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Supporting Information

Fragmentation Method Reveals a Wide Spectrum of Intramolecular Hydrogen Bond Energies in Antioxidant Natural Products

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Cartesian coordinates of various optimized antioxidant natural products:

1.curcumin

B3LYP/6-31G(d,p) E = -1263.61605156
B3LYPD3/6-311G(d,p) E: -1263.95756159
MP2/6-311G(d,p) E= 1260.3680336

C	6.545404000	1.140985000	-0.000293000
C	5.252326000	0.647506000	-0.000317000
C	7.652561000	0.259406000	0.000270000
C	5.020307000	-0.748504000	0.000241000
C	7.434021000	-1.113541000	0.000777000
C	6.130871000	-1.607750000	0.000748000
H	4.411565000	1.330149000	-0.000824000
H	8.291868000	-1.777224000	0.001180000
H	5.967398000	-2.681175000	0.001150000
O	6.910053000	2.465965000	-0.000810000
C	5.883119000	3.447194000	-0.001344000
H	5.253898000	3.364307000	-0.895896000
H	5.253574000	3.364936000	0.893039000
H	6.386707000	4.414570000	-0.001588000
O	8.915230000	0.755740000	0.000271000
H	8.841471000	1.723387000	-0.000170000
C	3.684436000	-1.328036000	0.000281000
H	3.638711000	-2.415868000	0.000423000
C	2.492733000	-0.693448000	0.000117000
H	2.417191000	0.390923000	0.000002000
C	1.228563000	-1.446524000	0.000110000
C	-0.006278000	-0.710381000	0.000049000
H	0.003294000	0.372722000	0.000007000
C	-1.217992000	-1.382186000	0.000028000
C	-2.490466000	-0.683275000	0.000014000
H	-2.428546000	0.401122000	0.000184000
O	1.234283000	-2.712271000	0.000173000
O	-1.260297000	-2.709626000	0.000072000
H	-0.281249000	-3.000692000	0.000118000
C	-3.679000000	-1.328388000	-0.000242000
H	-3.642066000	-2.415408000	-0.000481000
C	-5.013904000	-0.747106000	-0.000276000
C	-5.245705000	0.649114000	0.000325000
C	-6.125330000	-1.605633000	-0.000915000
C	-6.538661000	1.143079000	0.000258000
C	-7.428100000	-1.110793000	-0.001002000
C	-7.646366000	0.262200000	-0.000419000
H	-4.405945000	1.332938000	0.000869000
H	-5.963156000	-2.679297000	-0.001362000
H	-8.286055000	-1.774315000	-0.001503000
O	-6.902418000	2.468017000	0.000817000
C	-5.875349000	3.449263000	0.001489000
H	-5.246318000	3.366309000	0.896155000
H	-5.245879000	3.367099000	-0.892939000
H	-6.378954000	4.416597000	0.001798000
O	-8.908796000	0.758842000	-0.000466000
H	-8.835089000	1.726492000	0.000003000

2. demethoxy curcumin

B3LYP/6-31G(d,p) E = -1149.08896769
B3LYPD3/6-311G(d,p) E= -1149.39720024
MP2/6-311G(d,p) E = -1146.1109713

