

Supporting Information

Conformations of flavan-3-ols in water: Analysis using density functional theory

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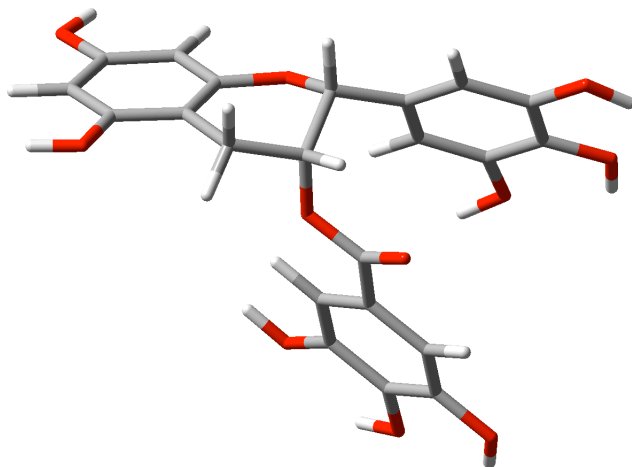
Cartesian coordinates and Gibbs energies of conformers.

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Cartesian coordinates and Gibbs energies of conformers.

1. Conformers in Figure 4.

Figure 4 (M06-2X), EGCg B-ring(p-eq)/3-O(p-ax) conformer



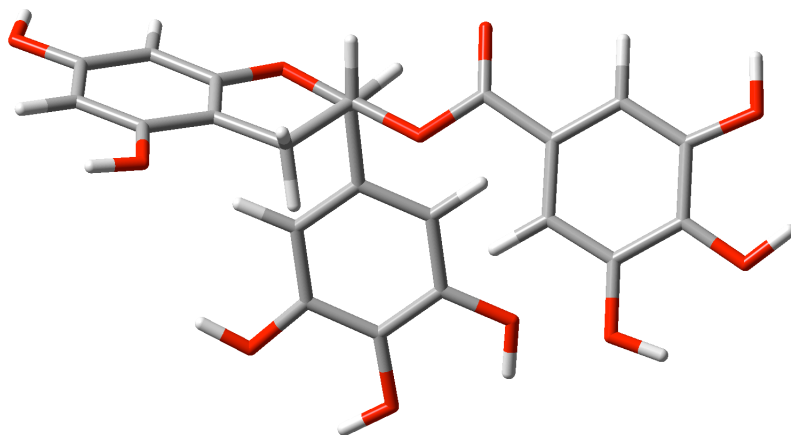
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Gibbs energy = -1676.344625 a.u.

C	-5.41577200	0.98410300	0.11832000
C	-4.69193200	0.41743800	-0.92129100
C	-3.50566200	-0.29355000	-0.70007500
C	-3.07640500	-0.42541000	0.61685900
C	-3.77806500	0.13598000	1.68557700
C	-4.94459300	0.84015500	1.42388000
H	-6.33257800	1.53162600	-0.06477500
H	-3.40417000	0.00543300	2.69389800
O	-1.93417000	-1.09220200	0.94829000
C	-1.33012000	-1.92144300	-0.04145300
H	-1.91817700	-2.84025100	-0.15224100
C	0.07061200	-2.23885300	0.41332500
C	0.81025600	-1.26485700	1.08120800
C	0.66642100	-3.43303100	0.02113800
C	2.16344800	-1.47325100	1.31032300
H	0.34307700	-0.33702400	1.38838000
C	2.01635200	-3.64604200	0.27897800
H	0.10611700	-4.19987300	-0.50120100
C	2.77036100	-2.66071100	0.91306900
C	-2.71777100	-0.86508000	-1.84827400
H	-2.67119300	-0.15079500	-2.67231800
H	-3.19527400	-1.76974500	-2.23697100
O	-0.57376200	0.01083800	-1.23712100
C	0.72392600	0.01921600	-1.59729800

O	1.23290300	-0.82672100	-2.28755700
C	1.45201000	1.18922800	-1.03787400
C	0.80747800	2.12459500	-0.22445700
C	2.81360400	1.28967800	-1.31238600
C	1.54515800	3.17267100	0.30505000
H	-0.24956600	2.03329200	-0.00709500
C	3.54438800	2.33967200	-0.77453500
H	3.30479200	0.55307800	-1.93438300
C	2.90985000	3.28252200	0.03381200
C	-1.30968400	-1.21085300	-1.40464800
H	-0.80269200	-1.84045800	-2.13394000
O	-5.08712200	0.52163000	-2.21700700
H	-5.89452200	1.04350000	-2.27126100
O	-5.68520700	1.41274600	2.40832100
H	-5.27150000	1.24971000	3.26223200
O	2.99183900	-0.56902600	1.90706300
H	2.54488000	0.27989100	1.99539300
O	4.09488700	-2.91242400	1.12019400
H	4.50135800	-2.12917400	1.51109100
O	2.60455200	-4.80912000	-0.10059800
H	3.53719300	-4.77344900	0.14661400
O	4.87065400	2.44923800	-1.03179600
H	5.20908700	3.23186700	-0.57865300
O	3.66692400	4.29128600	0.53399900
H	3.10875900	4.86795900	1.07133600
O	1.04812400	4.15392600	1.10599300
H	0.10428800	4.02998100	1.25016200

Figure 4 (M06-2X), EGCg B-ring(p-ax)/3-O(p-eq) conformer



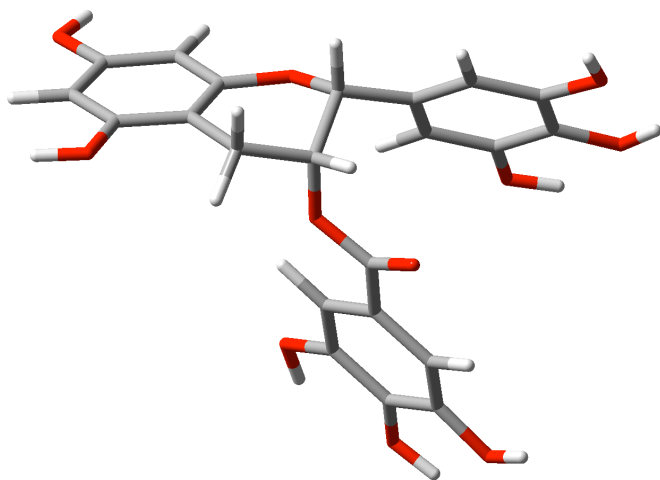
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C	5.44715500	-1.42871300	1.14797300
C	4.11786600	-1.42705800	1.54703100
C	3.07170400	-1.20881900	0.64127800
C	3.41456800	-0.97858700	-0.68817300
C	4.74083900	-0.97346900	-1.12221500
C	5.74819000	-1.20430200	-0.19577500
H	6.24865900	-1.60144900	1.85589100
H	4.95725300	-0.78632500	-2.16683500
O	2.48182700	-0.73727500	-1.65764800
C	1.13138900	-0.50455500	-1.26505300
H	0.53639000	-0.76788200	-2.14099200
C	0.87152400	0.94641900	-0.91310800
C	-0.43428200	1.42610600	-1.00070400
C	1.89641700	1.79144500	-0.48813500
C	-0.72566100	2.73305900	-0.63026900
H	-1.24589800	0.80436600	-1.36085000
C	1.59938100	3.10257100	-0.13195700
H	2.92360700	1.45067100	-0.43496500
C	0.29223500	3.57507800	-0.19129300
C	1.63433200	-1.23634100	1.08650600
H	1.34734000	-0.28867000	1.55565500
H	1.47917000	-2.02790500	1.82120200
O	-0.59570900	-1.27528000	0.26180400
C	-1.54876300	-1.81583800	-0.51624200
O	-1.30836500	-2.55545500	-1.43847400
C	-2.91032100	-1.37668500	-0.12217400
C	-3.99275900	-1.99223800	-0.75321200
C	-3.09956200	-0.35907100	0.81188100
C	-5.27725900	-1.58730000	-0.43177900
H	-3.82199800	-2.77462100	-1.48255600
C	-4.39087300	0.04630300	1.11972300
H	-2.26000800	0.12911800	1.28821200
C	-5.47901900	-0.56942300	0.50185800
C	0.76401200	-1.47670500	-0.12659900
H	0.88750200	-2.49456000	-0.50134800
O	3.75195400	-1.63637800	2.83758200
H	4.53391900	-1.79241700	3.37752100
O	7.06154600	-1.21669800	-0.53938400
H	7.15207500	-1.05355300	-1.48400800
O	-4.59424100	1.04071900	2.01844600
H	-5.54427300	1.19239900	2.10086500
O	-6.71892400	-0.13684200	0.84093800
H	-7.37568000	-0.63322700	0.33578800

O	-6.41961900	-2.10271700	-0.96182700
H	-6.21667600	-2.79058500	-1.60426500
O	-2.00299500	3.18772300	-0.70312300
H	-2.01557000	4.10941600	-0.41578900
O	-0.04319200	4.85165400	0.15253700
H	0.75547000	5.31864500	0.42726200
O	2.51724200	4.01686100	0.29258200
H	3.39584400	3.62483200	0.32437700

Figure 4 (ω B97X-D), EGCg B-ring(p-eq)/3-O(p-ax) conformer



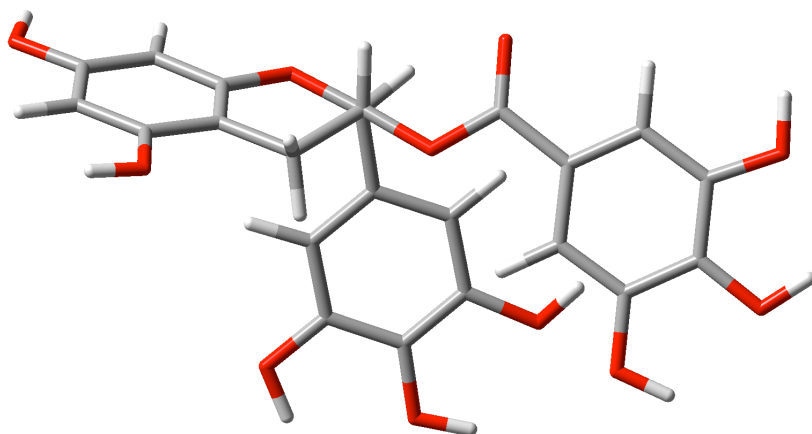
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C	-5.38199900	1.01387600	0.15260800
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C	-3.48413200	-0.23685100	-0.72999200
C	-3.07415600	-0.46565000	0.57983900
C	-3.77999900	0.03325700	1.67505100
C	-4.93106900	0.77440300	1.45015800
H	-6.28762900	1.58843600	-0.00454300
H	-3.41981600	-0.17089000	2.67657400
O	-1.95062100	-1.16966400	0.88087900
C	-1.31503600	-1.91281100	-0.15493600
H	-1.89479400	-2.82427700	-0.34629300
C	0.07187300	-2.27293600	0.31217000
C	0.66466100	-3.43888100	-0.16650900
C	0.79468500	-1.39181100	1.10763600
C	1.99128800	-3.70848700	0.14237300
H	0.10531600	-4.13066600	-0.78809900
C	2.12288700	-1.66460900	1.41026700

H	0.34434300	-0.48151600	1.47944200
C	2.72549500	-2.82159100	0.92579100
C	-2.68409000	-0.74323700	-1.89918100
H	-2.62969600	0.01242600	-2.68510000
H	-3.15551000	-1.62622900	-2.34309000
O	-0.54496500	0.09280300	-1.22137300
C	0.73394600	0.15376400	-1.62256300
O	1.23840300	-0.63813300	-2.38248700
C	1.45038500	1.30545500	-1.02034500
C	2.79066900	1.48148000	-1.36366200
C	0.82647400	2.15491000	-0.10925200
C	3.50692900	2.51744200	-0.78850300
H	3.25954100	0.80523000	-2.06813500
C	1.54893800	3.19276600	0.46045300
H	-0.20900600	2.01245400	0.16791900
C	2.88962700	3.37449600	0.12261300
C	-1.28019800	-1.11451600	-1.46524700
H	-0.76830600	-1.69732400	-2.22958900
O	-5.03459000	0.71040200	-2.20261900
H	-5.82536300	1.25416900	-2.22633600
O	-5.67205100	1.29101700	2.46224300
H	-5.26697600	1.07096100	3.30439000
O	2.67483500	-4.81195700	-0.26698900
H	2.12299500	-5.36331300	-0.82576100
O	4.03038400	-3.04062600	1.25156000
H	4.31866500	-3.86209500	0.84209400
O	2.83146500	-0.79336600	2.17069300
H	3.72773700	-1.13221300	2.26440900
O	0.95267400	4.02388200	1.34874100
H	1.59914300	4.67496600	1.64058000
O	3.55075500	4.40010700	0.71322800
H	4.46183500	4.40777600	0.40211000
O	4.81531000	2.79461600	-1.03261400
H	5.18895600	2.15903100	-1.64703700

Figure 4 (ω B97X-D), EGCg B-ring(p-ax)/3-O(p-eq) conformer



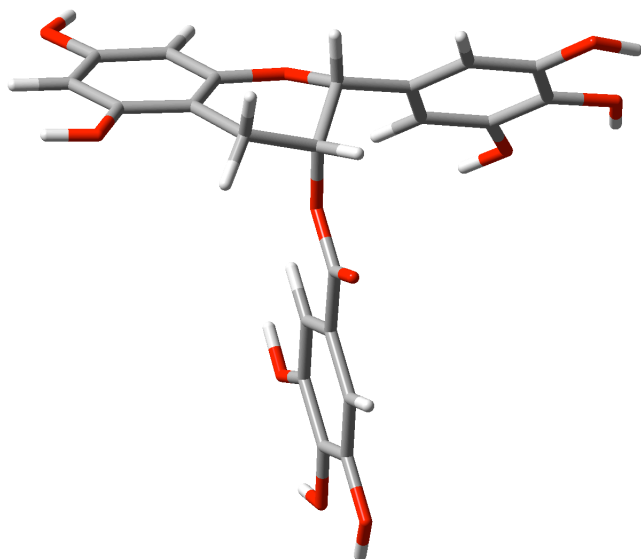
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C	5.64110100	-1.04148100	1.06652600
C	4.32832700	-1.17524300	1.49709400
C	3.24511000	-1.05275300	0.61855900
C	3.53106500	-0.77366800	-0.71453500
C	4.83899500	-0.63371300	-1.17794000
C	5.88714000	-0.77353300	-0.27948900
H	6.47176900	-1.14087400	1.75560700
H	5.01034800	-0.41446700	-2.22507700
O	2.56107600	-0.62503500	-1.65972300
C	1.19655500	-0.54526200	-1.25731000
H	0.63758700	-0.90575400	-2.12235400
C	0.74980500	0.86814000	-0.95079200
C	1.59750900	1.80568500	-0.36999300
C	-0.58013600	1.19853300	-1.20394000
C	1.10750700	3.05898000	-0.01914700
H	2.63829700	1.58557700	-0.16840800
C	-1.07448400	2.43636600	-0.82034100
H	-1.24559200	0.48979400	-1.68526600
C	-0.23231600	3.37357200	-0.23042900
C	1.82772600	-1.20787200	1.09473500
H	1.47557800	-0.28920400	1.57733300
H	1.75671000	-2.00884000	1.83257000
O	-0.41696800	-1.38633100	0.34482800
C	-1.37534400	-1.99899300	-0.36549000
O	-1.14684000	-2.82401200	-1.21837900
C	-2.72994700	-1.51388500	-0.00481000
C	-3.82653800	-2.18089100	-0.55113200
C	-2.90284100	-0.38510500	0.79540000

C	-5.10318400	-1.71597300	-0.28401000
H	-3.67351800	-3.04926500	-1.18055600
C	-4.18373600	0.08265300	1.04762100
H	-2.05329100	0.14372200	1.20493900
C	-5.28527400	-0.58398500	0.51125600
C	0.93825500	-1.52008400	-0.08787200
H	1.10681000	-2.53685600	-0.44698700
O	4.02113600	-1.43090000	2.79262300
H	4.82747600	-1.51787500	3.30637700
O	7.18471800	-0.65227000	-0.65349400
H	7.23469800	-0.47064900	-1.59495700
O	-4.36036600	1.18902300	1.80825100
H	-5.30343600	1.37449800	1.86640400
O	-6.51355700	-0.08524000	0.78856200
H	-7.17985800	-0.62389500	0.34916800
O	-6.25166000	-2.27402500	-0.74812800
H	-6.06126300	-3.03296300	-1.30395300
O	1.93797300	3.96834400	0.54873500
H	1.43091300	4.76359000	0.74218000
O	-0.66268700	4.60698200	0.15551900
H	-1.61281200	4.66203900	0.01411100
O	-2.36715900	2.83312300	-0.98120400
H	-2.91748700	2.08522900	-1.22562100

Figure 4 (B3LYP), EGCg B-ring(p-eq)/3-O(p-ax) conformer



Number of imaginary frequency = 0

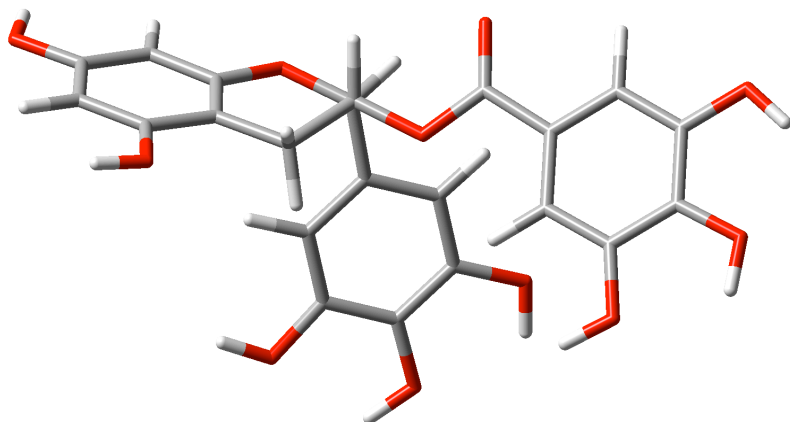
Gibbs energy = -1676.960392 a.u.

C	-4.69971100	2.40039700	0.30706900
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C	-3.96386200	1.98936700	-0.80078500
C	-3.09365200	0.88847100	-0.74991500
C	-3.00130000	0.20360900	0.46410900
C	-3.72536200	0.59397700	1.59527300
C	-4.56942600	1.69632900	1.50722400
H	-5.36700200	3.25266700	0.25341700
H	-3.62189600	0.02949800	2.51438300
O	-2.17930000	-0.87976700	0.63159700
C	-1.65820200	-1.50893000	-0.55221400
H	-2.48277000	-2.02294900	-1.06095500
C	-0.62843100	-2.53467800	-0.13594500
C	0.16920700	-2.34225900	0.99467100
C	-0.45969600	-3.67321600	-0.92660400
C	1.13102100	-3.29320400	1.32607700
H	0.03328200	-1.46804100	1.61806400
C	0.51216700	-4.61583300	-0.59651600
H	-1.07747100	-3.84885700	-1.79964500
C	1.31069800	-4.42762200	0.53281700
C	-2.27099500	0.47949500	-1.94770500
H	-1.85840600	1.35611500	-2.45121000
H	-2.89043800	-0.03495200	-2.69162700
O	-0.09502400	0.28827400	-0.86129100
C	0.91862500	0.77033300	-1.61387500
O	0.99989300	0.59238100	-2.81209700
C	1.90734800	1.53224100	-0.81078900
C	1.73770700	1.73828300	0.56560900
C	3.02418500	2.04893400	-1.47576700
C	2.69375600	2.46248200	1.26515200
H	0.87132800	1.34201500	1.07822400
C	3.97753100	2.77121700	-0.76928500
H	3.14927400	1.88892000	-2.53809900
C	3.81385100	2.97891100	0.60456700
C	-1.13735600	-0.45636000	-1.53775400
H	-0.70637200	-0.94755800	-2.40839100
O	-4.04392900	2.63870900	-1.99990600
H	-4.64360500	3.38997800	-1.92192700
O	-5.31002200	2.13723300	2.56613500
H	-5.13720300	1.58028200	3.33421100
O	1.96148700	-3.21503400	2.41336100
H	1.79757500	-2.40153500	2.90351400
O	2.24385800	-5.38931400	0.82086600
H	2.71835200	-5.12875400	1.62132200
O	0.67158600	-5.72683800	-1.37273300
H	1.37582600	-6.26582600	-0.98749100

O	5.06700500	3.27529300	-1.41373600
H	5.61352100	3.74555800	-0.76948100
O	4.77499600	3.69375900	1.25358900
H	4.53634300	3.76299200	2.18831600
O	2.64776600	2.73550700	2.60472500
H	1.85451800	2.35715900	3.00079900

Figure 4 (B3LYP), EGCg B-ring(p-ax)/3-O(p-eq) conformer



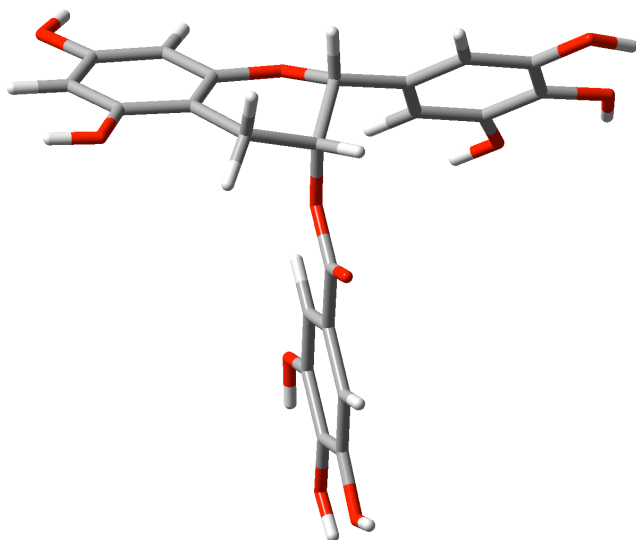
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Gibbs energy = -1676.955352 a.u.

