Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Solution-state conformations of natural products from chiroptical spectroscopy: the case of isocorilagin

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Supplementary Information

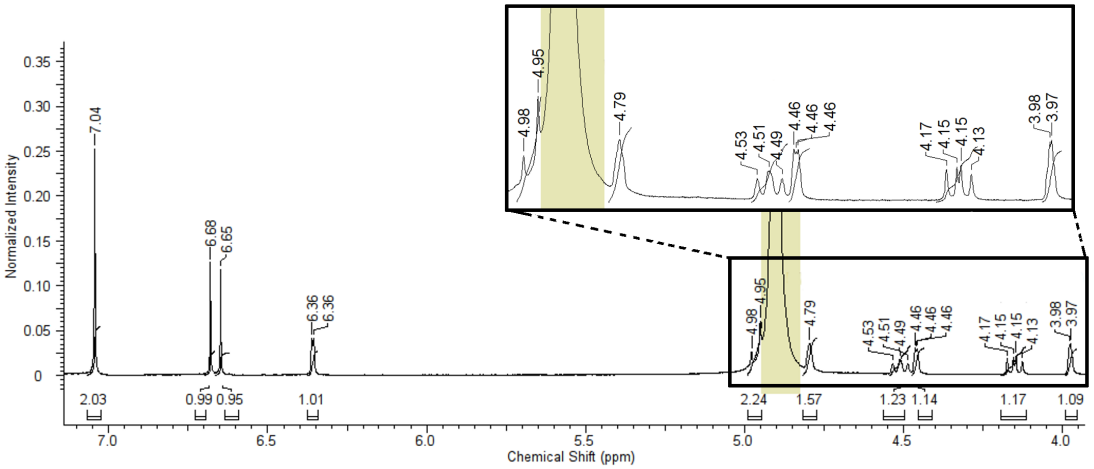

Figure S1. ^{1}H NMR (400 MHz) spectrum of corilagin in methanol-d_4 (20^{o}C).

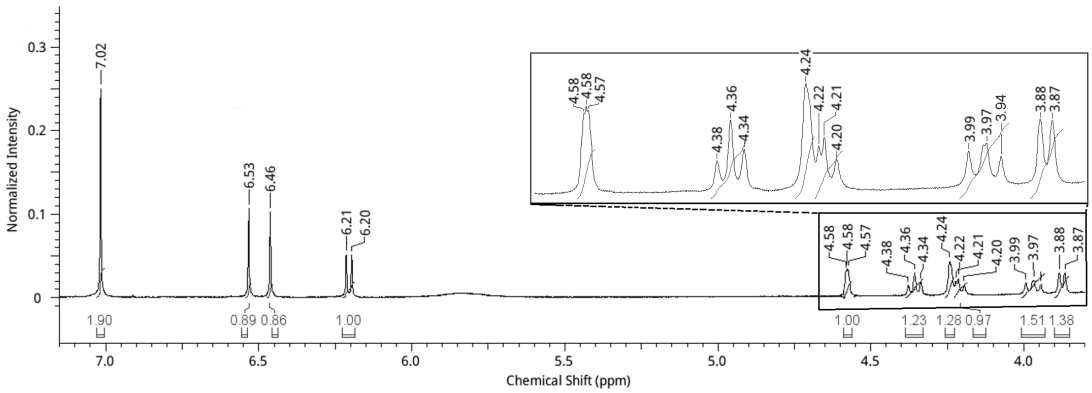

Figure S2. ^{1}H NMR (400 MHz) spectrum of corilagin in DMSO-d_6 (20^{o}C).

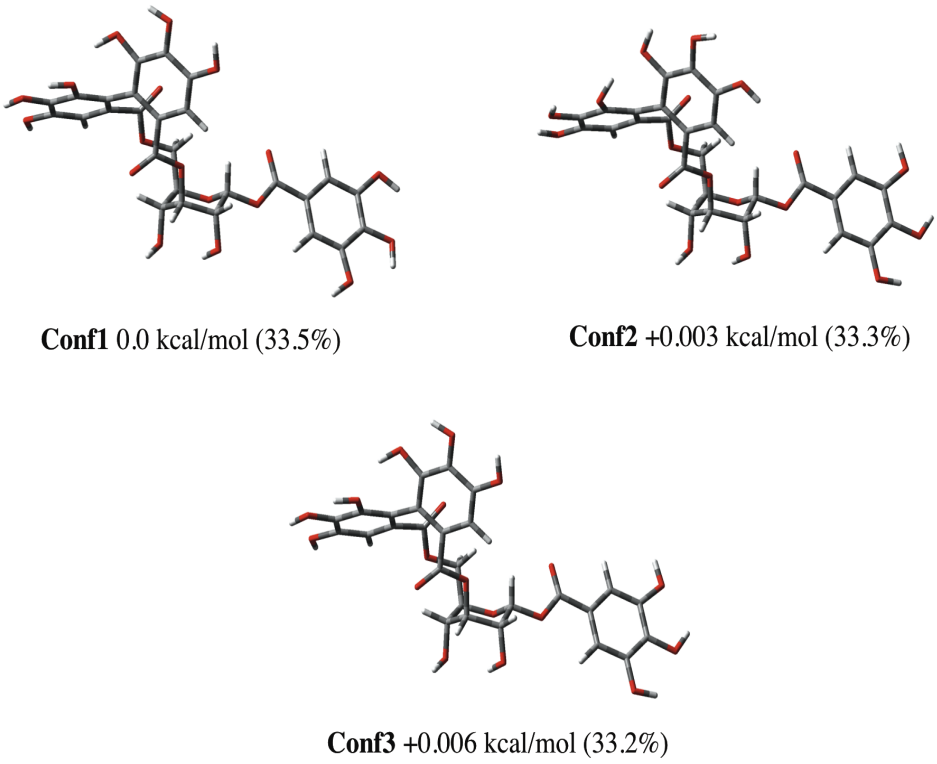

Figure S3. Optimized structures and relative energies of the three lowest-energy conformers of α-configured corilagin at the CAM-B3LYP/PCM(MeOH)/TZVP level.

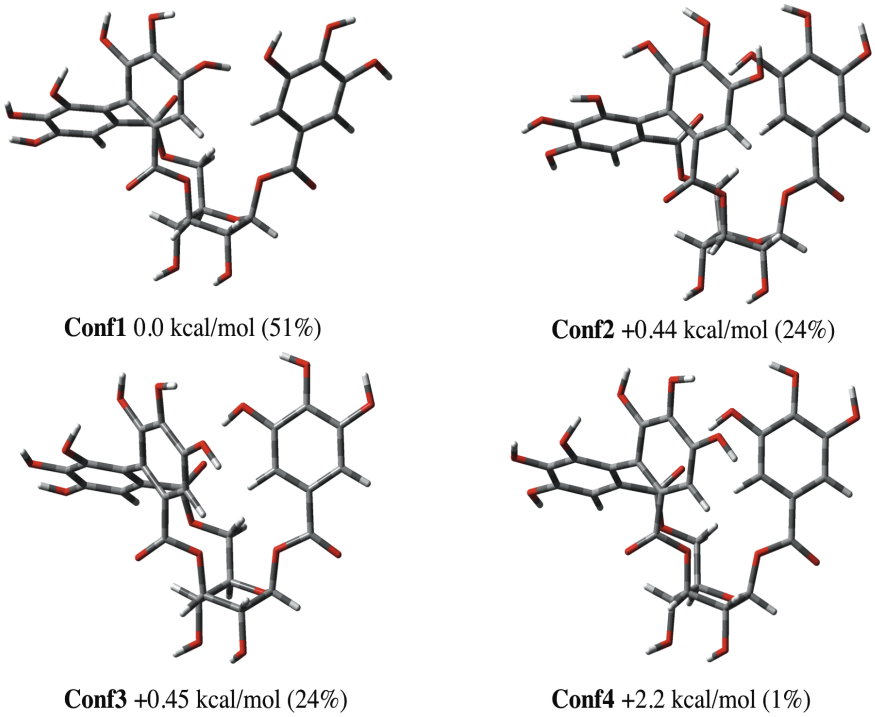

Figure S4. Optimized structures and relative energies of the four lowest-energy conformers of β-configured corilagin at the CAM-B3LYP/PCM(MeOH)/TZVP level.