C	-6.056893000	1.034575000	0.000086000
C	-4.735899000	0.621599000	0.000056000
C	-7.107756000	0.086537000	-0.000154000
C	-4.418659000	-0.757622000	-0.000219000
C	-6.805349000	-1.270490000	-0.000419000
C	-5.474312000	-1.683527000	-0.000448000
H	-3.938872000	1.354934000	0.000254000
H	-7.620827000	-1.985563000	-0.000597000
H	-5.245253000	-2.744872000	-0.000656000
O	-6.501619000	2.334730000	0.000345000
C	-5.535376000	3.376061000	0.000594000
H	-4.902299000	3.330951000	0.895075000
H	-4.902222000	3.331307000	-0.893850000
H	-6.096147000	4.311420000	0.000757000
O	-8.398443000	0.504273000	-0.000119000
H	-8.384529000	1.474639000	0.000083000
C	-3.049687000	-1.253694000	-0.000277000
H	-2.936732000	-2.336628000	-0.000424000
C	-1.899910000	-0.545808000	-0.000180000
H	-1.892813000	0.541090000	-0.000046000
C	-0.590784000	-1.216905000	-0.000261000
C	0.594652000	-0.402502000	-0.000121000
H	0.515573000	0.677708000	0.000008000
C	1.846330000	-0.995008000	-0.000152000
C	3.071057000	-0.214244000	-0.000020000
H	2.939429000	0.863821000	0.000106000
O	-0.514302000	-2.480225000	-0.000389000
O	1.975012000	-2.316808000	-0.000299000
H	1.016761000	-2.670495000	-0.000359000
C	4.298703000	-0.779483000	-0.000043000
H	4.334579000	-1.866704000	-0.000164000
C	5.591049000	-0.105306000	0.000085000
C	5.740576000	1.295221000	0.000184000
C	6.767045000	-0.882894000	0.000114000
C	6.996477000	1.886873000	0.000314000
C	8.028870000	-0.304878000	0.000243000
C	8.149627000	1.089063000	0.000346000
H	4.863589000	1.934618000	0.000155000
H	6.680267000	-1.966013000	0.000035000
H	8.928533000	-0.910676000	0.000267000
H	7.087812000	2.971053000	0.000387000
O	9.407248000	1.613711000	0.000471000
H	9.351445000	2.578543000	0.000531000

3. bis-demethoxy curcumin

B3LYP/6-31G(d,p) E = -1034.56181572
B3LYPD3/6-311G(d,p) E= -1034.83675637
MP2/6-311G(d,p) E= -1031.8537966

C	-6.461526000	-2.067024000	0.000000000
C	-5.195019000	-1.498590000	0.000000000
C	-7.599593000	-1.247619000	0.000000000
C	-5.020005000	-0.101113000	0.000000000
C	-7.453355000	0.143853000	0.000000000
C	-6.180918000	0.698400000	0.000000000
H	-4.328914000	-2.152637000	0.000000000
H	-8.341835000	0.765965000	0.000000000
H	-6.073295000	1.779607000	0.000000000
H	-6.573278000	-3.149295000	0.000000000
O	-8.866595000	-1.749075000	0.000000000
H	-8.828265000	-2.714767000	0.000000000
C	-3.714787000	0.547828000	0.000000000
H	-3.722106000	1.636769000	0.000000000
C	-2.494911000	-0.029065000	0.000000000
H	-2.369259000	-1.108625000	0.000000000
C	-1.267065000	0.782510000	0.000000000
C	0.000000000	0.104022000	0.000000000
H	0.040310000	-0.978284000	0.000000000
C	1.178808000	0.831483000	0.000000000
C	2.482299000	0.191071000	0.000000000
H	2.470916000	-0.894877000	0.000000000
O	-1.331471000	2.046671000	0.000000000
O	1.159761000	2.159097000	0.000000000
H	0.167815000	2.404718000	0.000000000
C	3.639313000	0.889636000	0.000000000
H	3.553355000	1.974058000	0.000000000
C	4.999071000	0.365015000	0.000000000
C	5.305862000	-1.009773000	0.000000000
C	6.079520000	1.270664000	0.000000000
C	6.620601000	-1.455525000	0.000000000
C	7.398489000	0.839119000	0.000000000
C	7.676105000	-0.532313000	0.000000000
H	4.506652000	-1.744039000	0.000000000
H	5.870906000	2.337017000	0.000000000
H	8.223956000	1.542679000	0.000000000
H	6.833995000	-2.522403000	0.000000000
O	8.984902000	-0.911106000	0.000000000
H	9.038942000	-1.876063000	0.000000000

4. garbogiol

B3LYP/6-31g(d,p) E = -1146.95903592
B3LYPD3/6-311G(d,p) E= -1147.27225028
MP2/6-311G(d,p) E = -1144.0871677

