862
H -3.027982 -1.093914 2.640765
C 0.196288 -3.506428 0.805347
H 0.617089 -4.196367 1.556750
H 0.856853 -3.566860 -0.075981
H -0.789407 -3.883285 0.500286
C 1.851661 -0.947981 -1.371144
H 0.995588 -1.510286 -0.978059
C 2.725405 -1.921187 -2.164491
H 2.108037 -2.461894 -2.898514
H 3.520301 -1.401764 -2.721748
H 3.203833 -2.674373 -1.519653
C 1.242814 0.119954 -2.298512
H 2.010013 0.830779 -2.647505
H 0.810998 -0.367482 -3.185560

1-c5, ΔG = 3.6145 kcal/mol, population = 0.19 %

O 1.126342 -0.166062 -0.510448
C 0.253211 -1.101002 -1.139183
H 0.815052 -1.925516 -1.596423
C -0.660200 -1.596294 -0.059665
C -1.811624 -0.989379 0.286925
C -2.389677 -1.732328 1.458207
H -2.504183 -1.106323 2.356801
H -3.364134 -2.195135 1.236425
O -1.442639 -2.772740 1.743714
C -0.410586 -2.703658 0.869504
O 0.524368 -3.482563 0.926906
C -2.435700 0.191525 -0.413639
C -3.757486 -0.302337 -1.051204
H -4.409174 -0.773191 -0.300715
H -3.566481 -1.039772 -1.845059
H -4.314101 0.539110 -1.486522
C -2.793575 1.309439 0.613761
H -3.671243 0.969456 1.188417
H -3.144392 2.182115 0.040506
C -1.730138 1.761133 1.643846
H -1.449918 0.908208 2.281139
H -2.235601 2.489127 2.304242
C -0.470313 2.381351 1.081377
C 0.703794 1.738575 1.199894
H 0.715636 0.800798 1.761426
C 1.995357 2.108268 0.502407
H 1.765906 2.430456 -0.525921
C 2.977684 0.925283 0.437080
H 3.122675 0.559664 1.469163
H 3.949866 1.314668 0.102042
C 2.551319 -0.256116 -0.476777
C 3.114661 -0.118451 -1.891298
H 2.789630 0.832286 -2.340579
H 4.215127 -0.140860 -1.877305
H 2.769429 -0.945774 -2.528093
C 3.031328 -1.557716 0.196174
H 4.125160 -1.471915 0.333539
H 2.579579 -1.600787 1.203066
O 2.751381 -2.735412 -0.526058
H 1.968277 -3.141317 -0.103161
O 2.636116 3.243751 1.098466
H 2.644685 3.097911 2.055308
C -0.619820 3.692555 0.352091
H -1.138141 3.573956 -0.614558
H 0.352200 4.168312 0.170536
H -1.231986 4.390956 0.947820
C -1.449190 0.732675 -1.510472
H -0.725707 1.359030 -0.979357
C -2.127194 1.602694 -2.570744
H -2.769639 2.377757 -2.125813
H -1.362810 2.115821 -3.174768
H -2.746840 1.008805 -3.260691
C -0.605979 -0.369705 -2.171140
H -1.244576 -1.103324 -2.692967
H 0.052612 0.083367 -2.928034

1-c9, ΔG = 3.9326 kcal/mol, population = 0.11 %

O 1.150478 0.219487 -0.553537
C 0.423974 -0.734661 -1.330609
H 1.109482 -1.426086 -1.837384
C -0.395773 -1.441054 -0.304273
C -1.634747 -1.070326 0.066586
C -2.066234 -1.987047 1.179266
H -2.363010 -1.462364 2.098652
H -2.892363 -2.651905 0.880397
O -0.909900 -2.790983 1.469614
C 0.094892 -2.467633 0.617419
O 1.199342 -2.972973 0.698966
C -2.457549 0.022357 -0.573304
C -3.655831 -0.683692 -1.254196
H -3.316913 -1.398666 -2.019012
H -4.320135 0.048859 -1.732244
H -4.254526 -1.236640 -0.514544
C -3.029711 0.992964 0.513385
H -3.379639 0.393517 1.369297
H -3.943026 1.447320 0.098055
C -2.152430 2.162151 1.021884
H -2.761826 2.683347 1.783006
H -2.006042 2.884923 0.205501
C -0.806994 1.811854 1.629055
C 0.320080 2.238553 1.030784
H 0.203673 2.872189 0.145323
C 1.766683 1.921182 1.360256
H 2.167160 2.734317 1.993637
C 2.664766 1.879684 0.092850
H 3.717845 1.967969 0.404015
H 2.441830 2.771176 -0.514298

C 2.510217 0.607724 -0.780010
C 2.781911 0.906885 -2.252516
H 2.057239 1.637378 -2.640632
H 3.791728 1.329790 -2.366383
H 2.730943 -0.009086 -2.858760
C 3.461923 -0.501120 -0.267326
H 4.496389 -0.186573 -0.490701
H 3.371912 -0.560908 0.828602
O 3.244027 -1.759263 -0.868651
H 2.572491 -2.234439 -0.341269
O 1.908589 0.738347 2.135826
H 1.464481 0.051268 1.615197
C -0.855613 0.971311 2.887233
H -0.038559 1.212451 3.577131
H -0.767034 -0.106012 2.673456
H -1.814991 1.116801 3.408908
C -1.571495 0.803014 -1.603693
H -0.967493 1.496798 -1.011909
C -2.382526 1.635483 -2.597406
H -1.713410 2.310647 -3.153436
H -2.903395 1.007623 -3.337023
H -3.137342 2.260339 -2.095012
C -0.539137 -0.076504 -2.323362
H -1.027882 -0.874470 -2.908944
H 0.025597 0.539573 -3.037785

Coordinates of the dominating conformers of **2**

2-c2, ΔG = 0.0000 kcal/mol, population = 40.09 %

O -1.416418 0.205634 -0.318966
C -0.512576 0.733107 -1.277428
C 0.571702 1.294138 -0.414522
C 1.682072 0.632962 -0.056150
C 2.459318 1.510123 0.914345
O 3.714862 1.907524 0.502827
H 3.666942 2.214196 -0.416474
H 2.583937 1.042268 1.901327
O 1.595758 2.663408 1.114904
C 0.466148 2.527066 0.380890
O -0.452567 3.316399 0.447186
C 2.069989 -0.752472 -0.512701
C 3.359125 -0.648319 -1.361631
H 4.150339 -0.128234 -0.806000
H 3.731854 -1.649165 -1.620460
H 3.176681 -0.096839 -2.296694
C 2.384100 -1.641667 0.729780
H 3.349417 -1.308609 1.146684
H 2.569071 -2.662696 0.360446
C 1.376380 -1.687489 1.903813
C -0.014756 -2.218570 1.617229
C -1.080981 -1.411704 1.758442
C -2.523829 -1.692766 1.423107
H -2.602851 -2.539433 0.723023
H -3.057943 -2.016590 2.336595
C -3.288087 -0.471838 0.874592
H -4.360924 -0.714300 0.805339
H -3.195842 0.360915 1.588953
C -2.828174 0.066686 -0.494134
C -3.172960 -0.887489 -1.638212
H -4.257364 -1.073363 -1.668666
H -2.660224 -1.851180 -1.508719
H -2.878319 -0.468729 -2.612387
C -3.461487 1.448905 -0.759223
H -4.556096 1.324194 -0.796280
H -3.152449 1.794508 -1.766010
O -3.177287 2.407299 0.227713
H -2.224835 2.618997 0.212618
H -0.887186 -0.393931 2.112400
C -0.094048 -3.660540 1.185106
H -1.113823 -3.968639 0.918119
H 0.557449 -3.868288 0.320730
H 0.253964 -4.322720 1.998127
H 1.850881 -2.317612 2.679362
H 1.280660 -0.684567 2.347941
C 0.887501 -1.370296 -1.343443
H 0.163097 -1.731287 -0.605471
C 1.304208 -2.556368 -2.214895
H 0.408311 -3.066104 -2.602240
H 1.889828 -3.301907 -1.656108
H 1.904572 -2.239995 -3.081958
C 0.120184 -0.333383 -2.176306
H -0.654686 -0.841991 -2.765328
H 0.785546 0.171041 -2.898455
H -0.981565 1.529632 -1.880227

2-c1, ΔG = 0.5371 kcal/mol, population = 16.17 %

O -1.460681 0.515362 0.563419
C -0.698718 -0.383680 1.360651
C 0.254945 -1.120304 0.455993
C 1.481078 -0.666301 0.135491
C 2.127939 -1.656733 -0.821460
O 3.311884 -2.235529 -0.413500
H 3.219496 -2.544727 0.501316
H 2.317479 -1.218754 -1.810155
O 1.112073 -2.672792 -1.009455
C 0.021810 -2.386500 -0.265104
O -0.942788 -3.126081 -0.260614
C 2.135422 0.588791 0.666375
C 3.347362 0.157213 1.530711
H 3.853187 1.040937 1.942001
H 3.034114 -0.480137 2.372175
H 4.078550 -0.397752 0.929814
C 2.687726 1.443230 -0.519407
H 3.218791 0.768728 -1.210435
H 3.473333 2.100909 -0.114227
C 1.720103 2.349813 -1.313174
C 0.474384 1.717137 -1.898474
C -0.739690 2.122750 -1.492927
C -2.079948 1.579944 -1.907833
H -2.510098 2.235865 -2.688613
H -1.970730 0.591558 -2.380616
C -3.099972 1.520051 -0.752313
H -3.092418 2.492098 -0.230972
H -4.116246 1.396766 -1.159017
C -2.860352 0.411601 0.295622
C -3.661233 0.686580 1.569707
H -4.738090 0.747120 1.346784
H -3.340306 1.639521 2.016074
H -3.515388 -0.120782 2.300620
C -3.262382 -0.953537 -0.295784
H -2.616896 -1.172342 -1.163627
H -4.295042 -0.852265 -0.676140
O -3.224542 -2.010729 0.637193
H -2.432574 -2.543619 0.427190
H -0.784206 2.926909 -0.749000
C 0.650070 0.633288 -2.940637
H 0.124132 0.882665 -3.876383
H 1.708996 0.483215 -3.198421
H 0.243894 -0.335538 -2.604113
H 1.418019 3.194188 -0.675305
H 2.323199 2.789268 -2.129748
C 1.090062 1.383974 1.517256
H 0.436020 1.890457 0.800422
C 1.710729 2.459890 2.408624
H 0.919830 3.109556 2.814983
H 2.410868 3.102320 1.851937
H 2.254878 2.031199 3.264604
C 0.150444 0.462224 2.314522
H -0.522708 1.074331 2.933769
H 0.712936 -0.199053 2.995487
H -1.345950 -1.086623 1.902992

2-c3, ΔG = 0.7511 kcal/mol, population = 11.27 %

O -1.462139 -0.518267 -0.581636
C -0.700600 0.381483 -1.379558
C 0.247709 1.124872 -0.475016
C 1.472657 0.673729 -0.146183
C 2.098939 1.654282 0.827896
O 3.264194 2.210816 0.345205
H 3.731023 2.647407 1.072919
H 2.239697 1.210754 1.824969
O 1.085135 2.677324 0.999332
C 0.009134 2.395661 0.234453
O -0.952378 3.139947 0.209266
C 2.132441 -0.579324 -0.673356
C 3.336309 -0.140065 -1.544859
H 3.857117 -1.022064 -1.941686
H 3.006658 0.478628 -2.393263
H 4.050074 0.448753 -0.957510
C 2.690024 -1.427590 0.513779
H 3.218066 -0.748590 1.202990
H 3.479022 -2.082049 0.109997
C 1.727230 -2.338651 1.309660
C 0.477239 -1.713401 1.894231
C -0.734837 -2.117495 1.481042
C -2.076502 -1.577628 1.895804
H -2.504865 -2.233318 2.677817
H -1.969236 -0.588451 2.367550
C -3.097409 -1.520694 0.741105
H -3.089096 -2.493721 0.221573
H -4.113487 -1.398103 1.148557

C -2.860673 -0.414094 -0.309731
C -3.665104 -0.692791 -1.580818
H -3.520150 0.112050 -2.314642
H -4.741545 -0.751683 -1.355329
H -3.345862 -1.647447 -2.024689
C -3.261945 0.952720 0.278757
H -2.611147 1.176827 1.141380
H -4.291637 0.850362 0.666892
O -3.234024 2.005904 -0.658861
H -2.440307 2.541021 -0.459959
H -0.776392 -2.916340 0.731386
C 0.644751 -0.639622 2.948041
H 0.224748 0.327861 2.624758
H 0.126376 -0.907048 3.883205
H 1.702907 -0.479940 3.202930
H 1.430554 -3.185458 0.672537
H 2.332450 -2.773865 2.126927
C 1.091089 -1.382795 -1.521710
H 0.435943 -1.887462 -0.804823
C 1.717498 -2.461135 -2.406125
H 2.418327 -3.098521 -1.844514
H 2.262712 -2.034720 -3.262463
H 0.929781 -3.115336 -2.811587
C 0.152265 -0.467329 -2.326955
H -0.518107 -1.083829 -2.944972
H 0.716214 0.191226 -3.009158
H -1.348909 1.079796 -1.926739

2-c8, ΔG = 0.7624 kcal/mol, population = 11.05 %

O -1.363014 -0.051954 0.386504
C -0.501098 -0.754829 1.262180
C 0.554806 -1.306934 0.355455
C 1.686574 -0.661499 0.031712
C 2.452981 -1.520284 -0.962925
O 3.683384 -1.980590 -0.541047
H 3.605661 -2.313091 0.367156
H 2.617677 -1.019071 -1.926914
O 1.553291 -2.632269 -1.230245
C 0.423636 -2.498325 -0.498622
O -0.513591 -3.262127 -0.614166
C 2.102539 0.697716 0.542723
C 3.406258 0.547301 1.360766
H 3.236311 -0.037991 2.277580
H 4.180787 0.040044 0.770875
H 3.794714 1.533615 1.650673
C 2.396083 1.639849 -0.666431
H 3.383635 1.365478 -1.073639
H 2.523102 2.657524 -0.264589
C 1.416937 1.668049 -1.863616
C -0.006666 2.145520 -1.649868
C -1.027649 1.292356 -1.845202
C -2.509915 1.537089 -1.687838
H -2.759435 2.568904 -1.985489
H -3.044426 0.885795 -2.399011
C -3.104085 1.330419 -0.272144
H -2.728394 2.132495 0.384171
H -4.198600 1.453817 -0.328553
C -2.788164 0.002120 0.442675
C -3.321932 0.035502 1.874458
H -3.114649 -0.908251 2.396557
H -4.413303 0.176821 1.862291
H -2.874470 0.866990 2.438180
C -3.348100 -1.216491 -0.314240
H -2.964662 -1.195171 -1.349507
H -4.447416 -1.127904 -0.367085
O -3.037651 -2.441284 0.314997
H -2.159523 -2.738529 0.007208
H -0.758733 0.267089 -2.115947
C -0.176474 3.585702 -1.242005
H 0.244230 3.775547 -0.239462
H 0.362199 4.256463 -1.934409
H -1.230746 3.894469 -1.217237
H 1.891892 2.324794 -2.616560
H 1.375465 0.670171 -2.325655
C 0.943937 1.292818 1.420508
H 0.207019 1.689820 0.711442
C 1.386170 2.441415 2.328106
H 1.957160 3.208981 1.783548
H 2.008289 2.091329 3.166322
H 0.501422 2.935447 2.759028
C 0.185502 0.221838 2.220864
H -0.571526 0.705896 2.855062
H 0.861878 -0.334881 2.891986
H -1.023643 -1.563413 1.794381

2-c12, ΔG = 1.1458 kcal/mol, population = 5.78 %

O 1.366711 0.059089 0.387978
C 0.509962 0.750026 1.278753
C -0.544146 1.318949 0.381138
C -1.677884 0.682486 0.048329
C -2.420860 1.542330 -0.957743
O -3.625656 1.990736 -0.459531
H -4.162674 2.334453 -1.188675
H -2.539704 1.043748 -1.932941
O -1.518800 2.658130 -1.205657
C -0.401250 2.518663 -0.457741
O 0.539416 3.281783 -0.554097
C -2.102044 -0.677819 0.548390
C -3.397138 -0.520254 1.378746
H -3.804342 -1.505959 1.645013
H -3.205813 0.036539 2.308715
H -4.159445 0.027175 0.810616
C -2.412528 -1.607776 -0.665421
H -3.395951 -1.314155 -1.069770
H -2.556754 -2.625136 -0.268596
C -1.435528 -1.648010 -1.864556
C -0.014533 -2.134633 -1.653004
C 1.011374 -1.286099 -1.843349
C 2.492396 -1.540729 -1.688304
H 2.735229 -2.572167 -1.992757
H 3.030370 -0.888213 -2.395774
C 3.089550 -1.347122 -0.272008
H 2.704412 -2.147616 0.380836
H 4.182485 -1.483848 -0.329611
C 2.790389 -0.018356 0.449060
C 3.321566 -0.066534 1.881329
H 2.863487 -0.895259 2.440431
H 3.125891 0.877089 2.408063
H 4.411053 -0.221739 1.869102
C 3.367409 1.197883 -0.299172
H 2.987222 1.186428 -1.335927
H 4.465895 1.098253 -0.348682
O 3.068658 2.422359 0.336266
H 2.187929 2.724679 0.040629
H 0.748168 -0.257804 -2.108096
C 0.146950 -3.578205 -1.253636
H -0.281279 -3.772710 -0.255238
H -0.389985 -4.242135 -1.953956
H 1.199739 -3.891604 -1.223996
H -1.916922 -2.303255 -2.614733
H -1.387638 -0.651963 -2.329558
C -0.944604 -1.292412 1.414485
H -0.212424 -1.686404 0.699115
C -1.393150 -2.447894 2.310329
H -0.511110 -2.953013 2.734065
H -1.971085 -3.205334 1.759015
H -2.011037 -2.102230 3.153419
C -0.177145 -0.236773 2.225994
H 0.579192 -0.733448 2.851242
H -0.848092 0.314437 2.907039
H 1.037064 1.549209 1.820902

2-c16, ΔG = 1.4847 kcal/mol, population = 3.26 %

O -1.432881 -0.136108 -0.251047
C -0.702974 0.652709 -1.190394
C 0.306968 1.363028 -0.346185
C 1.512951 0.861892 -0.033651
C 2.145903 1.773823 1.000066
O 3.346206 2.305735 0.584116
H 3.809125 2.681417 1.347528
H 2.235744 1.273534 1.978941
O 1.159429 2.827216 1.198082
C 0.069201 2.583685 0.438839
O -0.911998 3.301536 0.469898
C 2.115082 -0.403136 -0.597501
C 3.315061 0.006855 -1.486716
H 4.009401 0.649058 -0.931907
H 3.861914 -0.884058 -1.826082
H 2.974545 0.562265 -2.373682
C 2.658407 -1.303334 0.553512
H 3.548417 -0.805645 0.974210
H 3.040165 -2.226910 0.090487
C 1.736842 -1.667104 1.744583
C 0.457792 -2.413091 1.422920
C -0.731751 -1.821672 1.625091
C -2.097334 -2.302891 1.194251
H -2.020025 -2.881413 0.258636
H -2.512519 -3.003849 1.942353
C -3.115779 -1.160698 1.028611
H -4.125814 -1.581661 0.907247
H -3.133413 -0.589923 1.973113
C -2.854227 -0.172523 -0.140108
C -3.479253 -0.650138 -1.450496

H -3.257421 0.051708 -2.267486
H -4.573639 -0.720490 -1.356438
H -3.086572 -1.641776 -1.721950
C -3.412496 1.200498 0.290260
H -2.929249 1.468751 1.246065
H -4.492368 1.077057 0.491399
O -3.242124 2.234595 -0.654661
H -2.447756 2.732276 -0.379277
H -0.716783 -0.827539 2.082166
C 0.619524 -3.799175 0.852999
H 1.076933 -4.468458 1.603661
H -0.336761 -4.245473 0.547947
H 1.291900 -3.813084 -0.020143
H 2.357812 -2.274978 2.428921
H 1.478091 -0.752978 2.301482
C 1.033380 -1.169795 -1.442407
H 0.419209 -1.713622 -0.718728
C 1.626141 -2.192050 -2.414755
H 2.115769 -1.710729 -3.275764
H 0.825831 -2.837213 -2.809614
H 2.367078 -2.847192 -1.932395
C 0.050523 -0.242586 -2.172495
H -0.672921 -0.852961 -2.734255
H 0.572036 0.395923 -2.906705
H -1.360000 1.358653 -1.713368

2-c13, ΔG = 1.4885 kcal/mol, population = 3.24 %

O 1.432734 0.108523 -0.232928
C 0.686954 -0.669716 -1.167577
C -0.334568 -1.355521 -0.317701
C -1.536152 -0.838141 -0.015095
C -2.200960 -1.752303 1.003072
O -3.415821 -2.302898 0.653308
H -3.354629 -2.670368 -0.242537
H -2.349423 -1.251704 1.971215
O -1.216968 -2.800166 1.230121
C -0.113005 -2.567981 0.486014
O 0.863899 -3.289203 0.539277
C -2.117182 0.436138 -0.582316
C -3.334699 0.053612 -1.459213
H -4.061910 -0.532666 -0.883082
H -3.845338 0.956132 -1.822275
H -3.023424 -0.540833 -2.331768
C -2.633404 1.352139 0.569872
H -3.532811 0.877939 0.997419
H -2.995327 2.283275 0.106059
C -1.697568 1.697433 1.754761
C -0.412909 2.429716 1.423809
C 0.771584 1.827227 1.622257
C 2.138748 2.289656 1.176108
H 2.059636 2.860220 0.235755
H 2.568724 2.992545 1.913924
C 3.142059 1.133983 1.012106
H 4.155462 1.541758 0.874680
H 3.163722 0.573635 1.962672
C 2.856246 0.135770 -0.142141
C 3.467728 0.593828 -1.465734
H 4.563803 0.654482 -1.386527
H 3.081264 1.586422 -1.742475
H 3.228576 -0.114051 -2.272557
C 3.406889 -1.238012 0.295621
H 2.940176 -1.487513 1.264607
H 4.492139 -1.126125 0.472635
O 3.203812 -2.282373 -0.631510
H 2.404632 -2.760815 -0.337389
H 0.749065 0.836484 2.086069
C -0.563031 3.814717 0.847957
H 0.398423 4.255852 0.551833
H -1.225954 3.829804 -0.032422
H -1.025268 4.487995 1.592004
H -2.305381 2.309757 2.446858
H -1.445361 0.777075 2.304768
C -1.022958 1.177293 -1.434343
H -0.400890 1.716255 -0.713650
C -1.597206 2.202709 -2.414392
H -2.092557 1.723998 -3.273659
H -0.785457 2.831989 -2.811323
H -2.328225 2.873026 -1.937777
C -0.053734 0.229524 -2.156306
H 0.677979 0.824599 -2.723476
H -0.584438 -0.407523 -2.885304
H 1.329798 -1.391696 -1.686495

2-c4, ΔG = 2.0959 kcal/mol, population = 1.16 %

O 1.466917 -0.908551 0.908104
C 0.708660 0.141647 1.487571

C -0.080986 0.985016 0.515308
C -1.362834 0.758264 0.171768
C -1.827739 1.889719 -0.734914
O -2.913878 2.623111 -0.305212
H -2.790107 2.866860 0.625557
H -2.065085 1.544566 -1.748900
O -0.662940 2.744388 -0.849890
C 0.348334 2.250986 -0.103323
O 1.410396 2.833184 -0.011834
C -2.224456 -0.381606 0.660358
C -3.377084 0.211705 1.509269
H -4.012208 -0.595968 1.896536
H -2.994544 0.785822 2.367074
H -4.009131 0.873436 0.904773
C -2.877714 -1.112956 -0.551840
H -3.363634 -0.352381 -1.185302
H -3.706149 -1.725145 -0.161501
C -1.996652 -2.034811 -1.417725
C -0.766003 -1.416611 -2.047972
C 0.458504 -1.803242 -1.654065
C 1.782193 -1.299065 -2.158410
H 2.444236 -2.164636 -2.331543
H 1.660325 -0.813529 -3.139071
C 2.512781 -0.301490 -1.233535
H 3.503581 -0.087330 -1.666722
H 1.985076 0.660075 -1.235450
C 2.726604 -0.748308 0.223466
C 3.334166 -2.152290 0.301828
H 4.236773 -2.223098 -0.322952
H 2.613418 -2.910105 -0.032027
H 3.607060 -2.385123 1.342892
C 3.689289 0.209148 0.976558
H 4.710742 -0.178976 0.837199
H 3.465356 0.105638 2.058742
O 3.732273 1.547573 0.560525
H 2.842307 1.947662 0.520330
H 0.513750 -2.558482 -0.865841
C -0.986266 -0.402215 -3.150361
H -0.733101 -0.828680 -4.136334
H -2.038851 -0.088393 -3.208265
H -0.368185 0.500097 -3.025440
H -1.692698 -2.907937 -0.821675
H -2.651133 -2.427154 -2.217806
C -1.332123 -1.338508 1.518320
H -0.722157 -1.912835 0.811508
C -2.127133 -2.342039 2.354274
H -2.883304 -2.870227 1.753005
H -2.643098 -1.861754 3.200036
H -1.447312 -3.100730 2.772154
C -0.318644 -0.563361 2.380422
H 0.217785 -1.261829 3.039371
H -0.823471 0.177465 3.021664
H 1.356351 0.804148 2.089013

2-c35, ΔG = 2.1524 kcal/mol, population = 1.06 %

O 1.350200 0.093613 0.594063
C 0.363517 0.596463 1.471188
C -0.688977 1.160214 0.566013
C -1.745381 0.468896 0.109467
C -2.559277 1.386435 -0.790304
O -3.828660 1.691294 -0.342083
H -3.790382 1.905754 0.603486
H -2.669807 1.003512 -1.814200
O -1.746044 2.587562 -0.889583
C -0.624749 2.447573 -0.143860
O 0.267888 3.270323 -0.156541
C -2.035220 -0.984391 0.393069
C -3.396066 -1.102851 1.115734
H -3.351156 -0.665105 2.125062
H -4.182522 -0.581717 0.554176
H -3.690570 -2.157119 1.212618
C -2.134317 -1.753516 -0.963718
H -3.131305 -1.552495 -1.390161
H -2.132009 -2.830043 -0.729600
C -1.107837 -1.458716 -2.084008
C 0.357120 -1.782352 -1.861356
C 1.266066 -0.791174 -1.860034
C 2.761600 -0.875964 -1.662849
H 3.159918 -1.775745 -2.162185
H 3.218258 -0.007970 -2.158898
C 3.263398 -0.927223 -0.200172
H 2.962577 -1.895024 0.234401
H 4.366377 -0.911996 -0.202368
C 2.760743 0.159521 0.771781
C 3.194770 -0.188694 2.198021
H 2.783860 0.521025 2.931972
H 4.291831 -0.153382 2.280454

H 2.864386 -1.201973 2.468641
C 3.260057 1.581190 0.433069
H 4.362870 1.560527 0.400876
H 2.978702 2.253943 1.266226
O 2.794191 2.087979 -0.793532
H 1.914490 2.471856 -0.633753
H 0.886577 0.228308 -1.973499
C 0.698534 -3.237669 -1.672016
H 0.275928 -3.851925 -2.486934
H 1.782659 -3.413876 -1.637771
H 0.271492 -3.634144 -0.734350
H -1.458740 -2.036454 -2.959990
H -1.180185 -0.401864 -2.380617
C -0.869071 -1.577425 1.262305
H -0.054549 -1.793969 0.560038
C -1.232361 -2.883117 1.970298
H -1.679588 -3.617898 1.283249
H -1.939338 -2.724440 2.799430
H -0.325089 -3.341027 2.394450
C -0.278254 -0.557174 2.249615
H 0.483880 -1.047914 2.871986
H -1.049603 -0.161189 2.932025
H 0.759674 1.379853 2.139428

2-c18, ΔG = 2.3299 kcal/mol, population = 0.78 %

O 1.440580 0.665250 -0.831506
C 0.616267 -0.339660 -1.398226
C -0.224002 -1.093383 -0.399026
C -1.488180 -0.776549 -0.063754
C -2.017779 -1.844720 0.881586
O -3.129423 -2.542955 0.458893
H -3.005856 -2.817853 -0.463332
H -2.256236 -1.449258 1.878532
O -0.892228 -2.745565 1.054619
C 0.150003 -2.331838 0.303237
O 1.199147 -2.943730 0.274617
C -2.249474 0.433155 -0.551053
C -3.484677 -0.033250 -1.357126
H -4.099207 0.832507 -1.640296
H -3.188670 -0.558675 -2.278140
H -4.110457 -0.708859 -0.760942
C -2.760447 1.280955 0.658263
H -3.729163 0.866989 0.982792
H -2.990882 2.285287 0.271209
C -1.891426 1.398846 1.931492
C -0.448760 1.837300 1.792248
C 0.536270 0.963927 2.064126
C 2.024815 1.158815 2.045825
H 2.291513 2.191271 1.781024
H 2.392402 1.009993 3.077696
C 2.782439 0.158069 1.150956
H 3.833643 0.099845 1.477470
H 2.371093 -0.851317 1.298831
C 2.786916 0.481987 -0.352648
C 3.436709 1.841255 -0.635194
H 4.424203 1.916979 -0.156602
H 2.801062 2.656129 -0.263932
H 3.557471 1.980802 -1.720728
C 3.579889 -0.577273 -1.155997
H 4.640915 -0.282637 -1.122343
H 3.269235 -0.481065 -2.217380
O 3.534676 -1.904606 -0.702996
H 2.626080 -2.198016 -0.497512
H 0.231262 -0.047905 2.360673
C -0.229998 3.276019 1.403604
H -0.838799 3.552694 0.527533
H -0.543614 3.948782 2.221713
H 0.818509 3.498331 1.166123
H -2.416572 2.114052 2.590753
H -1.908667 0.441450 2.471628
C -1.291242 1.288770 -1.451519
H -0.628171 1.831031 -0.766423
C -2.013310 2.320241 -2.319447
H -2.571101 1.848097 -3.142983
H -1.279167 3.006300 -2.769383
H -2.722472 2.932401 -1.741547
C -0.361095 0.411358 -2.304768
H 0.219999 1.042997 -2.992202
H -0.935411 -0.304759 -2.915568
H 1.213411 -1.060216 -1.981878

2-c36, ΔG = 2.4027 kcal/mol, population = 0.69 %

O 1.353957 0.098815 0.599633
C 0.369917 0.594635 1.484428
C -0.686079 1.163717 0.587261
C -1.741893 0.474471 0.127367

C -2.542260 1.390479 -0.780693
O -3.785482 1.668014 -0.251809
H -4.343038 2.057800 -0.941231
H -2.609760 1.014213 -1.813810
O -1.735715 2.598209 -0.864478
C -0.623118 2.458607 -0.106970
O 0.266368 3.285727 -0.103312
C -2.030663 -0.979848 0.405812
C -3.385169 -1.098099 1.139860
H -3.681477 -2.152509 1.231590
H -3.327093 -0.666679 2.150863
H -4.172520 -0.564236 0.593178
C -2.140430 -1.746014 -0.951343
H -3.137362 -1.536002 -1.373985
H -2.146541 -2.822774 -0.718401
C -1.115686 -1.459662 -2.075842
C 0.350208 -1.781242 -1.855751
C 1.257521 -0.788480 -1.854644
C 2.753981 -0.871138 -1.663079
H 3.151706 -1.769370 -2.165674
H 3.207240 -0.001656 -2.159835
C 3.262374 -0.924124 -0.202779
H 2.962484 -1.892104 0.232011
H 4.365359 -0.909962 -0.210078
C 2.764768 0.162147 0.772364
C 3.205060 -0.187850 2.196266
H 4.302516 -0.152437 2.273720
H 2.876132 -1.201468 2.467351
H 2.797437 0.520999 2.932857
C 3.263917 1.584057 0.433088
H 4.366222 1.561241 0.387536
H 2.993763 2.254450 1.271791
O 2.784344 2.096529 -0.785974
H 1.906613 2.479539 -0.613945
H 0.875866 0.230544 -1.964700
C 0.694060 -3.236384 -1.669363
H 0.276916 -3.849031 -2.488329
H 1.778340 -3.410556 -1.629931
H 0.262724 -3.636356 -0.735183
H -1.468880 -2.042620 -2.947456
H -1.188812 -0.404742 -2.378517
C -0.860128 -1.578487 1.265473
H -0.048356 -1.789453 0.558514
C -1.219145 -2.889414 1.966090
H -0.309357 -3.349800 2.382234
H -1.669692 -3.619704 1.276430
H -1.921790 -2.737223 2.800103
C -0.266359 -0.564999 2.257713
H 0.498840 -1.059220 2.873682
H -1.035518 -0.174745 2.945838
H 0.768266 1.374126 2.155882

2-c6, ΔG = 2.4159 kcal/mol, population = 0.68 %

O 1.701062 0.690200 -0.710048
C 0.866644 -0.272076 -1.363783
C -0.091323 -1.027948 -0.481680
C -1.372488 -0.674999 -0.269994
C -2.027038 -1.738197 0.600475
O -3.154546 -2.355170 0.091358
H -2.978264 -2.646770 -0.816778
H -2.309647 -1.344765 1.585035
O -0.981164 -2.707977 0.818611
C 0.151763 -2.337970 0.161411
O 1.140102 -3.032630 0.159309
C -2.074603 0.525854 -0.861187
C -3.145398 0.009346 -1.856132
H -3.658282 0.856969 -2.329951
H -2.697485 -0.607055 -2.650376
H -3.902667 -0.591491 -1.338225
C -2.828228 1.318955 0.248684
H -3.444110 0.605081 0.820140
H -3.553768 1.980825 -0.250282
C -1.999295 2.189855 1.212891
C -0.930246 1.475833 2.011732
C 0.369566 1.703951 1.760990
C 1.547980 1.058385 2.433513
H 2.288069 1.836855 2.684242
H 1.246848 0.611029 3.392940
C 2.242241 -0.041469 1.605012
H 3.107483 -0.409363 2.182278
H 1.570079 -0.900667 1.504436
C 2.763065 0.358451 0.212533
C 3.596513 1.639934 0.276995
H 4.090660 1.816308 -0.687832
H 4.369854 1.554913 1.055062
H 2.962911 2.507331 0.504776
C 3.605528 -0.785342 -0.377155

H 3.015837 -1.717740 -0.358213
H 4.490257 -0.941689 0.259990
O 4.066035 -0.494093 -1.685403
H 3.374396 0.023873 -2.122172
H 0.613912 2.410287 0.963035
C -1.401347 0.544477 3.108518
H -2.465609 0.289956 2.995554
H -0.829266 -0.394796 3.143063
H -1.299977 1.021464 4.098887
H -1.538761 3.016107 0.650932
H -2.717476 2.658342 1.910347
C -1.010390 1.405343 -1.595117
H -0.441826 1.924266 -0.814752
C -1.612282 2.475669 -2.506152
H -2.068823 2.043022 -3.409718
H -0.824683 3.170546 -2.836526
H -2.382296 3.069616 -1.990099
C 0.024931 0.548473 -2.344543
H 0.699155 1.201347 -2.918577
H -0.463852 -0.130175 -3.062526
H 1.487164 -1.004978 -1.908430

2-c9, ΔG = 2.4523 kcal/mol, population = 0.64 %

O 1.633244 0.673015 -0.730717
C 0.836786 -0.334226 -1.347835
C -0.105548 -1.056606 -0.416661
C -1.386371 -0.700151 -0.205957
C -2.026494 -1.721423 0.723467
O -3.134339 -2.390865 0.236362
H -2.943498 -2.713222 -0.658232
H -2.329312 -1.282604 1.682338
O -0.962950 -2.654400 1.006502
C 0.162323 -2.311131 0.320775
O 1.163250 -2.986094 0.373045
C -2.102509 0.468318 -0.845601
C -3.195844 -0.096300 -1.787785
H -3.933467 -0.680240 -1.223982
H -3.728583 0.725410 -2.285327
H -2.764193 -0.744783 -2.565456
C -2.827610 1.321032 0.239416
H -3.427150 0.640033 0.866163
H -3.567601 1.953346 -0.276329
C -1.977955 2.249425 1.130340
C -0.858032 1.605776 1.918925
C 0.424321 1.889415 1.636137
C 1.639765 1.320523 2.314262
H 2.383735 2.123163 2.450774
H 1.384400 0.972327 3.327360
C 2.308564 0.141811 1.576825
H 3.197786 -0.163420 2.154110
H 1.635343 -0.725049 1.589193
C 2.752859 0.393156 0.120695
C 3.615647 1.652896 0.010558
H 3.987128 1.773643 -1.018771
H 4.474297 1.603886 0.696669
H 3.027289 2.549957 0.245487
C 3.550836 -0.834174 -0.366577
H 2.958441 -1.744644 -0.208601
H 4.457952 -0.918321 0.261599
O 3.871427 -0.797988 -1.743203
H 4.427796 -0.025789 -1.910855
H 0.621146 2.581087 0.812469
C -1.249755 0.677448 3.050102
H -1.027210 1.131828 4.030859
H -2.328061 0.460924 3.042033
H -0.710751 -0.281900 3.015404
H -1.561929 3.059981 0.513671
H -2.679557 2.733598 1.834448
C -1.053900 1.309107 -1.644238
H -0.472350 1.865266 -0.900177
C -1.674388 2.330786 -2.597189
H -2.138235 1.853776 -3.474478
H -0.895920 3.014599 -2.969807
H -2.442834 2.944323 -2.101932
C -0.028103 0.417215 -2.362376
H 0.633528 1.038613 -2.983942
H -0.525530 -0.305002 -3.030347
H 1.485152 -1.062885 -1.857060

2-c11, ΔG = 2.5025 kcal/mol, population = 0.58 %

O -1.599212 0.899810 0.823544
C -0.763260 -0.050456 1.486508
C 0.085085 -0.919640 0.582073
C 1.366773 -0.652207 0.262986
C 1.926536 -1.817277 -0.538004
O 3.018893 -2.467749 -0.000876

H 2.857988 -2.645644 0.939037
H 2.205519 -1.530960 -1.559387
O 0.808546 -2.726563 -0.655325
C -0.266245 -2.233739 0.000110
O -1.313935 -2.848946 0.021217
C 2.152933 0.572313 0.667227
C 3.313496 0.126885 1.591522
H 2.940179 -0.386038 2.490879
H 3.993821 -0.553654 1.065236
H 3.895904 1.000443 1.913665
C 2.795787 1.227399 -0.594098
H 3.354593 0.447886 -1.137793
H 3.565914 1.932005 -0.242390
C 1.880867 1.997001 -1.567669
C 0.721359 1.228418 -2.166829
C -0.539809 1.537210 -1.822791
C -1.805852 0.882478 -2.299906
H -2.506216 1.672311 -2.622074
H -1.610467 0.272496 -3.195163
C -2.526795 -0.020324 -1.272013
H -3.495808 -0.317462 -1.706781
H -1.965393 -0.951704 -1.152217
C -2.811180 0.590905 0.117582
C -3.499878 1.953666 -0.028160
H -4.418961 1.867520 -0.626352
H -2.834327 2.675963 -0.517330
H -3.758988 2.353934 0.962967
C -3.770591 -0.293008 0.946553
H -4.713907 -0.365386 0.367411
H -4.008600 0.258188 1.871820
O -3.322808 -1.565909 1.344523
H -2.749970 -1.990208 0.677363
H -0.676578 2.347429 -1.102337
C 1.055260 0.152836 -3.179204
H 2.128470 -0.088755 -3.175652
H 0.496529 -0.779889 -3.008188
H 0.814982 0.487554 -4.203098
H 1.492628 2.895043 -1.064844
H 2.530878 2.362775 -2.383594
C 1.187223 1.552399 1.407111
H 0.563583 2.017302 0.634518
C 1.899279 2.678668 2.156879
H 2.418153 2.314627 3.057056
H 1.164827 3.431119 2.483664
H 2.639723 3.191849 1.523881
C 0.202864 0.799278 2.316576
H -0.390332 1.519176 2.899482
H 0.736699 0.154926 3.034458
H -1.370733 -0.700704 2.131295

2-c15, ΔG = 2.5370 kcal/mol, population = 0.55 %

O 1.642869 -0.671014 0.759114
C 0.849851 0.341568 1.375454
C -0.083436 1.067144 0.439681
C -1.360626 0.708488 0.213317
C -1.971070 1.699290 -0.760477
O -3.077600 2.342396 -0.238967
H -3.542601 2.795245 -0.957445
H -2.196973 1.232911 -1.730673
O -0.912349 2.647078 -1.016450
C 0.193515 2.321279 -0.293406
O 1.188892 3.007142 -0.317106
C -2.089210 -0.445206 0.863860
C -3.166838 0.150272 1.805720
H -3.726898 -0.657385 2.296970
H -2.712558 0.780616 2.584697
H -3.874373 0.770825 1.244871
C -2.830684 -1.296334 -0.210657
H -3.420180 -0.611524 -0.842751
H -3.580411 -1.912027 0.311357
C -1.996179 -2.246811 -1.093585
C -0.882176 -1.621020 -1.905292
C 0.402877 -1.871921 -1.604145
C 1.617878 -1.313545 -2.291562
H 2.353916 -2.123073 -2.432056
H 1.360021 -0.963042 -3.302984
C 2.301418 -0.142165 -1.555978
H 3.189253 0.156766 -2.138749
H 1.634525 0.729468 -1.563915
C 2.755260 -0.397559 -0.102864
C 3.611978 -1.662221 -0.002751
H 4.465019 -1.616073 -0.696180
H 3.016663 -2.555373 -0.235129
H 3.991982 -1.787612 1.022940
C 3.564426 0.824738 0.378459
H 2.976408 1.738737 0.224031
H 4.468293 0.902821 -0.255244

O 3.893413 0.787101 1.753097
H 4.441432 0.008503 1.918887
H 0.604545 -2.527097 -0.752708
C -1.286959 -0.753929 -3.079350
H -2.354923 -0.492830 -3.042513
H -0.709948 0.181656 -3.132650
H -1.128265 -1.284613 -4.034239
H -1.576148 -3.046344 -0.465176
H -2.706614 -2.741635 -1.781014
C -1.053770 -1.292615 1.672633
H -0.478456 -1.866962 0.937754
C -1.691124 -2.293578 2.636591
H -2.155869 -1.797360 3.502456
H -0.921972 -2.979168 3.025139
H -2.462721 -2.906653 2.145655
C -0.019689 -0.406407 2.387865
H 0.637470 -1.032282 3.009943
H -0.512093 0.318912 3.056194
H 1.502747 1.065600 1.885725

2-c17, ΔG = 2.6763 kcal/mol, population = 0.44 %

O -1.609855 -0.898732 -0.862995
C -0.771457 0.053732 -1.523194
C 0.064259 0.927029 -0.613055
C 1.340526 0.660442 -0.272310
C 1.865572 1.803258 0.574405
O 2.961845 2.420630 0.009656
H 3.387382 2.978847 0.676823
H 2.061767 1.491011 1.609975
O 0.752573 2.724375 0.653371
C -0.300246 2.239832 -0.039601
O -1.345400 2.859222 -0.093124
C 2.141290 -0.551511 -0.684448
C 3.285182 -0.079647 -1.617094
H 2.889395 0.409815 -2.519293
H 3.935217 0.638240 -1.104836
H 3.894935 -0.938780 -1.928531
C 2.801855 -1.207483 0.566503
H 3.355041 -0.425336 1.112303
H 3.578098 -1.899409 0.203565
C 1.901823 -1.998084 1.538146
C 0.747876 -1.240694 2.163235
C -0.514172 -1.514335 1.792161
C -1.781623 -0.866967 2.274325
H -2.475134 -1.661237 2.601021
H -1.588152 -0.253789 3.167530
C -2.514070 0.026568 1.245938
H -3.480574 0.321431 1.687564
H -1.958809 0.960216 1.118076
C -2.811376 -0.591752 -0.139003
C -3.492239 -1.956706 0.024302
H -3.757029 -2.367428 -0.960909
H -4.407032 -1.868374 0.628838
H -2.820404 -2.671614 0.515782
C -3.787515 0.283090 -0.959303
H -4.716237 0.369828 -0.358481
H -4.050884 -0.283303 -1.868291
O -3.344136 1.545338 -1.392843
H -2.768393 1.988669 -0.739993
H -0.651961 -2.289730 1.035006
C 1.095287 -0.227191 3.231988
H 0.470276 0.676632 3.181103
H 0.961154 -0.660135 4.238850
H 2.149154 0.083313 3.170769
H 1.509254 -2.886619 1.021816
H 2.561199 -2.377796 2.339800
C 1.188001 -1.540377 -1.429097
H 0.565289 -2.013780 -0.661346
C 1.915529 -2.657992 -2.177308
H 2.435736 -2.286355 -3.073496
H 1.190839 -3.417472 -2.509823
H 2.657956 -3.165087 -1.541728
C 0.201464 -0.796789 -2.343912
H -0.386599 -1.523320 -2.923916
H 0.733274 -0.154141 -3.064745
H -1.378055 0.697972 -2.174609

2-c21, ΔG = 2.7002 kcal/mol, population = 0.42 %

O -1.573459 0.496695 0.680474
C -0.721182 -0.484931 1.261326
C 0.226865 -1.140823 0.289607
C 1.497379 -0.748056 0.080939
C 2.153591 -1.723787 -0.883399
O 3.256337 -2.406808 -0.401943
H 3.054853 -2.755705 0.480655
H 2.471973 -1.246969 -1.820872

