Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

VCD to determine absolute configuration of natural product molecules: secolignans from *Peperomia blanda*

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Supplementary Information:

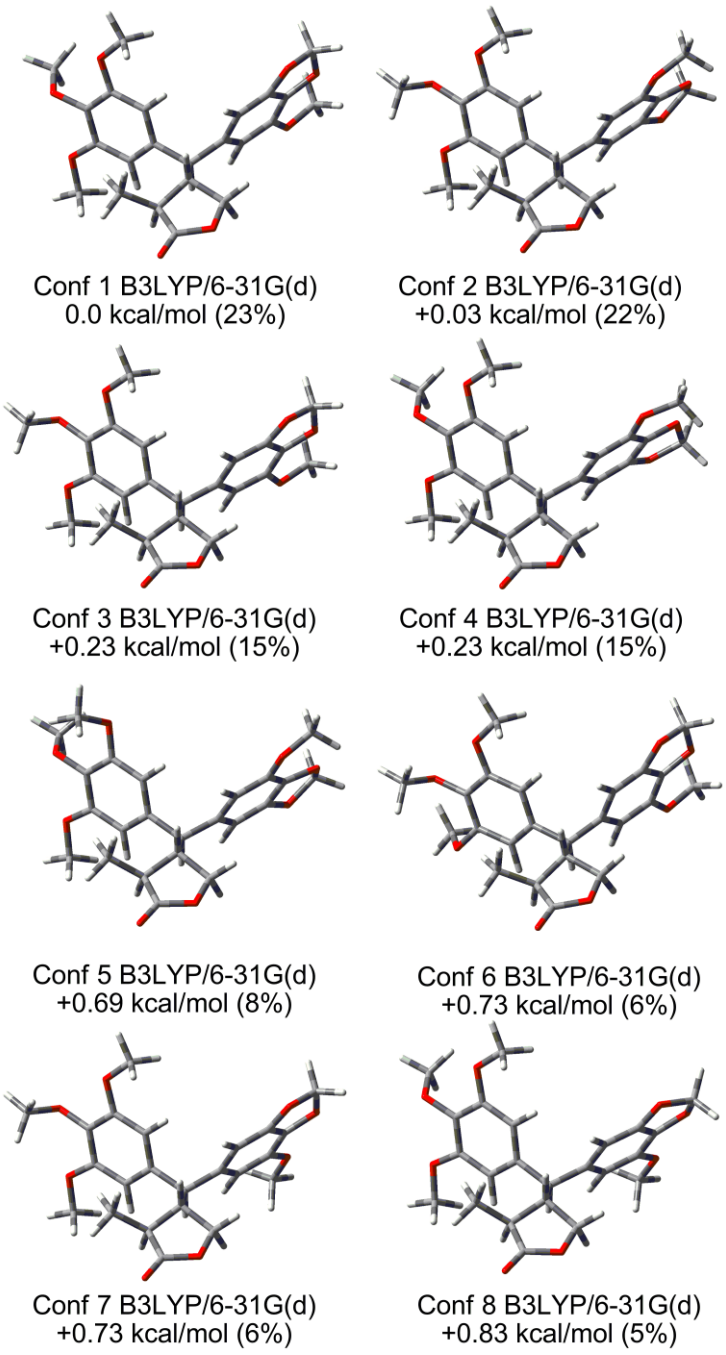

Figure 1. Optimized structures, relative energies, and Boltzmann factors of the eight lowest-energy conformers of (2*S*,3*S*,5*S*)-**2** used for VCD and ECD spectral calculations

Atomic coordinates - (2*S*,3*S*,5*S*)-**2**

B3LYP/6-31G(d) opt

Total energy = –937136.1505 kcal/mol

Conf 1

C	3.07459900	-1.14650900	-0.99546000
C	3.19431000	-1.76987300	0.25690100
C	2.01645800	-0.25937300	-1.24153700
C	1.06986900	0.00451000	-0.24669700
C	1.17297400	-0.63143400	0.99526800
C	2.22620700	-1.51878800	1.24583400
C	-0.05301900	1.00378000	-0.53408500
C	0.12580400	2.34044700	0.22844700
C	-1.44069700	0.38713800	-0.33640900
C	-2.05632700	-0.22960400	-1.42614600
C	-3.31454100	-0.86215200	-1.34499000
C	-3.93204100	-0.85080300	-0.09778200
C	-3.31599200	-0.23591800	0.98973400
C	-2.08853200	0.39160100	0.91856500
O	-3.79359100	-1.39697000	-2.49957000
O	-5.17849900	-1.32262400	0.28782300
C	-5.17245400	-1.23519400	1.71428300
O	-4.14171600	-0.31933800	2.08831200
C	-4.96768200	-2.20785000	-2.45659100
O	2.40500900	-2.19547200	2.41576500
C	1.48570100	-1.96403600	3.47062400
O	4.26580800	-2.58151000	0.52814100
O	4.03615200	-1.47451700	-1.90472500
C	1.42186700	3.12266200	-0.07017200
C	0.98482200	4.58497200	0.06699900
O	-0.37417300	4.67147900	0.04369200
C	-0.96314900	3.37058600	-0.13911300
O	1.68811100	5.55535100	0.18367600
C	2.64851400	2.83177800	0.79770800
H	1.92303600	0.22567500	-2.20657000
H	0.42248000	-0.44990600	1.75433100
H	0.02230100	1.25435400	-1.60038300
H	0.08779100	2.15644200	1.31008400
H	-1.56316100	-0.25139000	-2.39327900
H	-1.66502400	0.86753800	1.79514500
H	-6.13833600	-0.85778600	2.05719800
H	-4.95676500	-2.22520600	2.14505900
H	-5.11761900	-2.55427800	-3.48082200
H	-5.84060000	-1.63560900	-2.12830200
H	-4.83169800	-3.06966700	-1.79372000
H	1.82296500	-2.58758900	4.30064900
H	0.46415700	-2.25373300	3.19039700
H	1.48815900	-0.91175200	3.78416700
H	1.69201800	2.98484500	-1.12933600
H	-1.85311400	3.31780900	0.49005600
H	-1.27260000	3.27334500	-1.18778900
H	3.42650300	3.57231700	0.59000800
H	3.04487300	1.83270400	0.60416300
H	2.39638400	2.90242100	1.86220000
C	4.06048400	-3.95902200	0.21347300
C	4.00171200	-0.84391800	-3.17457700
H	4.98602700	-4.47460400	0.48108300
H	3.86583200	-4.09485300	-0.85764100
H	3.23027200	-4.37781400	0.79580200
H	3.08214400	-1.08621500	-3.72406000
H	4.86161200	-1.23294900	-3.72288900
H	4.09223600	0.24670900	-3.08612200

B3LYP/6-31G(d) opt

Total energy = –937136.1147 kcal/mol

Conf 2

C	3.05233600	-1.22046800	-1.07190200
C	3.07017300	-1.95934900	0.12205200
C	2.02468900	-0.29626200	-1.31160000
C	1.02201100	-0.09284700	-0.35846400
C	1.03757600	-0.82363700	0.83409400
C	2.05897700	-1.74928000	1.07732700
C	-0.06353800	0.95206500	-0.62560600
C	0.12399300	2.23673500	0.21935900
C	-1.46874200	0.35332200	-0.51683300
C	-2.20369200	0.38202100	0.66910400
C	-3.48227600	-0.20637200	0.79382600
C	-3.98882800	-0.83606900	-0.33727200
C	-3.25021500	-0.86540900	-1.52002000
C	-2.00548500	-0.28882700	-1.65341300
O	-4.07979600	-0.07765900	2.00952500
O	-5.21624800	-1.44698500	-0.54843500
C	-5.07999200	-2.10506500	-1.81043600
O	-3.98009800	-1.50483400	-2.49557900
C	-5.32848800	-0.72821300	2.24449500
O	2.16612600	-2.50224700	2.20882000
C	1.15893300	-2.36974300	3.19901800
O	4.02791100	-2.91969300	0.32386500
O	4.07745800	-1.47742800	-1.93298500
C	1.46378100	2.97838600	0.03011700
C	1.07784600	4.45089400	0.20431800
O	-0.27277200	4.59496300	0.11701000
C	-0.90541400	3.32834100	-0.14544200
O	1.81292300	5.38550000	0.39539800
C	2.62230600	2.60342700	0.95779500
H	2.00361200	0.27100000	-2.23529000
H	0.24516200	-0.67977700	1.55826300
H	0.05791700	1.26307000	-1.67227100
H	0.02298300	1.99610500	1.28543000
H	-1.81737300	0.86667800	1.55932400
H	-1.46169100	-0.33881500	-2.59039700
H	-4.87229000	-3.17403100	-1.64952800
H	-5.99371500	-1.96337400	-2.39183000
H	-5.58537900	-0.49617000	3.27975500
H	-5.24245500	-1.81325300	2.12092200
H	-6.10936900	-0.35140500	1.57679100
H	1.43134400	-3.06575600	3.99453500
H	0.16930200	-2.63627500	2.80606000
H	1.12175400	-1.35044200	3.60618500
H	1.79467600	2.87193200	-1.01507900
H	-1.82199000	3.28724500	0.44470800
H	-1.17485100	3.28952000	-1.20885100
H	3.44166500	3.31617600	0.82527500
H	2.98738100	1.59524100	0.74976400
H	2.30858800	2.64701700	2.00730300
C	5.18239900	-2.46562500	1.03071400
C	4.10680500	-0.78010000	-3.16740500
H	5.85144500	-3.32613900	1.10776700
H	4.91898200	-2.11920400	2.03769400
H	5.68876900	-1.66026100	0.48376200
H	3.21538600	-0.99152800	-3.77258200
H	4.99227400	-1.14284600	-3.69254900
H	4.19291200	0.30480100	-3.01908700

B3LYP/6-31G(d) opt

Total energy = –937135.9177 kcal/mol

Conf 3

C	2.94266100	-1.30902200	-1.13128000

C	3.06774600	-1.96525100	0.10362600
C	1.91153400	-0.37967800	-1.33273100
C	1.01025700	-0.09002300	-0.30366400
C	1.13464800	-0.73766500	0.93030800
C	2.16082700	-1.66709100	1.13653000
C	-0.08656000	0.94936200	-0.54574800
C	0.15214200	2.26594700	0.23408000
C	-1.48762900	0.37213300	-0.32360500
C	-2.15088900	-0.20218400	-1.40844900
C	-3.42615700	-0.79635500	-1.30592600
C	-4.01005700	-0.79079600	-0.04263800
C	-3.34630700	-0.21850100	1.04005900
C	-2.10169500	0.37136500	0.94822400
O	-3.95340900	-1.29063900	-2.45738400
O	-5.26080000	-1.23003800	0.36650500
C	-5.21406300	-1.17392000	1.79375600
O	-4.14545600	-0.29841700	2.15842800
C	-5.13846600	-2.08429600	-2.39535400
O	2.36893900	-2.34252300	2.30241300
C	1.46797300	-2.12050200	3.37503100
O	4.02463200	-2.93167900	0.27909900
O	3.87188200	-1.64833700	-2.06925300
C	1.46029500	3.01704900	-0.09075700
C	1.07050500	4.48784700	0.09132700
O	-0.28506700	4.61336200	0.10925700
C	-0.91647300	3.33345200	-0.08280900
O	1.80536000	5.43455400	0.20893600
C	2.70638900	2.67326800	0.72841800
H	1.80690200	0.12219900	-2.28796400
H	0.42391400	-0.52851800	1.71986100
H	-0.02968500	1.21635600	-1.60913600
H	0.14042700	2.06435900	1.31318700
H	-1.68391800	-0.22020400	-2.38855800
H	-1.63997100	0.81474300	1.82260800
H	-6.15813600	-0.77439400	2.17063800
H	-5.01805200	-2.17916700	2.19776000
H	-5.32528000	-2.40592800	-3.42159500
H	-5.99166700	-1.50633300	-2.02775400
H	-4.99539800	-2.96243700	-1.75576200
H	1.80647700	-2.76788500	4.18608300
H	0.43961000	-2.38951600	3.10071400
H	1.48875700	-1.07562900	3.71306400
H	1.69059000	2.89499300	-1.16128700
H	-1.78995400	3.29335900	0.56981600
H	-1.25706100	3.26635400	-1.12414700
H	3.49659800	3.39835800	0.51213400
H	3.06875100	1.66903500	0.49795000
H	2.49154300	2.72439800	1.80216800
C	5.26247900	-2.45160300	0.80429100
C	3.78484300	-1.04401700	-3.34922600
H	5.91796100	-3.32212900	0.88554200
H	5.12493300	-2.00701000	1.79780800
H	5.71875900	-1.71563400	0.13040000
H	2.83265700	-1.27859800	-3.84296700
H	4.60583700	-1.46466900	-3.93271400
H	3.90274000	0.04651400	-3.29263400

B3LYP/6-31G(d) opt

Total energy = –937135.9139 kcal/mol

Conf 4

C	-3.20893800	-1.00746800	0.91927400
C	-3.26145100	-1.68367200	-0.31013800
C	-2.13038800	-0.15906600	1.21004300
C	-1.09799100	0.01281500	0.28270700
C	-1.13445300	-0.67648600	-0.93389200
C	-2.20796900	-1.52481700	-1.22895200
C	0.04796200	0.97412700	0.60778400
C	-0.03017400	2.29328400	-0.19976800

C	1.41152300	0.28342800	0.51072000
C	2.16931200	0.28888800	-0.66148100
C	3.41008200	-0.37675800	-0.77578000
C	3.86069200	-1.04872600	0.35460200
C	3.10578300	-1.04522300	1.52685600
C	1.89210300	-0.40256900	1.64686700
O	4.02031300	-0.30001500	-1.98977800
O	4.99610800	-1.82246500	0.54210700
C	5.05012200	-2.05141300	1.95256600
O	3.74927700	-1.79581700	2.48400200
C	5.38279500	-0.71038500	-2.10806200
O	-2.32861400	-2.24722200	-2.37852300
C	-1.31347600	-2.11656100	-3.36109900
O	-4.34865300	-2.45611900	-0.62866800
O	-4.25372500	-1.24649700	1.76200700
C	-1.31541400	3.12624500	-0.01068200
C	-0.81989200	4.56988400	-0.14086000
O	0.53655900	4.61175100	-0.02620500
C	1.06832400	3.29586300	0.21483300
O	-1.47989700	5.56093200	-0.32018100
C	-2.48364900	2.85873900	-0.96279000
H	-2.08927000	0.36835700	2.15637800
H	-0.31628700	-0.56622800	-1.63482000
H	-0.07849700	1.26001300	1.66090600
H	0.07313200	2.07682600	-1.27076600
H	1.83545300	0.82215700	-1.54512400
H	1.33062500	-0.43396200	2.57419400
H	5.32255800	-3.09265400	2.13890300
H	5.77592500	-1.36258000	2.41150900
H	5.66351000	-0.48938000	-3.13955700
H	5.50016900	-1.78054800	-1.91356100
H	6.02756800	-0.14723900	-1.42373600
H	-1.61436300	-2.76438300	-4.18647200
H	-0.33614300	-2.44183800	-2.98091700
H	-1.23321300	-1.08301800	-3.72266900
H	-1.66895600	3.01947500	1.02717400
H	1.99225800	3.20171300	-0.35757800
H	1.31046200	3.20970800	1.28216800
H	-3.25371600	3.62261700	-0.82036100
H	-2.92057600	1.87323000	-0.78799100
H	-2.15290700	2.90922300	-2.00668600
C	-4.22366900	-3.83284500	-0.27101000
C	-4.28938900	-0.55413100	2.99901400
H	-5.15344000	-4.31480300	-0.58296000
H	-4.10038600	-3.94964400	0.81300200
H	-3.37939900	-4.30144700	-0.79158500
H	-3.42981600	-0.80950600	3.63331300
H	-5.20848500	-0.87496700	3.49273200
H	-4.31821600	0.53357300	2.85190600

B3LYP/6-31G(d) opt

Total energy = –937135.4533 kcal/mol

Conf 5

C	-3.08945100	-1.00588900	0.98674000
C	-3.17974800	-1.65757900	-0.25940700
C	-2.00412000	-0.16475300	1.25770000
C	-0.99981600	0.03915300	0.30018000
C	-1.09191100	-0.60966700	-0.93183500
C	-2.17164800	-1.45220200	-1.21129900
C	0.15868100	0.98717400	0.61916500
C	0.07152800	2.32190900	-0.16112400
C	1.51533700	0.29095200	0.47896400
C	2.23452600	0.29544500	-0.71693800
C	3.46580200	-0.37878100	-0.87321700
C	3.93974600	-1.07061800	0.23577500
C	3.21581800	-1.07811300	1.42732500
C	2.01810300	-0.41597500	1.59238400
O	4.06241900	-0.25805500	-2.08955000