H	4.229887000	-3.281909000	0.032618000
C	3.748645000	-2.309462000	0.022341000
C	2.353391000	-2.270008000	0.002976000
C	4.510165000	-1.142641000	0.029527000
C	3.890033000	0.110264000	0.021415000
C	2.471021000	0.178086000	-0.000952000
C	1.734120000	-1.020185000	-0.013332000
H	5.593135000	-1.184814000	0.045425000
C	1.760939000	1.445647000	-0.000865000
O	0.358855000	-1.035034000	-0.038925000
C	-0.349095000	0.138832000	-0.055851000
C	0.318804000	1.391300000	-0.023174000
C	-0.464628000	2.590023000	-0.002469000
C	-1.859595000	2.529907000	-0.021453000
H	-2.449054000	3.437529000	-0.005650000
C	-1.728709000	0.063450000	-0.103313000
C	-2.444628000	1.269812000	-0.067766000
O	-3.783410000	1.077847000	-0.072358000
C	-4.028800000	-0.324535000	-0.402406000
C	-5.319391000	-0.755995000	0.265962000
H	-6.143682000	-0.124092000	-0.075186000
H	-5.555819000	-1.791685000	0.002558000
H	-5.255310000	-0.677067000	1.353601000
H	-4.154496000	-0.356577000	-1.493600000
O	0.126876000	3.788677000	0.029166000
H	1.106773000	3.629550000	0.032561000
O	1.638788000	-3.435613000	-0.001927000
H	0.698530000	-3.211439000	0.035058000
O	2.389702000	2.546286000	0.021826000
O	4.648012000	1.220925000	0.036057000
H	4.029855000	1.990687000	0.034205000
C	-2.709695000	-1.099259000	-0.050910000
C	-2.458497000	-2.194985000	-1.101515000
H	-1.534345000	-2.740483000	-0.894312000
H	-3.278581000	-2.922000000	-1.101721000
H	-2.376747000	-1.771046000	-2.106701000
C	-2.722819000	-1.714399000	1.365233000
H	-2.962046000	-0.965077000	2.125224000
H	-3.450445000	-2.529076000	1.442219000
H	-1.735813000	-2.122298000	1.602311000

5. rheediaxanthone-A

B3LYP/6-31G(d,p) E = -1339.88014746
B3LYPD3/6-311G(d,p) E= -1340.23878189
MP2/6-311G(d,p) E= -1336.4522639

O	4.257138000	-1.343269000	-0.325184000
C	3.256755000	-0.421720000	-0.194376000
C	1.960878000	-0.935806000	-0.228313000
C	3.511755000	0.963119000	-0.105624000
C	2.431166000	1.835758000	-0.038959000
C	1.115243000	1.350058000	-0.059924000
C	0.888257000	-0.033842000	-0.158141000
C	4.911246000	1.372590000	-0.123107000
H	2.577287000	2.908504000	0.026745000
C	-0.036116000	2.256793000	0.004506000
O	-0.359181000	-0.581131000	-0.183423000
C	-1.463523000	0.223934000	-0.124796000
C	5.888342000	0.461445000	-0.027885000
H	5.137266000	2.430247000	-0.225403000
H	6.935018000	0.752015000	-0.041798000
C	-1.338853000	1.624757000	-0.035863000
C	-2.532995000	2.407739000	0.002849000
C	-3.780308000	1.786591000	-0.035504000
H	-4.685758000	2.379502000	-0.002990000
C	-2.700251000	-0.422854000	-0.164520000
C	-2.875733000	-1.857212000	-0.330604000
C	-3.852946000	0.395013000	-0.111741000
C	-4.097544000	-2.397251000	-0.233726000
O	-5.088638000	-0.149210000	-0.192443000
H	-2.002978000	-2.461638000	-0.553006000
H	-4.259712000	-3.462071000	-0.373294000
C	-5.304595000	-1.563155000	0.129689000
C	-5.596353000	-1.649131000	1.636583000
H	-6.464008000	-1.033005000	1.892737000
H	-5.803672000	-2.684326000	1.926064000
H	-4.734081000	-1.301424000	2.212003000
C	-6.530587000	-1.956031000	-0.697489000
H	-6.315301000	-1.866581000	-1.765266000
H	-6.815486000	-2.990575000	-0.483217000
H	-7.375283000	-1.305336000	-0.454930000
O	-2.461669000	3.739671000	0.085809000
H	-1.489803000	3.967080000	0.105990000
O	1.726647000	-2.270819000	-0.331997000
H	2.597016000	-2.698983000	-0.362510000
C	5.599038000	-1.012362000	0.167396000
O	0.105970000	3.498225000	0.085387000
C	6.536900000	-1.883239000	-0.669992000
H	7.572624000	-1.741339000	-0.347585000
H	6.280927000	-2.940010000	-0.551552000
H	6.460577000	-1.620048000	-1.727862000
C	5.661081000	-1.386472000	1.656282000
H	4.929287000	-0.808311000	2.226838000
H	5.454285000	-2.452907000	1.791641000
H	6.654518000	-1.170874000	2.061747000