O 1.096585 -2.647545 -1.221705
C -0.034840 -2.346369 -0.526747
O -1.038781 -3.010732 -0.634879
C 2.167259 0.453184 0.707175
C 3.323409 -0.026014 1.617333
H 2.947122 -0.605334 2.474129
H 4.026149 -0.655839 1.057948
H 3.881191 0.836994 2.007193
C 2.781935 1.377480 -0.391087
H 3.779706 0.986557 -0.649356
H 2.968420 2.354240 0.080541
C 2.032266 1.578760 -1.727752
C 0.571552 1.973045 -1.683279
C -0.358820 1.089481 -2.082572
C -1.849664 1.236000 -2.166859
H -2.181839 2.209418 -1.779290
H -2.127555 1.231582 -3.237075
C -2.628597 0.088800 -1.494205
H -3.630190 0.019359 -1.948489
H -2.128504 -0.867709 -1.715881
C -2.819209 0.209579 0.032018
C -3.700881 1.412857 0.381521
H -3.855410 1.467850 1.469876
H -4.679128 1.348201 -0.118263
H -3.212981 2.349786 0.079468
C -3.473311 -1.087192 0.543112
H -2.839526 -1.943774 0.279121
H -4.432800 -1.212075 0.006713
O -3.651770 -1.133090 1.945956
H -4.259897 -0.427932 2.204204
H 0.003735 0.109434 -2.417736
C 0.274461 3.377843 -1.227451
H -0.791107 3.539411 -1.016061
H 0.841170 3.634590 -0.317790
H 0.581579 4.106958 -1.998509
H 2.595028 2.353010 -2.280659
H 2.121152 0.665676 -2.333722
C 1.094050 1.232885 1.542048
H 0.473605 1.772447 0.816031
C 1.681662 2.257986 2.513497
H 2.180378 1.776314 3.368960
H 0.875426 2.890162 2.916824
H 2.411803 2.925365 2.031282
C 0.133355 0.281306 2.269888
H -0.540122 0.855347 2.923239
H 0.685037 -0.429003 2.907997
H -1.319536 -1.251680 1.773402

2-c24, ΔG = 2.7673 kcal/mol, population = 0.37 %

O -1.418992 -0.386657 -0.530139
C -0.546594 0.139954 -1.514647
C 0.418367 1.001848 -0.757311
C 1.578457 0.561843 -0.242482
C 2.236483 1.716128 0.499864
O 3.463003 2.131243 0.024394
H 3.422448 2.209526 -0.941713
H 2.366375 1.512756 1.570866
O 1.264106 2.790549 0.407475
C 0.183546 2.378544 -0.293528
O -0.793142 3.086151 -0.439246
C 2.142885 -0.831618 -0.388726
C 3.446620 -0.727468 -1.218307
H 3.251822 -0.311074 -2.218782
H 4.178313 -0.082128 -0.715267
H 3.901311 -1.719444 -1.342213
C 2.524184 -1.395397 1.019887
H 3.070109 -0.609521 1.566508
H 3.270021 -2.190878 0.862690
C 1.425274 -2.000575 1.926939
C 0.184990 -1.175032 2.205398
C -1.020175 -1.614561 1.806643
C -2.343860 -0.905786 1.914070
H -2.886922 -1.283298 2.802198
H -2.204410 0.172344 2.066633
C -3.258414 -1.134836 0.692168
H -3.289192 -2.217949 0.482664
H -4.290486 -0.841386 0.941047
C -2.842726 -0.398521 -0.606968
C -3.321957 -1.169158 -1.840090
H -4.416710 -1.284029 -1.826493
H -2.869545 -2.171511 -1.855115
H -3.049830 -0.649948 -2.772540
C -3.418785 1.030373 -0.662902
H -4.516853 0.938291 -0.730406
H -3.085836 1.513491 -1.600268
O -3.110134 1.834106 0.449873
H -2.297942 2.323802 0.230732

H -1.061162 -2.589151 1.304093
C 0.354120 0.141830 2.931846
H 1.396775 0.306430 3.241441
H 0.045649 0.999743 2.311926
H -0.262703 0.182430 3.844207
H 1.111650 -2.968311 1.506490
H 1.928598 -2.237985 2.883097
C 1.080685 -1.740015 -1.097595
H 0.350693 -2.006056 -0.326630
C 1.660361 -3.042568 -1.649261
H 2.291935 -2.875156 -2.535580
H 0.843910 -3.717655 -1.950108
H 2.267167 -3.572519 -0.898560
C 0.259345 -0.992304 -2.162525
H -0.432661 -1.696296 -2.648443
H 0.905674 -0.574926 -2.953680
H -1.087975 0.733092 -2.269870

2-c14, ΔG = 2.7742 kcal/mol, population = 0.37 %

O 1.504571 0.632342 -0.838184
C 0.627970 -0.340814 -1.400696
C -0.232394 -1.067904 -0.392904
C -1.496479 -0.720583 -0.083581
C -2.079358 -1.774749 0.843346
O -3.175546 -2.463994 0.365241
H -3.011081 -2.732006 -0.552660
H -2.365743 -1.373818 1.825170
O -0.973020 -2.680970 1.076005
C 0.107693 -2.289845 0.364958
O 1.156429 -2.899437 0.436323
C -2.214114 0.519250 -0.559453
C -3.463100 0.112526 -1.375267
H -3.183389 -0.401885 -2.307525
H -4.110286 -0.557135 -0.795254
H -4.048976 1.003791 -1.639538
C -2.694979 1.365119 0.664933
H -3.682343 0.987444 0.977234
H -2.880196 2.385029 0.294730
C -1.830588 1.424833 1.946571
C -0.364487 1.785570 1.826964
C 0.567480 0.855111 2.097992
C 2.064501 0.965796 2.096156
H 2.389895 1.994213 1.889299
H 2.414591 0.742309 3.120356
C 2.781932 -0.025533 1.155495
H 3.826916 -0.137636 1.487542
H 2.324518 -1.018946 1.266809
C 2.821443 0.369075 -0.336161
C 3.546537 1.709667 -0.517407
H 4.540482 1.692288 -0.047107
H 2.961964 2.523196 -0.069317
H 3.663570 1.933905 -1.587923
C 3.605616 -0.661934 -1.174630
H 4.648938 -0.635899 -0.801375
H 3.634134 -0.288857 -2.213499
O 3.134348 -1.988306 -1.220447
H 2.571069 -2.221371 -0.458423
H 0.202170 -0.139770 2.382631
C -0.062719 3.215560 1.463042
H 0.999773 3.385360 1.245881
H -0.640953 3.537120 0.581624
H -0.354300 3.891682 2.286433
H -2.322775 2.161224 2.607813
H -1.904367 0.465290 2.477849
C -1.222514 1.355648 -1.438754
H -0.544661 1.862883 -0.741232
C -1.902062 2.425946 -2.293718
H -1.141214 3.091602 -2.729830
H -2.591731 3.054578 -1.709818
H -2.472327 1.986906 -3.127054
C -0.321494 0.455483 -2.295583
H 0.284089 1.070919 -2.976673
H -0.919009 -0.233644 -2.915332
H 1.195550 -1.080412 -1.982254

2-c20, ΔG = 2.7824 kcal/mol, population = 0.36 %

O 1.426153 0.187642 -0.535554
C 0.535991 -0.563435 -1.342338
C -0.432015 -1.183191 -0.379695
C -1.580404 -0.606084 0.011048
C -2.245609 -1.516943 1.032992
O -3.482946 -2.021819 0.690795
H -3.454402 -2.348694 -0.222137
H -2.360946 -1.039589 2.014893
O -1.289178 -2.593520 1.216466
C -0.210729 -2.395386 0.424659

O 0.754457 -3.132134 0.461449
C -2.127648 0.710063 -0.488869
C -3.441698 0.414235 -1.253441
H -3.884184 1.346855 -1.628347
H -3.263593 -0.251412 -2.112217
H -4.176541 -0.065946 -0.594402
C -2.485980 1.626852 0.727083
H -3.036526 1.019000 1.463191
H -3.222629 2.365791 0.373413
C -1.369186 2.429593 1.437715
C -0.137286 1.685067 1.912653
C 1.069217 1.986032 1.404360
C 2.384199 1.308503 1.683399
H 2.941625 1.894877 2.439464
H 2.231621 0.309303 2.111702
C 3.288773 1.197747 0.437894
H 3.332163 2.188595 -0.046163
H 4.319319 0.962450 0.747450
C 2.849134 0.155912 -0.622306
C 3.325449 0.571737 -2.016658
H 3.036205 -0.167650 -2.780041
H 4.421742 0.668789 -2.040979
H 2.886451 1.542764 -2.288727
C 3.404714 -1.247503 -0.308688
H 4.503101 -1.193965 -0.405973
H 3.054467 -1.952382 -1.085448
O 3.097812 -1.728925 0.977274
H 2.276995 -2.246330 0.899136
H 1.117817 2.795222 0.664831
C -0.316320 0.605602 2.958158
H 0.307288 0.795991 3.846685
H -1.358289 0.541667 3.304973
H -0.023145 -0.388391 2.581968
H -1.047010 3.249483 0.777693
H -1.858791 2.915537 2.302624
C -1.061219 1.385772 -1.417389
H -0.319219 1.831606 -0.747521
C -1.629398 2.508969 -2.284924
H -0.807315 3.069362 -2.757154
H -2.220485 3.225653 -1.693660
H -2.273092 2.126755 -3.092418
C -0.261933 0.373752 -2.256842
H 0.434018 0.915959 -2.914326
H -0.922595 -0.224889 -2.907236
H 1.060922 -1.341185 -1.920979

2-c26, ΔG = 2.8094 kcal/mol, population = 0.35 %

O 1.421576 -0.392107 0.546199
C 0.548988 0.137643 1.529710
C -0.413830 1.002710 0.773293
C -1.573202 0.564620 0.255656
C -2.213771 1.712029 -0.504365
O -3.420435 2.090618 0.043821
H -3.889157 2.657566 -0.586108
H -2.299105 1.503212 -1.581419
O -1.244919 2.790006 -0.401399
C -0.176705 2.381275 0.318866
O 0.795854 3.091828 0.482311
C -2.139590 -0.827320 0.401656
C -3.438924 -0.719190 1.237349
H -3.900321 -1.709249 1.353715
H -3.233949 -0.311063 2.238733
H -4.162111 -0.055702 0.747939
C -2.524049 -1.389517 -1.006496
H -3.068645 -0.602218 -1.552573
H -3.271756 -2.183189 -0.848833
C -1.427120 -1.998828 -1.914267
C -0.183583 -1.178740 -2.195846
C 1.019615 -1.617269 -1.789887
C 2.344729 -0.911448 -1.901096
H 2.886368 -1.293308 -2.788283
H 2.206692 0.166251 -2.057971
C 3.260061 -1.136124 -0.679050
H 3.290782 -2.218431 -0.465267
H 4.292069 -0.843700 -0.929677
C 2.845307 -0.394979 0.617586
C 3.333486 -1.156679 1.852906
H 2.886972 -2.161575 1.874544
H 3.060964 -0.634418 2.783542
H 4.428903 -1.265067 1.836568
C 3.414316 1.037160 0.664767
H 4.513373 0.950789 0.725295
H 3.084853 1.521505 1.602521
O 3.092961 1.836125 -0.448104
H 2.288882 2.333816 -0.217295
H 1.057647 -2.587471 -1.278824
C -0.345399 0.131848 -2.935279

H -1.386770 0.298394 -3.248209
H -0.033521 0.993971 -2.322749
H 0.273080 0.160347 -3.847082
H -1.116094 -2.966531 -1.491742
H -1.931595 -2.236842 -2.869678
C -1.078958 -1.739347 1.108077
H -0.348735 -2.005499 0.337586
C -1.660899 -3.042178 1.656888
H -0.845599 -3.718403 1.958638
H -2.266591 -3.570669 0.904211
H -2.294400 -2.875342 2.541891
C -0.257688 -0.994938 2.175322
H 0.433993 -1.700289 2.659983
H -0.904605 -0.578696 2.966543
H 1.091574 0.728688 2.285641

2-c30, ΔG = 3.0290 kcal/mol, population = 0.24 %

O -1.571445 0.491508 0.672345
C -0.733661 -0.512005 1.233538
C 0.218519 -1.147772 0.252203
C 1.491449 -0.753792 0.061016
C 2.149278 -1.704214 -0.927202
O 3.249242 -2.402710 -0.461658
H 3.044173 -2.776148 0.409981
H 2.471735 -1.201999 -1.849917
O 1.091828 -2.616184 -1.294446
C -0.042039 -2.331280 -0.596213
O -1.046152 -2.991520 -0.725337
C 2.162648 0.426405 0.725104
C 3.311919 -0.084416 1.626894
H 4.015212 -0.700362 1.052939
H 3.871065 0.764351 2.045017
H 2.928470 -0.687063 2.464259
C 2.787298 1.380257 -0.341922
H 3.785455 0.993685 -0.605306
H 2.973886 2.342225 0.159223
C 2.047132 1.623284 -1.676995
C 0.587557 2.021708 -1.630896
C -0.343147 1.153334 -2.061368
C -1.833029 1.306719 -2.151053
H -2.165342 2.270326 -1.739891
H -2.103810 1.330667 -3.222855
C -2.619366 0.145076 -1.513026
H -3.617818 0.089326 -1.975816
H -2.119364 -0.806850 -1.753884
C -2.820475 0.233466 0.014371
C -3.694150 1.433741 0.392035
H -4.650195 1.409752 -0.152781
H -3.177935 2.374555 0.155590
H -3.899757 1.411349 1.470185
C -3.484616 -1.061780 0.492141
H -2.854529 -1.920853 0.211282
H -4.443261 -1.162422 -0.051354
O -3.690752 -1.006097 1.894467
H -4.023091 -1.866443 2.181463
H 0.018551 0.181835 -2.421546
C 0.292161 3.413865 -1.136777
H 0.852038 3.641485 -0.215186
H 0.608711 4.164011 -1.883507
H -0.774569 3.573384 -0.929674
H 2.616541 2.411034 -2.203456
H 2.136675 0.727818 -2.308668
C 1.088577 1.186110 1.577383
H 0.475262 1.750953 0.864708
C 1.676011 2.177924 2.582973
H 0.870731 2.801753 3.000946
H 2.412413 2.855821 2.125516
H 2.167284 1.667490 3.425969
C 0.118139 0.218519 2.270659
H -0.556552 0.777026 2.936078
H 0.661886 -0.513444 2.890962
H -1.343940 -1.287562 1.718541

2-c28, ΔG = 3.2467 kcal/mol, population = 0.17 %

O -1.635162 -0.490650 -0.701663
C -0.735072 0.443442 -1.297551
C 0.234338 1.119477 -0.363288
C 1.499763 0.712654 -0.150838
C 2.176778 1.716413 0.764303
O 3.268724 2.310468 0.161502
H 3.785506 2.775246 0.835940
H 2.441912 1.279808 1.740576
O 1.152098 2.697990 1.037706
C 0.015724 2.393321 0.354636
O -0.962077 3.102619 0.396960
C 2.136929 -0.530286 -0.726378

C 3.274301 -0.115277 -1.690906
H 3.984212 0.553239 -1.190757
H 3.818927 -1.005898 -2.035514
H 2.880212 0.410339 -2.573486
C 2.768440 -1.408694 0.399267
H 3.779523 -1.022219 0.607206
H 2.925279 -2.410152 -0.028878
C 2.058250 -1.531721 1.767254
C 0.580071 -1.855955 1.783918
C -0.293663 -0.906743 2.160088
C -1.786398 -0.969638 2.288832
H -2.174406 -1.959239 2.011120
H -2.033782 -0.842025 3.358602
C -2.531378 0.139916 1.518972
H -3.504476 0.316982 2.004915
H -1.977736 1.087032 1.606823
C -2.825118 -0.143537 0.033642
C -3.715945 -1.378146 -0.126808
H -4.615313 -1.292691 0.501414
H -3.171740 -2.288286 0.159561
H -4.029508 -1.479057 -1.174211
C -3.512146 1.082289 -0.589760
H -2.861573 1.964689 -0.463673
H -4.441649 1.281871 -0.034551
O -3.874322 0.891447 -1.946297
H -3.137983 0.451067 -2.392292
H 0.125386 0.069287 2.434970
C 0.203231 -3.266105 1.410832
H -0.873736 -3.385946 1.232004
H 0.734590 -3.597241 0.503992
H 0.494566 -3.967590 2.212905
H 2.603499 -2.312156 2.328441
H 2.209534 -0.603498 2.336438
C 1.031858 -1.330131 -1.496886
H 0.405084 -1.807545 -0.733484
C 1.575093 -2.428723 -2.412160
H 2.074198 -2.015731 -3.302516
H 0.744857 -3.060222 -2.764714
H 2.292672 -3.086870 -1.899717
C 0.091350 -0.395033 -2.271725
H -0.598614 -0.987133 -2.890714
H 0.656250 0.267013 -2.947936
H -1.290656 1.228076 -1.838967

2-c34, ΔG = 3.3490 kcal/mol, population = 0.14 %

O 1.573567 -0.498597 0.678752
C 0.745011 0.509183 1.247812
C -0.202648 1.158946 0.271253
C -1.477000 0.772394 0.075382
C -2.115541 1.713813 -0.928351
O -3.186739 2.398990 -0.385798
H -3.683817 2.820904 -1.101875
H -2.395817 1.203095 -1.863433
O -1.055760 2.629181 -1.282748
C 0.067059 2.346864 -0.567094
O 1.071742 3.010208 -0.679182
C -2.156849 -0.403061 0.737836
C -3.290718 0.119212 1.652697
H -2.888048 0.694109 2.500085
H -3.970989 0.773387 1.095273
H -3.870387 -0.724306 2.053935
C -2.802670 -1.343709 -0.327367
H -3.791700 -0.933826 -0.590449
H -3.011503 -2.299921 0.175858
C -2.069663 -1.607482 -1.663161
C -0.613173 -2.017682 -1.619873
C 0.324037 -1.155608 -2.049181
C 1.812629 -1.320454 -2.141797
H 2.138652 -2.284599 -1.726873
H 2.080138 -1.351943 -3.214266
C 2.610640 -0.162123 -1.511822
H 3.606507 -0.114374 -1.981032
H 2.115627 0.792786 -1.752081
C 2.820371 -0.248491 0.014635
C 3.689856 -1.452953 0.389087
H 3.167837 -2.391453 0.156168
H 3.900985 -1.430548 1.466186
H 4.643385 -1.434446 -0.160418
C 3.494779 1.043554 0.486439
H 2.866778 1.905700 0.210899
H 4.449571 1.139186 -0.064857
O 3.712486 0.987432 1.887145
H 4.043312 1.849041 2.172084
H -0.030062 -0.180502 -2.406969
C -0.328614 -3.413179 -1.128697
H -0.886440 -3.636329 -0.204704
H -0.656003 -4.159271 -1.874818

H 0.737517 -3.583428 -0.927010
H -2.648138 -2.394804 -2.180182
H -2.153277 -0.717187 -2.302654
C -1.086822 -1.178921 1.579913
H -0.477698 -1.741031 0.861672
C -1.679021 -2.175984 2.577498
H -0.876958 -2.808272 2.989085
H -2.419745 -2.845631 2.114937
H -2.166612 -1.670681 3.425715
C -0.109600 -0.223487 2.280629
H 0.562293 -0.791622 2.940805
H -0.648215 0.507016 2.906857
H 1.363317 1.275901 1.736658

2-c5, ΔG = 3.6358 kcal/mol, population = 0.09 %

O 1.477979 0.851095 -0.944497
C 0.639560 -0.124464 -1.560576
C -0.148667 -0.989013 -0.608259
C -1.409442 -0.731392 -0.213766
C -1.882060 -1.876303 0.671049
O -3.010068 -2.556578 0.250327
H -2.913778 -2.783522 -0.687786
H -2.083566 -1.552904 1.700151
O -0.750454 -2.769578 0.724933
C 0.264586 -2.294698 -0.048178
O 1.293629 -2.911975 -0.190043
C -2.253014 0.448710 -0.639464
C -3.416630 -0.084723 -1.513265
H -3.045695 -0.631586 -2.393394
H -4.061141 -0.758348 -0.935481
H -4.036173 0.750398 -1.866573
C -2.894300 1.137472 0.602970
H -3.374716 0.357622 1.216485
H -3.724896 1.764521 0.242193
C -1.999983 2.027704 1.487797
C -0.774835 1.372664 2.088571
C 0.455169 1.733821 1.687038
C 1.761889 1.166289 2.165690
H 2.478765 1.991085 2.314262
H 1.636852 0.695262 3.153015
C 2.398990 0.119689 1.229481
H 3.361480 -0.184759 1.673442
H 1.778278 -0.785064 1.214205
C 2.685763 0.551661 -0.223157
C 3.475313 1.859941 -0.269664
H 3.704182 2.117665 -1.314687
H 4.420120 1.755439 0.280668
H 2.895300 2.685831 0.164139
C 3.486913 -0.548071 -0.956417
H 3.604309 -0.235378 -2.007315
H 2.928239 -1.495970 -0.938667
O 4.790240 -0.722451 -0.426168
H 4.728247 -1.314933 0.334000
H 0.529892 2.501467 0.911871
C -1.007218 0.339400 3.170842
H -0.741082 0.740681 4.164033
H -2.065056 0.043466 3.227259
H -0.407199 -0.571325 3.022971
H -1.690192 2.913776 0.914319
H -2.643184 2.404384 2.304248
C -1.347561 1.431343 -1.450642
H -0.710334 1.940856 -0.719025
C -2.125135 2.508226 -2.208348
H -1.429993 3.272237 -2.589931
H -2.856769 3.019315 -1.563599
H -2.667420 2.097073 -3.073934
C -0.373063 0.684494 -2.375880
H 0.181147 1.407853 -2.992270
H -0.911978 0.011487 -3.062691
H 1.228154 -0.776629 -2.226616

2-c10, ΔG = 3.9169 kcal/mol, population = 0.05 %

O -1.469710 -0.801083 -0.992199
C -0.632824 0.207113 -1.553056
C 0.150940 1.024098 -0.556070
C 1.409055 0.746454 -0.166951
C 1.876662 1.846007 0.776132
O 3.010725 2.542506 0.400321
H 2.923709 2.816571 -0.525991
H 2.067413 1.472038 1.790063
O 0.747286 2.739405 0.862443
C -0.262914 2.304329 0.059680
O -1.287401 2.932551 -0.064312
C 2.254643 -0.411762 -0.645744
C 3.423525 0.164531 -1.484949
H 4.045336 -0.651948 -1.875888

H 3.057484 0.754326 -2.339162
H 4.064567 0.808521 -0.870705
C 2.888331 -1.161823 0.564646
H 3.363921 -0.412971 1.219221
H 3.722267 -1.769133 0.178617
C 1.990627 -2.096149 1.399231
C 0.762217 -1.473910 2.027493
C -0.466043 -1.818921 1.606797
C -1.775264 -1.272453 2.103663
H -2.495974 -2.101073 2.206055
H -1.655974 -0.851462 3.114192
C -2.397376 -0.178173 1.214399
H -3.360516 0.128122 1.651622
H -1.761777 0.715966 1.239170
C -2.678186 -0.543069 -0.257353
C -3.457209 -1.854894 -0.371197
H -3.703406 -2.049608 -1.425879
H -4.390885 -1.801872 0.204449
H -2.855777 -2.697057 -0.002792
C -3.478599 0.583813 -0.932353
H -3.549261 0.349712 -2.013744
H -2.941586 1.538423 -0.819304
O -4.763044 0.652921 -0.336329
H -5.162840 1.495169 -0.587269
H -0.535984 -2.549208 0.795722
C 0.988495 -0.492092 3.158082
H 2.046368 -0.201163 3.236156
H 0.391072 0.425701 3.047831
H 0.713619 -0.937745 4.129726
H 1.684291 -2.952451 0.780474
H 2.631183 -2.512788 2.198239
C 1.353974 -1.351206 -1.511814
H 0.711632 -1.896909 -0.811356
C 2.136152 -2.388402 -2.318551
H 1.443261 -3.131524 -2.743090
H 2.863510 -2.931944 -1.695857
H 2.684137 -1.933809 -3.158456
C 0.385351 -0.557163 -2.404073
H -0.164092 -1.247731 -3.061064
H 0.928573 0.151085 -3.050835
H -1.222264 0.890855 -2.186471

Coordinates of the dominating conformers of **3**

3-c1, ΔG = 0.0000 kcal/mol, population = 83.43 %

C -0.614903 1.584914 1.985472
C 0.347177 2.416651 1.174777
C 1.674937 2.248558 1.035359
C 2.508868 3.276034 0.308215
H 1.885263 3.996449 -0.241060
H 3.215156 2.819637 -0.404489
H 3.132044 3.839486 1.025884
C 2.454339 1.127445 1.688552
C 3.169044 0.137943 0.748095
H 3.751372 0.694670 -0.004572
H 3.921408 -0.401192 1.343520
C 2.324002 -0.941325 0.013745
C 1.406177 -0.342497 -1.024126
C 0.131014 -0.711903 -1.249641
C -0.374693 0.007770 -2.432244
O -1.455694 -0.043367 -2.974004
O 0.623418 0.815371 -2.890547
C 1.790972 0.656728 -2.077344
H 2.622774 0.309880 -2.711321
H 2.061260 1.635455 -1.659227
C -0.632659 -1.702184 -0.420304
H -1.284871 -2.305022 -1.078528
C 0.367134 -2.592839 0.309377
H -0.178354 -3.197720 1.049542
H 0.814192 -3.294538 -0.413659
C 1.462271 -1.776998 1.016739
H 0.931684 -1.050340 1.647986
C 2.287010 -2.671374 1.944147
H 3.089321 -2.116263 2.452787
H 2.747772 -3.510628 1.400483
H 1.638154 -3.101569 2.722552
O -1.440092 -1.063901 0.568973
C -2.576448 -0.347850 0.110115
H -2.798195 -0.678406 -0.924651
O -3.653230 -0.647504 0.945033
C -4.090777 -1.987902 0.871563
H -4.379667 -2.259208 -0.161891
H -3.308897 -2.689296 1.209128
H -4.968573 -2.086913 1.525048
C -2.362067 1.171783 0.118531
C -3.559799 1.861668 -0.539552

H -4.473379 1.709844 0.055698
H -3.384377 2.944746 -0.630781
H -3.739728 1.460780 -1.549701
H -1.476766 1.360244 -0.508846
C -2.070756 1.730172 1.522921
H -2.331703 2.802754 1.530088
H -2.744974 1.245557 2.245757
C 3.320350 -1.844079 -0.759152
H 3.882967 -1.260239 -1.502256
H 4.051475 -2.290718 -0.070997
H 2.802340 -2.655093 -1.291057
H 1.821272 0.578643 2.397423
H 3.245578 1.596857 2.300927
H -0.093312 3.302158 0.696583
H -0.555642 1.903916 3.043766
H -0.334716 0.524606 1.965374

3-c2, ΔG = 1.4954 kcal/mol, population = 6.67 %

C -0.200278 -2.061603 -1.121216
C 1.089986 -2.566744 -0.538515
C 2.319486 -2.052915 -0.722520
C 3.533068 -2.708315 -0.110195
H 4.199858 -3.103820 -0.897075
H 3.256580 -3.538083 0.556482
H 4.142600 -1.994498 0.470558
C 2.607415 -0.852639 -1.601048
C 3.098626 0.420929 -0.884388
H 3.862342 0.152481 -0.136168
H 3.629972 1.043148 -1.619829
C 2.047029 1.338554 -0.197622
C 1.326271 0.620872 0.915001
C -0.000708 0.657014 1.147584
C -0.282078 -0.087104 2.389995
O -1.331866 -0.292556 2.957440
O 0.897915 -0.563035 2.874535
C 1.975522 -0.147442 2.029964
H 2.669200 0.474834 2.618499
H 2.514919 -1.038909 1.685976
C -0.999597 1.419335 0.322486
H -1.708045 1.919497 1.003804
C -0.249006 2.456042 -0.508511
H -0.943891 2.868733 -1.255004
H 0.052431 3.289549 0.146480
C 0.981182 1.862986 -1.216987
H 0.618315 0.984526 -1.771647
C 1.538611 2.852191 -2.242075
H 1.798888 3.816751 -1.779242
H 0.783192 3.053381 -3.017202
H 2.435791 2.465988 -2.747933
O -1.728602 0.588540 -0.588252
C -2.785327 -0.201634 -0.069040
H -2.698651 -0.224991 1.032852
O -4.030637 0.333662 -0.428656
C -4.335215 1.588200 0.137517
H -4.230800 1.574213 1.239555
H -3.691524 2.391070 -0.263824
H -5.379359 1.821701 -0.114550
C -2.719518 -1.629602 -0.623906
C -2.996501 -1.677061 -2.129244
H -2.941324 -2.711907 -2.502552
H -3.997568 -1.281762 -2.349061
H -2.266814 -1.074178 -2.689584
H -3.543838 -2.155926 -0.113171
C -1.411985 -2.340748 -0.220333
H -1.169008 -2.073130 0.820694
H -1.595128 -3.429091 -0.207989
C 2.826452 2.510581 0.450932
H 3.525330 2.141225 1.215399
H 3.420344 3.043839 -0.304582
H 2.149981 3.231011 0.933277
H 1.740808 -0.616001 -2.232057
H 3.409516 -1.148627 -2.300055
H 1.008341 -3.468093 0.083696
H -0.370393 -2.545188 -2.100892
H -0.140578 -0.986759 -1.321456

3-c4, ΔG = 1.7746 kcal/mol, population = 4.16 %

C 0.327410 2.165749 -0.956435
C -0.876245 2.690068 -0.222609
C -2.152737 2.290364 -0.370417
C -3.265990 2.951373 0.405310
H -3.945214 3.494587 -0.275716
H -2.879273 3.665705 1.146691
H -3.896342 2.217804 0.936938
C -2.595192 1.240468 -1.369636
C -3.180667 -0.066039 -0.795769

H -3.882472 0.169161 0.021039
H -3.801471 -0.530413 -1.576496
C -2.201242 -1.166185 -0.295287
C -1.377489 -0.691976 0.875798
C -0.058264 -0.903379 1.050687
C 0.335037 -0.366822 2.368071
O 1.415125 -0.345498 2.914997
O -0.774602 0.156900 2.958424
C -1.909838 -0.013426 2.104175
H -2.664595 -0.619694 2.630599
H -2.341229 0.973793 1.893596
C 0.834840 -1.589655 0.054425
H 1.568472 -2.226031 0.577309
C -0.032054 -2.426174 -0.880133
H 0.595353 -2.773369 -1.714563
H -0.379793 -3.322991 -0.342252
C -1.229410 -1.631984 -1.429876
H -0.807278 -0.718199 -1.873478
C -1.915121 -2.408711 -2.555593
H -2.243714 -3.405781 -2.223782
H -1.211442 -2.556230 -3.389192
H -2.792445 -1.878399 -2.954880
O 1.536664 -0.633643 -0.747454
C 2.670809 -0.055628 -0.169139
H 2.585014 -0.063454 0.932160
O 3.776505 -0.862596 -0.532588
C 4.886077 -0.764657 0.331071
H 5.620504 -1.519852 0.016382
H 5.370626 0.228668 0.287699
H 4.601686 -0.961674 1.382487
C 2.801395 1.399091 -0.640250
C 3.030468 1.501020 -2.148954
H 3.154661 2.550933 -2.458022
H 3.935730 0.946827 -2.436539
H 2.187312 1.076941 -2.713419
H 3.704284 1.783941 -0.135430
C 1.616149 2.242804 -0.122459
H 1.396635 1.931766 0.913542
H 1.931383 3.298109 -0.052427
C -3.068238 -2.343538 0.219106
H -3.697354 -2.027050 1.063627
H -3.739540 -2.703724 -0.572871
H -2.447509 -3.185096 0.558820
H -1.783885 1.009308 -2.072000
H -3.392884 1.697290 -1.982165
H -0.681772 3.499157 0.494236
H 0.470812 2.743468 -1.888706
H 0.161704 1.128071 -1.262989

3-c3, ΔG = 1.9020 kcal/mol, population = 3.35 %

C 0.799291 -1.559720 -1.875877
C -0.116552 -2.527628 -1.169999
C -1.440624 -2.385298 -0.976274
C -2.244213 -3.451332 -0.276189
H -2.690778 -3.078104 0.660404
H -1.624322 -4.324404 -0.024411
H -3.085356 -3.792844 -0.905394
C -2.227547 -1.214709 -1.528838
C -3.121331 -0.403777 -0.569993
H -3.791008 0.212869 -1.192175
H -3.788091 -1.078125 -0.010778
C -2.422782 0.542012 0.447947
C -1.422534 1.408917 -0.275117
C -0.135868 1.594552 0.075212
C 0.483478 2.545715 -0.866913
O 1.611101 2.982191 -0.909461
O -0.463408 2.909446 -1.778751
C -1.703118 2.257265 -1.483548
H -2.472605 3.022889 -1.294659
H -2.014992 1.672041 -2.362905
C 0.515943 0.944851 1.260731
H 1.239391 1.635310 1.722512
C -0.576769 0.547436 2.246508
H -0.121509 -0.048199 3.051964
H -0.994996 1.456613 2.709305
C -1.680588 -0.273104 1.558835
H -1.164880 -1.092529 1.039969
C -2.618362 -0.887108 2.600107
H -3.030212 -0.126399 3.281638
H -2.069078 -1.616813 3.214859
H -3.466278 -1.416743 2.140353
O 1.195412 -0.258086 0.892185
C 2.454253 -0.116688 0.311765
H 2.428353 0.630257 -0.504942
O 3.341200 0.355759 1.312241
C 4.374763 1.186970 0.829744
H 3.965839 2.058069 0.286335

H 4.948869 1.540427 1.698163
H 5.065949 0.646888 0.155043
C 2.887592 -1.480743 -0.238948
C 2.661243 -2.595282 0.786556
H 3.172608 -2.351121 1.730388
H 1.594822 -2.732559 1.006978
H 3.065265 -3.549785 0.414306
H 3.977918 -1.391622 -0.386382
C 2.304579 -1.760046 -1.641883
H 2.830667 -1.102385 -2.354610
H 2.580336 -2.790492 -1.927799
C -3.500328 1.471945 1.055397
H -3.946144 2.117720 0.284789
H -4.313808 0.880149 1.498047
H -3.078429 2.120376 1.837604
H -2.903429 -1.626469 -2.301670
H -1.554497 -0.532757 -2.065302
H 0.347258 -3.452720 -0.808678
H 0.521130 -0.526376 -1.621415
H 0.634229 -1.644380 -2.967176

3-c12, ΔG = 2.4303 kcal/mol, population = 1.37 %

C -0.357777 2.171853 -1.359415
C 0.982226 2.814491 -1.130461
C 2.190300 2.221721 -1.124816
C 3.435056 3.012953 -0.810028
H 4.168047 2.945786 -1.633323
H 3.944780 2.627940 0.089403
H 3.206877 4.074282 -0.634613
C 2.417385 0.776521 -1.516955
C 3.101232 -0.150284 -0.491244
H 3.617117 -0.947593 -1.050399
H 3.902772 0.388726 0.035252
C 2.201464 -0.847483 0.566084
C 1.102459 -1.612396 -0.126320
C -0.196866 -1.639007 0.232646
C -0.901991 -2.612328 -0.629233
O -2.050953 -2.983776 -0.614116
O -0.001429 -3.107036 -1.528905
C 1.289056 -2.543274 -1.289841
H 2.001689 -3.355689 -1.074462
H 1.629056 -2.026541 -2.201367
C -0.769556 -0.900705 1.412643
H -1.493226 -1.556258 1.925787
C 0.381072 -0.503858 2.335477
H -0.010345 0.198159 3.086799
H 0.738662 -1.392576 2.879600
C 1.534044 0.157808 1.555842
H 1.083549 0.945935 0.935740
C 2.518673 0.831604 2.512046
H 2.015369 1.646496 3.054880
H 3.376608 1.270205 1.981642
H 2.910545 0.128240 3.263347
O -1.419537 0.330072 1.079584
C -2.367653 0.359071 0.064572
H -1.972014 -0.123137 -0.852469
O -3.496628 -0.371169 0.491378
C -4.365992 -0.772703 -0.543342
H -4.886047 0.085003 -1.009257
H -3.825609 -1.333571 -1.325486
H -5.122233 -1.435476 -0.098979
C -2.680699 1.843030 -0.226926
C -3.607722 2.437109 0.836674
H -4.563911 1.898119 0.888175
H -3.137465 2.381537 1.831157
H -3.817647 3.495807 0.618516
H -3.199335 1.868165 -1.201785
C -1.390127 2.668369 -0.335527
H -1.656137 3.713593 -0.569210
H -0.919602 2.683921 0.659789
C 3.085035 -1.875949 1.314590
H 3.954580 -1.376158 1.764512
H 2.528407 -2.388100 2.112228
H 3.467959 -2.642367 0.625279
H 3.069415 0.796140 -2.408892
H 1.475335 0.323518 -1.855121
H 0.947887 3.888538 -0.904135
H -0.259929 1.080013 -1.298102
H -0.726145 2.389951 -2.380121

3-c19, ΔG = 3.3020 kcal/mol, population = 0.31 %

C -0.612071 1.606536 -1.754863
C 0.385353 2.599107 -1.216359
C 1.704174 2.393571 -1.043043
C 2.590059 3.455431 -0.444080
H 2.030902 4.379463 -0.236036

H 3.429936 3.701183 -1.117793
H 3.042214 3.117908 0.503826
C 2.403375 1.133282 -1.510724
C 3.202596 0.305857 -0.484244
H 3.862269 -0.370393 -1.052476
H 3.882564 0.959932 0.082688
C 2.408776 -0.566512 0.528705
C 1.415374 -1.427306 -0.211043
C 0.119924 -1.594563 0.113804
C -0.505079 -2.505824 -0.860860
O -1.649851 -2.887910 -0.944321
O 0.455579 -2.895376 -1.747657
C 1.705218 -2.280675 -1.414422
H 2.447112 -3.068188 -1.204163
H 2.058763 -1.704755 -2.283525
C -0.564524 -0.937193 1.274952
H -1.245303 -1.661017 1.756912
C 0.503951 -0.468008 2.258296
H 0.025065 0.168882 3.017173
H 0.913346 -1.344851 2.786816
C 1.630561 0.314652 1.562123
H 1.140567 1.108112 0.980737
C 2.534104 0.980403 2.602041
H 3.397737 1.485945 2.145064
H 2.921037 0.253316 3.333090
H 1.966704 1.740024 3.161620
O -1.310450 0.203985 0.860599
C -2.652003 0.043774 0.439133
H -2.932209 -1.024765 0.536138
O -3.476734 0.829210 1.251042
C -3.512293 0.434776 2.604562
H -3.806937 -0.627518 2.707192
H -2.534746 0.572693 3.098513
H -4.258125 1.060811 3.113905
C -2.821931 0.506538 -1.014361
C -4.301976 0.587718 -1.392504
H -4.827582 -0.354469 -1.165829
H -4.805406 1.393457 -0.838383
H -4.412708 0.785634 -2.470231
H -2.361754 -0.283713 -1.629954
C -2.057451 1.825300 -1.263106
H -2.609681 2.434283 -1.997150
H -2.054886 2.408395 -0.329078
C 3.416027 -1.506325 1.234671
H 4.223991 -0.923176 1.698706
H 2.928360 -2.106240 2.016829
H 3.879762 -2.199346 0.517166
H 3.128361 1.445629 -2.285025
H 1.687274 0.482019 -2.028765
H -0.018926 3.575512 -0.919175
H -0.291699 0.597022 -1.469551
H -0.605412 1.618062 -2.861752

3-c11, ΔG = 3.4337 kcal/mol, population = 0.25 %

C -1.245642 -0.210548 2.174175
C -0.617154 -1.550294 1.882161
C 0.690102 -1.865061 1.889218
C 1.145581 -3.290090 1.693128
H 0.292392 -3.968631 1.545891
H 1.718254 -3.643145 2.569642
H 1.814883 -3.400193 0.824271
C 1.778562 -0.852544 2.173874
C 2.904590 -0.687693 1.133082
H 3.663930 -0.025099 1.580764
H 3.417290 -1.649501 0.975978
C 2.534352 -0.109243 -0.263453
C 1.689485 1.127853 -0.095141
C 0.502264 1.362300 -0.684487
C 0.042101 2.711681 -0.313314
O -0.953346 3.314249 -0.643643
O 0.968054 3.254480 0.529625
C 2.054089 2.340362 0.714856
H 2.984115 2.818626 0.368423
H 2.161807 2.127562 1.790176
C -0.189504 0.391012 -1.596001
H -0.741499 0.942445 -2.377568
C 0.881707 -0.508665 -2.208698
H 0.390066 -1.290962 -2.806685
H 1.503499 0.086651 -2.898320
C 1.741566 -1.160483 -1.114399
H 1.027068 -1.628833 -0.426509
C 2.623427 -2.261598 -1.705745
H 1.993973 -3.073721 -2.101077
H 3.299087 -2.703771 -0.957839
H 3.242559 -1.889952 -2.537065
O -1.095897 -0.439450 -0.875072
C -2.474606 -0.133097 -0.883246

H -2.687309 0.461251 -1.799925
O -3.185132 -1.331183 -0.920440
C -3.017379 -2.076379 -2.108214
H -1.972529 -2.404230 -2.238179
H -3.666366 -2.960258 -2.038514
H -3.310160 -1.485119 -2.997018
C -2.924070 0.666851 0.341316
C -4.394387 1.068000 0.175890
H -5.045681 0.180798 0.195643
H -4.709448 1.744925 0.984960
H -4.562363 1.586605 -0.781928
H -2.321766 1.587467 0.325593
C -2.700120 -0.036599 1.691804
H -3.236009 0.567362 2.441694
H -3.209553 -1.014542 1.675535
C 3.845474 0.310886 -0.969790
H 4.545295 -0.534983 -1.019038
H 3.656374 0.663156 -1.994884
H 4.349253 1.120113 -0.421167
H 2.275071 -1.153131 3.115637
H 1.327523 0.126876 2.381790
H -1.328073 -2.365010 1.695976
H -0.625245 0.608567 1.779874
H -1.241103 -0.073729 3.272135

3-c17, ΔG = 3.6515 kcal/mol, population = 0.17 %

C 1.268088 -1.767016 -1.681203
C 0.479652 -2.941852 -1.176936
C -0.838043 -3.007630 -0.903947
C -1.441222 -4.284942 -0.372101
H -2.274801 -4.627571 -1.010691
H -1.862268 -4.149705 0.638544
H -0.695081 -5.090780 -0.315492
C -1.825685 -1.889005 -1.180877
C -2.718391 -1.425314 -0.007279
H -3.695911 -1.116900 -0.411396
H -2.942056 -2.270618 0.659655
C -2.181611 -0.252031 0.857118
C -1.985913 0.962639 -0.017291
C -0.899565 1.754302 -0.037781
C -1.092330 2.819386 -1.036703
O -0.354902 3.714928 -1.373116
O -2.335994 2.658000 -1.580169
C -2.975589 1.512514 -1.006450
H -3.922704 1.826538 -0.538425
H -3.212971 0.797766 -1.810650
C 0.349710 1.491336 0.738198
H 0.824075 2.442284 1.039342
C -0.019961 0.632046 1.952606
H 0.896306 0.318593 2.467260
H -0.604280 1.246962 2.658382
C -0.812708 -0.613097 1.521457
H -0.210913 -1.093547 0.739119
C -0.933976 -1.609609 2.675117
H 0.066105 -1.965912 2.967137
H -1.529912 -2.492779 2.399733
H -1.395596 -1.155445 3.565905
O 1.203990 0.790133 -0.167504
C 2.593885 0.840217 -0.011104
H 2.957248 1.872021 -0.197638
O 2.984201 0.452273 1.288725
C 3.577003 1.451858 2.092661
H 2.902304 2.311723 2.254534
H 3.799904 0.995948 3.067588
H 4.520968 1.823928 1.655807
C 3.182847 -0.135650 -1.042705
C 4.708426 -0.151776 -0.934257
H 5.148269 -0.767403 -1.733717
H 5.131576 0.862700 -1.017214
H 5.023036 -0.570728 0.034071
H 2.906629 0.259489 -2.035661
C 2.565503 -1.541649 -0.878797
H 3.307831 -2.301651 -1.176201
H 2.374473 -1.713340 0.192796
C -3.255215 0.098168 1.913154
H -3.497112 -0.784368 2.521790
H -2.911906 0.898943 2.584535
H -4.186397 0.434520 1.433231
H -2.500745 -2.260935 -1.972952
H -1.308972 -1.021673 -1.616433
H 1.070036 -3.849680 -0.991563
H 0.664548 -0.854224 -1.644070
H 1.539466 -1.923978 -2.743325

3-c7, ΔG = 3.7431 kcal/mol, population = 0.15 %

C -0.525266 2.962395 0.085830

C 0.708676 3.460811 -0.630827
C 1.688985 2.684195 -1.130417
C 2.890657 3.258424 -1.832144
H 2.854735 4.356987 -1.877991
H 2.966783 2.869717 -2.863501
H 3.827062 2.967989 -1.324163
C 1.626094 1.178719 -1.040693
C 2.761676 0.501464 -0.238876
H 3.568070 0.171854 -0.913152
H 3.221392 1.221209 0.456830
C 2.268121 -0.709219 0.613857
C 1.349118 -1.546738 -0.237409
C 0.035340 -1.751849 -0.025733
C -0.491882 -2.608785 -1.104755
O -1.607260 -3.036957 -1.290205
O 0.536181 -2.889003 -1.957750
C 1.739521 -2.271271 -1.493118
H 2.495135 -3.053032 -1.315579
H 2.123615 -1.596631 -2.275273
C -0.705561 -1.234146 1.173571
H -1.497422 -1.944636 1.457127
C 0.311756 -1.047752 2.295778
H -0.192898 -0.591578 3.161074
H 0.680019 -2.037218 2.613810
C 1.475142 -0.146954 1.851593
H 1.009566 0.788131 1.510484
C 2.368954 0.213705 3.039487
H 1.782393 0.759659 3.794486
H 3.208013 0.861467 2.742689
H 2.787093 -0.679826 3.528146
O -1.300453 0.052844 0.950887
C -2.348267 0.125021 0.031201
H -2.035017 -0.305351 -0.942445
O -3.422599 -0.639888 0.538104
C -4.283695 -1.188194 -0.438592
H -4.820744 -0.407258 -1.008462
H -3.727136 -1.830621 -1.141627
H -5.029182 -1.799164 0.090325
C -2.741479 1.597867 -0.175301
C -3.277932 2.228639 1.111564
H -2.508989 2.252916 1.896964
H -3.613803 3.261631 0.929441
H -4.129479 1.649062 1.495461
H -3.573608 1.553658 -0.899187
C -1.623463 2.419334 -0.853342
H -1.156381 1.794626 -1.633230
H -2.081219 3.268003 -1.389212
C 3.475490 -1.572368 1.031858
H 4.225785 -0.966228 1.557270
H 3.168727 -2.395195 1.695419
H 3.969248 -2.010931 0.152141
H 1.621236 0.768915 -2.066548
H 0.665041 0.889502 -0.605817
H 0.801449 4.546031 -0.761634
H -0.943972 3.780984 0.691533
H -0.256382 2.168599 0.795071