C	5.30193700	-1.99708900	1.04972400
C	3.95333700	-1.93971900	1.38916500
C	2.98690100	-1.42580900	0.50907900
C	3.43144200	-0.95884500	-0.73056900
C	4.77992900	-1.00550900	-1.09970600
C	5.70642700	-1.52906300	-0.20369500
H	6.03752400	-2.39674500	1.73797400
H	5.07687600	-0.63195300	-2.07229700
O	2.58476700	-0.43768300	-1.67403700
C	1.20553700	-0.17354300	-1.33507600
H	0.67837300	-0.27813200	-2.28346500
C	0.99952800	1.24540000	-0.83726100
C	-0.12645900	1.94453700	-1.27844800
C	1.89996500	1.86615800	0.03693100
C	-0.36890200	3.24411600	-0.83743200
H	-0.82655800	1.49780300	-1.97411500
C	1.65842600	3.16792700	0.46847300
H	2.79358700	1.35740600	0.37671800
C	0.52415700	3.85975800	0.04009700
C	1.52396800	-1.38612200	0.87368900
H	1.29814600	-0.53106800	1.52130500
H	1.24445900	-2.28491300	1.42697600

O	-0.67273100	-1.05248400	-0.02038300
C	-1.64470000	-1.52254000	-0.83885500
O	-1.41004500	-2.09041900	-1.88562200
C	-3.00481400	-1.26101900	-0.30942800
C	-3.20750100	-0.60934900	0.91550300
C	-4.09284100	-1.69031400	-1.07695900
C	-4.50446800	-0.39280800	1.36074600
H	-2.36542700	-0.27849600	1.50854200
C	-5.38770800	-1.47058600	-0.62517800
H	-3.93066900	-2.19251000	-2.02101300
C	-5.59581400	-0.82005300	0.59603100
C	0.69878700	-1.29206000	-0.39662000
H	0.74519200	-2.22866700	-0.95387400
O	3.49514700	-2.38054400	2.59723900
H	4.22941300	-2.73636900	3.11139000
O	7.03835600	-1.60718400	-0.49117200
H	7.19937100	-1.25679600	-1.37520100
O	-6.44971800	-1.88674800	-1.37001400
H	-7.26285400	-1.64979500	-0.90355400
O	-6.88320100	-0.62641000	0.99586500
H	-6.88171100	-0.16464600	1.84574800
O	-4.84026200	0.22762000	2.53242300
H	-4.04953400	0.50323600	3.01013300
O	-1.47354000	3.91409600	-1.27583700
H	-1.46758800	4.79723500	-0.88222500
O	0.24790200	5.14118200	0.43759500
H	0.95422400	5.44120700	1.02497100
O	2.47291000	3.87090200	1.31622400
H	3.22769800	3.33378100	1.58245900

Figure 4 (CAM-B3LYP), EGCg B-ring(p-eq)/3-O(p-ax) conformer



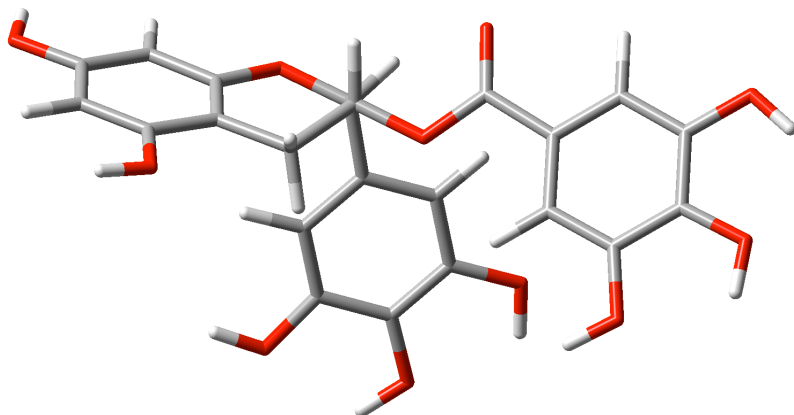
Number of imaginary frequency = 0

Gibbs energy = -1676.249812 a.u.

C	4.71877800	-2.26789300	0.35892500
C	3.99512100	-1.87410600	-0.75513300
C	3.10507600	-0.79657000	-0.71886300
C	2.97826800	-0.11728500	0.48703500
C	3.68876700	-0.49005500	1.62589900
C	4.55379400	-1.56899800	1.55158500
H	5.40442800	-3.10528300	0.31750100
H	3.55644000	0.07150100	2.54233100
O	2.13497300	0.94365100	0.63648300
C	1.62464500	1.55513000	-0.54866100
H	2.44174400	2.09084000	-1.04444900
C	0.55888300	2.54461900	-0.15283400
C	-0.23418600	2.33083600	0.96937900
C	0.35394100	3.66270000	-0.95299000
C	-1.23039600	3.24288700	1.28291900
H	-0.06755600	1.46745100	1.59964100
C	-0.65139300	4.56605000	-0.63802100
H	0.97023300	3.85360800	-1.82322700
C	-1.44549900	4.35688400	0.48193800
C	2.29573300	-0.41106900	-1.92730200
H	1.91134500	-1.29730000	-2.43331100
H	2.91352800	0.11646400	-2.66077100
O	0.12368800	-0.26460400	-0.85295300
C	-0.82024400	-0.84556800	-1.60558700
O	-0.85165600	-0.75822800	-2.81048800
C	-1.81004900	-1.59674100	-0.79736900

C	-2.85265400	-2.22445100	-1.47744800
C	-1.70968500	-1.67798600	0.58850700
C	-3.79662900	-2.93395400	-0.75979800
H	-2.91348600	-2.15110600	-2.55568600
C	-2.65970000	-2.39214400	1.29963200
H	-0.90209000	-1.19480400	1.11863700
C	-3.70331900	-3.01935200	0.62663600
C	1.14180500	0.49324600	-1.53140100
H	0.70190100	0.96921000	-2.40544200
O	4.10596700	-2.51763500	-1.94699000
H	4.72021300	-3.25485800	-1.86605300
O	5.28194200	-1.99122400	2.61798300
H	5.08834100	-1.44069500	3.38386500
O	-2.06330100	3.14413800	2.35851200
H	-1.87947300	2.34315300	2.85942400
O	-2.41381800	5.27932400	0.75532300
H	-2.88393900	5.00882500	1.55364300
O	-0.85238400	5.66019500	-1.41725500
H	-1.57866400	6.17236500	-1.03935300
O	-2.57450700	-2.48123500	2.65076000
H	-3.31470100	-3.01252100	2.97096000
O	-4.60803900	-3.70610200	1.36968200
H	-5.27234300	-4.08946700	0.78252000
O	-4.86157300	-3.59101000	-1.29693600
H	-4.87260700	-3.50261700	-2.25547800

Figure 4 (CAM-B3LYP), EGCg B-ring(p-ax)/3-O(p-eq)



Number of imaginary frequency = 0

Gibbs energy = -1676.244827 a.u.

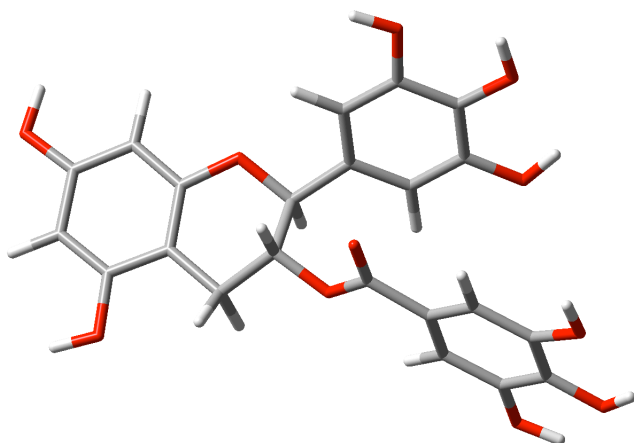
C	5.29240000	-1.93653700	1.06293700
C	3.95180800	-1.87556600	1.40742800
C	2.98174900	-1.39319400	0.52332500

C	3.41328800	-0.96243100	-0.72574800
C	4.75369500	-1.01309900	-1.10221800
C	5.68395800	-1.50448700	-0.20144100
H	6.03467500	-2.31300900	1.75596600
H	5.04109000	-0.66608300	-2.08670800
O	2.55968300	-0.47003700	-1.66936000
C	1.19244500	-0.21051300	-1.32931000
H	0.65398000	-0.33137600	-2.26824300
C	0.98357100	1.20724600	-0.84326500
C	-0.18805700	1.86382000	-1.20427500
C	1.92863800	1.86192900	-0.05614200
C	-0.42959300	3.15807400	-0.76592100
H	-0.92584200	1.38916800	-1.83910100
C	1.68453400	3.15782900	0.37324000
H	2.85882700	1.38205100	0.22014500
C	0.50711400	3.80734700	0.02681900
C	1.52658000	-1.35111500	0.89676300
H	1.29973500	-0.47571000	1.51364300
H	1.25815200	-2.23213200	1.48056500
O	-0.66309700	-1.06879000	0.00687800
C	-1.62425200	-1.50195100	-0.82642600
O	-1.38573300	-2.03587400	-1.88327700
C	-2.98637100	-1.24545100	-0.30498100
C	-3.19059100	-0.62553200	0.92789600
C	-4.06271600	-1.64618600	-1.09074800
C	-4.48512400	-0.41134500	1.36428400
H	-2.35013900	-0.31674800	1.53432300
C	-5.35471000	-1.42830100	-0.64579800
H	-3.89447100	-2.12575100	-2.04490900
C	-5.56603600	-0.80982700	0.58279700
C	0.69993700	-1.30421400	-0.36726300
H	0.75523100	-2.25498300	-0.89817600
O	3.50431900	-2.28131300	2.62386700
H	4.23870500	-2.61784600	3.14807000
O	7.00731300	-1.58450800	-0.49549800
H	7.16441800	-1.26140300	-1.38896200
O	-6.41283000	-1.81364500	-1.40162300
H	-7.22535500	-1.57976400	-0.93495800
O	-6.84998500	-0.61628800	0.97638400
H	-6.85329700	-0.17548400	1.83596400
O	-4.82814200	0.17977700	2.54211900
H	-4.04564300	0.44325000	3.03706500
O	-1.57524500	3.79397500	-1.12186400
H	-1.55978500	4.68236000	-0.74347800

O	0.22903000	5.08195700	0.42597000
H	0.96898700	5.41208700	0.95044300
O	2.53730900	3.89410800	1.14109500
H	3.32615300	3.38749200	1.35910800

2. Conformers in Figure 5.

Figure 5 (M06-2X), *ent*-GCg B-ring(p-eq)/3-*O*(p-eq) conformer



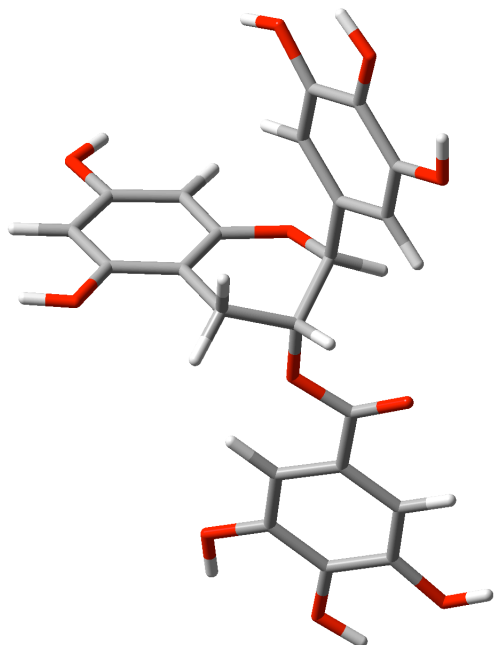
Number of imaginary frequency = 0

Gibbs energy = -1676.343754 a.u.

C	-6.13057300	-1.45271300	0.07243100
C	-4.86167100	-1.97312500	0.28414200
C	-3.70568700	-1.19542900	0.13430300
C	-3.87638400	0.13125500	-0.25213500
C	-5.13765900	0.68684200	-0.46924900
C	-6.25820700	-0.11406700	-0.30004100
H	-7.01748400	-2.06344700	0.19109300
H	-5.21769900	1.72440800	-0.77003100
O	-2.81572900	0.97508300	-0.42552400
C	-1.54293900	0.36056300	-0.59675100
H	-1.52840400	-0.18048700	-1.55143200
C	-0.47948800	1.42452400	-0.58838700
C	-0.62704600	2.55977600	0.20633900
C	0.70892300	1.18782400	-1.27202800
C	0.43248700	3.45037000	0.31792900
H	-1.55301400	2.74132200	0.73900900
C	1.77359200	2.07226800	-1.13554500
H	0.83943900	0.30656400	-1.88929100
C	1.63625900	3.20551300	-0.34015500
C	-2.34342800	-1.77845000	0.41306000

H	-2.03332700	-2.44523700	-0.39855800
H	-2.36665800	-2.37308300	1.32820700
O	-0.02315400	-1.21706400	0.40060800
C	0.97727800	-0.68150000	1.12902000
O	0.80210800	0.07369400	2.05076000
C	2.31361400	-1.13448500	0.66381200
C	2.45644600	-1.98028400	-0.43434400
C	3.42700200	-0.64430100	1.34814300
C	3.73005500	-2.34475400	-0.84950000
H	1.59588200	-2.35450400	-0.97150500
C	4.69358000	-1.01233700	0.92527700
H	3.29310800	0.01925100	2.19385500
C	4.84812300	-1.86139600	-0.17115800
C	-1.33061200	-0.65787500	0.53812900
H	-1.41360500	-0.13980300	1.49507500
O	-7.51959800	0.34969800	-0.49411900
H	-7.48890300	1.27794200	-0.74780900
O	-4.66286100	-3.26426500	0.65485000
H	-5.51041200	-3.70871200	0.76190800
O	2.94449900	1.82595500	-1.77692700
H	3.56341700	2.53580400	-1.56412800
O	2.70527300	4.04755000	-0.24511800
H	2.47552700	4.77418300	0.34705100
O	0.41255000	4.59634300	1.05577400
H	-0.42678900	4.68522300	1.51836900
O	3.88759800	-3.16827100	-1.91549700
H	4.83210300	-3.30801200	-2.05931200
O	6.06961200	-2.24697400	-0.61989700
H	6.75002000	-1.84624600	-0.06378100
O	5.86143700	-0.60926300	1.49657200
H	5.69092800	-0.03435500	2.24967400

Figure 5 (M06-2X), *ent*-GCg B-ring(p-ax)/3-*O*(p-ax) conformer



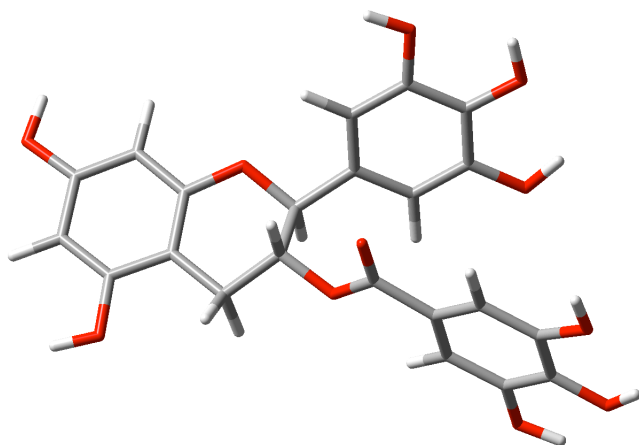
Number of imaginary frequency = 0

Gibbs energy = -1676.343707 a.u.

C	1.08082100	4.13855900	0.60770800
C	1.05075400	2.97576400	1.36504300
C	0.96111100	1.70824700	0.77635700
C	0.90626400	1.65181200	-0.61259700
C	0.93116300	2.80135000	-1.40434500
C	1.01475900	4.03927200	-0.78248400
H	1.15144500	5.11379200	1.07411900
H	0.88431100	2.70535100	-2.48241200
O	0.82280600	0.47219700	-1.29555600
C	1.02594800	-0.74289700	-0.58241500
H	0.52986600	-1.50271700	-1.18765700
C	2.49410300	-1.09387400	-0.44389000
C	3.49221500	-0.18552400	-0.78653800
C	2.82737900	-2.35713200	0.04311600
C	4.82646000	-0.54551600	-0.62198700
H	3.24749500	0.79137200	-1.18644800
C	4.16224500	-2.70888800	0.20091300
H	2.06490000	-3.08706200	0.29146400
C	5.16551800	-1.79981200	-0.12702400
C	0.89898600	0.46001000	1.61363800
H	0.26450800	0.61728000	2.48723000
H	1.89255800	0.18242500	1.97939400
O	-1.05587800	-0.43274800	0.60763700
C	-1.82285000	-1.47784400	0.26467700

O	-1.38665000	-2.59277600	0.10579400
C	-3.25273700	-1.10739300	0.11365200
C	-3.68529700	0.20564200	0.28977900
C	-4.14840800	-2.12754700	-0.21163700
C	-5.03309700	0.50145300	0.13898200
H	-2.99231700	0.99694600	0.54072200
C	-5.49143800	-1.82274900	-0.35697700
H	-3.78878400	-3.14054300	-0.34555700
C	-5.93582900	-0.51132000	-0.18284800
C	0.34697900	-0.68649400	0.79066000
H	0.47015800	-1.64236100	1.29787400
O	1.10726800	2.99724500	2.72215000
H	1.13903900	3.90813100	3.03273500
O	1.04422800	5.20348200	-1.48139800
H	0.99350900	5.01759500	-2.42468200
O	4.48967500	-3.93866100	0.67130600
H	5.45233500	-4.00512800	0.70604100
O	6.45940700	-2.19505700	0.04794400
H	7.04287000	-1.47612900	-0.22437200
O	5.88801300	0.25555800	-0.91971900
H	5.58787700	1.11607100	-1.22933300
O	-5.47248800	1.77337000	0.30616000
H	-6.42747800	1.79030800	0.16475500
O	-7.24169800	-0.16821800	-0.31578600
H	-7.75424700	-0.95777400	-0.53208900
O	-6.47183600	-2.71386500	-0.66853200
H	-6.11112000	-3.60249800	-0.75245300

Figure 5 (ω B97X-D), *ent*-GCg B-ring(p-eq)/3-O(p-eq) conformer



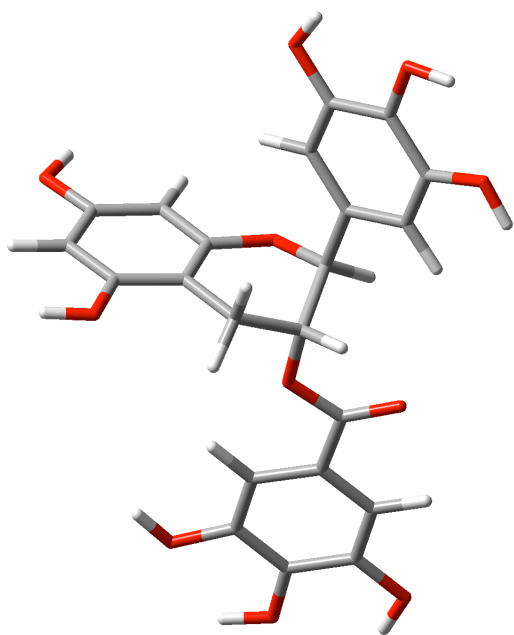
Number of imaginary frequency = 0

Gibbs energy = -1676.408974 a.u.