6. calebin-A

B3LYP/6-31G(d,p) E = -1338.83480259
B3LYPD3/6-311G(d,p) E= -1339.1995186
MP2/6-311G(d,p) E = -1335.4438085

C	7.242443000	1.006782000	-0.000021000
C	5.939037000	0.541739000	0.000050000
C	8.329695000	0.100197000	-0.000300000
C	5.678112000	-0.848723000	-0.000157000
C	8.081534000	-1.267677000	-0.000503000
C	6.767647000	-1.733265000	-0.000432000
H	5.112867000	1.241850000	0.000264000
H	8.924716000	-1.949829000	-0.000715000
H	6.580877000	-2.802947000	-0.000592000
O	7.635700000	2.322424000	0.000154000
C	6.629208000	3.326420000	0.000494000
H	5.998466000	3.257165000	-0.893843000
H	5.998707000	3.256797000	0.894973000
H	7.154011000	4.282322000	0.000618000
O	9.602391000	0.568825000	-0.000365000
H	9.549505000	1.537961000	-0.000191000
C	4.327784000	-1.395418000	-0.000098000
H	4.256357000	-2.482018000	-0.000274000
C	3.158145000	-0.725409000	0.000148000
H	3.088638000	0.357002000	0.000341000
C	1.885495000	-1.462740000	0.000166000
C	-1.528931000	-0.123714000	0.000282000
C	-2.909700000	-0.652196000	0.000248000
H	-3.037026000	-1.732289000	0.000296000
O	1.747851000	-2.673326000	-0.000045000
O	-1.259106000	1.067302000	0.000225000
C	-3.963638000	0.191397000	0.000145000
H	-3.711215000	1.251514000	0.000093000
C	-5.383700000	-0.129769000	0.000085000
C	-6.310010000	0.938219000	-0.000104000
C	-5.880559000	-1.444907000	0.000205000
C	-7.674342000	0.691006000	-0.000177000
C	-7.248400000	-1.695645000	0.000134000
C	-8.154486000	-0.636205000	-0.000058000
H	-5.935783000	1.955899000	-0.000193000
H	-5.193140000	-2.283915000	0.000360000
H	-7.637161000	-2.708262000	0.000228000
O	-8.672813000	1.633862000	-0.000359000
C	-8.301391000	3.006051000	-0.000482000
H	-7.720261000	3.260415000	0.894037000
H	-7.720112000	3.260215000	-0.894960000
H	-9.232992000	3.572834000	-0.000623000
O	-9.488310000	-0.878597000	-0.000129000
H	-9.935721000	-0.017251000	-0.000265000
O	0.834581000	-0.597358000	0.000460000
C	-0.450481000	-1.202647000	0.000391000
H	-0.571984000	-1.851708000	0.877955000
H	-0.571859000	-1.851780000	-0.877134000