3-c13, ΔG = 3.8535 kcal/mol, population = 0.12 %

C 0.609894 1.578592 1.869331
C -0.290267 2.528239 1.118787
C -1.603868 2.360762 0.881426
C -2.400410 3.392357 0.124801
H -2.826693 2.977783 -0.804116
H -1.781765 4.259127 -0.150690
H -3.255747 3.751939 0.723975
C -2.387883 1.187975 1.431385
C -3.157669 0.284446 0.448710
H -3.825078 -0.354333 1.050734
H -3.830292 0.892371 -0.175857
C -2.338432 -0.645694 -0.489891
C -1.326926 -1.421266 0.315414
C -0.018435 -1.558597 0.025859
C 0.602659 -2.434638 1.038222
O 1.746062 -2.816761 1.147207
O -0.362725 -2.799209 1.928287
C -1.617940 -2.223930 1.551612
H -2.341679 -3.034609 1.369320
H -1.994011 -1.614344 2.388002
C 0.652304 -0.949565 -1.172751
H 1.370312 -1.670527 -1.591108
C -0.422186 -0.620731 -2.205080
H 0.042494 -0.033723 -3.011364
H -0.787501 -1.558704 -2.654930
C -1.584673 0.173676 -1.588773
H -1.127944 1.028389 -1.071441
C -2.499647 0.717387 -2.687749
H -2.846269 -0.079032 -3.364899

H -1.954799 1.453863 -3.298243
H -3.389397 1.221060 -2.281672
O 1.314805 0.278859 -0.863745
C 2.563768 0.245127 -0.209874
H 2.549493 -0.526504 0.581823
O 3.620643 -0.034723 -1.095740
C 3.935310 -1.391854 -1.345454
H 5.027408 -1.478050 -1.461821
H 3.610496 -2.040832 -0.514671
H 3.464156 -1.757006 -2.276205
C 2.817265 1.634511 0.390091
C 2.566592 2.743396 -0.637237
H 1.519335 2.764251 -0.963737
H 2.817228 3.727059 -0.209760
H 3.194691 2.585831 -1.527097
H 3.897064 1.636589 0.611954
C 2.117571 1.840886 1.749954
H 2.618421 1.183294 2.480857
H 2.330360 2.872331 2.082463
C -3.318261 -1.665351 -1.119626
H -3.763711 -2.312716 -0.350108
H -4.142546 -1.144434 -1.626873
H -2.813249 -2.310473 -1.853338
H -3.148305 1.608991 2.115300
H -1.737648 0.571015 2.065759
H 0.173766 3.450935 0.753623
H 0.393307 0.544486 1.567193
H 0.362244 1.625381 2.946943

Coordinates of the dominating conformers of **4**

4-c3, ΔG = 0.0000 kcal/mol, population = 44.88 %

O -4.041401 -1.487924 -0.202838
H -3.291126 -2.045428 -0.482874
C -3.688733 -0.138404 -0.449973
H -2.979889 -0.076623 -1.290845
H -4.598056 0.418287 -0.734943
C -3.067562 0.517311 0.799766
C -4.093836 0.573128 1.934555
H -4.933392 1.239943 1.682482
H -3.617441 0.940437 2.856063
H -4.498342 -0.432843 2.122380
C -2.508457 1.916393 0.504100
C -1.486621 1.951555 -0.648576
C -0.537481 3.118440 -0.608719
C 0.719264 3.104018 -0.124918
C 1.593069 4.330746 -0.153651
H 2.514724 4.148399 -0.733792
H 1.919238 4.605853 0.865026
H 1.076572 5.194479 -0.597893
C 1.348763 1.867622 0.475260
H 1.755584 2.130361 1.466603
C 2.477092 1.252816 -0.385039
H 3.446205 1.708431 -0.130803
H 2.307485 1.498515 -1.446009
C 2.608374 -0.291508 -0.262095
C 1.325501 -0.916288 -0.754539
C 0.581001 -1.815796 -0.083845
C -0.643053 -2.067656 -0.852771
O -1.608098 -2.753943 -0.566038
O -0.586900 -1.360294 -2.007421
C 0.639920 -0.615477 -2.057059
H 0.395376 0.447720 -2.194522
H 1.219743 -0.950783 -2.932031
C 0.934998 -2.408343 1.237714
C 2.425293 -2.169372 1.502416
H 2.668506 -2.426259 2.545065
H 3.025210 -2.841684 0.864701
C 2.821702 -0.707281 1.234240
C 4.231431 -0.411817 1.748970
H 4.977934 -1.087330 1.303177
H 4.271828 -0.550615 2.840431
H 4.541354 0.622450 1.535230
H 2.122385 -0.094367 1.825126
H 0.685788 -3.481686 1.251606
H 0.318211 -1.937781 2.024384
C 3.765220 -0.763495 -1.168692
H 3.924867 -1.848727 -1.084030
H 4.701704 -0.253261 -0.903178
H 3.553202 -0.535205 -2.224082
H 0.573879 1.112201 0.663059
H -0.920394 4.068059 -1.003725
H -0.928686 1.010045 -0.608873
H -2.018764 1.959329 -1.614127
H -2.019742 2.264179 1.429067
H -3.342792 2.609887 0.310108
O -1.951805 -0.282355 1.219188

H -2.248643 -1.205174 1.193911

4-c2, ΔG = 0.5968 kcal/mol, population = 16.37 %

O 4.005002 1.639378 -0.064377
H 3.260208 2.242529 -0.253381
C 3.676125 0.372795 -0.607737
H 2.999036 0.484289 -1.469936
H 4.602721 -0.109620 -0.962338
C 3.004701 -0.530968 0.450045
C 4.032071 -0.964962 1.499638
H 3.541433 -1.479945 2.337846
H 4.553146 -0.078867 1.894635
H 4.785162 -1.640362 1.063582
C 2.314716 -1.711534 -0.238820
C 1.570447 -2.654745 0.725318
C 0.524966 -3.510320 0.055899
C -0.770730 -3.184166 -0.113074
C -1.744891 -4.146910 -0.741813
H -2.184906 -3.742104 -1.668631
H -2.591459 -4.346612 -0.060670
H -1.265317 -5.106521 -0.984182
C -1.337235 -1.863529 0.370883
H -1.812100 -2.029878 1.355324
C -2.368451 -1.214298 -0.568700
H -3.351134 -1.695284 -0.449305
H -2.083885 -1.394139 -1.618442
C -2.534916 0.318497 -0.379775
C -1.227764 0.987184 -0.728375
C -0.605607 1.930366 0.003210
C 0.676680 2.240767 -0.639540
O 1.573105 2.977630 -0.270207
O 0.768114 1.531426 -1.792297
C -0.384193 0.690490 -1.933196
H -0.046922 -0.356815 -1.975409
H -0.884156 0.928525 -2.885513
C -1.115577 2.500739 1.282772
C -2.601940 2.155218 1.429402
H -2.937665 2.369838 2.455780
H -3.198449 2.803396 0.764447
C -2.885077 0.677106 1.103564
C -4.309273 0.285665 1.500296
H -4.535469 -0.761941 1.249204
H -5.059209 0.921351 1.004477
H -4.444888 0.402725 2.586596
H -2.194956 0.091544 1.732327
H -0.948664 3.589712 1.310086
H -0.533010 2.080650 2.122704
C -3.613351 0.816946 -1.367066
H -3.802036 1.893822 -1.247353
H -4.559681 0.278524 -1.215577
H -3.299433 0.644164 -2.407497
H -0.517332 -1.153674 0.551327
H 0.858597 -4.484852 -0.321790
H 2.298516 -3.307793 1.232939
H 1.109266 -2.039192 1.510419
H 3.053110 -2.272007 -0.836229
H 1.591076 -1.288903 -0.952417
O 1.968413 0.226974 1.088337
H 2.363859 1.086191 1.304376

4-c5, ΔG = 0.9570 kcal/mol, population = 8.91 %

O 3.415914 1.687249 -0.305791
H 2.782705 1.543106 -1.040525
C 4.117013 0.492984 -0.009946
H 4.385541 -0.068153 -0.922273
H 5.052173 0.788798 0.493283
C 3.296487 -0.404030 0.948983
C 4.213703 -1.382470 1.675076
H 3.641920 -2.019276 2.366492
H 4.963707 -0.831929 2.262934
H 4.735529 -2.036285 0.959067
C 2.201071 -1.134214 0.147194
C 1.097910 -1.814269 0.963838
C 0.165995 -2.600112 0.083250
C -1.178243 -2.660863 0.098435
C -1.904278 -3.598756 -0.836671
H -2.682492 -3.086174 -1.427058
H -2.429183 -4.384247 -0.264274
H -1.214601 -4.087982 -1.539478
C -2.061620 -1.920055 1.079133
H -2.645334 -2.684645 1.622610
C -3.083055 -0.930034 0.481305
H -3.915405 -0.827540 1.193177
H -3.537371 -1.364812 -0.423391
C -2.607289 0.512535 0.144530
C -1.511353 0.502248 -0.893433

C -0.356127 1.192610 -0.815913
C 0.424015 0.926925 -2.031937
O 1.543880 1.302142 -2.335721
O -0.295557 0.121477 -2.844753
C -1.548163 -0.198926 -2.220585
H -1.620056 -1.291422 -2.140070
H -2.365205 0.158162 -2.867558
C 0.035045 2.091484 0.308601
C -1.220103 2.473517 1.095049
H -0.936509 2.979162 2.030953
H -1.817987 3.198037 0.515611
C -2.075613 1.239499 1.428353
C -3.174387 1.598267 2.431002
H -2.722434 1.933560 3.377140
H -3.827084 0.743598 2.663048
H -3.809491 2.418721 2.062521
H -1.396828 0.528135 1.926488
H 0.563589 2.976502 -0.078972
H 0.745655 1.567002 0.966618
C -3.815781 1.262416 -0.466664
H -4.130952 0.794138 -1.410686
H -3.571449 2.313838 -0.676583
H -4.676608 1.234693 0.215953
H -1.453571 -1.419882 1.843891
H 0.678078 -3.233399 -0.653718
H 1.561218 -2.508031 1.690034
H 0.565891 -1.059946 1.560130
H 2.691300 -1.877581 -0.504901
H 1.732578 -0.407688 -0.526183
O 2.714654 0.462045 1.927505
H 2.640657 1.318412 1.468516

4-c1, ΔG = 1.0053 kcal/mol, population = 8.21 %

O 4.178613 0.473606 -1.339753
H 3.416805 1.070901 -1.447437
C 4.482597 0.318320 0.029362
H 5.233342 -0.486495 0.090989
H 4.942263 1.233662 0.454414
C 3.286214 -0.044666 0.937524
C 3.816946 -0.456310 2.308627
H 2.985998 -0.568083 3.019922
H 4.494083 0.317460 2.703337
H 4.363669 -1.409419 2.255370
C 2.455620 -1.161508 0.278330
C 1.181393 -1.578070 1.019808
C 0.404175 -2.597368 0.229991
C -0.928317 -2.770923 0.158438
C -1.509966 -3.872877 -0.693396
H -2.180966 -3.478860 -1.476385
H -2.122287 -4.559768 -0.082664
H -0.723783 -4.458713 -1.191068
C -1.931487 -1.967966 0.959581
H -2.459388 -2.685851 1.611888
C -3.005355 -1.200520 0.152792
H -3.966977 -1.268479 0.681610
H -3.177501 -1.698346 -0.814300
C -2.750937 0.310594 -0.113493
C -1.441420 0.509823 -0.833942
C -0.487916 1.398206 -0.486908
C 0.621343 1.269570 -1.434214
O 1.701304 1.846851 -1.431644
O 0.310888 0.343571 -2.361064
C -0.991111 -0.200714 -2.076978
H -0.879509 -1.284507 -1.937741
H -1.644551 -0.013925 -2.943261
C -0.566388 2.353531 0.655582
C -2.027331 2.481339 1.092707
H -2.087077 3.015968 2.053069
H -2.579264 3.093795 0.358813
C -2.711379 1.110325 1.236061
C -4.084221 1.264567 1.895058
H -4.728008 1.959186 1.333571
H -3.967780 1.672994 2.910670
H -4.617771 0.306595 1.984936
H -2.080448 0.524335 1.925043
H -0.145683 3.327770 0.358397
H 0.068226 1.987553 1.481051
C -3.880216 0.820236 -1.039698
H -3.804755 1.904619 -1.207050
H -4.865712 0.603300 -0.604323
H -3.837781 0.322947 -2.019929
H -1.409746 -1.284290 1.641673
H 1.024175 -3.291311 -0.352948
H 1.450965 -2.003959 2.004189
H 0.573980 -0.686235 1.229583
H 3.107183 -2.042788 0.145729
H 2.193698 -0.841919 -0.740988

O 2.486684 1.121380 1.173842
H 2.266114 1.532484 0.320354

4-c6, ΔG = 1.4019 kcal/mol, population = 4.20 %

O -3.253973 1.001175 1.689455
H -2.393385 1.428203 1.527090
C -3.927292 0.872113 0.463070
H -4.906819 0.411789 0.673708
H -4.129825 1.862547 0.002514
C -3.187724 0.014265 -0.581072
C -4.056935 -0.125236 -1.831839
H -3.504119 -0.637451 -2.631726
H -4.356041 0.866963 -2.209097
H -4.972886 -0.697891 -1.619123
C -2.793385 -1.340789 0.018880
C -2.018638 -2.257837 -0.946478
C -1.186069 -3.301811 -0.250980
C 0.130257 -3.220288 0.020937
C 0.861406 -4.358147 0.686892
H 1.274335 -4.063545 1.666498
H 1.721787 -4.683300 0.074767
H 0.203393 -5.225465 0.843166
C 0.967030 -2.016025 -0.360195
H 1.543324 -2.266458 -1.269543
C 1.945844 -1.548242 0.728246
H 2.809020 -2.228678 0.782799
H 1.460307 -1.614580 1.716342
C 2.467050 -0.096836 0.551261
C 1.308628 0.861131 0.686320
C 1.057919 1.910666 -0.117117
C -0.179340 2.565957 0.332871
O -0.794653 3.492800 -0.136527
O -0.603266 1.925127 1.472560
C 0.241409 0.797999 1.737963
H -0.366182 -0.117620 1.665888
H 0.630900 0.877410 2.764897
C 1.888900 2.315294 -1.288542
C 3.249099 1.611521 -1.211826
H 3.775926 1.708106 -2.173828
H 3.881673 2.112634 -0.459313
C 3.108048 0.119311 -0.860046
C 4.433915 -0.620735 -1.043442
H 4.752206 -0.571864 -2.096314
H 4.355782 -1.684076 -0.770131
H 5.236492 -0.174128 -0.436205
H 2.393235 -0.296642 -1.588729
H 2.001738 3.411316 -1.315724
H 1.362209 2.040856 -2.220748
C 3.467636 0.195544 1.692516
H 3.899048 1.203102 1.604906
H 4.287859 -0.536290 1.686869
H 2.971541 0.126198 2.672276
H 0.311032 -1.178451 -0.635793
H -1.714502 -4.210021 0.066030
H -2.729283 -2.760648 -1.623470
H -1.382518 -1.627168 -1.581446
H -3.700190 -1.845424 0.390683
H -2.177109 -1.128695 0.904306
O -1.947266 0.658177 -0.918315
H -2.142410 1.522105 -1.309545

4-c4, ΔG = 1.5117 kcal/mol, population = 3.49 %

O -5.407222 0.987080 -0.139451
H -4.745416 1.692980 -0.242404
C -4.645320 -0.158300 0.173148
H -4.382011 -0.183712 1.251238
H -5.257313 -1.050005 -0.039320
C -3.337183 -0.188728 -0.643940
C -3.644760 -0.330672 -2.132558
H -4.043964 -1.332100 -2.353609
H -2.739307 -0.170837 -2.734850
H -4.395456 0.416485 -2.426867
C -2.428718 -1.308540 -0.117684
C -1.100660 -1.494515 -0.859689
C -0.207187 -2.494326 -0.170351
C 1.124867 -2.637343 -0.295639
C 1.850119 -3.736277 0.441801
H 2.362186 -4.410717 -0.267035
H 1.162349 -4.336203 1.055049
H 2.637384 -3.342635 1.108085
C 1.977363 -1.798486 -1.224841
H 2.432219 -2.495208 -1.951573
C 3.132681 -1.001344 -0.578010
H 3.953029 -0.918322 -1.306151
H 3.554625 -1.572774 0.263686
C 2.820839 0.444350 -0.090258

C 1.656847 0.429793 0.867501
C 0.546188 1.185645 0.759687
C -0.374095 0.805684 1.839286
O -1.519684 1.168906 2.043281
O 0.231809 -0.111073 2.628528
C 1.541638 -0.397870 2.115418
H 1.609729 -1.478758 1.941948
H 2.287089 -0.114376 2.875923
C 0.315995 2.241528 -0.269250
C 1.658426 2.607376 -0.905612
H 1.495150 3.237914 -1.793287
H 2.251458 3.211622 -0.197064
C 2.459250 1.359407 -1.313246
C 3.670859 1.751406 -2.162397
H 4.311864 2.480502 -1.643155
H 3.335167 2.219458 -3.100549
H 4.293671 0.885038 -2.431204
H 1.788359 0.765066 -1.955487
H -0.160346 3.116962 0.202031
H -0.405364 1.883399 -1.022549
C 4.063679 0.967110 0.665279
H 3.937694 2.017335 0.967507
H 4.962782 0.891426 0.037937
H 4.247290 0.374037 1.573469
H 1.343619 -1.127793 -1.820338
H -0.723467 -3.202474 0.490537
H -1.304381 -1.831837 -1.892024
H -0.596049 -0.522794 -0.957474
H -2.995648 -2.255389 -0.147380
H -2.225753 -1.114744 0.948472
O -2.728983 1.102299 -0.487911
H -2.403341 1.192275 0.431761

4-c12, ΔG = 1.8875 kcal/mol, population = 1.85 %

O -3.287537 0.674667 1.505146
H -2.419197 1.103281 1.421448
C -3.930679 0.682530 0.254069
H -4.899034 0.172430 0.384543
H -4.158224 1.720452 -0.069748
C -3.162422 0.000802 -0.895287
C -3.972398 0.154518 -2.186256
H -4.944908 -0.356773 -2.114206
H -3.414820 -0.275063 -3.031595
H -4.162310 1.218168 -2.404348
C -2.853916 -1.486456 -0.652306
C -1.971168 -1.791113 0.575337
C -1.177196 -3.063964 0.459247
C 0.100689 -3.160588 0.045398
C 0.814731 -4.486160 -0.014724
H 1.706066 -4.490372 0.636999
H 1.179501 -4.692917 -1.036511
H 0.164062 -5.317104 0.295797
C 0.912638 -1.958387 -0.385546
H 1.370013 -2.185130 -1.363479
C 2.023810 -1.565188 0.609662
H 2.882985 -2.246438 0.512034
H 1.654130 -1.704099 1.639086
C 2.534195 -0.102592 0.470216
C 1.377315 0.832402 0.729512
C 0.984363 1.838929 -0.072664
C -0.255867 2.414017 0.463850
O -0.984299 3.267839 0.012137
O -0.549956 1.771836 1.639510
C 0.448911 0.775596 1.909285
H -0.051259 -0.195050 2.033236
H 0.950998 1.025887 2.857777
C 1.675839 2.257363 -1.325750
C 3.085728 1.658589 -1.336317
H 3.543870 1.790666 -2.328801
H 3.723719 2.205237 -0.620288
C 3.068660 0.161891 -0.979943
C 4.426247 -0.488013 -1.252361
H 5.237107 0.018329 -0.706004
H 4.665058 -0.428529 -2.325475
H 4.440386 -1.551350 -0.968354
H 2.340224 -0.300546 -1.665249
H 1.700061 3.356953 -1.395834
H 1.097305 1.907540 -2.200032
C 3.618074 0.143156 1.541812
H 4.432279 -0.589032 1.447609
H 3.197842 0.040062 2.553636
H 4.046876 1.152547 1.455746
H 0.251645 -1.096928 -0.555439
H -1.698183 -3.992348 0.726706
H -1.294551 -0.942516 0.704141
H -2.594437 -1.816747 1.480674
H -2.331832 -1.843813 -1.555054

H -3.803498 -2.043312 -0.599501
O -1.887128 0.639201 -1.053936
H -2.023808 1.587473 -1.200343

4-c11, ΔG = 1.8913 kcal/mol, population = 1.84 %

O -2.786727 1.395696 -1.004897
H -2.270312 2.197369 -0.789944
C -3.303339 0.867286 0.199433
H -2.565962 0.921677 1.019459
H -4.202210 1.426890 0.524890
C -3.703223 -0.590435 -0.058452
C -4.536669 -1.124088 1.101659
H -5.461993 -0.536828 1.198917
H -3.988664 -1.068916 2.053569
H -4.812251 -2.174649 0.921543
C -2.479865 -1.484330 -0.351016
C -1.436038 -1.616624 0.764451
C -0.383424 -2.644348 0.441025
C 0.917502 -2.641251 0.785820
C 1.817178 -3.785915 0.392406
H 1.256518 -4.582942 -0.117102
H 2.312836 -4.221388 1.277896
H 2.622904 -3.458903 -0.284314
C 1.548791 -1.572764 1.653047
H 0.800835 -0.811784 1.913757
C 2.831976 -0.887368 1.143367
H 3.563432 -1.643652 0.820349
H 3.301632 -0.386352 2.005734
C 2.690664 0.169617 0.011881
C 1.661241 1.196364 0.413660
C 0.641131 1.629317 -0.353197
C -0.116250 2.632569 0.410960
O -1.118837 3.252586 0.102947
O 0.476970 2.803304 1.615455
C 1.618444 1.940435 1.717987
H 1.483064 1.288714 2.594812
H 2.514595 2.558438 1.887257
C 0.373631 1.192090 -1.754219
C 1.632918 0.529371 -2.317232
H 1.396939 0.020678 -3.264919
H 2.381176 1.304842 -2.557388
C 2.243757 -0.489367 -1.338758
C 3.360486 -1.278272 -2.027210
H 3.892820 -1.947203 -1.335190
H 4.106813 -0.609446 -2.483658
H 2.940553 -1.901362 -2.831815
H 1.439552 -1.194659 -1.081754
H 0.065914 2.057820 -2.362957
H -0.484291 0.500800 -1.766266
C 4.051670 0.889857 -0.135549
H 4.038780 1.605227 -0.970809
H 4.856818 0.163101 -0.313409
H 4.306524 1.443986 0.779930
H 1.816638 -2.060500 2.608627
H -0.746777 -3.509425 -0.128780
H -0.972999 -0.638577 0.965014
H -1.943877 -1.909829 1.702239
H -1.991414 -1.100414 -1.261517
H -2.872784 -2.482091 -0.609139
O -4.548096 -0.607096 -1.213346
H -4.116455 -0.012968 -1.848068

4-c13, ΔG = 1.8951 kcal/mol, population = 1.83 %

O 3.285141 -0.651257 1.499436
H 2.421460 -1.088203 1.410774
C 3.933436 -0.648538 0.251015
H 4.896041 -0.129110 0.387133
H 4.172802 -1.683041 -0.075212
C 3.163129 0.029198 -0.899341
C 3.980074 -0.112036 -2.187357
H 4.947138 0.408654 -2.109453
H 3.421818 0.314852 -3.033622
H 4.181469 -1.173006 -2.408208
C 2.838558 1.512444 -0.652811
C 1.947851 1.804163 0.572245
C 1.141325 3.069200 0.456854
C -0.135659 3.154098 0.037682
C -0.863010 4.472474 -0.021114
H -0.222074 5.309046 0.294524
H -1.756848 4.465531 0.627161
H -1.225925 4.678688 -1.043672
C -0.933372 1.945071 -0.400690
H -1.388582 2.170195 -1.380009
C -2.044995 1.537538 0.588240
H -2.910568 2.210392 0.488884
H -1.681339 1.676891 1.619748

C -2.539906 0.070314 0.441870
C -1.374711 -0.853680 0.703331
C -0.967972 -1.853548 -0.100294
C 0.275771 -2.417560 0.439800
O 1.014927 -3.262388 -0.011416
O 0.558137 -1.776190 1.618778
C -0.452101 -0.791156 1.887359
H 0.037509 0.184163 2.016685
H -0.955784 -1.049717 2.832786
C -1.649643 -2.275001 -1.357743
C -3.065491 -1.690537 -1.372697
H -3.517880 -1.824082 -2.367622
H -3.701035 -2.245935 -0.661235
C -3.065238 -0.194905 -1.011479
C -4.428144 0.442059 -1.287884
H -5.236230 -0.074272 -0.746777
H -4.661558 0.383632 -2.362250
H -4.454356 1.504276 -1.000544
H -2.338517 0.277140 -1.692046
H -1.662407 -3.374555 -1.431373
H -1.070846 -1.916559 -2.228353
C -3.625949 -0.189852 1.507859
H -4.447143 0.534321 1.412314
H -3.211246 -0.085685 2.521858
H -4.044067 -1.203281 1.416740
H -0.262925 1.090875 -0.570187
H 1.651550 4.001980 0.729724
H 1.279499 0.948259 0.695787
H 2.567251 1.833417 1.480120
H 2.316458 1.867391 -1.556500
H 3.782184 2.078781 -0.594400
O 1.895061 -0.621481 -1.065560
H 2.041879 -1.567936 -1.213924

4-c9, ΔG = 2.0419 kcal/mol, population = 1.42 %

O -5.426709 0.508359 -0.227164
H -5.859159 0.592060 0.633248
C -4.516411 -0.571457 -0.160130
H -5.000291 -1.499855 0.199037
H -4.170486 -0.756210 -1.190857
C -3.276304 -0.311179 0.723660
C -3.696950 -0.099142 2.176251
H -4.292450 -0.956850 2.526379
H -4.294960 0.818113 2.288255
H -2.815911 -0.011457 2.827767
C -2.500468 0.893353 0.161692
C -1.245744 1.313654 0.933914
C -0.495944 2.402286 0.210618
C 0.816400 2.693921 0.262249
C 1.372151 3.854510 -0.526943
H 1.861486 4.585295 0.140892
H 0.585388 4.373891 -1.092757
H 2.145988 3.534121 -1.246248
C 1.809377 1.973020 1.148973
H 2.221516 2.730733 1.839271
C 3.009392 1.299573 0.446260
H 3.881617 1.348925 1.114341
H 3.298075 1.882004 -0.442846
C 2.852755 -0.191524 0.029201
C 1.646074 -0.368622 -0.856656
C 0.672105 -1.282483 -0.676618
C -0.335382 -1.095848 -1.729060
O -1.403913 -1.659932 -1.885502
O 0.078246 -0.110547 -2.559994
C 1.343090 0.399706 -2.111236
H 1.238670 1.480565 -1.952813
H 2.092432 0.228262 -2.900856
C 0.647736 -2.321256 0.394004
C 2.055357 -2.462649 0.976407
H 2.024691 -3.073040 1.892283
H 2.698903 -3.003614 0.261131
C 2.683843 -1.097089 1.301213
C 3.977222 -1.277654 2.099613
H 4.695881 -1.920114 1.567634
H 3.757177 -1.760278 3.064361
H 4.474786 -0.320517 2.315772
H 1.963980 -0.578727 1.956201
H 0.285033 -3.274652 -0.024045
H -0.084832 -2.038207 1.168496
C 4.106767 -0.586457 -0.783977
H 4.093778 -1.654143 -1.048401
H 5.022495 -0.381600 -0.211816
H 4.166467 -0.007498 -1.717530
H 1.290284 1.248163 1.789952
H -1.120851 3.045190 -0.423123
H -1.538204 1.674730 1.937096
H -0.604439 0.436405 1.102963

H -3.199987 1.742477 0.098311
H -2.222026 0.661851 -0.879765
O -2.490045 -1.500524 0.708564
H -2.206810 -1.675706 -0.209811

4-c31, ΔG = 2.2477 kcal/mol, population = 1.01 %

O 5.080067 -0.797781 1.028595
H 4.494410 -0.235609 1.563935
C 4.196684 -1.606189 0.285310
H 4.766871 -2.083631 -0.527113
H 3.764514 -2.412417 0.911817
C 3.036869 -0.778640 -0.297038
C 1.986046 -1.711969 -0.895828
H 2.411395 -2.288398 -1.732038
H 1.119821 -1.151515 -1.277273
H 1.619694 -2.415319 -0.136090
C 3.576495 0.226811 -1.329160
C 2.568149 1.282372 -1.818633
C 2.298546 2.378599 -0.820271
C 1.137492 2.699967 -0.212657
C 1.063650 3.899847 0.697738
H 2.017843 4.444765 0.724265
H 0.802462 3.615524 1.730017
H 0.276649 4.595756 0.358270
C -0.156038 1.941647 -0.434554
H -0.731027 2.476914 -1.210859
C -1.026856 1.800494 0.820558
H -1.434761 2.783312 1.098915
H -0.398261 1.493575 1.673027
C -2.205424 0.797871 0.711400
C -1.678434 -0.614786 0.621826
C -2.139507 -1.566993 -0.210786
C -1.415488 -2.822696 0.060744
O -1.519682 -3.907535 -0.462505
O -0.533421 -2.589777 1.077908
C -0.613034 -1.218646 1.491156
H 0.379745 -0.757232 1.357835
H -0.869892 -1.187386 2.562702
C -3.234394 -1.387532 -1.209312
C -4.016379 -0.110503 -0.881493
H -4.662328 0.163070 -1.730250
H -4.688675 -0.298394 -0.027150
C -3.082817 1.069255 -0.556875
C -3.859163 2.385386 -0.487758
H -4.664709 2.342677 0.261572
H -4.326375 2.600604 -1.461188
H -3.210087 3.238049 -0.236563
H -2.382754 1.142437 -1.405636
H -3.889859 -2.273547 -1.213327
H -2.802612 -1.326045 -2.224805
C -3.031112 0.906785 2.015004
H -3.896476 0.228871 2.003774
H -3.394941 1.933923 2.159874
H -2.414187 0.649784 2.888977
H 0.053376 0.945658 -0.850684
H 3.171047 3.003489 -0.590297
H 2.994664 1.754779 -2.720474
H 1.637182 0.798793 -2.148158
H 3.944695 -0.350742 -2.191755
H 4.452515 0.729218 -0.887894
O 2.489111 -0.092936 0.849595
H 2.276287 0.825305 0.605246

4-c32, ΔG = 2.3657 kcal/mol, population = 0.82 %

O -3.136491 2.195917 -1.016252
H -2.769408 1.485069 -1.568685
C -4.339406 1.658542 -0.508074
H -4.676926 2.295801 0.323474
H -5.131197 1.665594 -1.283054
C -4.147758 0.208519 -0.027194
C -5.505908 -0.441862 0.234427
H -6.040049 0.069804 1.050923
H -5.390996 -1.499955 0.512399
H -6.127127 -0.397808 -0.672717
C -3.240355 0.182217 1.216606
C -2.934017 -1.201082 1.825914
C -2.370001 -2.245273 0.884368
C -1.141529 -2.252122 0.327579
C -0.697020 -3.376380 -0.571563
H -0.393365 -3.004321 -1.565007
H -1.489442 -4.124478 -0.717281
H 0.185751 -3.884227 -0.145320
C -0.128310 -1.154364 0.555797
H -0.386869 -0.581186 1.456298
C 0.002141 -0.203426 -0.647762
H -0.935132 0.356619 -0.766331

H 0.100708 -0.796355 -1.571594
C 1.187338 0.795963 -0.595089
C 2.480772 0.024213 -0.502824
C 3.490723 0.281776 0.347615
C 4.568867 -0.698173 0.112856
O 5.640307 -0.818136 0.658600
O 4.172384 -1.529462 -0.896445
C 2.870444 -1.151749 -1.354583
H 2.192169 -2.012717 -1.242242
H 2.926537 -0.903290 -2.427122
C 3.514747 1.391426 1.344079
C 2.427653 2.410794 0.988472
H 2.280443 3.111988 1.824686
H 2.761586 3.018132 0.129445
C 1.082518 1.743034 0.648463
C -0.020986 2.796401 0.520030
H -0.980468 2.382137 0.179414
H 0.265500 3.588391 -0.190025
H -0.192524 3.279768 1.494609
H 0.833017 1.098500 1.507659
H 4.513662 1.856574 1.367746
H 3.347176 0.982637 2.357134
C 1.189617 1.593073 -1.919249
H 1.976592 2.361146 -1.925207
H 0.220301 2.087348 -2.075367
H 1.362560 0.926565 -2.777329
H 0.851983 -1.619278 0.759669
H -3.029054 -3.090283 0.652229
H -2.231723 -1.039001 2.661774
H -3.850181 -1.605613 2.281728
H -3.717498 0.799620 1.995102
H -2.301583 0.691226 0.958282
O -3.507387 -0.426736 -1.147203
H -2.998795 -1.187018 -0.818287

4-c21, ΔG = 2.3745 kcal/mol, population = 0.81 %

O 2.527810 1.538240 0.995094
H 1.994548 2.341258 0.861925
C 3.380629 1.373667 -0.124696
H 2.821616 1.461943 -1.070524
H 4.173895 2.146118 -0.120411
C 4.043438 -0.008876 -0.030440
C 5.249264 -0.053692 -0.966530
H 4.937325 0.069518 -2.015132
H 5.765216 -1.021107 -0.871806
H 5.962738 0.744875 -0.713881
C 3.078355 -1.164667 -0.392430
C 1.958125 -1.466057 0.612745
C 1.233735 -2.741221 0.276773
C -0.089427 -2.990190 0.269160
C -0.620814 -4.356820 -0.084719
H -1.270398 -4.319605 -0.976218
H -1.243382 -4.760158 0.733860
H 0.190399 -5.071704 -0.286436
C -1.136939 -1.961198 0.621568
H -1.676624 -2.301564 1.522817
C -2.155894 -1.697678 -0.506622
H -2.979711 -2.425573 -0.460594
H -1.673912 -1.863002 -1.484344
C -2.753171 -0.265288 -0.507584
C -1.614271 0.711642 -0.659426
C -1.408640 1.806204 0.098165
C -0.127024 2.406683 -0.297500
O 0.486156 3.332165 0.198384
O 0.370385 1.706444 -1.351157
C -0.486990 0.596745 -1.643873
H 0.095101 -0.330731 -1.527526
H -0.817470 0.666064 -2.692464
C -2.309603 2.277398 1.190108
C -3.657221 1.555195 1.076572
H -4.245932 1.714950 1.993012
H -4.242290 1.994165 0.250136
C -3.484834 0.043693 0.841461
C -4.817756 -0.692248 0.990261
H -5.582507 -0.290755 0.307259
H -5.200111 -0.577776 2.016321
H -4.720637 -1.770497 0.791939
H -2.818297 -0.315932 1.643015
H -2.431687 3.371440 1.136828
H -1.839500 2.071712 2.168762
C -3.691809 -0.125600 -1.725490
H -4.470193 -0.901503 -1.706369
H -3.131205 -0.243596 -2.664987
H -4.181594 0.858727 -1.747560
H -0.648417 -1.018941 0.905224
H 1.895150 -3.579440 0.017821
H 2.430884 -1.573625 1.606328

H 1.279177 -0.607745 0.695721
H 3.692394 -2.075785 -0.499817
H 2.647528 -0.967218 -1.389303
O 4.535725 -0.173590 1.300928
H 3.881816 0.263209 1.870257

4-c24, ΔG = 2.4730 kcal/mol, population = 0.69 %

O -3.198685 1.175446 1.903539
H -2.639080 1.854749 1.498146
C -4.216884 0.808695 0.990379
H -4.894978 0.129440 1.531169
H -4.804725 1.690149 0.671238
C -3.682524 0.104010 -0.271633
C -4.842105 -0.201049 -1.214326
H -5.575857 -0.866282 -0.735461
H -4.477837 -0.688392 -2.130696
H -5.348103 0.731779 -1.506631
C -2.917719 -1.174735 0.133305
C -2.012509 -1.757247 -0.962031
C -1.275468 -2.985179 -0.506115
C 0.048556 -3.146078 -0.320190
C 0.609497 -4.459924 0.163634
H 1.378483 -4.839361 -0.532490
H -0.173238 -5.225754 0.266247
H 1.106868 -4.349572 1.142673
C 1.071431 -2.059908 -0.562523
H 1.790082 -2.412527 -1.322766
C 1.842817 -1.658497 0.709801
H 2.624644 -2.400592 0.929620
H 1.158875 -1.692461 1.574330
C 2.494608 -0.250772 0.669628
C 1.408170 0.782631 0.498466
C 1.447242 1.829633 -0.347256
C 0.176513 2.563669 -0.260163
O -0.218002 3.537917 -0.845819
O -0.619509 1.910307 0.669450
C 0.100412 0.801070 1.232244
H -0.491491 -0.112850 1.088977
H 0.214080 0.965344 2.315499
C 2.587601 2.168202 -1.248542
C 3.823616 1.362649 -0.832632
H 4.582225 1.405914 -1.629170
H 4.282708 1.823703 0.058407
C 3.484639 -0.109280 -0.533996
C 4.756229 -0.944999 -0.377167
H 5.409640 -0.547618 0.415065
H 5.332806 -0.934103 -1.314961
H 4.535292 -1.995997 -0.137016
H 2.947299 -0.487204 -1.420024
H 2.783927 3.252353 -1.219712
H 2.307413 1.939059 -2.292505
C 3.191795 -0.006892 2.026700
H 3.927217 -0.797964 2.231208
H 2.459581 -0.017193 2.848027
H 3.708431 0.963302 2.048655
H 0.586315 -1.173906 -0.995251
H -1.917485 -3.847802 -0.282549
H -2.630766 -2.015817 -1.840015
H -1.323641 -0.971217 -1.300258
H -3.647428 -1.931881 0.466429
H -2.306857 -0.940857 1.019532
O -2.831744 1.012600 -0.977287
H -2.101848 1.275532 -0.393913

4-c10, ΔG = 2.4893 kcal/mol, population = 0.67 %

O -4.401434 1.229912 -1.454029
H -3.650283 0.830576 -1.924609
C -4.534201 0.458383 -0.280949
H -5.165244 1.017843 0.428202
H -5.042583 -0.506286 -0.488739
C -3.160030 0.156246 0.345625
C -3.292588 -0.864529 1.469979
H -3.914322 -0.461327 2.284277
H -2.310825 -1.135768 1.880502
H -3.768684 -1.788599 1.103967
C -2.477162 1.455305 0.795537
C -1.070419 1.245221 1.389988
C -0.150305 2.426723 1.227529
C 0.607250 2.680107 0.143426
C 1.513118 3.882657 0.085878
H 1.277102 4.515772 -0.787560
H 2.570021 3.585986 -0.023464
H 1.430133 4.497865 0.993766
C 0.557875 1.825536 -1.107283
H -0.239662 1.076866 -1.020852
C 1.860086 1.144404 -1.576315

H 2.679852 1.878343 -1.613754
H 1.705742 0.833040 -2.622794
C 2.360300 -0.102219 -0.792287
C 1.245577 -1.114024 -0.676586
C 0.882130 -1.754251 0.450386
C -0.252354 -2.641300 0.146582
O -0.901396 -3.352233 0.878407
O -0.523164 -2.543869 -1.190517
C 0.366186 -1.595588 -1.796324
H -0.237254 -0.793043 -2.245068
H 0.929786 -2.100630 -2.597027
C 1.527519 -1.586431 1.783971
C 2.898526 -0.930461 1.595706
H 3.298770 -0.608958 2.569981
H 3.609167 -1.675954 1.198298
C 2.840206 0.282325 0.650016
C 4.174100 1.033231 0.667811
H 4.199564 1.862616 -0.054601
H 5.020402 0.365997 0.440817
H 4.351426 1.461054 1.666717
H 2.073888 0.959145 1.054704
H 1.609475 -2.561876 2.290120
H 0.883821 -0.961292 2.428992
C 3.504427 -0.743587 -1.612560
H 3.135721 -1.117441 -2.579339
H 3.959388 -1.588750 -1.075610
H 4.289873 -0.004179 -1.824242
H 0.248016 2.494614 -1.931154
H -0.101874 3.136906 2.062036
H -1.153060 0.992814 2.459043
H -0.627171 0.370198 0.897669
H -3.132254 1.975335 1.513049
H -2.412742 2.101546 -0.092086
O -2.334125 -0.358024 -0.719456
H -2.478364 -1.309732 -0.824777

4-c19, ΔG = 2.5433 kcal/mol, population = 0.61 %

O -1.561636 -0.929298 1.965490
H -2.147823 -0.558493 2.645672
C -2.414939 -1.355287 0.923110
H -1.790624 -1.567636 0.045388
H -2.926238 -2.303378 1.187588
C -3.491263 -0.303963 0.609983
C -4.438184 -0.816865 -0.471544
H -4.920878 -1.755912 -0.154064
H -3.901357 -1.021336 -1.410082
H -5.225277 -0.074756 -0.673682
C -2.882656 1.061072 0.262339
C -1.944701 1.093722 -0.952311
C -1.331903 2.457645 -1.149428
C -0.225290 2.928394 -0.543731
C 0.253635 4.339378 -0.766500
H 1.281321 4.359806 -1.167831
H 0.284002 4.894037 0.188211
H -0.395859 4.887797 -1.464434
C 0.603138 2.096577 0.408660
H 0.607744 2.593408 1.394459
C 2.063988 1.880282 -0.058334
H 2.750656 2.532344 0.501667
H 2.168845 2.186790 -1.111717
C 2.568530 0.417480 0.054874
C 1.684676 -0.460005 -0.797021
C 1.138729 -1.629883 -0.416708
C 0.321993 -2.149451 -1.529900
O -0.354936 -3.150055 -1.595019
O 0.412400 -1.269854 -2.570957
C 1.257080 -0.171304 -2.207909
H 0.680276 0.762739 -2.300452
H 2.103637 -0.123687 -2.912298
C 1.336690 -2.279693 0.911877
C 2.535424 -1.632331 1.615223
H 2.557433 -1.936603 2.673418
H 3.474606 -1.999586 1.166082
C 2.492509 -0.095049 1.532212
C 3.544732 0.533883 2.447232
H 3.553439 1.632199 2.375755
H 4.557751 0.172405 2.211210
H 3.338128 0.272065 3.496514
H 1.501314 0.204219 1.910766
H 1.478536 -3.365398 0.785202
H 0.423868 -2.145812 1.516744
C 4.006665 0.354630 -0.504794
H 4.659657 1.067322 0.018886
H 4.022799 0.616978 -1.573215
H 4.436401 -0.652363 -0.399802
H 0.116523 1.126271 0.573211
H -1.883194 3.142252 -1.805534

H -1.161570 0.334690 -0.819066
H -2.496187 0.807714 -1.861925
H -2.324984 1.406939 1.145308
H -3.711498 1.773158 0.118682
O -4.208404 -0.060928 1.834364
H -4.745011 -0.843772 2.027735

4-c8, ΔG = 2.6901 kcal/mol, population = 0.48 %

O 3.947857 -1.343323 0.771043
H 3.199407 -1.968802 0.785247
C 3.425109 -0.029357 0.832470
H 2.513501 -0.003800 1.451706
H 4.174618 0.616971 1.320343
C 3.114280 0.538142 -0.567023
C 4.392862 0.592086 -1.408535
H 4.860708 -0.402914 -1.440312
H 5.121548 1.301051 -0.984722
H 4.154328 0.905467 -2.436070
C 2.460121 1.925051 -0.492175
C 1.174567 1.993280 0.341249
C 0.357562 3.233107 0.072530
C -0.967594 3.347866 0.271849
C -1.726120 4.606912 -0.049520
H -2.540595 4.403037 -0.767391
H -1.075488 5.382612 -0.480074
H -2.208687 5.020365 0.853881
C -1.782544 2.183872 0.802287
H -1.192137 1.655502 1.561716
C -2.195562 1.208731 -0.317280
H -1.368100 1.150111 -1.035244
H -3.053291 1.630931 -0.867030
C -2.577597 -0.243166 0.108377
C -1.341791 -0.951054 0.611464
C -0.522265 -1.687990 -0.166869
C 0.600725 -2.147693 0.656094
O 1.598596 -2.770772 0.332470
O 0.413336 -1.727265 1.929957
C -0.804418 -0.974545 2.013050
H -0.563969 0.017670 2.422240
H -1.487475 -1.476690 2.717169
C -0.724038 -1.999255 -1.611357
C -1.906984 -1.197122 -2.180381
H -1.546489 -0.211913 -2.509926
H -2.293601 -1.695991 -3.082169
C -3.060444 -1.015624 -1.170402
C -3.718397 -2.363867 -0.850686
H -3.061078 -3.008636 -0.245624
H -3.946292 -2.903294 -1.783399
H -4.662992 -2.242184 -0.302429
H -3.821257 -0.377351 -1.650440
H -0.892177 -3.085901 -1.715037
H 0.198231 -1.778806 -2.170686
C -3.667658 -0.196516 1.190928
H -3.931707 -1.199809 1.552201
H -4.578623 0.275539 0.790907
H -3.342033 0.391622 2.061283
H -2.676729 2.561363 1.321704
H 0.902560 4.102829 -0.316134
H 0.583824 1.091616 0.124205
H 1.424257 1.940460 1.417618
H 2.230120 2.222388 -1.529487
H 3.198259 2.653453 -0.117192
O 2.162924 -0.317039 -1.214811
H 2.435894 -1.234192 -1.058559