O	5.12528300	-1.76791200	0.41547100
C	4.95915700	-2.44735400	1.66213100
O	3.91125700	-1.79110600	2.37730200
C	5.18550200	-1.08376200	-2.39744900
O	-2.18601700	-2.11984400	-2.41170500
C	-3.23456300	-1.75252300	-3.31466300
O	-4.25544100	-2.46280300	-0.55026200
O	-4.10099000	-1.27478100	1.86195200
C	-1.19793200	3.16478800	0.08245500
C	-0.69062000	4.60522300	-0.03959300
O	0.66815200	4.63075700	0.03591800
C	1.19270900	3.30497700	0.23915900
O	-1.34588500	5.60534000	-0.18352300
C	-2.39917400	2.92654200	-0.83553100
H	-1.93029000	0.33552300	2.21703500
H	-0.32335200	-0.50062900	-1.68966700
H	0.05783500	1.25351800	1.68037100
H	0.14128400	2.12433200	-1.23843500
H	1.86965800	0.82337900	-1.59136800
H	1.48556900	-0.44780400	2.53668700
H	4.67655600	-3.49524600	1.47776400
H	5.88735600	-2.38350400	2.23431900
H	5.43909200	-0.85270900	-3.43371900
H	4.93310800	-2.14645300	-2.30930300
H	6.03860500	-0.86147000	-1.74943900
H	-3.08133000	-2.35512000	-4.21299600
H	-3.16470500	-0.68836500	-3.57690100
H	-4.21945600	-1.96331000	-2.88879300
H	-1.51874000	3.04487400	1.12956500
H	2.09862200	3.21109400	-0.36115500
H	1.46411000	3.19812300	1.29744200
H	-3.15343500	3.69901100	-0.65873300
H	-2.84416900	1.94467900	-0.66008500
H	-2.10026900	2.98618000	-1.88847900
C	-4.15380500	-3.79271300	-0.03235500
C	-4.08520000	-0.62758200	3.12454600
H	-5.05787400	-4.31487200	-0.35448800
H	-4.10822400	-3.78502500	1.06242000
H	-3.27164800	-4.30306500	-0.43815600
H	-4.12171200	0.46433800	3.01710700
H	-3.19842500	-0.90345400	3.71061200
H	-4.98192300	-0.96869800	3.64488600

B3LYP/6-31G(d) opt

Total energy = –937135.4213 kcal/mol

Conf 6

C	-2.26537200	-1.40915800	-1.14751800
C	-3.18127400	-1.70718700	-0.11487200
C	-1.18679400	-0.55565300	-0.90536300
C	-1.00163800	0.01660600	0.36287300
C	-1.89647200	-0.29488500	1.38553700
C	-2.98320100	-1.14730600	1.15193000
C	0.15552100	0.97875400	0.63782700
C	-0.02351500	2.34803500	-0.06354700
C	1.51698100	0.33724400	0.35386400
C	2.16723600	-0.33119000	1.39162400
C	3.40423000	-0.98964100	1.22912700
C	3.96276900	-0.94883800	-0.04501700
C	3.31170800	-0.28284300	-1.08080300
C	2.10466400	0.36974600	-0.93007800
O	3.92287600	-1.57586800	2.34052100
O	5.17727300	-1.43653900	-0.50552500
C	5.10587300	-1.30068900	-1.92627000
O	4.08211600	-0.34835600	-2.22012400
C	5.07441100	-2.41016900	2.21536300
O	-3.86989700	-1.36544800	2.17742300
C	-3.93719300	-2.70816500	2.67005900
O	-4.22726800	-2.57132300	-0.33671200

O	-2.53225800	-2.00065300	-2.34782900
C	-1.27902100	3.15349200	0.33139800
C	-0.80962500	4.60680700	0.20672900
O	0.55089900	4.65636900	0.16497400
C	1.11023000	3.33495600	0.28470600
O	-1.49071700	5.59787900	0.14591700
C	-2.56235300	2.91947900	-0.46864700
H	-0.47789500	-0.34272200	-1.69591900
H	-1.78272900	0.12253700	2.38162200
H	0.13120900	1.18713600	1.71531200
H	-0.04573200	2.20686800	-1.15224900
H	1.71952900	-0.37499400	2.37989500
H	1.65257300	0.88520400	-1.76933800
H	6.06369900	-0.93498500	-2.30283500
H	4.84492300	-2.27011800	-2.37835700
H	5.26244000	-2.79593900	3.21901500
H	5.94470700	-1.84574200	1.86710200
H	4.88839200	-3.24472000	1.53012400
H	-4.66445900	-2.69151300	3.48515700
H	-2.96174200	-3.02599400	3.06176300
H	-4.26585000	-3.40210500	1.89172200
H	-1.49030600	2.99231800	1.40053300
H	1.96990600	3.27636100	-0.38467900
H	1.46154300	3.19751100	1.31550000
H	-3.30421800	3.67603200	-0.19667100
H	-2.97584300	1.92763600	-0.27385700
H	-2.37183700	3.01002900	-1.54450300
C	-5.35466200	-1.98031700	-0.99045500
C	-1.64449500	-1.75569500	-3.42746600
H	-6.10376800	-2.77068200	-1.07906500
H	-5.08525300	-1.62009200	-1.98943200
H	-5.76273500	-1.15458300	-0.39451800
H	-0.62711600	-2.09747600	-3.19741000
H	-1.61546000	-0.69071200	-3.69384500
H	-2.03622400	-2.32804300	-4.27025100

B3LYP/6-31G(d) opt

Total energy = –937135.4163 kcal/mol

Conf 7

C	2.95733200	-1.16902600	-1.06438800
C	3.06922300	-1.86875700	0.14775900
C	1.89010000	-0.28203800	-1.26878600
C	0.94086100	-0.07525600	-0.26261400
C	1.05206400	-0.76540700	0.94899800
C	2.11281000	-1.65485300	1.15696200
C	-0.19159600	0.92660100	-0.49920700
C	0.00379100	2.24545000	0.29017700
C	-1.57124000	0.29726100	-0.28323300
C	-2.17917300	-0.35005700	-1.37070400
C	-3.42341800	-0.99888900	-1.25991800
C	-4.02956100	-0.97115600	-0.00774300
C	-3.43191400	-0.32989000	1.06387000
C	-2.21013100	0.31628800	0.97106100
O	-4.08516500	-1.63921000	-2.26073800
O	-5.25328300	-1.48103100	0.36221600
C	-5.29456200	-1.33037700	1.78404400
O	-4.25518800	-0.41787200	2.16290300
C	-3.47497600	-1.68268800	-3.54225000
O	2.31064600	-2.36701500	2.30210800
C	1.36299000	-2.22976700	3.34904400
O	4.06378200	-2.79672900	0.31990800
O	3.93546100	-1.42576600	-1.97904900
C	1.29937600	3.02798700	-0.00971000
C	0.87083500	4.49015700	0.15284100
O	-0.48733500	4.58308600	0.15113000
C	-1.08653200	3.28772500	-0.03885600
O	1.58111500	5.45533800	0.27128400
C	2.53194100	2.72033600	0.84400500

H	1.79671400	0.25384100	-2.20674700
H	0.30281700	-0.62170100	1.71742800
H	-0.14044600	1.20463000	-1.56059200
H	-0.01861800	2.03708200	1.36768000
H	-1.65873900	-0.36077500	-2.32179100
H	-1.78591900	0.81320600	1.83558900
H	-6.26342600	-0.91916600	2.07848600
H	-5.11621900	-2.30427100	2.26355200
H	-4.16583800	-2.23620400	-4.18026800
H	-2.51017600	-2.20539300	-3.51119700
H	-3.32892400	-0.67519000	-3.95324000
H	1.70389900	-2.89247400	4.14653000
H	0.35897100	-2.53518800	3.02719900
H	1.32227700	-1.19929600	3.72681100
H	1.56069500	2.90446300	-1.07269900
H	-1.96382300	3.23035600	0.60718200
H	-1.41811600	3.20851000	-1.08228000
H	3.31160200	3.46010500	0.63963600
H	2.92108800	1.72180100	0.63344400
H	2.28872800	2.77798300	1.91136400
C	5.25438900	-2.28585600	0.92029700
C	3.87698800	-0.75796800	-3.22829600
H	5.70252800	-1.49870300	0.30096800
H	5.94666900	-3.12835700	0.99045800
H	5.05446000	-1.89566700	1.92589400
H	2.95991100	-1.00787000	-3.77820300
H	4.74191500	-1.10914900	-3.79398400
H	3.94011000	0.33209600	-3.10943700

B3LYP/6-31G(d) opt

Total energy = –937135.3140 kcal/mol

Conf 8

C	3.11155800	-0.94113300	-0.91658900
C	3.24445400	-1.58482300	0.32416400
C	1.99564900	-0.13057900	-1.17259100
C	1.00508100	0.03625800	-0.19941800
C	1.12188700	-0.62208000	1.02931100
C	2.23319500	-1.43210100	1.29019700
C	-0.18100000	0.95876000	-0.49226000
C	-0.09085700	2.30648200	0.26676100
C	-1.52460300	0.25003100	-0.29569600
C	-2.07267600	-0.44348900	-1.38648400
C	-3.28105500	-1.15956700	-1.29231300
C	-3.92057000	-1.14040900	-0.05678500
C	-3.38216700	-0.45366300	1.01796100
C	-2.19226100	0.25147700	0.94389400
O	-3.87762900	-1.85995500	-2.29426700
O	-5.08798000	-1.76869500	0.31322100
C	-5.37707500	-1.26036400	1.61887000
O	-4.19564700	-0.61694300	2.11556300
C	-3.22378700	-1.90997800	-3.55364100
O	2.43200600	-2.12071600	2.44962000
C	1.46790900	-1.98814600	3.48232600
O	4.36994400	-2.31577800	0.60443300
O	4.11986300	-1.17130000	-1.80495300
C	1.16171400	3.16184800	-0.01608700
C	0.63766000	4.59742700	0.09029600
O	-0.72374400	4.60381900	0.04832000
C	-1.23442700	3.26858500	-0.12068400
O	1.28143600	5.60909900	0.19901700
C	2.38156000	2.95500900	0.88512200
H	1.89316600	0.37185500	-2.12794600
H	0.33803100	-0.51873600	1.76904200
H	-0.11687700	1.21251000	-1.55909000
H	-0.13226100	2.12355300	1.34828200
H	-1.53657200	-0.43076000	-2.32875800
H	-1.81375500	0.78018800	1.81075600
H	-6.19294600	-0.52524900	1.55630600

H	-5.64456900	-2.08813100	2.28065600
H	-3.86000700	-2.52389200	-4.19327200
H	-2.23184600	-2.37342300	-3.47416400
H	-3.12250700	-0.90993200	-3.99529700
H	1.83086600	-2.60334800	4.30764300
H	0.48091500	-2.35033600	3.16569400
H	1.37892100	-0.94685000	3.81871400
H	1.46615200	3.02603600	-1.06592700
H	-2.12446400	3.17205700	0.50303500
H	-1.53044000	3.14053000	-1.17001900
H	3.12519300	3.73023800	0.67826900
H	2.83296300	1.97385400	0.72302400
H	2.10098100	3.03525100	1.94178400
C	4.25673500	-3.71210300	0.32754300
C	4.07988000	-0.49968800	-3.05288100
H	3.46312700	-4.17177200	0.92910400
H	5.21826800	-4.15545900	0.59751600
H	4.06233200	-3.88876000	-0.73793500
H	3.20051900	-0.79023700	-3.64367900
H	4.98473100	-0.80273300	-3.58283300
H	4.08326200	0.59076300	-2.92462600

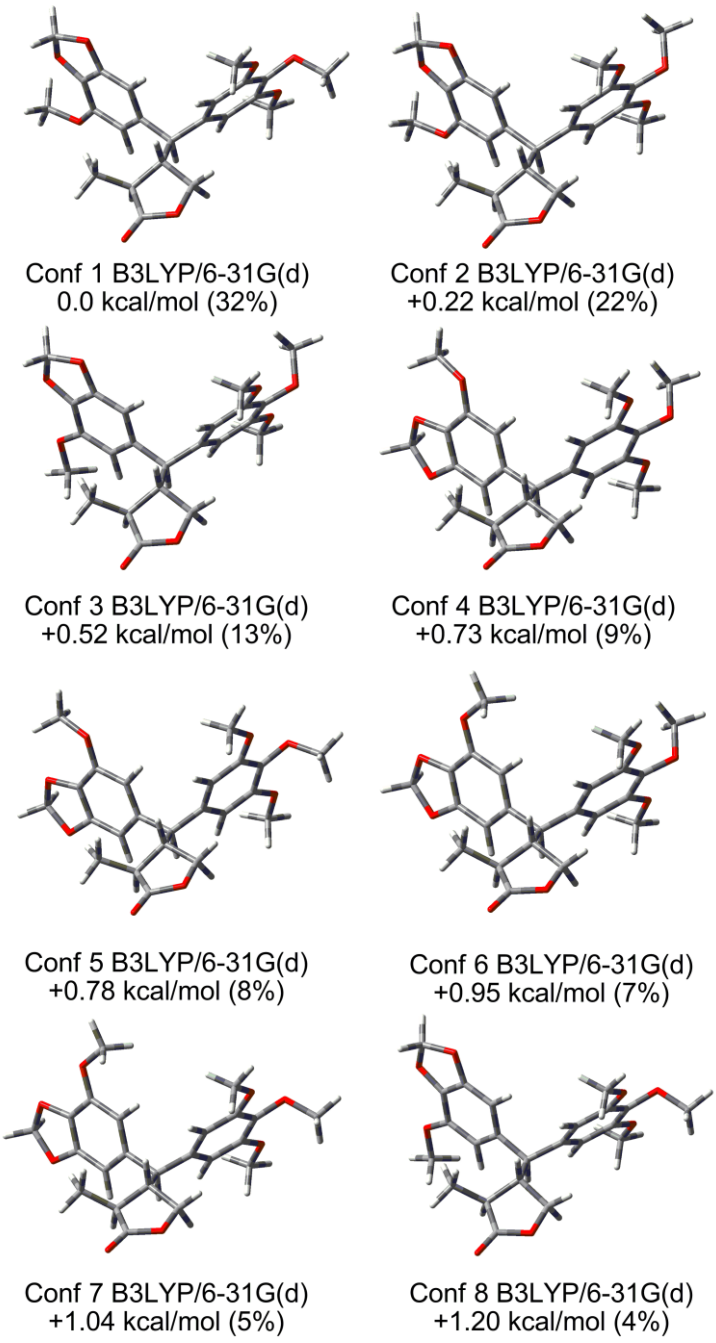

Figure 2. Optimized structures, relative energies, and Boltzmann factors of the eight lowest-energy conformers of (2*S*,3*S*,5*R*)-**2** used for VCD and ECD spectral calculations

Atomic coordinates - (2*S*,3*S*,5*R*)-**2**

B3LYP/6-31G(d) opt

Total energy = –1493.42034 kcal/mol

Conf 1

C	3.16680400	-0.33549800	-1.09600000
C	3.72870500	-1.15969700	-0.10760000
C	1.94510300	0.31400000	-0.86720000
C	1.27860300	0.15139900	0.35350000
C	1.84430400	-0.65800000	1.34470000
C	3.06390500	-1.30889800	1.12180000
C	-0.07919800	0.80229600	0.63740000
C	-0.21160100	2.22769600	0.04740000
C	-1.23869700	-0.11190600	0.23920000
C	-2.18629600	-0.46990700	1.19740000
C	-3.30209500	-1.28630900	0.90670000
C	-3.42179400	-1.72100900	-0.40860000
C	-2.47029500	-1.36040800	-1.36330000
C	-1.37319600	-0.57300600	-1.08770000
O	-4.12549400	-1.57111100	1.95140000
O	-4.35509300	-2.56701100	-0.98900000
C	-4.10689300	-2.47011100	-2.39350000
O	-2.78839400	-1.94980800	-2.56580000
C	-5.37719300	-2.20761300	1.69500000
O	3.69480700	-2.10349700	2.03130000
C	3.05380700	-2.33869800	3.27470000
O	4.88710600	-1.85009500	-0.35490000
O	3.89420300	-0.22929700	-2.24460000
C	-1.47410200	3.01479400	0.45690000
C	-0.98360500	4.46579500	0.48870000
O	0.37789500	4.49859700	0.50890000
C	0.91769800	3.16369800	0.52700000
O	-1.65040600	5.46849400	0.49280000
C	-2.71990200	2.87569200	-0.42110000
H	1.52350100	0.94739900	-1.63780000
H	1.32130400	-0.78190100	2.28620000
H	-0.14329900	0.92349600	1.72690000
H	-0.18970100	2.17949600	-1.04910000
H	-2.09599700	-0.11890700	2.22110000
H	-0.64539600	-0.34220500	-1.85610000
H	-4.16849100	-3.46491100	-2.84040000
H	-4.83519400	-1.78281200	-2.85110000
H	-5.87199300	-2.27511400	2.66560000
H	-5.24159100	-3.21021300	1.27830000
H	-5.99239400	-1.61331400	1.01000000
H	3.71460800	-3.00929700	3.82710000
H	2.07700800	-2.82120000	3.14000000
H	2.92150500	-1.40969800	3.84540000
H	-1.73920200	2.75989400	1.49540000
H	1.80209800	3.15420000	-0.11180000
H	1.22819800	2.92739900	1.55300000
H	-3.46710300	3.61339100	-0.11390000
H	-3.15140000	1.87539100	-0.34130000
H	-2.47720200	3.06389200	-1.47340000
C	6.08230500	-1.13979300	-0.02990000
C	3.36610200	0.54480200	-3.30860000
H	6.91100600	-1.80869200	-0.27440000
H	6.11760500	-0.89409300	1.03900000
H	6.17000300	-0.22129300	-0.62330000
H	2.39680300	0.15670100	-3.64840000
H	4.09000200	0.46550400	-4.12160000
H	3.25350000	1.60080200	-3.02760000