7. (S)-[3]-gingerol

B3LYP/6-31G(d,p) E = -844.032102135
B3LYPD3/6-311G(d,p) E= -844.261166408
MP2/6-311G(d,p) E= -841.8412593

C	-3.918604000	0.262275000	0.052377000
C	-2.598369000	0.685182000	0.019495000
C	-4.222643000	-1.115460000	0.033169000
C	-1.541089000	-0.251752000	-0.033189000
C	-3.187027000	-2.046906000	-0.018602000
C	-1.863649000	-1.620121000	-0.051256000
H	-2.359923000	1.742743000	0.033647000
H	-3.440994000	-3.101428000	-0.032563000
H	-1.073664000	-2.362217000	-0.091493000
O	-5.030507000	1.067338000	0.104254000
C	-4.839547000	2.475541000	0.130048000
H	-4.268164000	2.783186000	1.014104000
H	-4.324423000	2.823617000	-0.773335000
H	-5.836038000	2.916636000	0.171335000
O	-5.513942000	-1.530206000	0.064918000
H	-6.068629000	-0.734492000	0.098582000
C	-0.175195000	0.253628000	-0.066728000
H	-0.064035000	1.336968000	-0.049434000
C	0.976807000	-0.448582000	-0.117454000
H	0.987996000	-1.534767000	-0.138844000
C	2.280620000	0.231263000	-0.148443000
C	3.474648000	-0.576836000	-0.207579000
H	3.402256000	-1.657073000	-0.225922000
C	4.710390000	0.024927000	-0.244276000
O	2.350786000	1.493193000	-0.124998000
O	4.839171000	1.343029000	-0.222742000
H	3.881942000	1.697351000	-0.176387000
C	6.011673000	-0.724320000	-0.305134000
H	6.522949000	-0.429460000	-1.230813000
H	5.806437000	-1.796723000	-0.373787000
C	6.925814000	-0.421194000	0.894012000
H	7.878463000	-0.948952000	0.791878000
H	7.128822000	0.650178000	0.960702000
H	6.459968000	-0.738280000	1.832225000

8. (S)-[4]-Gingerol

B3LYP/6-31G(d,p) E = -883.348843172
B3LYPD3/6-311G(d,p) E= -883.588401608
MP2/6-311G(d,p) E = -881.0366064

C	4.406779000	0.193576000	0.091143000
C	3.101545000	0.660290000	0.051554000
C	4.666624000	-1.192148000	0.034954000
C	2.015664000	-0.239627000	-0.045633000
C	3.602504000	-2.087311000	-0.060145000
C	2.294281000	-1.616626000	-0.099888000
H	2.897100000	1.724200000	0.094067000
H	3.822430000	-3.148730000	-0.101538000
H	1.481408000	-2.330939000	-0.173571000
O	5.543076000	0.960058000	0.183820000
C	5.397180000	2.372214000	0.251537000
H	4.906654000	2.765014000	-0.647183000
H	4.823260000	2.670608000	1.137122000
H	6.406662000	2.779040000	0.320142000
O	5.943259000	-1.649667000	0.073635000
H	6.522717000	-0.873905000	0.139555000
C	0.667429000	0.310825000	-0.085099000
H	0.590469000	1.395865000	-0.029996000
C	-0.505196000	-0.351025000	-0.183221000
H	-0.550813000	-1.434703000	-0.246311000
C	-1.785609000	0.372263000	-0.212630000
C	-3.003468000	-0.392811000	-0.328292000
H	-2.965454000	-1.473219000	-0.389770000
C	-4.218431000	0.250074000	-0.366463000
O	-1.815076000	1.633886000	-0.140354000
O	-4.305213000	1.570219000	-0.294570000
H	-3.338794000	1.891066000	-0.214427000
C	-5.540865000	-0.452116000	-0.479532000
H	-5.371803000	-1.524249000	-0.623953000
H	-6.046097000	-0.075955000	-1.379448000
C	-6.452624000	-0.213087000	0.740536000
H	-5.951860000	-0.592152000	1.640001000
H	-6.572173000	0.866065000	0.881586000
C	-7.821235000	-0.880405000	0.586710000
H	-8.354346000	-0.494401000	-0.289385000
H	-7.726299000	-1.965459000	0.464961000
H	-8.448909000	-0.698634000	1.464718000