4-c7, ΔG = 2.7999 kcal/mol, population = 0.40 %

O 4.021256 0.976873 -1.551787
H 3.194288 1.470687 -1.408533
C 4.555395 0.561823 -0.312787
H 5.333829 -0.184494 -0.542640
H 5.047246 1.399803 0.221625
C 3.537949 -0.058048 0.670604
C 4.297436 -0.688948 1.835107
H 4.971060 0.050630 2.295931
H 4.895243 -1.549801 1.500994
H 3.594460 -1.029696 2.609056
C 2.657780 -1.084608 -0.069277
C 1.485189 -1.643608 0.739948
C 0.557492 -2.467107 -0.110550
C -0.774314 -2.612641 0.017938
C -1.534393 -3.525837 -0.911948
H -2.279565 -2.982131 -1.517907
H -2.100823 -4.285334 -0.344565
H -0.857445 -4.045989 -1.604643
C -1.572180 -1.976992 1.137255
H -1.795960 -2.779226 1.865769

C -2.926505 -1.356048 0.755879
H -3.527707 -1.257081 1.672535
H -3.473484 -2.076692 0.131535
C -2.967161 0.046325 0.039672
C -1.661218 0.380187 -0.633836
C -0.698195 1.150957 -0.084330
C 0.368914 1.315280 -1.072978
O 1.413805 1.947328 -0.980049
O 0.054321 0.628839 -2.187668
C -1.237219 0.018177 -2.025549
H -1.129887 -1.063072 -2.187897
H -1.912449 0.427620 -2.793180
C -0.754062 1.808327 1.255433
C -2.006866 1.354348 2.023590
H -1.796683 0.409947 2.546155
H -2.245403 2.089182 2.807500
C -3.229852 1.171662 1.103623
C -3.653914 2.513293 0.492161
H -2.937686 2.870106 -0.264788
H -3.713759 3.281224 1.279396
H -4.642181 2.454958 0.015390
H -4.065471 0.814284 1.727828
H -0.755823 2.902495 1.106816
H 0.163099 1.588600 1.825724
C -4.100893 -0.000543 -1.002767
H -4.171652 0.926382 -1.588424
H -5.067055 -0.161973 -0.499944
H -3.949084 -0.834153 -1.705558
H -0.950693 -1.254585 1.679660
H 1.045675 -3.031316 -0.916046
H 1.871036 -2.263260 1.571017
H 0.950588 -0.809398 1.215775
H 3.302036 -1.910723 -0.416783
H 2.272815 -0.613687 -0.984990
O 2.741865 0.981081 1.254023
H 2.281264 1.461263 0.542536

4-c15, ΔG = 2.8062 kcal/mol, population = 0.39 %

O -3.664603 -0.608112 -1.361229
H -3.002976 -1.324264 -1.340699
C -4.263654 -0.474567 -0.090630
H -5.096462 0.237331 -0.209710
H -4.701046 -1.435550 0.247196
C -3.359098 0.040442 1.048647
C -4.233271 0.224862 2.290773
H -4.947632 1.051708 2.159286
H -3.595131 0.451872 3.157887
H -4.794980 -0.695968 2.511646
C -2.667329 1.385758 0.712679
C -1.489683 1.287997 -0.266038
C -0.763593 2.583014 -0.493481
C 0.486639 2.904653 -0.105954
C 1.083792 4.250833 -0.427641
H 0.395354 4.877643 -1.013332
H 2.022062 4.146832 -1.000068
H 1.346571 4.793504 0.497872
C 1.382190 1.977337 0.686744
H 1.714792 2.515355 1.590562
C 2.632720 1.461984 -0.077674
H 3.550372 1.866436 0.374541
H 2.626269 1.841826 -1.111979
C 2.777860 -0.087084 -0.131104
C 1.549934 -0.653549 -0.796761
C 0.732888 -1.590729 -0.275862
C -0.423846 -1.723532 -1.165486
O -1.471723 -2.329473 -0.979435
O -0.227329 -0.972765 -2.265847
C 0.987369 -0.218687 -2.118067
H 0.725252 0.850351 -2.140137
H 1.648905 -0.439439 -2.969814
C 0.953470 -2.295029 1.019756
C 2.424422 -2.133111 1.416826
H 2.578541 -2.495041 2.445001
H 3.051501 -2.764593 0.763370
C 2.888756 -0.668739 1.322343
C 4.277441 -0.492897 1.939725
H 4.247108 -0.745115 3.010845
H 4.640753 0.542656 1.854376
H 5.021016 -1.152471 1.466407
H 2.184295 -0.089403 1.941030
H 0.673088 -3.356508 0.927038
H 0.285833 -1.867064 1.788911
C 4.008157 -0.439438 -0.994612
H 3.866680 -0.106106 -2.033460
H 4.189080 -1.524595 -1.009667
H 4.910084 0.057420 -0.611342
H 0.793134 1.127179 1.053342

H -1.329934 3.347563 -1.041978
H -0.802987 0.533522 0.131600
H -1.864411 0.906598 -1.226219
H -2.294007 1.814438 1.658685
H -3.427493 2.089393 0.331580
O -2.383123 -0.948783 1.404594
H -2.130826 -1.467938 0.624092

4-c22, ΔG = 2.9505 kcal/mol, population = 0.31 %

O 2.207407 -0.532959 -1.630641
H 2.206991 -1.274695 -0.996549
C 3.237958 0.370039 -1.302500
H 4.236079 -0.053310 -1.530392
H 3.101577 1.237845 -1.969768
C 3.257175 0.884025 0.154203
C 4.259194 2.046934 0.212121
H 3.985594 2.836942 -0.505633
H 5.281593 1.711417 -0.022851
H 4.260864 2.484514 1.221091
C 3.684608 -0.182205 1.191867
C 2.612886 -1.174381 1.678479
C 2.299955 -2.336446 0.777075
C 1.097818 -2.689842 0.273862
C 0.939683 -3.961280 -0.519515
H 0.173285 -4.610296 -0.060672
H 1.882068 -4.524955 -0.572817
H 0.600044 -3.761006 -1.548880
C -0.155122 -1.869308 0.506048
H -0.681261 -2.301515 1.375755
C -1.120847 -1.810462 -0.685605
H -1.599192 -2.789613 -0.837062
H -0.551124 -1.611993 -1.607981
C -2.235304 -0.732597 -0.572198
C -1.592537 0.632093 -0.527227
C -1.884546 1.609363 0.351669
C -1.000548 2.757588 0.093266
O -0.913201 3.820217 0.660827
O -0.193031 2.438085 -0.971456
C -0.520265 1.121508 -1.452070
H 0.390334 0.501801 -1.440993
H -0.871736 1.207547 -2.493805
C -2.937214 1.531272 1.407142
C -3.867671 0.351965 1.102168
H -4.506892 0.142198 1.973897
H -4.546542 0.621023 0.274665
C -3.079582 -0.917883 0.733862
C -3.991775 -2.145193 0.699630
H -4.829239 -2.010149 -0.002451
H -4.423923 -2.323283 1.696507
H -3.449411 -3.056833 0.406029
H -2.354866 -1.068411 1.550614
H -3.492519 2.482159 1.457040
H -2.463917 1.404221 2.397729
C -3.110792 -0.817443 -1.842256
H -3.940210 -0.096069 -1.808759
H -3.531428 -1.826337 -1.958877
H -2.514073 -0.603195 -2.741584
H 0.125657 -0.846267 0.792938
H 3.149369 -2.999405 0.564620
H 2.986532 -1.601238 2.626851
H 1.707632 -0.610063 1.933141
H 4.036836 0.365330 2.080627
H 4.563023 -0.722060 0.799427
O 1.966285 1.340151 0.549626
H 1.628726 1.975572 -0.101556

4-c20, ΔG = 2.9687 kcal/mol, population = 0.30 %

O -5.716620 0.859586 -0.706468
H -5.372794 1.296659 0.091992
C -4.972513 -0.335644 -0.780031
H -5.357266 -1.091968 -0.066159
H -5.078267 -0.749930 -1.795229
C -3.488311 -0.082863 -0.459518
C -2.871280 0.830946 -1.522323
H -3.504052 1.720235 -1.652953
H -2.798387 0.309207 -2.488458
H -1.865995 1.166204 -1.233097
C -2.746339 -1.427463 -0.340648
C -1.328785 -1.298859 0.223820
C -0.590958 -2.600979 0.347634
C 0.650294 -2.896823 -0.085216
C 1.249191 -4.261185 0.143925
H 2.196118 -4.194182 0.707419
H 1.496968 -4.745145 -0.817526
H 0.568222 -4.922571 0.699440
C 1.539751 -1.924415 -0.828699

H 1.865180 -2.403773 -1.767452
C 2.796056 -1.463693 -0.038631
H 3.708987 -1.853539 -0.512753
H 2.785269 -1.898834 0.973528
C 2.956806 0.078026 0.100465
C 1.728631 0.621456 0.785766
C 0.924580 1.592913 0.311358
C -0.235623 1.705750 1.206074
O -1.262569 2.343530 1.065457
O -0.045967 0.884171 2.268575
C 1.161899 0.131520 2.086372
H 0.903249 -0.938406 2.067715
H 1.828392 0.315308 2.943640
C 1.174651 2.375204 -0.934019
C 2.647756 2.214352 -1.324190
H 2.820891 2.638856 -2.325136
H 3.276864 2.791720 -0.624325
C 3.085842 0.739081 -1.316423
C 4.474390 0.575291 -1.937522
H 5.225852 1.196348 -1.426143
H 4.453283 0.885819 -2.993431
H 4.821286 -0.468876 -1.906801
H 2.374444 0.208438 -1.970411
H 0.909478 3.432907 -0.776163
H 0.517927 2.014108 -1.746137
C 4.183924 0.367872 0.990944
H 4.375332 1.448499 1.069414
H 5.084203 -0.115533 0.587040
H 4.030833 -0.022499 2.008088
H 0.952913 -1.048163 -1.131944
H -1.140229 -3.392858 0.874172
H -0.753651 -0.588568 -0.384078
H -1.422081 -0.846038 1.224150
H -2.718882 -1.906399 -1.334171
H -3.333687 -2.092799 0.315512
O -3.527456 0.586336 0.810399
H -2.783717 1.212340 0.888578

4-c17, ΔG = 3.1852 kcal/mol, population = 0.21 %

O -5.667699 -0.314630 0.047459
H -5.340151 0.158123 0.830529
C -4.922951 0.220397 -1.025514
H -5.056291 -0.441149 -1.896445
H -5.290933 1.228323 -1.304272
C -3.431670 0.333820 -0.664754
C -2.704500 1.168494 -1.717348
H -3.129242 2.183035 -1.762109
H -2.800496 0.705744 -2.711577
H -1.633761 1.263729 -1.488641
C -2.824778 -1.079598 -0.521447
C -1.457834 -1.094496 0.165890
C -0.859245 -2.461658 0.330942
C 0.366071 -2.880711 -0.042002
C 0.822005 -4.292654 0.223707
H 1.748351 -4.307833 0.824127
H 1.060496 -4.810771 -0.722250
H 0.059858 -4.878906 0.757737
C 1.377291 -2.005938 -0.750342
H 1.709148 -2.530966 -1.661982
C 2.625055 -1.641635 0.101259
H 3.520039 -2.140553 -0.298835
H 2.509279 -2.030555 1.125581
C 2.931923 -0.118870 0.198028
C 1.733210 0.565918 0.804763
C 1.062476 1.604569 0.269306
C -0.128199 1.854997 1.093473
O -1.075995 2.588836 0.882290
O -0.081953 1.044743 2.180242
C 1.047495 0.165744 2.078403
H 0.677232 -0.870827 2.060031
H 1.681497 0.295357 2.969610
C 1.457913 2.327056 -0.974881
C 2.919297 1.991931 -1.293098
H 3.181364 2.364175 -2.295421
H 3.579835 2.516471 -0.580699
C 3.187528 0.477940 -1.229180
C 4.571078 0.142023 -1.789762
H 5.368074 0.690294 -1.264123
H 4.624235 0.423274 -2.852876
H 4.797363 -0.932833 -1.720326
H 2.444829 0.010502 -1.896326
H 1.308704 3.411203 -0.846260
H 0.801566 2.026395 -1.811508
C 4.140864 0.081916 1.136342
H 4.429034 1.141921 1.196881
H 5.008279 -0.494260 0.785198
H 3.907807 -0.262924 2.154827

H 0.888354 -1.088268 -1.100790
H -1.508810 -3.191341 0.832740
H -0.764902 -0.440738 -0.379461
H -1.592906 -0.640003 1.160518
H -2.754310 -1.538141 -1.522438
H -3.535301 -1.688814 0.060636
O -3.435214 0.994110 0.608431
H -2.661731 1.580599 0.700588

4-c29, ΔG = 3.6835 kcal/mol, population = 0.09 %

O -2.890042 1.728943 -0.943527
H -3.387362 1.520097 -1.751937
C -3.801199 1.526503 0.115718
H -3.222572 1.456647 1.049159
H -4.487389 2.391340 0.222904
C -4.649789 0.263337 -0.111018
C -5.719211 0.129854 0.968745
H -6.385283 1.008473 0.967864
H -5.271392 0.053472 1.970859
H -6.330564 -0.767800 0.791164
C -3.781626 -0.995099 -0.242568
C -2.965228 -1.389382 0.997251
C -2.045601 -2.538870 0.695790
C -0.707138 -2.484326 0.581783
C 0.096251 -3.693005 0.178162
H 0.659181 -3.496981 -0.752401
H -0.538542 -4.574902 0.007231
H 0.848057 -3.945958 0.946101
C 0.092221 -1.213163 0.792099
H -0.303710 -0.653717 1.652576
C 0.100298 -0.304048 -0.448696
H -0.877781 0.188158 -0.553614
H 0.209638 -0.926688 -1.352836
C 1.209353 0.782110 -0.478498
C 2.562983 0.117096 -0.532803
C 3.641523 0.468263 0.191460
C 4.765151 -0.415763 -0.172268
O 5.901137 -0.436798 0.240138
O 4.325044 -1.288169 -1.127476
C 2.946872 -1.035398 -1.417433
H 2.369272 -1.949204 -1.205512
H 2.841133 -0.808623 -2.490970
C 3.688854 1.580100 1.184984
C 2.469907 2.487667 0.988568
H 2.357742 3.159191 1.854187
H 2.633727 3.137593 0.111903
C 1.166936 1.689363 0.797018
C -0.046789 2.619171 0.839070
H 0.056904 3.445008 0.117687
H -0.146960 3.067283 1.839908
H -0.981540 2.095631 0.600296
H 1.095326 1.005245 1.659131
H 4.631913 2.141187 1.080874
H 3.699240 1.159551 2.207044
C 1.015738 1.606555 -1.772017
H 1.736384 2.434622 -1.838211
H -0.001977 2.019967 -1.809344
H 1.149785 0.972903 -2.661776
H 1.128152 -1.483432 1.057884
H -2.539095 -3.498522 0.494832
H -2.388393 -0.524044 1.354440
H -3.652832 -1.668412 1.814425
H -3.093784 -0.835495 -1.086534
H -4.444999 -1.825833 -0.534403
O -5.259561 0.402441 -1.407833
H -5.944346 1.084873 -1.345657

4-c25, ΔG = 3.7098 kcal/mol, population = 0.09 %

O -4.906227 -0.180640 -0.668026
H -4.713727 0.692099 -1.036470
C -3.684089 -0.791930 -0.306012
H -3.914183 -1.847995 -0.085067
H -2.958761 -0.790825 -1.138387
C -3.030187 -0.163249 0.941144
C -3.950742 -0.309262 2.153668
H -3.506598 0.177093 3.035619
H -4.105673 -1.375005 2.386811
H -4.931676 0.144625 1.950579
C -2.669045 1.315620 0.716442
C -1.842051 1.569260 -0.556900
C -1.099107 2.879296 -0.562886
C 0.162019 3.076062 -0.134003
C 0.814084 4.432693 -0.189048
H 1.723479 4.413501 -0.814835
H 1.138593 4.754104 0.816570
H 0.137086 5.198020 -0.596378

C 1.010642 1.962679 0.434426
H 1.358371 2.268263 1.436122
C 2.234506 1.595051 -0.434189
H 3.092314 2.238181 -0.185046
H 2.010418 1.801062 -1.493811
C 2.674722 0.108801 -0.314396
C 1.527311 -0.758149 -0.774535
C 0.981074 -1.772518 -0.080540
C -0.188421 -2.270888 -0.820492
O -1.003534 -3.112808 -0.505828
O -0.282220 -1.579768 -1.990652
C 0.768614 -0.606450 -2.062781
H 0.314303 0.387903 -2.188546
H 1.387605 -0.814894 -2.950466
C 1.470069 -2.273036 1.235415
C 2.894070 -1.754472 1.463653
H 3.205052 -1.948811 2.501942
H 3.596823 -2.308144 0.816767
C 3.001158 -0.246317 1.177546
C 4.342783 0.314072 1.652814
H 4.447172 1.386402 1.427089
H 5.191722 -0.212671 1.190066
H 4.436555 0.194890 2.743311
H 2.214718 0.228569 1.786007
H 1.428777 -3.374046 1.261788
H 0.792689 -1.920171 2.033684
C 3.879314 -0.129077 -1.249057
H 4.700789 0.562486 -1.014793
H 3.597150 0.038907 -2.299476
H 4.256833 -1.158835 -1.163042
H 0.393340 1.068131 0.592388
H -1.653570 3.750305 -0.933711
H -1.143016 0.731072 -0.659871
H -2.498822 1.531384 -1.442517
H -2.086739 1.636823 1.595113
H -3.587052 1.925462 0.715105
O -1.790777 -0.835137 1.187433
H -1.875744 -1.774554 0.961068

4-c18, ΔG = 3.7374 kcal/mol, population = 0.08 %

O 3.152131 2.148809 0.315845
H 2.488886 2.839540 0.139759
C 2.526314 0.906111 0.060922
H 1.596814 0.807031 0.654198
H 2.261285 0.809476 -1.004767
C 3.483046 -0.215882 0.481549
C 4.696107 -0.272840 -0.453439
H 4.405341 -0.529920 -1.483636
H 5.413690 -1.024677 -0.091632
H 5.194911 0.707558 -0.476622
C 2.733421 -1.553633 0.558084
C 2.050130 -2.011698 -0.742805
C 1.152028 -3.211149 -0.561556
C -0.117607 -3.189703 -0.115051
C -0.923418 -4.455524 0.024996
H -1.804296 -4.448438 -0.640082
H -1.312571 -4.563359 1.052885
H -0.326460 -5.347487 -0.215257
C -0.816912 -1.917283 0.307144
H -1.101095 -2.029221 1.367545
C -2.071202 -1.572613 -0.513063
H -2.876063 -2.290227 -0.293868
H -1.849537 -1.696531 -1.586415
C -2.620986 -0.135055 -0.289971
C -1.565956 0.862839 -0.703498
C -1.143971 1.910977 0.030506
C -0.040585 2.567035 -0.686609
O 0.687535 3.471818 -0.328777
O 0.119230 1.950362 -1.888235
C -0.795645 0.851701 -1.992935
H -0.214185 -0.071059 -2.146657
H -1.435014 1.001477 -2.877424
C -1.692435 2.307129 1.360070
C -3.038242 1.605669 1.569844
H -3.360714 1.718049 2.616477
H -3.809966 2.094412 0.950396
C -2.960757 0.109010 1.220994
C -4.213124 -0.633995 1.689143
H -5.129251 -0.197325 1.262367
H -4.299629 -0.574066 2.785022
H -4.188709 -1.700136 1.417107
H -2.108892 -0.288362 1.796154
H -1.792521 3.403158 1.415600
H -0.979139 2.025844 2.155766
C -3.856007 0.057463 -1.197755
H -4.614278 -0.710731 -0.990823
H -3.579675 -0.031138 -2.259050

H -4.313760 1.046518 -1.050303
H -0.119202 -1.069525 0.276032
H 1.590833 -4.187580 -0.799412
H 1.467838 -1.177018 -1.160372
H 2.816593 -2.245524 -1.498164
H 1.975529 -1.451459 1.351323
H 3.437938 -2.328602 0.903572
O 3.918379 0.069981 1.812417
H 4.046630 1.032913 1.830141

4-c16, ΔG = 3.7475 kcal/mol, population = 0.08 %

O -5.382579 0.661245 0.087361
H -5.301400 0.012511 -0.632093
C -4.577414 0.139114 1.122085
H -4.366783 0.950464 1.836971
H -5.104146 -0.665879 1.672926
C -3.263467 -0.433988 0.568349
C -2.533919 -1.224052 1.654492
H -2.319070 -0.603141 2.537003
H -1.583518 -1.624247 1.275650
H -3.156307 -2.074263 1.971429
C -2.405726 0.686384 -0.060915
C -1.533392 1.508209 0.898029
C -0.813136 2.617810 0.185214
C 0.509012 2.871829 0.133535
C 1.021761 4.073651 -0.622355
H 0.198484 4.668776 -1.043124
H 1.687413 3.786642 -1.453737
H 1.618807 4.725806 0.039616
C 1.557715 2.064466 0.872198
H 1.955551 2.708145 1.676560
C 2.752268 1.557110 0.023701
H 3.696654 1.892075 0.476112
H 2.737295 2.019938 -0.974703
C 2.856583 0.018642 -0.170107
C 1.599397 -0.500050 -0.820732
C 0.894670 -1.577524 -0.421704
C -0.265460 -1.726179 -1.311277
O -1.196523 -2.506695 -1.248861
O -0.201877 -0.766387 -2.270150
C 0.933201 0.079879 -2.033622
H 0.568466 1.105581 -1.865906
H 1.574402 0.073558 -2.928832
C 1.251492 -2.462295 0.726074
C 2.712084 -2.213460 1.116159
H 2.926769 -2.688394 2.085838
H 3.376528 -2.696591 0.379360
C 3.046380 -0.713400 1.202184
C 4.431055 -0.503892 1.819326
H 4.715488 0.558442 1.855137
H 5.211256 -1.044361 1.261278
H 4.443115 -0.884147 2.852336
H 2.309200 -0.271045 1.893364
H 1.078253 -3.517003 0.458415
H 0.584068 -2.252906 1.580888
C 4.037206 -0.259255 -1.129400
H 4.208521 -1.338191 -1.255509
H 4.961688 0.197658 -0.749124
H 3.843429 0.169295 -2.123848
H 1.081182 1.219582 1.385393
H -1.472827 3.303731 -0.362492
H -2.173754 1.948209 1.685652
H -0.823343 0.847676 1.414599
H -3.093533 1.352528 -0.606216
H -1.760818 0.237953 -0.827162
O -3.700305 -1.317453 -0.472515
H -2.915100 -1.738852 -0.869271

Coordinates of the dominating conformers of **5**

5-c12, ΔG = 0.0000 kcal/mol, population = 32.04 %

O -2.685060 -1.979803 1.242478
C -3.564008 -1.518190 0.536096
O -3.716407 -0.212195 0.329181
C -2.697688 0.674177 0.828512
C -2.911301 2.044814 0.196449
C -4.190005 2.700997 0.722306
H -5.057554 2.036432 0.593394
H -4.095309 2.931473 1.796925
H -4.397968 3.643057 0.191679
H -3.024372 1.872217 -0.888991
C -1.677421 2.939902 0.403372
C -0.459961 2.511799 -0.431000
C 0.737096 3.406215 -0.272031
C 1.923582 3.098911 0.286617

C 3.039164 4.108620 0.364374
H 2.756680 5.071302 -0.086439
H 3.944664 3.741961 -0.149926
H 3.332055 4.287663 1.414028
C 2.242548 1.741475 0.870027
H 2.614397 1.880915 1.899169
C 3.285534 0.931355 0.057387
H 4.267361 0.959732 0.553254
H 3.441372 1.401879 -0.926909
C 2.900576 -0.555394 -0.178339
C 1.601405 -0.597158 -0.943688
C 0.491205 -1.270524 -0.587392
C -0.553946 -1.026423 -1.604555
O -1.698889 -1.409784 -1.672303
O -0.025292 -0.203325 -2.558662
C 1.327561 0.124491 -2.231568
H 1.416425 1.218362 -2.135801
H 1.983793 -0.202844 -3.053841
C 0.377867 -2.139869 0.639411
C 1.793167 -2.526573 1.064374
H 1.745437 -3.056924 2.028002
H 2.195305 -3.238527 0.322883
C 2.706814 -1.297775 1.188080
C 4.024044 -1.654403 1.879758
H 4.554199 -2.464762 1.356239
H 3.828273 -1.998305 2.907008
H 4.703166 -0.790382 1.942349
H 2.177971 -0.592120 1.849375
H -0.079864 -1.538484 1.447974
O -0.398583 -3.297611 0.418927
H -1.321529 -3.040732 0.599879
C 3.993655 -1.218215 -1.044633
H 4.979863 -1.119028 -0.570354
H 4.055382 -0.739621 -2.033141
H 3.788611 -2.288001 -1.199350
H 1.318347 1.157673 0.966883
H 0.608644 4.427776 -0.653423
H -0.761365 2.497222 -1.494039
H -0.196663 1.476642 -0.181578
H -1.947150 3.977185 0.142570
H -1.404389 2.957368 1.474061
H -2.765307 0.721808 1.927972
H -1.719775 0.249166 0.571479
C -4.565623 -2.335970 -0.225698
H -4.142145 -2.508110 -1.228111
H -4.714718 -3.304181 0.267784
H -5.518079 -1.802295 -0.339254

5-c1, ΔG = 0.4876 kcal/mol, population = 14.06 %

O -1.098628 0.693464 -0.918504
C -1.842648 1.613979 -1.184740
O -2.984665 1.858453 -0.535444
C -3.318032 1.082437 0.638349
C -4.185604 -0.144785 0.339848
C -5.381768 0.225498 -0.541892
H -5.048687 0.524069 -1.548176
H -6.064738 -0.630806 -0.651826
H -5.953377 1.065005 -0.114703
H -4.573170 -0.444525 1.331901
C -3.425899 -1.358725 -0.223688
C -2.316102 -1.887943 0.696674
C -1.718824 -3.190034 0.239433
C -0.494355 -3.395790 -0.281155
C -0.036320 -4.777850 -0.673380
H 0.862120 -5.077458 -0.105945
H 0.248131 -4.810735 -1.740091
H -0.815135 -5.534906 -0.498791
C 0.509739 -2.289117 -0.511003
H 0.879247 -2.375111 -1.547101
C 1.711890 -2.330101 0.452112
H 2.393575 -3.151437 0.182755
H 1.353370 -2.566982 1.467839
C 2.528445 -1.010504 0.526823
C 1.625275 0.091644 1.021630
C 1.484062 1.294738 0.444669
C 0.469262 2.060924 1.172348
O 0.037761 3.172883 0.943691
O 0.032140 1.307190 2.218021
C 0.711860 0.041499 2.214515
H -0.041107 -0.757516 2.149942
H 1.253167 -0.072353 3.167344
C 2.194510 1.772654 -0.781750
C 3.425968 0.895833 -0.980652
H 3.879096 1.109775 -1.961008
H 4.170053 1.170141 -0.213599
C 3.067695 -0.598694 -0.888769
C 4.227710 -1.471702 -1.370730

H 5.148162 -1.276652 -0.799189
H 4.445695 -1.260606 -2.428963
H 3.998707 -2.544981 -1.287283
H 2.231113 -0.750617 -1.589239
H 1.509281 1.637662 -1.643636
O 2.575131 3.135576 -0.669874
H 1.787889 3.620677 -0.372857
C 3.671177 -1.198054 1.548607
H 3.267887 -1.386378 2.555021
H 4.311788 -0.305654 1.604100
H 4.297596 -2.059861 1.278757
H 0.020164 -1.309193 -0.448561
H -2.375252 -4.064645 0.341584
H -2.740095 -2.029694 1.708240
H -1.541149 -1.118131 0.782418
H -4.161182 -2.162474 -0.403551
H -2.992263 -1.113010 -1.207054
H -2.392733 0.818823 1.166301
H -3.886578 1.785965 1.261963
C -1.563607 2.648242 -2.240277
H -0.980500 2.200357 -3.054819
H -2.487434 3.100912 -2.621813
H -0.954361 3.437420 -1.770077

5-c14, ΔG = 0.6275 kcal/mol, population = 11.10 %

O -1.666019 1.552992 1.907847
C -2.484710 2.121066 1.213553
O -3.527053 1.500153 0.652831
C -3.667202 0.080263 0.865684
C -4.591134 -0.488602 -0.201142
C -6.025619 0.023877 -0.044200
H -6.688679 -0.424195 -0.800558
H -6.430792 -0.219781 0.950786
H -6.063554 1.118013 -0.166708
H -4.589649 -1.578002 -0.019728
C -4.068980 -0.240622 -1.627297
C -2.615979 -0.663536 -1.890188
C -2.351440 -2.114000 -1.582272
C -1.206114 -2.656844 -1.133852
C -1.091910 -4.133499 -0.854999
H -0.339543 -4.601407 -1.514365
H -2.049228 -4.656346 -0.996545
H -0.750984 -4.317275 0.179128
C 0.050136 -1.853519 -0.865642
H 0.917481 -2.476255 -1.136475
C 0.167309 -1.418439 0.603377
H 0.009571 -2.289653 1.257238
H -0.652472 -0.722514 0.838096
C 1.497495 -0.736963 1.020068
C 1.756030 0.467216 0.150437
C 2.935149 0.770881 -0.418269
C 2.809650 2.048804 -1.130973
O 3.656256 2.669410 -1.740553
O 1.533073 2.492950 -0.988324
C 0.785185 1.562723 -0.190465
H -0.073649 1.207028 -0.780809
H 0.392807 2.078115 0.698421
C 4.201471 -0.023913 -0.313268
C 4.067608 -0.970917 0.874979
H 4.892604 -1.699608 0.862181
H 4.180155 -0.373043 1.794890
C 2.717898 -1.711344 0.873616
C 2.723293 -2.841072 1.905887
H 3.496503 -3.581599 1.649903
H 1.759789 -3.370681 1.947099
H 2.947805 -2.466417 2.916369
H 2.622318 -2.177858 -0.121106
H 4.318641 -0.622898 -1.241063
O 5.329164 0.818086 -0.134389
H 5.262040 1.520125 -0.803002
C 1.329205 -0.239358 2.475557
H 1.061436 -1.075358 3.137500
H 0.520731 0.502250 2.536299
H 2.253719 0.220630 2.853993
H 0.096144 -0.971920 -1.522215
H -3.196199 -2.791729 -1.761864
H -1.929666 -0.013983 -1.324834
H -2.395891 -0.462278 -2.955510
H -4.730723 -0.779881 -2.326776
H -4.176350 0.830281 -1.865753
H -2.675558 -0.386576 0.828335
H -4.074937 -0.081555 1.876322
C -2.428037 3.576210 0.835236
H -1.845656 4.131363 1.580568
H -1.922525 3.663797 -0.140694
H -3.435447 4.000093 0.731508

5-c13, ΔG = 0.6790 kcal/mol, population = 10.17 %

O -0.877089 -1.739895 -0.311875
C -1.676598 -2.648848 -0.231490
O -2.881859 -2.528035 0.339579
C -3.264597 -1.251558 0.887134
C -3.978384 -0.370556 -0.140171
C -5.191987 -1.092157 -0.731232
H -4.910022 -2.063074 -1.164345
H -5.953000 -1.276837 0.046173
H -5.659030 -0.485186 -1.522220
H -3.264375 -0.154056 -0.953978
C -4.383367 0.962611 0.513416
C -3.231143 1.964102 0.718652
C -2.783471 2.618825 -0.559663
C -1.602581 2.468726 -1.185336
C -1.279180 3.216033 -2.452710
H -2.094071 3.889152 -2.757817
H -1.077788 2.514887 -3.281767
H -0.362415 3.820206 -2.331375
C -0.504110 1.576345 -0.651699
H -0.934933 0.691312 -0.171461
C 0.428114 2.304300 0.328088
H -0.169871 2.710579 1.158469
H 0.872442 3.183072 -0.169716
C 1.573734 1.443539 0.923088
C 2.409156 0.879595 -0.197203
C 2.787181 -0.404346 -0.310848
C 3.610853 -0.555912 -1.517313
O 4.155673 -1.549431 -1.951672
O 3.709134 0.658225 -2.122981
C 2.985195 1.636675 -1.362173
H 2.215926 2.089185 -2.007480
H 3.683102 2.431170 -1.053056
C 2.458261 -1.510726 0.644354
C 2.038235 -0.877781 1.967324
H 1.617395 -1.651363 2.628306
H 2.945605 -0.489880 2.461356
C 1.003436 0.242644 1.758593
C 0.386006 0.666231 3.092890
H 1.150708 0.989735 3.816197
H -0.154474 -0.181596 3.541719
H -0.335686 1.488617 2.974057
H 0.202236 -0.201939 1.151690
H 1.601888 -2.080380 0.232346
O 3.572663 -2.367155 0.851375
H 3.914390 -2.597331 -0.028309
C 2.471642 2.361765 1.782376
H 1.874792 2.873494 2.550631
H 2.948103 3.137160 1.164029
H 3.267815 1.791568 2.283033
H 0.083064 1.184879 -1.499170
H -3.523931 3.287271 -1.018786
H -2.389605 1.473493 1.229924
H -3.582589 2.751271 1.408732
H -5.155938 1.441011 -0.112315
H -4.869268 0.752800 1.483135
H -3.946984 -1.495885 1.714555
H -2.373431 -0.757156 1.295957
C -1.432779 -4.052091 -0.717205
H -1.193795 -4.690703 0.148539
H -2.333047 -4.462677 -1.194598
H -0.586014 -4.062540 -1.413667

5-c11, ΔG = 0.8365 kcal/mol, population = 7.80 %

O -1.730400 1.339204 1.524591
C -2.799315 1.884226 1.708909
O -3.733038 2.022876 0.759918
C -3.490626 1.454673 -0.541220
C -4.116400 0.066878 -0.678123
C -5.625157 0.119578 -0.426953
H -6.129248 0.718054 -1.205019
H -6.060300 -0.891630 -0.445233
H -5.852569 0.573818 0.548815
H -3.653855 -0.585936 0.083680
C -3.791384 -0.510172 -2.068020
C -2.390810 -1.127380 -2.205699
C -2.253565 -2.414593 -1.436583
C -1.194447 -2.865928 -0.742393
C -1.236257 -4.200593 -0.041349
H -1.014166 -4.095965 1.034699
H -0.468436 -4.881610 -0.449364
H -2.217510 -4.687363 -0.140587
C 0.104218 -2.103240 -0.592552
H 0.935012 -2.819825 -0.697674

C 0.201328 -1.389162 0.764306
H 0.045738 -2.118300 1.573995
H -0.628753 -0.671828 0.848216
C 1.522566 -0.628563 1.052126
C 1.736900 0.447941 0.018654
C 2.907700 0.712498 -0.586607
C 2.738560 1.867985 -1.476306
O 3.566181 2.427381 -2.166665
O 1.444838 2.276330 -1.403661
C 0.725338 1.438497 -0.485452
H -0.106401 0.959768 -1.024354
H 0.288310 2.058465 0.310433
C 4.201629 -0.014004 -0.376344
C 4.096773 -0.806755 0.922421
H 4.942971 -1.506809 0.998608
H 4.191402 -0.094975 1.759316
C 2.768531 -1.580162 1.016071
C 2.805115 -2.582283 2.171526
H 3.011219 -2.086839 3.132804
H 3.603191 -3.322102 2.004828
H 1.858388 -3.133982 2.270763
H 2.684226 -2.160811 0.082198
H 4.346195 -0.721985 -1.219837
O 5.297067 0.885285 -0.307138
H 5.210182 1.488075 -1.064398
C 1.367788 0.063360 2.427780
H 2.275861 0.616538 2.708376
H 1.161298 -0.682948 3.208431
H 0.521515 0.763335 2.409412
H 0.227309 -1.375838 -1.408661
H -3.138537 -3.063650 -1.479241
H -1.620877 -0.400679 -1.905097
H -2.210956 -1.325111 -3.279013
H -4.535803 -1.287869 -2.308478
H -3.927721 0.278849 -2.828335
H -3.957280 2.153910 -1.250637
H -2.409376 1.429593 -0.723748
C -3.252997 2.468941 3.018451
H -3.992215 1.789971 3.473173
H -2.398220 2.575478 3.696586
H -3.746679 3.437591 2.859346

5-c10, ΔG = 1.0981 kcal/mol, population = 5.01 %

O -2.440177 -0.639216 -1.816936
C -3.622006 -0.722172 -1.557209
O -4.109527 -0.779822 -0.311115
C -3.199621 -0.680443 0.800829
C -3.136881 0.746407 1.348282
C -4.519816 1.220678 1.800887
H -4.874826 0.625530 2.659529
H -4.488518 2.276230 2.112656
H -5.259795 1.122920 0.992784
H -2.789459 1.405024 0.532891
C -2.109841 0.816447 2.491636
C -0.641542 0.858691 2.028611
C -0.234611 2.196803 1.475760
C -0.002622 2.541828 0.194950
C 0.413546 3.947468 -0.158346
H -0.268718 4.383921 -0.908590
H 1.421159 3.968943 -0.606482
H 0.426032 4.603014 0.724426
C -0.194835 1.604796 -0.976008
H -0.622635 0.655051 -0.639060
C 1.009460 1.326765 -1.896818
H 1.452892 2.272857 -2.243823
H 0.614467 0.841191 -2.804263
C 2.149853 0.425935 -1.343544
C 1.555652 -0.827439 -0.753863
C 1.826288 -1.308806 0.471188
C 1.062518 -2.544566 0.681825
O 1.048442 -3.277505 1.649877
O 0.325132 -2.785322 -0.433833
C 0.587617 -1.767120 -1.418101
H -0.368665 -1.301676 -1.697050
H 1.018635 -2.249940 -2.310031
C 2.785957 -0.720795 1.459853
C 3.732396 0.198987 0.696503
H 4.346547 0.772609 1.407887
H 4.420973 -0.435952 0.113101
C 2.968478 1.165695 -0.225688
C 3.914494 2.236519 -0.774055
H 4.786664 1.791889 -1.277944
H 4.292813 2.861336 0.049512
H 3.416713 2.904291 -1.492916
H 2.224046 1.672130 0.405364
H 2.214202 -0.119088 2.196310
O 3.525149 -1.731026 2.127769

H 2.882702 -2.398964 2.420443
C 3.055324 0.015136 -2.527496
H 3.416064 0.902994 -3.065671
H 2.502496 -0.605025 -3.248666
H 3.927286 -0.560887 -2.184112
H -0.975326 2.053023 -1.616990
H -0.127072 2.985853 2.231800
H -0.452318 0.056614 1.302294
H -0.000632 0.633907 2.898394
H -2.314850 1.713667 3.099418
H -2.262004 -0.045756 3.165096
H -3.602658 -1.362033 1.564675
H -2.212438 -1.043162 0.487405
C -4.726302 -0.761089 -2.578577
H -4.303483 -0.900761 -3.580244
H -5.437429 -1.565584 -2.343076
H -5.280710 0.190188 -2.544433

5-c27, ΔG = 1.1967 kcal/mol, population = 4.24 %

O -0.939426 -1.882043 -0.973415
C -1.830278 -2.255585 -0.237915
O -3.064308 -1.738014 -0.258358
C -3.331237 -0.652102 -1.170959
C -4.501031 0.167528 -0.642995
C -5.823511 -0.599421 -0.730146
H -6.047451 -0.895522 -1.767301
H -5.783504 -1.514485 -0.117659
H -6.660747 0.015069 -0.363682
H -4.557955 1.037957 -1.320855
C -4.261748 0.690457 0.784737
C -2.891285 1.338157 1.035842
C -2.570581 2.474408 0.105362
C -1.417345 2.670762 -0.559349
C -1.205083 3.874570 -1.438628
H -0.325580 4.455079 -1.107667
H -2.077440 4.544798 -1.441448
H -0.998078 3.569024 -2.479452
C -0.232761 1.734486 -0.429278
H -0.571550 0.690461 -0.396986
C 0.616007 2.040673 0.816132
H -0.050619 2.164148 1.682795
H 1.114936 3.015722 0.686229
C 1.683591 0.974916 1.185483
C 2.551871 0.689826 -0.011884
C 2.833847 -0.532814 -0.491563
C 3.727922 -0.397357 -1.649671
O 4.220792 -1.264112 -2.341042
O 3.967419 0.926145 -1.852001
C 3.274076 1.699329 -0.861354
H 2.598251 2.404492 -1.370256
H 4.012792 2.285073 -0.291172
C 2.361113 -1.836203 0.077279
C 1.924719 -1.584161 1.517002
H 1.413980 -2.477598 1.908408
H 2.832268 -1.437043 2.127234
C 0.992194 -0.365002 1.627318
C 0.360819 -0.293349 3.019434
H -0.263738 -1.182576 3.195732
H -0.284771 0.589322 3.138360
H 1.123459 -0.266795 3.812702
H 0.179936 -0.541373 0.907061
H 1.483716 -2.178573 -0.505368
O 3.389799 -2.815900 0.052645
H 3.761279 -2.807822 -0.844839
C 2.575471 1.551660 2.307420
H 1.962794 1.877901 3.159639
H 3.136373 2.428451 1.951319
H 3.301732 0.807328 2.665941
H 0.390462 1.811764 -1.334161
H -3.368147 3.218725 -0.019151
H -2.104683 0.570370 0.997942
H -2.883290 1.710131 2.077503
H -5.057841 1.418853 1.016290
H -4.390462 -0.141803 1.496394
H -2.427213 -0.040696 -1.272786
H -3.559704 -1.081250 -2.159744
C -1.681175 -3.302161 0.832276
H -2.596622 -3.900177 0.932477
H -0.818944 -3.943025 0.612530
H -1.507113 -2.793106 1.794093

5-c5, ΔG = 1.3404 kcal/mol, population = 3.33 %

O -1.104842 -1.365086 -0.979646
C -1.553079 -2.300003 -0.348443
O -2.282879 -2.158896 0.765000
C -2.562432 -0.827237 1.244245

C -3.750122 -0.178208 0.527791
C -4.954412 -1.123172 0.482229
H -5.790326 -0.658558 -0.063340
H -4.707641 -2.071631 -0.016401
H -5.307616 -1.360240 1.500459
H -3.434593 0.043628 -0.505445
C -4.133893 1.147596 1.207513
C -3.086127 2.277310 1.152140
C -2.791788 2.737066 -0.249033
C -1.661959 2.569376 -0.961824
C -1.580776 3.042734 -2.391332
H -0.814012 3.825287 -2.520859
H -2.542151 3.450244 -2.736472
H -1.296118 2.215044 -3.065274
C -0.456433 1.832507 -0.421100
H -0.525403 1.784863 0.672345
C 0.913126 2.395300 -0.811231
H 1.019151 3.429606 -0.445955
H 0.997184 2.458440 -1.908008
C 2.116978 1.557835 -0.298709
C 1.991767 0.143227 -0.807709
C 2.124001 -0.963571 -0.059080
C 1.965820 -2.142616 -0.917078
O 2.020676 -3.318864 -0.611249
O 1.757053 -1.724578 -2.188004
C 1.712996 -0.290001 -2.220485
H 0.712942 0.014533 -2.564344
H 2.461594 0.069885 -2.943397
C 2.414250 -1.007424 1.409421
C 3.002832 0.341648 1.809308
H 3.070739 0.406025 2.906259
H 4.033340 0.388623 1.418296
C 2.161681 1.512685 1.270746
C 2.604950 2.833958 1.902540
H 3.675178 3.027408 1.732206
H 2.445034 2.803524 2.991266
H 2.038691 3.691076 1.508304
H 1.128656 1.323460 1.603871
H 1.455809 -1.158056 1.951040
O 3.322808 -2.047709 1.731819
H 3.004143 -2.846693 1.279551
C 3.412543 2.164432 -0.883585
H 3.420373 2.085115 -1.980817
H 4.307010 1.651140 -0.501250
H 3.488188 3.231241 -0.630139
H -0.527766 0.786382 -0.761180
H -3.634836 3.229734 -0.751604
H -2.169481 1.968437 1.675657
H -3.490725 3.126912 1.730409
H -5.062901 1.510338 0.735213
H -4.389940 0.946015 2.263322
H -2.789032 -0.964212 2.311875
H -1.653014 -0.221612 1.146094
C -1.324916 -3.744942 -0.698936
H -1.387664 -3.865272 -1.788893
H -0.299279 -4.010472 -0.397471
H -2.039147 -4.405287 -0.192680

5-c8, ΔG = 1.4960 kcal/mol, population = 2.56 %

O -2.258198 0.830893 -2.003797
C -3.300371 0.924273 -1.390019
O -3.975273 -0.140587 -0.927745
C -3.350241 -1.429361 -1.090152
C -2.326571 -1.686203 0.014292
C -2.997140 -1.777038 1.385903
H -3.628035 -2.679414 1.456024
H -2.254147 -1.811503 2.195277
H -3.632416 -0.896466 1.561337
H -1.651162 -0.813759 0.015112
C -1.460009 -2.905136 -0.335289
C -0.354069 -3.172266 0.708851
C 0.879871 -3.850255 0.167238
C 1.904292 -3.226908 -0.445019
C 3.112504 -3.979334 -0.937195
H 4.033788 -3.618803 -0.447228
H 3.258225 -3.825669 -2.021020
H 3.027776 -5.059582 -0.748040
C 1.915493 -1.734194 -0.689113
H 2.117002 -1.561787 -1.759852
C 2.950273 -0.959212 0.150896
H 3.956249 -1.071455 -0.281581
H 3.010294 -1.405811 1.157172
C 2.644597 0.557722 0.313025
C 1.328921 0.706884 1.034656
C 0.287404 1.441089 0.606945
C -0.822388 1.293137 1.558416
O -1.933136 1.782078 1.524307