B3LYP/6-31G(d) opt

Total energy = –1493.419984 kcal/mol

Conf 2

C	3.24970600	-0.03319500	-0.97360700
C	3.84830500	-0.78339600	0.05139300
C	1.97850600	0.53000600	-0.78970700
C	1.29020600	0.33750700	0.41439300
C	1.88090500	-0.41849400	1.43269300
C	3.14910500	-0.98449500	1.25399300
C	-0.11859300	0.89370800	0.64909300
C	-0.33899200	2.29070800	0.02079300
C	-1.19509400	-0.11489100	0.24549300
C	-2.12869500	-0.53419000	1.19259300
C	-3.16809600	-1.44408900	0.89649300
C	-3.22669600	-1.90828900	-0.41290700
C	-2.28979600	-1.48579000	-1.35660700
C	-1.26609500	-0.60689100	-1.07530700
O	-3.98489600	-1.77908800	1.93129300
O	-4.07649700	-2.83728800	-0.99510700
C	-3.81149700	-2.74028800	-2.39640700
O	-2.53559600	-2.11889000	-2.55410700
C	-5.17609700	-2.51898700	1.66399300
O	3.79710400	-1.74159600	2.18339300
C	3.15820400	-1.96449500	3.43029300
O	5.12250400	-1.26699700	-0.09790700
O	3.99230600	0.09150400	-2.11040700
C	-1.66499100	2.99360900	0.38209300
C	-1.28199000	4.47720900	0.37989300
O	0.07191000	4.60980800	0.43129300
C	0.70640900	3.31880700	0.50169300
O	-2.01998900	5.42781000	0.33709300
C	-2.88029200	2.73861100	-0.51220700
H	1.53310700	1.11610600	-1.58400700
H	1.33670500	-0.57359300	2.35749300
H	-0.21979300	1.03370800	1.73339300
H	-0.28709200	2.21770800	-1.07350700
H	-2.08759400	-0.16049000	2.21139300
H	-0.54539500	-0.32899200	-1.83490700
H	-3.78569800	-3.74278800	-2.82900700
H	-4.58369600	-2.11958800	-2.87660700
H	-5.68119700	-2.61258700	2.62709300
H	-4.95229800	-3.51298700	1.26529300
H	-5.82489600	-1.98628700	0.95949300
H	3.84930300	-2.57659600	4.01259300
H	2.20910300	-2.50329400	3.30929300
H	2.97270500	-1.02229500	3.96239300
H	-1.93079200	2.75011000	1.42329300
H	1.60670900	3.35830600	-0.11310700
H	1.00450900	3.13370700	1.54169300
H	-3.68119100	3.43431100	-0.24510700
H	-3.24549300	1.71511100	-0.40340700
H	-2.62999200	2.90611000	-1.56630700
C	5.19570300	-2.57699700	-0.66180700
C	3.46610700	0.86020500	-3.17910700
H	6.25830300	-2.82439800	-0.72200700
H	4.76020300	-2.59869700	-1.66850700
H	4.68740300	-3.31049700	-0.02370700
H	2.52630600	0.43820500	-3.56030700
H	4.22010600	0.82800400	-3.96760700
H	3.29850800	1.90430500	-2.88310700

B3LYP/6-31G(d) opt

Total energy = –1493.419496 kcal/mol

Conf 3

C	-3.22700400	0.14481200	0.96230200

C	-3.85980600	-0.54738600	-0.08299800
C	-1.91320300	0.61130800	0.80970200
C	-1.21630300	0.37810600	-0.38209800
C	-1.84160500	-0.32149200	-1.41999800
C	-3.15260700	-0.79038900	-1.27309800
C	0.23439800	0.82920200	-0.58219800
C	0.53780200	2.20860100	0.05200200
C	1.22989500	-0.25180100	-0.15539800
C	2.17119400	-0.71550400	-1.08659800
C	3.13719100	-1.68810700	-0.75519800
C	3.11498900	-2.16480700	0.55010200
C	2.17779100	-1.70950400	1.46570200
C	1.21949300	-0.76210100	1.15580200
O	4.07738900	-2.20101000	-1.59529800
O	3.90798600	-3.13430900	1.12040200
C	3.57628600	-3.10290800	2.51180200
O	2.35168900	-2.37280500	2.65840200
C	4.10869100	-1.72321000	-2.93139800
O	-3.83740900	-1.48668700	-2.22399800
C	-3.19201000	-1.74658800	-3.45989800
O	-5.17090700	-0.92978300	0.03590200
O	-3.98130300	0.31571400	2.08480200
C	1.91880400	2.81509700	-0.27359800
C	1.64180800	4.32199700	-0.28979800
O	0.30230900	4.54990100	-0.37419800
C	-0.42079500	3.30700300	-0.45429800
O	2.44461100	5.21799500	-0.23619800
C	3.08560300	2.48109300	0.65880200
H	-1.44060100	1.15320600	1.61950200
H	-1.29180600	-0.50869400	-2.33549800
H	0.36909800	0.96250100	-1.66419800
H	0.45300200	2.14020100	1.14440200
H	2.15619500	-0.30680400	-2.09069800
H	0.48719400	-0.44819900	1.89000200
H	3.43588300	-4.12410800	2.87510200
H	4.37458800	-2.59111100	3.06950200
H	4.92328900	-2.26091200	-3.41959800
H	4.31129400	-0.64481000	-2.96969800
H	3.16809000	-1.93380700	-3.45719800
H	-3.91531100	-2.29928600	-4.06219800
H	-2.28921100	-2.35739100	-3.32559800
H	-2.92460700	-0.81658900	-3.97859800
H	2.19760300	2.54739600	-1.30539800
H	-1.32879400	3.41190600	0.14110200
H	-0.70969500	3.13950400	-1.49989800
H	3.94540500	3.10909100	0.40730200
H	3.37310000	1.43069200	0.57490200
H	2.81890400	2.68289400	1.70270200
C	-5.36031100	-2.24748200	0.55260200
C	-3.42000100	1.03111200	3.17270200
H	-4.90991300	-2.99928300	-0.10719800
H	-6.44071100	-2.40537900	0.59670200
H	-4.93851100	-2.34088300	1.56110200
H	-2.52480300	0.53311000	3.56910200
H	-4.19150100	1.05081500	3.94460200
H	-3.16489800	2.06151200	2.89150200

B3LYP/6-31G(d) opt

Total energy = –1493.419263 kcal/mol

Conf 4

C	3.02999500	-1.15240600	1.24120400
C	3.70979500	-1.01090800	0.02550400
C	1.79279700	-0.53070200	1.43550400
C	1.21409900	0.24310000	0.42880400
C	1.89250000	0.38689800	-0.79269600
C	3.13059800	-0.23240600	-0.99699600
C	-0.16059800	0.87120500	0.68010400
C	-0.30349400	2.29110500	0.07950400

C	-1.29560200	-0.06519100	0.26280400
C	-2.23060300	-0.46968800	1.21470400
C	-3.31810600	-1.31928500	0.91130400
C	-3.41520700	-1.74928400	-0.40739600
C	-2.47030600	-1.35098700	-1.35329600
C	-1.40740300	-0.52129100	-1.06819600
O	-4.15580700	-1.61058200	1.94230400
O	-4.37731000	-2.53598100	-1.02389600
C	-3.82841100	-2.84018300	-2.30819600
O	-2.80070800	-1.88608600	-2.57799600
C	-5.17091000	-2.59677900	1.75660400
O	3.86799800	-0.13400800	-2.14029600
C	3.33730100	0.61349300	-3.22289600
O	4.91049300	-1.64801200	-0.17969600
O	3.58619300	-1.84770700	2.28710400
C	-1.58069100	3.06561000	0.46760400
C	-1.10898600	4.52330800	0.48120400
O	0.25191400	4.57320400	0.51950400
C	0.80620900	3.24520200	0.56810400
O	-1.78768300	5.51761000	0.45870400
C	-2.81889200	2.89571400	-0.41539600
H	1.29779600	-0.66530000	2.39270400
H	1.46240200	0.98970000	-1.58339600
H	-0.24759800	0.99530500	1.76730400
H	-0.26619400	2.23770500	-1.01659600
H	-2.14620200	-0.14048900	2.24590400
H	-0.68970200	-0.25409300	-1.83429600
H	-3.39521400	-3.85228400	-2.29519600
H	-4.61201000	-2.75658000	-3.06449600
H	-5.67231000	-2.68127700	2.72250400
H	-4.73911300	-3.56518000	1.48060400
H	-5.89170900	-2.29327600	0.99130400
H	4.07310000	0.53789100	-4.02549600
H	3.19850400	1.67029400	-2.95789600
H	2.38099900	0.19929700	-3.56819600
H	-1.84809200	2.82231000	1.50840400
H	1.70340900	3.23719900	-0.05289600
H	1.09840900	3.02650100	1.60330400
H	-3.57638900	3.63011600	-0.12619600
H	-3.23939500	1.89241500	-0.31959600
H	-2.57199100	3.06741300	-1.46959600
C	6.05999600	-0.82721600	0.04930400
C	3.70518800	-3.26190800	2.09600400
H	6.92959400	-1.46361800	-0.13089600
H	6.08019700	-0.46351600	1.08400400
H	6.08069900	0.02168400	-0.64359600
H	4.34888700	-3.49511000	1.24330400
H	2.71648600	-3.71660500	1.94940400
H	4.14908700	-3.65240900	3.01470400

B3LYP/6-31G(d) opt

Total energy = –1493.419162 kcal/mol

Conf 5

C	3.13550100	-0.12400500	-1.03210600
C	3.80230000	-0.74750500	0.03509400
C	1.87020200	0.44849700	-0.83900600
C	1.25520200	0.39239800	0.41759400
C	1.91450100	-0.23560300	1.47979400
C	3.17720000	-0.81160500	1.29209400
C	-0.14279800	0.96789900	0.66649400
C	-0.38769600	2.30990000	-0.06600600
C	-1.24419900	-0.06109900	0.39839400
C	-1.36770000	-0.67879900	-0.84660600
C	-2.38300100	-1.61209800	-1.13870600
C	-3.27170100	-1.90709700	-0.10780600
C	-3.13650000	-1.30049700	1.13819400
C	-2.14889900	-0.38069800	1.43169400
O	-2.39330100	-2.11259800	-2.40380600

O	-4.38680200	-2.73249600	-0.09780600
C	-4.75550200	-2.82709500	1.28019400
O	-4.14280100	-1.73649600	1.97009400
C	-3.23530300	-3.22519700	-2.70460600
O	3.88790000	-1.45220600	2.26269400
C	3.32779900	-1.52920500	3.56349400
O	5.07190000	-1.23810700	-0.13130600
O	3.80890100	-0.12590500	-2.21770600
C	-1.69179500	3.05250100	0.29499400
C	-1.30059300	4.52760100	0.15469400
O	0.05500700	4.65129900	0.12969400
C	0.68530500	3.36479800	0.27669400
O	-2.03449200	5.47880200	0.07169400
C	-2.94659500	2.73760300	-0.52250600
H	1.37000200	0.93439700	-1.66750600
H	1.42930100	-0.28350300	2.44819400
H	-0.19359700	1.19969900	1.73879400
H	-0.38699600	2.14360000	-1.15120600
H	-0.65779900	-0.47270000	-1.64000600
H	-2.08119900	0.07160200	2.41519400
H	-5.84160200	-2.75149400	1.36929400
H	-4.38820300	-3.77759600	1.69719400
H	-3.02100300	-3.47749700	-3.74490600
H	-4.29390200	-2.97099600	-2.59650600
H	-3.00390400	-4.08349700	-2.06380600
H	4.05879900	-2.06700600	4.16999400
H	2.37849900	-2.08130400	3.56479400
H	3.16520100	-0.53180500	3.99269400
H	-1.91209500	2.89870100	1.36359400
H	1.55420500	3.34359700	-0.38250600
H	1.03330500	3.26419800	1.31279400
H	-3.73159500	3.45930400	-0.27770600
H	-3.31249700	1.72910300	-0.31770600
H	-2.74139500	2.81790200	-1.59620600
C	5.12909800	-2.59760700	-0.56390600
C	3.20640200	0.50589500	-3.33530600
H	6.18969800	-2.84620800	-0.65000600
H	4.64639800	-2.72200600	-1.54120600
H	4.65799700	-3.26520600	0.16829400
H	2.25300100	0.03199600	-3.60470600
H	3.91250200	0.38869400	-4.15930600
H	3.03900300	1.57579500	-3.15310600

B3LYP/6-31G(d) opt

Total energy = –1493.419093 kcal/mol

Conf 6

C	3.04180900	-0.45750400	-1.12739700
C	3.66420900	-1.17230500	-0.09079700
C	1.83491000	0.21809600	-0.89629700
C	1.24451000	0.19329700	0.37310300
C	1.87210900	-0.50420400	1.41090300
C	3.07600900	-1.18300400	1.18530300
C	-0.09249000	0.88189700	0.66380300
C	-0.23318900	2.25849800	-0.03179700
C	-1.28519000	-0.03990200	0.39550300
C	-1.49179100	-0.60530200	-0.86309700
C	-2.59109100	-1.43790100	-1.15529700
C	-3.47639100	-1.68840100	-0.10959700
C	-3.25909100	-1.13470100	1.14940300
C	-2.18939100	-0.31180100	1.44270300
O	-2.67659100	-1.89380100	-2.43399700
O	-4.65889200	-2.41380000	-0.09379700
C	-4.99959200	-2.52070000	1.29040300
O	-4.27959100	-1.50750000	1.99470300
C	-3.61439200	-2.92460100	-2.74359700
O	3.76220900	-1.87860500	2.13590300
C	3.20170900	-1.96940400	3.43570300
O	4.80640900	-1.89070500	-0.33429700

O	3.69750900	-0.47900500	-2.32249700
C	-1.45908900	3.10299800	0.37520300
C	-0.94298800	4.54109800	0.26060300
O	0.41801200	4.54649700	0.20750300
C	0.93501100	3.20639700	0.31090300
O	-1.59158700	5.55459800	0.21610300
C	-2.75228900	2.91839900	-0.42219700
H	1.36311000	0.76379700	-1.70389700
H	1.41010900	-0.52050300	2.39160300
H	-0.10299000	1.09029700	1.74220300
H	-0.26948900	2.12029800	-1.12019700
H	-0.78629100	-0.43690200	-1.66939700
H	-2.05929000	0.10269900	2.43660300
H	-6.07279200	-2.35709900	1.41180300
H	-4.70319200	-3.51110000	1.66900300
H	-3.44779200	-3.16090100	-3.79619700
H	-4.64549200	-2.58850000	-2.59869700
H	-3.43779300	-3.81840100	-2.13459700
H	3.89590800	-2.57960500	4.01650300
H	2.21820800	-2.45670400	3.41770300
H	3.10630900	-0.98190400	3.90690300
H	-1.67168900	2.94149800	1.44420300
H	1.78511100	3.12459600	-0.36789700
H	1.29351100	3.05009700	1.33660300
H	-3.46938800	3.69449900	-0.13889700
H	-3.19558900	1.93749900	-0.23819700
H	-2.56298900	3.01409900	-1.49759700
C	6.01890900	-1.17130600	-0.10809700
C	3.10131000	0.17709600	-3.42929700
H	6.83220900	-1.86270700	-0.34169700
H	6.10130900	-0.85470600	0.93900300
H	6.08730900	-0.29550600	-0.76549700
H	2.11551000	-0.24460400	-3.66539700
H	3.77531000	0.01079500	-4.27159700
H	2.99991000	1.25709600	-3.25579700

B3LYP/6-31G(d) opt

Total energy = –1493.418816 kcal/mol

Conf 7

C	3.13299400	0.19907500	-0.89589800
C	3.78768800	-0.50553000	0.12690200
C	1.82249700	0.66418500	-0.70969800
C	1.15169500	0.41929000	0.49480200
C	1.79959000	-0.29201500	1.51080200
C	3.10628600	-0.76002500	1.33010200
C	-0.29400100	0.86670100	0.73520200
C	-0.63489100	2.22520400	0.07520200
C	-1.29681000	-0.23479100	0.38150200
C	-1.31111400	-0.80569100	-0.90059800
C	-2.23742200	-1.80168400	-1.26109800
C	-3.13892500	-2.20357700	-0.27939800
C	-3.11702000	-1.64547700	0.98710200
C	-2.21461300	-0.66138400	1.35770200
O	-2.32892600	-2.40708300	-2.47649800
O	-4.15193200	-3.13016900	-0.37699800
C	-4.64423300	-3.27816500	0.95850200
O	-4.11682500	-2.20406900	1.74890200
C	-1.42562300	-1.99889000	-3.49239800
O	3.81158100	-1.46523000	2.25890200
C	3.19567900	-1.73152500	3.50920200
O	5.09628500	-0.88394000	-0.02669800
O	3.86249500	0.38357000	-2.03329800
C	-2.01528600	2.82171400	0.42230200
C	-1.75897500	4.33201300	0.39220200
O	-0.42057300	4.57990200	0.43450200
C	0.32121800	3.34939700	0.52770200
O	-2.57466800	5.21571900	0.33550200
C	-3.20018900	2.44922400	-0.47179800