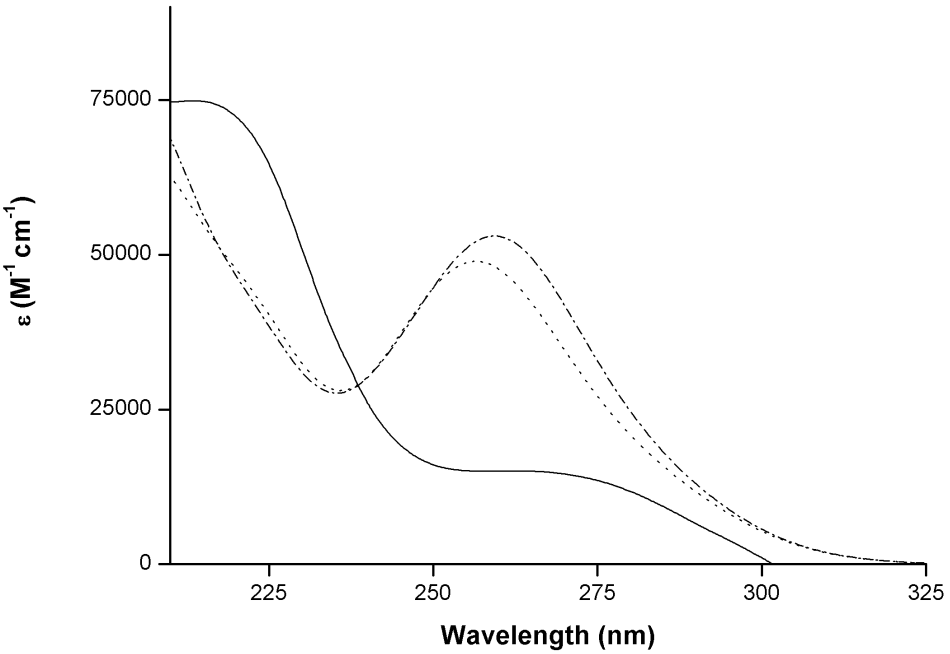

Figure S5. Experimental UV spectrum of corilagin in MeOH (solid line) and calculated [CAM-B3LYP/PCM(MeOH)/TZVP//B3LYP/PCM(MeOH)/6-31G(d)] UV spectra for the β-anomer (dotted line) and α-anomer (dash-dotted line) of corilagin.

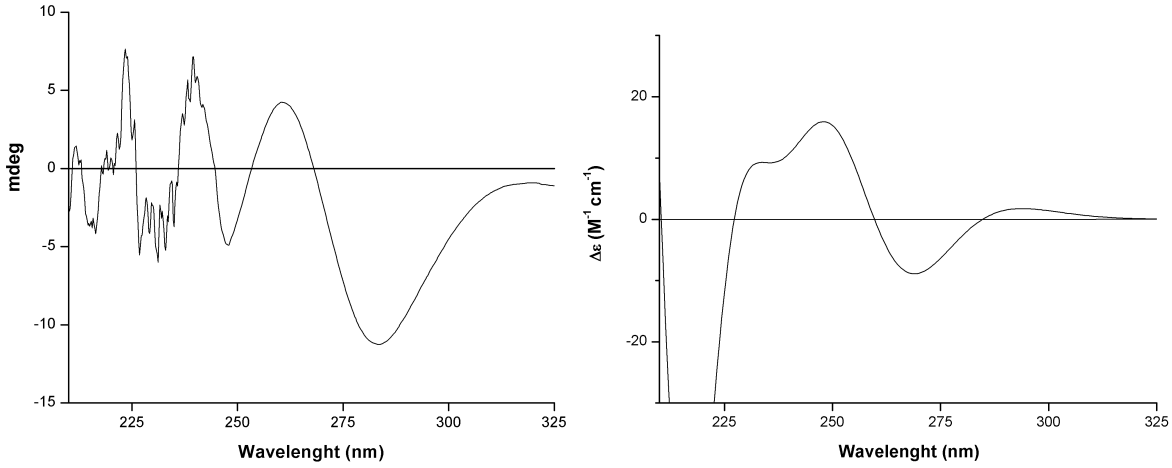

Figure S6. (Left) Experimental ECD spectrum of corilagin in DMSO. (Right) Calculated [CAM-B3LYP/PCM(DMSO)/TZVP//B3LYP/PCM(DMSO)/6-311G(d,p)] ECD spectra of the Boltzmann average of the lowest-energy conformers identified for β-configured corilagin.

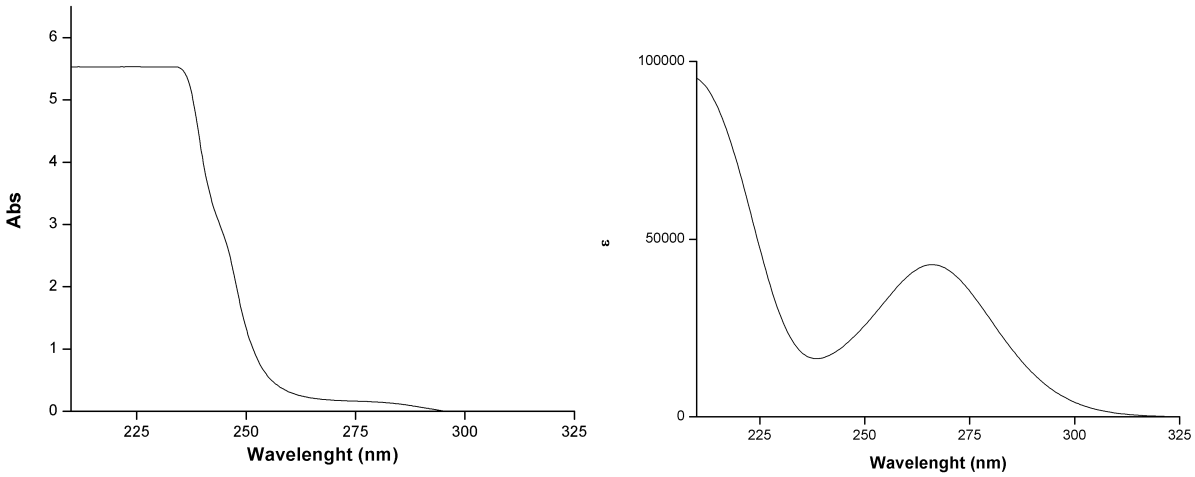

Figure S7. (Left) Experimental UV spectrum of corilagin in DMSO (Right) Calculated [CAM-B3LYP/PCM(DMSO)/TZVP//B3LYP/PCM(DMSO)/6-311G(d,p)] UV spectra of the Boltzmann average of the lowest-energy conformers identified for β-configured corilagin.