O -0.416704 0.471978 2.563893
C 0.944347 0.072775 2.342466
H 0.993003 -1.026112 2.332845
H 1.559116 0.433837 3.182362
C 0.265327 2.301577 -0.620857
C 1.712325 2.569279 -1.021542
H 1.738311 3.070428 -2.001489
H 2.153252 3.265239 -0.287556
C 2.517508 1.258540 -1.085562
C 3.863321 1.466692 -1.781604
H 3.703947 1.785820 -2.822983
H 4.460906 0.542662 -1.804924
H 4.463087 2.245522 -1.286010
H 1.927855 0.575063 -1.717200
H -0.245828 1.748911 -1.429563
O -0.411948 3.528195 -0.378843
H -1.254609 3.304082 0.047298
C 3.752545 1.192354 1.181250
H 3.600358 2.275601 1.297456
H 4.741521 1.026781 0.731825
H 3.768689 0.743337 2.185583
H 0.916916 -1.315442 -0.504483
H 0.934823 -4.939834 0.278006
H -0.764330 -3.766107 1.540217
H -0.073584 -2.205402 1.150171
H -2.090855 -3.803219 -0.459649
H -0.988422 -2.722406 -1.314801
H -4.173729 -2.156648 -1.049544
H -2.875483 -1.473356 -2.079885
C -3.976839 2.216432 -1.028762
H -3.493368 3.044980 -1.559928
H -5.050117 2.176452 -1.262498
H -3.865415 2.365211 0.055650

5-c18, ΔG = 1.6579 kcal/mol, population = 1.95 %

O 1.000410 -1.347833 -0.534437
C 1.752413 -1.989675 -1.237346
O 2.961085 -1.549175 -1.612774
C 3.378996 -0.259505 -1.113071
C 3.914484 -0.360789 0.315201
C 5.166927 -1.239955 0.365515
H 5.496511 -1.399721 1.404002
H 4.979609 -2.224609 -0.088433
H 5.998593 -0.766801 -0.183869
H 3.124776 -0.839513 0.919197
C 4.176482 1.023483 0.931802
C 2.919649 1.885804 1.186925
C 2.539516 2.831229 0.080907
C 1.383349 2.884083 -0.604798
C 1.137793 3.951361 -1.640193
H 1.969649 4.668314 -1.703444
H 0.215049 4.514279 -1.413531
H 0.987448 3.503251 -2.638380
C 0.246663 1.904181 -0.407353
H -0.266755 1.784668 -1.374440
C -0.769119 2.345128 0.657527
H -1.143625 3.354667 0.425609
H -0.249251 2.439016 1.625925
C -1.989034 1.400253 0.845675
C -1.506584 0.003256 1.149256
C -1.926087 -1.112218 0.532918
C -1.223826 -2.268865 1.099932
O -1.329646 -3.443862 0.807340
O -0.407357 -1.829549 2.089858
C -0.486573 -0.400058 2.177842
H 0.510868 0.013691 1.967947
H -0.769276 -0.123051 3.205534
C -2.943561 -1.186552 -0.561172
C -3.764665 0.098001 -0.522240
H -4.411773 0.152821 -1.411399
H -4.428353 0.048635 0.357770
C -2.865950 1.346183 -0.456472
C -3.688292 2.615861 -0.688322
H -4.514237 2.703068 0.034264
H -4.132743 2.598083 -1.695310
H -3.075233 3.526535 -0.613762
H -2.160068 1.257458 -1.297899
H -2.406278 -1.243982 -1.531864
O -3.792554 -2.313218 -0.408841
H -3.213305 -3.073759 -0.233212
C -2.805042 1.900188 2.059012
H -3.085483 2.955299 1.931902
H -2.214708 1.825706 2.984470
H -3.722965 1.309752 2.195962
H 0.631426 0.907608 -0.156809
H 3.303286 3.583920 -0.156023
H 3.108903 2.496624 2.087527

H 2.078375 1.227221 1.450216
H 4.685956 0.854029 1.894034
H 4.895913 1.582447 0.305862
H 4.169000 0.069077 -1.803622
H 2.538491 0.439388 -1.181137
C 1.440521 -3.349633 -1.799174
H 2.288360 -4.032386 -1.645196
H 0.536263 -3.741593 -1.318350
H 1.276472 -3.266114 -2.885268

5-c17, ΔG = 1.8712 kcal/mol, population = 1.36 %

O 2.520526 -1.688010 -0.951060
C 3.657994 -1.701557 -1.372223
O 4.532342 -0.706212 -1.177751
C 4.109874 0.431463 -0.396426
C 4.212085 0.169336 1.107178
C 5.607442 -0.339919 1.482325
H 6.372257 0.427265 1.272470
H 5.659535 -0.582074 2.555158
H 5.873713 -1.243339 0.914796
H 3.473538 -0.612729 1.355425
C 3.857462 1.422456 1.926371
C 2.402937 1.916695 1.841674
C 2.065321 2.690702 0.594659
C 0.932124 2.631074 -0.126789
C 0.734844 3.483345 -1.353548
H 0.527648 2.861380 -2.242131
H 1.616326 4.104404 -1.571044
H -0.137764 4.149621 -1.233571
C -0.205200 1.688042 0.203115
H -0.204754 1.455899 1.276182
C -0.121000 0.388620 -0.611045
H 0.845374 -0.097849 -0.423984
H -0.116477 0.634937 -1.686455
C -1.240600 -0.654977 -0.361448
C -2.585376 -0.042914 -0.651136
C -3.667454 -0.136831 0.139624
C -4.794136 0.549969 -0.504651
O -5.941423 0.658779 -0.124191
O -4.359437 1.069201 -1.684102
C -2.972628 0.748062 -1.870342
H -2.402974 1.684883 -1.975268
H -2.865387 0.174998 -2.805087
C -3.744665 -0.861890 1.449146
C -2.564372 -1.825459 1.525377
H -2.483651 -2.232397 2.545188
H -2.782448 -2.674610 0.855849
C -1.239375 -1.150175 1.127349
C -0.049045 -2.051763 1.464088
H 0.015680 -2.199284 2.553241
H 0.904259 -1.627289 1.119182
H -0.154431 -3.045867 1.002503
H -1.153600 -0.246390 1.752926
H -3.657199 -0.117657 2.268745
O -4.962173 -1.579844 1.574445
H -5.674769 -0.966107 1.330300
C -1.015042 -1.827027 -1.345875
H -1.151590 -1.493759 -2.385766
H -1.719912 -2.650952 -1.161417
H 0.012098 -2.204726 -1.253476
H -1.163712 2.197768 0.003781
H 2.838755 3.398573 0.268216
H 2.232373 2.577241 2.712956
H 1.722141 1.061761 1.975581
H 4.078606 1.191565 2.981060
H 4.543502 2.244497 1.649607
H 4.793736 1.239966 -0.693374
H 3.089564 0.707168 -0.687214
C 4.274657 -2.829364 -2.155635
H 4.828345 -2.439323 -3.021282
H 4.995873 -3.359786 -1.513544
H 3.495441 -3.529414 -2.479082

5-c6, ΔG = 2.0369 kcal/mol, population = 1.03 %

O -2.048669 -1.218974 -1.278283
C -2.549250 -1.834434 -0.356197
O -3.848087 -1.772442 -0.047130
C -4.703900 -0.862614 -0.773602
C -5.192527 0.254295 0.148214
C -6.067843 -0.303829 1.275405
H -5.486339 -0.983745 1.917805
H -6.460844 0.507011 1.907985
H -6.924332 -0.868936 0.874294
H -5.819957 0.901005 -0.493047
C -4.051187 1.114075 0.713022
C -3.181682 1.844258 -0.325487

C -2.245760 2.823895 0.327616
C -0.932769 2.666285 0.573241
C -0.143024 3.730788 1.293563
H 0.268459 3.337048 2.239942
H -0.756770 4.613532 1.525183
H 0.724053 4.066187 0.699113
C -0.133055 1.446468 0.169522
H 0.483979 1.149026 1.033821
C 0.778027 1.700696 -1.054048
H 0.952104 2.780153 -1.178198
H 0.247432 1.385251 -1.967031
C 2.170532 1.011809 -1.017007
C 2.001291 -0.460577 -0.745875
C 2.624220 -1.146263 0.228328
C 2.219563 -2.555166 0.157286
O 2.572316 -3.488469 0.849427
O 1.341681 -2.694358 -0.871589
C 1.146999 -1.422486 -1.519632
H 0.072063 -1.185315 -1.501710
H 1.467455 -1.517310 -2.569665
C 3.628833 -0.593613 1.193415
C 4.175377 0.700070 0.599335
H 4.799619 1.216137 1.345032
H 4.834626 0.429695 -0.243164
C 3.051204 1.636605 0.125382
C 3.618649 3.013819 -0.227436
H 4.045591 3.485324 0.670873
H 2.848468 3.693115 -0.622011
H 4.422190 2.943926 -0.976572
H 2.379237 1.776022 0.988754
H 3.117757 -0.363765 2.152147
O 4.690239 -1.507812 1.415649
H 4.283203 -2.374573 1.582439
C 2.835438 1.175326 -2.401500
H 2.876997 2.234935 -2.689837
H 2.261800 0.646643 -3.176961
H 3.859625 0.773592 -2.404611
H -0.791096 0.593301 -0.037469
H -2.715671 3.749335 0.686179
H -3.846848 2.388162 -1.020368
H -2.625121 1.115254 -0.929692
H -4.496042 1.861907 1.391409
H -3.401214 0.488054 1.349951
H -4.155155 -0.474548 -1.639766
H -5.551918 -1.465852 -1.129028
C -1.782057 -2.714104 0.590857
H -2.423661 -3.490091 1.026767
H -0.918130 -3.152918 0.076855
H -1.403411 -2.080428 1.410087

5-c28, ΔG = 2.2967 kcal/mol, population = 0.66 %

O -2.643224 1.282824 -0.703706
C -3.770625 1.488951 -1.100548
O -4.858438 1.425507 -0.322279
C -4.721261 1.030295 1.059086
C -5.172569 -0.417117 1.262910
C -6.625933 -0.605699 0.815937
H -7.296339 0.110209 1.317890
H -6.721481 -0.451326 -0.270198
H -6.978758 -1.622487 1.047043
H -5.121931 -0.581140 2.355488
C -4.245331 -1.443452 0.593517
C -2.836836 -1.535371 1.193562
C -2.007659 -2.601545 0.529264
C -0.699419 -2.550027 0.223555
C -0.011503 -3.698672 -0.469612
H 0.815402 -4.094210 0.146219
H 0.440113 -3.376003 -1.424532
H -0.705003 -4.523567 -0.689331
C 0.181592 -1.356259 0.524661
H -0.213066 -0.797494 1.384280
C 0.329673 -0.410954 -0.679176
H -0.612713 0.134558 -0.824421
H 0.470995 -1.006288 -1.596955
C 1.497376 0.606406 -0.594346
C 2.811252 -0.132592 -0.566553
C 3.837939 0.143199 0.255353
C 4.957674 -0.754726 -0.056018
O 6.064311 -0.796551 0.439923
O 4.573060 -1.581929 -1.064524
C 3.227020 -1.272655 -1.455198
H 2.605821 -2.171757 -1.318800
H 3.219841 -1.009909 -2.525114
C 3.870558 1.213921 1.303617
C 2.744549 2.199790 1.010350
H 2.612704 2.876729 1.868437
H 3.057275 2.822091 0.155085

C 1.415850 1.485437 0.701599
C 0.255156 2.482033 0.689005
H 0.138438 2.934115 1.686425
H -0.698049 2.009616 0.415578
H 0.439562 3.303421 -0.021463
H 1.240627 0.784626 1.534719
H 3.687581 0.740542 2.291473
O 5.116609 1.892714 1.315195
H 5.806937 1.209188 1.326987
C 1.459441 1.472483 -1.874617
H 2.240496 2.246386 -1.865122
H 0.480555 1.962431 -1.972922
H 1.609592 0.851607 -2.770647
H 1.177274 -1.723358 0.831390
H -2.550142 -3.521640 0.273526
H -2.937273 -1.760241 2.273741
H -2.336531 -0.560121 1.120128
H -4.724872 -2.434903 0.666041
H -4.174211 -1.229414 -0.487634
H -3.682819 1.187099 1.376449
H -5.373687 1.713630 1.620925
C -4.133668 1.826036 -2.521616
H -3.232846 2.103158 -3.081613
H -4.593822 0.941512 -2.990381
H -4.873700 2.637895 -2.549369

5-c21, ΔG = 2.3500 kcal/mol, population = 0.60 %

O -4.500358 1.470355 -0.040882
C -3.491661 1.307695 0.609745
O -2.403088 0.675907 0.129271
C -2.476790 0.165422 -1.213411
C -3.131155 -1.219112 -1.288338
C -3.579278 -1.482933 -2.730196
H -4.049454 -2.474099 -2.820169
H -4.306099 -0.728521 -3.069799
H -2.718911 -1.459152 -3.420455
H -4.030591 -1.186907 -0.649255
C -2.208442 -2.346061 -0.801515
C -1.730275 -2.257021 0.658682
C -0.774869 -3.368985 1.018008
C 0.533095 -3.412691 0.702316
C 1.397330 -4.593298 1.060946
H 1.877677 -5.015818 0.160451
H 0.816543 -5.389650 1.549121
H 2.216857 -4.304018 1.741141
C 1.216236 -2.295709 -0.051938
H 1.518209 -2.673819 -1.044822
C 2.447739 -1.710606 0.659911
H 3.338023 -2.325879 0.460930
H 2.298861 -1.755047 1.751781
C 2.757665 -0.238264 0.287039
C 1.618140 0.637577 0.745403
C 1.061407 1.625256 0.024933
C 0.050930 2.304517 0.846258
O -0.624625 3.276747 0.576409
O -0.004606 1.683700 2.052957
C 0.933756 0.599194 2.083551
H 0.383525 -0.340570 2.252454
H 1.622720 0.751625 2.929148
C 1.435286 2.020483 -1.371543
C 2.808870 1.431636 -1.682425
H 3.016685 1.526788 -2.759249
H 3.561423 2.040976 -1.154691
C 2.913552 -0.046083 -1.261068
C 4.181893 -0.687632 -1.825488
H 4.286873 -1.736853 -1.510586
H 5.086795 -0.146516 -1.508781
H 4.156444 -0.671812 -2.925828
H 2.053164 -0.559043 -1.721752
H 0.688872 1.581864 -2.067707
O 1.469009 3.429689 -1.524134
H 0.647589 3.773623 -1.135118
C 4.027976 0.196816 1.052803
H 4.870827 -0.465347 0.809058
H 3.867335 0.138337 2.139628
H 4.314863 1.229849 0.809797
H 0.497963 -1.488159 -0.247566
H -1.202381 -4.234680 1.538365
H -2.607043 -2.288329 1.326434
H -1.265817 -1.275505 0.828341
H -2.722501 -3.311635 -0.946205
H -1.324504 -2.377617 -1.463296
H -3.034356 0.885053 -1.828206
H -1.434463 0.128989 -1.563937
C -3.276294 1.791913 2.015654
H -2.793115 1.015748 2.624267
H -2.589921 2.651787 1.983030

H -4.235579 2.092907 2.453065

5-c25, ΔG = 2.3538 kcal/mol, population = 0.60 %

O -2.502828 -1.317253 1.936930
C -3.514380 -1.269749 1.268115
O -4.091672 -0.122352 0.874456
C -3.345450 1.097699 1.069177
C -2.560397 1.407955 -0.206257
C -3.490999 1.821549 -1.347210
H -4.289021 1.077312 -1.490855
H -3.965648 2.794234 -1.133824
H -2.929292 1.906299 -2.288788
H -2.078705 0.463103 -0.499625
C -1.440423 2.433618 0.010406
C -0.395177 2.041555 1.068382
C 0.901539 2.785005 0.888521
C 2.141334 2.369946 1.206686
C 3.335519 3.256414 0.951897
H 4.077078 2.770840 0.293982
H 3.865660 3.481830 1.894037
H 3.043151 4.206784 0.482578
C 2.440315 1.059360 1.904994
H 2.967218 1.315921 2.841108
C 3.334500 0.051735 1.149457
H 3.897277 -0.537290 1.888285
H 4.100702 0.592888 0.571620
C 2.639146 -0.969555 0.204981
C 1.828518 -0.267673 -0.854765
C 0.553939 -0.557960 -1.169175
C 0.140930 0.274735 -2.304330
O -0.919284 0.280560 -2.899413
O 1.174176 1.086241 -2.640026
C 2.304058 0.803302 -1.797292
H 2.597385 1.729832 -1.285522
H 3.138768 0.470396 -2.434266
C -0.299638 -1.583291 -0.488760
C 0.625377 -2.611926 0.146545
H 0.032522 -3.300924 0.767501
H 1.095087 -3.210288 -0.652377
C 1.690437 -1.923284 1.019614
C 2.440056 -2.957928 1.862709
H 1.739146 -3.459708 2.547154
H 3.231357 -2.502908 2.477009
H 2.901573 -3.736593 1.236421
H 1.135186 -1.278281 1.720423
H -0.858018 -1.090558 0.327492
O -1.218405 -2.200177 -1.380770
H -1.543666 -1.507476 -1.981751
C 3.749238 -1.768089 -0.519511
H 4.348091 -1.109634 -1.165729
H 3.324288 -2.564369 -1.148002
H 4.435565 -2.225810 0.206544
H 1.508463 0.573080 2.222856
H 0.806814 3.784939 0.445482
H -0.220013 0.956988 1.024430
H -0.799698 2.236925 2.078688
H -0.932344 2.572263 -0.958451
H -1.872962 3.418932 0.261828
H -4.089811 1.877327 1.286348
H -2.687938 0.971562 1.936942
C -4.226815 -2.475922 0.724600
H -5.269206 -2.256825 0.462788
H -3.680036 -2.772627 -0.186151
H -4.165234 -3.303216 1.443482

5-c20, ΔG = 2.3613 kcal/mol, population = 0.59 %

O 4.546839 -1.311339 -0.061975
C 3.537291 -1.176902 0.593758
O 2.424592 -0.587783 0.114375
C 2.472009 -0.088630 -1.233752
C 3.075542 1.317774 -1.326105
C 3.506006 1.583138 -2.773030
H 2.643275 1.521658 -3.457995
H 3.939769 2.589586 -2.875398
H 4.257576 0.851934 -3.109518
H 3.979036 1.324316 -0.691939
C 2.115429 2.415585 -0.844989
C 1.648567 2.323958 0.618731
C 0.654721 3.403568 0.972445
C -0.655657 3.395737 0.663879
C -1.561018 4.547170 1.015753
H -1.007540 5.369111 1.493121
H -2.365924 4.234597 1.703060
H -2.061119 4.942879 0.113822
C -1.301001 2.246778 -0.075503
H -1.621945 2.603532 -1.070351

C -2.506206 1.623641 0.648889
H -3.419565 2.203996 0.449566
H -2.353028 1.683715 1.739416
C -2.764017 0.137497 0.291315
C -1.590850 -0.691867 0.751265
C -1.002320 -1.665361 0.036793
C 0.036658 -2.299603 0.858579
O 0.745935 -3.248942 0.593825
O 0.075876 -1.665872 2.059216
C -0.901137 -0.615942 2.085061
H -0.384556 0.344770 2.242007
H -1.579525 -0.785210 2.935991
C -1.369109 -2.087281 -1.353748
C -2.764805 -1.551640 -1.662335
H -2.974746 -1.664471 -2.737035
H -3.491905 -2.182885 -1.124739
C -2.920956 -0.074794 -1.254062
C -4.214756 0.514862 -1.817257
H -5.097667 -0.055821 -1.490522
H -4.194527 0.489631 -2.917530
H -4.356246 1.562477 -1.511442
H -2.082242 0.464738 -1.724273
H -0.642844 -1.628688 -2.058286
O -1.352571 -3.498205 -1.492791
H -0.516731 -3.808318 -1.106077
C -4.013525 -0.336428 1.068157
H -3.849293 -0.262128 2.153481
H -4.263894 -1.381407 0.836093
H -4.881246 0.292353 0.823261
H -0.554396 1.464411 -0.267299
H 1.052722 4.289629 1.481819
H 2.527103 2.394262 1.281163
H 1.221467 1.327828 0.800829
H 2.593515 3.397557 -1.002089
H 1.227410 2.408713 -1.501997
H 3.051749 -0.793826 -1.844712
H 1.427079 -0.093410 -1.578331
C 3.347650 -1.654632 2.005556
H 2.696755 -2.542054 1.984381
H 4.320144 -1.912339 2.441479
H 2.835656 -0.892834 2.608626

5-c19, ΔG = 2.4674 kcal/mol, population = 0.50 %

O -1.610698 -1.490065 -2.289704
C -2.494385 -0.663281 -2.390854
O -3.519361 -0.574741 -1.537705
C -3.563522 -1.474189 -0.413841
C -4.473567 -0.869757 0.649089
C -4.674624 -1.871822 1.789697
H -3.717925 -2.159242 2.254581
H -5.312853 -1.441738 2.577115
H -5.157648 -2.793416 1.428599
H -5.452347 -0.704208 0.165466
C -3.975730 0.506795 1.125226
C -2.696360 0.503341 1.979026
C -2.204527 1.901704 2.227161
C -0.972415 2.387398 1.998126
C -0.642294 3.839432 2.228531
H -0.238211 4.300595 1.309627
H 0.141944 3.949658 2.998265
H -1.522160 4.419392 2.543828
C 0.169341 1.546943 1.461326
H 1.116033 1.981850 1.816397
C 0.173855 1.480434 -0.074333
H 0.044810 2.493967 -0.483742
H -0.714177 0.917415 -0.405283
C 1.430039 0.850466 -0.732672
C 1.669528 -0.530654 -0.175623
C 2.862821 -1.005997 0.219629
C 2.706565 -2.403629 0.642578
O 3.553240 -3.181523 1.032886
O 1.399359 -2.746524 0.507173
C 0.656110 -1.627637 -0.002581
H -0.128533 -1.371080 0.726946
H 0.156232 -1.915664 -0.938989
C 4.164511 -0.263685 0.202513
C 4.013592 0.936060 -0.727008
H 4.878391 1.606922 -0.609329
H 4.035687 0.561558 -1.764218
C 2.711919 1.713534 -0.460692
C 2.720228 3.045371 -1.214884
H 2.858429 2.897851 -2.297004
H 3.551342 3.673700 -0.859697
H 1.790176 3.613889 -1.066170
H 2.705764 1.947143 0.616779
H 4.373183 0.100568 1.230752
O 5.228109 -1.089422 -0.243971

H 5.160673 -1.922906 0.251298
C 1.155191 0.709092 -2.248293
H 0.843297 1.673247 -2.675306
H 0.351036 -0.015931 -2.432768
H 2.050429 0.365398 -2.786415
H 0.130750 0.529998 1.879670
H -2.963456 2.597243 2.609229
H -1.915607 -0.097897 1.490242
H -2.906719 0.005297 2.942724
H -3.810133 1.140411 0.239161
H -4.782873 0.990531 1.701702
H -3.948125 -2.446633 -0.760430
H -2.542261 -1.636453 -0.041251
C -2.551643 0.409675 -3.443887
H -2.103729 1.327618 -3.029562
H -1.969544 0.102192 -4.320936
H -3.589066 0.636570 -3.722429

5-c16, ΔG = 2.4762 kcal/mol, population = 0.49 %

O -2.095972 0.193066 1.913527
C -2.925982 1.064804 1.755144
O -4.157568 0.847532 1.280412
C -4.544370 -0.482250 0.872791
C -4.702251 -0.552362 -0.646559
C -5.732151 0.468832 -1.140684
H -5.912006 0.352337 -2.220404
H -6.695741 0.350614 -0.619700
H -5.377687 1.496230 -0.963851
H -5.095625 -1.565936 -0.847881
C -3.367727 -0.410496 -1.394854
C -2.405822 -1.591246 -1.220284
C -1.139319 -1.437179 -2.020896
C 0.084249 -1.896243 -1.701341
C 1.242211 -1.732689 -2.652042
H 0.961595 -1.151601 -3.542903
H 1.612206 -2.718831 -2.985034
H 2.095060 -1.228382 -2.172738
C 0.357782 -2.663783 -0.417859
H -0.445950 -3.403733 -0.270319
C 0.441942 -1.851156 0.888294
H 0.501834 -2.574709 1.716834
H -0.500220 -1.308741 1.048638
C 1.604332 -0.839543 1.082852
C 1.464262 0.356638 0.174354
C 2.474323 0.925813 -0.506516
C 1.972353 2.112616 -1.208975
O 2.578851 2.896412 -1.911492
O 0.649816 2.244111 -0.933183
C 0.234758 1.190666 -0.047364
H -0.581231 0.631107 -0.521869
H -0.142074 1.635671 0.884378
C 3.901096 0.468074 -0.530989
C 4.125608 -0.447146 0.668777
H 5.097527 -0.954828 0.571235
H 4.181617 0.186967 1.569275
C 3.003474 -1.491083 0.810872
C 3.388122 -2.560612 1.835402
H 4.290874 -3.095100 1.501739
H 2.592785 -3.308028 1.973983
H 3.612317 -2.119064 2.818703
H 2.922582 -1.993853 -0.166411
H 4.071321 -0.111781 -1.463458
O 4.798877 1.564962 -0.477909
H 4.489277 2.209800 -1.136093
C 1.488616 -0.306838 2.533729
H 1.570537 -1.132289 3.254852
H 0.508637 0.167886 2.685210
H 2.271814 0.431529 2.758523
H 1.277450 -3.256041 -0.543285
H -1.253138 -0.920469 -2.982824
H -2.930481 -2.511516 -1.545103
H -2.177043 -1.736128 -0.155642
H -3.584303 -0.289308 -2.469806
H -2.874567 0.529229 -1.087770
H -3.803328 -1.199197 1.246777
H -5.508079 -0.673537 1.366222
C -2.692419 2.526160 2.028933
H -1.894715 2.644392 2.772382
H -2.373401 3.009971 1.091066
H -3.614087 3.019562 2.363750

5-c4, ΔG = 2.5684 kcal/mol, population = 0.42 %

O -1.667733 -0.894812 1.827114
C -2.664207 -1.438599 1.395974
O -3.705824 -0.763536 0.887405
C -3.586958 0.673693 0.830736

C -2.778881 1.109807 -0.392051
C -3.541624 0.846227 -1.689376
H -2.909760 1.060219 -2.564054
H -3.851071 -0.207833 -1.751898
H -4.445420 1.475815 -1.750747
H -1.871040 0.489137 -0.393267
C -2.299505 2.563890 -0.273163
C -1.375535 2.794435 0.948451
C -0.239336 3.744949 0.693480
C 1.074634 3.450921 0.643193
C 2.105031 4.529293 0.422724
H 2.835069 4.546998 1.251834
H 1.643192 5.524817 0.349917
H 2.688519 4.356191 -0.497489
C 1.618293 2.052325 0.838971
H 2.112246 1.998833 1.825875
C 2.618516 1.599994 -0.242243
H 3.634691 1.940184 0.008471
H 2.377190 2.087706 -1.201157
C 2.648333 0.068458 -0.489796
C 1.313536 -0.361991 -1.042539
C 0.599200 -1.416312 -0.614527
C -0.601354 -1.546831 -1.448296
O -1.483071 -2.381291 -1.394436
O -0.595440 -0.547601 -2.368749
C 0.564381 0.276878 -2.178355
H 0.232516 1.301830 -1.946579
H 1.136443 0.304055 -3.118669
C 0.973489 -2.329945 0.511928
C 2.478106 -2.206570 0.732982
H 2.760827 -2.738629 1.654519
H 2.994185 -2.708882 -0.102560
C 2.909244 -0.730309 0.835408
C 4.348411 -0.609947 1.339106
H 4.680555 0.438297 1.386966
H 5.052628 -1.159624 0.695900
H 4.430083 -1.031249 2.352811
H 2.257604 -0.276711 1.599645
H 0.441360 -1.979677 1.416386
O 0.615364 -3.679948 0.239128
H -0.252984 -3.659568 -0.196706
C 3.720638 -0.231382 -1.561990
H 4.703667 0.138928 -1.239235
H 3.475684 0.268328 -2.511012
H 3.802319 -1.310101 -1.759881
H 0.786311 1.336758 0.880617
H -0.527232 4.792431 0.533606
H -0.989106 1.821170 1.282226
H -1.974790 3.179527 1.791964
H -1.750887 2.807269 -1.198246
H -3.164314 3.250264 -0.246564
H -4.620285 1.045557 0.779405
H -3.125867 1.021339 1.763621
C -2.900277 -2.924274 1.402761
H -3.468410 -3.231840 0.516401
H -1.937700 -3.447872 1.439441
H -3.484568 -3.187607 2.299423

5-c9, ΔG = 2.6519 kcal/mol, population = 0.36 %

O 1.187195 1.355912 -0.225995
C 1.731323 2.084295 0.578830
O 2.686196 1.657065 1.419210
C 3.037408 0.263085 1.335639
C 4.061275 -0.021194 0.230189
C 5.469658 0.386666 0.663823
H 5.490471 1.436393 0.997095
H 5.819412 -0.240854 1.501114
H 6.188452 0.277670 -0.163372
H 3.776069 0.584386 -0.646871
C 3.955035 -1.501580 -0.170800
C 2.714512 -1.778775 -1.057521
C 2.097841 -3.126683 -0.820936
C 0.893009 -3.394230 -0.282000
C 0.442959 -4.817709 -0.064582
H 1.237377 -5.537559 -0.310346
H -0.438691 -5.064057 -0.680747
H 0.141066 -4.978619 0.985662
C -0.090579 -2.330333 0.155361
H -0.234443 -2.421846 1.246782
C -1.456875 -2.444466 -0.539823
H -2.000565 -3.322215 -0.159463
H -1.298055 -2.642511 -1.613583
C -2.378813 -1.205417 -0.416044
C -1.762927 -0.023959 -1.123503
C -1.777642 1.237573 -0.667610
C -1.153117 2.114721 -1.663602
O -1.026568 3.323729 -1.643847

O -0.750823 1.353364 -2.711602
C -1.059232 -0.024188 -2.451711
H -0.117276 -0.595508 -2.423847
H -1.675236 -0.411700 -3.278589
C -2.308098 1.696931 0.653242
C -3.228236 0.614188 1.209082
H -3.451350 0.824111 2.266575
H -4.184085 0.671671 0.662627
C -2.610370 -0.791078 1.077848
C -3.416958 -1.818186 1.873917
H -4.467406 -1.851887 1.545967
H -3.413984 -1.556309 2.943184
H -3.000545 -2.832324 1.779610
H -1.608662 -0.731146 1.535275
H -1.440958 1.818813 1.337005
O -3.010585 2.925032 0.541475
H -2.454486 3.511918 0.001978
C -3.709086 -1.537141 -1.132937
H -4.428539 -0.709390 -1.058447
H -4.167151 -2.438090 -0.700368
H -3.534838 -1.735242 -2.201236
H 0.321299 -1.325820 -0.013289
H 2.732674 -3.984614 -1.079988
H 3.018364 -1.689291 -2.115693
H 1.975695 -0.982682 -0.894799
H 4.874034 -1.813149 -0.693150
H 3.906778 -2.116094 0.746177
H 3.454857 0.012312 2.321202
H 2.118641 -0.317607 1.184199
C 1.415391 3.540590 0.775095
H 0.677697 3.859196 0.030117
H 1.013534 3.690302 1.789374
H 2.334607 4.139818 0.695959

5-c24, ΔG = 2.6707 kcal/mol, population = 0.35 %

O -1.589514 1.286098 1.532216
C -2.649286 1.756134 1.892986
O -3.671317 2.003831 1.065052
C -3.555107 1.621202 -0.319431
C -4.228914 0.274438 -0.580884
C -5.724855 0.339867 -0.265567
H -6.190222 -0.653163 -0.364102
H -5.900589 0.700890 0.758865
H -6.240566 1.025051 -0.959879
H -3.761045 -0.467928 0.089758
C -3.964969 -0.163760 -2.032252
C -2.581382 -0.802652 -2.257432
C -2.481481 -2.177169 -1.657540
C -1.733988 -2.586645 -0.616391
C -1.784010 -4.019876 -0.148005
H -2.496207 -4.617996 -0.735031
H -2.077992 -4.073751 0.915037
H -0.795232 -4.504833 -0.219283
C -0.800925 -1.683253 0.159089
H -1.041012 -0.630438 -0.024930
C 0.681147 -1.971872 -0.132697
H 0.855565 -1.921554 -1.220834
H 0.890101 -3.012571 0.153775
C 1.729307 -1.065246 0.577474
C 1.893744 0.226424 -0.188863
C 3.072007 0.760932 -0.556717
C 2.831139 2.036772 -1.241311
O 3.638676 2.827073 -1.687296
O 1.491587 2.247251 -1.292573
C 0.807121 1.149032 -0.667985
H 0.159695 0.674416 -1.422283
H 0.164759 1.530013 0.139157
C 4.431937 0.186804 -0.305342
C 4.307285 -0.861447 0.792470
H 5.239217 -1.443583 0.858849
H 4.192987 -0.328510 1.751423
C 3.115826 -1.808378 0.564637
C 3.189534 -2.974854 1.554201
H 3.240190 -2.616339 2.593823
H 4.096604 -3.569808 1.367179
H 2.327285 -3.653143 1.474215
H 3.220604 -2.224486 -0.454085
H 4.779707 -0.305402 -1.238347
O 5.357544 1.188710 0.086187
H 5.261186 1.918341 -0.548641
C 1.292831 -0.721161 2.019492
H 2.101293 -0.203181 2.555882
H 1.040054 -1.633703 2.578382
H 0.410920 -0.067291 2.027950
H -0.988201 -1.840376 1.233608
H -3.134402 -2.923301 -2.129885
H -1.793890 -0.140068 -1.869898

H -2.406595 -0.876037 -3.344990
H -4.739246 -0.890116 -2.331710
H -4.090159 0.703796 -2.704335
H -4.061280 2.418342 -0.883878
H -2.494329 1.606031 -0.598914
C -2.990974 2.110478 3.314107
H -3.560042 3.049232 3.355210
H -3.628793 1.314878 3.732109
H -2.074494 2.184290 3.911420

5-c23, ΔG = 2.8464 kcal/mol, population = 0.26 %

O 2.602837 2.537297 0.239739
C 2.850895 2.162179 -0.885733
O 3.529502 1.039327 -1.167489
C 3.980774 0.215988 -0.073164
C 3.894590 -1.250932 -0.482366
C 4.862710 -1.558464 -1.628226
H 5.908279 -1.451861 -1.292492
H 4.729142 -2.588238 -1.994704
H 4.706335 -0.870029 -2.472124
H 2.866154 -1.426846 -0.845696
C 4.130936 -2.174205 0.727599
C 2.917031 -2.381661 1.657457
C 2.500023 -1.164598 2.434666
C 1.346000 -0.478115 2.350164
C 1.129032 0.777751 3.155206
H 1.027882 1.653685 2.490886
H 1.968448 0.976287 3.837671
H 0.202248 0.716072 3.751740
C 0.215061 -0.849317 1.416510
H 0.256372 -1.918831 1.169889
C 0.217819 -0.022472 0.120194
H 1.069921 -0.329342 -0.502375
H 0.403556 1.036727 0.354790
C -1.072899 -0.107262 -0.731655
C -2.230154 0.460295 0.048362
C -3.454369 -0.087124 0.119875
C -4.321146 0.783035 0.926249
O -5.496772 0.652674 1.194883
O -3.584643 1.847051 1.346075
C -2.244244 1.734980 0.845669
H -1.547961 1.715653 1.698845
H -2.015841 2.625434 0.238247
C -3.894948 -1.362240 -0.533884
C -2.877622 -1.726123 -1.612209
H -3.055361 -2.756851 -1.955207
H -3.052977 -1.064791 -2.477060
C -1.430125 -1.586569 -1.105200
C -0.439042 -2.220665 -2.082568
H 0.601533 -2.116162 -1.739877
H -0.511584 -1.772223 -3.085277
H -0.646183 -3.296664 -2.186785
H -1.376369 -2.160161 -0.165259
H -3.905257 -2.162201 0.236173
O -5.183423 -1.230964 -1.112881
H -5.758189 -0.844344 -0.431859
C -0.870793 0.767397 -1.989992
H 0.016254 0.435758 -2.548055
H -0.714919 1.820249 -1.712557
H -1.740525 0.720292 -2.660435
H -0.742783 -0.695300 1.944480
H 3.259555 -0.785460 3.131433
H 3.186005 -3.179792 2.373042
H 2.079903 -2.773630 1.059213
H 4.433167 -3.164204 0.348865
H 4.992355 -1.802024 1.312340
H 5.024325 0.493722 0.153562
H 3.366406 0.431825 0.805633
C 2.432033 2.871865 -2.145858
H 3.310677 3.070627 -2.777124
H 1.753396 2.225720 -2.722390
H 1.925219 3.810493 -1.894200

5-c7, ΔG = 3.0158 kcal/mol, population = 0.20 %

O 0.946033 1.685130 0.383253
C 1.868456 2.097957 -0.289905
O 3.158924 1.899922 0.010865
C 3.518973 1.216826 1.227455
C 4.437469 0.028922 0.936860
C 5.285083 -0.269315 2.179923
H 5.904257 0.595889 2.464360
H 4.644526 -0.524003 3.041189
H 5.955124 -1.123768 2.000480
H 5.114302 0.340740 0.120908
C 3.685420 -1.236800 0.498579
C 2.827585 -1.142020 -0.775922

C 2.281142 -2.493414 -1.149508
C 1.077743 -3.002769 -0.826353
C 0.724082 -4.427654 -1.172801
H 1.575683 -4.956652 -1.624832
H -0.122523 -4.482141 -1.877694
H 0.411228 -4.983468 -0.270869
C 0.025449 -2.225207 -0.064314
H 0.016758 -2.588214 0.979502
C -1.389473 -2.362479 -0.646732
H -1.799739 -3.354916 -0.407436
H -1.337328 -2.328064 -1.748110
C -2.404399 -1.285251 -0.191165
C -1.991859 0.063527 -0.723649
C -2.065467 1.215835 -0.040630
C -1.643029 2.317282 -0.911198
O -1.605788 3.508360 -0.679515
O -1.306553 1.797781 -2.122811
C -1.461680 0.371942 -2.095533
H -0.478334 -0.091237 -2.278865
H -2.140498 0.072553 -2.909764
C -2.463779 1.370724 1.392636
C -3.205275 0.110602 1.829329
H -3.309746 0.104139 2.925312
H -4.224599 0.157165 1.411329
C -2.487259 -1.172801 1.369702
C -3.097067 -2.407549 2.035078
H -4.173860 -2.493827 1.822273
H -2.981664 -2.345043 3.128128
H -2.611565 -3.337565 1.702924
H -1.446677 -1.086684 1.724076
H -1.529666 1.468322 1.984458
O -3.286361 2.510400 1.592220
H -2.844078 3.251464 1.145960
C -3.775396 -1.632019 -0.817788
H -4.552660 -0.916597 -0.514194
H -4.094163 -2.641646 -0.521265
H -3.714126 -1.615125 -1.916397
H 0.302803 -1.162366 -0.007348
H 2.985085 -3.157468 -1.667701
H 3.444394 -0.744719 -1.600207
H 2.008012 -0.429298 -0.619611
H 4.426996 -2.042270 0.359089
H 3.037206 -1.567784 1.330303
H 4.043517 1.963122 1.843033
H 2.605992 0.905452 1.754260
C 1.710072 2.858159 -1.578033
H 2.639292 3.366674 -1.861348
H 1.430505 2.146248 -2.369851
H 0.881518 3.570969 -1.476140

5-c26, ΔG = 3.0698 kcal/mol, population = 0.18 %

O -1.774704 -1.513623 -1.808172
C -2.683900 -2.171164 -1.343282
O -3.881784 -1.668036 -1.017029
C -4.104604 -0.246067 -1.140358
C -4.140836 0.418946 0.235137
C -5.394867 0.032305 1.024118
H -5.431739 -1.057986 1.179127
H -5.409447 0.514773 2.013335
H -6.311417 0.331522 0.491397
H -4.176884 1.502263 0.022199
C -2.850723 0.130199 1.022474
C -2.505790 1.169740 2.103704
C -2.238044 2.545734 1.543462
C -1.105041 2.957341 0.944105
C -0.973473 4.354839 0.394786
H -0.719834 4.341856 -0.679267
H -0.154209 4.898326 0.898000
H -1.900416 4.933589 0.518715
C 0.112326 2.075909 0.762975
H 1.007385 2.672277 1.004547
C 0.239636 1.524502 -0.667787
H 0.171368 2.353427 -1.388059
H -0.624884 0.878582 -0.885476
C 1.527452 0.720957 -0.988334
C 1.677875 -0.437749 -0.034579
C 2.820906 -0.784954 0.581726
C 2.593178 -2.006966 1.363623
O 3.382938 -2.644245 2.030531
O 1.294514 -2.374277 1.212472
C 0.626844 -1.442826 0.346154
H -0.215860 -0.999235 0.896887
H 0.211290 -1.980249 -0.519059
C 4.141504 -0.085892 0.465003
C 4.104509 0.787786 -0.784377
H 4.977457 1.458465 -0.793601
H 4.198470 0.124740 -1.660752

C 2.810073 1.616573 -0.869869
C 2.920574 2.672183 -1.972313
H 3.737922 3.372520 -1.741735
H 1.998586 3.263392 -2.075182
H 3.143172 2.216999 -2.949641
H 2.722556 2.153628 0.089368
H 4.275110 0.563694 1.355870
O 5.213108 -1.011092 0.375259
H 5.076708 -1.665334 1.080971
C 1.364371 0.135657 -2.411658
H 1.168331 0.939122 -3.136091
H 0.511305 -0.556371 -2.446177
H 2.265980 -0.407199 -2.730616
H 0.095725 1.243101 1.481578
H -3.061858 3.266223 1.607126
H -1.626766 0.803901 2.660565
H -3.325476 1.227513 2.837875
H -2.923197 -0.870779 1.481527
H -2.010879 0.085873 0.316841
H -3.309667 0.181116 -1.764873
H -5.068931 -0.138341 -1.657653
C -2.592535 -3.637227 -1.019523
H -3.569772 -4.129236 -1.105850
H -1.852745 -4.116653 -1.672488
H -2.250659 -3.737369 0.023999

5-c2, ΔG = 3.4745 kcal/mol, population = 0.09 %

O 1.177131 1.314271 1.417107
C 2.019289 2.183910 1.333117
O 3.336995 1.925915 1.298434
C 3.724504 0.538235 1.271246
C 3.930462 0.041245 -0.168472
C 5.356654 0.315774 -0.648711
H 5.616592 1.378776 -0.521364
H 6.084888 -0.281636 -0.074475
H 5.475129 0.061045 -1.713508
H 3.238325 0.620320 -0.804762
C 3.525384 -1.439184 -0.280607
C 2.006310 -1.592878 -0.443210
C 1.508949 -3.007282 -0.326208
C 0.349312 -3.429098 0.214657
C -0.001231 -4.893952 0.269771
H 0.789119 -5.523491 -0.164833
H -0.941293 -5.103561 -0.269430
H -0.166834 -5.215434 1.313522
C -0.696065 -2.495613 0.783149
H -0.908550 -2.785488 1.826630
C -2.019641 -2.500034 -0.023647
H -2.758413 -3.164139 0.449590
H -1.841520 -2.927769 -1.023755
C -2.665344 -1.102466 -0.222073
C -1.669189 -0.219744 -0.929035
C -1.303373 1.010689 -0.534772
C -0.287153 1.524423 -1.462587
O 0.280345 2.597398 -1.465360
O -0.055440 0.575704 -2.410820
C -0.899718 -0.561206 -2.173349
H -0.269251 -1.455471 -2.060368
H -1.549320 -0.706368 -3.051394
C -1.837922 1.740027 0.658973
C -3.160695 1.092298 1.052061
H -3.499266 1.499634 2.017462
H -3.921787 1.363819 0.300702
C -3.018386 -0.438705 1.155051
C -4.242662 -1.059200 1.829998
H -5.173746 -0.798832 1.303485
H -4.333168 -0.687703 2.862290
H -4.175360 -2.156694 1.876949
H -2.153195 -0.623506 1.813820
H -1.110038 1.611918 1.479160
O -2.018533 3.125394 0.387688
H -1.217644 3.424163 -0.073538
C -3.910709 -1.258680 -1.121441
H -3.629135 -1.621836 -2.121078
H -4.438753 -0.301977 -1.246865
H -4.611455 -1.988506 -0.691972
H -0.296138 -1.473825 0.827550
H 2.177488 -3.774562 -0.739100
H 1.752890 -1.181904 -1.438019
H 1.493931 -0.935629 0.274863
H 4.033819 -1.901764 -1.143440
H 3.876816 -1.991953 0.609613
H 4.660832 0.482686 1.844709
H 2.955479 -0.046383 1.790405
C 1.727512 3.653514 1.223169
H 2.460708 4.248252 1.784233
H 1.791777 3.928378 0.159172