C	-6.13622500	-1.42228200	0.06728400
C	-4.87248200	-1.96048400	0.26670500
C	-3.70887000	-1.19729000	0.10765100
C	-3.86620800	0.13227600	-0.27422100
C	-5.12187200	0.70332000	-0.47819700
C	-6.25170200	-0.08249900	-0.30107800
H	-7.02918900	-2.02354100	0.19314900
H	-5.19111100	1.74328200	-0.77499000
O	-2.80282300	0.96531600	-0.45371800
C	-1.52534600	0.35657200	-0.61016900
H	-1.49352000	-0.16574000	-1.57472200
C	-0.46660800	1.42513600	-0.57383400
C	-0.60039200	2.52013600	0.27637300
C	0.70346100	1.23669500	-1.29999700
C	0.44981300	3.41887200	0.39853200
H	-1.51173900	2.66517100	0.84447600
C	1.76086500	2.12732500	-1.15647700
H	0.82509100	0.38448700	-1.95778300
C	1.63500700	3.22179100	-0.30722200
C	-2.34905200	-1.79134300	0.36872600
H	-2.04792400	-2.44889400	-0.45435100
H	-2.36748800	-2.40085600	1.27459000
O	-0.02235200	-1.24368400	0.36457200
C	0.96263900	-0.78531600	1.15778400
O	0.77050200	-0.11898000	2.14563700
C	2.30462500	-1.19193600	0.67377000
C	2.46813300	-1.91947200	-0.50293600
C	3.40864000	-0.77648100	1.41847400
C	3.74659800	-2.23663800	-0.93722800
H	1.61580300	-2.23332000	-1.08921700
C	4.68193600	-1.09600800	0.97895100
H	3.26271100	-0.20310700	2.32591700
C	4.85477800	-1.82526300	-0.19750100
C	-1.32759800	-0.68190200	0.50801900
H	-1.40530400	-0.18150400	1.47459300
O	-7.50675100	0.39766600	-0.48233600
H	-7.46574600	1.32242900	-0.73693100
O	-4.69241900	-3.25379200	0.63216300
H	-5.54408900	-3.68147900	0.74866300
O	2.91148900	1.92277400	-1.84404300
H	3.52918700	2.62546600	-1.61704600
O	2.69593200	4.07054600	-0.20593400
H	2.47899400	4.76363000	0.42512700

O	0.43527700	4.52567100	1.19071100
H	-0.39156900	4.58320000	1.67417800
O	3.91603500	-2.94137500	-2.08165500
H	4.85960300	-3.06241900	-2.23014700
O	6.08101700	-2.15849000	-0.66924500
H	6.75303300	-1.81243400	-0.07299600
O	5.83569200	-0.75004100	1.60886500
H	5.64964000	-0.25049300	2.40692700

Figure 5 (ω B97X-D), *ent*-GCg B-ring(p-ax)/3-*O*(p-ax) conformer



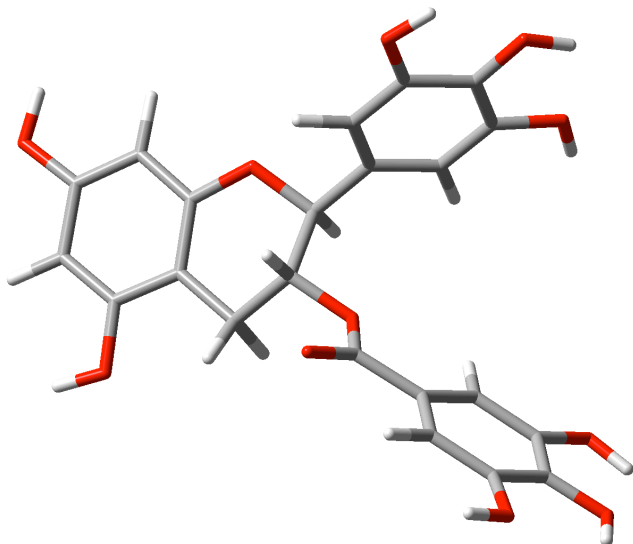
Number of imaginary frequency = 0

Gibbs energy = -1676.408854 a.u.

C	0.97713700	4.19128200	0.57346300
C	0.96570100	3.03449000	1.34107200
C	0.92275000	1.76158500	0.76121100
C	0.89695200	1.69316000	-0.62797700
C	0.90408600	2.83599000	-1.42749200
C	0.94140300	4.08095200	-0.81591200
H	1.01266700	5.17156000	1.03443400
H	0.88249500	2.73019600	-2.50577100
O	0.85666900	0.51084800	-1.30312800
C	1.05576000	-0.70171200	-0.58605000
H	0.56341900	-1.46025600	-1.19559400
C	2.52176000	-1.06208300	-0.44401700
C	2.84245300	-2.35099600	-0.01507300
C	3.52840700	-0.14687100	-0.72029600

C	4.17277500	-2.70978200	0.14995900
H	2.06190100	-3.07970300	0.18021700
C	4.86069000	-0.51319300	-0.55380700
H	3.30664700	0.85392100	-1.06676800
C	5.18640400	-1.79185900	-0.11543500
C	0.88642600	0.51429600	1.59966300
H	0.24906200	0.65425200	2.47418700
H	1.88553400	0.26095300	1.96889200
O	-1.04166000	-0.44043400	0.59902200
C	-1.79042700	-1.50356700	0.28114400
O	-1.33739400	-2.61712600	0.14605400
C	-3.22338500	-1.15394800	0.12239400
C	-4.10845200	-2.17788600	-0.20596600
C	-3.67354300	0.15639400	0.29652100
C	-5.45683400	-1.89600600	-0.36136300
H	-3.75079200	-3.19046200	-0.33942100
C	-5.02280700	0.43003100	0.14225100
H	-2.97900800	0.94752100	0.54908300
C	-5.91531300	-0.59060800	-0.18653600
C	0.36826000	-0.65087900	0.78257200
H	0.51804400	-1.59887100	1.29768900
O	0.99667600	3.07333900	2.69672200
H	0.99812100	3.98575700	2.99532100
O	0.95204800	5.23785700	-1.52377000
H	0.92934100	5.04226200	-2.46340900
O	5.84031600	0.38457900	-0.82336000
H	6.69085900	-0.03666500	-0.66154000
O	6.50680500	-2.09612300	0.02928500
H	6.58506400	-3.00870900	0.32351900
O	4.60121300	-3.93365100	0.56026900
H	3.85590300	-4.51239200	0.73468300
O	-6.32460900	-2.88584100	-0.67972600
H	-7.20904300	-2.51033600	-0.74162200
O	-7.24198100	-0.36620100	-0.34699400
H	-7.42511000	0.56572100	-0.18850600
O	-5.59282900	1.65573800	0.28555600
H	-4.93835700	2.30861800	0.54322800

Figure 5 (B3LYP), *ent*-GCg B-ring(p-eq)/3-*O*(p-eq) conformer



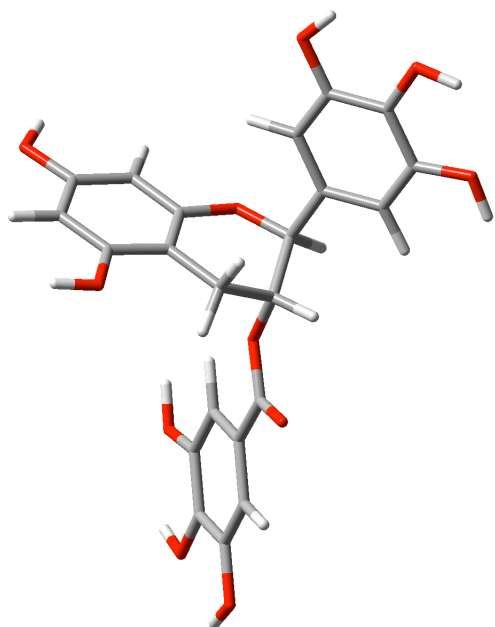
Number of imaginary frequency = 0

Gibbs energy = -1676.960701 a.u.

C	-5.61052700	-2.36721100	-0.19874600
C	-4.24384300	-2.62756900	-0.16033800
C	-3.29127100	-1.59569800	-0.16643600
C	-3.76807700	-0.28524000	-0.22432800
C	-5.13485800	0.00873000	-0.26110900
C	-6.04858300	-1.04061700	-0.24377200
H	-6.33557900	-3.17282300	-0.19404100
H	-5.45519600	1.04290600	-0.30562900
O	-2.92505400	0.79602000	-0.22028700
C	-1.53723900	0.56863200	-0.54832600
H	-1.46796200	0.31984900	-1.61337000
C	-0.78979700	1.85270700	-0.28166800
C	0.05862300	2.37407100	-1.26130500
C	-0.92958700	2.50681000	0.94460400
C	0.77163100	3.54433500	-1.00714200
H	0.16676000	1.87618900	-2.21867600
C	-0.22118800	3.67967500	1.19168000
H	-1.59466300	2.12810200	1.71025900
C	0.63440100	4.19965700	0.21672400
C	-1.81308100	-1.89060100	-0.09110100
H	-1.44101400	-2.26540200	-1.05194300
H	-1.61762300	-2.67129000	0.64719600
O	0.36136000	-0.80806700	-0.06252300
C	1.18269700	-1.28932600	0.89901100
O	0.80262400	-1.57147900	2.01661400
C	2.58245600	-1.43129700	0.42838500

C	2.96330400	-1.09662200	-0.87576200
C	3.52416000	-1.92133500	1.34360300
C	4.28864500	-1.25221500	-1.26591200
H	2.24414700	-0.71901800	-1.58825100
C	4.84468500	-2.07395400	0.94754200
H	3.21314400	-2.17618300	2.34910900
C	5.23159900	-1.74118300	-0.35577200
C	-1.03259700	-0.63069500	0.26898900
H	-1.11578000	-0.40735800	1.33311000
O	-7.39808000	-0.83797200	-0.27885400
H	-7.58217300	0.10815600	-0.30732100
O	-3.75279800	-3.90048800	-0.10926600
H	-4.48386200	-4.52845800	-0.07460300
O	-0.36483300	4.32107300	2.38718200
H	0.19413100	5.11001600	2.37657300
O	1.30627500	5.35598600	0.51279100
H	1.85185200	5.59965500	-0.24674300
O	1.62980800	4.14565600	-1.88931700
H	1.67937100	3.64290200	-2.71018900
O	4.66552700	-0.92869200	-2.53483800
H	5.61299200	-1.09913300	-2.62565500
O	6.51580900	-1.87545100	-0.78972300
H	7.05635700	-2.22449600	-0.06762600
O	5.85676900	-2.54041300	1.74019400
H	5.52653800	-2.75932500	2.61907800

Figure 5 (B3LYP), *ent*-GCg B-ring(p-ax)/3-*O*(p-ax) conformer

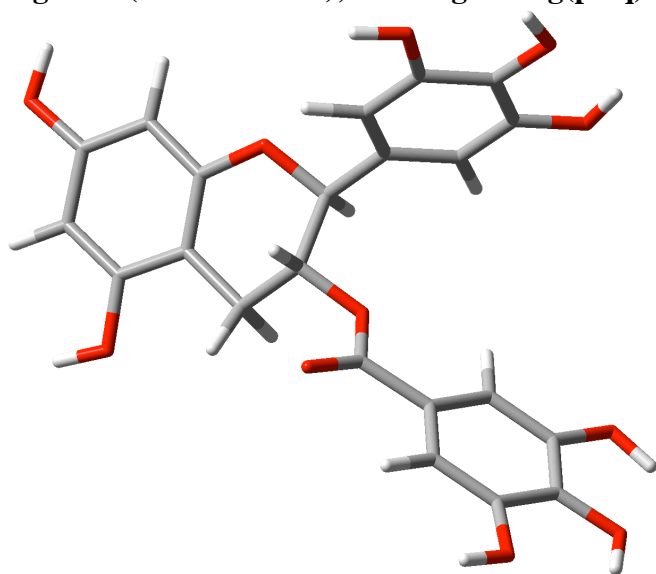


Number of imaginary frequency = 0
 Gibbs energy = -1676.958595 a.u.

C	0.70739800	4.05281300	1.14489100
C	0.68891800	2.77700600	1.70176600
C	0.80821400	1.62056800	0.91492700
C	0.95399600	1.79527800	-0.46205300
C	0.97203800	3.06350600	-1.05238200
C	0.84614000	4.18563200	-0.23944700
H	0.61575700	4.93805600	1.76358500
H	1.08282000	3.14875700	-2.12702200
O	1.07223300	0.74226800	-1.33259600
C	1.21943300	-0.59227700	-0.81919100
H	0.78510700	-1.22149600	-1.59878000
C	2.68166500	-0.97646200	-0.63138300
C	2.99642800	-2.32256300	-0.40225600
C	3.70010600	-0.02897700	-0.70818600
C	4.32398800	-2.70432200	-0.23469600
H	2.21901600	-3.07850100	-0.36533600
C	5.02963200	-0.41775200	-0.53906700
H	3.48851600	1.01267400	-0.90476500
C	5.34585000	-1.75403400	-0.29876700
C	0.76176100	0.24055000	1.51790200
H	0.04049200	0.19631800	2.33502100
H	1.73165200	-0.03613500	1.94731500
O	-0.99015200	-0.64295100	0.05805000
C	-1.92204500	-1.29703500	0.78565200
O	-1.64797600	-1.99371800	1.74171200
C	-3.29799800	-1.06738200	0.27955000
C	-4.35128600	-1.70047100	0.94756000
C	-3.54631800	-0.24552400	-0.82880400
C	-5.65706000	-1.51588300	0.51116800
H	-4.15405700	-2.33298500	1.80247300
C	-4.85390100	-0.06446100	-1.25883700
H	-2.72999800	0.24291300	-1.34391100
C	-5.91076300	-0.69635300	-0.59414600
C	0.39853600	-0.79240500	0.45778100
H	0.53837400	-1.80254700	0.83725100
O	0.55444500	2.57946600	3.04667300
H	0.45478400	3.42978800	3.49024200
O	0.85662800	5.45608700	-0.73957600
H	0.95907700	5.42433500	-1.69787600
O	6.01910900	0.51881800	-0.61392300
H	6.86712900	0.07407300	-0.47977900

O	6.66760400	-2.08063800	-0.14257900
H	6.73471400	-3.03230100	0.01098200
O	4.74599700	-3.98686500	-0.00815700
H	3.99419800	-4.58863300	0.03461600
O	-6.68618500	-2.13086600	1.15850500
H	-7.51254500	-1.88895700	0.71849800
O	-7.20778000	-0.54609100	-0.98261500
H	-7.23910800	0.03915500	-1.75203100
O	-5.23158300	0.70897400	-2.32188800
H	-4.46305100	1.12290700	-2.73123800

Figure 5 (CAM-B3LYP), *ent*-GCg B-ring(p-eq)/3-*O*(p-eq) conformer



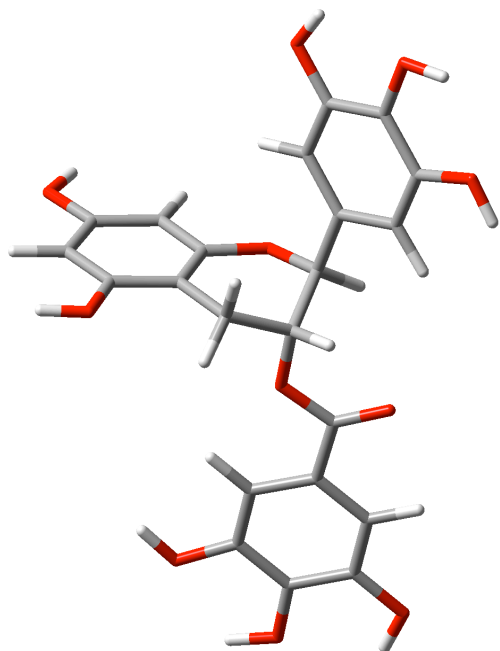
Number of imaginary frequency = 0

Gibbs energy = -1676.249334 a.u.

C	-5.58514800	-2.34292500	-0.22159500
C	-4.22470200	-2.60173400	-0.18351700
C	-3.27606700	-1.57448200	-0.18538000
C	-3.75015100	-0.27031500	-0.23802100
C	-5.11106600	0.02400100	-0.27379500
C	-6.02041000	-1.02091200	-0.26162800
H	-6.31071100	-3.14717300	-0.22008900
H	-5.42990500	1.05809100	-0.31484300
O	-2.90779400	0.80349000	-0.23158600
C	-1.53382700	0.57344100	-0.56190100
H	-1.46347400	0.32378400	-1.62593500
C	-0.77984900	1.84787700	-0.29284900
C	-0.98542600	2.53661100	0.90054600
C	0.13752100	2.31720900	-1.22247200

C	-0.26634400	3.69344900	1.15259700
H	-1.71499700	2.18532500	1.62007900
C	0.86052300	3.47390000	-0.96045400
H	0.30469000	1.79874900	-2.15809400
C	0.65935900	4.16273900	0.22747800
C	-1.80375000	-1.87283000	-0.10855100
H	-1.43090100	-2.24297400	-1.06924600
H	-1.61165000	-2.65383300	0.62793400
O	0.35682900	-0.78291700	-0.07106700
C	1.14902900	-1.34421100	0.85544200
O	0.74425200	-1.71655700	1.93077400
C	2.55737400	-1.45367600	0.40853000
C	3.46523800	-2.04265900	1.28771400
C	2.96736400	-0.98993200	-0.83818600
C	4.78857700	-2.16551400	0.90966200
H	3.12645800	-2.39628900	2.25306200
C	4.29589000	-1.11687600	-1.20848700
H	2.26788400	-0.53160200	-1.52189100
C	5.20633600	-1.70431800	-0.33581600
C	-1.03004000	-0.61789700	0.25338500
H	-1.12027500	-0.39286900	1.31655800
O	-3.73479800	-3.86765900	-0.13624500
H	-4.46066500	-4.49976100	-0.10740700
O	-7.36288500	-0.81756100	-0.29628300
H	-7.55042600	0.12646200	-0.32238500
O	1.75868300	3.93492000	-1.86887700
H	2.15526600	4.74350800	-1.52022600
O	1.38761500	5.29762800	0.43503900
H	1.14002800	5.67432100	1.28851700
O	-0.38564200	4.45678600	2.27585100
H	-1.03467600	4.07983400	2.87844500
O	4.71093400	-0.67023800	-2.42033900
H	5.65806400	-0.84019800	-2.50243300
O	6.49577000	-1.80550400	-0.74679300
H	7.01582000	-2.22933500	-0.05177700
O	5.77535700	-2.71911300	1.66730900
H	5.43031600	-3.02790300	2.51125600

Figure 5 (CAM-B3LYP), *ent*-GCg B-ring(p-ax)/3-*O*(p-ax)



Number of imaginary frequency = 0

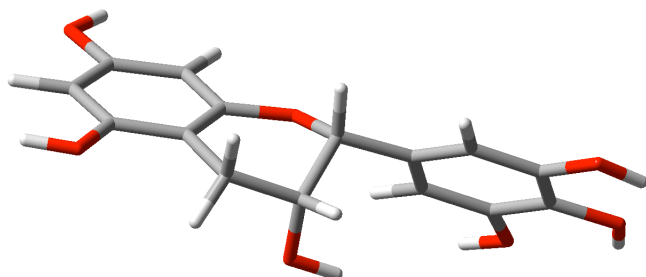
Gibbs energy = -1676.247940 a.u.

C	0.96801700	4.27076800	0.57413100
C	0.93219500	3.11909000	1.34388700
C	0.92002700	1.84472000	0.76975600
C	0.94957300	1.76975600	-0.61639100
C	0.98162900	2.90830600	-1.41906100
C	0.98783600	4.15363900	-0.81298500
H	0.97990500	5.25269800	1.03088100
H	0.99970700	2.79860800	-2.49628300
O	0.93800100	0.58169800	-1.28640000
C	1.07892800	-0.64029400	-0.56332000
H	0.56909100	-1.37801000	-1.18219200
C	2.52914000	-1.05568600	-0.41095600
C	2.80252700	-2.35103500	0.02949200
C	3.56923000	-0.19029100	-0.71494300
C	4.11702000	-2.76195900	0.17855400
H	1.99761200	-3.04585700	0.24276700
C	4.88538000	-0.61054100	-0.56312300
H	3.38468300	0.81090800	-1.07753200
C	5.16205200	-1.89311900	-0.11358000
C	0.85695800	0.60113600	1.60992900
H	0.19298800	0.74631300	2.46238700
H	1.84136700	0.35047800	2.01592000
O	-1.04653300	-0.37166500	0.56899500
C	-1.78281100	-1.45556200	0.28373000

O	-1.30979900	-2.56372200	0.18165400
C	-3.22083400	-1.14157900	0.11550900
C	-4.07810400	-2.19192300	-0.19745400
C	-3.70487700	0.15781000	0.26751800
C	-5.43027800	-1.94738700	-0.36097100
H	-3.69347900	-3.19568700	-0.31269400
C	-5.05788300	0.39263800	0.10392600
H	-3.03287800	0.96944300	0.51127300
C	-5.92049300	-0.65387100	-0.20990700
C	0.36536600	-0.57074500	0.78764900
H	0.50155300	-1.51248400	1.31402900
O	0.90753300	3.16449600	2.70188500
H	0.89260200	4.08040800	2.99877600
O	1.01883300	5.30886300	-1.52721600
H	1.03031400	5.11012500	-2.46927800
O	5.90327500	0.23794700	-0.85987500
H	6.73774300	-0.22274900	-0.70459000
O	6.47177700	-2.25492400	0.01592900
H	6.51289200	-3.16968800	0.32089300
O	4.50449300	-3.99902800	0.59847200
H	3.74044600	-4.55216900	0.79029800
O	-6.27740800	-2.96176100	-0.66609100
H	-7.17165700	-2.60414300	-0.73787000
O	-7.25343000	-0.46319400	-0.37849500
H	-7.45784600	0.47092200	-0.24121100
O	-5.66435900	1.60608100	0.22464500
H	-5.02770400	2.28933600	0.45809800

3. Conformers in Figure 6.

Figure 6 (M06-2X), EGC B-ring(p-eq)/3-O(p-ax) conformer



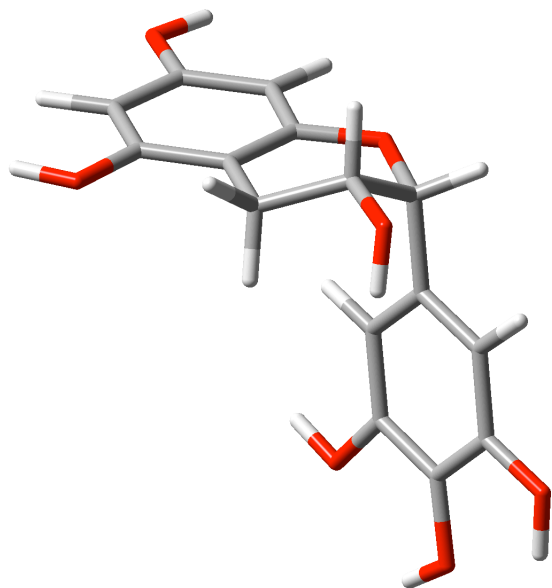
Number of imaginary frequency = 0

Gibbs energy = -1106.358784 a.u.