H	1.33290100	1.21678900	-1.50189800
H	1.27028800	-0.48811100	2.43640200
H	-0.38940000	1.02950200	1.81730200
H	-0.57919200	2.13020400	-1.01719800
H	-0.56991200	-0.48649700	-1.62289800
H	-2.22371000	-0.24208400	2.35810200
H	-5.73613200	-3.22135700	0.95220200
H	-4.30214000	-4.23766800	1.37330200
H	-1.67832800	-2.59518800	-4.37079800
H	-0.38332500	-2.19369800	-3.20789800
H	-1.54301500	-0.93338900	-3.73019800
H	3.93307500	-2.28793100	4.09060200
H	2.28947400	-2.34071800	3.39340200
H	2.94198600	-0.80392300	4.03870200
H	-2.26448800	2.57641600	1.46710200
H	1.21231800	3.45149000	-0.09329800
H	0.63901700	3.21249400	1.56930200
H	-4.06328400	3.06883000	-0.21129800
H	-3.46859700	1.39672600	-0.35799800
H	-2.96378800	2.63312200	-1.52639800
C	5.27787500	-2.21554100	-0.50909800
C	3.29330100	1.14657400	-3.08319800
H	4.85497000	-2.95003800	0.18710200
H	6.35727400	-2.36794900	-0.58439800
H	4.82397400	-2.34163800	-1.50029800
H	2.38499700	0.67598100	-3.48409800
H	4.05190100	1.18626800	-3.86699800
H	3.05530900	2.16827600	-2.75869800

B3LYP/6-31G(d) opt

Total energy = –1493.418668 kcal/mol

Conf 8

C	3.07890200	-0.13061800	-1.00480300
C	3.66909800	-0.95902100	-0.03720300
C	1.82450500	0.45188900	-0.76940300
C	1.15640400	0.22349200	0.43979700
C	1.75230000	-0.58701100	1.41249700
C	3.00079700	-1.17591700	1.18069700
C	-0.23389300	0.79909900	0.73079700
C	-0.46008600	2.20150000	0.11549700
C	-1.34429800	-0.19309500	0.37519700
C	-1.43560100	-0.73219500	-0.91720300
C	-2.45960600	-1.62719000	-1.27900300
C	-3.37850700	-1.96088500	-0.28780300
C	-3.28090500	-1.43488600	0.98899700
C	-2.28130000	-0.55019100	1.36099700
O	-2.62960900	-2.19568900	-2.50330300
O	-4.47691200	-2.78477900	-0.38310300
C	-4.94701200	-2.92367700	0.96099700
O	-4.31570700	-1.91328000	1.75899700
C	-1.69570700	-1.87189400	-3.52230300
O	3.65969300	-1.96992100	2.07089700
C	3.02389100	-2.26691800	3.30419700
O	4.86059500	-1.58442700	-0.29910300
O	3.81120300	0.04797800	-2.14140300
C	-1.77268300	2.91180700	0.51049700
C	-1.37827500	4.39230500	0.51979700
O	-0.02187400	4.51489800	0.53839700
C	0.60471900	3.21939500	0.57659700
O	-2.10907000	5.34910900	0.50929700
C	-3.00448400	2.67861300	-0.36730300
H	1.38030800	1.08839100	-1.52460300
H	1.22829900	-0.76250800	2.34519700
H	-0.28779300	0.93979900	1.81889700
H	-0.43618700	2.13230000	-0.97990300
H	-0.67860000	-0.47109900	-1.64670300
H	-2.23079800	-0.15499100	2.36999700
H	-6.03031100	-2.77967200	0.98429700

H	-4.67251700	-3.91657800	1.34669700
H	-2.01671000	-2.42689200	-4.40540300
H	-0.67810800	-2.17949900	-3.24890300
H	-1.70200100	-0.79699400	-3.74660300
H	3.71078800	-2.92342100	3.84139700
H	2.06968800	-2.78731300	3.15069700
H	2.84909600	-1.36051700	3.89909700
H	-2.02358400	2.65770800	1.55259700
H	1.48751900	3.26019000	-0.06320300
H	0.93151800	3.02109300	1.60559700
H	-3.79798000	3.37211700	-0.07390300
H	-3.37228900	1.65481500	-0.27200300
H	-2.77128300	2.86521200	-1.42210300
C	6.01569800	-0.87383300	0.14849700
C	3.27600700	0.86718100	-3.16650300
H	6.09030300	0.10586700	-0.33990300
H	6.87729500	-1.48413700	-0.13270300
H	6.00259900	-0.74373300	1.23759700
H	2.32640500	0.46978600	-3.54960300
H	4.01630700	0.86167700	-3.96860300
H	3.12171200	1.89958200	-2.82460300

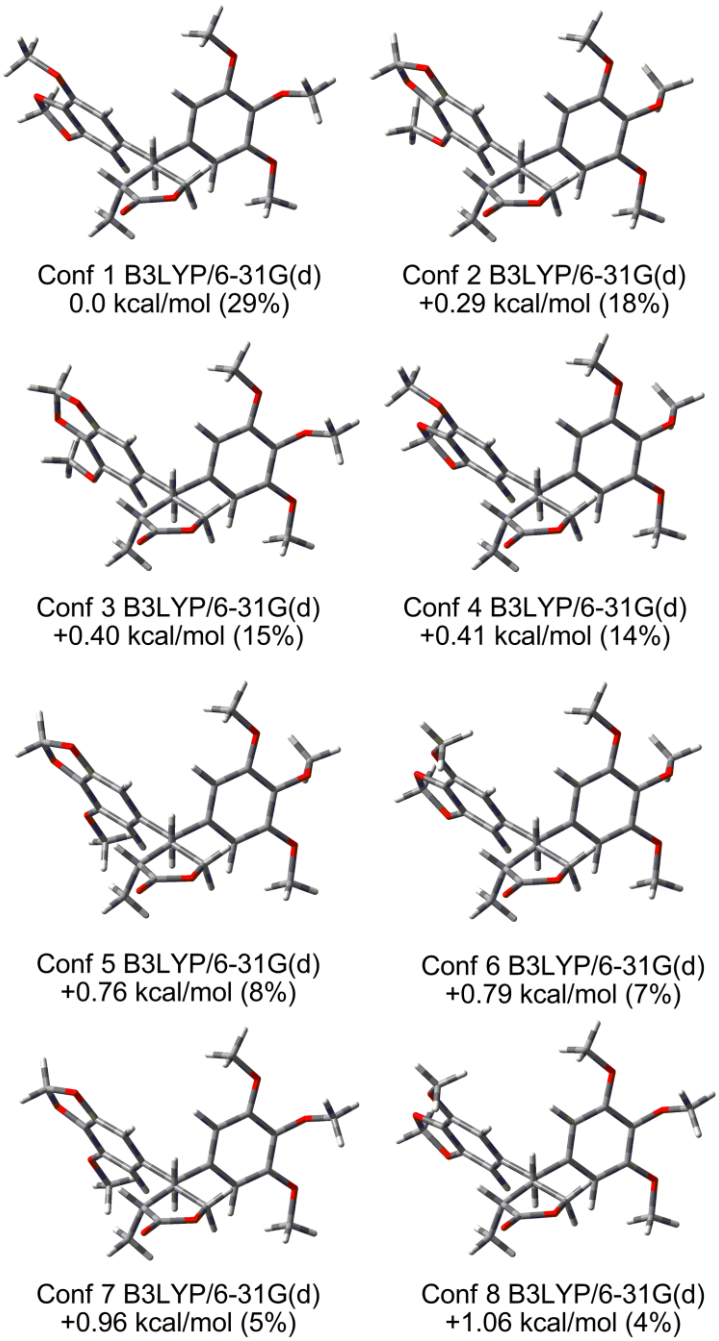

Figure 3. Optimized structures, relative energies, and Boltzmann factors of the eight lowest-energy conformers of (2*R*,3*S*,5*R*)-**3** at the B3LYP/6-31G(d) level

Atomic coordinates - (2*R*,3*S*,5*R*)-**3**

B3LYP/6-31G(d) opt

Total energy = –1493.41721 kcal/mol

Conf 1

C	3.37459000	-0.75352300	1.01379900
C	3.50378700	-1.48692400	-0.17610100
C	2.22409400	0.01478300	1.24579900
C	1.20369400	0.06258800	0.29079900
C	1.33169100	-0.65991300	-0.90080100
C	2.47838700	-1.42691900	-1.13750100
C	-0.03220200	0.93299400	0.54859900
C	-0.02259500	2.18639400	-0.35220100
C	-1.32510600	0.11880000	0.46639900
C	-2.09390600	0.04710400	-0.69540100
C	-3.26591000	-0.73659100	-0.79260100
C	-3.62791300	-1.45608900	0.34019900
C	-2.85701300	-1.38199300	1.50029900
C	-1.71590900	-0.61669800	1.60679900
O	-3.91191000	-0.69068800	-1.98920100
O	-4.73291700	-2.26158400	0.57519900
C	-4.45402000	-2.90398500	1.82149900
O	-3.44291700	-2.14419000	2.48479900
C	-5.09321300	-1.46988200	-2.17520100
O	2.69988300	-2.15772000	-2.26640100
C	1.68918300	-2.17521500	-3.26200100
O	4.58938300	-2.30132900	-0.37330100
O	4.42359000	-0.85612800	1.87909900
C	-1.10899000	3.25869900	-0.10580100
C	-0.43398400	4.52969600	-0.62840100
O	0.91611500	4.33938900	-0.70110100
C	1.26730900	3.02038700	-0.23910100
O	-0.95137900	5.57679800	-0.91970100
C	-1.53338900	3.47990100	1.35819900
H	2.11689700	0.57408300	2.16849900
H	0.52719100	-0.64100900	-1.62600100
H	0.05050000	1.28449300	1.58429900
H	-0.09919700	1.86939400	-1.39980100
H	-1.82220300	0.60090200	-1.58730100
H	-1.13990900	-0.59300100	2.52549900
H	-5.36002000	-2.91718000	2.43159900
H	-4.08402500	-3.92428700	1.63709900
H	-5.41861200	-1.26248000	-3.19640100
H	-5.87971200	-1.17937800	-1.47140100
H	-4.88851900	-2.53998300	-2.06400100
H	2.06628000	-2.82211700	-4.05630100
H	1.50308800	-1.17231400	-3.66910100
H	0.74808100	-2.58651000	-2.87460100
H	-2.00739100	3.07670300	-0.70170100
H	2.08360700	2.65268300	-0.86290100
H	1.62570900	3.09538600	0.79569900
H	-2.06969300	2.60710300	1.74209900
H	-2.19638500	4.34820400	1.41799900
H	-0.67398800	3.67119700	2.01159900
C	5.69138600	-1.67193400	-1.02750100
C	4.33909300	-0.17432800	3.11949900
H	6.46928200	-2.43413800	-1.11690100
H	6.07399000	-0.83073600	-0.43610100
H	5.40968700	-1.32193300	-2.02840100
H	4.26379800	0.91277300	2.98169900
H	5.26439200	-0.40633200	3.64989900
H	3.48399100	-0.52202400	3.71409900

B3LYP/6-31G(d) opt

Total energy = –1493.416745 kcal/mol

Conf 2

C	-2.63240200	-1.10310000	1.28430000
C	-3.64630200	-1.13539900	0.31000000
C	-1.43090100	-0.43050100	1.03230000
C	-1.22620100	0.20509900	-0.19770000
C	-2.22370100	0.16110000	-1.17670000
C	-3.42910100	-0.51219900	-0.92890000
C	0.06850000	0.97849900	-0.47490000
C	0.10950000	2.28689900	0.34380000
C	1.30839900	0.10009800	-0.29290000
C	1.73119900	-0.67880200	-1.37160000
C	2.83299800	-1.55660300	-1.30460000
C	3.50739800	-1.60930300	-0.08770000
C	3.08869900	-0.82630300	0.98480000
C	2.00869900	0.03239800	0.93060000
O	3.11009800	-2.25820300	-2.43570000
O	4.58679800	-2.38780400	0.30650000
C	4.98879800	-1.83790400	1.56310000
O	3.89389900	-1.07550400	2.07340000
C	4.26229700	-3.10000400	-2.47060000
O	-4.45250100	-0.62119900	-1.82360000
C	-4.31280100	0.01380100	-3.08370000
O	-4.85050200	-1.73099900	0.58470000
O	-2.92080200	-1.76240000	2.44190000
C	1.27000100	3.27249800	0.07390000
C	0.66140200	4.61179800	0.49860000
O	-0.69939800	4.51119900	0.53040000
C	-1.11969900	3.19079900	0.13300000
O	1.23640200	5.63929800	0.74960000
C	1.75210100	3.38069800	-1.38510000
H	-0.64350100	-0.42350100	1.77590000
H	-2.05340100	0.64310000	-2.13280000
H	0.03800000	1.26409900	-1.53310000
H	0.13070000	2.03369900	1.41130000
H	1.20059900	-0.63540200	-2.31800000
H	1.73609900	0.62199800	1.79750000
H	5.22179800	-2.65030400	2.25510000
H	5.85819800	-1.17840500	1.41730000
H	4.27269700	-3.53460400	-3.47180000
H	4.19999700	-3.89680400	-1.72280000
H	5.18129800	-2.52630400	-2.30920000
H	-5.24090100	-0.18709800	-3.62220000
H	-3.46770100	-0.39519900	-3.65360000
H	-4.18420000	1.09900100	-2.97730000
H	2.13610100	3.07119700	0.71030000
H	-1.97879900	2.91360000	0.74560000
H	-1.43599900	3.22499900	-0.91750000
H	2.24470100	2.45629700	-1.70090000
H	2.46890100	4.20299700	-1.47130000
H	0.92630100	3.58499800	-2.07680000
C	-4.91950300	-3.11529900	0.24170000
C	-1.95330200	-1.74880000	3.47940000
H	-5.92240300	-3.44889800	0.51930000
H	-4.17580300	-3.69819900	0.79900000
H	-4.77300300	-3.26299900	-0.83550000
H	-1.01640200	-2.22890100	3.16740000
H	-2.39280200	-2.31500000	4.30260000
H	-1.73890100	-0.72630000	3.81730000

B3LYP/6-31G(d) opt

Total energy = –1493.416561 kcal/mol

Conf 3

C	-3.28280600	-0.84860100	-1.07890400

C	-3.47640600	-1.52790000	0.13399600
C	-2.13440500	-0.06680100	-1.27200400
C	-1.17970500	0.04899800	-0.25670400
C	-1.37320600	-0.61880200	0.95799600
C	-2.51810600	-1.39970100	1.15569600
C	0.05239500	0.93319700	-0.48270400
C	-0.03220400	2.22569700	0.35809600
C	1.35959500	0.16229600	-0.28690400
C	1.88439400	-0.53780500	-1.37490400
C	3.05899400	-1.31420500	-1.29830400
C	3.68839400	-1.36150600	-0.05750400
C	3.16199400	-0.66530500	1.02739600
C	2.01749500	0.10389500	0.96059600
O	3.45889300	-1.91590600	-2.45020400
O	4.87459300	-1.97300700	0.32139600
C	4.89779300	-1.86590700	1.74649600
O	3.98389400	-0.83280600	2.11909600
C	4.51299300	-2.87730700	-2.40310400
O	-2.80010700	-2.08160100	2.30199600
C	-1.85580700	-2.03460200	3.35929600
O	-4.55650700	-2.35670000	0.29899600
O	-4.26960600	-1.01530000	-2.00520400
C	1.04489700	3.30969600	0.12219600
C	0.31889800	4.58519700	0.55899600
O	-1.02940200	4.36959800	0.56529600
C	-1.32990300	3.02559800	0.14089600
O	0.79969900	5.65299600	0.83749600
C	1.53539700	3.48349600	-1.32760400
H	-1.97650500	0.44869800	-2.21260400
H	-0.62150600	-0.54750300	1.73439600
H	0.02309600	1.23529700	-1.53620400
H	-0.00480400	1.95779700	1.42209600
H	1.37849400	-0.51470400	-2.33550400
H	1.66589500	0.63669600	1.83589600
H	4.57609300	-2.81860700	2.19479600
H	5.90509400	-1.59710800	2.07229600
H	4.60569200	-3.25530700	-3.42300400
H	4.26739200	-3.70350600	-1.72650400
H	5.45809300	-2.42410700	-2.08930400
H	-2.27170700	-2.65340100	4.15649600
H	-1.71390600	-1.01120200	3.73199600
H	-0.88450700	-2.44340200	3.05159600
H	1.91579700	3.17029500	0.76829600
H	-2.17130300	2.66609900	0.73529600
H	-1.63250300	3.04959800	-0.91370400
H	2.10389700	2.60719500	-1.65260400
H	2.18529800	4.36149500	-1.38940400
H	0.70459800	3.63409600	-2.02720400
C	-5.71270700	-1.72209900	0.84559600
C	-4.11510600	-0.39190000	-3.26950400
H	-6.48060700	-2.49619800	0.91769600
H	-6.06930600	-0.91759800	0.19039600
H	-5.50770600	-1.32029900	1.84579600
H	-4.06890500	0.70190000	-3.18050400
H	-4.99880600	-0.66869900	-3.84730400
H	-3.21630600	-0.74950100	-3.78880400

B3LYP/6-31G(d) opt

Total energy = –1493.416558 kcal/mol

Conf 4

C	2.55560200	-1.15258600	-1.28469600
C	3.62710200	-1.13368400	-0.37329600
C	1.36570100	-0.47698900	-0.99029600
C	1.23160000	0.21501100	0.21860400
C	2.28630000	0.22221300	1.13650400
C	3.48020100	-0.45518400	0.84680400
C	-0.05080200	0.99510800	0.53280400
C	-0.14680500	2.26090800	-0.34609600