H 0.706583 3.855931 1.569014

5-c15, ΔG = 3.6797 kcal/mol, population = 0.06 %

O -1.571022 1.728761 0.634913
C -2.090712 2.398851 -0.236198
O -3.053303 1.935734 -1.037561
C -3.460311 0.557976 -0.865897
C -4.368381 0.360406 0.347541
C -5.604405 1.260773 0.261861
H -6.222575 1.166143 1.168137
H -5.323849 2.318560 0.149720
H -6.230039 0.984420 -0.603943
H -3.784791 0.646455 1.238158
C -4.775097 -1.113099 0.519284
C -3.634416 -2.119225 0.765695
C -2.932249 -2.584110 -0.482430
C -1.618191 -2.796150 -0.673097
C -1.095655 -3.284231 -2.000675
H -0.333807 -2.597176 -2.408418
H -1.896790 -3.384431 -2.747509
H -0.598403 -4.264175 -1.890543
C -0.557882 -2.551762 0.379991
H -0.985614 -2.618887 1.389753
C 0.124962 -1.184748 0.195220
H -0.573512 -0.397027 0.511209
H 0.304678 -1.004402 -0.874421
C 1.467274 -0.986670 0.966023
C 1.890479 0.439053 0.732087
C 2.720229 0.832988 -0.250544
C 2.923767 2.284377 -0.148778
O 3.648251 3.004635 -0.801915
O 2.150087 2.750960 0.870791
C 1.468171 1.653436 1.503633
H 0.382538 1.829476 1.452972
H 1.779821 1.610056 2.559858
C 3.434423 -0.052842 -1.224853
C 2.963085 -1.503483 -1.057384
H 2.093705 -1.659919 -1.712407
H 3.758645 -2.161281 -1.439203
C 2.601513 -1.902115 0.388566
C 3.850830 -1.948199 1.278600
H 4.283756 -0.947657 1.423627
H 4.625398 -2.570974 0.805155
H 3.635324 -2.382001 2.265314
H 2.195686 -2.925489 0.345307
H 3.198243 0.282315 -2.253420
O 4.846378 0.023066 -1.023840
H 5.089881 0.958281 -1.101423
C 1.229828 -1.237847 2.465612
H 1.071614 -2.308132 2.661829
H 0.334894 -0.696900 2.810890
H 2.080777 -0.907780 3.077277
H 0.190293 -3.358163 0.306038
H -3.601748 -2.795091 -1.327137
H -4.080150 -3.004846 1.256554
H -2.922259 -1.698969 1.493460
H -5.467836 -1.155890 1.375342
H -5.364857 -1.435614 -0.358819
H -3.992344 0.310972 -1.795802
H -2.560952 -0.064484 -0.799075
C -1.745624 3.836060 -0.515863
H -0.687880 4.007358 -0.276391
H -1.959288 4.104986 -1.557983
H -2.355100 4.478267 0.140564

Coordinates of the dominating conformers of **6**

6-c19, ΔG = 0.0000 kcal/mol, population = 22.83 %

O 0.476218 -1.825321 -0.300020
C -0.679021 -1.666118 0.428986
C -1.360159 -0.313659 0.252224
C -2.549941 -0.515571 -0.332399
C -2.749380 -1.961983 -0.526560
O -3.717649 -2.535891 -0.978917
O -1.658778 -2.615093 -0.062298
C -3.565550 0.529327 -0.686354
C -3.259166 1.786161 0.121745
H -3.843474 2.630995 -0.273922
H -3.605456 1.612931 1.154183
C -1.760200 2.135623 0.101536
C -1.524908 3.531175 0.682480
H -0.460459 3.808144 0.681240
H -1.894999 3.609303 1.716524
H -2.062145 4.282932 0.084081
H -1.465726 2.168778 -0.960495

C -0.872743 1.022614 0.761381
C -1.044251 0.998151 2.301164
H -0.472362 0.168313 2.742464
H -2.096804 0.874995 2.592493
H -0.665143 1.929525 2.745405
C 0.635157 1.248427 0.478984
H 0.931722 2.177829 0.988395
C 1.065119 1.312343 -0.994515
C 2.533317 1.654664 -1.140117
C 3.503484 0.753498 -1.381256
C 3.353895 -0.732319 -1.549089
C 4.162032 -1.535336 -0.501432
C 3.704585 -1.253794 0.914963
O 2.581479 -1.568335 1.294808
C 4.653238 -0.540890 1.831334
H 5.607851 -1.087867 1.892751
H 4.882369 0.444808 1.391069
H 4.215503 -0.414881 2.829532
H 4.023011 -2.613654 -0.685025
H 5.234780 -1.312711 -0.599960
H 3.732752 -1.033819 -2.541310
H 2.300933 -1.035818 -1.505245
H 4.533326 1.126925 -1.457233
C 2.864677 3.118010 -0.986002
H 2.508338 3.510403 -0.018074
H 3.946371 3.305160 -1.051844
H 2.360249 3.715898 -1.765404
H 0.484765 2.089435 -1.517674
H 0.824893 0.355656 -1.476258
H 1.204132 0.449257 0.974578
H -3.461325 0.760913 -1.767591
O -4.885232 0.090915 -0.408134
H -4.966733 -0.804999 -0.776303
H -0.521247 -1.900149 1.496271
H 1.258576 -1.884777 0.299915

6-c1, ΔG = 0.1029 kcal/mol, population = 19.18 %

O 0.652164 -1.266021 1.736517
C -0.704409 -1.219386 1.561918
C -1.298521 -0.161932 0.633448
C -2.071604 -0.787440 -0.267663
C -1.997610 -2.242267 -0.046961
O -2.567589 -3.126140 -0.652210
O -1.184307 -2.478516 1.006278
C -2.966860 -0.136232 -1.279808
C -3.259707 1.276125 -0.786826
H -3.793687 1.837937 -1.568591
H -3.940649 1.195739 0.077405
C -1.973664 2.021005 -0.397091
C -2.268611 3.504505 -0.160063
H -1.374777 4.061886 0.156973
H -3.047120 3.647097 0.605020
H -2.633093 3.966935 -1.090144
H -1.307813 1.960533 -1.273027
C -1.198304 1.340026 0.790945
C -1.821074 1.708964 2.157232
H -1.322494 1.166919 2.974176
H -2.893528 1.465894 2.191962
H -1.701566 2.782467 2.359321
C 0.284100 1.805753 0.799711
H 0.293357 2.904725 0.870010
C 1.119604 1.353439 -0.404842
C 2.507327 1.960482 -0.439038
C 3.568818 1.433225 0.197107
C 3.593217 0.196983 1.057670
C 4.194970 -1.031310 0.351764
C 3.294062 -1.648197 -0.700675
O 2.095900 -1.816484 -0.505437
C 3.926801 -2.068464 -1.995006
H 4.274978 -1.163380 -2.521951
H 4.820899 -2.682822 -1.802211
H 3.210463 -2.613355 -2.622562
H 5.174487 -0.791432 -0.088433
H 4.372742 -1.836322 1.089401
H 2.592421 -0.050827 1.430090
H 4.209559 0.399894 1.948779
H 4.532378 1.947298 0.089665
C 2.626528 3.236631 -1.231644
H 2.382738 3.063826 -2.294696
H 1.904613 3.989993 -0.869211
H 3.635155 3.671232 -1.172120
H 0.606239 1.631013 -1.338060
H 1.179102 0.259876 -0.409263
H 0.762835 1.438084 1.719636
H -2.428879 -0.078098 -2.249383
O -4.180810 -0.850650 -1.435678
H -3.947285 -1.791132 -1.516134

H -1.158646 -1.130538 2.562623
H 1.120504 -1.441800 0.883888

6-c5, ΔG = 0.2303 kcal/mol, population = 15.47 %

O 0.533478 -0.951839 2.053241
C -0.777067 -1.187257 1.752327
C -1.403435 -0.435816 0.580826
C -1.966136 -1.335976 -0.240428
C -1.693584 -2.692952 0.264873
O -2.049083 -3.754994 -0.204835
O -0.979955 -2.595182 1.406080
C -2.841151 -1.040030 -1.423854
C -3.397770 0.368119 -1.239804
H -3.921194 0.682709 -2.155866
H -4.148011 0.333373 -0.431990
C -2.274773 1.364489 -0.911229
C -2.762947 2.809202 -1.031738
H -3.073715 3.018348 -2.066860
H -1.977206 3.533223 -0.767774
H -3.630602 3.001303 -0.382079
H -1.510899 1.212719 -1.689369
C -1.565047 1.063444 0.454857
C -2.423466 1.518820 1.659786
H -2.581643 2.605729 1.633041
H -1.916785 1.286641 2.608418
H -3.405996 1.024060 1.669498
C -0.196378 1.803352 0.550439
H -0.405709 2.852749 0.806742
C 0.686090 1.751325 -0.705445
C 2.088376 2.294462 -0.511873
C 3.177397 1.766527 -1.102087
C 3.259819 0.563051 -2.003390
C 3.985285 -0.612526 -1.333703
C 3.207933 -1.189053 -0.173079
O 1.984560 -1.133042 -0.164147
C 3.979692 -1.809150 0.955856
H 4.484472 -1.001245 1.513250
H 3.314732 -2.360142 1.633434
H 4.771739 -2.468456 0.568090
H 4.133507 -1.442763 -2.050016
H 4.993582 -0.326901 -0.993203
H 3.818216 0.831463 -2.915979
H 2.264453 0.232045 -2.328299
H 4.140521 2.257360 -0.909660
C 2.212388 3.537069 0.334566
H 1.539562 4.332100 -0.033284
H 1.922983 3.347350 1.381566
H 3.240252 3.927691 0.330992
H 0.209413 2.353838 -1.499419
H 0.735200 0.719068 -1.074607
H 0.355591 1.384519 1.404275
H -2.221744 -1.064976 -2.345121
O -3.905797 -1.970214 -1.523845
H -3.520701 -2.854509 -1.398775
H -1.367998 -1.016796 2.667392
H 1.078083 -1.059368 1.233230

6-c14, ΔG = 0.4443 kcal/mol, population = 10.77 %

O 0.884562 -1.298764 -0.281523
C -0.248960 -1.550575 0.435686
C -1.278303 -0.443035 0.274719
C -2.354534 -0.954932 -0.339668
C -2.144091 -2.396370 -0.566868
O -2.912158 -3.197949 -1.057692
O -0.928061 -2.736614 -0.088430
C -3.609044 -0.222251 -0.709198
C -3.677138 1.058119 0.115897
H -4.463112 1.715578 -0.286280
H -3.982872 0.781691 1.138513
C -2.331686 1.806354 0.134514
C -2.503188 3.202159 0.737080
H -2.899175 3.155291 1.763290
H -3.217441 3.785477 0.135970
H -1.558103 3.763999 0.763080
H -2.034445 1.937114 -0.919473
C -1.186515 0.969105 0.805589
C -1.377755 0.877009 2.340743
H -2.365090 0.473011 2.605250
H -1.270833 1.868828 2.802914
H -0.615218 0.222147 2.788240
C 0.206176 1.606205 0.563907
H 0.222141 2.575509 1.085089
C 0.653589 1.804992 -0.893582
C 1.964358 2.561952 -0.963386
C 3.174322 1.973432 -0.995748

C 3.462863 0.497829 -0.985209
C 3.824059 -0.008439 0.436755
C 4.138264 -1.488646 0.443885
O 3.247036 -2.329126 0.387953
C 5.582579 -1.897293 0.493897
H 6.014613 -1.578941 1.457533
H 5.686109 -2.983498 0.378131
H 6.148260 -1.370247 -0.291726
H 4.678449 0.563145 0.828257
H 2.963939 0.158965 1.101539
H 4.309232 0.284107 -1.659849
H 2.601582 -0.076322 -1.348840
H 4.056721 2.625651 -0.995403
C 1.834275 4.063606 -0.942554
H 1.286031 4.420788 -1.832094
H 1.251298 4.399179 -0.066960
H 2.812768 4.565124 -0.914163
H -0.107896 2.381496 -1.442418
H 0.730223 0.822702 -1.376893
H 0.957187 0.985607 1.073693
H -3.546038 0.045448 -1.785324
O -4.764068 -1.009505 -0.470780
H -4.588113 -1.886312 -0.852120
H -0.038472 -1.779729 1.495027
H 1.669502 -1.793969 0.063461

6-c3, ΔG = 0.6087 kcal/mol, population = 8.16 %

O -0.375656 1.088637 2.077921
C 0.939829 0.803207 1.805915
C 1.194159 -0.155978 0.652479
C 1.892718 0.492010 -0.290651
C 2.212853 1.846270 0.190709
O 2.898418 2.691941 -0.342328
O 1.648005 2.015942 1.409888
C 2.395220 -0.062297 -1.587598
C 1.982484 -1.534396 -1.725477
H 1.017545 -1.577067 -2.250394
H 2.716460 -2.027544 -2.380615
C 1.878002 -2.287593 -0.384890
C 3.259046 -2.457557 0.260571
H 3.229563 -3.139279 1.122029
H 3.678375 -1.496040 0.590928
H 3.961972 -2.881913 -0.472622
H 1.491154 -3.296199 -0.607638
C 0.810033 -1.614355 0.555676
C 0.813348 -2.267697 1.947349
H 0.593014 -3.343473 1.863991
H 0.056999 -1.816595 2.603435
H 1.786657 -2.158500 2.444430
C -0.593469 -1.767327 -0.118609
H -0.675557 -1.037278 -0.936683
C -1.821722 -1.609395 0.792372
C -3.118877 -1.558122 0.017406
C -3.963438 -0.510112 0.034270
C -3.810213 0.801375 0.755247
C -3.608340 1.972192 -0.223471
C -2.295809 1.901153 -0.976707
O -1.247768 1.628836 -0.405421
C -2.318188 2.177500 -2.450986
H -1.299884 2.208787 -2.858562
H -2.896649 1.378281 -2.945410
H -2.848443 3.121459 -2.655380
H -4.445023 2.033990 -0.935617
H -3.592664 2.929910 0.328565
H -2.983080 0.777843 1.476805
H -4.723771 1.009501 1.337367
H -4.876492 -0.590499 -0.570166
C -3.441448 -2.786232 -0.796943
H -3.406755 -3.693994 -0.169190
H -4.437725 -2.720438 -1.257859
H -2.704847 -2.939530 -1.603812
H -1.704113 -0.715843 1.412655
H -1.870096 -2.468411 1.483913
H -0.619118 -2.765958 -0.583001
H 1.937125 0.515342 -2.414684
O 3.814709 0.057162 -1.659584
H 4.021890 0.992666 -1.505159
H 1.413282 0.458065 2.738357
H -0.816169 1.317756 1.222823

6-c41, ΔG = 0.6796 kcal/mol, population = 7.24 %

O 0.972896 0.475953 -2.317616
C -0.337689 0.853944 -2.162740
C -1.070815 0.301328 -0.945354
C -1.460692 1.333966 -0.183893
C -1.044903 2.593063 -0.827073

O -1.237157 3.729936 -0.449616
O -0.418546 2.299254 -1.988316
C -2.258577 1.259203 1.083666
C -2.969116 -0.090034 1.111510
H -3.409318 -0.255518 2.106921
H -3.804374 -0.046329 0.392862
C -2.008938 -1.241931 0.768568
C -2.647162 -2.596740 1.080461
H -2.873042 -2.668551 2.155436
H -1.982521 -3.435028 0.824182
H -3.593590 -2.736003 0.535592
H -1.145431 -1.124182 1.442854
C -1.434840 -1.143503 -0.688740
C -2.495223 -1.531777 -1.747692
H -3.398281 -0.909987 -1.666154
H -2.785511 -2.585750 -1.634640
H -2.091688 -1.410877 -2.764025
C -0.219780 -2.092290 -0.880672
H -0.595807 -3.126081 -0.861926
C 0.916301 -1.931908 0.138625
C 2.108932 -2.825044 -0.121983
C 3.337750 -2.348956 -0.392230
C 3.719892 -0.890523 -0.513496
C 3.704294 -0.098923 0.811042
C 2.886364 1.175427 0.823089
O 2.076325 1.456089 -0.049848
C 3.094581 2.096374 1.994874
H 4.067836 2.601935 1.875202
H 2.298029 2.850061 2.034561
H 3.141503 1.530452 2.937550
H 3.280212 -0.711451 1.628205
H 4.720389 0.149245 1.158439
H 3.047717 -0.398029 -1.229033
H 4.724017 -0.819521 -0.955294
H 4.145059 -3.076408 -0.534223
C 1.849932 -4.306854 -0.024703
H 2.775309 -4.890683 -0.135454
H 1.390775 -4.562769 0.946539
H 1.141856 -4.644814 -0.800540
H 0.539426 -2.173163 1.147325
H 1.215611 -0.878070 0.165346
H 0.189390 -1.932930 -1.889591
H -1.556122 1.315269 1.942209
O -3.210619 2.306517 1.163196
H -2.745552 3.127508 0.929012
H -0.871177 0.618708 -3.097179
H 1.460537 0.745713 -1.503511

6-c8, ΔG = 0.9375 kcal/mol, population = 4.68 %

O -0.464400 1.554691 1.372884
C 0.821934 1.110167 1.475843
C 1.281640 0.000884 0.530968
C 2.353680 0.452986 -0.140618
C 2.648449 1.836143 0.273512
O 3.551675 2.555617 -0.103036
O 1.750600 2.208565 1.205507
C 3.208068 -0.319566 -1.100101
C 3.005774 -1.797271 -0.800126
H 3.494594 -2.405745 -1.576439
H 3.514216 -2.019851 0.153496
C 1.516688 -2.160686 -0.714331
C 1.361707 -3.683981 -0.660286
H 1.942488 -4.116355 0.168796
H 1.736403 -4.132156 -1.593191
H 0.315180 -3.999404 -0.538778
H 1.047905 -1.810484 -1.651785
C 0.743627 -1.416038 0.441354
C 0.983572 -2.098029 1.805456
H 2.059921 -2.197152 2.010473
H 0.534054 -3.100276 1.829746
H 0.539430 -1.519533 2.627719
C -0.765963 -1.438600 0.045620
H -0.930772 -0.658558 -0.710942
C -1.820713 -1.303085 1.157587
C -3.227823 -1.350927 0.596720
C -4.021239 -0.273359 0.449456
C -3.710340 1.157445 0.790891
C -3.699895 2.071127 -0.453526
C -2.621050 1.701845 -1.451836
O -1.442731 1.623316 -1.122956
C -3.043690 1.414447 -2.861832
H -3.695683 0.523828 -2.850574
H -3.652640 2.244041 -3.255674
H -2.173229 1.233976 -3.504969
H -4.683210 2.059456 -0.946700
H -3.503114 3.112677 -0.144022
H -2.754028 1.249108 1.318297

H -4.485846 1.550038 1.471138
H -5.016973 -0.436184 0.016196
C -3.712116 -2.719793 0.187233
H -3.046182 -3.175904 -0.564992
H -3.716027 -3.406220 1.052252
H -4.727767 -2.688276 -0.233457
H -1.654625 -0.379162 1.720762
H -1.706652 -2.139682 1.866472
H -0.947059 -2.393606 -0.467532
H 2.860320 -0.107931 -2.133425
O 4.578118 0.015621 -0.965547
H 4.627451 0.986278 -0.923455
H 0.997935 0.826370 2.526141
H -0.754834 1.627761 0.428995

6-c16, ΔG = 1.3272 kcal/mol, population = 2.42 %

O -0.923975 -0.131290 2.148914
C 0.410327 0.202954 2.115520
C 1.177281 -0.220299 0.868965
C 1.643311 0.881712 0.267258
C 1.251965 2.064059 1.054555
O 1.501060 3.230936 0.834521
O 0.572355 1.649481 2.147365
C 2.450613 0.930705 -0.993472
C 3.064894 -0.447751 -1.215485
H 3.505929 -0.497810 -2.222979
H 3.892278 -0.566515 -0.495799
C 2.028318 -1.572259 -1.043452
C 2.593646 -2.909200 -1.526746
H 2.831007 -2.852725 -2.600251
H 1.878625 -3.734071 -1.388540
H 3.522482 -3.174213 -0.998330
H 1.184459 -1.316703 -1.705379
C 1.435603 -1.635763 0.407380
C 2.429366 -2.273245 1.405777
H 2.597657 -3.331552 1.160730
H 2.031120 -2.233319 2.430716
H 3.399582 -1.755557 1.400734
C 0.121355 -2.458710 0.446600
H 0.365118 -3.510936 0.236092
C -0.974161 -1.958819 -0.514306
C -2.406099 -2.004170 -0.001222
C -3.367225 -1.221955 -0.526306
C -3.242233 -0.261008 -1.677748
C -3.582896 1.195689 -1.339795
C -2.516372 1.937229 -0.566591
O -1.562586 1.362175 -0.063641
C -2.661649 3.433226 -0.459777
H -1.951291 3.833530 0.274869
H -2.454622 3.881508 -1.446392
H -3.693417 3.710386 -0.193957
H -3.793768 1.776298 -2.254206
H -4.513137 1.260613 -0.744164
H -3.942245 -0.582604 -2.469064
H -2.238725 -0.299051 -2.124729
H -4.379410 -1.307863 -0.109545
C -2.732936 -2.969907 1.108787
H -2.368634 -3.985846 0.878378
H -2.250950 -2.666975 2.052603
H -3.817040 -3.023914 1.285153
H -0.917327 -2.536911 -1.453862
H -0.757410 -0.919910 -0.800009
H -0.238738 -2.438641 1.481691
H 1.762489 1.159102 -1.835198
O 3.473789 1.910133 -0.921505
H 3.058920 2.723043 -0.587391
H 0.871044 -0.184259 3.037511
H -1.332839 0.176851 1.314022

6-c24, ΔG = 1.4069 kcal/mol, population = 2.12 %

O -0.925377 -1.586090 -2.067829
C -0.575054 -0.262881 -2.083260
C -0.787660 0.548157 -0.812226
C 0.369652 1.155156 -0.502222
C 1.401911 0.753472 -1.473153
O 2.563697 1.101767 -1.527284
O 0.853640 -0.109492 -2.356404
C 0.582407 2.155609 0.595666
C -0.773687 2.769999 0.919582
H -0.687595 3.402576 1.816295
H -1.055684 3.431239 0.082708
C -1.845977 1.692696 1.148909
C -3.118467 2.324177 1.720197
H -3.920445 1.586667 1.871504
H -3.506327 3.119020 1.065051
H -2.901063 2.780768 2.697791

H -1.442038 1.023875 1.925927
C -2.105578 0.793655 -0.115868
C -3.023889 1.510489 -1.135768
H -3.152630 0.901820 -2.042772
H -2.609395 2.484159 -1.435354
H -4.022465 1.673527 -0.708018
C -2.819915 -0.527997 0.293347
H -3.785111 -0.232989 0.728862
C -2.092287 -1.459695 1.293287
C -1.354409 -2.638583 0.696240
C -0.013126 -2.787963 0.737458
C 0.995942 -1.845825 1.332735
C 2.298578 -1.806276 0.533081
C 3.258135 -0.710606 0.962731
O 2.948835 0.118642 1.798667
C 4.601609 -0.687801 0.275070
H 5.098001 -1.667815 0.351184
H 4.444025 -0.475144 -0.794127
H 5.235542 0.094717 0.711744
H 2.829141 -2.772565 0.590355
H 2.101951 -1.667019 -0.544757
H 1.229726 -2.157231 2.367219
H 0.590859 -0.829989 1.415281
H 0.400159 -3.716218 0.322181
C -2.230934 -3.713206 0.101905
H -1.639801 -4.522714 -0.349803
H -2.878932 -4.149019 0.881872
H -2.903188 -3.306476 -0.671186
H -2.855123 -1.880832 1.969382
H -1.421248 -0.878869 1.937987
H -3.069422 -1.083102 -0.622400
H 0.972231 1.622626 1.485102
O 1.488629 3.172098 0.202638
H 2.268585 2.726814 -0.168427
H -1.090939 0.205129 -2.936432
H -0.673174 -1.983014 -1.207585

6-c45, ΔG = 1.5813 kcal/mol, population = 1.58 %

O 0.268083 1.195627 -2.283266
C -0.972036 1.281780 -1.711666
C -1.312397 0.266118 -0.631288
C -1.673375 0.925676 0.478107
C -1.611672 2.376371 0.217239
O -1.930646 3.287046 0.949660
O -1.158352 2.568558 -1.045154
C -2.193550 0.328985 1.747638
C -2.082232 -1.197669 1.692144
H -1.098656 -1.472856 2.086042
H -2.822098 -1.610866 2.394646
C -2.296161 -1.828076 0.295462
C -3.783517 -1.751695 -0.081388
H -4.394703 -2.150929 0.742603
H -4.019028 -2.337438 -0.980263
H -4.103760 -0.712012 -0.246089
H -2.031344 -2.896319 0.381179
C -1.346295 -1.228742 -0.806384
C -1.866709 -1.546222 -2.226704
H -2.818089 -1.043522 -2.446939
H -2.017495 -2.630242 -2.340641
H -1.131790 -1.226224 -2.979880
C 0.095777 -1.827668 -0.756874
H 0.012062 -2.860345 -1.131105
C 0.852529 -1.835705 0.577838
C 2.304988 -2.241405 0.437012
C 3.328768 -1.565585 0.990462
C 3.287844 -0.301045 1.805555
C 3.918013 0.888181 1.070686
C 3.109148 1.363798 -0.112332
O 1.924824 1.071517 -0.210283
C 3.808363 2.191110 -1.154440
H 3.082537 2.702429 -1.800300
H 4.493436 2.916403 -0.690289
H 4.426353 1.515237 -1.770695
H 4.018095 1.761111 1.743436
H 4.943935 0.663365 0.733136
H 3.852408 -0.457056 2.740369
H 2.261610 -0.039559 2.096321
H 4.338183 -1.967211 0.830089
C 2.562246 -3.509233 -0.339871
H 3.619754 -3.807062 -0.292050
H 1.949640 -4.341727 0.049500
H 2.289656 -3.395847 -1.402688
H 0.371641 -2.559426 1.258937
H 0.784208 -0.846685 1.044226
H 0.697679 -1.277740 -1.496584
H -1.580874 0.697832 2.592840
O -3.552702 0.716919 1.952066

H -3.569653 1.686261 1.963153
H -1.718807 1.250183 -2.521655
H 0.942732 1.172893 -1.558864

6-c9, ΔG = 1.8631 kcal/mol, population = 0.98 %

O 0.996310 0.056721 2.520799
C 0.814899 -1.166604 1.917625
C -0.125823 -1.213720 0.713735
C 0.588123 -1.590959 -0.357907
C 1.979961 -1.850544 0.053364
O 2.908281 -2.229099 -0.628850
O 2.082271 -1.642123 1.385361
C 0.071656 -1.796689 -1.749740
C -1.433722 -2.021134 -1.664619
H -1.869332 -1.981704 -2.674906
H -1.595680 -3.044649 -1.286546
C -2.133724 -0.991325 -0.760835
C -3.652337 -1.136234 -0.893921
H -4.199888 -0.467075 -0.215147
H -3.982161 -2.166398 -0.688784
H -3.963515 -0.889327 -1.920533
H -1.866871 0.003857 -1.143323
C -1.628940 -1.033548 0.725299
C -2.213712 -2.258293 1.474161
H -3.300634 -2.148699 1.595671
H -1.779737 -2.350163 2.480630
H -2.016529 -3.194915 0.933625
C -2.058529 0.230893 1.516635
H -3.157856 0.282633 1.508927
C -1.458120 1.588926 1.108631
C -1.952848 2.260167 -0.155128
C -1.139374 2.520986 -1.195828
C 0.305287 2.098749 -1.274504
C 1.270942 3.020825 -0.480812
C 2.545424 2.271650 -0.161927
O 2.557944 1.415400 0.713618
C 3.768662 2.566087 -0.980726
H 4.074488 3.612779 -0.816289
H 4.589075 1.887145 -0.716296
H 3.526263 2.476111 -2.052505
H 1.472602 3.945133 -1.040563
H 0.804320 3.293374 0.477005
H 0.631223 2.056305 -2.324982
H 0.412894 1.079687 -0.876784
H -1.545169 3.071942 -2.051473
C -3.394694 2.692159 -0.157973
H -3.660157 3.221831 -1.084376
H -4.072761 1.828575 -0.056058
H -3.607909 3.356040 0.698019
H -0.369050 1.491321 1.090928
H -1.675184 2.284356 1.939597
H -1.779734 0.066038 2.568660
H 0.268583 -0.872818 -2.333462
O 0.685175 -2.908873 -2.378938
H 1.641021 -2.832428 -2.218856
H 0.505574 -1.881655 2.695870
H 1.449039 0.652505 1.878725

6-c27, ΔG = 2.0043 kcal/mol, population = 0.77 %

O -0.191534 0.665791 2.429984
C 1.002450 0.872001 1.793056
C 1.348582 0.046804 0.558703
C 1.690677 0.889410 -0.428344
C 1.556937 2.276439 0.052736
O 1.830094 3.304956 -0.527482
O 1.104544 2.248198 1.328843
C 2.313292 0.538836 -1.747455
C 2.577729 -0.975208 -1.839456
H 1.758966 -1.441998 -2.403216
H 3.483464 -1.108636 -2.449423
C 2.755883 -1.687893 -0.481577
C 4.092816 -1.300204 0.161171
H 4.127968 -0.229081 0.410793
H 4.914780 -1.494255 -0.544994
H 4.298867 -1.877400 1.073543
H 2.782283 -2.771645 -0.686448
C 1.513440 -1.452483 0.455506
C 1.711908 -2.084150 1.841930
H 2.570003 -1.652224 2.374956
H 1.883865 -3.167104 1.742508
H 0.824301 -1.931040 2.470565
C 0.267066 -2.080842 -0.230989
H 0.154173 -1.629819 -1.223914
C -1.069337 -1.919199 0.510412
C -2.265408 -2.125417 -0.397095
C -2.652499 -1.192547 -1.285490

C -2.008854 0.147767 -1.525500
C -2.961336 1.320699 -1.276403
C -3.233964 1.603769 0.185447
O -2.438917 1.305062 1.063333
C -4.525700 2.301579 0.515110
H -5.354062 1.586468 0.371978
H -4.522554 2.652714 1.554808
H -4.705462 3.137921 -0.178151
H -2.530083 2.259616 -1.673768
H -3.917724 1.189630 -1.808061
H -1.669404 0.202946 -2.574616
H -1.115379 0.285496 -0.903762
H -3.520271 -1.412247 -1.920965
C -2.975145 -3.447071 -0.276478
H -2.274505 -4.284073 -0.445692
H -3.378875 -3.585179 0.742130
H -3.804239 -3.541038 -0.993527
H -1.119870 -0.915091 0.944439
H -1.121613 -2.619061 1.358059
H 0.476578 -3.150232 -0.401276
H 1.621121 0.829658 -2.561490
O 3.542531 1.247429 -1.892915
H 3.337787 2.188811 -1.769867
H 1.797727 0.736211 2.545354
H -0.943995 0.861190 1.828938

6-c40, ΔG = 2.0382 kcal/mol, population = 0.73 %

O -0.962007 -1.189332 0.090164
C 0.144839 -1.496190 -0.651382
C 1.283717 -0.519884 -0.383366
C 2.267341 -1.190059 0.235517
C 1.900777 -2.614590 0.333324
O 2.557498 -3.528728 0.787332
O 0.684167 -2.787078 -0.226417
C 3.565813 -0.628688 0.731901
C 3.815873 0.704521 0.037121
H 4.627791 1.241347 0.551144
H 4.172677 0.488564 -0.983357
C 2.554752 1.585948 -0.004337
C 2.911047 2.998166 -0.474168
H 3.644983 3.447406 0.212337
H 2.035629 3.663017 -0.501644
H 3.363101 2.989799 -1.478112
H 2.193253 1.665736 1.034902
C 1.385712 0.927271 -0.819149
C 1.698045 0.904097 -2.337050
H 2.662288 0.421440 -2.548473
H 1.722428 1.926238 -2.741326
H 0.919128 0.352429 -2.884396
C 0.059494 1.709805 -0.645294
H 0.215834 2.727561 -1.034911
C -0.523616 1.794149 0.772512
C -1.749532 2.687933 0.848645
C -2.960925 2.334054 0.380583
C -3.319189 1.035319 -0.289498
C -3.966822 0.000348 0.661904
C -4.307164 -1.271764 -0.088650
O -3.428472 -1.980565 -0.567501
C -5.757824 -1.616838 -0.264365
H -6.223568 -1.755438 0.725562
H -6.282248 -0.771761 -0.740662
H -5.873962 -2.525928 -0.867723
H -3.246171 -0.254837 1.455344
H -4.863946 0.420401 1.139210
H -2.434502 0.564348 -0.731086
H -4.022128 1.238629 -1.115294
H -3.781890 3.053074 0.492826
C -1.519453 4.042875 1.464942
H -1.178282 3.946832 2.510936
H -0.716787 4.580440 0.928761
H -2.423965 4.668705 1.449844
H 0.237304 2.190230 1.461942
H -0.764823 0.778093 1.111157
H -0.688247 1.257720 -1.312881
H 3.461824 -0.451989 1.823645
O 4.648551 -1.509954 0.483776
H 4.363279 -2.391733 0.777454
H -0.078924 -1.610440 -1.726035
H -1.792009 -1.598621 -0.261434

6-c7, ΔG = 2.1210 kcal/mol, population = 0.63 %

O -0.845527 -1.328286 2.120175
C 0.001833 -0.259386 2.284182
C 0.819743 0.125338 1.058048
C 0.441454 1.352613 0.671583
C -0.558054 1.870645 1.623635

O -1.104220 2.955383 1.619032
O -0.756918 0.948216 2.587754
C 0.996499 2.136498 -0.479845
C 2.378854 1.579590 -0.807646
H 2.726089 1.994929 -1.766089
H 3.074671 1.937952 -0.031165
C 2.383447 0.042348 -0.878824
C 3.703967 -0.467252 -1.459881
H 3.733787 -1.564940 -1.520784
H 4.566598 -0.136712 -0.861188
H 3.842026 -0.074911 -2.479078
H 1.591089 -0.229437 -1.593769
C 1.993507 -0.631944 0.482641
C 3.131905 -0.474686 1.527085
H 3.376978 0.581671 1.705286
H 4.039904 -0.991897 1.187170
H 2.841546 -0.921181 2.489571
C 1.754943 -2.163643 0.331714
H 2.751405 -2.614111 0.215164
C 0.873042 -2.687106 -0.823917
C -0.602305 -2.879469 -0.546376
C -1.569337 -2.127231 -1.098581
C -1.380750 -0.936790 -2.002925
C -2.554865 0.043338 -1.995261
C -2.867335 0.663452 -0.650038
O -2.537442 0.137600 0.400656
C -3.596685 1.981487 -0.658011
H -2.856064 2.771195 -0.873100
H -4.358459 2.020556 -1.450908
H -4.041085 2.179652 0.325545
H -2.399825 0.849255 -2.730178
H -3.487193 -0.462103 -2.314004
H -1.235342 -1.271826 -3.046076
H -0.464626 -0.390664 -1.734557
H -2.609442 -2.398170 -0.881804
C -0.940671 -4.036043 0.358722
H -2.026835 -4.141014 0.497617
H -0.547450 -4.984696 -0.047186
H -0.486842 -3.899538 1.353978
H 1.268972 -3.682848 -1.089207
H 1.019775 -2.074098 -1.722581
H 1.374435 -2.547728 1.289785
H 0.329975 1.988360 -1.356746
O 1.096285 3.517195 -0.177371
H 0.266140 3.770594 0.261673
H 0.631388 -0.462367 3.163350
H -1.377872 -1.169309 1.313237

6-c35, ΔG = 2.2327 kcal/mol, population = 0.52 %

O 0.580410 1.255564 -2.005088
C -0.742306 1.297842 -1.633074
C -1.232929 0.200914 -0.701860
C -1.712438 0.768125 0.413856
C -1.625087 2.233855 0.279671
O -2.028127 3.086671 1.038633
O -1.035444 2.523523 -0.908741
C -2.360549 0.074177 1.572940
C -2.361878 -1.446472 1.351271
H -1.464734 -1.871815 1.818900
H -3.219443 -1.858075 1.904585
C -2.438316 -1.881342 -0.126288
C -3.831212 -1.576789 -0.695744
H -4.013285 -0.494031 -0.764776
H -4.602179 -1.991646 -0.028345
H -3.981405 -2.021399 -1.689093
H -2.301122 -2.975365 -0.150470
C -1.265334 -1.277752 -0.983019
C -1.502112 -1.523732 -2.486648
H -2.410611 -1.028138 -2.854230
H -1.598840 -2.603315 -2.680737
H -0.650535 -1.148560 -3.072416
C 0.108646 -1.946715 -0.631602
H -0.075259 -3.020008 -0.459747
C 0.923467 -1.356275 0.529665
C 2.274229 -2.023550 0.691679
C 3.352729 -1.672792 -0.032027
C 3.417264 -0.603188 -1.091625
C 4.111340 0.686556 -0.608554
C 3.285505 1.446278 0.411376
O 2.120336 1.749701 0.180949
C 3.932284 1.806053 1.715085
H 4.190673 0.871819 2.242817
H 4.880804 2.337464 1.535503
H 3.259200 2.413252 2.333193
H 5.107749 0.461797 -0.200731
H 4.254890 1.371879 -1.462940
H 2.418505 -0.351444 -1.471977

H 3.987769 -0.984388 -1.954270
H 4.294262 -2.202576 0.159645
C 2.333657 -3.134474 1.706350
H 3.322068 -3.615923 1.738978
H 2.096150 -2.756465 2.716233
H 1.579128 -3.909211 1.482426
H 0.375050 -1.443037 1.477129
H 1.057449 -0.283416 0.360109
H 0.743576 -1.890702 -1.528061
H -1.780232 0.299361 2.489026
O -3.698640 0.541093 1.736735
H -3.648547 1.505496 1.829998
H -1.345023 1.322989 -2.555429
H 1.155758 1.393581 -1.212483

6-c18, ΔG = 2.4090 kcal/mol, population = 0.39 %

O -0.678783 0.580480 2.503465
C 0.656195 0.477535 2.172186
C 0.971332 -0.188496 0.838198
C 1.537575 0.726636 0.037094
C 1.719312 1.980071 0.792816
O 2.253123 3.005944 0.429474
O 1.234039 1.804526 2.043914
C 2.089268 0.510472 -1.339495
C 1.950515 -0.967367 -1.738032
H 1.011047 -1.092977 -2.294107
H 2.762093 -1.196111 -2.444848
C 1.991844 -1.950694 -0.550969
C 3.388163 -1.984078 0.082563
H 4.144477 -2.161201 -0.697426
H 3.486147 -2.788455 0.824902
H 3.641146 -1.029390 0.566445
H 1.786697 -2.956110 -0.955009
C 0.832074 -1.650346 0.472061
C 0.952799 -2.532332 1.725475
H 1.895851 -2.356852 2.260310
H 0.913344 -3.596446 1.444654
H 0.132573 -2.337443 2.429920
C -0.521778 -1.934038 -0.247515
H -0.675134 -1.169113 -1.020116
C -1.787683 -1.996628 0.624652
C -3.041359 -2.067683 -0.223238
C -3.736013 -0.974504 -0.590541
C -3.388537 0.440889 -0.217231
C -2.536812 1.167127 -1.270580
C -1.597991 2.217476 -0.720520
O -1.327112 2.292711 0.469445
C -0.961453 3.155329 -1.711616
H -0.053402 3.600396 -1.284482
H -0.735525 2.643627 -2.658854
H -1.681790 3.959031 -1.942436
H -1.871836 0.451307 -1.789014
H -3.144210 1.612480 -2.075265
H -2.832450 0.448376 0.728138
H -4.306119 1.024735 -0.038849
H -4.607824 -1.111761 -1.241589
C -3.439798 -3.445469 -0.683109
H -4.322045 -3.423366 -1.339705
H -2.615747 -3.933851 -1.232221
H -3.663858 -4.097292 0.179699
H -1.810815 -1.126073 1.291817
H -1.744582 -2.886098 1.272783
H -0.411421 -2.890632 -0.784687
H 1.511493 1.127430 -2.055593
O 3.460154 0.897640 -1.382952
H 3.501290 1.813146 -1.062261
H 1.171789 -0.020354 3.007222
H -1.108650 1.134933 1.813511

6-c13, ΔG = 2.5376 kcal/mol, population = 0.31 %

O 0.582091 0.487702 -2.573389
C -0.602990 0.941894 -2.081504
C -1.180211 0.354453 -0.796186
C -1.555198 1.371719 -0.004014
C -1.147879 2.644858 -0.620411
O -1.308948 3.771468 -0.197490
O -0.541324 2.381066 -1.798915
C -2.387643 1.266709 1.241465
C -3.155313 -0.049453 1.158414
H -3.682069 -0.231761 2.107810
H -3.923062 0.054538 0.372876
C -2.203942 -1.217296 0.856641
C -2.888995 -2.567086 1.077307
H -3.188844 -2.670466 2.131443
H -2.223155 -3.410328 0.837613
H -3.797689 -2.669000 0.464425

H -1.402615 -1.138434 1.606272
C -1.503501 -1.100408 -0.543262
C -2.426832 -1.565046 -1.693539
H -3.356459 -0.977394 -1.729400
H -2.690273 -2.624711 -1.575062
H -1.919433 -1.461956 -2.664223
C -0.210107 -1.969396 -0.594166
H -0.514243 -3.016189 -0.744790
C 0.701668 -1.875428 0.637529
C 2.075226 -2.488104 0.457359
C 3.189477 -1.959110 0.993913
C 3.308419 -0.722265 1.838526
C 3.908920 0.501980 1.091346
C 2.913115 1.053330 0.101288
O 2.667037 0.431961 -0.925701
C 2.198924 2.330245 0.448125
H 1.572263 2.667161 -0.385455
H 1.574291 2.168310 1.343485
H 2.929079 3.111046 0.711913
H 4.197300 1.274128 1.818435
H 4.809182 0.186422 0.540835
H 3.979493 -0.935033 2.686666
H 2.342065 -0.436984 2.281169
H 4.138137 -2.476886 0.804039
C 2.137408 -3.777319 -0.320870
H 3.151181 -4.202908 -0.315601
H 1.445714 -4.527379 0.102164
H 1.832756 -3.633144 -1.370981
H 0.212916 -2.393834 1.481915
H 0.794100 -0.823540 0.942137
H 0.352193 -1.681973 -1.493909
H -1.718430 1.239115 2.126944
O -3.296513 2.348130 1.345585
H -2.796669 3.159773 1.153122
H -1.352010 0.833795 -2.884194
H 1.306900 0.529037 -1.898445

6-c23, ΔG = 2.7359 kcal/mol, population = 0.22 %

O 0.694699 0.790869 -1.941025
C -0.674603 0.757435 -1.851765
C -1.255570 -0.019726 -0.676520
C -1.948334 0.832743 0.092775
C -1.913346 2.172611 -0.520034
O -2.452243 3.189621 -0.137260
O -1.191675 2.107209 -1.662721
C -2.714436 0.494772 1.337184
C -2.986230 -1.006379 1.332878
H -3.361026 -1.316553 2.320331
H -3.794046 -1.198994 0.607764
C -1.727059 -1.815739 0.976924
C -1.941345 -3.305375 1.250228
H -2.152450 -3.466691 2.318487
H -1.055648 -3.905459 0.993494
H -2.796005 -3.703687 0.682057
H -0.937000 -1.465933 1.661427
C -1.206506 -1.516669 -0.472541
C -2.132155 -2.135603 -1.549884
H -3.167431 -1.779116 -1.452783
H -2.131500 -3.232110 -1.473765
H -1.779322 -1.877534 -2.559532
C 0.214832 -2.095293 -0.704640
H 0.119134 -3.187692 -0.789666
C 1.259550 -1.752659 0.362875
C 2.670577 -2.193672 0.022299
C 3.752321 -1.439546 0.291227
C 3.731120 -0.075020 0.926012
C 3.643479 1.080043 -0.123025
C 2.781627 2.189306 0.426856
O 1.590638 2.254447 0.140645
C 3.405567 3.162847 1.384912
H 2.644280 3.824047 1.817450
H 3.940995 2.622514 2.182074
H 4.160508 3.760988 0.847943
H 4.649891 1.449437 -0.369503
H 3.177194 0.703747 -1.043279
H 4.632669 0.066381 1.540913
H 2.878196 -0.002357 1.617712
H 4.738209 -1.832024 0.015956
C 2.817757 -3.562507 -0.590420
H 2.348505 -3.614292 -1.587071
H 3.875074 -3.844759 -0.697097
H 2.315977 -4.326761 0.029097
H 0.977965 -2.243656 1.311909
H 1.232946 -0.671644 0.556525
H 0.574212 -1.742547 -1.682880
H -2.080089 0.744177 2.214109
O -3.940448 1.203279 1.404215

H -3.740761 2.131512 1.195657
H -1.073085 0.396368 -2.813268
H 1.040765 1.256380 -1.136719

6-c43, ΔG = 2.7661 kcal/mol, population = 0.21 %

O 0.466593 1.563424 0.435106
C -0.522779 1.399867 -0.501860
C -1.411982 0.202415 -0.188587
C -2.620499 0.669717 0.159366
C -2.643620 2.134410 -0.007573
O -3.576178 2.893323 0.157354
O -1.431973 2.539375 -0.443552
C -3.801516 -0.131819 0.611831
C -3.595218 -1.573994 0.172097
H -4.327001 -2.223426 0.676394
H -3.816083 -1.624327 -0.907112
C -2.170777 -2.089255 0.444647
C -2.125013 -3.593832 0.157303
H -1.121244 -4.023992 0.282987
H -2.461474 -3.815566 -0.867252
H -2.799470 -4.125830 0.845486
H -1.966090 -1.944173 1.521057
C -1.059259 -1.267129 -0.310448
C -1.059703 -1.609027 -1.818995
H -0.690069 -2.630731 -1.988264
H -0.416559 -0.924526 -2.389394
H -2.073215 -1.532911 -2.237279
C 0.316398 -1.603998 0.338506
H 0.380392 -1.093465 1.311545
C 1.580027 -1.296259 -0.481077
C 2.843150 -1.820612 0.176615
C 3.543108 -1.136617 1.099756
C 3.216207 0.224795 1.652143
C 4.119890 1.350788 1.099245
C 3.893254 1.601628 -0.378545
O 2.804918 1.978524 -0.799962
C 5.036370 1.350195 -1.315933
H 5.915769 1.939000 -1.008340
H 5.324270 0.288128 -1.232910
H 4.756501 1.586754 -2.350127
H 3.886137 2.293362 1.623061
H 5.178685 1.118356 1.285824
H 3.350186 0.209978 2.746449
H 2.166319 0.484540 1.470465
H 4.451491 -1.603622 1.500945
C 3.265894 -3.199177 -0.260451
H 4.144367 -3.560465 0.293964
H 2.444921 -3.923682 -0.116424
H 3.503294 -3.213362 -1.338738
H 1.663879 -0.219834 -0.657299
H 1.497658 -1.769244 -1.470465
H 0.321205 -2.681114 0.560336
H -3.835264 -0.090408 1.721323
O -5.015065 0.363437 0.070128
H -5.004276 1.327400 0.196734
H -0.124845 1.382947 -1.529895
H 1.300138 1.879601 0.010518