9. (S)-[5]-gingerol

B3LYP/6-31G(d,p) E = -922.665408005
B3LYPD3/6-311G(d,p) E= -922.915464953
MP2/6-311G(d,p) E= -920.2318211

C	4.882231000	0.157082000	0.189205000
C	3.586053000	0.644012000	0.112541000
C	5.127277000	-1.228220000	0.080527000
C	2.494630000	-0.234791000	-0.074293000
C	4.057625000	-2.102599000	-0.103872000
C	2.758488000	-1.611711000	-0.180135000
H	3.393085000	1.707739000	0.195017000
H	4.266102000	-3.164013000	-0.185294000
H	1.941167000	-2.309982000	-0.324528000
O	6.022564000	0.901986000	0.368187000
C	5.891487000	2.311388000	0.496570000
H	5.447644000	2.753508000	-0.403541000
H	5.281543000	2.576244000	1.368639000
H	6.901849000	2.699534000	0.629962000
O	6.395163000	-1.705271000	0.155073000
H	6.980291000	-0.941636000	0.283095000
C	1.156239000	0.335868000	-0.148063000
H	1.090620000	1.419176000	-0.056459000
C	-0.019546000	-0.305844000	-0.316601000
H	-0.075962000	-1.386062000	-0.418405000
C	-1.288903000	0.435311000	-0.371086000
C	-2.511042000	-0.309808000	-0.552101000
H	-2.484061000	-1.388466000	-0.643126000
C	-3.716166000	0.349709000	-0.612578000
O	-1.305225000	1.694588000	-0.262607000
O	-3.789232000	1.668297000	-0.505917000
H	-2.822357000	1.974064000	-0.383241000
C	-5.042317000	-0.332222000	-0.788966000
H	-4.880127000	-1.401775000	-0.957667000
H	-5.512274000	0.074777000	-1.694484000
C	-5.990565000	-0.115139000	0.406524000
H	-5.526653000	-0.526577000	1.312679000
H	-6.103041000	0.961666000	0.575962000
C	-7.366388000	-0.757178000	0.195613000
H	-7.821926000	-0.343427000	-0.714238000
H	-7.242903000	-1.833150000	0.011002000
C	-8.311440000	-0.547716000	1.382356000
H	-8.481513000	0.518357000	1.569483000
H	-9.285679000	-1.013942000	1.203747000
H	-7.897936000	-0.981696000	2.299650000

10. E)-1,3,6-trihydroxy-8-(3-hydroxy-3-methylbut-1-en-1-yl)-7-methoxy-2-(3-methylbut-2-en-1-yl)-9H-xanthen-9-one

B3LYP/6-31G(d,p) E = -1496.11094812
B3LYPD3/6-311G(d,p) E= -1496.52505585
MP2/6-311G(d,p) E = -1492.2570419