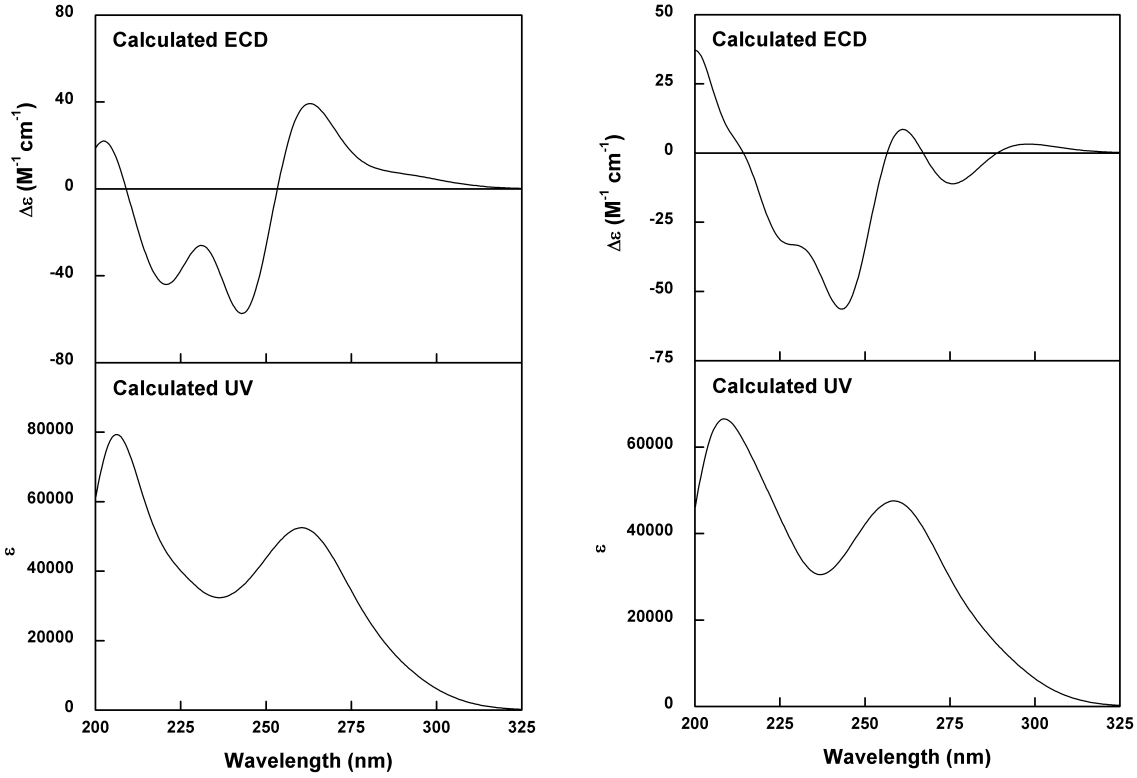

Figure S8. (Left) Calculated [wB97XD/PCM(MeOH)/TZVP// B3LYP/PCM(MeOH)/6-31G(d)] UV and ECD spectra of the Boltzmann average of the three lowest-energy conformers identified for α-configured corilagin. (Right) Calculated [wB97XD/PCM(MeOH)/TZVP// B3LYP/PCM(MeOH)/6-31G(d)] UV and ECD spectra of the Boltzmann average of the four lowest-energy conformers identified for β-configured corilagin.

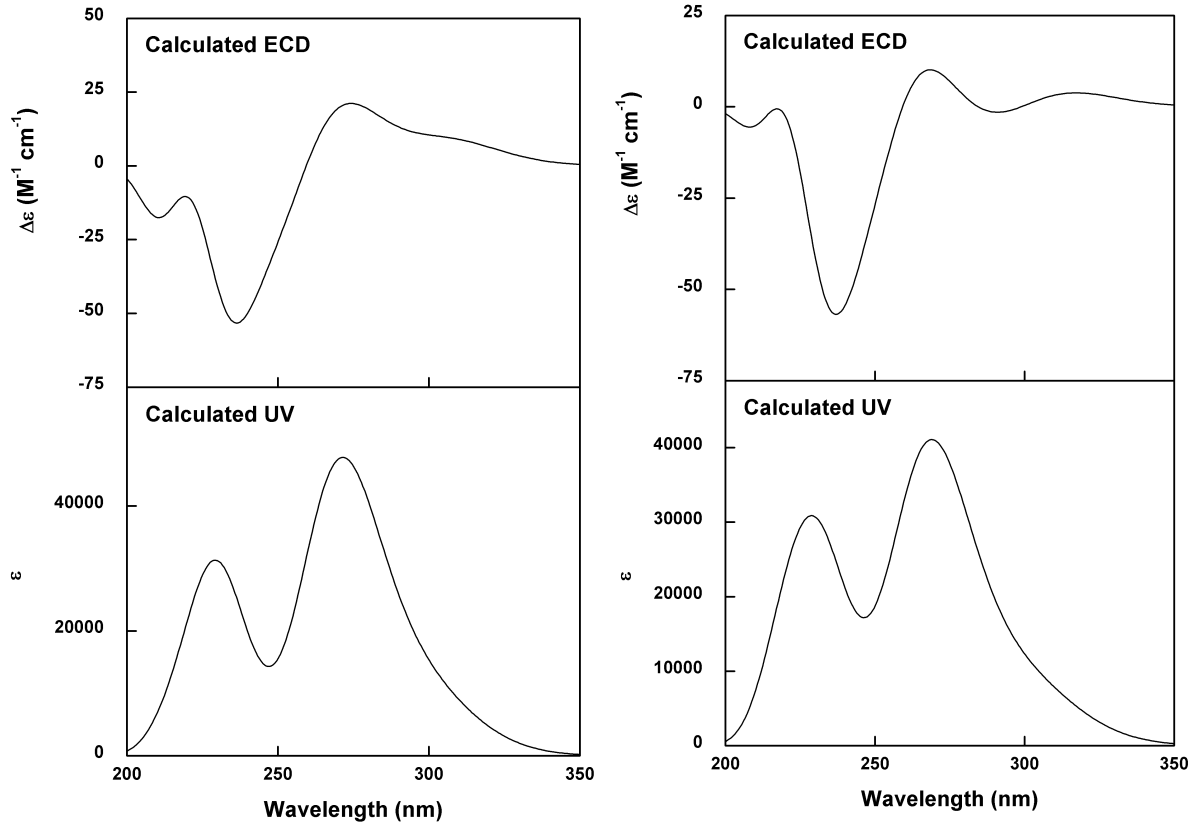

Figure S9. (Left) Calculated [B3LYP/PCM(MeOH)/TZVP// B3LYP/PCM(MeOH)/6-31G(d)] UV and ECD spectra of the Boltzmann average of the three lowest-energy conformers identified for α-configured corilagin. (Right) Calculated [B3LYP/PCM(MeOH)/TZVP// B3LYP/PCM(MeOH)/6-31G(d)] UV and ECD spectra of the Boltzmann average of the four lowest-energy conformers identified for β-configured corilagin.