C	-1.28690000	0.09590600	0.47610400
C	-2.09820000	0.00120400	-0.65449600
C	-3.21279800	-0.86479800	-0.72829600
C	-3.47169700	-1.64189900	0.39460400
C	-2.65809700	-1.54469700	1.52350400
C	-1.57299900	-0.69979500	1.60740400
O	-3.91219800	-0.83280000	-1.89489600
O	-4.50309500	-2.53480100	0.64910400
C	-4.12179300	-3.19220000	1.85970400
O	-3.14239500	-2.37819800	2.50580400
C	-5.03939600	-1.69340200	-2.05659600
O	4.55720100	-0.51558200	1.68090400
C	4.49230000	0.18411800	2.91260400
O	4.81830400	-1.73298200	-0.69339600
O	2.77910400	-1.86238600	-2.42659600
C	-1.29030700	3.26030600	-0.05459600
C	-0.70791000	4.57890700	-0.57069600
O	0.64839100	4.47331000	-0.68139600
C	1.09239300	3.17111100	-0.25239600
O	-1.29671200	5.59660600	-0.82899600
C	-1.69180700	3.43240500	1.42240400
H	0.53260100	-0.50869100	-1.68209600
H	2.17089800	0.75001300	2.07660400
H	0.04089700	1.33470800	1.57190400
H	-0.23170400	1.95540800	-1.39649600
H	-1.90680100	0.59940400	-1.53849600
H	-0.96019900	-0.66039400	2.50140400
H	-4.99629300	-3.29400200	2.50620400
H	-3.68459100	-4.17499900	1.62500400
H	-5.42549700	-1.47980300	-3.05499600
H	-5.81239700	-1.48580400	-1.30989600
H	-4.75039400	-2.74770200	-1.99109600
H	5.45380000	0.01572000	3.40110400
H	3.68780000	-0.19758400	3.55550400
H	4.34909700	1.26181700	2.75800400
H	-2.19060600	3.03350400	-0.63199600
H	1.91209400	2.86441200	-0.90369600
H	1.47329300	3.25111100	0.77380400
H	-2.16870500	2.52440400	1.80320400
H	-2.40190900	4.26000300	1.51210400
H	-0.82970800	3.66270700	2.05960400
C	4.92110600	-3.09978100	-0.29389600
C	1.75450400	-1.89248800	-3.40769600
H	5.91020700	-3.43747900	-0.61289600
H	4.15330800	-3.71308300	-0.78169600
H	4.83720700	-3.20008200	0.79540400
H	1.51610200	-0.88488800	-3.77249600
H	0.83900500	-2.36249000	-3.02469600
H	2.14990500	-2.48968700	-4.23139600

B3LYP/6-31G(d) opt

Total energy = –1493.416357 kcal/mol

Conf 5

C	3.39229900	-0.51628200	1.04850600
C	3.59120100	-1.15118200	-0.18189400
C	2.18719600	0.14721400	1.31460600
C	1.17229600	0.18951000	0.35980600
C	1.36119800	-0.45848900	-0.87119400
C	2.55820100	-1.12358500	-1.14469400
C	-0.12160600	0.95940600	0.64720600
C	-0.17661000	2.26180600	-0.17949400
C	-1.35540300	0.06800200	0.49230600
C	-2.10610300	0.02180000	-0.68259400
C	-3.21830000	-0.83420400	-0.84909400
C	-3.53869800	-1.65300500	0.22740600
C	-2.78639800	-1.60350200	1.40120600
C	-1.70370100	-0.76889900	1.57520600
O	-3.85280100	-0.75470600	-2.05009400

O	-4.58409500	-2.55040800	0.39090600
C	-4.27169300	-3.25490700	1.59500600
O	-3.32509500	-2.47170400	2.32290600
C	-4.99699800	-1.57331000	-2.29079400
O	2.83710300	-1.76978400	-2.31319400
C	1.83730300	-1.79248700	-3.32079400
O	4.76000300	-1.83057800	-0.43219400
O	4.38229800	-0.47167900	1.99920600
C	-1.33351400	3.24870200	0.10170600
C	-0.73071800	4.58640400	-0.33569400
O	0.62948200	4.48530900	-0.38789400
C	1.05518700	3.16721000	0.01070600
O	-1.30882100	5.61320200	-0.58209400
C	-1.79771400	3.36060100	1.56610600
H	2.07499500	0.63061300	2.28080600
H	0.55969800	-0.45709200	-1.60039400
H	-0.07630700	1.25300600	1.70290600
H	-0.21301000	2.00250600	-1.24519400
H	-1.86660500	0.65400100	-1.53039400
H	-1.13900100	-0.76719700	2.50110600
H	-5.18029200	-3.37501000	2.18930600
H	-3.82698900	-4.23100600	1.34740600
H	-5.32929900	-1.31701100	-3.29849400
H	-5.79729900	-1.36311200	-1.57409400
H	-4.74459500	-2.63800900	-2.24549400
H	2.26420500	-2.35908600	-4.15019400
H	1.58539900	-0.78018800	-3.66349400
H	0.92480400	-2.29169000	-2.97069400
H	-2.20751300	3.04559900	-0.52289400
H	1.90618800	2.88761300	-0.61229400
H	1.38658700	3.20631100	1.05620600
H	-2.28901100	2.43789900	1.88880600
H	-2.51231700	4.18399800	1.65930600
H	-0.96371500	3.56430300	2.24800600
C	5.70120100	-1.11177500	-1.23539400
C	4.74090300	-1.72707800	2.58730600
H	6.57330300	-1.76187200	-1.33759400
H	5.99749700	-0.17597400	-0.74549400
H	5.28840000	-0.89767600	-2.22739400
H	5.51750200	-1.50227600	3.32200600
H	5.12730500	-2.42217700	1.83720600
H	3.87830400	-2.17538100	3.09810600

B3LYP/6-31G(d) opt

Total energy = –1493.416074 kcal/mol

Conf 6

C	3.41429500	-0.45008400	1.00580100
C	3.59299700	-1.14558300	-0.19459900
C	2.21629400	0.23181300	1.25610100
C	1.18319400	0.22211100	0.32010100
C	1.35669500	-0.47518900	-0.88599900
C	2.54949700	-1.15288600	-1.14649900
C	-0.10820800	1.00160800	0.59370100
C	-0.18101100	2.26420700	-0.29169900
C	-1.34110600	0.10070500	0.50350100
C	-2.11470600	-0.00219700	-0.65269900
C	-3.22650400	-0.86870000	-0.75689900
C	-3.52210200	-1.63780100	0.36250100
C	-2.74690200	-1.53129900	1.51730100
C	-1.66440400	-0.68629600	1.63080100
O	-3.88500400	-0.84750200	-1.94749900
O	-4.56009900	-2.53040300	0.58810100
C	-4.22179800	-3.17620300	1.81790100
O	-3.26350000	-2.35750000	2.48900100
C	-5.03600200	-1.67310500	-2.12309900
O	2.80489900	-1.86538500	-2.28139900
C	1.80399900	-1.90388800	-3.28739900
O	4.78199900	-1.78388000	-0.45609900

O	4.37309500	-0.46308100	1.98910100
C	-1.33541400	3.26110500	-0.03679900
C	-0.74291700	4.57850600	-0.54399900
O	0.61668300	4.47730900	-0.61369900
C	1.05188600	3.17891000	-0.16449900
O	-1.32712000	5.59240500	-0.82679900
C	-1.77661400	3.43910400	1.42820100
H	2.11529200	0.75251300	2.20390100
H	0.54499600	-0.50559100	-1.60329900
H	-0.04490900	1.34390800	1.63380100
H	-0.23481100	1.95590700	-1.34349900
H	-1.89500700	0.59090300	-1.53349900
H	-1.08150400	-0.64009500	2.54420100
H	-5.11819800	-3.27010500	2.43510100
H	-3.77909500	-4.16200100	1.60800100
H	-5.38970200	-1.46500500	-3.13459900
H	-5.82000200	-1.42550600	-1.40019900
H	-4.78529900	-2.73510400	-2.03139900
H	2.22020000	-2.50518700	-4.09769900
H	1.57339700	-0.89868800	-3.66319900
H	0.88090000	-2.37279000	-2.92249900
H	-2.21881300	3.02810200	-0.63709900
H	1.89178700	2.87221300	-0.78969900
H	1.40138600	3.26491100	0.87220100
H	-2.26041200	2.53130200	1.80080100
H	-2.49181600	4.26450200	1.49470100
H	-0.93281500	3.67540600	2.08700100
C	4.75620200	-3.19868000	-0.24249900
C	5.59979400	0.20372200	1.67230100
H	5.76220300	-3.55877800	-0.47049900
H	4.03560300	-3.68348200	-0.90999900
H	4.51190300	-3.43148100	0.80140100
H	6.09679500	-0.26177700	0.81700100
H	6.22779400	0.11432300	2.56180100
H	5.41949100	1.26662100	1.46240100

B3LYP/6-31G(d) opt

Total energy = –1493.415998 kcal/mol

Conf 7

C	-3.41278700	-0.24270800	-0.82330000
C	-3.64778600	-0.88400800	0.40300000
C	-2.16318800	0.33799500	-1.08600000
C	-1.14088800	0.27269700	-0.13360000
C	-1.36548700	-0.37940300	1.08390000
C	-2.61058600	-0.96110600	1.35020000
C	0.20681000	0.94250000	-0.42740000
C	0.36030800	2.24650000	0.38660000
C	1.37701200	-0.03009800	-0.26250000
C	1.68821400	-0.86879700	-1.34580000
C	2.71471600	-1.82919500	-1.28330000
C	3.42331600	-1.90479300	-0.08780000
C	3.11821500	-1.07679400	0.97850000
C	2.10781300	-0.12939600	0.93560000
O	3.07561800	-2.68139400	-2.28040000
O	4.44691800	-2.76139100	0.24850000
C	4.92461700	-2.27969000	1.50840000
O	3.94561500	-1.37499200	2.03680000
C	2.34121800	-2.63359600	-3.49460000
O	-2.92228400	-1.62960700	2.49600000
C	-1.93068400	-1.72600400	3.50650000
O	-4.88898500	-1.39031100	0.69190000
O	-4.46418700	-0.24271000	-1.69180000
C	1.59020600	3.13800300	0.09580000
C	1.09330300	4.52330200	0.51760000
O	-0.27059700	4.52819900	0.57050000
C	-0.79779400	3.24249800	0.18800000
O	1.74940100	5.50520300	0.75130000
C	2.06100600	3.19680400	-1.36930000

H	-1.97918900	0.83489500	-2.03210000
H	-0.56028700	-0.45730200	1.80430000
H	0.18321000	1.23010000	-1.48560000
H	0.37570800	1.99510000	1.45460000
H	1.10431400	-0.77519800	-2.25470000
H	1.91131100	0.49960400	1.79550000
H	5.04991900	-3.12039000	2.19560000
H	5.87411600	-1.74388800	1.36230000
H	2.78181900	-3.39739500	-4.13750000
H	2.43071600	-1.65359500	-3.98140000
H	1.27981800	-2.86179800	-3.33210000
H	-2.39378300	-2.28060500	4.32460000
H	-1.62588600	-0.73500400	3.86770000
H	-1.04418300	-2.26970300	3.15450000
H	2.44610600	2.87410500	0.72290000
H	-1.66679400	3.03659600	0.81460000
H	-1.12639500	3.29599700	-0.85800000
H	2.46650800	2.23080500	-1.68420000
H	2.84590400	3.95260500	-1.46970000
H	1.24750500	3.46940200	-2.05210000
C	-5.06998200	-2.75951100	0.32980000
C	-4.31358900	0.43269100	-2.92910000
H	-6.09178100	-3.01881300	0.61720000
H	-4.36618100	-3.40701000	0.86720000
H	-4.95028200	-2.90081100	-0.75170000
H	-4.09809100	1.49949100	-2.78370000
H	-5.26988800	0.32598900	-3.44450000
H	-3.52008800	-0.01450800	-3.54330000

B3LYP/6-31G(d) opt

Total energy = –1493.415942 kcal/mol

Conf 8

C	3.48860100	-0.18339900	0.83419800
C	3.68380100	-0.84729900	-0.38720200
C	2.23920000	0.37680000	1.13879800
C	1.17760000	0.26650000	0.23519800
C	1.36260100	-0.40920000	-0.97620200
C	2.60790100	-0.96900000	-1.28500200
C	-0.17200000	0.90949900	0.57699800
C	-0.40480100	2.18519900	-0.26190200
C	-1.31990000	-0.10110200	0.50909800
C	-2.11889900	-0.25190200	-0.63510200
C	-3.14619900	-1.21580200	-0.70860200
C	-3.32869900	-2.02120200	0.40869800
C	-2.54039900	-1.86940200	1.53899800
C	-1.53409900	-0.92570200	1.63029800
O	-3.97319900	-1.42130300	-1.77030200
O	-4.27559800	-2.99850300	0.61439800
C	-3.90149800	-3.61370300	1.85079800
O	-2.95689800	-2.75610200	2.50429800
C	-3.82999900	-0.57860300	-2.90320200
O	2.88420100	-1.65830000	-2.42820200
C	1.85080100	-1.80580000	-3.38810200
O	4.92110100	-1.33579900	-0.71980200
O	4.57630100	-0.14179900	1.65519800
C	-1.64100100	3.05169800	0.07339800
C	-1.20720200	4.43619900	-0.41520200
O	0.15129800	4.47639900	-0.54050200
C	0.73419900	3.21639900	-0.15280200
O	-1.90280200	5.39139800	-0.64520200
C	-2.03020100	3.14019800	1.56099800
H	2.08520000	0.89010000	2.08139800
H	0.52660100	-0.52440100	-1.65520200
H	-0.10180000	1.22849900	1.62409800
H	-0.47010000	1.90589900	-1.32150200
H	-1.95030000	0.38949800	-1.49050200
H	-0.92919900	-0.83480100	2.52619800
H	-4.78619800	-3.72740300	2.48259800

H	-3.43119700	-4.58770300	1.65059800
H	-4.59239900	-0.90380300	-3.61300200
H	-2.83849900	-0.68460200	-3.36350200
H	-3.99870000	0.47549700	-2.64680200
H	2.28980200	-2.37020000	-4.21280200
H	1.50430100	-0.83240000	-3.76020200
H	0.99550200	-2.36190000	-2.98200200
H	-2.52340100	2.74679800	-0.49560200
H	1.57389900	3.01580000	-0.81980200
H	1.11659900	3.30740000	0.87179800
H	-2.38620100	2.17219800	1.92559800
H	-2.83200100	3.87439800	1.68479800
H	-1.18880100	3.45739900	2.18819800
C	5.15480200	-2.68439800	-0.31240200
C	4.45760000	0.53850100	2.89379800
H	6.16830200	-2.93049800	-0.63860200
H	4.44340200	-3.36999900	-0.78920200
H	5.09020200	-2.78419800	0.77819800
H	4.21200000	1.59910100	2.75049800
H	5.43540000	0.45760200	3.37209800
H	3.69910000	0.07690100	3.54019800

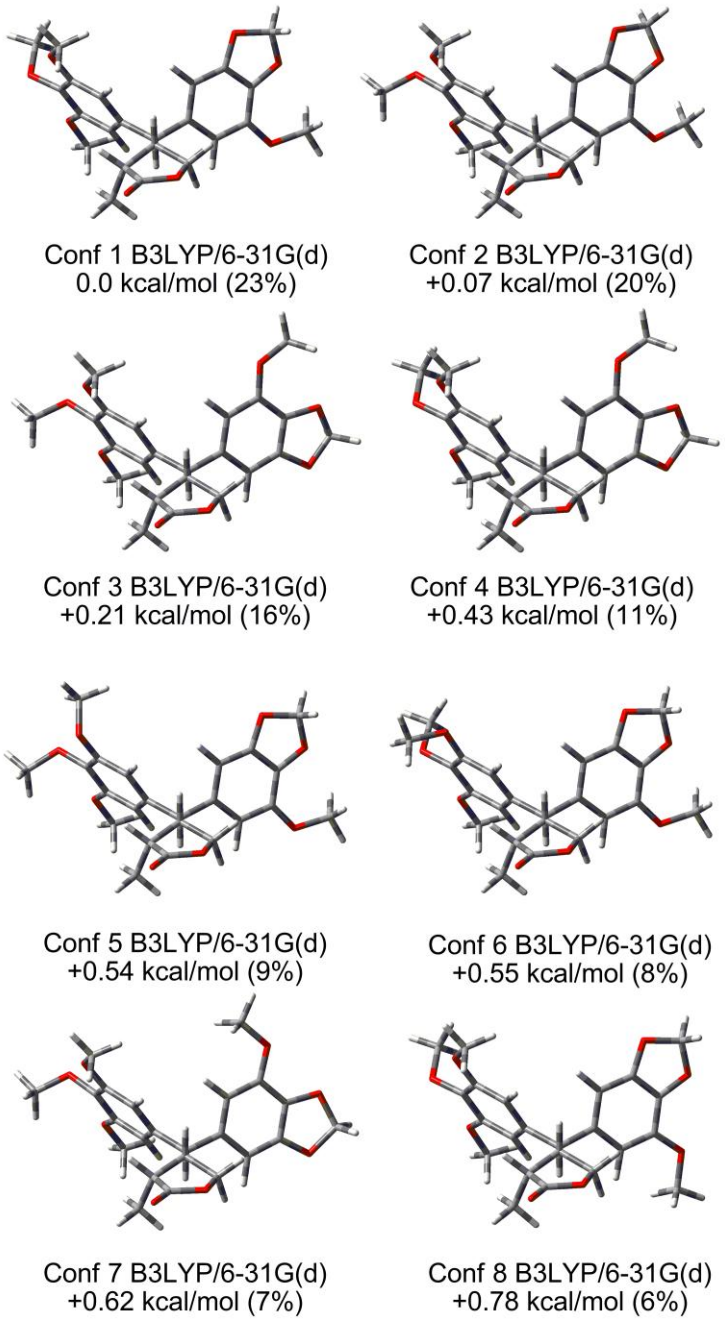

Figure 4. Optimized structures, relative energies, and Boltzmann factors of the eight lowest-energy conformers of (2*R*,3*S*,5*S*)-**3** at the B3LYP/6-31G(d) level