O	4.140983000	-3.773128000	1.002317000
C	3.200179000	-2.868210000	0.655920000
C	1.863539000	-3.230723000	0.615521000
C	3.596285000	-1.550648000	0.331101000
C	2.669058000	-0.565967000	-0.006183000
C	1.282321000	-0.930679000	-0.052072000
C	0.928141000	-2.263507000	0.252823000
C	0.204001000	0.021731000	-0.354453000
O	-0.361760000	-2.711103000	0.232587000
C	-1.387240000	-1.865857000	-0.079501000
C	-1.145788000	-0.515535000	-0.368517000
C	-2.274062000	0.310833000	-0.670715000
C	-3.571318000	-0.208775000	-0.693467000
C	-2.661747000	-2.416853000	-0.086233000
C	-3.739996000	-1.576203000	-0.392869000
O	-5.027055000	-2.015483000	-0.426137000
O	-2.089446000	1.609690000	-0.952052000
H	-1.105795000	1.768030000	-0.879775000
H	1.547789000	-4.237206000	0.859466000
O	0.407330000	1.239224000	-0.591212000
H	-2.781700000	-3.464715000	0.149508000
C	-4.757832000	0.682173000	-1.013158000
H	-4.406077000	1.523440000	-1.610990000
H	-5.459079000	0.111713000	-1.633367000
C	-5.488732000	1.158360000	0.223234000
H	-6.016121000	0.371864000	0.762186000
C	-5.553703000	2.404559000	0.714902000
C	-4.869792000	3.607810000	0.112959000
H	-5.606801000	4.315632000	-0.290311000
H	-4.311545000	4.151224000	0.886036000
H	-4.164968000	3.349995000	-0.677809000
C	-6.359369000	2.696778000	1.958798000
H	-6.849462000	1.800600000	2.349456000
H	-5.724235000	3.112448000	2.752568000
H	-7.135465000	3.448225000	1.759585000
H	4.978620000	-3.277589000	1.043232000
O	4.967209000	-1.333252000	0.402619000
C	5.628592000	-1.287461000	-0.874909000
H	5.465696000	-2.217322000	-1.432518000
H	5.273431000	-0.437594000	-1.463302000
H	6.692727000	-1.166800000	-0.663802000
C	-5.294895000	-3.386677000	-0.163406000
H	-4.989613000	-3.668548000	0.851337000
H	-6.374912000	-3.502506000	-0.260122000
H	-4.793305000	-4.039749000	-0.887424000
C	3.100059000	0.808940000	-0.330323000
H	2.598350000	1.279228000	-1.165632000
C	3.989497000	1.526485000	0.367006000
H	4.488941000	1.097655000	1.233113000
C	4.316190000	2.977427000	0.058961000
C	4.165337000	3.817021000	1.343007000
H	3.142413000	3.750220000	1.729303000
H	4.843448000	3.472525000	2.130949000
H	4.385790000	4.866058000	1.125504000
C	5.740717000	3.101382000	-0.501540000
H	6.476147000	2.702076000	0.203213000
H	5.819431000	2.551364000	-1.442915000
H	5.975062000	4.152740000	-0.693917000
O	3.463474000	3.500727000	-0.961484000
H	2.548708000	3.375170000	-0.667996000

11. 2-hydroxy-6-pentadecylbenzoic-acid

B3LYP/6-31G(d,p) E = -1085.81160896
B3LYPD3/6-311G(d,p) E= -1086.1058364
MP2/6-311G(d,p) E= -1082.7740681