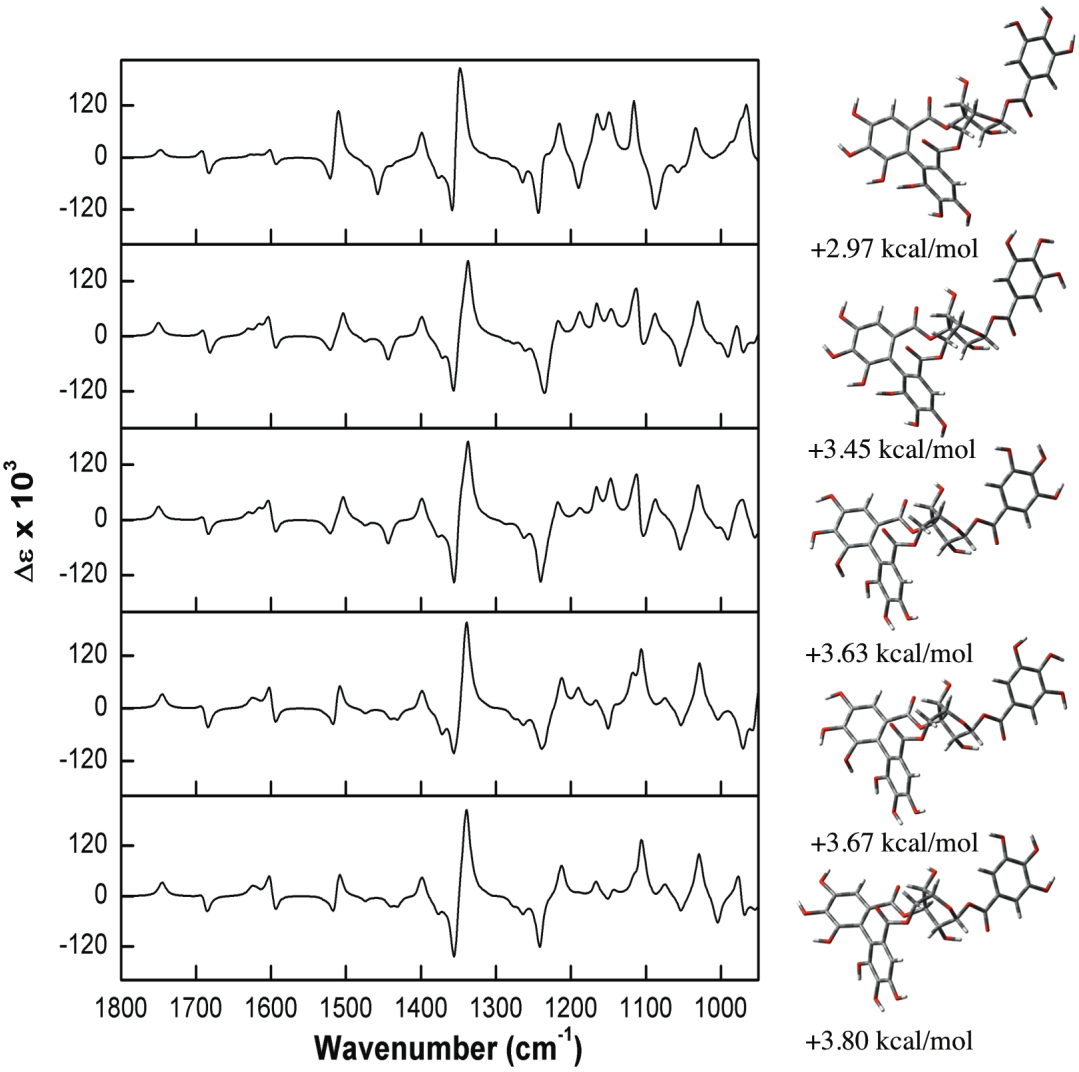

Figure S10. (Left) Calculated [B3LYP/PCM(MeOH)/ 6-31G(d)] VCD spectra of different conformers of α-configured corilagin containing (a*S*)-HHDP moiety. (Right) Optimized structures and relative energies of different conformers of α-configured corilagin containing (a*S*)-HHDP moiety.

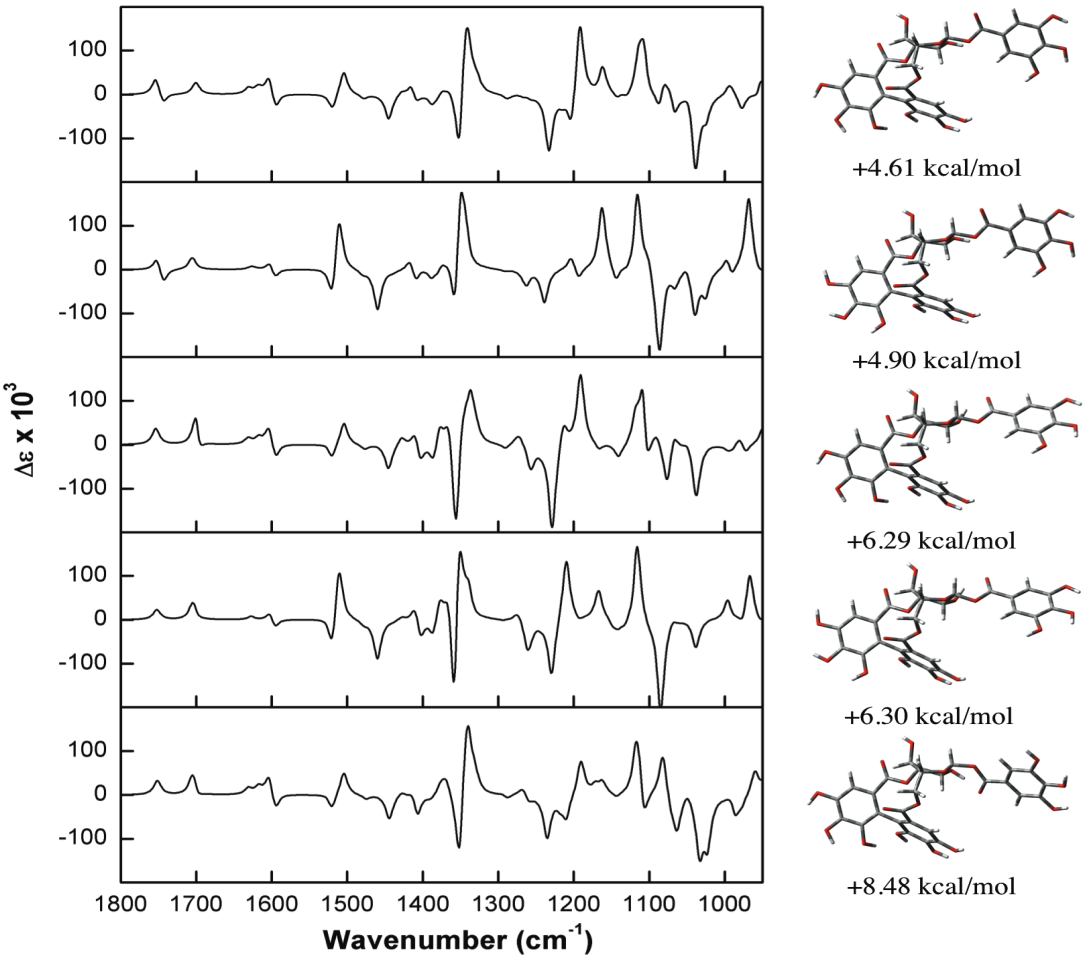

Figure S11. (Left) Calculated [B3LYP/PCM(MeOH)/ 6-31G(d)] VCD spectra of different conformers of β-configured corilagin containing (a*S*)-HHDP moiety. (Right) Optimized structures and relative energies of different conformers of β-configured corilagin containing (a*S*)-HHDP moiety.

Conf1 α-configured corilagin

CAM-B3LYP/PCM(MeOH)/TZVP SPE

Total energy = -1503571.543 kcal/mol

C	-0.04106800	-2.38991900	0.91796800
C	0.65379000	-2.33091900	-0.45172000
O	2.01424900	-1.90746900	-0.33168000
C	1.68193300	-0.74049800	1.78683300
C	2.20166800	-0.66824800	0.34429600
C	0.18539200	-1.11532800	1.76026200
C	-0.07253300	-1.49059900	-1.52432800
O	0.55308400	-3.51043300	1.59923000
O	-0.52661000	0.01080200	1.20144800
H	-0.16711200	-1.28672300	2.78250000
H	-1.10978600	-2.55922200	0.77829600
H	1.80174800	0.24408700	2.25016600
O	2.40675000	-1.65955200	2.57762600
H	1.72756700	0.15117900	-0.20357000
O	3.59234600	-0.45426400	0.39120100
C	4.16995900	0.12832300	-0.70810700
O	3.53643800	0.50969600	-1.66850200
C	5.63975400	0.23674800	-0.54744500
C	6.36724100	0.84441100	-1.57811700
C	7.74897200	0.96971900	-1.46598200
C	8.39781300	0.48644900	-0.32249800
C	7.66399400	-0.11988700	0.70206000
C	6.28514300	-0.25046700	0.60119100
O	8.46977900	1.55886700	-2.46066900
O	9.75726100	0.63072200	-0.25482500
O	8.42075400	-0.55230000	1.76832200
H	0.72298600	-3.36683200	-0.79628100
H	5.85705800	1.21612000	-2.45885400
H	5.70842400	-0.72115600	1.39062800
H	9.40505400	1.54820000	-2.19407100
H	10.05476800	0.25124900	0.58979100
H	7.84112900	-0.95488500	2.43256400
O	-1.49095900	-1.72212500	-1.39490700
C	-2.30379000	-0.64145700	-1.57538100
H	0.11783100	-0.42307500	-1.42021200
H	0.25714800	-1.79760100	-2.52083300
H	0.05431400	-3.65054600	2.42052100
H	2.22029800	-2.54258700	2.20534700
C	-1.88317800	0.04021200	1.38727300
O	-1.93469000	0.39910400	-2.06693700
C	-3.68398100	-0.92632700	-1.07058100
C	-4.27743300	-2.14167700	-1.43307200
C	-5.59310900	-2.40948600	-1.07491300
C	-6.31267600	-1.46141000	-0.34934800
C	-5.70197300	-0.27035500	0.04156000
C	-4.37354100	0.03088900	-0.28986800
H	-3.70981300	-2.86389200	-2.01237100
O	-6.28853000	-3.55146300	-1.38998600
O	-7.61683700	-1.65103600	0.02535900
O	-6.44924900	0.63611000	0.76188900