Atomic coordinates - (2*R*,3*S*,5*S*)-**3**

B3LYP/6-31G(d) opt

Total energy = –1493.4172 kcal/mol

Conf 1

C	-2.72876800	-1.53274400	1.21432700
C	-3.49884500	-1.42423700	0.04308200
C	-1.57443400	-0.75735200	1.37181700
C	-1.16731800	0.12367200	0.36258500
C	-1.92484400	0.22634200	-0.80927100
C	-3.08239900	-0.54952300	-0.97272900
C	0.12897000	0.90988100	0.57563800
C	0.15707200	2.28302700	-0.13017300
C	1.36117000	0.08018000	0.19936600
C	2.37735600	-0.10677500	1.13586700
C	3.55698500	-0.83145300	0.85388000
C	3.66773400	-1.35378200	-0.42969800
C	2.64957200	-1.16064600	-1.36409800
C	1.49131900	-0.46305400	-1.09705400
O	4.44604400	-0.95136900	1.87666500
O	4.65805400	-2.14801400	-0.98899700
C	4.34774000	-2.18490600	-2.38391500
O	2.97882300	-1.80744500	-2.53383500
C	5.74187200	-1.48754300	1.61052300
O	-3.87765000	-0.52522700	-2.07974100
C	-3.53835700	0.35897000	-3.13485100
O	-4.67398400	-2.11902100	-0.08402600
O	-3.19768000	-2.42033600	2.13679800
C	-0.92827200	3.31504300	0.25543800
C	-0.24080700	4.64381700	-0.06917900
O	1.10939800	4.45790200	-0.14868700
C	1.44823600	3.08360400	0.12277600
O	-0.75014200	5.72460200	-0.21639100
C	-1.37241500	3.32247600	1.73016700
H	-0.97459200	-0.84351900	2.27078300
H	-1.62149800	0.90601900	-1.59517000
H	0.20584200	1.10336700	1.65226400
H	0.09461100	2.12552600	-1.21479000
H	2.29048600	0.30933400	2.13523100
H	0.71204100	-0.36461400	-1.84364900
H	4.98698700	-1.46959000	-2.92419700
H	4.48972900	-3.20113500	-2.75835200
H	6.28091900	-1.42632700	2.55779700
H	6.26734100	-0.89870400	0.85032500
H	5.68693400	-2.53004600	1.28285800
H	-4.30647200	0.21961600	-3.89770400
H	-2.55532000	0.12204300	-3.56400300
H	-3.54431800	1.40599300	-2.80384900
H	-1.81928600	3.22590300	-0.37160600
H	2.27308500	2.80617800	-0.53542100
H	1.79003000	3.00474800	1.16260900
H	-1.91325400	2.40381200	1.97538200
H	-2.03719700	4.17365000	1.90561700
H	-0.52202000	3.41723900	2.41579600
C	-4.53144600	-3.43248000	-0.62582600
C	-2.48132100	-2.56478800	3.35265100
H	-5.53829900	-3.85468300	-0.67091800
H	-3.90295200	-4.05995100	0.01794600
H	-4.10662600	-3.39878500	-1.63701700
H	-2.44144300	-1.62061000	3.91151000
H	-1.45842900	-2.92530700	3.18066400
H	-3.03200100	-3.30525400	3.93566300

B3LYP/6-31G(d) opt

Total energy = –1493.4170 kcal/mol

Conf 2

C	-2.90629000	-0.82117600	-1.12420800
C	-3.28735400	-1.74259500	-0.13582700
C	-1.81534200	0.03472900	-0.91302500
C	-1.10170100	-0.01704800	0.28977500
C	-1.48991600	-0.92438100	1.28270500
C	-2.57800300	-1.78099700	1.07704100
C	0.12382400	0.86140400	0.55506600
C	0.04392900	2.25735800	-0.10043500
C	1.42695800	0.15025900	0.17666000
C	2.42356500	-0.01225100	1.13838300
C	3.65830200	-0.64276400	0.86610700
C	3.84064100	-1.10619100	-0.43173700
C	2.83763300	-0.94676000	-1.38859900
C	1.63076800	-0.33157400	-1.13450700
O	4.53608000	-0.71311900	1.90306400
O	4.94006100	-1.71621900	-1.01771000
C	4.46245500	-2.18571700	-2.28093900
O	3.27005100	-1.46334600	-2.58903100
C	5.72202900	-1.49403900	1.75773300
O	-3.03557800	-2.68464300	1.98923300
C	-2.34744700	-2.79727700	3.22438800
O	-4.30976000	-2.62599700	-0.36887600
O	-3.66956100	-0.83453000	-2.25395800
C	-1.13212100	3.17528300	0.30553900
C	-0.56083400	4.56947300	0.03435000
O	0.80114000	4.50578400	-0.02877900
C	1.25669100	3.15736500	0.20129600
O	-1.16233300	5.60543500	-0.08601100
C	-1.58616800	3.09422200	1.77498300
H	-1.53317700	0.74086300	-1.68355000
H	-0.92989900	-0.96293400	2.21019400
H	0.16641500	1.02018200	1.63915400
H	0.00866400	2.13687300	-1.19080300
H	2.27282700	0.33984900	2.15460900
H	0.87076800	-0.25375500	-1.90285700
H	5.21622400	-1.99021800	-3.04687800
H	4.23344200	-3.26041100	-2.21353900
H	6.22918800	-1.43269800	2.72246100
H	6.37221000	-1.09659600	0.97249800
H	5.48480900	-2.53993300	1.53309500
H	-2.86889900	-3.57526500	3.78500100
H	-2.37841800	-1.85815000	3.79301400
H	-1.30102700	-3.09524400	3.07793600
H	-2.00626800	3.02955200	-0.33468200
H	2.11151700	2.97673500	-0.45227700
H	1.59008300	3.07240600	1.24340800
H	-2.04469900	2.12346500	1.98497500
H	-2.32440000	3.87744900	1.97211900
H	-0.75185000	3.23990000	2.47128800
C	-5.59975800	-2.15746100	0.02544400
C	-3.32363500	0.04322000	-3.31252500
H	-6.30276700	-2.95787700	-0.21770400
H	-5.87703100	-1.25090900	-0.52676100
H	-5.63532200	-1.95854800	1.10382100
H	-3.39484300	1.09631900	-3.00852000
H	-4.04640900	-0.15049200	-4.10713600
H	-2.31130100	-0.15597500	-3.68834100

B3LYP/6-31G(d) opt

Total energy = –1493.4168 kcal/mol

Conf 3

C	-2.81668000	-0.86019900	-1.13424100

C	-3.24519800	-1.74249000	-0.12973000
C	-1.74105100	0.00974400	-0.90245300
C	-1.09020800	0.01087600	0.33625500
C	-1.52724200	-0.85603500	1.34509800
C	-2.59989200	-1.72669100	1.11891100
C	0.11828800	0.90392400	0.62682500
C	0.08047100	2.26623500	-0.09832500
C	1.44350400	0.18075800	0.35670000
C	1.72236100	-0.35458200	-0.90187500
C	2.93654700	-1.00424000	-1.20269600
C	3.86381200	-1.09879500	-0.16762900
C	3.57766200	-0.57399000	1.08964700
C	2.39433500	0.07093300	1.39217300
O	3.07941300	-1.45289100	-2.47878400
O	5.14782800	-1.62424600	-0.16401900
C	5.51638500	-1.66563500	1.21643500
O	4.65712000	-0.76837100	1.92196100
C	4.14716100	-2.34972500	-2.78475300
O	-3.10137600	-2.59443700	2.04310600
C	-2.47578800	-2.65438400	3.31440800
O	-4.25043700	-2.64132600	-0.37823200
O	-3.51998900	-0.92369800	-2.30055400
C	-1.11768000	3.20187800	0.18480800
C	-0.52734600	4.58212300	-0.11512900
O	0.83578700	4.51712500	-0.08684500
C	1.27248900	3.18217700	0.23731600
O	-1.11773000	5.61043200	-0.32360700
C	-1.66879600	3.19099300	1.62314700
H	-1.42048300	0.68388400	-1.68634100
H	-1.01701200	-0.85235500	2.30171100
H	0.09841500	1.11548700	1.70275200
H	0.11690200	2.09097100	-1.18105300
H	0.98507300	-0.31239800	-1.69657100
H	2.21187500	0.46689400	2.38546000
H	5.37920100	-2.68646300	1.60551100
H	6.55296200	-1.33852500	1.32345200
H	4.00425200	-2.62335200	-3.83182000
H	4.10077500	-3.24968700	-2.16105100
H	5.12367900	-1.87323800	-2.65696500
H	-3.02220100	-3.41209200	3.87903900
H	-2.53802700	-1.69357000	3.84292200
H	-1.42239000	-2.95269600	3.23241500
H	-1.94827700	3.02512000	-0.50386800
H	2.16766800	2.97085700	-0.34952000
H	1.53597800	3.14907300	1.30234600
H	-2.14372900	2.23145600	1.84766800
H	-2.41613200	3.98269800	1.73289100
H	-0.88283300	3.37008700	2.36646600
C	-5.56153700	-2.16263000	-0.07714800
C	-3.11868100	-0.09124600	-3.37630200
H	-6.24789000	-2.97630600	-0.32392300
H	-5.80977500	-1.28224800	-0.68285700
H	-5.65782100	-1.91734900	0.98794200
H	-3.20791700	0.97366700	-3.12238100
H	-3.79744500	-0.32188000	-4.19935300
H	-2.08728400	-0.30272200	-3.68774200

B3LYP/6-31G(d) opt

Total energy = –1493.4165 kcal/mol

Conf 4

C	-2.70919000	-1.50110700	1.24986500
C	-3.40197800	-1.49710500	0.02678900
C	-1.59017700	-0.67903100	1.42710100
C	-1.14007400	0.14272900	0.38671400
C	-1.82093300	0.14159000	-0.83567100
C	-2.94353700	-0.67946500	-1.01833100
C	0.11663900	0.98330600	0.62522500
C	0.13378000	2.32075700	-0.14515400

C	1.39857800	0.18526800	0.35572400
C	1.62152400	-0.40909100	-0.88724000
C	2.79663000	-1.12600500	-1.19090400
C	3.74334900	-1.22662700	-0.17406400
C	3.51303100	-0.64086200	1.06782100
C	2.36853900	0.06966100	1.37266300
O	2.88288500	-1.63052700	-2.45117900
O	5.00039000	-1.81459300	-0.17760300
C	5.40019300	-1.81954200	1.19468700
O	4.60166700	-0.85554500	1.88294900
C	3.94720400	-2.52552500	-2.77285500
O	-3.66528100	-0.75362100	-2.17247500
C	-3.28758700	0.07627900	-3.25861800
O	-4.54668300	-2.23672900	-0.12434700
O	-3.21368200	-2.33833400	2.20031500
C	-1.00801300	3.32666600	0.12976800
C	-0.35283000	4.66404500	-0.22541400
O	1.00557900	4.52783500	-0.22341100
C	1.37898000	3.18299800	0.13542800
O	-0.89267500	5.71548200	-0.45395800
C	-1.53124400	3.39010900	1.57717300
H	-1.05102900	-0.68283100	2.36769000
H	-1.48372300	0.77399300	-1.64685200
H	0.12817700	1.23154100	1.69346500
H	0.13770800	2.10770600	-1.22170700
H	0.86813400	-0.35987300	-1.66632500
H	2.22922700	0.51090500	2.35376100
H	5.22476400	-2.81670400	1.62739400
H	6.45334300	-1.53864700	1.26515800
H	3.77081900	-2.82446300	-3.80783500
H	3.93201000	-3.41087400	-2.12744600
H	4.92298700	-2.03732400	-2.69049200
H	-4.00208600	-0.13516000	-4.05618700
H	-2.27301200	-0.15227500	-3.61184300
H	-3.34637500	1.14031600	-2.99397400
H	-1.86002000	3.17276400	-0.53784100
H	2.24873400	2.90597000	-0.46231900
H	1.66416200	3.16967500	1.19529400
H	-2.05598900	2.46677100	1.83955700
H	-2.23030500	4.22612800	1.67511800
H	-0.72200900	3.54599300	2.30052800
C	-4.33593600	-3.56385500	-0.60672400
C	-2.58351800	-2.36761300	3.47044900
H	-5.32477300	-4.02350200	-0.67752700
H	-3.71528100	-4.14318300	0.08812100
H	-3.86844600	-3.55410400	-1.59930000
H	-1.54022400	-2.70317900	3.39887500
H	-3.15214600	-3.08264700	4.06785000
H	-2.61282900	-1.38422500	3.95790800

B3LYP/6-31G(d) opt

Total energy = –1493.4163 kcal/mol

Conf 5

C	-3.02117900	-0.51073900	-1.06393200
C	-3.44803400	-1.38855200	-0.06269800
C	-1.85748600	0.25123100	-0.89376700
C	-1.10786600	0.15315600	0.27828000
C	-1.53158300	-0.73220900	1.28341300
C	-2.68665500	-1.49945100	1.12102100
C	0.19038000	0.93059600	0.50465400
C	0.25231900	2.28061700	-0.24196700
C	1.41995900	0.07412400	0.18358800
C	2.41372100	-0.09465300	1.14714100
C	3.59056000	-0.84047200	0.91248500
C	3.72161000	-1.40402400	-0.35151500
C	2.72547000	-1.22899200	-1.31303500
C	1.56998700	-0.51088700	-1.09235900
O	4.45668300	-0.93922100	1.95716900

O	4.71394600	-2.22626400	-0.86427100
C	4.43186300	-2.30503400	-2.26370000
O	3.07142400	-1.91607500	-2.45443800
C	5.75861500	-1.47866300	1.72971200
O	-3.17755900	-2.37172100	2.04780200
C	-2.44420700	-2.55640900	3.24887600
O	-4.57294900	-2.15713300	-0.24535500
O	-3.75632100	-0.32061700	-2.20829600
C	-0.82396700	3.33987700	0.09333000
C	-0.10721200	4.65005100	-0.24399000
O	1.24057500	4.43979400	-0.29718000
C	1.55209000	3.06724900	0.01152000
O	-0.59492700	5.73684400	-0.41743900
C	-1.30360400	3.39117900	1.55603400
H	-1.58257900	0.92185100	-1.70042300
H	-0.94030300	-0.82112700	2.18813000
H	0.24261100	1.15541200	1.57687300
H	0.20492100	2.08982200	-1.32154600
H	2.31137300	0.35423400	2.13074600
H	0.80773200	-0.42585000	-1.85814100
H	5.09133800	-1.61572100	-2.81328800
H	4.56839500	-3.33468300	-2.60174700
H	6.27874600	-1.39348300	2.68569000
H	6.29782600	-0.90659500	0.96621400
H	5.71240500	-2.52870300	1.42580900
H	-2.99978500	-3.29821500	3.82534100
H	-2.37344100	-1.62555300	3.82711000
H	-1.43342400	-2.93420100	3.04820300
H	-1.70044000	3.25163800	-0.55397700
H	2.38193100	2.76063400	-0.62720500
H	1.87725300	3.00824500	1.05802800
H	-1.86848000	2.48931800	1.81004800
H	-1.95540000	4.25904300	1.69450700
H	-0.46845400	3.48585500	2.26026900
C	-5.74487000	-1.65628800	0.40540300
C	-3.83981300	-1.44459700	-3.09146400
H	-6.55141600	-2.34943100	0.15501300
H	-5.99682900	-0.65364900	0.03844400
H	-5.61014600	-1.63141100	1.49236500
H	-4.43155900	-1.10968100	-3.94656000
H	-4.32960100	-2.29474300	-2.60910800
H	-2.84023300	-1.74052200	-3.43691900

B3LYP/6-31G(d) opt

Total energy = –1493.41627 kcal/mol

Conf 6

C	3.04221900	-0.49565600	1.00246400
C	3.44496100	-1.39286000	0.00835500
C	1.88544300	0.27778300	0.83658600
C	1.11067700	0.16115900	-0.31726600
C	1.51790300	-0.73316100	-1.32118200
C	2.67052100	-1.50578900	-1.16665300
C	-0.19127800	0.93663900	-0.52847200
C	-0.23362500	2.30080500	0.19359200
C	-1.41356800	0.08835500	-0.16109400
C	-2.42907100	-0.09942800	-1.09824300
C	-3.59996200	-0.84012000	-0.82178100
C	-3.70186200	-1.37821500	0.45592100
C	-2.68425100	-1.18387300	1.39089000
C	-1.53423600	-0.47050500	1.12966600
O	-4.49007800	-0.96017100	-1.84404700
O	-4.68193100	-2.18999600	1.00748600
C	-4.36843400	-2.23945100	2.40169400
O	-3.00405100	-1.84778600	2.55336200
C	-5.78808800	-1.48909600	-1.57391700
O	3.13219500	-2.40526600	-2.08234500
C	2.39886500	-2.57271200	-3.28596800
O	4.59962200	-2.12393600	0.15693600