C	4.76634400	0.29591400	-0.08245000
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C	3.97869500	-0.82333500	0.15143800
C	2.58329300	-0.78856800	0.04079100
C	2.00395700	0.42217400	-0.32814400
C	2.76596200	1.56795800	-0.56650100
C	4.14525600	1.49386600	-0.43655700
H	5.84544800	0.25561700	0.00657400
H	2.26852900	2.48676300	-0.85313400
O	0.65681100	0.57033800	-0.47000500
C	-0.12998300	-0.61726300	-0.52903700
H	0.02648300	-1.10202200	-1.50037200
C	-1.57728900	-0.22118800	-0.38431300
C	-2.55932200	-1.02858300	-0.95254900
C	-1.93193100	0.88866800	0.38308100
C	-3.90206800	-0.72529200	-0.75826900
H	-2.30086200	-1.89155500	-1.55540300
C	-3.27802500	1.18874800	0.56520500
H	-1.16758100	1.52862900	0.80771300
C	-4.26346200	0.38412300	0.00244900
C	1.74697300	-2.00293100	0.34892400
H	2.11979500	-2.49854600	1.24745800
H	1.80215300	-2.73080900	-0.46609000
O	0.21293900	-0.99315100	1.84623000
C	0.29931000	-1.60114000	0.57111400
H	-0.35057000	-2.48110500	0.51087700
H	-0.69587600	-0.69957400	1.97693500
O	4.95511500	2.56386000	-0.65324600
H	4.42219600	3.33119800	-0.88549500
O	4.51678000	-2.02007400	0.50715100
H	5.47318000	-1.93762700	0.58145800
O	-4.86192000	-1.50487500	-1.31653400
H	-5.72465300	-1.13584200	-1.08858000
O	-5.59452400	0.64128600	0.15257800
H	-5.69850900	1.44310300	0.67956300
O	-3.74646900	2.25038100	1.27874500
H	-3.01584000	2.77073600	1.62804900

Figure 6 (M06-2X), EGC B-ring(p-ax)/3-O(p-eq) conformer



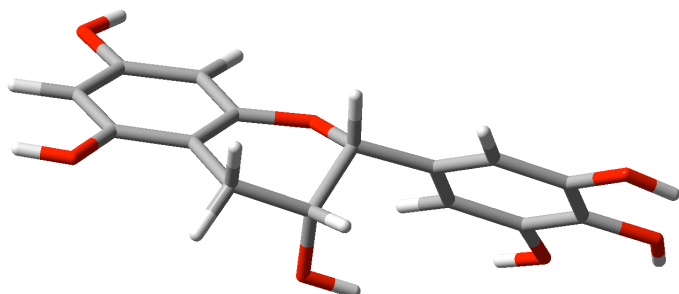
Number of imaginary frequency = 0

Gibbs energy = -1106.356436 a.u.

C	-3.91375600	-0.71879700	0.76774000
C	-2.96466200	0.16482900	1.26334400
C	-1.92708100	0.66575300	0.46629200
C	-1.87099500	0.23222800	-0.85560500
C	-2.80960100	-0.65545900	-1.38526100
C	-3.82888900	-1.11974200	-0.56593300
H	-4.71330800	-1.09816300	1.39258500
H	-2.72204400	-0.96555600	-2.41937300
O	-0.89613700	0.63464700	-1.72277500
C	0.21644900	1.36980200	-1.21266900
H	0.59203500	1.93838400	-2.06489500
C	1.31950500	0.45806800	-0.71370800
C	1.05662000	-0.84700000	-0.29654900
C	2.62117700	0.95833000	-0.65854300
C	2.09601300	-1.63363000	0.18714800
H	0.05898900	-1.26647100	-0.35216400
C	3.65430800	0.16497200	-0.17001300
H	2.85385500	1.95660300	-1.01019200
C	3.39210100	-1.13231900	0.25907500
C	-0.92190200	1.64550900	1.00871600
H	-0.15489600	1.12677700	1.59896900
H	-1.40779800	2.36339000	1.67167000
O	0.79562700	3.21469800	0.27511900
C	-0.25795100	2.37647000	-0.14531800
H	-0.98837500	3.02956000	-0.62993400

H	1.42270800	2.67652000	0.77222700
O	-2.98587000	0.59648900	2.55105700
H	-3.74472300	0.21984300	3.00870300
O	-4.78033600	-1.98238400	-1.00801100
H	-4.62742200	-2.18714500	-1.93634600
O	4.91906300	0.65377100	-0.12139900
H	5.49860400	-0.03514200	0.22775200
O	4.43983200	-1.87142200	0.72390400
H	4.11715400	-2.74745900	0.96873500
O	1.95877400	-2.91908500	0.61721200
H	1.03958200	-3.19893300	0.55911000

Figure 6 (ω B97X-D), EGC B-ring(p-eq)/3-O(p-ax) conformer



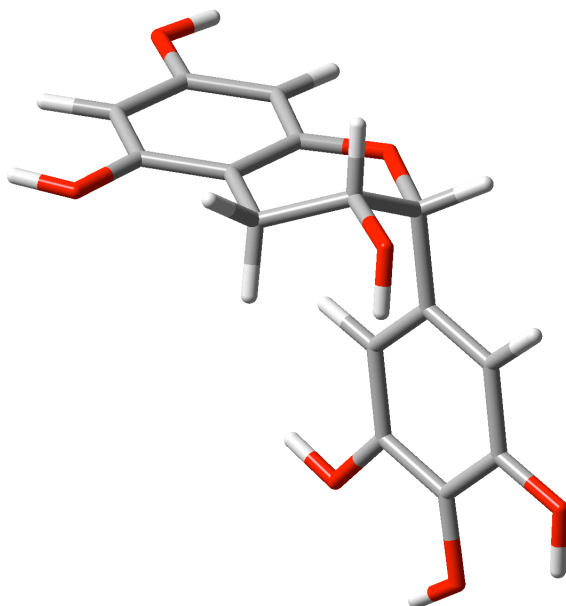
Number of imaginary frequency = 0

Gibbs energy = -1106.409665 a.u.

C	4.76219900	0.31135500	-0.07120400
C	3.98180500	-0.81416900	0.15930800
C	2.58802500	-0.78997300	0.03541000
C	2.00349200	0.41526500	-0.34285600
C	2.75881700	1.56500300	-0.57744300
C	4.13740800	1.50321100	-0.43493000
H	5.84113800	0.27780600	0.02813400
H	2.25662900	2.47957500	-0.87084700
O	0.66032800	0.55629300	-0.49568900
C	-0.13384300	-0.62678100	-0.53414700
H	0.00951800	-1.11798300	-1.50463100
C	-1.57820500	-0.22285700	-0.38471200
C	-2.56479500	-1.01473800	-0.96424500
C	-1.92848300	0.87762300	0.39579500
C	-3.90563500	-0.70832100	-0.76618800
H	-2.30910900	-1.87139800	-1.57742800
C	-3.27179000	1.18347400	0.58303900
H	-1.16037900	1.50643900	0.83002800
C	-4.26193400	0.39232300	0.00960000

C	1.75177600	-2.00605400	0.33276400
H	2.12472800	-2.51613500	1.22330500
H	1.80630800	-2.72589900	-0.49047400
O	0.20084800	-1.04119600	1.84731300
C	0.30151400	-1.61676700	0.55906400
H	-0.33865700	-2.50349400	0.47712900
H	-0.70764100	-0.75399400	1.97466500
O	4.93896300	2.57783100	-0.64708200
H	4.40294500	3.33710000	-0.88749100
O	4.52993500	-2.00179400	0.52258300
H	5.48151400	-1.90713900	0.60705200
O	-4.86510900	-1.47718000	-1.33583400
H	-5.72492900	-1.11157200	-1.10292000
O	-5.59041500	0.65240900	0.16318200
H	-5.69255400	1.44355100	0.70097300
O	-3.72902300	2.23737200	1.31133900
H	-2.99583600	2.74169200	1.67047300

Figure 6 (ω B97X-D), EGC B-ring(p-ax)/3-O(p-eq) conformer



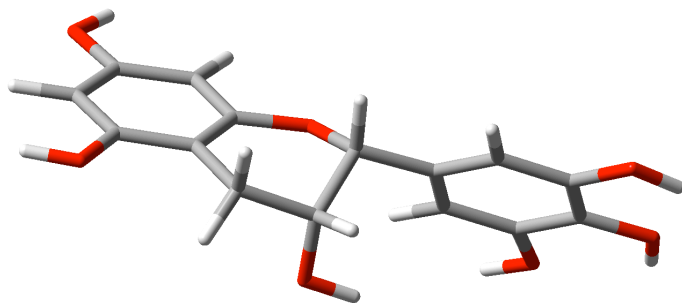
Number of imaginary frequency = 0

Gibbs energy = -1106.407644 a.u.

C	-3.95573600	-0.73325100	0.70558900
C	-3.01416500	0.13743000	1.23817800
C	-1.96039300	0.64950800	0.47178800
C	-1.87786200	0.23872000	-0.85606900
C	-2.80869600	-0.63397700	-1.42040900
C	-3.84654900	-1.11020800	-0.63220000

H	-4.76854900	-1.12130000	1.30863200
H	-2.70003000	-0.92654600	-2.45798800
O	-0.88823400	0.65241200	-1.69519500
C	0.22005100	1.37804600	-1.16161300
H	0.59107400	1.96791800	-2.00115100
C	1.33256900	0.46319400	-0.68997600
C	1.07561000	-0.81946100	-0.20798900
C	2.64035200	0.94513800	-0.71437200
C	2.12479900	-1.60222300	0.25683700
H	0.06986600	-1.22233600	-0.19177800
C	3.68604300	0.15859800	-0.24369700
H	2.86585800	1.92890100	-1.10890200
C	3.42944000	-1.11788500	0.24647100
C	-0.95499300	1.60704400	1.04996400
H	-0.20535600	1.06703600	1.64375600
H	-1.44171900	2.31677600	1.72148500
O	0.79076400	3.18025600	0.38643300
C	-0.26010900	2.36006400	-0.07216200
H	-0.97511800	3.03572200	-0.54926400
H	1.42949000	2.62045800	0.83785500
O	-3.06313000	0.54028000	2.53241600
H	-3.83135200	0.15775200	2.96264200
O	-4.78993400	-1.95987700	-1.10964200
H	-4.61895000	-2.14632400	-2.03587800
O	4.95405300	0.63583200	-0.27233800
H	5.54130000	-0.04188500	0.07829000
O	4.48814600	-1.85090000	0.69062800
H	4.16839600	-2.70604700	0.99403500
O	1.98709400	-2.86453200	0.74497300
H	1.06285900	-3.12231800	0.75802000

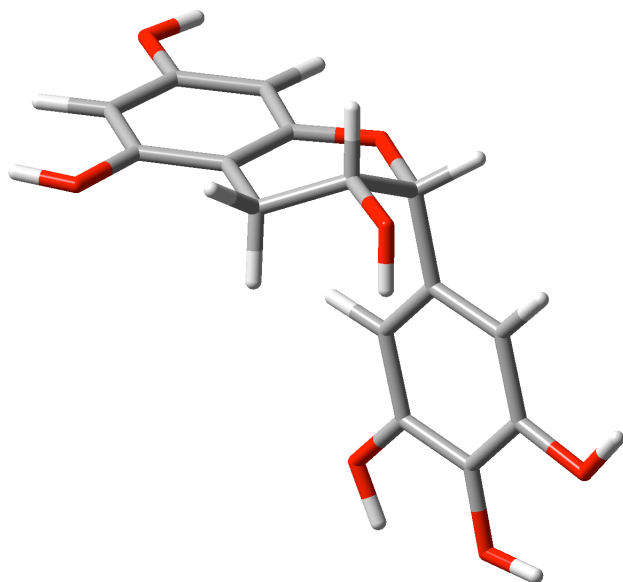
Figure 6 (B3LYP), EGC B-ring(p-eq)/3-O(p-ax) conformer



Number of imaginary frequency = 0
Gibbs energy = -1106.772211 a.u.

C	4.78512100	0.32908400	-0.10273500
C	4.01054500	-0.80197800	0.14233100
C	2.61065700	-0.78362800	0.04081300
C	2.01445800	0.42360400	-0.33014600
C	2.76482700	1.57812800	-0.57927400
C	4.14954300	1.52124400	-0.45932100
H	5.86549400	0.29835800	-0.02096000
H	2.25600100	2.49090500	-0.86631000
O	0.65887000	0.56169700	-0.45786400
C	-0.13916800	-0.63583900	-0.50038600
H	0.00603900	-1.11608800	-1.47553000
C	-1.58896600	-0.23448000	-0.35539200
C	-2.57073300	-0.98562000	-1.00486700
C	-1.95704000	0.83216200	0.47276600
C	-3.91806300	-0.67704200	-0.82797100
H	-2.30762500	-1.80946100	-1.65795200
C	-3.30602500	1.14157500	0.63772100
H	-1.19986500	1.43767900	0.95518600
C	-4.28921300	0.38776000	-0.00404000
C	1.77992300	-2.00575200	0.34849000
H	2.16074900	-2.51117600	1.23888900
H	1.83762200	-2.73230200	-0.46974100
O	0.21819800	-1.07570500	1.88995300
C	0.31973400	-1.63534300	0.58264500
H	-0.30752800	-2.53057900	0.49730000
H	-0.70069300	-0.81680300	2.03178300
O	4.94984900	2.60464700	-0.68849800
H	4.40373700	3.36406100	-0.92286900
O	4.57425000	-1.99453500	0.50072400
H	5.53060200	-1.89156400	0.56927000
O	-4.87178000	-1.41081500	-1.46942600
H	-5.73782700	-1.04503800	-1.24294700
O	-5.62683400	0.65444300	0.12615000
H	-5.73441600	1.42237600	0.70281300
O	-3.77964000	2.16888000	1.40896900
H	-3.04920000	2.64748400	1.81720000

Figure 6 (B3LYP), EGC B-ring(p-ax)/3-O(p-eq) conformer



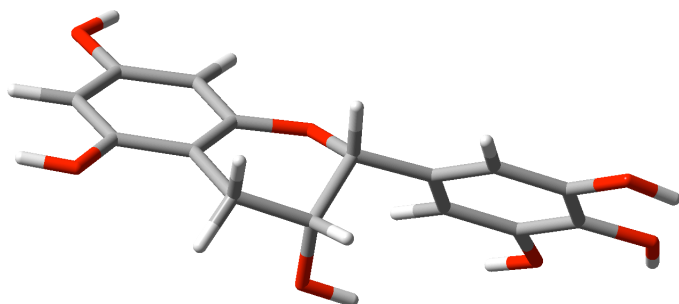
Number of imaginary frequency = 0

Gibbs energy = -1106.767595 a.u.

C	-4.07725300	-0.68459400	0.68194000
C	-3.14067400	0.20667100	1.19890900
C	-2.03758000	0.64568000	0.44881800
C	-1.90384800	0.14223600	-0.84749900
C	-2.82924900	-0.75377300	-1.39434100
C	-3.91374000	-1.15810400	-0.62270500
H	-4.92478600	-1.01431700	1.27140200
H	-2.68318400	-1.11651000	-2.40472600
O	-0.87011200	0.49042700	-1.67716900
C	0.22142200	1.28521200	-1.16971900
H	0.57507800	1.83882500	-2.04119200
C	1.36439500	0.42304600	-0.65977000
C	2.66792500	0.93409900	-0.73349200
C	1.15044600	-0.84679900	-0.12034300
C	3.73885400	0.18228800	-0.25531900
H	2.85378600	1.90734800	-1.17417500
C	2.22672600	-1.59689700	0.35125500
H	0.16134600	-1.28040400	-0.06445200
C	3.52328300	-1.08397300	0.28975700
C	-1.03718400	1.63020800	1.00065900
H	-0.30846400	1.12505800	1.64896400
H	-1.53675200	2.38019900	1.61726800
O	0.73901400	3.17723100	0.30638700
C	-0.30146400	2.31967700	-0.14265000
H	-0.99869300	2.97027200	-0.67713700

H	1.37357500	2.64237900	0.80004500
O	-3.24515900	0.70398400	2.46684300
H	-4.04558800	0.36289500	2.88273800
O	-4.85779900	-2.02880400	-1.08693600
H	-4.64292200	-2.28601400	-1.99127300
O	2.00629600	-2.83888600	0.87077100
H	2.85769800	-3.21075300	1.13876500
O	4.54260100	-1.86712800	0.76352000
H	5.37738100	-1.39643900	0.63915100
O	5.04785000	0.58252000	-0.28210800
H	5.12763600	1.45283000	-0.68885200

Figure 6 (CAM-B3LYP), EGC B-ring(p-eq)/3-O(p-ax) conformer



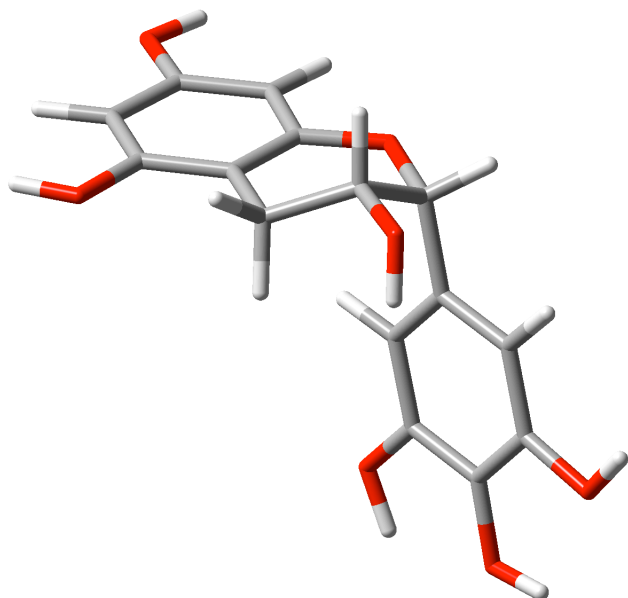
Number of imaginary frequency = 0

Gibbs energy = -1106.293955 a.u.

C	4.76240400	0.31979500	-0.09411500
C	3.98744000	-0.80447700	0.14464500
C	2.59402200	-0.78272500	0.03909700
C	2.00418700	0.42057500	-0.32823100
C	2.75420000	1.56988500	-0.57139700
C	4.13212400	1.50923500	-0.44809200
H	5.84178800	0.28770300	-0.00896200
H	2.24773400	2.48356600	-0.85721100
O	0.65559700	0.55750400	-0.46005200
C	-0.13511300	-0.63182800	-0.50990100
H	0.01160200	-1.11070700	-1.48432800
C	-1.58089000	-0.23386500	-0.36272000
C	-2.56173600	-1.00436800	-0.97699500
C	-1.93940000	0.85038400	0.43489700
C	-3.90193700	-0.69487400	-0.79448400
H	-2.30317400	-1.84565400	-1.60840700
C	-3.28212200	1.15830700	0.60499400
H	-1.17723300	1.46870200	0.89145800
C	-4.26406800	0.38712900	-0.00129800

C	1.76530800	-2.00111800	0.34305200
H	2.14278300	-2.50333600	1.23503400
H	1.82501300	-2.72630400	-0.47404600
O	0.21560800	-1.05082100	1.86478400
C	0.31351600	-1.62395700	0.57171900
H	-0.31930900	-2.51450100	0.49464900
H	-0.69816700	-0.78075100	2.00722400
O	4.54277200	-1.99358100	0.50076700
H	5.49847500	-1.90003100	0.57167800
O	4.93025400	2.58698900	-0.67092700
H	4.39034600	3.34910200	-0.90483000
O	-4.86113700	-1.44179900	-1.39765000
H	-5.72319200	-1.07080200	-1.16933800
O	-5.59513600	0.65400000	0.13675800
H	-5.69996300	1.43646100	0.69201400
O	-3.75060700	2.20019500	1.34800000
H	-3.02312900	2.69806500	1.73459300

Figure 6 (CAM-B3LYP), EGC B-ring(p-ax)/3-O(p-eq) conformer



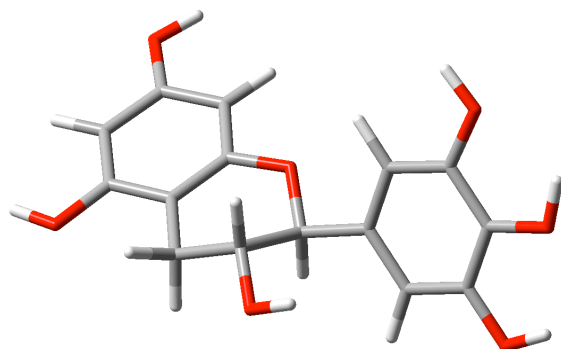
Number of imaginary frequency = 0

Gibbs energy = -1106.289474 a.u.