C	-3.73124600	1.28772100	0.19148800
C	-4.30242400	2.53367900	-0.10852300
C	-3.64016500	3.72886700	0.18563500
C	-2.37952500	3.71849600	0.78590700
C	-1.80743000	2.49639500	1.12583100
C	-2.48015700	1.29851900	0.85945100
O	-5.51363900	2.70212000	-0.74048100
O	-4.20206000	4.93698600	-0.11109500
O	-1.73666600	4.88387500	1.06999400
H	-0.84432000	2.48922500	1.62163200
O	-2.48633300	-0.85835900	1.93719500
H	-5.71835200	-4.15528100	-1.88958500
H	-7.89260400	-2.53370700	-0.27532400
H	-7.31748400	0.22942500	0.93651100
H	-6.15625700	2.09917800	-0.31219300
H	-5.06726400	4.74071500	-0.51720800
H	-2.29461500	5.61278800	0.74788600

Conf2 α-configured corilagin

CAM-B3LYP/PCM(MeOH)/TZVP SPE

Total energy = -1503571.540 kcal/mol

C	-0.06095100	-2.41191300	0.90175000
C	0.66033300	-2.35188600	-0.45469600
O	2.01820900	-1.92297500	-0.30834900
C	1.64664800	-0.76361400	1.80677600
C	2.18620100	-0.68662800	0.37212600
C	0.15163100	-1.14196600	1.75513700
C	-0.04691500	-1.51849200	-1.54560000
O	0.52092600	-3.53164100	1.59269100
O	-0.55980700	-0.01160200	1.19489300
H	-0.21470100	-1.32041600	2.77073100
H	-1.12689900	-2.58089200	0.73929600
H	1.75633800	0.22149800	2.27264600
O	2.35826100	-1.67840200	2.60994000
H	1.71226200	0.13089200	-0.17912800
O	3.57674500	-0.46003200	0.43464800
C	4.15351500	0.14121800	-0.64938500
O	3.52086300	0.54991900	-1.60184800
C	5.62517200	0.24318600	-0.50113100
C	6.33204900	0.86095500	-1.54496500
C	7.71120500	0.97773900	-1.45089400
C	8.38745000	0.48770800	-0.32828600
C	7.67857200	-0.12707600	0.71100800
C	6.29333200	-0.25149900	0.62660100
O	8.52370400	1.55751900	-2.39945000
O	9.74659600	0.58364300	-0.20008800
O	8.34356400	-0.60332400	1.80051800
H	0.74042500	-3.38861500	-0.79318300
H	5.78658900	1.23353300	-2.40686600
H	5.74939800	-0.73193700	1.43037400
H	7.98592300	1.84773600	-3.15152500
H	10.09174100	1.01417000	-1.00093800
H	9.29162600	-0.43214200	1.66698000

O	-1.46429000	-1.74737400	-1.44213200
C	-2.27260700	-0.65411300	-1.57009300
H	0.14480300	-0.45044800	-1.44744100
H	0.30082200	-1.83561400	-2.53287900
H	-0.01630500	-3.70170500	2.38337800
H	2.18021100	-2.56431900	2.24050800
C	-1.91225800	0.02259000	1.39408400
O	-1.88375000	0.41079900	-1.99765900
C	-3.65318100	-0.94696800	-1.08605600
C	-4.22711700	-2.18059800	-1.41177000
C	-5.54324300	-2.46092400	-1.05690700
C	-6.28185500	-1.48853100	-0.37854800
C	-5.70418400	-0.26551900	-0.02939900
C	-4.36870200	0.02832700	-0.34669700
H	-3.66161500	-2.92223600	-1.96335800
O	-6.11136400	-3.65146300	-1.39427600
O	-7.58124900	-1.76985900	-0.06491200
O	-6.54110500	0.57702200	0.66752000
C	-3.72735700	1.28067000	0.14675300
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C	-3.65866800	3.72677100	0.19952300
C	-2.42719200	3.70455600	0.85115100
C	-1.85376300	2.48373900	1.18498100
C	-2.50734200	1.28730600	0.86412000
O	-5.49061200	2.60166600	-0.81438800
O	-4.29069200	4.89149200	-0.14568500
O	-1.89375800	4.93914400	1.13017800
H	-0.90685500	2.45261600	1.71503700
O	-2.51718000	-0.85781600	1.96513800
H	-7.02571100	-3.64371200	-1.06206800
H	-7.92684200	-0.97829100	0.38897100
H	-6.45348600	1.46962300	0.27314800
H	-5.67754900	3.54246200	-0.98648200
H	-3.70582400	5.63266200	0.08775500
H	-1.00513300	4.83617200	1.50314300

Conf3 α-configured corilagin

CAM-B3LYP/PCM(MeOH)/TZVP SPE

Total energy = -1503571.536 Kcal/mol

C	-0.05905500	-2.41456200	0.91988000
C	0.64760200	-2.34537200	-0.44340600
O	2.00852200	-1.92725100	-0.30949600
C	1.66675800	-0.78362800	1.82041800
C	2.19480700	-0.69680200	0.38226500
C	0.16796200	-1.14956400	1.77636400
C	-0.06602100	-1.49312500	-1.51504100
O	0.52224500	-3.54623800	1.59136600
O	-0.53297700	-0.01395700	1.22053000
H	-0.19489500	-1.32743700	2.79380800
H	-1.12784100	-2.57496600	0.76939100
H	1.78764800	0.19521200	2.29550900
O	2.37872300	-1.71354000	2.60705700
H	1.72391200	0.12963200	-0.15760000

O	3.58718800	-0.48479800	0.43404400
C	4.16064900	0.10822400	-0.65673500
O	3.52563600	0.50029700	-1.61425500
C	5.63148900	0.22220500	-0.50860900
C	6.33219100	0.84898500	-1.55109800
C	7.70991900	0.98040000	-1.45610300
C	8.39106500	0.49345300	-0.33527800
C	7.68852600	-0.13160300	0.70222600
C	6.30438500	-0.26861400	0.61791300
O	8.51621300	1.57212900	-2.40285200
O	9.74933500	0.60358200	-0.20635700
O	8.35863400	-0.60396000	1.79025500
H	0.71637800	-3.37849400	-0.79628800
H	5.78282900	1.21900200	-2.41161300
H	5.76490900	-0.75373300	1.42186600
H	7.97078100	1.88745600	-3.13915000
H	10.08782200	1.05475400	-0.99860500
H	9.30394500	-0.41575500	1.66032200
O	-1.48677900	-1.71707100	-1.39870300
C	-2.29199500	-0.63092400	-1.57744300
H	0.13002900	-0.42759800	-1.40150400
H	0.26926100	-1.79468500	-2.51141000
H	0.03295800	-3.67851300	2.41965200
H	2.21239200	-2.59035300	2.21222900
C	-1.89019700	0.02404700	1.39526200
O	-1.91380600	0.41083800	-2.05991000
C	-3.67727000	-0.91122100	-1.08403600
C	-4.27520000	-2.12079100	-1.45818800
C	-5.59469800	-2.38335900	-1.11030200
C	-6.31387800	-1.43550700	-0.38406100
C	-5.69902900	-0.25042200	0.01838100
C	-4.36654700	0.04484100	-0.30173900
H	-3.70781700	-2.84280100	-2.03798600
O	-6.29440100	-3.51950500	-1.43694700
O	-7.62156800	-1.62002400	-0.01914200
O	-6.44574900	0.65578800	0.73956000
C	-3.71948400	1.29370400	0.19358500
C	-4.28028400	2.54558100	-0.10122600
C	-3.61230900	3.73393400	0.20682700
C	-2.35645600	3.71053900	0.81664100
C	-1.79516000	2.48214500	1.15206600
C	-2.47374900	1.29085000	0.87141600
O	-5.48586200	2.72664700	-0.74085200
O	-4.16396100	4.94818900	-0.08521800
O	-1.70804700	4.86977800	1.11388800
H	-0.83639800	2.46462300	1.65600100
O	-2.50566300	-0.87338700	1.93316000
H	-5.72107300	-4.12801100	-1.92714900
H	-7.89857300	-2.50144800	-0.32232200
H	-7.31686500	0.25243500	0.90743000
H	-6.13555100	2.12524500	-0.32105100
H	-5.02821300	4.76031200	-0.49728700
H	-2.26123400	5.60451300	0.79686500