H	-5.013959000	-2.370097000	0.000597000
C	-5.952729000	-1.832121000	0.000333000
C	-5.951048000	-0.440255000	0.000182000
C	-7.146293000	-2.567149000	0.000118000
C	-7.214461000	0.238320000	-0.000160000
C	-8.370835000	-1.931643000	-0.000300000
C	-8.421742000	-0.528803000	-0.000463000
H	-7.103573000	-3.652832000	0.000277000
H	-9.308561000	-2.475605000	-0.000504000
O	-9.642415000	0.021750000	-0.000855000
H	-9.517875000	1.005177000	-0.000929000
C	-7.390269000	1.696694000	-0.000073000
O	-8.488783000	2.267541000	-0.000576000
O	-6.275992000	2.455725000	0.000660000
H	-6.596692000	3.374039000	0.000637000
C	-4.622768000	0.306005000	0.000395000
H	-4.595182000	0.976559000	0.866749000
H	-4.595045000	0.976797000	-0.865756000
C	-3.349794000	-0.548678000	0.000379000
H	-3.335979000	-1.205970000	0.879767000
H	-3.336037000	-1.205989000	-0.878993000
C	-2.078892000	0.311265000	0.000354000
H	-2.087068000	0.973090000	0.877934000
H	-2.087094000	0.973080000	-0.877233000
C	-0.786768000	-0.514633000	0.000333000
H	-0.779621000	-1.176683000	0.877929000
H	-0.779676000	-1.176726000	-0.877232000
C	0.487409000	0.338842000	0.000270000
H	0.480779000	1.000935000	0.877877000
H	0.480682000	1.000953000	-0.877322000
C	1.778513000	-0.488889000	0.000186000
H	1.784437000	-1.151180000	0.877679000
H	1.784330000	-1.151163000	-0.877320000
C	3.054426000	0.361980000	0.000113000
H	3.048976000	1.024196000	0.877675000
H	3.048848000	1.024238000	-0.877417000
C	4.344424000	-0.467482000	-0.000005000
H	4.349547000	-1.129839000	0.877463000
H	4.349418000	-1.129789000	-0.877511000
C	5.621362000	0.381856000	-0.000076000
H	5.616566000	1.044135000	0.877456000
H	5.616447000	1.044170000	-0.877580000
C	6.910727000	-0.448579000	-0.000183000
H	6.915427000	-1.110963000	0.877274000
H	6.915343000	-1.110871000	-0.877710000
C	8.188091000	0.400115000	-0.000197000
H	8.183472000	1.062420000	0.877315000
H	8.183440000	1.062458000	-0.877681000
C	9.477330000	-0.430499000	-0.000242000
H	9.481910000	-1.092901000	0.877240000
H	9.481920000	-1.092796000	-0.877802000
C	10.754729000	0.417848000	-0.000177000
H	10.751083000	1.080373000	0.877350000
H	10.751187000	1.080370000	-0.877707000
C	12.044433000	-0.412118000	-0.000080000
H	12.048221000	-1.073579000	0.877002000
H	12.048303000	-1.073659000	-0.877100000
C	13.314777000	0.443477000	-0.000058000
H	13.356379000	1.090671000	0.883460000
H	14.216915000	-0.176956000	0.000081000
H	13.356522000	1.090507000	-0.883686000

12. 8-hydroxy myricetin

B3LYP/6-31G(d,p) E = -1254.64588068
B3LYPD3/6-311G(d,p) E= -1255.00125515
MP2/6-311G(d,p) E = -1251.6989102

C	-2.553932000	1.687448000	-0.142716000
C	-3.955967000	1.637780000	-0.127794000
C	-4.643210000	0.422870000	-0.009202000
C	-3.929833000	-0.768538000	0.077211000
C	-2.506531000	-0.741916000	0.051442000
C	-1.846221000	0.497389000	-0.040943000
O	-0.486141000	0.585721000	-0.068550000
C	0.318461000	-0.535683000	-0.002364000
C	-0.266487000	-1.770121000	0.078013000
C	-1.714396000	-1.934019000	0.116642000
H	-5.726037000	0.416238000	0.001681000
O	-2.181399000	-3.099585000	0.212845000
O	0.432986000	-2.926555000	0.154771000
H	-0.262925000	-3.614184000	0.226263000
O	-4.583602000	-1.937929000	0.177970000
H	-3.901410000	-2.651353000	0.221390000
O	-1.958775000	2.930159000	-0.235215000
H	-1.093579000	2.824251000	-0.654090000
O	-4.661286000	2.788224000	-0.231585000
H	-4.024087000	3.512937000	-0.337617000
C	1.743764000	-0.201458000	-0.003104000
C	2.718671000	-1.177101000	-0.276624000
C	2.142789000	1.123566000	0.272050000
C	4.068383000	-0.833714000	-0.274968000
C	3.492630000	1.449416000	0.275829000
C	4.461059000	0.480607000	0.000871000
H	2.443682000	-2.200020000	-0.489884000
H	1.402404000	1.882051000	0.500616000
O	5.006571000	-1.781769000	-0.543591000
H	5.877873000	-1.360550000	-0.491505000
O	5.800110000	0.762084000	-0.004397000
H	5.911525000	1.694701000	0.233025000
O	3.996058000	2.702615000	0.539734000
H	3.281299000	3.293057000	0.808208000