C	-4.01784500	-0.67934400	0.72289600
C	-3.08065000	0.21513700	1.21542100
C	-2.00025600	0.65624900	0.44523300
C	-1.88977100	0.15249400	-0.84535200
C	-2.81602900	-0.74714100	-1.36965700
C	-3.87750400	-1.15347200	-0.57839500

H	-4.85156900	-1.01236100	1.32867400
H	-2.68693400	-1.11160100	-2.38102100
O	-0.87590300	0.50206900	-1.68842600
C	0.21631700	1.28655500	-1.19796800
H	0.57579900	1.82938800	-2.07252900
C	1.34577600	0.42113400	-0.67768400
C	2.64153100	0.94067700	-0.68985800
C	1.12141600	-0.86194500	-0.19364000
C	3.69468800	0.18097600	-0.20226500
H	2.83526800	1.92852100	-1.09166900
C	2.18178700	-1.61786500	0.28821000
H	0.13454800	-1.30280300	-0.18823000
C	3.46877200	-1.09757700	0.28967400
C	-1.00141900	1.64649100	0.97508000
H	-0.26112100	1.14922900	1.61392900
H	-1.49682000	2.39660900	1.59260700
O	0.74938000	3.18260000	0.24338600
C	-0.29118200	2.32588700	-0.18094900
H	-0.99908800	2.96663300	-0.71130800
H	1.37265000	2.66464700	0.76516800
O	-3.16109500	0.71457800	2.47659600
H	-3.94581400	0.37054400	2.91607000
O	-4.81995600	-2.02674100	-1.02020400
H	-4.62502000	-2.28725000	-1.92654500
O	1.95945900	-2.87281500	0.75627000
H	2.80409900	-3.24614900	1.03903300
O	4.47351300	-1.88567400	0.77061800
H	5.30864000	-1.40841700	0.69087700
O	4.99588200	0.58408900	-0.16868000
H	5.09132900	1.46861600	-0.53600200

Figure 6 (M06-2X), *ent*-GC B-ring(p-eq)/3-*O*(p-eq) conformer

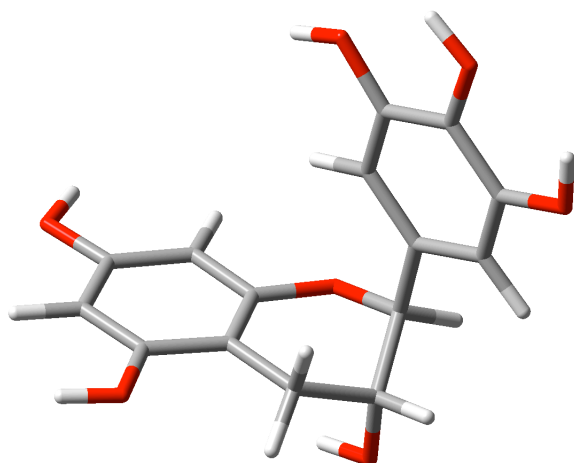


Number of imaginary frequency = 0
Gibbs energy = -1676.343754 a.u.

C	-6.13057300	-1.45271300	0.07243100
C	-4.86167100	-1.97312500	0.28414200
C	-3.70568700	-1.19542900	0.13430300
C	-3.87638400	0.13125500	-0.25213500
C	-5.13765900	0.68684200	-0.46924900
C	-6.25820700	-0.11406700	-0.30004100
H	-7.01748400	-2.06344700	0.19109300
H	-5.21769900	1.72440800	-0.77003100
O	-2.81572900	0.97508300	-0.42552400
C	-1.54293900	0.36056300	-0.59675100
H	-1.52840400	-0.18048700	-1.55143200
C	-0.47948800	1.42452400	-0.58838700
C	-0.62704600	2.55977600	0.20633900
C	0.70892300	1.18782400	-1.27202800
C	0.43248700	3.45037000	0.31792900
H	-1.55301400	2.74132200	0.73900900
C	1.77359200	2.07226800	-1.13554500
H	0.83943900	0.30656400	-1.88929100
C	1.63625900	3.20551300	-0.34015500
C	-2.34342800	-1.77845000	0.41306000
H	-2.03332700	-2.44523700	-0.39855800
H	-2.36665800	-2.37308300	1.32820700
O	-0.02315400	-1.21706400	0.40060800
C	0.97727800	-0.68150000	1.12902000
O	0.80210800	0.07369400	2.05076000
C	2.31361400	-1.13448500	0.66381200
C	2.45644600	-1.98028400	-0.43434400
C	3.42700200	-0.64430100	1.34814300
C	3.73005500	-2.34475400	-0.84950000
H	1.59588200	-2.35450400	-0.97150500
C	4.69358000	-1.01233700	0.92527700
H	3.29310800	0.01925100	2.19385500
C	4.84812300	-1.86139600	-0.17115800
C	-1.33061200	-0.65787500	0.53812900
H	-1.41360500	-0.13980300	1.49507500
O	-7.51959800	0.34969800	-0.49411900
H	-7.48890300	1.27794200	-0.74780900
O	-4.66286100	-3.26426500	0.65485000
H	-5.51041200	-3.70871200	0.76190800
O	2.94449900	1.82595500	-1.77692700
H	3.56341700	2.53580400	-1.56412800
O	2.70527300	4.04755000	-0.24511800
H	2.47552700	4.77418300	0.34705100

O	0.41255000	4.59634300	1.05577400
H	-0.42678900	4.68522300	1.51836900
O	3.88759800	-3.16827100	-1.91549700
H	4.83210300	-3.30801200	-2.05931200
O	6.06961200	-2.24697400	-0.61989700
H	6.75002000	-1.84624600	-0.06378100
O	5.86143700	-0.60926300	1.49657200
H	5.69092800	-0.03435500	2.24967400

Figure 6 (M06-2X), *ent*-GC B-ring(p-ax)/3-*O*(p-ax) conformer



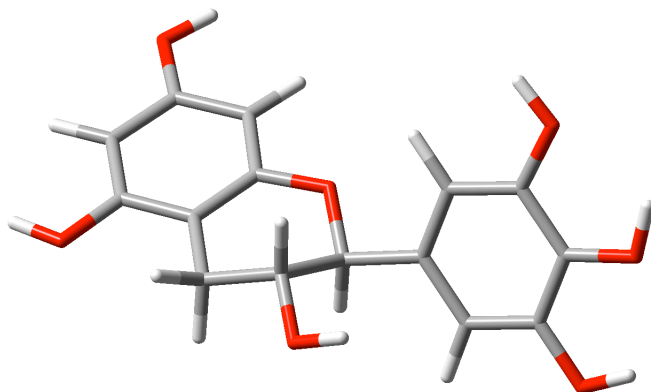
Number of imaginary frequency = 0

Gibbs energy = -1106.358924 a.u.

C	-4.81415000	0.33082500	-0.06787600
C	-4.01211900	-0.76999900	0.19990200
C	-2.61389700	-0.70253000	0.14493000
C	-2.04960600	0.52027400	-0.20864900
C	-2.82641900	1.64776500	-0.48078300
C	-4.20782700	1.54166500	-0.40398000
H	-5.89471800	0.26634500	-0.02119300
H	-2.33889800	2.57612600	-0.75291500
O	-0.69838000	0.69331100	-0.29522800
C	0.08725200	-0.49349100	-0.39946000
H	-0.10250700	-0.96723800	-1.37116400
C	1.53843600	-0.10799000	-0.29073900
C	1.92317000	0.93374100	0.55370600
C	2.49693400	-0.85366800	-0.97269700
C	3.27225400	1.23078200	0.69717600
H	1.17765100	1.51814800	1.07996600
C	3.84721600	-0.55407700	-0.81629900
H	2.21345800	-1.66083000	-1.63769100

C	4.23624100	0.48878000	0.01856400
C	-1.76555500	-1.90019500	0.48387700
H	-1.78328400	-2.63439200	-0.32919200
H	-2.15377800	-2.39944300	1.37388700
O	0.47090000	-2.64365000	0.67546500
C	-0.32539100	-1.47894000	0.70621400
H	-0.22617200	-0.95350700	1.66604200
H	1.38011400	-2.39307100	0.87304000
O	-4.53507200	-1.97743900	0.53803800
H	-5.49555500	-1.91896500	0.57210400
O	-5.03383800	2.59021200	-0.65723000
H	-4.51212200	3.36664600	-0.88464700
O	4.78300700	-1.27398900	-1.48515800
H	5.65410100	-0.92030100	-1.26500700
O	5.57066600	0.74733400	0.12918100
H	5.69376800	1.49817100	0.72295000
O	3.76950800	2.22957300	1.47906400
H	3.05436800	2.70183900	1.91744900

Figure 6 (ω B97X-D), *ent*-GC B-ring(p-eq)/3-*O*(p-eq) conformer



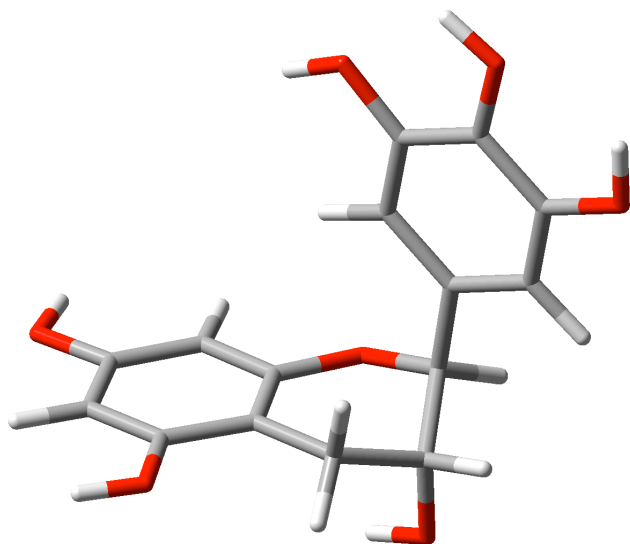
Number of imaginary frequency = 0

Gibbs energy = -1106.409892 a.u.

C	-4.80818100	0.35028000	-0.05143700
C	-4.01444600	-0.75719100	0.21563500
C	-2.61725300	-0.70471100	0.13890500
C	-2.04592300	0.50841900	-0.23572900
C	-2.81528800	1.63993600	-0.50768900
C	-4.19642600	1.55092200	-0.40896400
H	-5.88889900	0.29596700	0.01299800
H	-2.32208200	2.56081300	-0.79624700
O	-0.69879100	0.67127200	-0.34284200
C	0.09419800	-0.51302300	-0.41751100

H	-0.07805800	-0.99822400	-1.38680100
C	1.54132600	-0.11630100	-0.29773500
C	1.91903500	0.88871800	0.59172400
C	2.50555900	-0.81635600	-1.01593500
C	3.26395400	1.19399000	0.74717700
H	1.16868100	1.43937300	1.14702300
C	3.85294300	-0.51155800	-0.84940500
H	2.22724600	-1.59639300	-1.71465100
C	4.23406600	0.49490500	0.03223100
C	-1.77068900	-1.90382500	0.47331900
H	-1.79656800	-2.63876100	-0.33963800
H	-2.15530400	-2.40416900	1.36476700
O	0.46189300	-2.66067700	0.67362600
C	-0.32780000	-1.49181900	0.69211000
H	-0.22861600	-0.96376500	1.65142100
H	1.37071400	-2.41139400	0.86117100
O	-4.54910800	-1.95188600	0.57238400
H	-5.50501200	-1.87814200	0.62206500
O	-5.01289000	2.60500900	-0.65967300
H	-4.48671100	3.37087100	-0.90085900
O	4.79004700	-1.19183900	-1.55374400
H	5.65698000	-0.84448800	-1.31936300
O	5.56477700	0.75959100	0.15225500
H	5.68391500	1.47711400	0.78198400
O	3.74814700	2.15892700	1.57488100
H	3.03065400	2.59371200	2.04085500

Figure 6 (ω B97X-D), *ent*-GC B-ring(p-ax)/3-*O*(p-ax) conformer

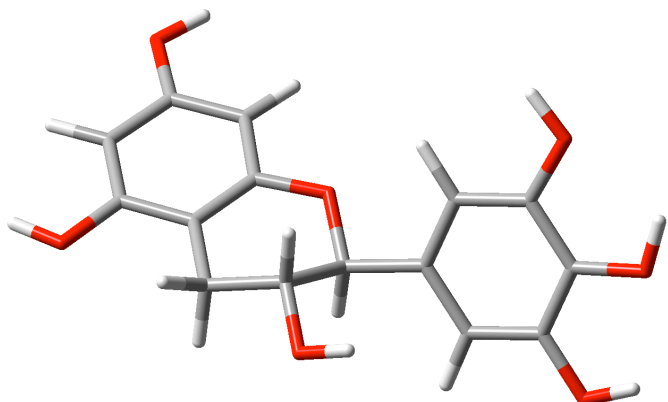


Number of imaginary frequency = 0

Gibbs energy = -1106.409448 a.u.

C	3.69186200	-0.98196100	0.90777500
C	2.80340400	-0.02884500	1.38610400
C	1.82639800	0.55150400	0.56690500
C	1.77507900	0.12942400	-0.75889100
C	2.65580100	-0.82347400	-1.27109000
C	3.61259800	-1.37114300	-0.42895700
H	4.44206600	-1.42581800	1.55197800
H	2.57594000	-1.11638400	-2.31135900
O	0.87346400	0.63078000	-1.65161200
C	-0.21215800	1.41717000	-1.15604400
H	-0.52640700	2.00652200	-2.01932000
C	-1.36933800	0.55970600	-0.68152300
C	-1.25316400	-0.82235900	-0.56971800
C	-2.56982000	1.18600300	-0.35176600
C	-2.33377600	-1.56870800	-0.11219400
H	-0.33378500	-1.32873800	-0.83755500
C	-3.64626700	0.43544400	0.10262300
H	-2.69290100	2.25864100	-0.44924000
C	-3.52930600	-0.94680800	0.22789500
C	0.87341600	1.59475600	1.08691400
H	1.38705400	2.27994600	1.76357100
H	0.06188100	1.12694300	1.65475000
O	1.21915300	3.30080400	-0.62719700
C	0.28853400	2.38629700	-0.07591700
H	-0.55051600	2.99244100	0.26608700
H	2.00227800	2.81076600	-0.89065900
O	2.82901600	0.39179900	2.67493100
H	3.54486500	-0.04252500	3.14467600
O	4.50267000	-2.30342400	-0.85000900
H	4.35398900	-2.49605500	-1.77873000
O	-4.81169400	1.05063200	0.42086800
H	-5.44022400	0.37973900	0.70702100
O	-4.61571200	-1.63561400	0.67898100
H	-4.39877500	-2.57235200	0.70802000
O	-2.32615300	-2.92160800	0.03713100
H	-1.47098400	-3.28211600	-0.20667400

Figure 6 (B3LYP), *ent*-GC B-ring(p-eq)/3-*O*(p-eq) conformer



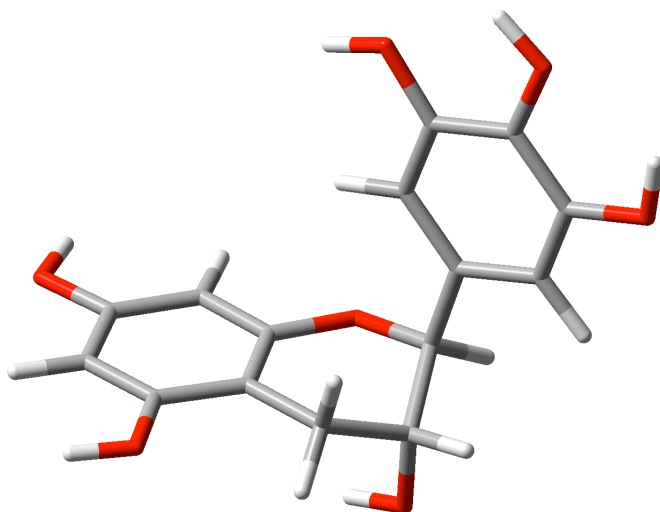
Number of imaginary frequency = 0

Gibbs energy = -1106.772924 a.u.

C	-4.82773400	0.36913200	-0.06668900
C	-4.04097200	-0.74725000	0.20373500
C	-2.63868700	-0.70308800	0.14075000
C	-2.05545300	0.51315100	-0.22271300
C	-2.81854600	1.65258200	-0.49841600
C	-4.20490400	1.57079600	-0.41413000
H	-5.90914800	0.31970600	-0.01306500
H	-2.31870900	2.57255400	-0.77789700
O	-0.69705300	0.67129600	-0.31099400
C	0.10187900	-0.52558100	-0.39363800
H	-0.06952300	-0.99591500	-1.36950800
C	1.55383900	-0.12926100	-0.27286400
C	1.94121900	0.88917700	0.60511200
C	2.51958000	-0.83210300	-0.99704500
C	3.29018500	1.20139000	0.74425500
H	1.19694200	1.44727900	1.16003400
C	3.87090100	-0.52032100	-0.84669200
H	2.24038800	-1.61542700	-1.69113900
C	4.25910800	0.49778000	0.02478300
C	-1.79705800	-1.91088300	0.47366700
H	-1.82607500	-2.64552700	-0.34038700
H	-2.18820900	-2.41553300	1.36038300
O	0.43017900	-2.71120400	0.66436400
C	-0.34397200	-1.51873900	0.70138500
H	-0.23659200	-1.01468000	1.67145700
H	1.34478400	-2.48075400	0.86706000
O	-4.59165600	-1.94776700	0.55216400
H	-5.55148900	-1.86366900	0.59246700
O	-5.01884000	2.63693300	-0.67074800
H	-4.48215600	3.40321100	-0.90447500

O	4.80790500	-1.20699500	-1.56143700
H	5.67887900	-0.85047800	-1.33938200
O	5.59742600	0.77126800	0.12900700
H	5.71639700	1.50079300	0.75148900
O	3.78259900	2.18349000	1.56171700
H	3.06372600	2.62159100	2.03138400

Figure 6 (B3LYP), *ent*-GC B-ring(p-ax)/3-*O*(p-ax) conformer



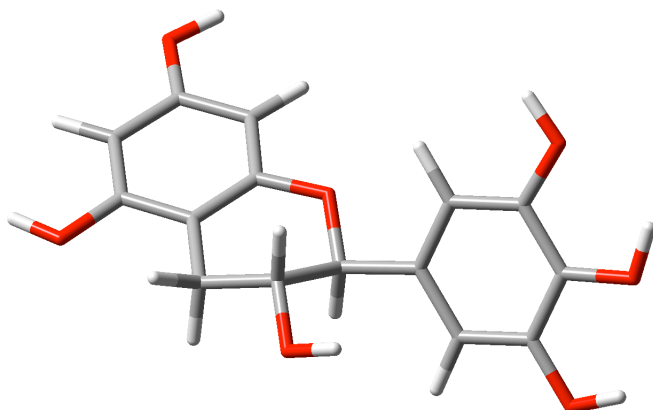
Number of imaginary frequency = 0

Gibbs energy = -1106.769266 a.u.

C	3.88494900	-0.88939200	0.85716800
C	2.98151400	0.05231000	1.34110500
C	1.92405300	0.54144900	0.55553300
C	1.80872300	0.04015800	-0.74367200
C	2.70318800	-0.90448200	-1.25888300
C	3.73940000	-1.36058300	-0.45081900
H	4.69538900	-1.25965800	1.47408600
H	2.57488400	-1.25939200	-2.27453600
O	0.82957200	0.45326000	-1.61151300
C	-0.23091900	1.30806000	-1.13491000
H	-0.52131700	1.87644900	-2.02097100
C	-1.42724100	0.50885500	-0.64176900
C	-1.35701200	-0.87228200	-0.44877700
C	-2.62778900	1.18363400	-0.39712300
C	-2.47893100	-1.56595400	0.00347900
H	-0.44436300	-1.41602300	-0.65616500
C	-3.74542400	0.48579400	0.05327000
H	-2.72018600	2.25109200	-0.55993500
C	-3.67307900	-0.89385200	0.25901900

C	0.95249900	1.57468500	1.07151100
H	1.46470700	2.29674300	1.71006600
H	0.17166900	1.10734900	1.68236400
O	1.21314700	3.22758000	-0.72136800
C	0.30774500	2.31384900	-0.10025600
H	-0.52276800	2.92687100	0.25003900
H	2.01038800	2.74161300	-0.96364300
O	3.07182900	0.55100400	2.60894400
H	3.83957100	0.17133000	3.05225500
O	4.65184300	-2.28051300	-0.88030500
H	4.45658700	-2.52818100	-1.79170400
O	-4.91247100	1.15234000	0.28817600
H	-5.57254400	0.51021000	0.58303700
O	-4.80314300	-1.53187600	0.70147200
H	-4.61036500	-2.47445800	0.79073300
O	-2.51761800	-2.91741800	0.22574700
H	-1.65697900	-3.31245600	0.04589500

Figure 6 (CAM-B3LYP), *ent*-GC B-ring(p-eq)/3-*O*(p-eq) conformer



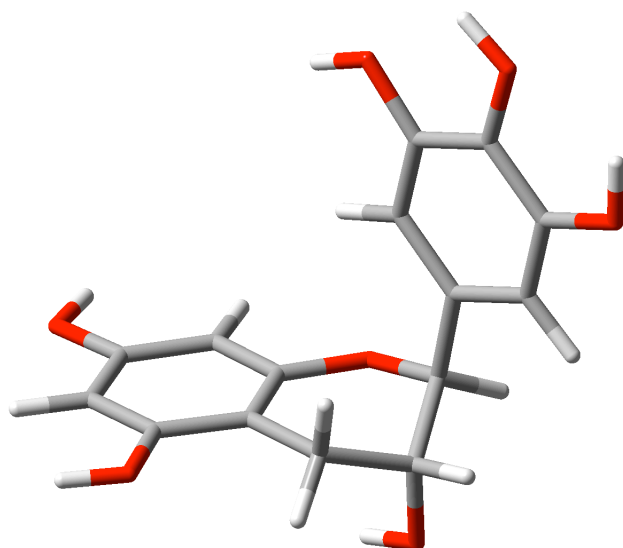
Number of imaginary frequency = 0

Gibbs energy = -1106.294419 a.u.