Conf1 β-configured corilagin

CAM-B3LYP/PCM(MeOH)/TZVP SPE

Total energy = -1503574.675 kcal/mol

C	0.76952900	3.42727600	0.54463900
C	-0.07954500	3.47827000	-0.72993800
O	-1.44941400	3.83156900	-0.47142200
C	-1.33621500	3.06453600	1.88392900
C	-2.13434000	3.19864700	0.57129700
C	0.11223900	2.59571900	1.66312600
C	-0.01858300	2.20267200	-1.59272300
O	0.90085700	4.78980600	0.99764400
O	0.10569200	1.19015200	1.32653400
H	0.67199800	2.73116800	2.59324600
H	1.75119400	3.02111900	0.29874100
H	-1.86043200	2.34943600	2.52405700
O	-1.33505400	4.30734800	2.56354100
H	-3.01496300	3.81539900	0.74616200
O	-2.58476700	1.86976200	0.20844400
C	-3.81978600	1.77153000	-0.35802700
O	-4.49075400	2.72805200	-0.68607100
C	-4.26580100	0.35789800	-0.48920400
C	-5.50999300	0.13802000	-1.09914200
C	-6.00116800	-1.15557000	-1.20193300
C	-5.26634800	-2.22859000	-0.68563800
C	-4.02966200	-1.99934800	-0.07808000
C	-3.51562200	-0.71129800	0.01783200
O	-7.19824300	-1.50902600	-1.77656200
O	-5.71149000	-3.51997100	-0.74983400
O	-3.33671400	-3.07531500	0.42925400
H	0.30127900	4.32259400	-1.31164100
H	-6.07007600	0.98985700	-1.47315300
H	-2.54736900	-0.54373300	0.47262100
H	-7.64776200	-0.71696500	-2.10843500
H	-6.56986800	-3.52110300	-1.20761300
H	-3.84917500	-3.87905000	0.23047900
O	1.35877100	1.78484900	-1.64673300
C	1.58736800	0.43928200	-1.61318100
H	-0.62189300	1.39970900	-1.17411600
H	-0.37999200	2.42203000	-2.60211600
H	1.63272700	4.81480100	1.63515800
H	-0.73316800	4.89090400	2.06048200
C	1.30241700	0.53552600	1.45210000
O	0.72575600	-0.38183600	-1.83813200
C	2.99944000	0.14477600	-1.22741900
C	4.02495300	0.89516400	-1.81249500
C	5.35698900	0.59797300	-1.53922100
C	5.65096000	-0.46306300	-0.67938500
C	4.62884600	-1.19771600	-0.07404400
C	3.27833100	-0.89532900	-0.30607800
H	3.79586200	1.69963700	-2.50160800
O	6.35867700	1.30994300	-2.12670700
O	6.96490000	-0.75990700	-0.44921200
O	5.06793700	-2.19199000	0.77064800

C	2.19353700	-1.60333000	0.43209300
C	2.08884900	-2.99672500	0.36468500
C	0.99402900	-3.67890700	0.89731000
C	-0.04740600	-2.97755900	1.50148500
C	0.05659700	-1.59769800	1.64566800
C	1.17164300	-0.91835500	1.13885000
O	3.07266400	-3.73050500	-0.26391700
O	0.95684700	-5.03682100	0.75534200
O	-1.09473000	-3.74220000	1.96277200
H	-0.71423600	-1.05415800	2.18048400
O	2.31940600	1.09311500	1.80508600
H	7.20197000	0.94036000	-1.81250800
H	6.96620300	-1.52738000	0.15326900
H	4.54141300	-2.99521200	0.57618700
H	2.79102900	-4.66317900	-0.25930600
H	0.09828200	-5.32258700	1.12104600
H	-1.93328000	-3.37264600	1.61415600

Conf2 β-configured corilagin

CAM-B3LYP/PCM(MeOH)/TZVP SPE

Total energy = -1503574.234 kcal/mol

C	0.17192200	3.62024200	0.20681200
C	-0.77093300	3.39870900	-0.98328100
O	-2.14905900	3.62886000	-0.65215100
C	-1.79173800	3.26072300	1.76089000
C	-2.67230300	3.03213400	0.51843200
C	-0.30973800	2.92907100	1.49764800
C	-0.62461200	2.03450300	-1.69793400
O	0.19459100	5.04398700	0.42202200
O	-0.16556700	1.49499400	1.40499700
H	0.28894800	3.28616900	2.34182400
H	1.17059400	3.26721000	-0.05567400
H	-2.17084600	2.62426400	2.56515900
O	-1.90886200	4.60114300	2.20165400
H	-3.64985700	3.49259000	0.66069900
O	-2.83034700	1.62437000	0.34652200
C	-4.06758100	1.12117500	0.00513600
O	-5.08044900	1.78584300	0.02490500
C	-3.95729700	-0.29995500	-0.39641800
C	-5.10918300	-0.97843300	-0.81960800
C	-5.00007200	-2.28783400	-1.28068800
C	-3.74085600	-2.90334200	-1.34484700
C	-2.59582200	-2.22062800	-0.92339700
C	-2.70535300	-0.93221900	-0.41943900
O	-6.10785200	-2.96321800	-1.70306000
O	-3.67287900	-4.17378600	-1.84886500
O	-1.41111900	-2.90157900	-1.04795300
H	-0.53738700	4.19780900	-1.69300600
H	-6.07460200	-0.48607900	-0.80574200
H	-1.82324000	-0.42679600	-0.05628100
H	-5.81789400	-3.84071600	-2.00588100
H	-2.72912700	-4.41233000	-1.88454000
H	-0.68106300	-2.25371700	-1.09456800

O	0.77760100	1.66659500	-1.72626600
C	1.09264600	0.37196200	-1.49326500
H	-1.18742900	1.25888300	-1.19142600
H	-0.98569400	2.11526200	-2.72707300
H	0.89512300	5.23022400	1.06839000
H	-1.46622000	5.15168300	1.52752800
C	1.09667100	0.98663600	1.51820400
O	0.27751500	-0.53100200	-1.50891900
C	2.55325900	0.21324800	-1.22051500
C	3.45089600	0.87923700	-2.06558700
C	4.81900800	0.69113700	-1.91443200
C	5.28847900	-0.16075500	-0.91479300
C	4.38980400	-0.78944200	-0.05343300
C	3.00357000	-0.61334000	-0.16441800
H	3.07116000	1.52565200	-2.85104800
O	5.79381200	1.26760300	-2.68979400
O	6.62044900	-0.40395900	-0.71756900
O	4.89525500	-1.61785000	0.92298000
C	2.07294000	-1.24361000	0.81475800
C	2.07841500	-2.63556400	0.99900700
C	1.10886500	-3.27145200	1.77957000
C	0.09805700	-2.53460000	2.40250900
C	0.09595900	-1.14876700	2.26818800
C	1.07991200	-0.50550500	1.50758500
O	2.98267400	-3.49119000	0.41126500
O	1.11710600	-4.62418800	1.95161900
O	-0.84398900	-3.15259400	3.16099400
H	-0.66938200	-0.57523500	2.77679300
O	2.08369200	1.68568200	1.62570400
H	5.38992300	1.85662200	-3.34502600
H	7.12550900	0.13555500	-1.34982700
H	5.86761400	-1.56723400	0.88074500
H	3.87547400	-3.10710500	0.53539700
H	1.88497400	-4.95927800	1.45178300
H	-0.68664200	-4.11111500	3.10699500