O	3.72671300	-0.38693600	2.18801500
C	0.83704700	3.35082100	-0.18517700
C	0.13173200	4.66857500	0.14643500
O	-1.21496100	4.46346200	0.23226900
C	-1.53676800	3.08639600	-0.04513800
O	0.62665200	5.75627200	0.29210600
C	1.28270300	3.37509800	-1.65921600
H	1.62257400	0.95387800	1.64264900
H	0.91256900	-0.82952000	-2.21574400
H	-0.26882400	1.14028800	-1.60340700
H	-0.16243700	2.13001300	1.27522300
H	-2.34925700	0.32978300	-2.09266500
H	-0.75520900	-0.37030900	1.87650700
H	-5.01519400	-1.53813100	2.95122300
H	-4.49779900	-3.26160900	2.76437200
H	-6.33083100	-1.42211600	-2.51871800
H	-6.30662900	-0.89860300	-0.81011300
H	-5.73857700	-2.53259400	-1.24875600
H	2.94248200	-3.32259000	-3.86339600
H	2.35000600	-1.63830800	-3.86009800
H	1.37923500	-2.93078600	-3.09207200
H	1.72808100	3.27089600	0.44307900
H	-2.35290500	2.79363000	0.61726000
H	-1.88532700	3.00989000	-1.08295300
H	1.83780900	2.46658300	-1.91082300
H	1.93453000	4.23762500	-1.82785900
H	0.43190600	3.46167700	-2.34545600
C	4.39376800	-3.47462300	0.58271500
C	5.05256500	0.14723600	2.09936500
H	5.38758600	-3.91895600	0.67534500
H	3.81142600	-4.03505500	-0.15690000
H	3.88713200	-3.50431100	1.55525000
H	5.69720300	-0.48710300	1.48517100
H	5.43024900	0.18132400	3.12388600
H	5.03335800	1.16498100	1.68728900

B3LYP/6-31G(d) opt

Total energy = –1493.4161 kcal/mol

Conf 7

C	-2.91994400	-0.54120300	-0.99550600
C	-3.32235100	-1.49711100	-0.05027300
C	-1.76813900	0.23079900	-0.77714400
C	-1.01986100	0.06573700	0.39342000
C	-1.43178900	-0.87362900	1.34713900
C	-2.57374800	-1.65219800	1.13038000
C	0.27131400	0.84176600	0.66498700
C	0.34406900	2.21803700	-0.03257400
C	1.51507800	0.00323300	0.34302500
C	1.65600400	-0.59985500	-0.91658700
C	2.79887800	-1.34479800	-1.26082200
C	3.79448000	-1.44606800	-0.29253000
C	3.65089700	-0.85398500	0.95062300
C	2.52837600	-0.12511700	1.30955400
O	3.01482500	-1.97551000	-2.44641000
O	4.98038500	-2.14265100	-0.35541700
C	5.68611000	-1.76431600	0.82985100
O	4.75056400	-1.14687500	1.72409800
C	1.98790900	-1.91919200	-3.42602200
O	-3.05087700	-2.58714000	1.99988700
C	-2.31115600	-2.84262400	3.18348400
O	-4.40171200	-2.30343300	-0.30358700
O	-3.71943100	-0.43906800	-2.09547200
C	-0.74181600	3.26355900	0.31486800
C	-0.02601500	4.58433100	0.02053200
O	1.32308900	4.38134600	-0.00900000
C	1.63397600	3.00241500	0.27340600
O	-0.51698700	5.67129000	-0.14335200
C	-1.24152400	3.27140200	1.77169600

H	-1.46791100	0.96186400	-1.51628800
H	-0.84285900	-1.00289100	2.24830500
H	0.30157500	1.03198200	1.74493800
H	0.32374200	2.06363100	-1.11926300
H	0.84599100	-0.50859000	-1.63032500
H	2.44058600	0.31894900	2.29548300
H	6.10649200	-2.65528700	1.30305300
H	6.47613800	-1.04241400	0.57456000
H	2.35636900	-2.49806200	-4.27450200
H	1.79481800	-0.88714700	-3.74747400
H	1.05507000	-2.36456600	-3.05739400
H	-2.85134600	-3.63410600	3.70606500
H	-2.25669200	-1.95495300	3.82780800
H	-1.29385200	-3.18618100	2.95588300
H	-1.60989000	3.19006300	-0.34550800
H	2.48137400	2.71561100	-0.35098100
H	1.93206400	2.91941300	1.32616400
H	-1.80548100	2.36010100	1.99164500
H	-1.89875100	4.13238000	1.92671000
H	-0.41632100	3.34880500	2.48945700
C	-5.63272700	-1.84473700	0.25675500
C	-3.36947100	0.49856500	-3.09924000
H	-6.38963800	-2.57958700	-0.02784000
H	-5.90938700	-0.86339400	-0.14902300
H	-5.57353200	-1.78923500	1.35043000
H	-3.36824000	1.52714300	-2.71381200
H	-4.13425400	0.40563900	-3.87243300
H	-2.38620200	0.27709700	-3.53578100

B3LYP/6-31G(d) opt

Total energy = –1493.4159 kcal/mol

Conf 8

C	3.10149400	-0.37021300	0.93206500
C	3.55686100	-1.19174300	-0.11116900
C	1.88128600	0.31271400	0.81523900
C	1.10123800	0.16993500	-0.33740100
C	1.54854000	-0.65829100	-1.37403300
C	2.76487100	-1.34152900	-1.26293500
C	-0.25797300	0.85457200	-0.50088200
C	-0.36935600	2.21309700	0.22623300
C	-1.41488400	-0.07001300	-0.10337300
C	-2.45802700	-0.29355900	-1.01471000
C	-3.56931900	-1.10154400	-0.69698600
C	-3.58502600	-1.66317900	0.57402600
C	-2.54987900	-1.44316400	1.47068800
C	-1.44988200	-0.65946900	1.17407600
O	-4.61751800	-1.38035700	-1.51965500
O	-4.51860700	-2.51314000	1.12155800
C	-4.13453100	-2.64191800	2.49381900
O	-2.79734700	-2.14387500	2.62823200
C	-4.61190700	-0.81446100	-2.82114300
O	3.27622700	-2.17302000	-2.21460000
C	2.53844000	-2.35530900	-3.41189800
O	4.78490300	-1.79589500	-0.03033300
O	3.92350900	-0.30144500	2.01722000
C	0.62584200	3.32859000	-0.17024800
C	-0.14927800	4.59785200	0.19211400
O	-1.47941000	4.31062800	0.30402100
C	-1.72277300	2.91877500	0.02106100
O	0.28189700	5.71173600	0.34163400
C	1.03095800	3.39086800	-1.65490700
H	1.54709000	0.95194900	1.62223800
H	0.93212200	-0.77698700	-2.25804900
H	-0.37845900	1.05712400	-1.57209700
H	-0.26647200	2.04524000	1.30607000
H	-2.40375600	0.17038100	-1.99330900
H	-0.64407100	-0.53051100	1.88714900
H	-4.81071700	-2.04500800	3.12352400

H	-4.15978700	-3.69630500	2.78093200
H	-5.52726300	-1.16490500	-3.30087000
H	-3.74451300	-1.15128200	-3.40405400
H	-4.61910800	0.28295300	-2.78434200
H	3.12962600	-3.03869000	-4.02422700
H	2.40549500	-1.40851200	-3.95187000
H	1.55375400	-2.80116300	-3.21786000
H	1.53699100	3.29783700	0.43311600
H	-2.50588300	2.57129300	0.69668400
H	-2.08673300	2.82969400	-1.01061200
H	1.63179400	2.51870900	-1.92856600
H	1.62656900	4.29153900	-1.83166400
H	0.15922300	3.43308200	-2.31874900
C	4.76196100	-3.11241700	0.52262800
C	3.54131500	0.52764100	3.10233300
H	5.79780500	-3.46027500	0.52537300
H	4.15342800	-3.78824800	-0.09085400
H	4.37964400	-3.10234900	1.55096800
H	3.45250300	1.57877700	2.79738300
H	4.33865400	0.43492600	3.84188000
H	2.59302900	0.20027100	3.54960900

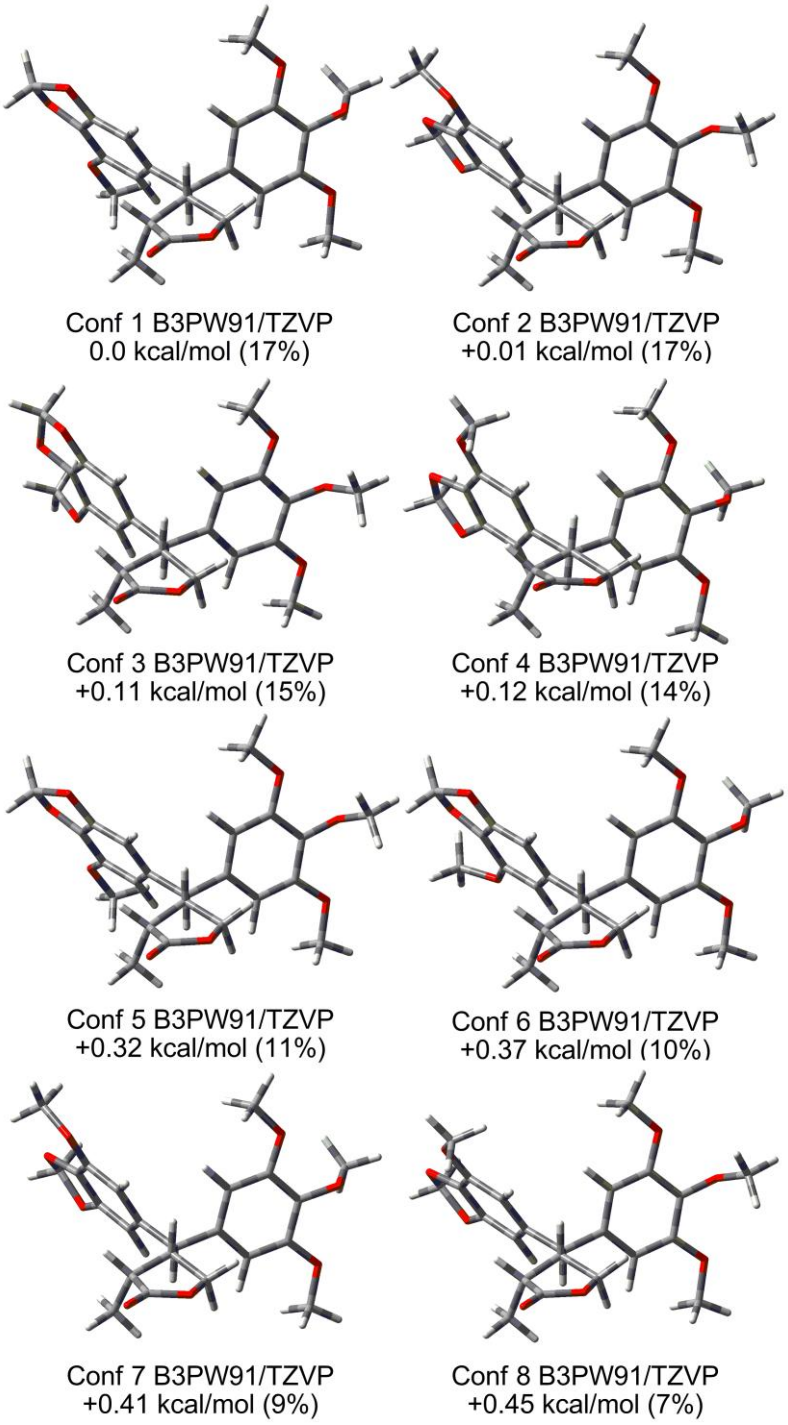

Figure 5. Optimized structures, relative energies, and Boltzmann factors of the eight lowest-energy conformers of (2*R*,3*S*,5*R*)-**3** at the B3PW91/TZVP level

Atomic coordinates - (2*R*,3*S*,5*R*)-**3**

B3PW91/TZVP opt

Total energy = –937088.8375 kcal/mol

Conf 1

C	-3.39610400	-0.23999400	-0.80826700
C	-3.62372100	-0.88317400	0.41242100
C	-2.15236000	0.33568300	-1.07682500
C	-1.13022100	0.26934400	-0.13562000
C	-1.34656500	-0.37922400	1.07624200
C	-2.58507800	-0.95601100	1.35070900
C	0.20788700	0.93603100	-0.43246800
C	0.36183000	2.23127300	0.37462800
C	1.36958000	-0.03161200	-0.26670900
C	1.66763000	-0.88080200	-1.33609500
C	2.68603500	-1.83971800	-1.27042700
C	3.40746000	-1.89511100	-0.08862500
C	3.11323100	-1.05467200	0.96452300
C	2.10736300	-0.11238700	0.91883300
O	3.02304000	-2.70526200	-2.25337800
O	4.41262300	-2.75747800	0.26236900
C	4.94293400	-2.19439000	1.45833900
O	3.93446200	-1.35439400	2.02010700
C	2.26889400	-2.67600200	-3.44987900
O	-2.88236600	-1.61651800	2.49512800
C	-1.88770100	-1.70016600	3.49624700
O	-4.85741900	-1.38139900	0.70879900
O	-4.44325100	-0.23206300	-1.66917100
C	1.58059400	3.11897100	0.07276600
C	1.08742300	4.49664000	0.49847000
O	-0.26830600	4.49941600	0.56352200
C	-0.79158700	3.21846600	0.18048300
O	1.73918800	5.47219700	0.73270400
C	2.02845500	3.17232200	-1.38965000
H	-1.97478100	0.83407800	-2.02124000
H	-0.53829800	-0.45778100	1.79062500
H	0.18291700	1.21936500	-1.48941000
H	0.38497600	1.98116500	1.44040400
H	1.07739700	-0.79688100	-2.23980400
H	1.91715800	0.52548600	1.77115700
H	5.18514900	-2.99099100	2.16019600
H	5.82492400	-1.58578900	1.21559800
H	2.68915500	-3.45322900	-4.08525500
H	2.35813600	-1.70966100	-3.95760700
H	1.21213100	-2.89383900	-3.26366900
H	-2.33890100	-2.25235300	4.31869100
H	-1.59052200	-0.70772600	3.85134900
H	-1.00232200	-2.23942800	3.14324800
H	2.44052800	2.86122500	0.69180700
H	-1.65892000	3.00944100	0.80385000
H	-1.11599800	3.27193200	-0.86414800
H	2.42388200	2.20505800	-1.70367900
H	2.81462800	3.91991000	-1.50638300
H	1.20923800	3.44510400	-2.06021900
C	-5.04921600	-2.74462900	0.34946500
C	-4.29540300	0.44849700	-2.89773200
H	-6.06612100	-3.00154900	0.64451500
H	-4.34582500	-3.39435500	0.87925800
H	-4.94190100	-2.88505400	-0.73072200
H	-4.08238900	1.51223000	-2.74659400
H	-5.24953000	0.34671200	-3.41188400
H	-3.50664900	0.00492100	-3.51568500

B3PW91/TZVP opt

Total energy = –937088.8193 kcal/mol

Conf 2

C	3.34719300	-0.76300600	0.99525500
C	3.47046800	-1.48007400	-0.19902400
C	2.20925900	0.01022200	1.23561000
C	1.19103600	0.07248800	0.29061900
C	1.30741700	-0.63815800	-0.90006600
C	2.44166000	-1.40836200	-1.14837100
C	-0.03222700	0.94268800	0.55544300
C	-0.02482900	2.18582100	-0.33977700
C	-1.31675000	0.13225400	0.47848000
C	-2.09654100	0.08286500	-0.66742300
C	-3.26130200	-0.69918700	-0.76695800
C	-3.60150000	-1.44315500	0.34901000
C	-2.81541000	-1.39201700	1.49504300
C	-1.68481900	-0.62492500	1.60337300
O	-3.93407700	-0.61576900	-1.93877800
O	-4.70951500	-2.22904700	0.59666200
C	-4.36751000	-2.93671000	1.78309300
O	-3.39668700	-2.15830800	2.47120800
C	-4.98331500	-1.53783300	-2.20639600
O	2.64201100	-2.12879300	-2.27799800
C	1.62337600	-2.13161100	-3.25770100
O	4.53935100	-2.30055200	-0.40549100
O	4.38553000	-0.88130000	1.85893900
C	-1.09833400	3.25594100	-0.08343400
C	-0.42683700	4.51687000	-0.61436500
O	0.91429400	4.32258200	-0.69959200
C	1.26060000	3.00976900	-0.23365600
O	-0.93958700	5.55686800	-0.90898800
C	-1.49818800	3.47482000	1.37763000
H	2.10940200	0.56054200	2.16239500
H	0.49875900	-0.61128600	-1.61799900
H	0.05568100	1.29061200	1.58969700
H	-0.11063000	1.86973200	-1.38440700
H	-1.83597500	0.65327200	-1.54997600
H	-1.09924300	-0.61439900	2.51382600
H	-5.25391700	-3.05054700	2.40491400
H	-3.93023000	-3.90937200	1.51635400
H	-5.31379600	-1.31680400	-3.21982000
H	-5.81716800	-1.41103400	-1.51382500
H	-4.62562900	-2.56974600	-2.15702900
H	1.98253000	-2.77568200	-4.05847400
H	1.44366400	-1.12769200	-3.65776000
H	0.68593900	-2.53715200	-2.86306500
H	-2.00095800	3.08066300	-0.66946800
H	2.07388400	2.63652100	-0.85334600
H	1.61549700	3.08748100	0.79949300
H	-2.03094800	2.60464300	1.76420800
H	-2.15745500	4.34106600	1.45211100
H	-0.63173200	3.66087100	2.01786300
C	5.65793200	-1.67372100	-1.02191500
C	4.29595600	-0.22366200	3.10590800
H	6.42428400	-2.44140100	-1.12483600
H	6.04524800	-0.85999500	-0.40099100
H	5.39715600	-1.29084300	-2.01364800
H	4.22960000	0.86351900	2.98743400
H	5.21316900	-0.46816900	3.63880100
H	3.43828800	-0.57813900	3.68757000