C	-4.80725000	0.35670200	-0.06801600
C	-4.01948500	-0.75210600	0.19749700
C	-2.62327900	-0.70148800	0.13982100
C	-2.04694300	0.51310500	-0.21265800
C	-2.81010800	1.64691700	-0.48297400
C	-4.19001900	1.55815600	-0.40459800
H	-5.88799300	0.30352600	-0.01858100
H	-2.31266400	2.56967500	-0.75484400
O	-0.69479900	0.67216900	-0.29615900
C	0.09578100	-0.51579200	-0.39068000
H	-0.08105400	-0.98273700	-1.36636000

C	1.54493500	-0.12552000	-0.27357700
C	1.92680300	0.92081400	0.56270400
C	2.50736500	-0.85978200	-0.95812200
C	3.27098600	1.22892700	0.69995400
H	1.17982900	1.50277700	1.08751800
C	3.85308900	-0.54963800	-0.80859900
H	2.22960900	-1.66838000	-1.62227700
C	4.23630800	0.49534600	0.02083800
C	-1.78312700	-1.90489700	0.47037700
H	-1.80705600	-2.63556400	-0.34519100
H	-2.17500500	-2.41079400	1.35431100
O	0.43890500	-2.68739800	0.65837500
C	-0.33880100	-1.50725900	0.69865700
H	-0.23396800	-1.00241000	1.66753000
H	1.34928000	-2.46035200	0.87538200
O	-4.56138400	-1.95140600	0.53622900
H	-5.52087500	-1.87899600	0.57321800
O	-5.00261900	2.61772800	-0.65644800
H	-4.47258100	3.38864600	-0.88395900
O	4.79317300	-1.26165400	-1.48088300
H	5.66153400	-0.89886900	-1.26379400
O	5.56937000	0.76648600	0.12610500
H	5.68795400	1.52017900	0.71727200
O	3.76212100	2.23498800	1.47745600
H	3.04732900	2.70508400	1.91863500

Figure 6 (CAM-B3LYP), *ent*-GC B-ring(p-ax)/3-*O*(p-ax) conformer



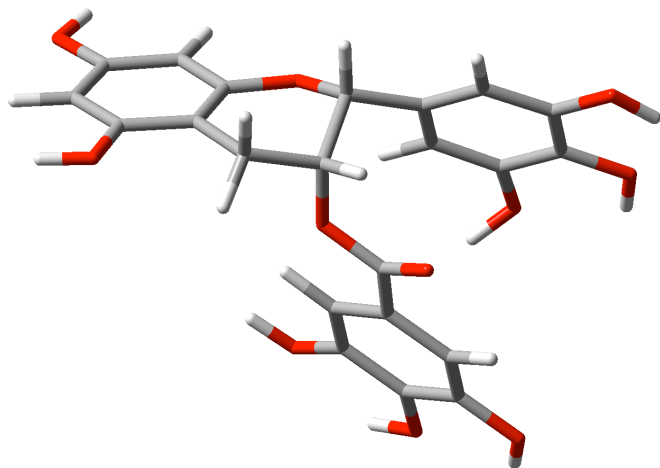
Number of imaginary frequency = 0

Gibbs energy = -1106.291704 a.u.

C	3.77864400	-0.91650600	0.91751500
C	2.89324400	0.05098800	1.36358300
C	1.87843400	0.56084700	0.54621000
C	1.78718100	0.05324500	-0.74436600
C	2.66455600	-0.91736300	-1.22439100
C	3.65779600	-1.39337500	-0.38521900
H	4.55931100	-1.30473700	1.56001400
H	2.55561900	-1.27609900	-2.24038200
O	0.84820700	0.48771400	-1.63682700
C	-0.21728300	1.32832400	-1.17677200
H	-0.51857600	1.87911400	-2.06871500
C	-1.39457900	0.52242800	-0.66522600
C	-1.32565400	-0.86020400	-0.53959200
C	-2.57303100	1.19038400	-0.34119900
C	-2.42849600	-1.56368100	-0.07340300
H	-0.42649800	-1.39804600	-0.80951000
C	-3.67090500	0.48088100	0.12094800
H	-2.66521600	2.26391500	-0.45072200
C	-3.59942500	-0.90012100	0.26003200
C	0.92970700	1.62433200	1.02812900
H	1.45506800	2.34960100	1.65025300
H	0.13709200	1.18874000	1.64419900
O	1.23801400	3.22077400	-0.78942400
C	0.31351300	2.34469800	-0.16169200
H	-0.51022400	2.97767600	0.16468600
H	2.01156800	2.70959400	-1.04959700
O	2.95932500	0.55795700	2.62203400
H	3.69781100	0.16249900	3.09704600
O	4.54986300	-2.33922000	-0.77794200
H	4.37321200	-2.59728000	-1.68861800
O	-4.81940900	1.13323300	0.43532900
H	-5.46831500	0.48070900	0.72838600
O	-4.70867100	-1.55035000	0.71927300
H	-4.52103700	-2.49624700	0.75692000
O	-2.46935500	-2.91682400	0.09072100
H	-1.62583200	-3.31496800	-0.14661400

4. Conformers in Figure 9.

Figure 9, EGCg B-ring(p-eq)/3-O(p-ax) conformer



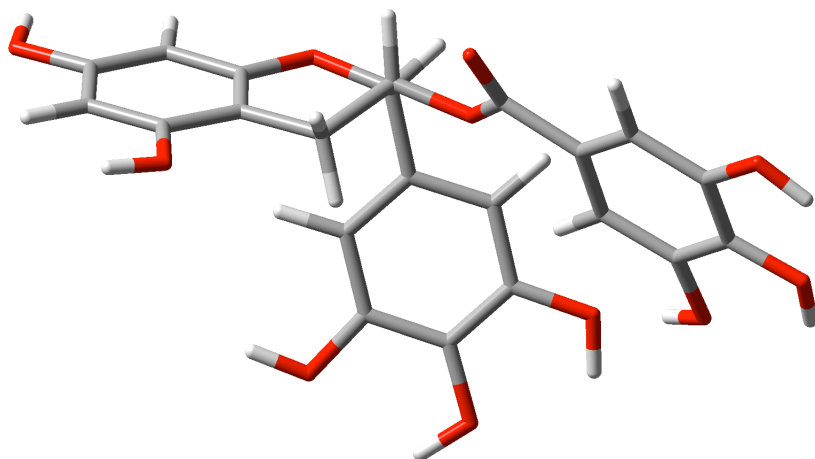
Number of imaginary frequency = 0

Gibbs energy = -1676.313553 a.u.

C	-5.42568500	0.95999700	0.07818200
C	-4.71196400	0.31816100	-0.92253100
C	-3.52263100	-0.37180100	-0.66391400
C	-3.07585700	-0.40346300	0.65267100
C	-3.76888500	0.23634600	1.68285400
C	-4.94069600	0.91354000	1.38470600
H	-6.34933200	1.48823200	-0.12617900
H	-3.38038400	0.17298300	2.69242700
O	-1.93128400	-1.03851300	1.02192300
C	-1.32434400	-1.92935800	0.09135200
H	-1.89964300	-2.86342000	0.05875100
C	0.08880000	-2.18511100	0.54340800
C	0.81116800	-1.14451400	1.11990600
C	0.71952000	-3.37655700	0.20105600
C	2.18236800	-1.27537900	1.27900300
H	0.31536000	-0.22238200	1.39495400
C	2.08610700	-3.51863300	0.40679400
H	0.17829600	-4.19777000	-0.25412700
C	2.82248900	-2.45622200	0.92916100
C	-2.74614400	-1.02389000	-1.77574400
H	-2.71908400	-0.37285500	-2.65135300
H	-3.22576700	-1.95698300	-2.08851000
O	-0.60868800	-0.08405500	-1.25847600
C	0.69605500	-0.10420100	-1.61261200
O	1.20650500	-0.97874700	-2.25369200
C	1.42586100	1.08714200	-1.08987100

C	0.76864600	2.06686200	-0.34159900
C	2.79880400	1.14366200	-1.30607000
C	1.50944200	3.11628700	0.17859600
H	-0.29972900	1.99753500	-0.17240100
C	3.53382000	2.19595300	-0.77377300
H	3.29383000	0.36595600	-1.87283900
C	2.88647800	3.18225200	-0.02917200
C	-1.32910200	-1.32149200	-1.32407700
H	-0.81715600	-1.99660500	-2.00979300
O	-5.12281200	0.32325900	-2.21946900
H	-5.93325400	0.83367900	-2.29452600
O	-5.67330800	1.55505500	2.33334700
H	-5.26432400	1.42015900	3.19207800
O	2.99512700	-0.27837400	1.75603200
H	2.63035000	0.57367400	1.49067500
O	4.16989100	-2.62239400	1.06284200
H	4.54360900	-1.77519900	1.33339900
O	2.71045200	-4.67239700	0.07131300
H	3.65292000	-4.55885100	0.24119900
O	4.86965400	2.26478400	-0.96851200
H	5.19687100	3.06640700	-0.54369400
O	3.64484000	4.19608300	0.46877700
H	3.06441700	4.81853600	0.92231800
O	0.99791600	4.14507200	0.91953200
H	0.04116700	4.07121500	0.96872800

Figure 9, EGCg B-ring(p-ax)/3-O(p-eq) conformer



Number of imaginary frequency = 0

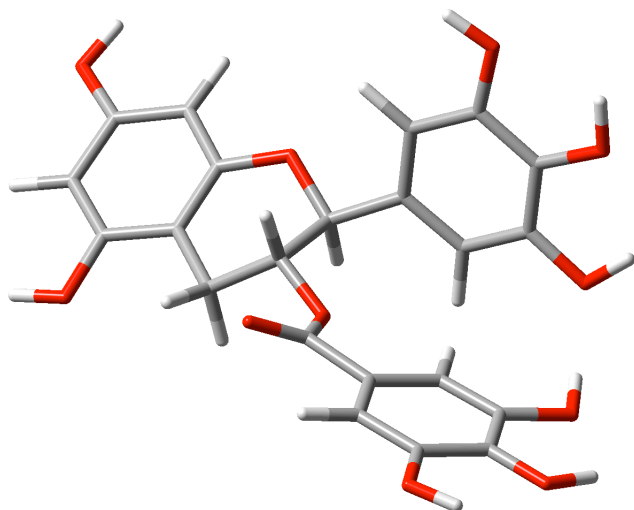
Gibbs energy = -1676.312734 a.u.

C	5.25369100	-1.60396400	1.11445800
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C	3.88092000	-1.70645300	1.28415900
C	2.97583400	-1.25356400	0.31643700
C	3.50712000	-0.68366200	-0.83573100
C	4.88379000	-0.56669700	-1.03783900
C	5.74685200	-1.03665400	-0.05985300
H	5.95042500	-1.95902400	1.86433100
H	5.24146400	-0.11811600	-1.95691900
O	2.72871300	-0.19502600	-1.84419800
C	1.32651300	-0.08497400	-1.63979500
H	0.89101200	-0.12636400	-2.63977100
C	0.93534600	1.23349700	-0.99717900
C	-0.36512300	1.69952300	-1.18252200
C	1.81778100	1.94375900	-0.18605800
C	-0.80937400	2.81382200	-0.48851000
H	-1.05639500	1.17210700	-1.82716200
C	1.37677900	3.08980000	0.46380100
H	2.84259600	1.61379800	-0.05473000
C	0.06065600	3.51766000	0.33540000
C	1.49066900	-1.39466400	0.50930800
H	1.10145900	-0.60139900	1.15784700
H	1.25610800	-2.35084100	0.97880300
O	-0.58728700	-1.07089800	-0.70221500
C	-1.40024600	-2.08746600	-0.33638800
O	-1.03637200	-3.22664300	-0.24458700
C	-2.77323100	-1.57098600	-0.09547100
C	-2.98125400	-0.19408100	-0.01238600
C	-3.83153700	-2.46571600	0.02637400
C	-4.26311500	0.29350800	0.15607200
H	-2.14814700	0.49086000	-0.05846600
C	-5.11620700	-1.96998200	0.21198900
H	-3.66536900	-3.53352000	-0.03157300
C	-5.33177200	-0.59168300	0.26683500
C	0.80751900	-1.29840800	-0.84312800
H	0.97962100	-2.20885800	-1.42362400
O	3.33085600	-2.24864300	2.40160600
H	4.02861300	-2.57988100	2.97300300
O	7.09761600	-0.96181400	-0.18377200
H	7.31633500	-0.58611700	-1.04050600
O	-6.16637200	-2.81882900	0.32305100
H	-6.96589200	-2.29180300	0.43508700
O	-6.61209700	-0.15729900	0.42931300
H	-6.60208400	0.80723000	0.41870500
O	-4.56988900	1.62020300	0.21974100
H	-3.79498500	2.13799500	-0.04696500

O	-2.11874900	3.21221500	-0.57744600
H	-2.19331200	4.06327700	-0.12584000
O	-0.42303000	4.61637800	0.98309100
H	0.29066400	4.99881200	1.50638700
O	2.15156200	3.86868300	1.27851500
H	3.01862700	3.46955200	1.38677000

Figure 9, *ent*-GCg B-ring(p-eq)/3-*O*(p-eq) conformer

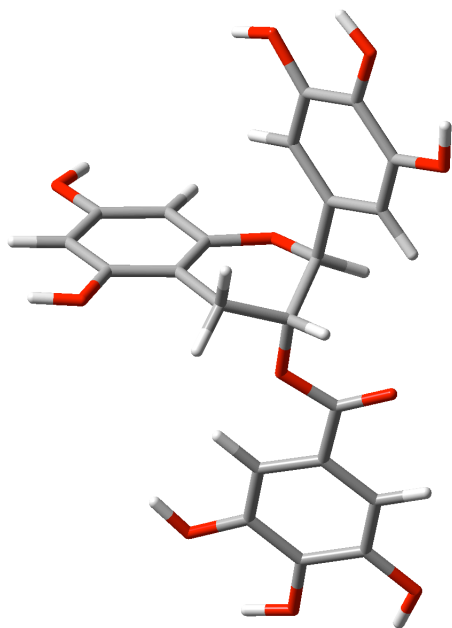


Number of imaginary frequency = 0
Gibbs energy = -1676.313752 a.u.

C	-6.08178500	-1.41691900	-0.16155200
C	-4.80049100	-1.93612900	-0.26562200
C	-3.66281000	-1.11993500	-0.24183300
C	-3.86821100	0.25079200	-0.12266700
C	-5.14343700	0.80540300	-0.01352200
C	-6.24322100	-0.03845000	-0.02957600
H	-6.95880200	-2.05285300	-0.17960100
H	-5.24312000	1.88090900	0.07044200
O	-2.82764800	1.13743400	-0.09017800
C	-1.58785400	0.65814900	-0.59371100
H	-1.68378000	0.47418700	-1.67192200
C	-0.52392500	1.69289800	-0.34502800
C	-0.54467500	2.46102300	0.81682100
C	0.54936000	1.77989300	-1.22435900
C	0.52389800	3.30148400	1.09529500
H	-1.39500200	2.40558900	1.48749600
C	1.63845300	2.57767400	-0.90603100
H	0.57215700	1.19427200	-2.13567700
C	1.62748900	3.34792900	0.24899100

C	-2.28153400	-1.72237600	-0.29933200
H	-2.04897300	-2.07086300	-1.31161500
H	-2.21176100	-2.58558100	0.36384000
O	0.05898600	-1.02333200	-0.30359900
C	0.77223500	-1.81510400	0.53198200
O	0.27009900	-2.43999800	1.42563500
C	2.22450100	-1.76164700	0.22678600
C	2.71832500	-0.77217500	-0.62148000
C	3.08257000	-2.64744300	0.87314900
C	4.08342800	-0.65029900	-0.80432000
H	2.04374800	-0.09107300	-1.11440800
C	4.44978700	-2.54462600	0.65583100
H	2.69557600	-3.40224400	1.54497500
C	4.94912700	-1.54092600	-0.17637900
C	-1.26061800	-0.67311600	0.10134000
H	-1.27408600	-0.51398400	1.18435500
O	-4.56844800	-3.26890700	-0.39059300
H	-5.40330600	-3.74323900	-0.35775900
O	-7.51763900	0.42228700	0.06941700
H	-7.50232000	1.37910400	0.15315300
O	2.75375900	2.57915900	-1.70275100
H	3.33745000	3.27981900	-1.38239300
O	2.71655500	4.12819700	0.50355300
H	2.57423400	4.58601300	1.33997700
O	0.61506000	4.11320200	2.19148900
H	-0.13576200	3.96666300	2.77232000
O	5.30626400	-3.39973300	1.26544600
H	6.20293300	-3.16093100	1.00390600
O	6.29948000	-1.46187000	-0.33259200
H	6.48777400	-0.71014400	-0.90706000
O	4.66932500	0.30852300	-1.57769300
H	4.01301300	0.98805200	-1.79379400

Figure 9, *ent*-GCg B-ring(p-ax)/3-*O*(p-ax) conformer



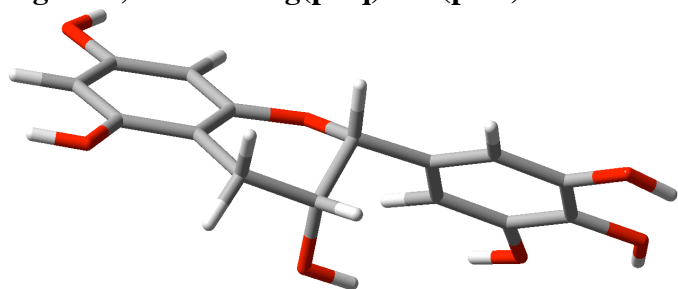
Number of imaginary frequency = 0

Gibbs energy = -1676.313864 a.u.

C	0.95065500	4.14250700	0.60172600
C	0.98112400	2.98263100	1.36262000
C	0.92891600	1.71047500	0.78364700
C	0.84794200	1.64260900	-0.60350900
C	0.81224500	2.79133300	-1.39820500
C	0.85894000	4.03372000	-0.78527800
H	0.99227500	5.12577900	1.05500600
H	0.74117800	2.68034200	-2.47386700
O	0.80321900	0.46408300	-1.28095700
C	1.03260700	-0.74620300	-0.56702500
H	0.53722500	-1.51552700	-1.16026000
C	2.50587800	-1.07603500	-0.44850900
C	3.48519700	-0.13772200	-0.76179100
C	2.86288500	-2.34561200	0.00129700
C	4.82323400	-0.47891400	-0.60649100
H	3.21677900	0.84470500	-1.13308600
C	4.20369100	-2.67734900	0.15013700
H	2.11369800	-3.09768200	0.22281400
C	5.18714800	-1.73767300	-0.14995500
C	0.92643900	0.46435400	1.62595000
H	0.31454700	0.61152700	2.51720200
H	1.93854900	0.21542900	1.95980600
O	-1.02922000	-0.46410500	0.66183300
C	-1.77762400	-1.52429500	0.30346300

O	-1.32376600	-2.62750000	0.14481800
C	-3.20964400	-1.16514800	0.13768400
C	-4.10118500	-2.18901400	-0.16701600
C	-3.63996500	0.15587700	0.27528100
C	-5.44678800	-1.89559200	-0.33400100
H	-3.74996200	-3.20677600	-0.27370200
C	-4.98403700	0.43690900	0.10294400
H	-2.93003200	0.94055600	0.50704000
C	-5.88632200	-0.57965200	-0.19840500
C	0.37700300	-0.69477000	0.81789900
H	0.52812900	-1.64951300	1.32100200
O	1.06285200	3.01416700	2.72037400
H	1.08095900	3.92793800	3.01629600
O	0.82578000	5.19574800	-1.49057500
H	0.74968000	4.99389800	-2.42673300
O	4.55823600	-3.90985600	0.58256500
H	5.52143200	-3.95087800	0.60714300
O	6.49154000	-2.11063600	0.01238000
H	7.05070400	-1.36898100	-0.24428300
O	5.87192800	0.35713200	-0.88139200
H	5.54004100	1.21368000	-1.16148700
O	-6.33181500	-2.87631000	-0.62846600
H	-7.20645600	-2.47811900	-0.70643400
O	-7.21406900	-0.33699200	-0.37303400
H	-7.36835200	0.60743600	-0.25468800
O	-5.54426100	1.68179800	0.20433200
H	-4.86383800	2.33133800	0.39843000

Figure 9, EGC B-ring(p-eq)/3-O(p-ax) conformer



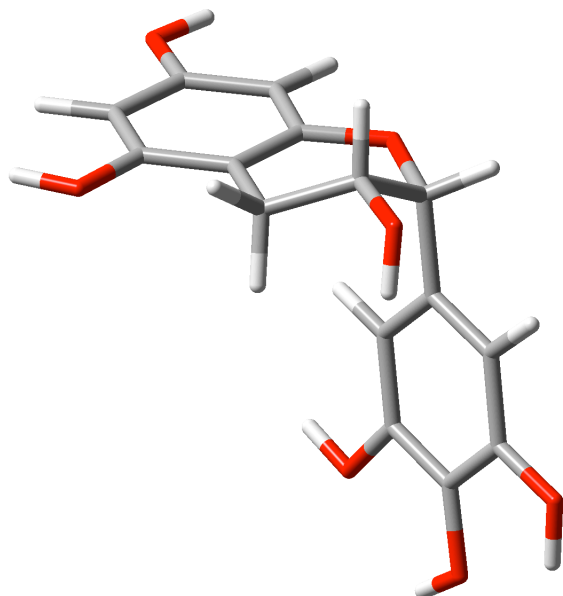
Number of imaginary frequency = 0

Gibbs energy = -1106.335715 a.u.