Conf3 β-configured corilagin

CAM-B3LYP/PCM(MeOH)/TZVP SPE

Total energy = -1503574.227 kcal/mol

C	0.30810600	3.63650600	0.19712200
C	-0.61357100	3.46982900	-1.01900700
O	-1.99496800	3.73005800	-0.71371800
C	-1.70204100	3.32785900	1.70131100
C	-2.55925500	3.13860600	0.43546400
C	-0.22834400	2.94403600	1.46550500
C	-0.48584900	2.12129200	-1.76809500
O	0.37603000	5.05408000	0.44110300
O	-0.13970100	1.50564300	1.34829200
H	0.36595100	3.26121300	2.32808600
H	1.29897200	3.25150300	-0.05025200
H	-2.12223000	2.69605800	2.48928600
O	-1.78331600	4.66478200	2.15563500
H	-3.53025200	3.61738000	0.56231300

O	-2.74487100	1.73280500	0.24383200
C	-3.99913700	1.23292300	-0.01426000
O	-5.01061100	1.89576900	0.06193900
C	-3.91251500	-0.19697200	-0.39920900
C	-5.08335400	-0.88909600	-0.73844800
C	-4.99330100	-2.20778900	-1.17935100
C	-3.73692500	-2.82120500	-1.30233800
C	-2.57285200	-2.12484700	-0.96280400
C	-2.66151700	-0.82528000	-0.48334000
O	-6.12035300	-2.89583200	-1.52066300
O	-3.69288800	-4.10274800	-1.78110000
O	-1.39066900	-2.79978300	-1.13551900
H	-0.34263900	4.28094200	-1.70054600
H	-6.04933700	-0.40088800	-0.68052400
H	-1.76130700	-0.30472600	-0.19652400
H	-5.84413100	-3.76980100	-1.84598600
H	-2.75268300	-4.32539200	-1.90469400
H	-0.66849700	-2.14532200	-1.23182400
O	0.89944800	1.70484300	-1.75085400
C	1.16550900	0.39855900	-1.51623400
H	-1.09846600	1.35430700	-1.30812900
H	-0.80128600	2.24572200	-2.80782200
H	1.10208200	5.21069900	1.06666400
H	-1.28410200	5.20545800	1.51328000
C	1.09249000	0.94152800	1.50907800
O	0.31011600	-0.47047900	-1.56291600
C	2.60164300	0.18260100	-1.18666200
C	3.56342400	0.86672100	-1.93935700
C	4.91855100	0.63133600	-1.72857200
C	5.30069600	-0.30262800	-0.76154900
C	4.34368200	-0.96710500	0.00987800
C	2.97267400	-0.72027800	-0.15811400
H	3.26589300	1.56669600	-2.71111400
O	5.85433700	1.27573900	-2.47656500
O	6.63309000	-0.54221600	-0.59284700
O	4.86828000	-1.82737500	0.94571900
C	1.96985400	-1.32306200	0.76496900
C	1.88974000	-2.71399000	0.91650800
C	0.87824000	-3.32247100	1.66000700
C	-0.10460500	-2.54335900	2.26878100
C	-0.03376900	-1.15850100	2.17509800
C	1.00351700	-0.55150200	1.45425000
O	2.82593300	-3.52134800	0.30910600
O	0.88356500	-4.68763100	1.72749100
O	-1.06462200	-3.24718800	2.94900700
H	-0.77665100	-0.54066200	2.66889400
O	2.10035100	1.58656900	1.69860400
H	6.72956000	0.96972300	-2.18160000
H	6.70299700	-1.22011100	0.10551500
H	4.34871600	-2.65708200	0.90972800
H	2.56848700	-4.44702000	0.47357000
H	0.05983700	-4.97025900	2.16182700
H	-1.81068600	-2.66621500	3.16371100

Conf4 β-configured corilagin

CAM-B3LYP/PCM(MeOH)/TZVP SPE

Total energy = -1503572.386 kcal/mol

C	0.32664500	3.62244100	0.21020500
C	-0.59834300	3.47100300	-1.00554200
O	-1.97709100	3.73985900	-0.69715400
C	-1.68445700	3.32304100	1.71487900
C	-2.54420400	3.14506700	0.44940800
C	-0.21372000	2.92975300	1.47678100
C	-0.48287500	2.12697800	-1.76484700
O	0.41001600	5.03825900	0.45923000
O	-0.13136700	1.49141700	1.35592700
H	0.38280600	3.24173900	2.33974900
H	1.31314900	3.22805900	-0.04001200
H	-2.10860400	2.69207700	2.50134100
O	-1.75498800	4.65929200	2.17346200
H	-3.51224000	3.62898400	0.57931500
O	-2.73738800	1.74194400	0.25071000
C	-3.99481800	1.24994300	-0.00889100
O	-5.00205900	1.91905400	0.06797200
C	-3.91610900	-0.17955800	-0.39604200
C	-5.09017000	-0.86386900	-0.74002200
C	-5.00675500	-2.18227000	-1.18304800
C	-3.75369500	-2.80303400	-1.30355400
C	-2.58649000	-2.11432700	-0.95919200
C	-2.66867300	-0.81524000	-0.47744000
O	-6.13690600	-2.86278800	-1.52894300
O	-3.71623400	-4.08389200	-1.78449700
O	-1.40777100	-2.79579500	-1.12986900
H	-0.32179600	4.28469100	-1.68195100
H	-6.05340100	-0.37005800	-0.68382800
H	-1.76617300	-0.30060800	-0.18699200
H	-5.86531300	-3.73855700	-1.85331600
H	-2.77712500	-4.31344400	-1.90348800
H	-0.68140200	-2.14527400	-1.21978300
O	0.90066300	1.70406900	-1.76521100
C	1.16168200	0.39700900	-1.51502000
H	-1.09390600	1.35896300	-1.30438700
H	-0.80901200	2.26040800	-2.80021100
H	1.12694300	5.18273900	1.09827000
H	-1.25627700	5.19892400	1.52997000
C	1.10032500	0.92400000	1.51560500
O	0.29999200	-0.46638600	-1.54963800
C	2.59443100	0.17715000	-1.18645600
C	3.56419900	0.86340300	-1.92888200
C	4.92252700	0.63404100	-1.72688100
C	5.31610800	-0.30781600	-0.76538400
C	4.34268600	-0.97125900	-0.00352900
C	2.97104000	-0.72899900	-0.16659500
H	3.24812000	1.56877400	-2.69224400
O	5.90950300	1.25218600	-2.43495200
O	6.62850800	-0.57067400	-0.57104900
O	4.85847800	-1.83752000	0.93271600

C	1.97148600	-1.33741200	0.75678900
C	1.88974100	-2.72911800	0.89876700
C	0.88144500	-3.34048100	1.64454800
C	-0.09583000	-2.56347000	2.26493200
C	-0.02409800	-1.17808600	2.17869900
C	1.00987600	-0.56852600	1.45542000
O	2.82011700	-3.53331400	0.27942200
O	0.88476600	-4.70593800	1.70340900
O	-1.05201800	-3.27006100	2.94762900
H	-0.76319600	-0.56223300	2.68068600
O	2.10876600	1.56768800	1.70627900
H	5.50203200	1.86486300	-3.06670900
H	6.65874500	-1.25233800	0.12758900
H	4.34709900	-2.67104700	0.87975200
H	2.56539400	-4.45993900	0.44258200
H	0.06555300	-4.98999200	2.14522100
H	-1.79302200	-2.68812400	3.17664600