6-c37, ΔG = 2.8997 kcal/mol, population = 0.17 %

O 0.083855 -1.974122 -1.714895
C 1.308723 -1.412048 -1.463598
C 1.345598 -0.146050 -0.624909
C 2.160553 -0.341554 0.420805
C 2.724182 -1.702266 0.338530
O 3.553033 -2.221055 1.052295
O 2.179309 -2.328841 -0.735972
C 2.541298 0.674756 1.453960
C 1.711847 1.951742 1.261463
H 0.781462 1.840668 1.836904
H 2.262876 2.783998 1.725134
C 1.377516 2.298326 -0.205973
C 2.637964 2.727221 -0.967877
H 2.402139 3.121564 -1.966195
H 3.343819 1.891052 -1.078177
H 3.160756 3.520908 -0.412304
H 0.692329 3.162539 -0.182255
C 0.600572 1.131429 -0.903954
C 0.468142 1.343800 -2.422627
H 0.046331 2.334810 -2.643236
H -0.194830 0.582820 -2.860215
H 1.440078 1.273061 -2.930340
C -0.810207 0.935944 -0.275639
H -1.139849 -0.071684 -0.536883
C -1.914870 1.910713 -0.701084
C -3.172218 1.706214 0.128117
C -3.945306 0.608270 0.041155

C -3.740597 -0.583825 -0.853050
C -3.620062 -1.926940 -0.083276
C -2.484821 -1.954908 0.922219
O -1.329070 -2.177574 0.583311
C -2.817697 -1.672215 2.358991
H -3.551036 -2.407302 2.728290
H -1.911395 -1.693564 2.977071
H -3.299106 -0.682573 2.423560
H -4.568999 -2.128439 0.436621
H -3.446297 -2.736424 -0.808893
H -2.864710 -0.457256 -1.503254
H -4.609141 -0.693701 -1.525539
H -4.824206 0.550940 0.696114
C -3.482953 2.804123 1.109879
H -3.647571 3.763825 0.589233
H -4.371590 2.580892 1.718438
H -2.627834 2.965352 1.790363
H -2.140668 1.771059 -1.769535
H -1.573617 2.951547 -0.589541
H -0.721461 0.938846 0.819799
H 2.326385 0.259774 2.457482
O 3.932885 0.979068 1.361562
H 4.412655 0.143587 1.468649
H 1.793997 -1.241061 -2.438695
H -0.433700 -2.083540 -0.881515

6-c47, ΔG = 3.0302 kcal/mol, population = 0.14 %

O -0.885467 0.985666 -0.296919
C 0.167318 1.174741 0.557216
C 1.331366 0.255815 0.218048
C 2.352967 1.022232 -0.193682
C 1.976578 2.442893 -0.086293
O 2.655170 3.419395 -0.328801
O 0.714716 2.519401 0.386952
C 3.690405 0.556933 -0.680620
C 3.894477 -0.877582 -0.215190
H 4.759368 -1.317626 -0.734767
H 4.148829 -0.845723 0.857437
C 2.651025 -1.754679 -0.440511
C 3.006333 -3.216901 -0.151799
H 3.432594 -3.333580 0.856500
H 3.762928 -3.567839 -0.870140
H 2.139547 -3.888869 -0.230202
H 2.382658 -1.676944 -1.509966
C 1.384284 -1.251710 0.347195
C 1.509314 -1.585392 1.851554
H 2.465890 -1.222877 2.253929
H 1.452966 -2.669934 2.019136
H 0.706486 -1.116050 2.436512
C 0.123228 -1.917399 -0.284782
H -0.163115 -1.343061 -1.178534
C -1.103949 -2.079368 0.626668
C -2.316089 -2.619933 -0.099813
C -3.492412 -1.971204 -0.189057
C -3.825409 -0.612844 0.355379
C -4.028427 0.434308 -0.768197
C -4.124639 1.822903 -0.175158
O -3.124108 2.378928 0.265301
C -5.474463 2.473711 -0.100210
H -6.188945 1.792944 0.391162
H -5.420738 3.427754 0.439171
H -5.852665 2.639191 -1.122955
H -3.152914 0.409595 -1.434368
H -4.923201 0.194070 -1.360926
H -3.031542 -0.250912 1.020999
H -4.748910 -0.665685 0.958113
H -4.304789 -2.465273 -0.737188
C -2.145464 -3.981313 -0.727329
H -1.408286 -3.957310 -1.547788
H -1.765473 -4.709980 0.010163
H -3.092133 -4.362975 -1.136504
H -1.342297 -1.124883 1.107910
H -0.854339 -2.787071 1.436083
H 0.417697 -2.914485 -0.639997
H 3.674775 0.579984 -1.791023
O 4.741308 1.374478 -0.192378
H 4.473838 2.295528 -0.351102
H -0.127707 1.118703 1.620596
H -1.657324 1.539635 -0.013882

6-c42, ΔG = 3.2417 kcal/mol, population = 0.10 %

O 0.599864 -0.998996 2.035505
C -0.715075 -0.631575 1.943002
C -1.163465 0.063062 0.658600
C -2.122396 -0.690388 0.096258
C -2.375128 -1.873133 0.938979

O -3.187313 -2.758667 0.765964
O -1.562466 -1.819631 2.013162
C -2.904018 -0.375724 -1.143273
C -2.829070 1.127971 -1.361939
H -3.252383 1.382512 -2.345696
H -3.467597 1.609082 -0.601682
C -1.388921 1.652589 -1.264087
C -1.347388 3.113795 -1.722409
H -0.349776 3.564597 -1.618205
H -2.057705 3.732254 -1.152568
H -1.631416 3.181219 -2.783700
H -0.782575 1.061077 -1.973974
C -0.723234 1.421916 0.147370
C -1.198544 2.480458 1.165880
H -2.296925 2.517095 1.208498
H -0.830020 3.479680 0.895147
H -0.833469 2.257583 2.178132
C 0.819563 1.491906 -0.073657
H 1.137249 0.536646 -0.514960
C 1.732000 1.838447 1.114676
C 3.169353 2.028530 0.658238
C 3.988712 1.001812 0.367651
C 3.614761 -0.452875 0.437620
C 3.367567 -1.076599 -0.948794
C 2.354793 -2.201979 -0.989132
O 1.443276 -2.295011 -0.177607
C 2.480191 -3.187973 -2.117527
H 3.370704 -3.814944 -1.940615
H 1.588483 -3.824764 -2.175476
H 2.646173 -2.664619 -3.072149
H 2.944577 -0.317403 -1.634887
H 4.302245 -1.403491 -1.429834
H 2.713014 -0.570252 1.047094
H 4.408709 -1.029375 0.941735
H 4.998756 1.230728 0.005626
C 3.609199 3.458416 0.487135
H 2.931900 3.994689 -0.201559
H 3.565012 4.002631 1.447102
H 4.632885 3.534726 0.091570
H 1.662913 1.056860 1.882283
H 1.388589 2.774125 1.579247
H 1.002965 2.248181 -0.851266
H -2.424024 -0.892176 -2.001524
O -4.257834 -0.776581 -1.025013
H -4.254423 -1.674873 -0.651896
H -0.960407 -0.028971 2.831799
H 0.890081 -1.454700 1.207981

6-c36, ΔG = 3.3409 kcal/mol, population = 0.08 %

O -0.864368 -0.481083 -2.200331
C 0.401588 -0.953557 -1.943529
C 1.149431 -0.359296 -0.753622
C 1.413368 -1.349435 0.113444
C 0.934445 -2.624771 -0.452182
O 1.065713 -3.743216 -0.005126
O 0.348589 -2.374355 -1.647077
C 2.248851 -1.270239 1.356012
C 2.818110 0.147288 1.522843
H 2.142854 0.722193 2.171744
H 3.768783 0.057768 2.069461
C 3.044046 0.903065 0.197279
C 4.186610 0.268077 -0.604771
H 4.471393 0.879810 -1.472178
H 3.926355 -0.740277 -0.958888
H 5.076824 0.165783 0.034447
H 3.350805 1.929875 0.458205
C 1.699910 1.043639 -0.612311
C 1.941827 1.668706 -1.996020
H 2.618567 1.059179 -2.609605
H 2.390367 2.668317 -1.885683
H 1.000746 1.776610 -2.552180
C 0.740426 1.951991 0.211550
H 0.500088 1.447062 1.156980
C -0.579931 2.357358 -0.462158
C -1.506419 3.070594 0.502786
C -2.312768 2.395700 1.341453
C -2.411756 0.895299 1.399444
C -3.497915 0.327275 0.448322
C -3.348161 -1.172673 0.350501
O -2.483697 -1.663127 -0.365877
C -4.239632 -2.034051 1.197303
H -3.940110 -3.087609 1.132335
H -4.212023 -1.689849 2.243946
H -5.282191 -1.917911 0.856626
H -4.499691 0.610135 0.802744
H -3.352376 0.751737 -0.556503
H -2.632389 0.570566 2.429088

H -1.450746 0.434661 1.128683
H -2.964701 2.960682 2.017678
C -1.441233 4.573548 0.496257
H -1.736791 4.974644 -0.489189
H -2.091695 5.020326 1.262589
H -0.408265 4.921598 0.673512
H -1.059927 1.463950 -0.882260
H -0.373980 3.020308 -1.316086
H 1.300449 2.862206 0.484254
H 1.612301 -1.504860 2.231547
O 3.316564 -2.212264 1.281448
H 2.912121 -3.078019 1.108570
H 0.996963 -0.841100 -2.864097
H -1.469614 -0.808727 -1.488513

6-c17, ΔG = 3.3409 kcal/mol, population = 0.08 %

O -0.213703 1.827943 -1.875845
C -1.410276 1.181671 -1.679362
C -1.374107 0.035999 -0.683178
C -2.166763 0.345757 0.353200
C -2.864402 1.611822 0.060876
O -3.729109 2.162598 0.704235
O -2.406373 2.090289 -1.124051
C -2.374222 -0.467561 1.593536
C -1.424027 -1.670626 1.580243
H -0.463063 -1.349403 2.010593
H -1.831400 -2.433867 2.260436
C -1.186690 -2.275097 0.182646
C -2.467568 -2.908607 -0.377511
H -3.226096 -2.151767 -0.623960
H -2.912084 -3.579670 0.373290
H -2.266363 -3.506307 -1.277800
H -0.452632 -3.086965 0.301999
C -0.542824 -1.218851 -0.777906
C -0.486491 -1.724889 -2.230137
H -1.488475 -1.879528 -2.653274
H 0.052761 -2.682649 -2.283175
H 0.043482 -1.002805 -2.868962
C 0.893475 -0.820466 -0.322423
H 1.329817 -0.214572 -1.128675
C 1.864175 -1.956548 0.035129
C 3.317594 -1.510248 -0.017816
C 3.854435 -0.583561 0.796690
C 3.176315 0.190414 1.892401
C 3.145371 1.726346 1.647438
C 2.354988 2.100926 0.411881
O 1.137946 2.236168 0.474588
C 3.104464 2.252784 -0.881176
H 2.421161 2.418843 -1.723282
H 3.807727 3.097637 -0.795439
H 3.711715 1.350844 -1.056533
H 2.669597 2.212467 2.512054
H 4.177673 2.098509 1.558272
H 3.726934 0.042933 2.837331
H 2.153937 -0.170141 2.072294
H 4.911949 -0.331370 0.645733
C 4.140179 -2.154006 -1.102649
H 5.172162 -1.774258 -1.124908
H 4.173425 -3.250250 -0.974757
H 3.681462 -1.972469 -2.091074
H 1.732809 -2.799537 -0.659948
H 1.625275 -2.348174 1.037521
H 0.806999 -0.149748 0.537629
H -2.131164 0.167579 2.467614
O -3.726145 -0.908790 1.696130
H -4.283602 -0.116201 1.666145
H -1.790128 0.870275 -2.664825
H 0.207268 2.036296 -1.005415

6-c28, ΔG = 3.3427 kcal/mol, population = 0.08 %

O 0.695336 -0.650942 2.225412
C -0.617397 -0.853725 1.868654
C -1.143423 -0.099009 0.651337
C -1.536622 -0.999338 -0.263344
C -1.364349 -2.355302 0.291170
O -1.683880 -3.415827 -0.200019
O -0.827938 -2.250413 1.530063
C -2.247706 -0.730289 -1.555727
C -2.509095 0.775721 -1.713724
H -1.687954 1.214859 -2.297203
H -3.416820 0.889630 -2.324997
C -2.674156 1.536775 -0.382224
C -3.975180 1.130342 0.320695
H -3.947800 0.083783 0.658177
H -4.819617 1.221617 -0.379417
H -4.193569 1.770616 1.186762

H -2.750036 2.609009 -0.629402
C -1.390773 1.388478 0.519312
C -1.601512 2.024029 1.903336
H -0.700354 1.929454 2.524265
H -2.428872 1.552575 2.450328
H -1.831803 3.095474 1.795808
C -0.212419 2.099550 -0.208939
H -0.010578 1.573945 -1.152104
C 1.110536 2.217892 0.563989
C 2.227544 2.747313 -0.313626
C 2.940969 1.939173 -1.117981
C 2.742349 0.450854 -1.217314
C 3.621908 -0.341212 -0.214355
C 3.168920 -1.781730 -0.174410
O 2.174333 -2.100381 0.466133
C 3.929500 -2.790184 -0.985745
H 3.421647 -3.762750 -0.974702
H 4.047596 -2.429225 -2.020380
H 4.946616 -2.892511 -0.571595
H 4.682820 -0.259773 -0.491873
H 3.492368 0.085925 0.791539
H 2.967313 0.106836 -2.239736
H 1.691767 0.188407 -1.026432
H 3.739260 2.373478 -1.730856
C 2.463275 4.232249 -0.263183
H 3.243048 4.552732 -0.969747
H 1.535968 4.784302 -0.497557
H 2.761511 4.547719 0.752139
H 1.370906 1.238476 0.985909
H 0.980549 2.892929 1.423367
H -0.558095 3.108867 -0.488748
H -1.609393 -1.071864 -2.393991
O -3.484485 -1.439218 -1.583572
H -3.274464 -2.371748 -1.412410
H -1.243492 -0.640784 2.750264
H 1.272935 -1.080037 1.545261

6-c26, ΔG = 3.4199 kcal/mol, population = 0.07 %

O 0.342201 -1.082487 2.304960
C -0.928137 -0.943292 1.807821
C -1.169007 0.016751 0.646455
C -1.763265 -0.662667 -0.346351
C -1.935260 -2.067454 0.066972
O -2.485749 -2.966422 -0.531424
O -1.416386 -2.219371 1.307996
C -2.379475 -0.098060 -1.592326
C -2.288357 1.438251 -1.592535
H -1.415671 1.738311 -2.188342
H -3.170147 1.815426 -2.131518
C -2.219112 2.083798 -0.191780
C -3.568264 1.962842 0.527134
H -3.586406 2.523014 1.472392
H -3.823752 0.913698 0.738108
H -4.367616 2.367741 -0.112397
H -2.013630 3.157449 -0.341043
C -1.006715 1.519815 0.640245
C -0.995824 2.073080 2.074529
H -0.133345 1.689356 2.636177
H -1.899991 1.794010 2.632181
H -0.934524 3.172161 2.055000
C 0.303462 1.938794 -0.086602
H 0.257131 1.589698 -1.125858
C 1.616269 1.424857 0.516037
C 2.817706 1.777221 -0.339091
C 3.181421 1.065881 -1.422400
C 2.501917 -0.162238 -1.971230
C 3.166577 -1.500304 -1.550073
C 2.869495 -1.769386 -0.093346
O 1.733189 -2.092654 0.236414
C 3.959424 -1.538469 0.909189
H 4.313212 -0.498894 0.801714
H 3.608949 -1.719061 1.933409
H 4.820414 -2.187592 0.680535
H 2.724080 -2.318786 -2.138669
H 4.249178 -1.470573 -1.740521
H 2.519585 -0.118232 -3.071726
H 1.442830 -0.208071 -1.676864
H 4.070956 1.394945 -1.973380
C 3.574688 3.008720 0.081551
H 4.394568 3.248994 -0.610928
H 2.900227 3.881447 0.136471
H 3.997603 2.881735 1.093509
H 1.540537 0.341495 0.649157
H 1.760431 1.841581 1.523986
H 0.322306 3.040549 -0.132361
H -1.834447 -0.487563 -2.474132
O -3.747301 -0.495391 -1.667088

H -3.759617 -1.464131 -1.598325
H -1.582654 -0.662705 2.650032
H 0.911878 -1.493020 1.610599

6-c32, ΔG = 3.9339 kcal/mol, population = 0.03 %

O 1.007892 -0.692148 -2.191041
C -0.116734 0.090289 -2.227251
C -0.941682 0.137304 -0.947140
C -0.944116 1.400556 -0.494155
C -0.188566 2.250961 -1.431457
O 0.004201 3.447234 -1.370484
O 0.250153 1.484135 -2.453616
C -1.637287 1.916495 0.731503
C -2.717331 0.916849 1.134784
H -3.067772 1.144829 2.152913
H -3.577351 1.063823 0.461492
C -2.220717 -0.539068 1.073226
C -3.237518 -1.481386 1.720563
H -3.399393 -1.194757 2.770895
H -2.899529 -2.527785 1.711775
H -4.213620 -1.435479 1.213720
H -1.305921 -0.577619 1.687854
C -1.792595 -0.971315 -0.371831
C -3.021938 -1.064890 -1.317345
H -3.552901 -0.106263 -1.392633
H -3.724885 -1.829578 -0.958219
H -2.708155 -1.356384 -2.330708
C -1.134617 -2.382631 -0.394222
H -1.961397 -3.094728 -0.263201
C -0.044233 -2.746382 0.642969
C 1.396567 -2.689170 0.185885
C 2.353276 -1.988074 0.820886
C 2.184515 -1.093865 2.021013
C 1.763649 0.357814 1.671670
C 2.712389 0.994781 0.684819
O 2.635488 0.748083 -0.511749
C 3.772008 1.914954 1.222958
H 4.311639 1.428784 2.052024
H 4.471642 2.208520 0.430300
H 3.288409 2.811707 1.645541
H 0.772100 0.332960 1.202808
H 1.703692 0.956193 2.592698
H 3.129215 -1.064074 2.587307
H 1.425155 -1.490356 2.712252
H 3.369370 -2.046452 0.414859
C 1.740955 -3.552355 -1.000276
H 1.246383 -3.182739 -1.911504
H 2.824485 -3.563886 -1.188357
H 1.403166 -4.591450 -0.841132
H -0.231289 -3.794828 0.936583
H -0.179207 -2.162077 1.561350
H -0.760017 -2.565773 -1.411038
H -0.887620 1.987763 1.548038
O -2.224203 3.186836 0.505152
H -1.547212 3.735744 0.074504
H -0.721588 -0.221408 -3.093011
H 1.584684 -0.364881 -1.460532

6-c20, ΔG = 3.9709 kcal/mol, population = 0.03 %

O 0.015666 1.827196 -1.591622
C -1.192297 1.184131 -1.603585
C -1.383235 0.014579 -0.637983
C -2.421295 0.301937 0.161344
C -2.981660 1.612223 -0.212868
O -3.944013 2.180089 0.261471
O -2.260132 2.113953 -1.236434
C -2.993769 -0.583090 1.224126
C -2.572933 -2.007773 0.897177
H -2.853374 -2.677209 1.724825
H -3.149096 -2.329371 0.012545
C -1.064226 -2.135593 0.621172
C -0.726122 -3.627951 0.510796
H 0.326764 -3.818451 0.275454
H -1.337639 -4.116521 -0.263317
H -0.949171 -4.128366 1.465794
H -0.538891 -1.732565 1.505917
C -0.573087 -1.268199 -0.599261
C -0.762437 -1.999618 -1.944543
H -0.111618 -2.882194 -2.009623
H -0.504772 -1.339653 -2.786319
H -1.802895 -2.331016 -2.079333
C 0.911214 -0.837744 -0.422817
H 1.212511 -0.292592 -1.328714
C 1.974763 -1.904874 -0.121711
C 3.376328 -1.341392 -0.288176
C 3.955395 -0.500886 0.587927

C 3.361898 0.056660 1.851663
C 3.309094 1.608859 1.863560
C 2.448596 2.142681 0.738178
O 1.226358 2.116737 0.835782
C 3.136760 2.631690 -0.503422
H 3.773932 1.822106 -0.895292
H 2.414233 2.942730 -1.267798
H 3.808022 3.468070 -0.249122
H 2.871086 1.944565 2.815742
H 4.329924 2.012331 1.785710
H 3.977020 -0.243141 2.717976
H 2.352499 -0.339542 2.032974
H 4.969250 -0.147682 0.359203
C 4.081888 -1.753115 -1.552959
H 5.066025 -1.273084 -1.656598
H 4.220380 -2.847863 -1.590120
H 3.472839 -1.488779 -2.435892
H 1.863758 -2.761616 -0.802827
H 1.840076 -2.293835 0.898935
H 0.939018 -0.104509 0.391263
H -2.558209 -0.289317 2.202578
O -4.407743 -0.498587 1.271626
H -4.634860 0.446249 1.234436
H -1.401456 0.884058 -2.642777
H 0.324843 1.986956 -0.666965

Coordinates of the dominating conformers of **7**

7-c2, ΔG = 0.0000 kcal/mol, population = 33.35 %

O -4.691987 0.817052 0.584160
H -4.534702 1.712414 0.928111
C -3.476928 0.101613 0.740927
C -2.307239 0.894774 0.243043
C -1.267779 0.418192 -0.462809
C -0.366244 1.572615 -0.795747
H 0.657708 1.462625 -0.409556
H -0.288131 1.745585 -1.881429
O -0.991640 2.719251 -0.194949
C -2.146893 2.344503 0.411853
O -2.884205 3.134236 0.967054
C -1.080065 -1.021451 -0.868159
C -1.246870 -1.110518 -2.402295
H -0.552613 -0.424927 -2.910199
H -2.269185 -0.849376 -2.712983
H -1.023969 -2.126607 -2.756883
C 0.362280 -1.478130 -0.516621
H 0.479521 -2.520805 -0.849217
C 0.757781 -1.353434 0.963511
C 2.179907 -1.789083 1.236578
C 3.182679 -0.945118 1.537851
C 3.144930 0.554106 1.650137
C 4.175239 1.227905 0.737211
C 3.861666 1.125717 -0.743988
O 2.727661 0.945145 -1.149880
C 5.025207 1.277033 -1.692691
H 5.660511 2.128866 -1.403120
H 5.654776 0.373170 -1.627202
H 4.667534 1.396782 -2.723605
H 4.236837 2.310707 0.956468
H 5.189744 0.836101 0.920603
H 3.375921 0.848321 2.689437
H 2.146302 0.952200 1.425797
H 4.171055 -1.386692 1.723567
C 2.423178 -3.276067 1.157924
H 1.770772 -3.819288 1.864240
H 3.468216 -3.532757 1.385007
H 2.187813 -3.670565 0.154628
H 0.088915 -1.978723 1.578569
H 0.598948 -0.318504 1.297110
H 1.071781 -0.884986 -1.113614
C -2.155127 -1.885508 -0.118232
C -2.283433 -3.307186 -0.668971
H -2.910989 -3.915879 -0.000028
H -1.307199 -3.807713 -0.753320
H -2.756577 -3.316238 -1.662956
H -1.807826 -1.969710 0.924379
C -3.531782 -1.198865 -0.054509
H -4.267331 -1.880788 0.399463
H -3.895729 -0.959323 -1.068026
H -3.313547 -0.138684 1.812828

7-c1, ΔG = 0.0860 kcal/mol, population = 28.84 %

O 1.380387 -3.111843 -0.159940
H 2.166804 -2.691630 0.225673
C 0.509945 -2.061839 -0.553662
C 0.295748 -1.081535 0.560694

C -0.863901 -0.481039 0.882715
C -0.622312 0.370022 2.098879
H -0.818513 1.436802 1.924580
H -1.205652 0.038005 2.972340
O 0.775335 0.207037 2.395081
C 1.329414 -0.665873 1.514419
O 2.497381 -0.997072 1.569098
C -2.178333 -0.711045 0.181960
C -3.087028 -1.503106 1.152549
H -4.091055 -1.630524 0.724310
H -3.202110 -0.967368 2.106260
H -2.672338 -2.497798 1.371134
C -2.896697 0.630399 -0.136911
H -3.844022 0.369061 -0.630280
C -2.147635 1.655783 -1.017609
C -1.336326 2.709416 -0.293016
C -0.003561 2.849399 -0.412869
C 0.949736 1.976802 -1.182348
C 2.300745 1.856894 -0.476205
C 3.199970 0.756578 -1.007754
O 2.830436 -0.013045 -1.876058
C 4.565659 0.645516 -0.373366
H 5.088841 1.614248 -0.390767
H 4.433519 0.355922 0.681355
H 5.161692 -0.118485 -0.889388
H 2.858972 2.808536 -0.522468
H 2.166453 1.674111 0.604255
H 1.118182 2.386705 -2.195436
H 0.532247 0.973438 -1.335007
H 0.458935 3.694072 0.114033
C -2.135260 3.676589 0.545346
H -1.493275 4.438322 1.010776
H -2.684700 3.161155 1.352305
H -2.898576 4.189554 -0.065769
H -2.909388 2.196741 -1.605928
H -1.526784 1.135476 -1.758702
H -3.192967 1.100730 0.814237
C -1.902084 -1.527906 -1.131919
C -3.167147 -2.106454 -1.770842
H -3.956492 -1.350390 -1.892986
H -3.579858 -2.935441 -1.175623
H -2.932886 -2.504354 -2.770022
H -1.470820 -0.814325 -1.853396
C -0.848765 -2.633132 -0.938454
H -0.754196 -3.220474 -1.864792
H -1.161006 -3.331964 -0.144054
H 0.942149 -1.519631 -1.417269

7-c10, ΔG = 0.8214 kcal/mol, population = 8.32 %

O -4.416431 1.795198 -0.859052
H -5.028037 1.059548 -1.028135
C -3.103628 1.270051 -0.978312
C -2.943412 0.008747 -0.184541
C -1.885809 -0.323309 0.574293
C -2.164095 -1.665439 1.193120
H -1.444474 -2.439527 0.882985
H -2.181399 -1.635525 2.294297
O -3.468703 -2.032304 0.720426
C -3.952178 -1.054796 -0.092603
O -5.050979 -1.111923 -0.603977
C -0.663785 0.533170 0.780371
C -0.719390 1.108279 2.214954
H -1.580860 1.777464 2.352189
H 0.198929 1.669873 2.437178
H -0.799088 0.299629 2.956852
C 0.613842 -0.337330 0.673273
H 1.490897 0.282828 0.902213
C 0.845081 -1.027638 -0.679905
C 2.004087 -1.998549 -0.637251
C 3.232584 -1.714179 -1.104773
C 3.709725 -0.444616 -1.756166
C 4.946697 0.139366 -1.065055
C 4.663247 0.813474 0.266492
O 3.570011 1.277891 0.532468
C 5.818160 0.901911 1.234610
H 5.573762 1.577389 2.064764
H 6.024350 -0.106608 1.632294
H 6.734917 1.235414 0.723185
H 5.731105 -0.623812 -0.930891
H 5.405811 0.923111 -1.697065
H 2.921211 0.319560 -1.775055
H 3.979078 -0.656481 -2.806316
H 3.999924 -2.494673 -1.013175
C 1.699828 -3.336015 -0.010546
H 2.588421 -3.982574 0.035528
H 0.915392 -3.865524 -0.579902
H 1.311080 -3.220394 1.016149

H 1.013433 -0.269144 -1.455120
H -0.066248 -1.574784 -0.980946
H 0.568687 -1.098343 1.470298
C -0.687900 1.670621 -0.299432
C 0.367141 2.752989 -0.063611
H 0.124555 3.367326 0.817580
H 0.409711 3.429652 -0.931422
H 1.370118 2.326724 0.079828
H -0.449268 1.184341 -1.259849
C -2.088450 2.288288 -0.467484
H -2.038836 3.140986 -1.162008
H -2.459282 2.678830 0.494944
H -2.881827 1.042563 -2.042466

7-c27, ΔG = 0.9111 kcal/mol, population = 7.15 %

O 4.119333 2.067819 0.306778
H 4.562544 1.632977 1.054022
C 2.791955 1.568259 0.272448
C 2.765969 0.071348 0.346192
C 1.980239 -0.746393 -0.373707
C 2.301573 -2.161750 0.020431
H 1.444438 -2.689155 0.468377
H 2.675294 -2.767954 -0.820262
O 3.339016 -2.049455 1.005700
C 3.634684 -0.737836 1.211456
O 4.498496 -0.373631 1.981455
C 0.988750 -0.298379 -1.416653
C 1.568833 -0.649591 -2.806402
H 0.840894 -0.419430 -3.597256
H 1.799576 -1.723247 -2.873569
H 2.494670 -0.093497 -3.011692
C -0.340588 -1.075496 -1.242753
H -1.021806 -0.799105 -2.062183
C -1.061879 -0.874221 0.097560
C -2.246074 -1.803900 0.252167
C -3.475304 -1.496665 -0.197723
C -3.899775 -0.231365 -0.893293
C -4.905877 0.588028 -0.078213
C -4.300732 1.318145 1.108705
O -3.108807 1.549706 1.186892
C -5.266332 1.763133 2.182187
H -6.162361 2.226697 1.740550
H -5.608354 0.874915 2.740530
H -4.775703 2.459195 2.875044
H -5.367446 1.373529 -0.706399
H -5.747073 -0.035020 0.269832
H -4.373276 -0.493840 -1.855061
H -3.034796 0.403362 -1.130324
H -4.274678 -2.234745 -0.049398
C -1.954375 -3.126785 0.910830
H -1.149848 -3.664723 0.377864
H -2.838307 -3.780912 0.940779
H -1.594095 -2.979994 1.944335
H -1.399721 0.164913 0.199399
H -0.355409 -1.050934 0.926698
H -0.132019 -2.148613 -1.390987
C 0.782616 1.247814 -1.247495
C -0.016694 1.882347 -2.386774
H 0.558706 1.903163 -3.325063
H -0.274275 2.922228 -2.134006
H -0.957889 1.345697 -2.578482
H 0.195882 1.379163 -0.323602
C 2.110844 1.994578 -1.024511
H 1.929767 3.080275 -1.006959
H 2.811586 1.798716 -1.853210
H 2.213262 1.968860 1.131405

7-c35, ΔG = 1.3448 kcal/mol, population = 3.44 %

O 4.252767 2.054365 0.881199
H 4.946422 1.380454 0.974002
C 3.010543 1.384194 1.022170
C 2.941577 0.166150 0.151559
C 1.885968 -0.230909 -0.578080
C 2.272546 -1.491161 -1.302259
H 1.658756 -2.359356 -1.014522
H 2.227268 -1.388403 -2.398246
O 3.632318 -1.741667 -0.917631
C 4.051563 -0.772427 -0.060531
O 5.175178 -0.741891 0.395726
C 0.571302 0.501491 -0.668899
C 0.492814 1.168112 -2.062054
H 1.268589 1.936760 -2.188117
H -0.490175 1.637350 -2.209603
H 0.624655 0.421945 -2.859679
C -0.600408 -0.506347 -0.560112
H -1.543068 0.038945 -0.714767

C -0.690198 -1.301165 0.751331
C -1.727898 -2.403551 0.676230
C -3.039397 -2.179984 0.873757
C -3.674266 -0.851504 1.172306
C -4.471507 -0.300868 -0.016428
C -4.863450 1.159942 0.121482
O -4.302102 1.903605 0.904477
C -5.968407 1.645830 -0.787234
H -6.924266 1.203873 -0.458528
H -6.041932 2.740526 -0.750478
H -5.800591 1.307307 -1.821901
H -3.866272 -0.360170 -0.941020
H -5.369409 -0.905667 -0.225650
H -2.921088 -0.104530 1.456835
H -4.357317 -0.942718 2.035277
H -3.727574 -3.028099 0.766561
C -1.203154 -3.766026 0.307829
H -0.660718 -3.731792 -0.654223
H -2.008640 -4.509542 0.216532
H -0.478088 -4.127192 1.058203
H -0.922906 -0.618042 1.580540
H 0.292903 -1.741520 0.987276
H -0.530470 -1.210523 -1.406410
C 0.534444 1.563524 0.485263
C -0.637033 2.541993 0.379011
H -0.683712 3.168650 1.282973
H -1.606786 2.031094 0.288858
H -0.525071 3.217873 -0.482783
H 0.401882 0.994419 1.420500
C 1.869776 2.317218 0.627308
H 1.768352 3.115457 1.378345
H 2.146374 2.802903 -0.323280
H 2.868070 1.067143 2.076887

7-c20, ΔG = 1.3811 kcal/mol, population = 3.23 %

O -4.327621 0.991220 1.034217
H -4.100116 1.933455 1.106451
C -3.104236 0.273991 1.068763
C -2.091497 0.870207 0.138977
C -1.242302 0.194225 -0.653454
C -0.424723 1.200559 -1.416607
H 0.645024 1.164307 -1.159415
H -0.537074 1.112705 -2.508620
O -0.930052 2.481678 -1.003438
C -1.907421 2.310850 -0.077732
O -2.505138 3.240082 0.426647
C -1.177577 -1.309266 -0.766920
C -1.756292 -1.706474 -2.144919
H -2.826410 -1.464491 -2.219627
H -1.630207 -2.784351 -2.320653
H -1.233085 -1.177746 -2.955407
C 0.298437 -1.784743 -0.714512
H 0.310620 -2.884550 -0.767865
C 1.109420 -1.316126 0.502267
C 2.509071 -1.897736 0.531564
C 3.530691 -1.406333 -0.191896
C 3.506890 -0.235955 -1.138502
C 4.265372 0.986174 -0.606860
C 3.505356 1.779912 0.442769
O 2.287542 1.807060 0.470892
C 4.335353 2.560445 1.430823
H 3.703036 3.244678 2.011294
H 4.831359 1.849814 2.114023
H 5.135104 3.116431 0.916358
H 5.256609 0.706011 -0.215429
H 4.461739 1.704543 -1.425712
H 2.478981 0.064353 -1.379043
H 3.973061 -0.541327 -2.090350
H 4.506171 -1.900496 -0.094936
C 2.685515 -3.107093 1.412666
H 1.971240 -3.901774 1.132169
H 2.471041 -2.859974 2.467444
H 3.702381 -3.522346 1.352821
H 0.591417 -1.613690 1.426810
H 1.161129 -0.218957 0.517769
H 0.803959 -1.443063 -1.632586
C -2.017309 -1.925028 0.407117
C -2.276203 -3.425179 0.250382
H -2.716253 -3.829113 1.175016
H -1.352409 -3.988319 0.051241
H -2.983076 -3.632191 -0.567787
H -1.412806 -1.790345 1.319264
C -3.338615 -1.172783 0.647666
H -3.927377 -1.692661 1.418982
H -3.950700 -1.159725 -0.269940
H -2.685431 0.286530 2.097393

7-c9, ΔG = 1.6171 kcal/mol, population = 2.17 %

O 4.439420 -1.671696 -0.865575
H 5.022580 -0.911674 -1.027214
C 3.107810 -1.201045 -1.001524
C 2.884917 0.050933 -0.208157
C 1.804767 0.337486 0.537356
C 2.020298 1.688330 1.162564
H 1.274874 2.434199 0.843961
H 2.023614 1.656206 2.263836
O 3.315069 2.108801 0.708721
C 3.848726 1.154161 -0.100045
O 4.950924 1.257126 -0.596414
C 0.616767 -0.569636 0.726203
C 0.673852 -1.143297 2.161066
H 1.559649 -1.777149 2.310172
H -0.223887 -1.742644 2.368477
H 0.709554 -0.333051 2.904569
C -0.694780 0.247007 0.599442
H -1.541949 -0.413939 0.827432
C -0.934222 0.919444 -0.761828
C -2.104902 1.876945 -0.739577
C -3.334345 1.564305 -1.188444
C -3.798457 0.256627 -1.766236
C -4.908992 -0.407714 -0.919537
C -4.373955 -0.805367 0.445991
O -3.573581 -1.717631 0.556412
C -4.822249 0.009861 1.630433
H -4.364718 -0.363576 2.555805
H -4.533192 1.061418 1.463595
H -5.921217 -0.007644 1.712999
H -5.768661 0.272237 -0.819818
H -5.250336 -1.323968 -1.427015
H -2.968521 -0.456988 -1.867645
H -4.206400 0.422267 -2.778583
H -4.111782 2.335822 -1.113161
C -1.812894 3.237042 -0.158454
H -2.709146 3.873568 -0.127271
H -1.037999 3.756922 -0.748845
H -1.417854 3.157437 0.869318
H -1.085998 0.149523 -1.529425
H -0.028820 1.475082 -1.063651
H -0.695049 1.012447 1.393215
C 0.701906 -1.703510 -0.354484
C -0.307500 -2.831820 -0.135036
H -0.049761 -3.437417 0.748027
H -0.306765 -3.507603 -1.004601
H -1.332424 -2.456767 -0.003919
H 0.455963 -1.225972 -1.317390
C 2.129363 -2.261400 -0.505277
H 2.124216 -3.113982 -1.201666
H 2.503974 -2.638714 0.460978
H 2.890690 -0.981020 -2.068166

7-c38, ΔG = 1.6246 kcal/mol, population = 2.14 %

O -2.736362 1.601902 2.117434
H -2.587700 2.474387 1.716712
C -1.727687 0.743452 1.607357
C -1.652769 0.821810 0.113007
C -1.498948 -0.209454 -0.734578
C -1.584883 0.329978 -2.136058
H -0.693080 0.128583 -2.742086
H -2.468762 -0.049074 -2.674482
O -1.718975 1.751456 -1.980986
C -1.774706 2.062866 -0.659722
O -1.906809 3.201304 -0.258695
C -1.346606 -1.651180 -0.322441
C -2.637779 -2.394996 -0.739516
H -3.516028 -2.008280 -0.202415
H -2.550274 -3.471168 -0.534645
H -2.824387 -2.281005 -1.817584
C -0.159770 -2.325841 -1.067831
H -0.145618 -3.380737 -0.755098
C 1.255732 -1.747136 -0.865085
C 1.598254 -0.520881 -1.684185
C 1.766448 0.714072 -1.177484
C 1.654427 1.160725 0.251899
C 2.999765 1.604511 0.834990
C 3.935399 0.452440 1.162902
O 3.522633 -0.675842 1.354533
C 5.404393 0.788910 1.261935
H 5.961993 -0.049605 1.699183
H 5.789837 0.994659 0.248671
H 5.559683 1.704989 1.853373
H 3.514575 2.319455 0.171840
H 2.848167 2.145528 1.788210
H 1.240105 0.369371 0.887864

H 0.956005 2.012198 0.309052
H 2.040446 1.511314 -1.881022
C 1.794585 -0.773956 -3.159077
H 0.912789 -1.258118 -3.613636
H 2.638410 -1.467027 -3.323533
H 1.995909 0.154315 -3.713078
H 1.965006 -2.539393 -1.162452
H 1.457550 -1.564895 0.197324
H -0.399290 -2.352283 -2.143680
C -1.136474 -1.697098 1.233193
C -1.276899 -3.099100 1.830162
H -0.942238 -3.095216 2.878806
H -0.669962 -3.842879 1.293220
H -2.322769 -3.442505 1.820466
H -0.098438 -1.373076 1.411024
C -2.036890 -0.700738 1.985208
H -1.913658 -0.834719 3.070804
H -3.099364 -0.888655 1.755797
H -0.743336 1.026421 2.032789

7-c6, ΔG = 1.9014 kcal/mol, population = 1.34 %

O 4.323289 1.229103 -0.041350
H 4.090913 2.114804 -0.367189
C 3.264939 0.366209 -0.425908
C 1.926889 0.945872 -0.082754
C 0.869769 0.282209 0.418154
C -0.257712 1.263815 0.568702
H -1.111973 1.005128 -0.072046
H -0.622660 1.362388 1.602097
O 0.281000 2.524057 0.135481
C 1.569360 2.358365 -0.258204
O 2.258281 3.274857 -0.659337
C 0.884689 -1.172705 0.818720
C 0.988480 -1.194688 2.365688
H 1.902288 -0.697900 2.720805
H 0.984509 -2.228867 2.738088
H 0.126148 -0.679498 2.813959
C -0.435139 -1.909718 0.460188
H -0.399659 -2.883197 0.973636
C -0.782858 -2.187922 -1.016233
C -1.231541 -0.997579 -1.845118
C -2.481628 -0.501985 -1.790701
C -3.644604 -1.010733 -0.979916
C -4.419759 0.104801 -0.270181
C -3.754286 0.656039 0.978121
O -2.950820 0.004830 1.621624
C -4.145557 2.053717 1.389256
H -3.820507 2.257837 2.417719
H -3.649111 2.764917 0.706116
H -5.229653 2.214187 1.285147
H -4.648632 0.935180 -0.958559
H -5.404024 -0.268990 0.070146
H -3.327430 -1.755699 -0.237862
H -4.348682 -1.522918 -1.660758
H -2.715021 0.354192 -2.437583
C -0.211116 -0.410819 -2.786885
H 0.709527 -0.120483 -2.257690
H -0.597879 0.474493 -3.312773
H 0.089168 -1.158227 -3.542581
H -1.588409 -2.938694 -1.007585
H 0.065911 -2.678687 -1.517581
H -1.269160 -1.363363 0.923653
C 2.134791 -1.837219 0.145662
C 2.400266 -3.266469 0.622590
H 2.738468 -3.287752 1.670116
H 3.192780 -3.726189 0.012282
H 1.508026 -3.904477 0.541603
H 1.907521 -1.889843 -0.932273
C 3.405389 -0.977788 0.280651
H 4.268704 -1.523139 -0.130447
H 3.628524 -0.778861 1.341792
H 3.295182 0.199535 -1.524293

7-c23, ΔG = 1.9641 kcal/mol, population = 1.21 %

O -4.561469 -0.761658 0.008270
H -4.466382 -1.608326 -0.459349
C -3.391173 -0.009475 -0.268480
C -2.152120 -0.827135 -0.060916
C -1.012246 -0.414559 0.519246
C -0.061757 -1.579340 0.547825
H 0.862897 -1.421752 -0.026193
H 0.222489 -1.873015 1.571081
O -0.782593 -2.665021 -0.056041
C -2.021202 -2.245335 -0.420767
O -2.840083 -2.981009 -0.932851
C -0.786939 0.960905 1.097025

C -0.788859 0.827071 2.638283
H -1.763102 0.482034 3.013181
H -0.555917 1.791902 3.110605
H -0.025860 0.106311 2.967827
C 0.604619 1.499714 0.674818
H 0.778613 2.455104 1.193067
C 0.838076 1.687300 -0.832769
C 2.225703 2.217029 -1.128324
C 3.281353 1.425110 -1.389211
C 3.284443 -0.076153 -1.430414
C 3.975496 -0.701791 -0.211836
C 3.780599 -2.203607 -0.093999
O 2.828653 -2.764352 -0.606030
C 4.808029 -2.956220 0.715721
H 5.764419 -2.962567 0.165903
H 4.996390 -2.445857 1.673666
H 4.479157 -3.988876 0.890107
H 5.050737 -0.461705 -0.185689
H 3.561948 -0.274445 0.721862
H 3.804564 -0.426196 -2.339225
H 2.262522 -0.472594 -1.496438
H 4.252249 1.908029 -1.557958
C 2.364283 3.716539 -1.070190
H 3.404289 4.041390 -1.220485
H 2.018862 4.110012 -0.098058
H 1.734864 4.198941 -1.838746
H 0.100396 2.399114 -1.234638
H 0.660545 0.734341 -1.353708
H 1.372535 0.813654 1.068759
C -1.947118 1.890361 0.596836
C -1.986413 3.247712 1.301750
H -2.708171 3.911418 0.801468
H -1.008058 3.750811 1.285552
H -2.300882 3.151884 2.352383
H -1.748439 2.081593 -0.470425
C -3.321577 1.200386 0.658523
H -4.111461 1.918544 0.390138
H -3.537211 0.851455 1.682210
H -3.406600 0.343212 -1.321447

7-c13, ΔG = 2.0061 kcal/mol, population = 1.12 %

O 3.779736 -1.578875 1.273906
H 3.441655 -2.478578 1.131210
C 2.654745 -0.714145 1.244274
C 1.786786 -0.982223 0.053472
C 1.190045 -0.058671 -0.715254
C 0.427183 -0.777527 -1.791945
H -0.657302 -0.607161 -1.721929
H 0.758703 -0.513697 -2.808816
O 0.686818 -2.170110 -1.569407
C 1.462630 -2.317037 -0.463060
O 1.816560 -3.402292 -0.050336
C 1.309779 1.433401 -0.531746
C 2.199789 1.976040 -1.673842
H 2.276488 3.071135 -1.618895
H 1.769183 1.724968 -2.654847
H 3.213998 1.552983 -1.633249
C -0.091040 2.086484 -0.665732
H 0.037525 3.174778 -0.768259
C -1.075120 1.776851 0.474254
C -2.532008 2.010016 0.121459
C -3.535145 1.246489 0.594220
C -3.461394 0.088084 1.555026
C -3.705325 -1.276899 0.896125
C -2.467580 -1.869640 0.243676
O -1.349599 -1.585559 0.634854
C -2.689135 -2.841232 -0.887807
H -3.101559 -2.289945 -1.750283
H -1.744573 -3.318197 -1.177174
H -3.441220 -3.596442 -0.608900
H -4.013725 -2.022398 1.653795
H -4.531119 -1.236939 0.167580
H -4.231892 0.238520 2.329485
H -2.494008 0.054401 2.075066
H -4.552456 1.503932 0.271081
C -2.832305 3.201752 -0.754213
H -2.409144 4.123105 -0.315856
H -3.914879 3.348227 -0.879665
H -2.383618 3.104236 -1.756416
H -0.820601 2.414194 1.341008
H -0.941645 0.737207 0.802896
H -0.517515 1.754633 -1.626323
C 1.945630 1.693195 0.877014
C 2.349295 3.151527 1.098633
H 2.627792 3.312177 2.151526
H 1.527972 3.845494 0.863156
H 3.216842 3.432392 0.481821