C	4.76352100	0.29397100	-0.07650100
C	3.97440400	-0.82398600	0.14866200
C	2.58042100	-0.78706500	0.04031600
C	2.00286800	0.42670200	-0.31331700

C	2.76704000	1.57187800	-0.54385800
C	4.14493100	1.49527700	-0.41854700
H	5.84320300	0.25870600	0.00744200
H	2.26478500	2.49013500	-0.82421100
O	0.65589700	0.57847700	-0.45138800
C	-0.12451800	-0.60589300	-0.54212700
H	0.03820600	-1.06817300	-1.52469300
C	-1.57346400	-0.21642800	-0.39557100
C	-2.55888900	-1.03727900	-0.93610500
C	-1.92385900	0.90576500	0.35491200
C	-3.90083800	-0.73558600	-0.73687000
H	-2.30825300	-1.91009500	-1.52763400
C	-3.26840100	1.20339600	0.54151000
H	-1.14903000	1.55239300	0.75057900
C	-4.25605500	0.38770900	0.00601400
C	1.74786300	-2.00461700	0.34066300
H	2.11088000	-2.49039700	1.24823300
H	1.82773600	-2.73573500	-0.47005300
O	0.17903500	-1.04112100	1.82550700
C	0.29358100	-1.61457600	0.54217900
H	-0.35115200	-2.49735300	0.44542300
H	-0.72467400	-0.72572700	1.93052600
O	4.51077300	-2.02692000	0.49231300
H	5.46316900	-1.93543400	0.57797700
O	4.95730900	2.56569200	-0.62982700
H	4.41907000	3.32826500	-0.85637100
O	-4.86287700	-1.52498400	-1.26842000
H	-5.71972000	-1.14691300	-1.03790600
O	-5.58750600	0.64692700	0.16451200
H	-5.67848800	1.46241800	0.66993900
O	-3.73404300	2.28265100	1.24181600
H	-2.99605300	2.81653000	1.54647500

Figure 9, EGC B-ring(p-ax)/3-O(p-eq) conformer



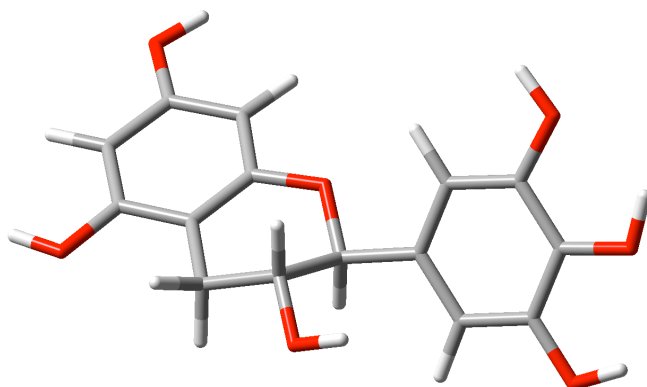
Number of imaginary frequency = 0

Gibbs energy = -1106.334921 a.u.

C	-3.88893400	-0.72038300	0.78865200
C	-2.93704800	0.16431900	1.27425300
C	-1.90895200	0.66852900	0.46953500
C	-1.86608200	0.23995400	-0.85419500
C	-2.80960800	-0.64963500	-1.37353100
C	-3.81946400	-1.11640300	-0.54625700
H	-4.68649200	-1.10307500	1.41420100
H	-2.73010000	-0.94796800	-2.41215600
O	-0.90258800	0.64151900	-1.72914000
C	0.21379200	1.37363900	-1.22696800
H	0.58838800	1.93805400	-2.08236000
C	1.31414500	0.45936100	-0.72736500
C	1.04726800	-0.85191700	-0.33517500
C	2.61342400	0.96103800	-0.64084900
C	2.08006800	-1.64039100	0.15471000
H	0.05059200	-1.26923700	-0.42077000
C	3.64050000	0.16321100	-0.14731000
H	2.85259400	1.96300100	-0.97685400
C	3.37131500	-1.14010300	0.25832300
C	-0.90343000	1.65252300	1.00260200
H	-0.13071200	1.13429000	1.58614300
H	-1.38557500	2.36705200	1.67157200
O	0.80204500	3.22503900	0.24862700
C	-0.25038300	2.38436600	-0.15783700
H	-0.98756400	3.03376600	-0.63751600

H	1.43167200	2.69014100	0.74412700
O	-2.94691000	0.59472300	2.56415000
H	-3.70858100	0.22324700	3.01674200
O	-4.77510600	-1.97992600	-0.97998400
H	-4.64284900	-2.15284000	-1.91569600
O	4.90110100	0.64991400	-0.06668400
H	5.46855000	-0.04917700	0.27892100
O	4.41200600	-1.88687000	0.73227900
H	4.07893500	-2.76494800	0.94861900
O	1.93525800	-2.93791700	0.56385300
H	1.01503100	-3.20280800	0.48871100

Figure 9, *ent*-GC B-ring(p-eq)/3-*O*(p-eq) conformer



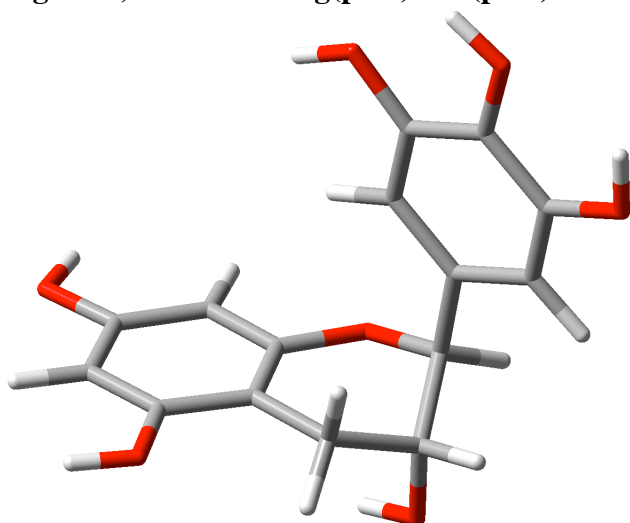
Number of imaginary frequency = 0

Gibbs energy = -1106.336453 a.u.

C	-4.80992100	0.33099500	-0.05640400
C	-4.00951200	-0.77344100	0.19425000
C	-2.61234300	-0.70924600	0.13840200
C	-2.04708200	0.51652500	-0.19763000
C	-2.82330600	1.64765300	-0.45449600
C	-4.20323600	1.54428800	-0.37745100
H	-5.89105600	0.27553900	-0.01090200
H	-2.32884700	2.57447700	-0.71976300
O	-0.69655300	0.69036600	-0.28037900
C	0.08655700	-0.49270400	-0.40631600
H	-0.10453900	-0.95105800	-1.38545300
C	1.53839200	-0.10897800	-0.29373000
C	1.91277200	0.99884400	0.46536000
C	2.50763900	-0.91467400	-0.88786600
C	3.26025200	1.29669100	0.61156200
H	1.15403200	1.63193400	0.91032700
C	3.85630600	-0.61138900	-0.72852700

H	2.23530000	-1.77092700	-1.49322900
C	4.23277100	0.49602500	0.02524200
C	-1.76651100	-1.91310100	0.45824400
H	-1.78664100	-2.63759900	-0.36283500
H	-2.15438500	-2.42676600	1.33978500
O	0.46332800	-2.66508000	0.63229200
C	-0.32437300	-1.49966400	0.68309000
H	-0.22325200	-0.98580800	1.65018800
H	1.37608900	-2.42222800	0.81785800
O	-4.53469500	-1.98525100	0.51849900
H	-5.49256500	-1.91822400	0.54865400
O	-5.02833400	2.59833100	-0.61555300
H	-4.49888700	3.36973600	-0.83300200
O	4.80128700	-1.38675800	-1.30975000
H	5.66464500	-1.01039400	-1.10203600
O	5.56777000	0.75834500	0.14499300
H	5.67186000	1.56191400	0.66669100
O	3.74816300	2.36292800	1.31738600
H	3.02007500	2.87941900	1.67144800

Figure 9, *ent*-GC B-ring(p-ax)/3-*O*(p-ax) conformer



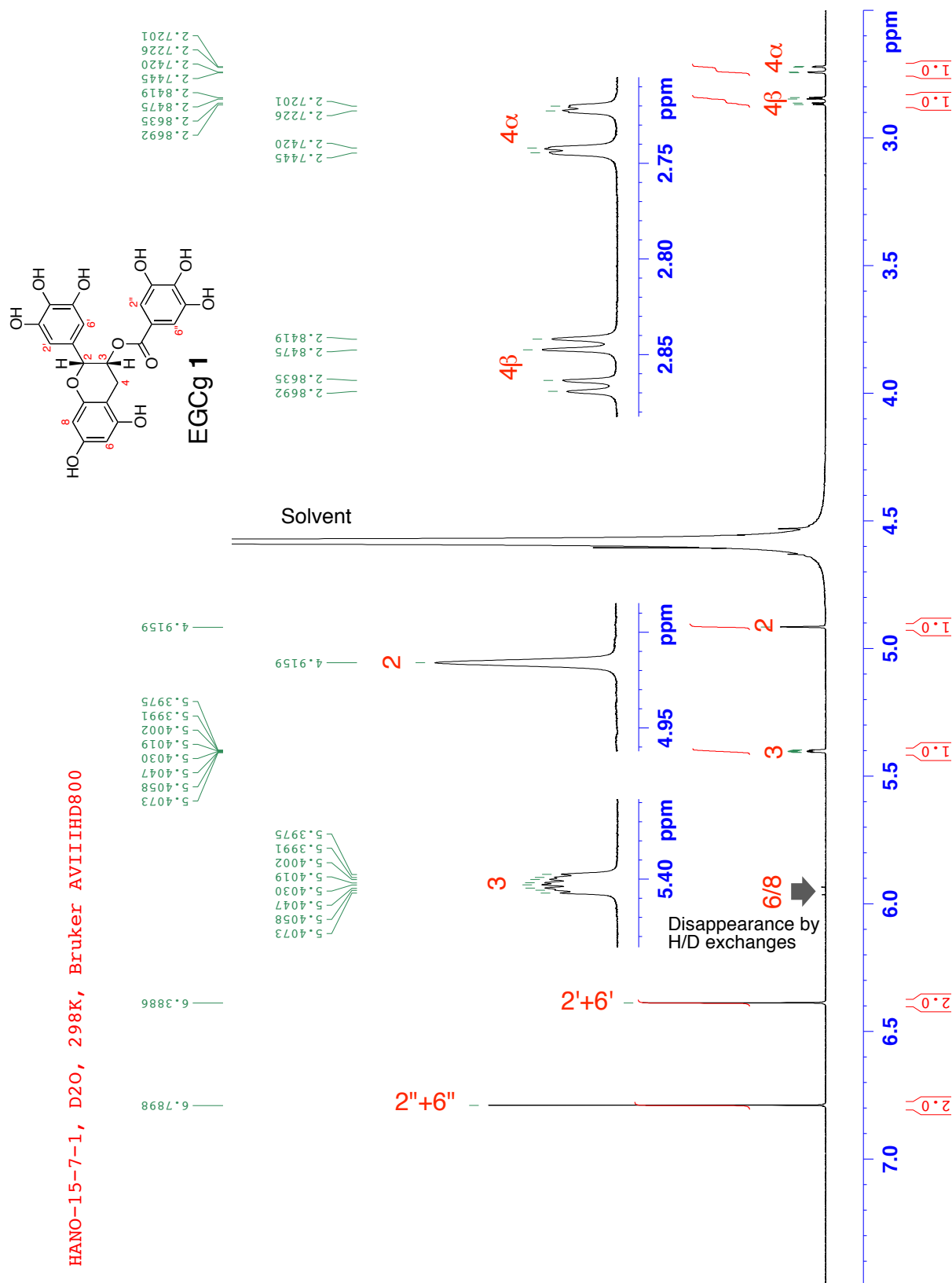
Number of imaginary frequency = 0

Gibbs energy = -1106.336704 a.u.

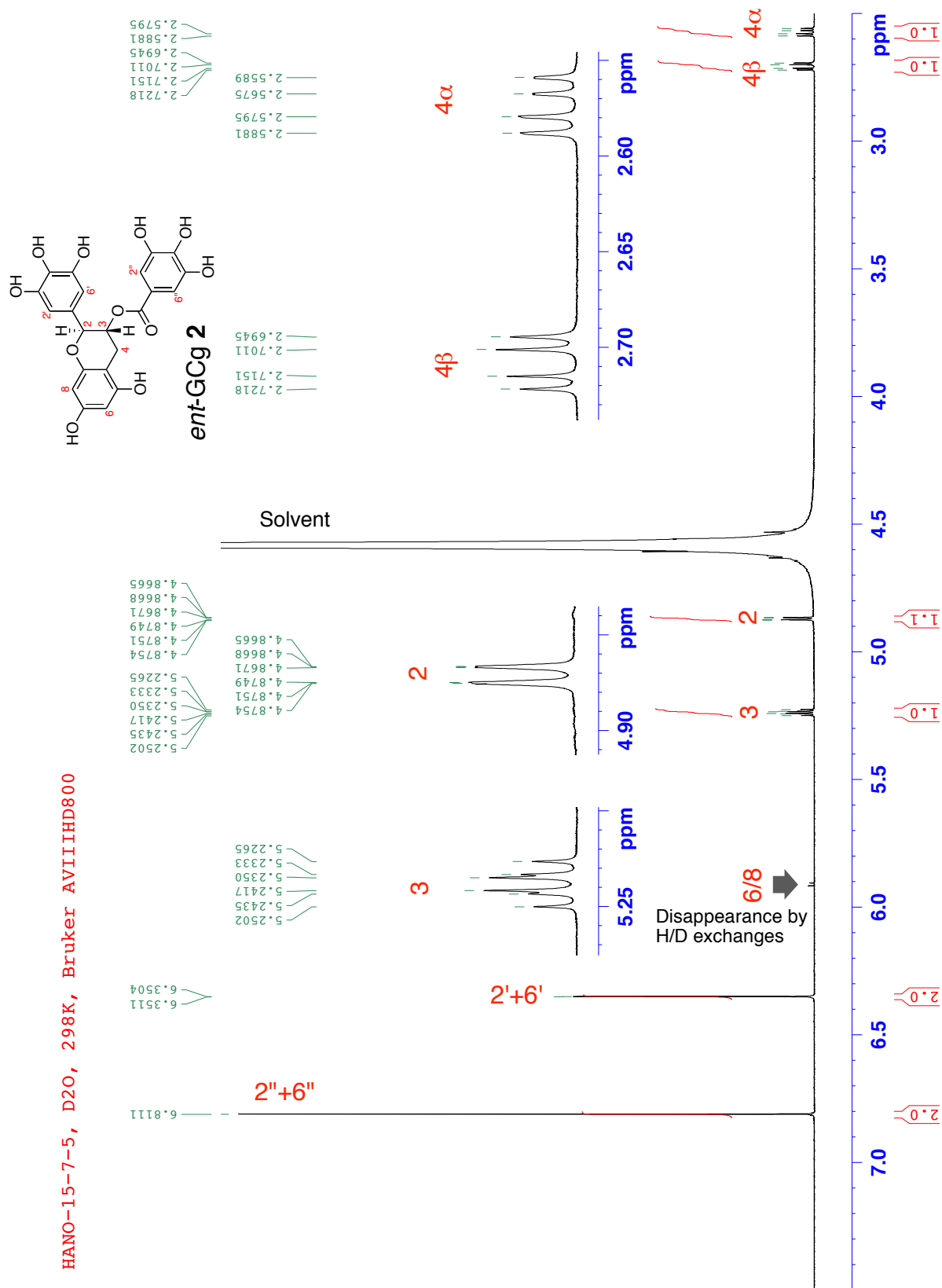
C	3.65232700	-1.00426900	0.91122500
C	2.75267100	-0.06775800	1.39820600
C	1.79050100	0.53781100	0.57987100
C	1.76653800	0.15814700	-0.75905100
C	2.66162800	-0.77873700	-1.28210700
C	3.60271600	-1.34900200	-0.43902500

H	4.39526000	-1.46865600	1.54873400
H	2.60194900	-1.02865900	-2.33493100
O	0.88064100	0.68262000	-1.65409500
C	-0.21156700	1.45422400	-1.14893200
H	-0.52219200	2.06356800	-1.99945300
C	-1.36071700	0.58062200	-0.69197200
C	-1.22716800	-0.80188600	-0.59514100
C	-2.56618800	1.19179400	-0.35127700
C	-2.30042200	-1.55905000	-0.14120900
H	-0.30351200	-1.29330600	-0.87789400
C	-3.63536900	0.42623400	0.09596500
H	-2.70556300	2.26303700	-0.43836800
C	-3.49972600	-0.95522400	0.20726700
C	0.83406300	1.57059900	1.11657000
H	1.34815500	2.23091600	1.81656200
H	0.01229400	1.08885900	1.65620500
O	1.24761100	3.28639100	-0.56456300
C	0.28516600	2.39512400	-0.04233300
H	-0.54685800	3.01463600	0.29360100
H	2.00509900	2.76674800	-0.85298200
O	2.75004300	0.31786800	2.70106500
H	3.46148900	-0.12920900	3.16694200
O	4.50793600	-2.26586600	-0.87068800
H	4.39745400	-2.39899700	-1.81567900
O	-4.80800800	1.01824600	0.42406500
H	-5.42129800	0.32838200	0.70344700
O	-4.57764400	-1.66534100	0.65533000
H	-4.33363700	-2.59720100	0.68205900
O	-2.28211400	-2.92098700	-0.00344500
H	-1.40306800	-3.25533900	-0.19794700

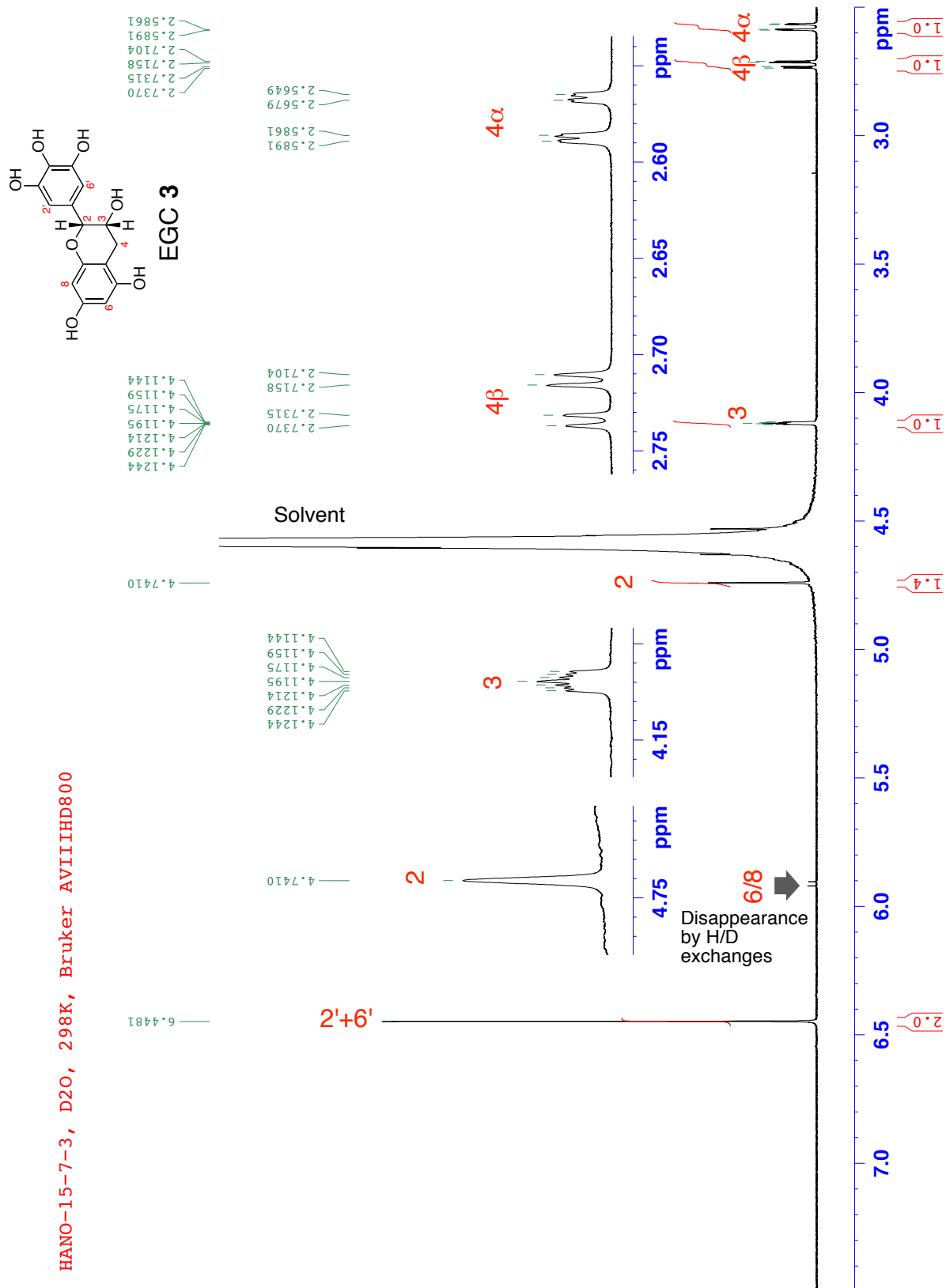
HANO-15-7-1, D2O, 298K, Bruker AVIIIHD800