Conf1a β-configured corilagin

B3LYP/PCM(DMSO)/6-311G(d,p) SPE

Total energy = -1504028.255 kcal/mol

C	-0.03790000	-2.18090000	0.83310000
C	0.63320000	-2.14000000	-0.55400000
O	1.90480000	-1.46970000	-0.54180000
C	1.63810000	-0.39650000	1.62120000
C	2.50920000	-1.27980000	0.72330000
C	0.16160000	-0.87590000	1.61660000
C	-0.16690000	-1.39370000	-1.63870000
O	0.55450000	-3.18450000	1.65970000
O	-0.63570000	0.18690000	1.03290000
H	-0.16760000	-1.04220000	2.64400000
H	-1.10590000	-2.37300000	0.70720000
H	1.66240000	0.61890000	1.20600000
O	2.21570000	-0.44410000	2.91650000
H	2.73970000	-2.23090000	1.20530000
O	3.70900000	-0.56640000	0.47130000
C	4.82860000	-1.30020000	0.20070000
O	4.83790000	-2.51750000	0.19170000
C	6.00620000	-0.44400000	-0.06940000
C	5.92900000	0.95610000	-0.04170000
C	7.06910000	1.71140000	-0.30430000
C	8.28120000	1.07130000	-0.59390000
C	8.35190000	-0.32880000	-0.62070000
C	7.21960000	-1.09000000	-0.35940000
O	7.00390000	3.07390000	-0.27920000
O	9.36630000	1.85870000	-0.84360000
O	9.59190000	-0.82850000	-0.91680000
H	0.79100000	-3.18250000	-0.86490000
H	4.99780000	1.46200000	0.17990000
H	7.25960000	-2.17410000	-0.37710000
H	7.88950000	3.42290000	-0.48390000

H	10.13060000	1.28310000	-1.02500000
H	9.57300000	-1.79890000	-0.91730000
O	-1.56470000	-1.71360000	-1.49230000
C	-2.44580000	-0.70050000	-1.70350000
H	-0.03090000	-0.31870000	-1.52450000
H	0.17230000	-1.68800000	-2.63580000
H	0.36850000	-4.05000000	1.26080000
H	1.87880000	0.31050000	3.42500000
C	-1.95920000	0.21910000	1.33710000
O	-2.14480000	0.34050000	-2.25210000
C	-3.77950000	-1.02170000	-1.11940000
C	-4.34880000	-2.27850000	-1.35200000
C	-5.60480000	-2.59520000	-0.83450000
C	-6.27680000	-1.65740000	-0.03950000
C	-5.68060000	-0.41610000	0.21840000
C	-4.43690000	-0.05980000	-0.32200000
H	-3.81930000	-3.00820000	-1.95720000
O	-6.23300000	-3.78730000	-1.04720000
O	-7.49090000	-1.97470000	0.49090000
O	-6.41380000	0.39150000	1.04500000
C	-3.84000000	1.26710000	0.01430000
C	-4.43350000	2.44150000	-0.48500000
C	-3.86170000	3.69660000	-0.24440000
C	-2.64290000	3.81100000	0.42540000
C	-2.01860000	2.65840000	0.90890000
C	-2.62490000	1.41390000	0.72470000
O	-5.57330000	2.36020000	-1.21890000
O	-4.45830000	4.82830000	-0.79070000
O	-2.06680000	5.02390000	0.61440000
H	-1.07660000	2.74620000	1.43720000
O	-2.51110000	-0.61390000	2.02680000
H	-5.67090000	-4.34550000	-1.60910000
H	-7.77750000	-1.21540000	1.03000000
H	-5.90160000	1.19030000	1.25800000
H	-5.77800000	3.26300000	-1.52950000
H	-5.07690000	5.21520000	-0.14430000
H	-2.60390000	5.68110000	0.13350000

Conf1b β-configured corilagin

CAM-B3LYP/PCM(DMSO)/6-311G(d,p) SPE

Total energy = -1504027.195 kcal/mol

C	-0.52120000	-3.05710000	0.60130000
C	0.29790000	-2.87320000	-0.71690000
O	1.23360000	-1.79290000	-0.59310000
C	1.05920000	-1.36760000	1.75450000
C	1.94950000	-1.87550000	0.62320000
C	-0.41110000	-1.82450000	1.51440000
C	-0.53140000	-2.62300000	-1.99300000
O	0.00630000	-4.12420000	1.38960000
O	-1.15610000	-0.75110000	0.88500000
H	-0.86740000	-2.06140000	2.47690000

H	-1.57480000	-3.23270000	0.36730000
H	1.08610000	-0.27280000	1.71750000
O	1.58440000	-1.84710000	2.97820000
H	2.28900000	-2.89910000	0.80950000
O	3.06610000	-1.00960000	0.51840000
C	4.18520000	-1.51350000	-0.08440000
O	4.25560000	-2.65800000	-0.49290000
C	5.27510000	-0.51560000	-0.16780000
C	5.12910000	0.78830000	0.32790000
C	6.18920000	1.68500000	0.22190000
C	7.38970000	1.28180000	-0.37770000
C	7.52900000	-0.02260000	-0.87260000
C	6.47730000	-0.92410000	-0.76920000
O	6.05650000	2.95560000	0.70060000
O	8.39460000	2.20020000	-0.45710000
O	8.74860000	-0.28910000	-1.43520000
H	0.87240000	-3.79950000	-0.86480000
H	4.20570000	1.11240000	0.79110000
H	6.57190000	-1.93690000	-1.14640000
H	6.89080000	3.42970000	0.53600000
H	9.15550000	1.78750000	-0.90320000
H	8.77170000	-1.19820000	-1.77510000
O	-1.88690000	-2.25290000	-1.69740000
C	-2.23450000	-0.93920000	-1.69940000
H	-0.05110000	-1.85060000	-2.59610000
H	-0.61080000	-3.54510000	-2.57090000
H	-0.17950000	-4.95550000	0.92470000
H	1.16050000	-1.34270000	3.69180000
C	-1.42230000	0.32040000	1.66620000
O	-1.52790000	-0.05340000	-2.13540000
C	-3.57940000	-0.77360000	-1.08240000
C	-4.53590000	-1.78460000	-1.24720000
C	-5.79860000	-1.67930000	-0.66710000
C	-6.10060000	-0.56160000	0.12050000
C	-5.13170000	0.43460000	0.29720000
C	-3.86350000	0.36370000	-0.30090000
H	-4.29430000	-2.66060000	-1.84000000
O	-6.77790000	-2.61890000	-0.80960000
O	-7.32530000	-0.46120000	0.70730000
O	-5.54130000	1.46880000	1.09640000
C	-2.92950000	1.50860000	-0.06400000
C	-3.17640000	2.71250000	-0.75450000
C	-2.43050000	3.86680000	-0.49220000
C	-1.39970000	3.85040000	0.44800000
C	-1.14040000	2.67400000	1.15180000
C	-1.88470000	1.51790000	0.88770000
O	-4.16460000	2.75800000	-1.68410000
O	-2.67770000	5.01580000	-1.23600000
O	-0.65780000	4.96090000	0.68670000
H	-0.34560000	2.65870000	1.88830000
O	-1.18850000	0.34340000	2.86060000
H	-6.44480000	-3.33870000	-1.37000000
H	-7.33320000	0.36870000	1.21780000
H	-4.80220000	2.08790000	1.22820000
H	-4.14180000	3.65000000	-2.08040000
H	-3.30100000	5.58950000	-0.75340000

H	-0.92970000	5.64020000	0.04190000