H 1.161619 1.454419 1.613784
C 3.116146 0.739234 1.178587
H 3.590859 1.020955 2.131116
H 3.891219 0.812353 0.397486
H 2.043162 -0.856523 2.160469

7-c15, ΔG = 2.0501 kcal/mol, population = 1.04 %

O -4.496825 0.805893 -0.431415
H -4.949492 -0.020156 -0.659641
C -3.182688 0.725637 -0.984732
C -2.469471 -0.491637 -0.480547
C -1.387985 -0.506236 0.317865
C -1.036075 -1.935874 0.606599
H -0.029227 -2.211490 0.253307
H -1.091533 -2.171922 1.681784
O -2.029279 -2.708870 -0.084070
C -2.909090 -1.875503 -0.709168
O -3.876325 -2.284043 -1.314087
C -0.654117 0.719224 0.787437
C -0.091217 0.483091 2.202219
H 0.732530 -0.245166 2.164265
H -0.861100 0.100656 2.886860
H 0.298257 1.417587 2.631171
C 0.526728 0.907234 -0.212218
H 1.082324 -0.038226 -0.244246
C 1.532890 2.020888 0.120696
C 2.718867 1.968534 -0.818681
C 3.857027 1.309245 -0.536274
C 4.208870 0.559241 0.721012
C 4.623234 -0.893636 0.452039
C 3.474043 -1.849346 0.179473
O 2.363327 -1.668297 0.647589
C 3.787068 -3.049834 -0.677417
H 3.918380 -2.710563 -1.719426
H 4.738772 -3.512620 -0.372356
H 2.971121 -3.782901 -0.633651
H 5.356547 -0.956111 -0.368411
H 5.137380 -1.313006 1.337781
H 3.379433 0.563683 1.440757
H 5.060639 1.063113 1.211651
H 4.644766 1.310189 -1.301573
C 2.527501 2.667582 -2.140187
H 2.364867 3.749711 -1.991266
H 1.630706 2.290505 -2.662095
H 3.392354 2.536154 -2.807029
H 1.868062 1.916691 1.160577
H 1.049159 3.008600 0.042454
H 0.122872 1.064002 -1.223164
C -1.658705 1.918624 0.740122
C -2.660507 1.910469 1.902363
H -2.160362 2.017726 2.875191
H -3.256907 0.986466 1.915333
H -3.365680 2.749443 1.797219
H -1.058150 2.838807 0.829388
C -2.385738 1.985364 -0.619623
H -1.654144 2.169669 -1.420426
H -3.080461 2.839059 -0.631791
H -3.259830 0.660991 -2.087452

7-c21, ΔG = 2.0513 kcal/mol, population = 1.04 %

O 2.906449 2.342376 -0.929693
H 2.481590 3.043908 -0.408914
C 1.996114 1.254898 -0.969827
C 1.466215 0.929984 0.392815
C 1.251994 -0.301660 0.883230
C 0.725422 -0.157326 2.284336
H -0.285329 -0.576480 2.405617
H 1.383582 -0.613838 3.040593
O 0.670433 1.258731 2.518054
C 1.109156 1.922718 1.414970
O 1.176519 3.132793 1.361509
C 1.501155 -1.590436 0.141964
C 2.671482 -2.324882 0.831553
H 3.609566 -1.756531 0.746623
H 2.824242 -3.316965 0.384201
H 2.463270 -2.474849 1.901377
C 0.228994 -2.475013 0.241100
H 0.442231 -3.441287 -0.240152
C -1.040697 -1.827359 -0.367472
C -2.252482 -1.852803 0.533527
C -2.797363 -0.748070 1.078560
C -2.343124 0.681723 0.937699
C -3.231969 1.518234 0.008743
C -2.903431 1.358531 -1.467665
O -1.798363 1.016563 -1.847971
C -4.011387 1.680628 -2.440372

H -3.620735 1.736461 -3.464776
H -4.774862 0.886012 -2.382442
H -4.512254 2.622770 -2.166859
H -4.303336 1.321025 0.175709
H -3.094328 2.596888 0.214974
H -1.317959 0.739972 0.553469
H -2.337363 1.151291 1.934480
H -3.693724 -0.884521 1.697691
C -2.839889 -3.217197 0.787301
H -3.156723 -3.687426 -0.160446
H -3.707497 -3.176278 1.462085
H -2.091317 -3.895666 1.232253
H -1.298981 -2.352203 -1.303161
H -0.836311 -0.792847 -0.664130
H 0.062944 -2.710951 1.305013
C 1.825053 -1.248210 -1.355975
C 2.429286 -2.423401 -2.127137
H 1.840666 -3.344704 -2.001453
H 3.461272 -2.634034 -1.806959
H 2.458546 -2.193081 -3.203188
H 0.859755 -1.010177 -1.831026
C 2.697305 0.010703 -1.506663
H 2.954604 0.159498 -2.566737
H 3.646625 -0.105200 -0.956480
H 1.134734 1.498973 -1.625977

7-c30, ΔG = 2.1160 kcal/mol, population = 0.93 %

O -2.772752 -1.948653 -1.827874
H -2.266812 -2.774831 -1.751131
C -1.918316 -0.907429 -1.380650
C -1.273785 -1.250634 -0.072907
C -1.083162 -0.418513 0.964576
C -0.416299 -1.201008 2.064194
H 0.588254 -0.827309 2.309857
H -1.016945 -1.242075 2.986703
O -0.280055 -2.533406 1.545137
C -0.769232 -2.583816 0.280768
O -0.776263 -3.601095 -0.382164
C -1.508725 1.028735 1.001400
C -2.706576 1.142966 1.973811
H -2.978267 2.196717 2.130122
H -2.455699 0.718713 2.957276
H -3.588775 0.609496 1.591459
C -0.355640 1.904808 1.562017
H -0.667128 2.959799 1.521060
C 1.041893 1.724836 0.940194
C 1.312164 2.319337 -0.424180
C 1.677614 1.588102 -1.494304
C 1.768019 0.086727 -1.608277
C 3.182500 -0.486320 -1.430540
C 3.545031 -0.843604 0.002449
O 2.696470 -1.097162 0.838579
C 5.017550 -0.906830 0.324928
H 5.568253 -1.452568 -0.457259
H 5.419320 0.120812 0.339216
H 5.177611 -1.373976 1.305346
H 3.280460 -1.441334 -1.981579
H 3.953834 0.175445 -1.856116
H 1.401834 -0.199507 -2.606988
H 1.111441 -0.406566 -0.879979
H 1.927886 2.136386 -2.411595
C 1.214664 3.820868 -0.512529
H 1.509588 4.193445 -1.504305
H 1.852234 4.305096 0.247707
H 0.184606 4.164670 -0.316956
H 1.308276 0.663418 0.936171
H 1.755526 2.204531 1.634963
H -0.263608 1.674883 2.636481
C -1.911934 1.459790 -0.452807
C -2.653228 2.798004 -0.507576
H -2.721547 3.147296 -1.549331
H -2.142367 3.582573 0.069961
H -3.680810 2.711660 -0.121639
H -0.967972 1.584306 -1.003571
C -2.718652 0.376200 -1.191246
H -3.042641 0.758484 -2.171566
H -3.632195 0.121013 -0.628012
H -1.118019 -0.728270 -2.128392

7-c32, ΔG = 2.2484 kcal/mol, population = 0.75 %

O -0.248077 -2.671841 1.946232
H -1.160003 -2.747063 1.620017
C 0.273050 -1.453574 1.442931
C 0.022927 -1.317311 -0.029235
C 0.889888 -0.845438 -0.942107
C 0.254084 -0.992238 -2.298353

H 0.137893 -0.044280 -2.844273
H 0.806495 -1.691867 -2.946056
O -1.050277 -1.536520 -2.042942
C -1.200420 -1.755438 -0.711565
O -2.208063 -2.239971 -0.236560
C 2.269608 -0.321810 -0.635095
C 3.300735 -1.314490 -1.222387
H 4.319389 -0.912934 -1.125750
H 3.115560 -1.486913 -2.292862
H 3.260535 -2.287010 -0.710638
C 2.493020 1.056502 -1.323220
H 3.427318 1.483250 -0.927704
C 1.366787 2.108404 -1.264254
C 0.944669 2.638485 0.087468
C -0.319920 2.570732 0.545739
C -1.522377 1.970742 -0.130495
C -2.437335 1.218147 0.833256
C -3.668915 0.620902 0.178255
O -3.933495 0.823602 -0.991670
C -4.529262 -0.260131 1.053004
H -4.004953 -1.222658 1.169595
H -4.664345 0.171961 2.056059
H -5.501611 -0.437916 0.574904
H -1.901989 0.405072 1.350607
H -2.786679 1.882615 1.644907
H -1.235992 1.299001 -0.950912
H -2.118439 2.771025 -0.606044
H -0.525206 3.038471 1.517625
C 2.013895 3.357223 0.871978
H 1.630028 3.735929 1.830405
H 2.407588 4.212541 0.294779
H 2.877758 2.707452 1.085524
H 0.488572 1.734801 -1.803999
H 1.725225 2.970575 -1.856235
H 2.692878 0.869557 -2.391254
C 2.417005 -0.212226 0.925001
C 3.861279 -0.013831 1.390956
H 4.454295 -0.935151 1.283124
H 3.876137 0.263910 2.455943
H 4.377511 0.783415 0.835868
H 1.842533 0.678143 1.218445
C 1.778765 -1.398962 1.666921
H 1.989130 -1.320940 2.744484
H 2.207979 -2.354817 1.322003
H -0.192555 -0.593642 1.967407

7-c39, ΔG = 2.3676 kcal/mol, population = 0.61 %

O 4.142738 -1.495184 0.778888
H 3.787811 -2.393252 0.890790
C 3.039587 -0.607680 0.862565
C 1.896715 -1.072219 0.011272
C 1.104823 -0.300486 -0.752945
C 0.136234 -1.202159 -1.469399
H -0.921720 -1.027695 -1.221814
H 0.243491 -1.152482 -2.564858
O 0.474487 -2.530655 -1.037664
C 1.510045 -2.478336 -0.163148
O 2.001327 -3.471177 0.334909
C 1.246547 1.194491 -0.905495
C 1.791452 1.472287 -2.326198
H 2.800085 1.055511 -2.459904
H 1.832441 2.553491 -2.519249
H 1.137583 1.026307 -3.090046
C -0.139188 1.882249 -0.788436
H -0.005290 2.961140 -0.962157
C -0.896479 1.667777 0.531124
C -2.205852 2.430137 0.570709
C -3.363347 1.900626 0.137785
C -3.521598 0.506836 -0.408270
C -3.841174 -0.539836 0.666185
C -3.661899 -1.975161 0.202572
O -2.968117 -2.255847 -0.757679
C -4.364883 -3.037273 1.013160
H -4.201826 -2.876378 2.090576
H -5.451760 -2.959497 0.840697
H -4.019227 -4.036637 0.718605
H -3.156256 -0.420876 1.527279
H -4.852149 -0.405228 1.083838
H -2.608547 0.192013 -0.930199
H -4.319944 0.489209 -1.168134
H -4.271124 2.512113 0.203930
C -2.121745 3.836445 1.102129
H -1.793555 3.839217 2.156609
H -3.086821 4.360197 1.037951
H -1.372440 4.426231 0.545107
H -0.274494 2.004411 1.374552
H -1.062051 0.591002 0.689291

H -0.772630 1.530587 -1.619741
C 2.236541 1.706028 0.200019
C 2.686480 3.153560 -0.009372
H 3.229331 3.511363 0.878858
H 1.836664 3.832798 -0.173354
H 3.366458 3.246445 -0.870116
H 1.680361 1.670584 1.150934
C 3.451941 0.779621 0.381212
H 4.157437 1.226455 1.098548
H 3.994472 0.658097 -0.571298
H 2.689224 -0.535248 1.914020

7-c36, ΔG = 2.5671 kcal/mol, population = 0.44 %

O 3.211688 1.648218 -1.209597
H 3.420759 2.283934 -0.507372
C 1.878681 1.193633 -0.964835
C 1.781891 0.621457 0.416237
C 1.457292 -0.640596 0.746611
C 1.620000 -0.786762 2.233221
H 0.688788 -1.052960 2.757090
H 2.383442 -1.537074 2.495643
O 2.061279 0.498227 2.691385
C 2.195524 1.340776 1.628653
O 2.622556 2.469676 1.741980
C 1.074227 -1.700039 -0.254002
C 1.499791 -3.094337 0.234003
H 1.289672 -3.846177 -0.542576
H 0.947709 -3.385473 1.139256
H 2.571120 -3.140361 0.472037
C -0.464973 -1.672545 -0.484609
H -0.741082 -0.692991 -0.889363
C -1.354705 -1.910699 0.746133
C -2.822090 -1.742149 0.415758
C -3.513013 -0.616204 0.668565
C -3.025677 0.647255 1.325893
C -3.334195 1.901960 0.502596
C -2.450198 2.096595 -0.715900
O -1.373342 1.538881 -0.824489
C -2.966987 3.037408 -1.777476
H -3.791051 2.540230 -2.317463
H -3.385905 3.951007 -1.327699
H -2.169748 3.289311 -2.488906
H -4.392049 1.931747 0.190962
H -3.189520 2.810632 1.117100
H -1.945396 0.609704 1.521176
H -3.524926 0.759114 2.305146
H -4.571402 -0.597466 0.375444
C -3.475538 -2.924324 -0.253277
H -4.525861 -2.723431 -0.510838
H -3.442849 -3.812945 0.401744
H -2.943877 -3.204549 -1.179050
H -1.073366 -1.208044 1.541128
H -1.193151 -2.924364 1.148883
H -0.691538 -2.424791 -1.258742
C 1.783785 -1.319555 -1.604417
C 3.295488 -1.579308 -1.593002
H 3.734313 -1.269376 -2.553940
H 3.535038 -2.642380 -1.448622
H 3.797802 -0.997330 -0.806025
H 1.336826 -1.968344 -2.377151
C 1.483011 0.139812 -2.008657
H 0.411614 0.261647 -2.212007
H 2.012525 0.382514 -2.942561
H 1.175805 2.042726 -1.045538

7-c7, ΔG = 2.5759 kcal/mol, population = 0.43 %

O 2.774764 -2.842648 0.794886
H 2.007729 -3.432111 0.881132
C 2.287233 -1.515164 0.904224
C 1.121668 -1.282693 -0.008628
C 0.905835 -0.181428 -0.747993
C -0.354813 -0.386887 -1.537436
H -1.146708 0.341929 -1.309508
H -0.182387 -0.381180 -2.625531
O -0.820130 -1.691787 -1.154301
C 0.038337 -2.243671 -0.255796
O -0.133014 -3.348529 0.216212
C 1.782959 1.044197 -0.763263
C 2.447479 1.148124 -2.153157
H 3.007180 2.089200 -2.247120
H 1.689508 1.134830 -2.950425
H 3.139362 0.312006 -2.331993
C 0.881425 2.290639 -0.549712
H 1.508482 3.191290 -0.627268
C 0.089337 2.288370 0.782179
C -1.371958 2.649078 0.641068

C -2.372578 1.809467 0.963902
C -2.246791 0.418846 1.532086
C -3.411726 -0.527903 1.214574
C -3.607521 -0.856562 -0.257131
O -3.451755 -0.018591 -1.126588
C -4.016476 -2.272537 -0.578305
H -4.277788 -2.365504 -1.640462
H -3.164725 -2.935294 -0.351435
H -4.858509 -2.591905 0.056381
H -3.302097 -1.461250 1.787118
H -4.365514 -0.078380 1.550918
H -2.181671 0.484242 2.633962
H -1.305073 -0.054090 1.216232
H -3.399111 2.174316 0.841001
C -1.651041 4.038367 0.127574
H -2.729961 4.239083 0.052787
H -1.205698 4.197109 -0.869880
H -1.201827 4.799471 0.790502
H 0.559756 3.000374 1.482585
H 0.179696 1.305234 1.261670
H 0.183868 2.345737 -1.400767
C 2.841842 0.907489 0.385503
C 3.986579 1.916816 0.276380
H 4.594423 1.898614 1.193899
H 3.617302 2.945021 0.143526
H 4.655204 1.685259 -0.566930
H 2.306752 1.125320 1.324773
C 3.385238 -0.526398 0.522783
H 4.184503 -0.551515 1.279315
H 3.829290 -0.866513 -0.428135
H 1.965827 -1.312601 1.947541

7-c11, ΔG = 2.5866 kcal/mol, population = 0.42 %

O 3.820561 -1.080118 1.048051
H 3.575586 -2.010946 0.917038
C 2.608894 -0.342911 1.093478
C 1.712249 -0.682693 -0.056366
C 0.982359 0.185465 -0.773501
C 0.215109 -0.594556 -1.803195
H -0.875200 -0.507688 -1.676494
H 0.460814 -0.307444 -2.838086
O 0.597869 -1.961391 -1.598812
C 1.482972 -2.039266 -0.566419
O 1.974412 -3.088000 -0.205580
C 0.965229 1.680029 -0.575234
C 1.745672 2.323151 -1.744606
H 2.802609 2.020111 -1.741315
H 1.697373 3.419769 -1.685657
H 1.313070 2.025785 -2.711682
C -0.498765 2.188093 -0.636974
H -0.489510 3.288078 -0.665348
C -1.405346 1.692092 0.501415
C -2.886572 1.782759 0.198370
C -3.750097 0.793441 0.495000
C -3.416686 -0.515296 1.166284
C -3.097715 -1.683164 0.208929
C -1.796121 -2.411481 0.516625
O -0.934425 -1.918413 1.222200
C -1.618346 -3.764571 -0.126989
H -0.587786 -4.118185 -0.001028
H -2.318446 -4.476627 0.341940
H -1.873901 -3.719149 -1.196744
H -3.912613 -2.422633 0.155545
H -2.984354 -1.319918 -0.829468
H -4.262354 -0.808791 1.807896
H -2.552454 -0.390903 1.833124
H -4.804417 0.946240 0.232974
C -3.364192 3.070972 -0.421660
H -4.458889 3.089051 -0.525119
H -2.925047 3.234616 -1.420232
H -3.060921 3.936478 0.194242
H -1.196697 2.291032 1.406875
H -1.138347 0.656542 0.754782
H -0.919080 1.876231 -1.607658
C 1.632567 1.984089 0.809374
C 1.895789 3.472830 1.040244
H 2.205912 3.645772 2.082237
H 0.998098 4.082286 0.855799
H 2.700254 3.849759 0.390048
H 0.911000 1.655512 1.575016
C 2.908289 1.152777 1.042003
H 3.390808 1.465745 1.980721
H 3.638383 1.322296 0.232935
H 2.060399 -0.570864 2.031733

7-c25, ΔG = 2.6688 kcal/mol, population = 0.37 %

O -2.946824 -2.655071 0.030217
H -3.301199 -2.545393 0.928428
C -1.845555 -1.768283 -0.087477
C -2.184448 -0.402005 0.427296
C -1.796659 0.763394 -0.116840
C -2.417202 1.875608 0.683580
H -1.676960 2.545284 1.148589
H -3.109617 2.491903 0.088324
O -3.163875 1.220067 1.719583
C -3.049428 -0.127759 1.582242
O -3.611472 -0.910822 2.319754
C -0.900215 0.908082 -1.318605
C -1.697160 1.591750 -2.449718
H -1.041135 1.825227 -3.299950
H -2.136518 2.539769 -2.105270
H -2.514913 0.948934 -2.808620
C 0.312545 1.807176 -0.943262
H 1.023766 1.780003 -1.782997
C 1.033962 1.391483 0.351698
C 2.435796 1.948929 0.476347
C 3.510213 1.328150 -0.043187
C 3.531394 0.042243 -0.829637
C 4.096696 -1.151441 -0.047660
C 3.112740 -1.821937 0.897211
O 1.907977 -1.762447 0.726164
C 3.710076 -2.601492 2.042682
H 4.542042 -3.234161 1.695196
H 4.134227 -1.889445 2.771150
H 2.941996 -3.212224 2.534654
H 4.408296 -1.953468 -0.744257
H 5.009134 -0.876038 0.505871
H 4.162088 0.191633 -1.721818
H 2.531054 -0.221586 -1.197592
H 4.491476 1.798041 0.103493
C 2.558971 3.263419 1.201312
H 1.924203 4.032508 0.726236
H 3.594261 3.635149 1.217509
H 2.204620 3.173215 2.243367
H 1.076206 0.298353 0.413922
H 0.444569 1.722081 1.221856
H -0.021415 2.855785 -0.869515
C -0.391778 -0.519765 -1.741665
C 0.184214 -0.564006 -3.158748
H -0.601124 -0.475395 -3.925216
H 0.699536 -1.522875 -3.323110
H 0.918484 0.236804 -3.333019
H 0.427000 -0.774191 -1.052063
C -1.451185 -1.618665 -1.553024
H -1.061509 -2.576991 -1.929982
H -2.364666 -1.389784 -2.128655
H -0.973974 -2.156608 0.479251

7-c40, ΔG = 2.8401 kcal/mol, population = 0.27 %

O -3.179045 -1.801822 -0.645657
H -2.811312 -2.549241 -0.145031
C -2.122592 -0.867875 -0.811146
C -1.409345 -0.612990 0.480046
C -0.967636 0.576878 0.917883
C -0.317123 0.366401 2.257666
H 0.749533 0.639496 2.264356
H -0.820343 0.915123 3.069841
O -0.437955 -1.041818 2.512307
C -1.101728 -1.639807 1.485095
O -1.382432 -2.819114 1.486914
C -1.123695 1.886634 0.185890
C -2.136664 2.753464 0.966667
H -3.138555 2.299713 0.966163
H -2.209642 3.757934 0.526304
H -1.821783 2.875352 2.013748
C 0.240982 2.626531 0.167965
H 0.092938 3.611752 -0.297968
C 1.388344 1.858366 -0.537719
C 2.650423 1.732022 0.286118
C 3.108798 0.549749 0.740489
C 2.467690 -0.791540 0.503296
C 2.982773 -1.519859 -0.743956
C 2.035687 -2.597016 -1.249132
O 0.855684 -2.603526 -0.949969
C 2.629191 -3.636354 -2.169508
H 3.256117 -3.162749 -2.941332
H 3.290477 -4.296482 -1.582792
H 1.835770 -4.236053 -2.634257
H 3.080380 -0.805712 -1.583925
H 3.991856 -1.939887 -0.603366
H 1.383827 -0.689689 0.382731
H 2.615019 -1.439070 1.383055
H 4.046144 0.549941 1.310018

C 3.380861 3.020469 0.558857
H 2.732380 3.747194 1.078185
H 3.688166 3.501903 -0.386507
H 4.278213 2.862176 1.174835
H 1.639671 2.370944 -1.481890
H 1.038044 0.860221 -0.829611
H 0.519039 2.838610 1.213010
C -1.621722 1.580738 -1.269932
C -2.116382 2.822165 -2.015138
H -2.279680 2.583824 -3.077371
H -1.391231 3.648687 -1.969052
H -3.072417 3.187000 -1.609173
H -0.745440 1.199224 -1.820152
C -2.677794 0.460965 -1.314338
H -3.048660 0.341780 -2.344151
H -3.546935 0.722638 -0.687262
H -1.381156 -1.258302 -1.537051

7-c14, ΔG = 2.9098 kcal/mol, population = 0.24 %

O 4.355287 -1.038223 -0.489417
H 4.853653 -0.242669 -0.730792
C 3.031194 -0.867608 -0.996278
C 2.422723 0.393862 -0.463988
C 1.371273 0.481204 0.368902
C 1.141696 1.929041 0.686991
H 0.145696 2.288950 0.381345
H 1.258421 2.142141 1.762235
O 2.165283 2.633012 -0.032605
C 2.958913 1.743285 -0.693467
O 3.935216 2.084045 -1.325238
C 0.564551 -0.693663 0.850011
C 0.044402 -0.427934 2.275555
H -0.723328 0.360960 2.260036
H 0.850556 -0.107432 2.949833
H -0.406177 -1.334386 2.704710
C -0.646634 -0.800183 -0.125851
H -1.139054 0.179350 -0.133832
C -1.702439 -1.865278 0.212575
C -2.891266 -1.772469 -0.720730
C -3.989666 -1.044249 -0.446931
C -4.266308 -0.231580 0.787818
C -4.425330 1.284210 0.510509
C -3.111919 1.902281 0.065012
O -2.224758 2.121152 0.873888
C -2.934577 2.164528 -1.406605
H -3.066314 1.214273 -1.951018
H -3.720619 2.847481 -1.767976
H -1.942249 2.584223 -1.616777
H -5.208797 1.447966 -0.245214
H -4.730067 1.785363 1.442276
H -3.479143 -0.364578 1.543748
H -5.208833 -0.576450 1.247489
H -4.783686 -1.017902 -1.204463
C -2.751250 -2.517158 -2.022817
H -3.613246 -2.355118 -2.686331
H -2.647588 -3.601906 -1.844474
H -1.839412 -2.204297 -2.560716
H -2.027533 -1.745742 1.254324
H -1.259507 -2.871408 0.135081
H -0.278068 -0.959339 -1.149647
C 1.484137 -1.957536 0.776189
C 2.517872 -2.016934 1.908750
H 2.040559 -2.086927 2.896397
H 3.178622 -1.137725 1.900276
H 3.157967 -2.904186 1.785943
H 0.827249 -2.835835 0.885176
C 2.164431 -2.072146 -0.604256
H 1.398836 -2.209474 -1.382096
H 2.801304 -2.969269 -0.634878
H 3.073404 -0.804679 -2.100914

7-c33, ΔG = 2.9267 kcal/mol, population = 0.24 %

O 3.171300 1.646228 -1.695114
H 2.912755 2.516057 -1.348744
C 2.086600 0.766999 -1.437118
C 1.640922 0.851400 -0.010558
C 1.289251 -0.183041 0.768529
C 0.938754 0.357362 2.127571
H -0.091684 0.126457 2.437451
H 1.620315 -0.000848 2.916073
O 1.078751 1.781125 2.009453
C 1.516796 2.096551 0.757779
O 1.757994 3.234470 0.417592
C 1.220398 -1.623997 0.327468
C 2.292905 -2.429454 1.089594
H 3.307895 -2.107510 0.813105

H 2.199329 -3.503612 0.876499
H 2.181218 -2.298227 2.176437
C -0.185035 -2.172653 0.701170
H -0.234934 -3.240606 0.439996
C -1.334950 -1.390296 0.036717
C -2.650982 -1.427256 0.772175
C -3.234497 -0.328664 1.288664
C -2.706342 1.085383 1.297930
C -3.130375 1.956365 0.088111
C -2.338670 1.590063 -1.157087
O -1.163786 1.901826 -1.252284
C -3.050236 0.795107 -2.219375
H -2.361013 0.511098 -3.025007
H -3.496760 -0.101721 -1.758799
H -3.886169 1.386660 -2.628526
H -4.212693 1.864796 -0.087571
H -2.901236 3.009065 0.316857
H -1.608805 1.115068 1.353110
H -3.070341 1.584912 2.209025
H -4.215474 -0.458531 1.761896
C -3.298260 -2.783212 0.877883
H -2.655445 -3.485353 1.436552
H -3.444762 -3.226767 -0.122588
H -4.272830 -2.736574 1.385188
H -1.502188 -1.788304 -0.978609
H -1.016151 -0.351230 -0.102573
H -0.290936 -2.128652 1.797699
C 1.438680 -1.669892 -1.226679
C 1.715904 -3.077802 -1.756087
H 1.673643 -3.082723 -2.856096
H 0.976155 -3.807074 -1.392119
H 2.715277 -3.434801 -1.463127
H 0.491846 -1.333917 -1.678381
C 2.508282 -0.673740 -1.708564
H 2.687002 -0.811843 -2.786155
H 3.468574 -0.850809 -1.194648
H 1.220563 1.026542 -2.078781

7-c34, ΔG = 2.9857 kcal/mol, population = 0.21 %

O -4.946430 -0.197100 -0.240437
H -5.169327 0.642534 0.195712
C -3.688190 -0.601761 0.275836
C -2.709968 0.530538 0.292773
C -1.404972 0.452059 -0.017481
C -0.817360 1.831403 0.120055
H -0.047476 1.892634 0.904162
H -0.369338 2.210751 -0.810516
O -1.921135 2.672787 0.491872
C -3.048392 1.924592 0.603907
O -4.127124 2.400915 0.895286
C -0.668288 -0.801773 -0.426691
C -0.214914 -0.619534 -1.892762
H 0.341105 -1.496484 -2.249234
H 0.449081 0.251009 -1.981775
H -1.079233 -0.474441 -2.558032
C 0.567275 -0.884217 0.515840
H 1.124474 0.053558 0.398285
C 1.578946 -2.022730 0.301235
C 2.848487 -1.771317 1.088733
C 3.931279 -1.162155 0.573522
C 4.129947 -0.648790 -0.827650
C 4.570069 0.820470 -0.860107
C 3.461241 1.823981 -0.591615
O 2.298127 1.582460 -0.861927
C 3.878229 3.146740 0.001008
H 4.167369 2.983649 1.053524
H 4.766335 3.546078 -0.513746
H 3.051874 3.868119 -0.041797
H 5.408827 1.002962 -0.168613
H 4.954981 1.081467 -1.864285
H 3.219767 -0.759534 -1.431973
H 4.917759 -1.244820 -1.322102
H 4.791741 -1.012522 1.239471
C 2.811543 -2.212768 2.529234
H 1.962152 -1.751860 3.063106
H 3.735320 -1.951313 3.066063
H 2.664734 -3.304921 2.601800
H 1.809212 -2.118070 -0.768204
H 1.147016 -2.983726 0.620784
H 0.202537 -0.911109 1.556366
C -1.634542 -2.030216 -0.250043
C -1.219876 -3.278756 -1.038537
H -1.376408 -3.135500 -2.118848
H -1.839547 -4.135116 -0.730260
H -0.170097 -3.556533 -0.886136
H -1.603722 -2.283193 0.825433
C -3.100156 -1.702356 -0.597350

H -3.712452 -2.613064 -0.508618
H -3.173076 -1.367047 -1.646195
H -3.807958 -0.983892 1.311769

7-c26, ΔG = 3.1030 kcal/mol, population = 0.18 %

O -4.093096 1.414683 1.027688
H -3.748010 2.321451 1.085850
C -2.970922 0.547546 1.050266
C -1.912317 1.001079 0.089840
C -1.181846 0.212255 -0.716761
C -0.318953 1.094834 -1.574556
H 0.765295 0.923886 -1.478715
H -0.582800 1.017358 -2.642229
O -0.607640 2.433958 -1.133580
C -1.564834 2.404313 -0.170513
O -2.021165 3.410090 0.333955
C -1.279139 -1.291540 -0.775978
C -1.888998 -1.674402 -2.143257
H -2.908167 -1.276655 -2.256484
H -1.926498 -2.766513 -2.258723
H -1.277849 -1.277693 -2.967556
C 0.147202 -1.900814 -0.696778
H 0.083693 -2.970978 -0.945106
C 0.862401 -1.720522 0.652948
C 2.354685 -1.950038 0.585913
C 3.252426 -1.090301 1.099641
C 2.970304 0.215148 1.809533
C 2.557060 1.385868 0.882736
C 3.428929 1.495526 -0.352060
O 2.979107 1.290602 -1.466143
C 4.883091 1.845350 -0.143198
H 5.376304 1.059177 0.451092
H 5.391646 1.943147 -1.110772
H 4.972211 2.781606 0.430557
H 1.518917 1.264268 0.549581
H 2.617066 2.330053 1.449593
H 3.868134 0.507640 2.374969
H 2.170807 0.091449 2.557843
H 4.311343 -1.355192 0.997387
C 2.796861 -3.232871 -0.069845
H 2.537440 -3.251477 -1.141741
H 2.289907 -4.101016 0.387247
H 3.882958 -3.379922 0.018518
H 0.438325 -2.436781 1.379356
H 0.648103 -0.719328 1.052700
H 0.755995 -1.447671 -1.496525
C -2.173087 -1.770501 0.420055
C -2.586470 -3.239315 0.315738
H -3.054411 -3.568406 1.256168
H -1.724243 -3.896691 0.126309
H -3.318159 -3.399668 -0.490837
H -1.552508 -1.670531 1.324838
C -3.394238 -0.862244 0.647354
H -4.040049 -1.292826 1.428043
H -4.002077 -0.784413 -0.269760
H -2.536218 0.514241 2.071618

7-c12, ΔG = 3.1972 kcal/mol, population = 0.15 %

O 4.069525 1.241625 -1.070079
H 3.823492 2.179539 -1.005256
C 2.859303 0.502516 -1.094934
C 1.927233 0.940979 -0.004834
C 1.173879 0.140867 0.769704
C 0.446954 1.002456 1.762682
H -0.650779 0.957802 1.674400
H 0.723165 0.771309 2.804045
O 0.871692 2.345788 1.467165
C 1.751343 2.331778 0.429355
O 2.275071 3.339376 0.000612
C 1.153558 -1.364925 0.692269
C 1.899570 -1.899679 1.938050
H 2.949017 -1.572508 1.953545
H 1.876029 -2.998254 1.960245
H 1.420695 -1.541508 2.861382
C -0.305403 -1.889245 0.758399
H -0.267238 -2.974014 0.935423
C -1.181326 -1.598376 -0.466693
C -2.646457 -1.935850 -0.272483
C -3.650417 -1.196380 -0.776396
C -3.564324 0.049417 -1.610054
C -3.997511 1.336225 -0.856374
C -2.909750 1.765002 0.105454
O -2.788337 1.230722 1.195374
C -1.954169 2.826803 -0.382596
H -1.180266 3.039917 0.363998
H -1.483835 2.501803 -1.325958

H -2.515358 3.746376 -0.615817
H -4.202695 2.135614 -1.583545
H -4.917238 1.135304 -0.285540
H -4.237995 -0.061476 -2.476090
H -2.555858 0.190903 -2.028238
H -4.674468 -1.533847 -0.571695
C -2.946332 -3.204307 0.486893
H -4.022388 -3.429803 0.482349
H -2.616771 -3.141368 1.537439
H -2.412217 -4.064255 0.045285
H -0.806739 -2.192237 -1.319740
H -1.066553 -0.543534 -0.757485
H -0.781500 -1.460940 1.656126
C 1.869088 -1.786840 -0.637780
C 2.132924 -3.290423 -0.733551
H 2.475330 -3.550336 -1.746962
H 1.228160 -3.881890 -0.526819
H 2.915460 -3.611852 -0.029140
H 1.177310 -1.523451 -1.454362
C 3.154631 -0.981152 -0.895711
H 3.671896 -1.378325 -1.782632
H 3.852246 -1.074006 -0.046789
H 2.349722 0.641214 -2.071865

7-c19, ΔG = 3.3164 kcal/mol, population = 0.12 %

O -4.751337 0.321219 0.203060
H -4.769564 1.094271 0.791908
C -3.512009 -0.332019 0.425759
C -2.369904 0.638548 0.408152
C -1.168336 0.444883 -0.162097
C -0.360222 1.699016 0.030075
H 0.551242 1.542639 0.625543
H -0.051333 2.170645 -0.914406
O -1.225888 2.595674 0.744474
C -2.420134 1.992251 0.975188
O -3.338648 2.548263 1.542148
C -0.756037 -0.800269 -0.906552
C -0.669092 -0.441067 -2.408785
H -1.650884 -0.160125 -2.816817
H -0.281564 -1.291845 -2.986893
H 0.019885 0.402237 -2.562813
C 0.658520 -1.249721 -0.455972
H 0.926328 -2.159852 -1.015120
C 0.857386 -1.505100 1.046399
C 2.227624 -2.084636 1.351920
C 3.352144 -1.346301 1.356721
C 3.433477 0.119522 1.040884
C 4.023843 0.381349 -0.372072
C 3.612154 1.752130 -0.877502
O 2.498645 1.926082 -1.343056
C 4.605352 2.876292 -0.736290
H 4.961303 2.933149 0.305695
H 5.490431 2.664693 -1.359361
H 4.156583 3.831842 -1.036972
H 5.118331 0.270224 -0.352974
H 3.615052 -0.360082 -1.073991
H 4.051956 0.643875 1.788502
H 2.432828 0.571118 1.092147
H 4.305570 -1.852019 1.552716
C 2.257761 -3.568678 1.602254
H 3.280630 -3.944907 1.750992
H 1.807969 -4.114449 0.753657
H 1.656335 -3.831307 2.490416
H 0.091150 -2.204287 1.412780
H 0.702605 -0.569705 1.607698
H 1.369340 -0.478185 -0.785763
C -1.829134 -1.911705 -0.634204
C -1.694770 -3.126683 -1.555039
H -0.668085 -3.521503 -1.575373
H -1.986936 -2.886599 -2.588958
H -2.353263 -3.937274 -1.207076
H -1.653709 -2.261944 0.396830
C -3.268082 -1.366250 -0.667719
H -3.984049 -2.195502 -0.560139
H -3.476519 -0.884158 -1.637564
H -3.524370 -0.843796 1.411288

7-c42, ΔG = 3.5574 kcal/mol, population = 0.08 %

O -3.596108 1.590122 1.192561
H -3.356391 2.465506 0.847036
C -2.427212 0.789815 1.129150
C -1.800577 0.841258 -0.231275
C -1.291567 -0.201506 -0.907418
C -0.799169 0.302387 -2.236128
H 0.278774 0.139463 -2.391216
H -1.337514 -0.144831 -3.087176

O -1.055296 1.714566 -2.217589
C -1.660363 2.055665 -1.046518
O -1.998674 3.191177 -0.789925
C -1.222054 -1.618895 -0.398969
C -2.196790 -2.485129 -1.225968
H -1.983867 -2.394508 -2.301570
H -3.241755 -2.183983 -1.061964
H -2.094600 -3.546215 -0.958256
C 0.220386 -2.146517 -0.619602
H 0.266298 -3.200401 -0.307073
C 1.306411 -1.322547 0.096060
C 2.682383 -1.448779 -0.509992
C 3.377677 -0.399839 -0.986484
C 2.962351 1.047787 -1.012494
C 3.444412 1.852063 0.224423
C 2.710878 1.420998 1.479225
O 3.178533 0.596106 2.241156
C 1.359641 2.056412 1.728766
H 0.773078 1.446568 2.428083
H 1.524592 3.051388 2.177232
H 0.798445 2.220964 0.797321
H 4.520799 1.685530 0.378697
H 3.270838 2.924945 0.043293
H 1.871527 1.161915 -1.106248
H 3.391270 1.528167 -1.905750
H 4.387502 -0.596755 -1.366835
C 3.256499 -2.841342 -0.531649
H 3.265147 -3.274881 0.483877
H 4.283516 -2.854560 -0.924386
H 2.645218 -3.518333 -1.152749
H 1.367224 -1.630847 1.153210
H 1.001049 -0.268534 0.115440
H 0.418468 -2.150956 -1.704367
C -1.596172 -1.605673 1.124480
C -1.845285 -3.001672 1.697903
H -2.783426 -3.435564 1.319121
H -1.924786 -2.950529 2.794570
H -1.027949 -3.698033 1.456761
H -0.722700 -1.187291 1.651109
C -2.774436 -0.664206 1.432969
H -3.063603 -0.762070 2.490501
H -3.657407 -0.934445 0.829621
H -1.683157 1.144857 1.872355

7-c17, ΔG = 3.7400 kcal/mol, population = 0.06 %

O 3.388528 1.393890 -0.861895
H 3.062501 2.266737 -0.588517
C 2.256147 0.539772 -0.933388
C 1.451897 0.595002 0.329928
C 0.889889 -0.453734 0.953104
C 0.225641 0.049940 2.205199
H -0.855640 -0.153222 2.241013
H 0.680377 -0.360761 3.120993
O 0.429653 1.470998 2.187857
C 1.175650 1.815500 1.100067
O 1.514947 2.958083 0.878916
C 0.922601 -1.879669 0.462601
C 1.761239 -2.716505 1.452190
H 1.727344 -3.782800 1.188169
H 1.371242 -2.619095 2.476480
H 2.812665 -2.393438 1.459411
C -0.531462 -2.426324 0.451647
H -0.507399 -3.493342 0.183577
C -1.483083 -1.649318 -0.486064
C -2.904776 -1.544295 0.014095
C -3.472889 -0.364808 0.329152
C -2.793866 0.980651 0.248570
C -2.691027 1.549966 -1.194479
C -1.491117 2.469877 -1.315653
O -0.495990 2.118028 -1.924645
C -1.553171 3.794364 -0.594724
H -2.404632 4.388112 -0.964596
H -1.724434 3.625998 0.480938
H -0.613160 4.343048 -0.729818
H -2.546895 0.732241 -1.913490
H -3.619012 2.082867 -1.456535
H -1.776742 0.909025 0.659467
H -3.322382 1.701803 0.889309
H -4.518646 -0.367339 0.657140
C -3.658073 -2.842571 0.126872
H -3.699645 -3.356638 -0.849619
H -4.687165 -2.691007 0.484014
H -3.153252 -3.536920 0.820610
H -1.497117 -2.138806 -1.475167
H -1.074029 -0.646053 -0.661102
H -0.914929 -2.390950 1.484455
C 1.534217 -1.887556 -0.982708

C 1.922506 -3.286042 -1.465627
H 1.103223 -4.009076 -1.333773
H 2.803803 -3.671176 -0.930093
H 2.172664 -3.259726 -2.537263
H 0.740570 -1.520240 -1.653310
C 2.707153 -0.903045 -1.136949
H 3.155350 -1.012526 -2.136535
H 3.499814 -1.120804 -0.400932
H 1.599368 0.844959 -1.770644

7-c22, ΔG = 3.9288 kcal/mol, population = 0.04 %

O -2.038469 -2.995185 -0.318130
H -1.340778 -3.508275 0.120519
C -1.487640 -1.717534 -0.605582
C -0.891786 -1.093706 0.620109
C -1.005514 0.193116 0.991246
C -0.280383 0.366415 2.296782
H 0.554552 1.081733 2.233500
H -0.944985 0.678903 3.117873
O 0.250989 -0.932886 2.602098
C -0.097556 -1.811802 1.626197
O 0.240228 -2.978028 1.644230
C -1.738437 1.259615 0.219631
C -2.991710 1.660644 1.029313
H -3.506263 2.506873 0.552967
H -2.716718 1.972459 2.047914
H -3.700895 0.824188 1.112178
C -0.825578 2.509875 0.084095
H -1.403788 3.297470 -0.420542
C 0.515957 2.267924 -0.656766
C 1.756347 2.639345 0.127219
C 2.678192 1.732006 0.504040
C 2.599660 0.252149 0.230019
C 3.064224 -0.147482 -1.198339
C 2.392212 -1.442317 -1.608531
O 1.469070 -1.435759 -2.406002
C 2.820087 -2.712577 -0.912656
H 2.523847 -3.585943 -1.509270
H 3.899478 -2.729687 -0.704306
H 2.290403 -2.771401 0.054354
H 2.757377 0.622300 -1.919438
H 4.161111 -0.241924 -1.230751
H 1.560964 -0.081733 0.343495
H 3.183819 -0.303201 0.978779
H 3.569108 2.089071 1.033103
C 1.922798 4.104189 0.432621
H 1.064875 4.494694 1.006358
H 1.964673 4.693803 -0.500243
H 2.837747 4.301670 1.009781
H 0.519025 2.854572 -1.591196
H 0.578605 1.220249 -0.974482
H -0.633766 2.896760 1.097646
C -2.116307 0.676020 -1.187788
C -3.131558 1.533433 -1.945738
H -3.219213 1.182841 -2.985414
H -2.836037 2.592949 -1.977352
H -4.132828 1.473915 -1.492199
H -1.185951 0.671761 -1.779577
C -2.585409 -0.788828 -1.116098
H -2.916793 -1.121154 -2.111879
H -3.451420 -0.885583 -0.439328
H -0.695077 -1.808925 -1.374309

7-c44, ΔG = 3.9621 kcal/mol, population = 0.04 %

O -2.994413 1.406746 2.080451
H -2.627130 2.305513 2.046832
C -2.019907 0.542215 1.520159
C -1.514615 1.062082 0.208708
C -1.255377 0.327954 -0.886253
C -0.826191 1.267690 -1.980795
H 0.180808 1.060844 -2.373780
H -1.527814 1.273424 -2.830311
O -0.826275 2.570778 -1.376594
C -1.258944 2.477913 -0.088236
O -1.390658 3.445659 0.629792
C -1.399125 -1.169075 -0.983728
C -2.558066 -1.476594 -1.959873
H -2.623666 -2.556431 -2.153889
H -2.400571 -0.976963 -2.927201
H -3.523245 -1.136647 -1.556726
C -0.095192 -1.774699 -1.576171
H -0.183719 -2.871567 -1.561955
C 1.242798 -1.340223 -0.946576
C 1.607157 -1.894254 0.413730
C 1.893452 -1.123267 1.479125
C 1.837716 0.376673 1.569526

C 3.211813 1.068992 1.374602
C 3.694536 0.928928 -0.056125
O 4.420648 0.014242 -0.396373
C 3.208943 1.969789 -1.041945
H 2.145450 2.212676 -0.895442
H 3.768432 2.904721 -0.865987
H 3.387028 1.634589 -2.071942
H 3.115137 2.134804 1.635350
H 3.957929 0.606320 2.037888
H 1.465238 0.660450 2.566875
H 1.117480 0.791217 0.850159
H 2.223467 -1.630901 2.393740
C 1.708217 -3.395256 0.499348
H 2.373746 -3.790253 -0.287658
H 0.727264 -3.875384 0.347327
H 2.092649 -3.720961 1.476511
H 1.298779 -0.244967 -0.932486
H 2.039980 -1.662027 -1.639693
H -0.057380 -1.502653 -2.643759
C -1.691619 -1.736632 0.451207
C -2.217596 -3.173881 0.438499
H -2.196615 -3.591053 1.456902
H -1.613221 -3.834346 -0.200886
H -3.258242 -3.223340 0.082811
H -0.725526 -1.740591 0.976519
C -2.628922 -0.833233 1.271759
H -2.859237 -1.314646 2.234596
H -3.587725 -0.685660 0.746219
H -1.159922 0.436965 2.213834