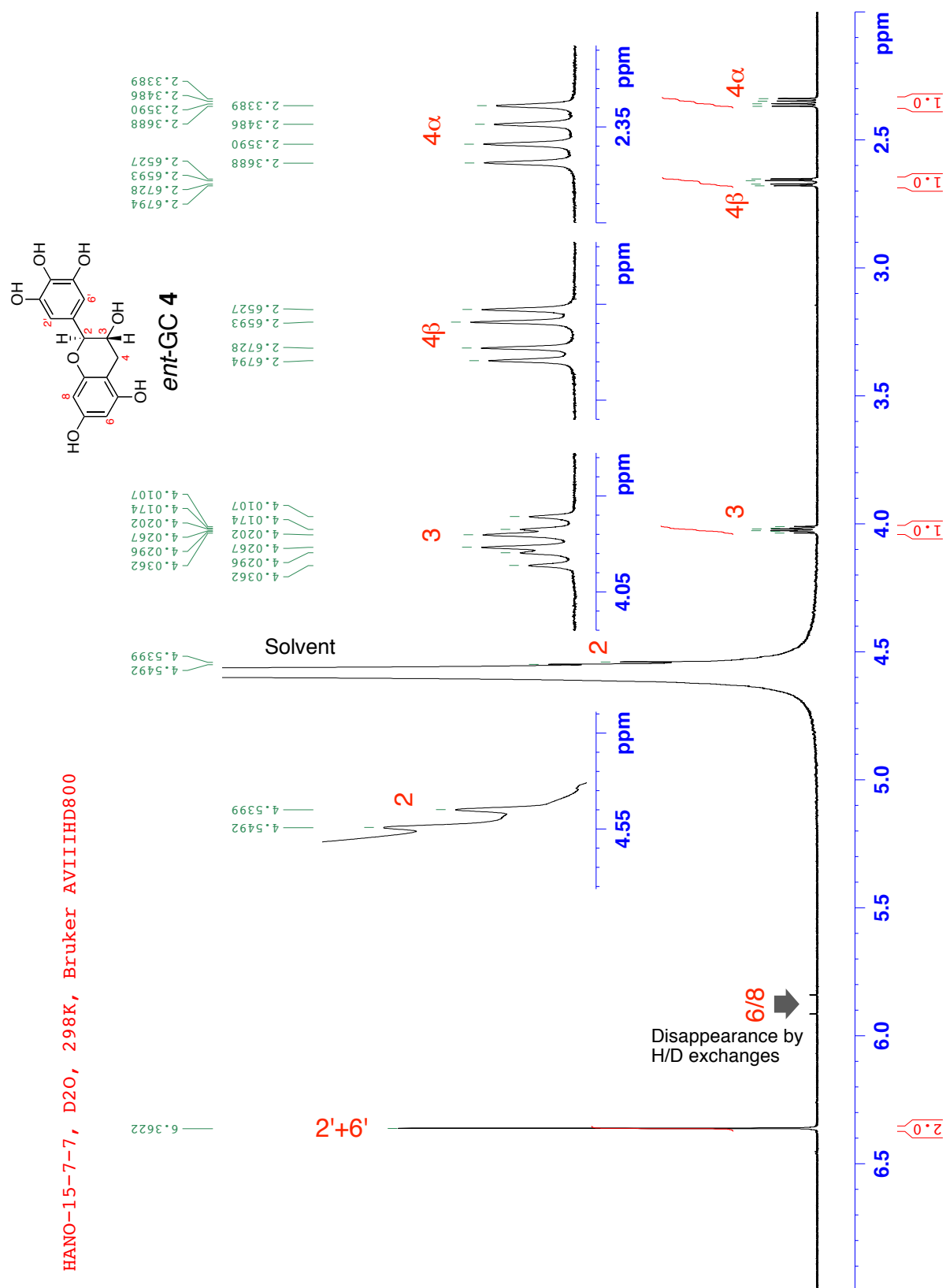
HANO-15-7-5, D2O, 298K, Bruker AVIIIHD800



HANO-15-7-3, D2O, 298K, Bruker AVIIIHD800

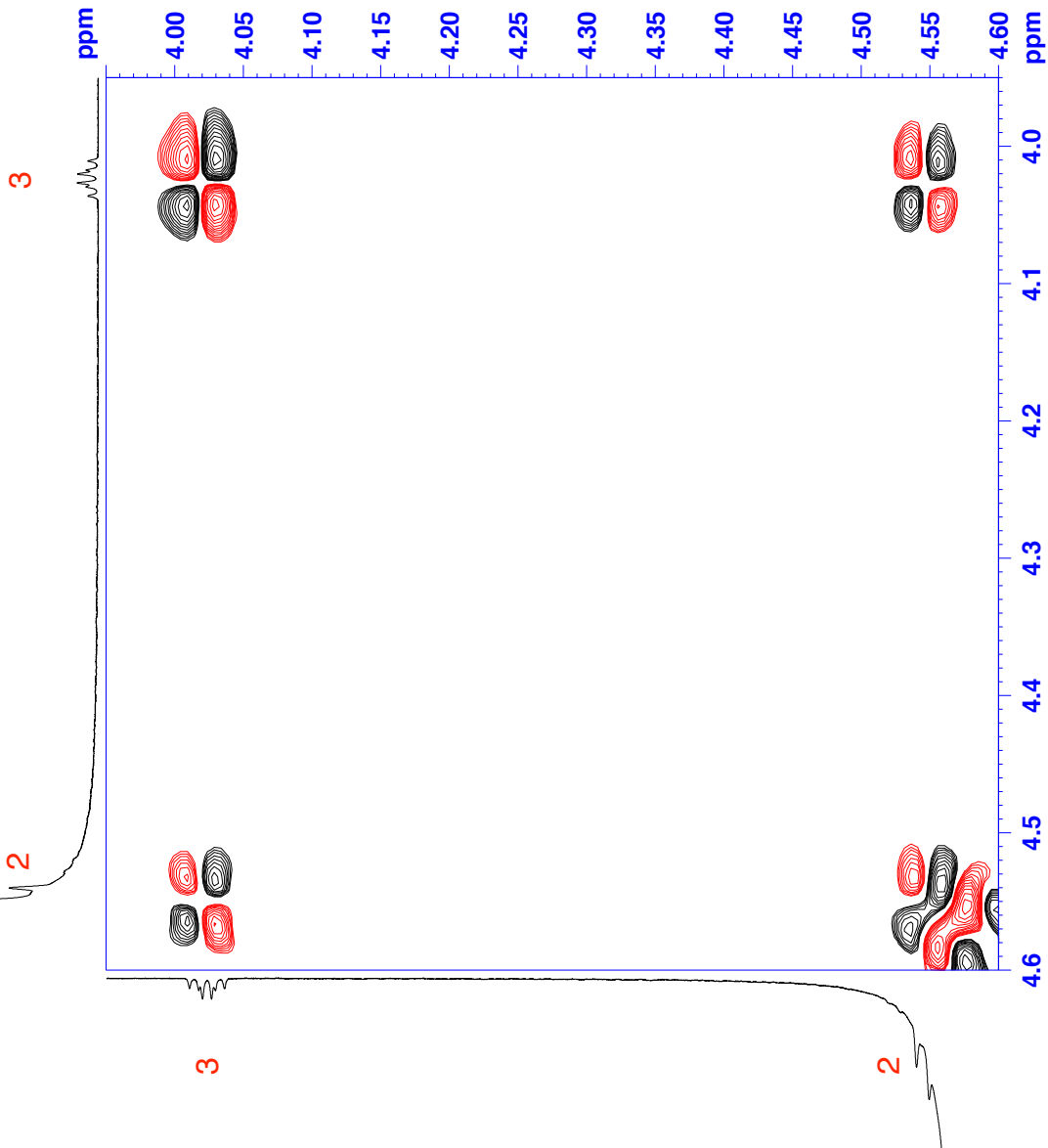
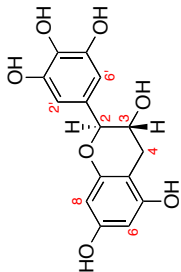


HANO-15-7-7, D2O, 298K, Bruker AVIIIHD800

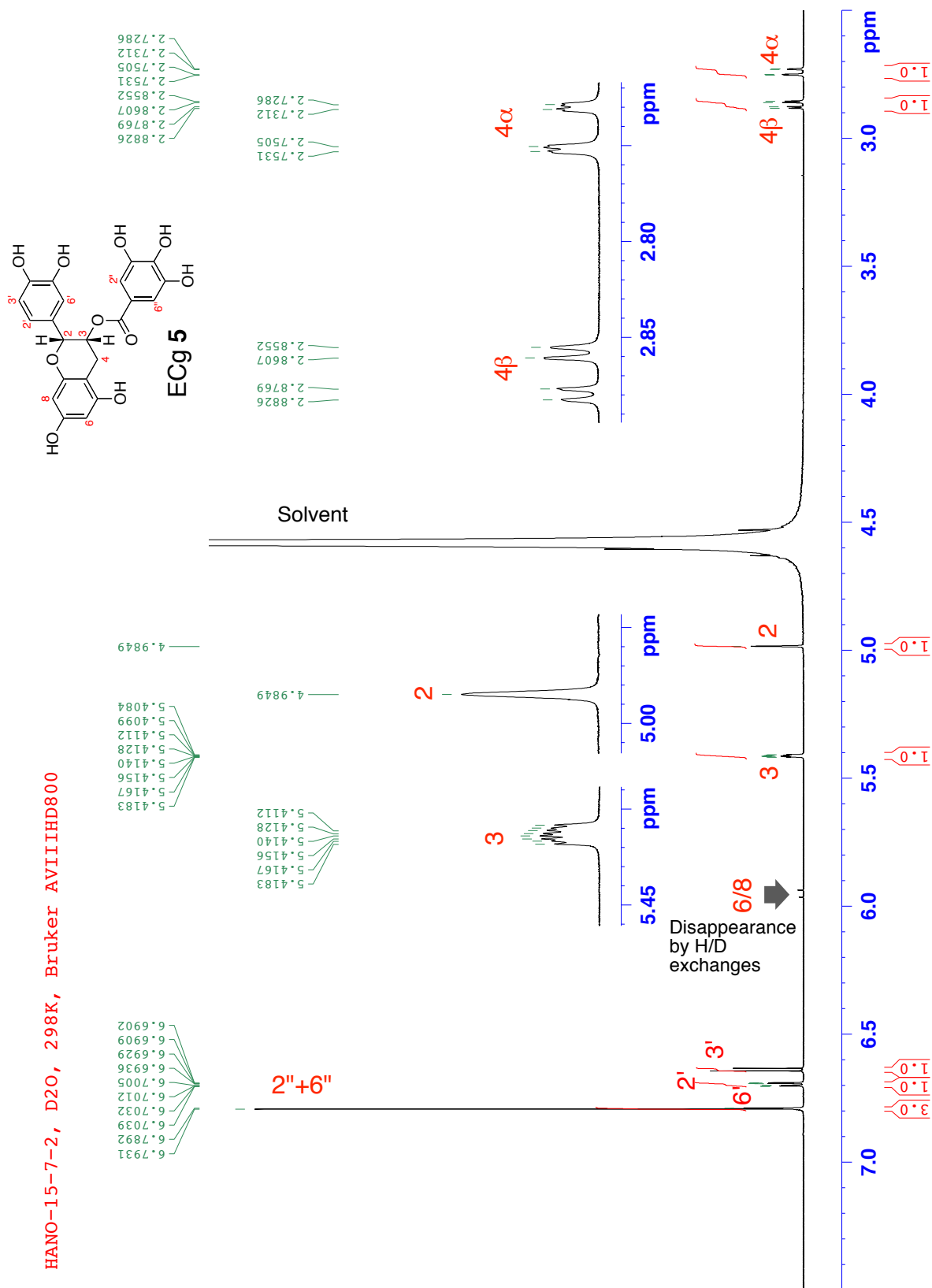


HANO-15-7-7, D20, 298K, Bruker AVIIIHD800

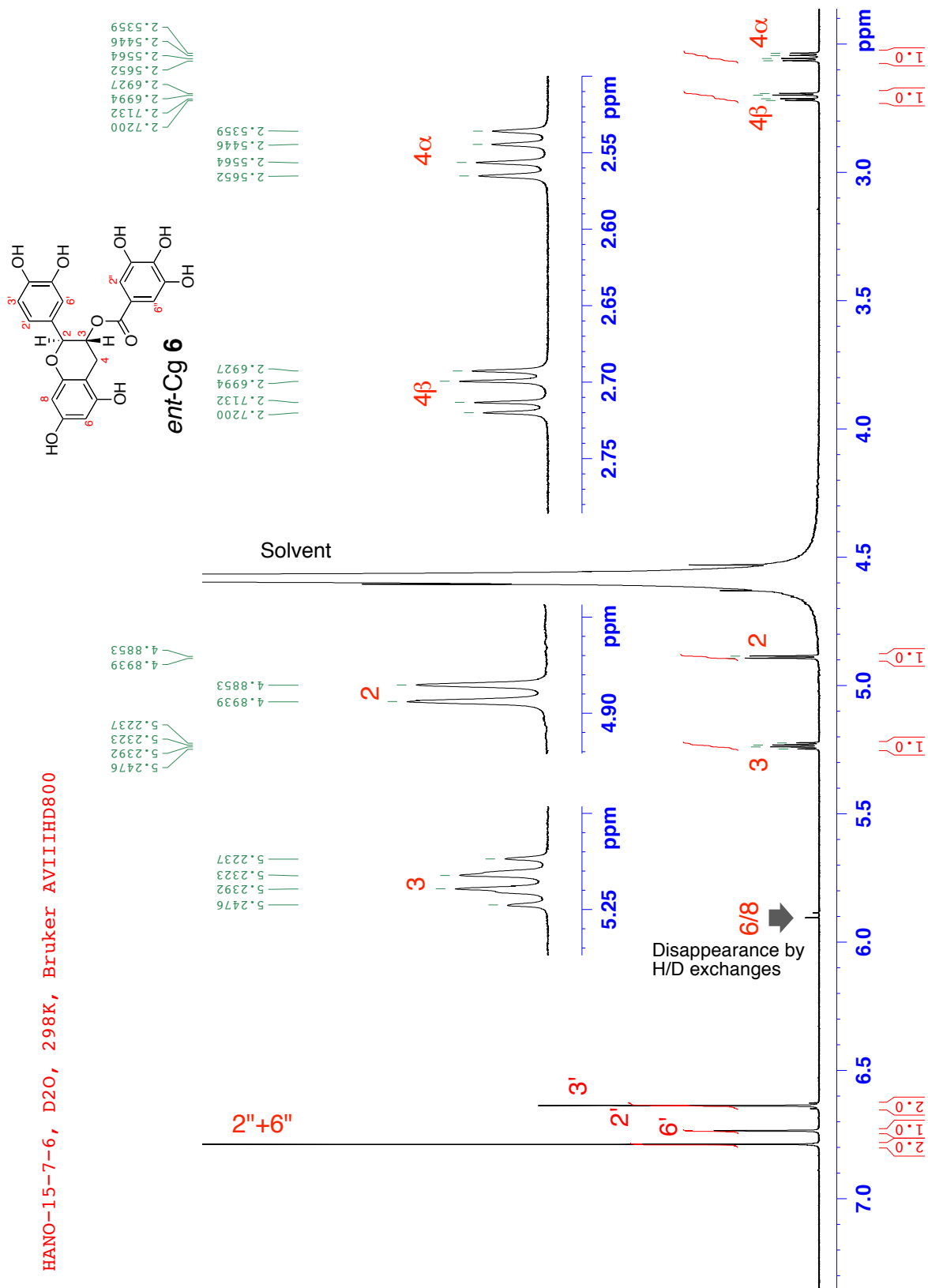
dqfCOSY



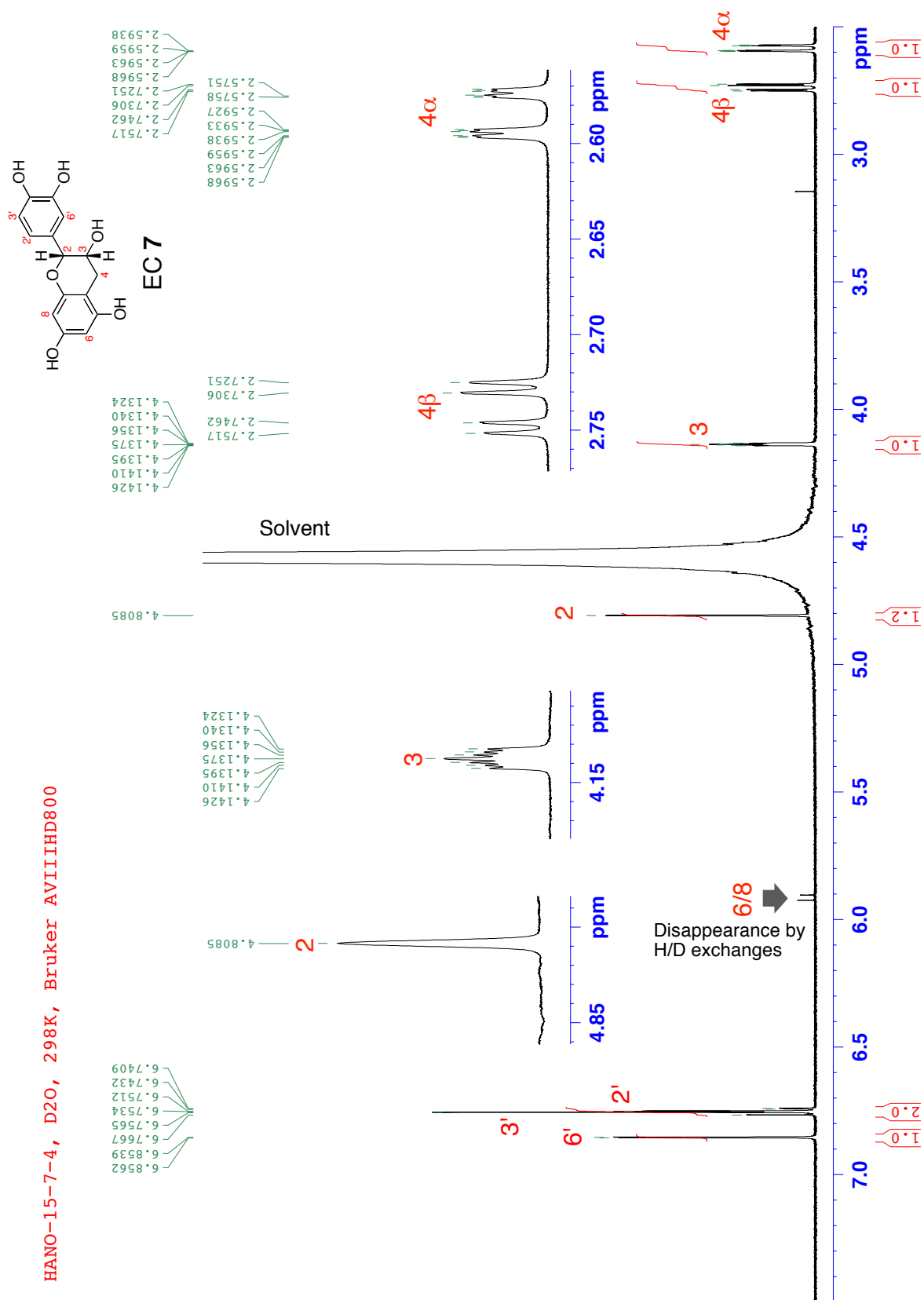
HANO-15-7-2, D2O, 298K, Bruker AVIIIHD800



HANO-15-7-6, D2O, 298K, Bruker AVIIHD800



HANO-15-7-4, D2O, 298K, Bruker AVIIIHD800



HANO-15-7-8, D2O, 298K, Bruker AVIIIHD800