B3PW91/TZVP opt

Total energy = –937088.7277 kcal/mol

Conf 3

C	-3.21791200	-0.91013500	-1.08542700
C	-3.45617300	-1.48585400	0.16649800
C	-2.07445500	-0.13596800	-1.29502200
C	-1.16569400	0.07054200	-0.26314000

C	-1.39921000	-0.49651500	0.98633600
C	-2.53666600	-1.27130700	1.20240000
C	0.06420200	0.93669800	-0.50945600
C	-0.01219300	2.24155300	0.29006400
C	1.35308100	0.15983000	-0.28886100
C	1.86913100	-0.57359000	-1.34944500
C	3.02365400	-1.36383700	-1.24642900
C	3.64207600	-1.38786100	-0.00645200
C	3.12223900	-0.65682500	1.05253300
C	1.99934400	0.12818600	0.95675200
O	3.43543600	-1.98594900	-2.37550300
O	4.82649800	-1.97665300	0.38803400
C	4.79841600	-1.88147600	1.80755200
O	3.94841900	-0.78995700	2.13887600
C	4.33703900	-3.08149800	-2.26885400
O	-2.84324400	-1.86422900	2.38226300
C	-1.93348900	-1.72861800	3.45511200
O	-4.52834800	-2.30740400	0.34968700
O	-4.15454100	-1.15823100	-2.03280900
C	1.06830000	3.30337700	0.02906500
C	0.35404400	4.58897400	0.42945900
O	-0.98859400	4.38590900	0.43506700
C	-1.29325000	3.03981100	0.03987700
O	0.83850800	5.65152500	0.68934800
C	1.55650700	3.42973900	-1.41630300
H	-1.88516400	0.30437700	-2.26542400
H	-0.67964300	-0.35733200	1.78136300
H	0.04219500	1.20720800	-1.56932000
H	0.00772300	2.00474500	1.35902200
H	1.36784000	-0.56797500	-2.31058600
H	1.65376100	0.69339500	1.81151900
H	4.38074700	-2.80732800	2.22834800
H	5.80384800	-1.68850200	2.17788800
H	4.43058800	-3.48189900	-3.27683300
H	3.93875700	-3.85545800	-1.60664900
H	5.31669700	-2.76512300	-1.90742400
H	-2.36180400	-2.29234800	4.28205000
H	-1.81658400	-0.68204000	3.75726700
H	-0.95219100	-2.14577800	3.20609600
H	1.93320800	3.17834700	0.68136200
H	-2.14400500	2.70049100	0.62792500
H	-1.57647300	3.04001300	-1.01792700
H	2.11569500	2.54090500	-1.71234600
H	2.21465000	4.29530500	-1.50692900
H	0.72958900	3.56652100	-2.11828000
C	-5.67706600	-1.67176700	0.89805300
C	-3.94234200	-0.64860900	-3.33308700
H	-6.44506900	-2.44020700	0.98090300
H	-6.03639900	-0.87417300	0.23987100
H	-5.46658400	-1.26486100	1.89172700
H	-3.90789300	0.44650100	-3.33947500
H	-4.79279800	-0.98097700	-3.92580100
H	-3.02128200	-1.04297500	-3.77539500

B3PW91/TZVP opt

Total energy = –937088.7158 kcal/mol

Conf 4

C	3.47354200	-0.17869000	0.81821800
C	3.66032600	-0.85280400	-0.39286800
C	2.23053900	0.37800700	1.12637500
C	1.16831300	0.26000200	0.23635500
C	1.34357300	-0.42149800	-0.96402500
C	2.58194900	-0.97747900	-1.27908600
C	-0.17104500	0.90216000	0.57884600
C	-0.40446600	2.16627000	-0.25705700
C	-1.31233900	-0.10184400	0.51494600
C	-2.11523400	-0.24157200	-0.61847600
C	-3.13995000	-1.19824500	-0.69379800

C	-3.31207300	-2.01196900	0.41149200
C	-2.51857500	-1.86795300	1.53353600
C	-1.51845400	-0.92811400	1.62690500
O	-3.97197700	-1.38334400	-1.74524700
O	-4.26502300	-2.97164500	0.62937300
C	-3.81627500	-3.63788500	1.80525700
O	-2.94243900	-2.74577300	2.49590000
C	-3.84153000	-0.52282700	-2.85974300
O	2.84279400	-1.66699900	-2.41597700
C	1.80678500	-1.80548700	-3.36637900
O	4.88983200	-1.33386900	-0.73169300
O	4.55757700	-0.12316700	1.62961700
C	-1.62586300	3.03272800	0.09078400
C	-1.19714300	4.40535500	-0.41362100
O	0.15209600	4.44098100	-0.55604200
C	0.73108900	3.18769300	-0.16110300
O	-1.88876300	5.35293700	-0.64895700
C	-1.98208500	3.12730800	1.57627900
H	2.08356000	0.89904300	2.06374300
H	0.50325000	-0.54355300	-1.63387700
H	-0.09834300	1.22042400	1.62367300
H	-0.48231700	1.88453000	-1.31272600
H	-1.95041300	0.40448100	-1.46907700
H	-0.91209900	-0.84060500	2.51966800
H	-4.67021100	-3.87378800	2.43850000
H	-3.25886200	-4.54158700	1.52278500
H	-4.61030600	-0.83149100	-3.56548600
H	-2.85941100	-0.62268100	-3.33455100
H	-4.00752900	0.52359500	-2.58307100
H	2.23377300	-2.37182100	-4.19223200
H	1.46856300	-0.83179300	-3.73712900
H	0.95232900	-2.35523200	-2.95715700
H	-2.51611300	2.73121800	-0.46182900
H	1.56765300	2.97927600	-0.82542100
H	1.11170400	3.28435500	0.86092700
H	-2.32806600	2.16190700	1.94884700
H	-2.78132100	3.85665500	1.71705300
H	-1.13089800	3.44675200	2.18337100
C	5.13671800	-2.67379700	-0.32112200
C	4.44316300	0.57218700	2.85404000
H	6.14606500	-2.91692600	-0.65163000
H	4.42868100	-3.36518200	-0.78847600
H	5.08235500	-2.76775400	0.76789200
H	4.19879200	1.62822200	2.69678900
H	5.41960600	0.50061700	3.32987700
H	3.69100000	0.11907700	3.50921700

B3PW91/TZVP opt

Total energy = –937088.5187 kcal/mol

Conf 5

C	-3.27841600	-0.64261400	-0.97989200
C	-3.49228300	-1.29248500	0.23986100
C	-2.08456100	0.04626000	-1.20763500
C	-1.10287000	0.09553900	-0.22378900
C	-1.30946500	-0.54896500	0.99207800
C	-2.49566200	-1.24152300	1.22454800
C	0.17662000	0.88596700	-0.47373600
C	0.17820500	2.18670200	0.33624000
C	1.41419400	0.02640500	-0.26141200
C	1.81603200	-0.80825100	-1.30774800
C	2.90990300	-1.67555800	-1.19697800
C	3.59907600	-1.65062700	0.00525100
C	3.20226300	-0.82396600	1.03528100
C	2.12034300	0.02611200	0.94593700
O	3.34827300	-2.52331000	-2.15462800
O	4.66503700	-2.41635300	0.39952200
C	5.10973900	-1.78937900	1.59823600
O	4.01513600	-1.03509200	2.11850500

C	2.62219700	-2.58628000	-3.36741400
O	-2.78049600	-1.90252600	2.37261500
C	-1.79576800	-1.93667900	3.38671000
O	-4.62196800	-2.03086000	0.42934200
O	-4.28768400	-0.73728600	-1.87931900
C	1.31253000	3.19121000	0.07508500
C	0.67158700	4.51237900	0.48379400
O	-0.67940200	4.38120200	0.50371800
C	-1.05979400	3.05626700	0.10340900
O	1.21540200	5.54686600	0.73941100
C	1.80296200	3.29560400	-1.37109100
H	-1.91588700	0.54537200	-2.15330800
H	-0.52981200	-0.53648000	1.74170400
H	0.16492600	1.16721900	-1.53150400
H	0.19118100	1.93791400	1.40252300
H	1.24702100	-0.78893000	-2.22845900
H	1.84940900	0.65557400	1.78244700
H	5.40317800	-2.54979100	2.32035800
H	5.93987900	-1.10746400	1.36751100
H	3.12314100	-3.33751200	-3.97492200
H	2.63919700	-1.62703400	-3.89574200
H	1.58440500	-2.89144800	-3.19815800
H	-2.22069400	-2.52973100	4.19456200
H	-1.56572300	-0.93312400	3.76086200
H	-0.87463500	-2.41338800	3.03644000
H	2.17237600	3.01845700	0.72312500
H	-1.92248500	2.75995400	0.69721900
H	-1.35259100	3.08010700	-0.95157800
H	2.31742200	2.38060300	-1.66897600
H	2.50285100	4.12775400	-1.46213900
H	0.98230300	3.47413300	-2.07108000
C	-5.64957700	-1.36942000	1.15848400
C	-4.11419700	-0.13690500	-3.14548300
H	-6.47973500	-2.07168000	1.22734300
H	-5.98352800	-0.46805500	0.63436300
H	-5.31380200	-1.10855900	2.16634100
H	-3.98584900	0.94841300	-3.06645400
H	-5.02535200	-0.34755700	-3.70271700
H	-3.25993600	-0.56464400	-3.68152600

B3PW91/TZVP opt

Total energy = –937088.4648 kcal/mol

Conf 6

C	-2.62627600	-1.06516300	1.28925300
C	-3.62841700	-1.12349900	0.31121700
C	-1.42932400	-0.39992100	1.03186100
C	-1.21742200	0.20749400	-0.20215700
C	-2.20237100	0.14416700	-1.18172200
C	-3.40409100	-0.52182400	-0.93100800
C	0.07236400	0.97037100	-0.48103200
C	0.11768400	2.27247200	0.32565400
C	1.29715100	0.08855600	-0.29014400
C	1.70664100	-0.70807800	-1.35134500
C	2.79346800	-1.59244500	-1.27379900
C	3.47152200	-1.62634300	-0.06505300
C	3.06635200	-0.82083600	0.98980500
C	1.99840400	0.04059900	0.92466800
O	3.04820400	-2.33183400	-2.37769900
O	4.51746700	-2.42615500	0.35257600
C	4.95790600	-1.80912000	1.55680500
O	3.85703500	-1.07667000	2.08067300
C	4.28780700	-3.02170300	-2.48040300
O	-4.41208400	-0.64157700	-1.82952000
C	-4.26102500	-0.02425300	-3.09106700
O	-4.82721900	-1.70959200	0.58955400
O	-2.91418800	-1.69370200	2.45430400
C	1.27471100	3.24642000	0.04962000
C	0.67451900	4.58262500	0.47056700

O	-0.67887400	4.48820800	0.50398400
C	-1.09970200	3.17396100	0.10691600
O	1.24942700	5.60080000	0.72451900
C	1.74492300	3.34190700	-1.40398000
H	-0.64883800	-0.37734500	1.78015000
H	-2.02723100	0.60894900	-2.14343000
H	0.04638100	1.24703000	-1.53928000
H	0.13763400	2.02550300	1.39222900
H	1.17416500	-0.67339700	-2.29495500
H	1.73186100	0.64480700	1.78101400
H	5.25922600	-2.57637100	2.26802800
H	5.78154000	-1.11601800	1.33338900
H	4.29250400	-3.46615800	-3.47413800
H	4.37582100	-3.80695700	-1.72771500
H	5.13235100	-2.33366800	-2.38622600
H	-5.18016600	-0.23134000	-3.63636700
H	-3.41295900	-0.43934200	-3.64673400
H	-4.13754500	1.05999900	-2.99699300
H	2.13917600	3.04872500	0.68445700
H	-1.96321500	2.90041100	0.71026600
H	-1.40331600	3.20648100	-0.94479000
H	2.22899000	2.41426000	-1.71319500
H	2.46553300	4.15518700	-1.50394100
H	0.91842000	3.54487600	-2.09013400
C	-4.90545300	-3.08956700	0.25141000
C	-1.95914700	-1.64203900	3.49480100
H	-5.90430300	-3.42050500	0.53425200
H	-4.16289100	-3.67287300	0.80479200
H	-4.76752400	-3.23963000	-0.82378900
H	-1.01731400	-2.11995400	3.20472200
H	-2.39642400	-2.18976100	4.32775500
H	-1.76138100	-0.61140700	3.80832000

B3PW91/TZVP opt

Total energy = –937088.4258 kcal/mol

Conf 7

C	2.51651400	-1.15191600	-1.28208000
C	3.58737400	-1.15035200	-0.37781100
C	1.33873000	-0.47207600	-0.97922500
C	1.21689200	0.21401000	0.22526300
C	2.26992300	0.21031800	1.13328100
C	3.45236000	-0.47185400	0.83766300
C	-0.05114500	0.99895700	0.54153000
C	-0.14121300	2.25200900	-0.33631300
C	-1.28236900	0.10908600	0.48982900
C	-2.10113400	0.03270500	-0.62673500
C	-3.21270100	-0.82611000	-0.70264000
C	-3.45786000	-1.61731200	0.40580000
C	-2.63247900	-1.53884100	1.52223200
C	-1.55374000	-0.69803900	1.60779300
O	-3.93546300	-0.76351900	-1.84564700
O	-4.49882300	-2.48416400	0.67476700
C	-4.06220800	-3.19423500	1.82797400
O	-3.12052300	-2.36699600	2.49923900
C	-4.92330000	-1.75500600	-2.09837000
O	4.52404100	-0.53509800	1.66532000
C	4.46770000	0.17053700	2.88778300
O	4.76617700	-1.75139800	-0.70553200
O	2.72153500	-1.85063000	-2.42459200
C	-1.26774000	3.25597400	-0.04217300
C	-0.68152900	4.55933400	-0.57165100
O	0.66563500	4.44321200	-0.69003400
C	1.09753600	3.14694600	-0.24986200
O	-1.26011300	5.57151400	-0.84035500

C	-1.64680600	3.43562500	1.42978400
H	0.50349800	-0.49444700	-1.66631000
H	2.16457200	0.73814800	2.07247100
H	0.04508100	1.33829500	1.57800100
H	-0.23370800	1.94341400	-1.38272500
H	-1.91498400	0.64008000	-1.50335700
H	-0.93464500	-0.66838200	2.49541000
H	-4.91324900	-3.38455600	2.47977200
H	-3.57010400	-4.12759300	1.51914900
H	-5.30858700	-1.53573000	-3.09261300
H	-5.73642300	-1.70752600	-1.37205800
H	-4.48844000	-2.75807500	-2.08948200
H	5.42582900	-0.00062100	3.37537000
H	3.66501600	-0.20102000	3.53431200
H	4.33537800	1.24584300	2.72688300
H	-2.17228200	3.03658000	-0.61027200
H	1.91540700	2.82785200	-0.89314000
H	1.47200900	3.23230800	0.77569600
H	-2.12492900	2.53427200	1.81636300
H	-2.34925200	4.26470000	1.52899700
H	-0.77797300	3.66027200	2.05424100
C	4.87016800	-3.11243000	-0.30441300
C	1.69900100	-1.84956400	-3.40033700
H	5.85120500	-3.45635200	-0.63077200
H	4.09759700	-3.72341900	-0.78160300
H	4.79882000	-3.20849700	0.78346500
H	1.48241500	-0.83613000	-3.75451100
H	0.77767200	-2.30582500	-3.02265300
H	2.07850900	-2.44357300	-4.22990300

B3PW91/TZVP opt

Total energy = –937088.3788 kcal/mol

Conf 8

C	3.36334100	-0.61092700	0.98795500
C	3.52236500	-1.28875600	-0.22507400
C	2.17006600	0.06074600	1.26444400
C	1.13472100	0.06422600	0.33634000
C	1.28561300	-0.61021400	-0.87152100
C	2.47196300	-1.28403300	-1.15311500
C	-0.14345300	0.83979000	0.63492300
C	-0.20475500	2.11969700	-0.20484400
C	-1.37524000	-0.04591900	0.51899600
C	-2.17559400	-0.06450800	-0.62450200
C	-3.28074900	-0.92211900	-0.74667600
C	-3.53432200	-1.76462100	0.32028200
C	-2.74243000	-1.74006500	1.45285800
C	-1.66515700	-0.89677700	1.59315300
O	-4.11607200	-0.98620400	-1.81012500
O	-4.56953800	-2.64534400	0.48931500
C	-4.19082900	-3.40074300	1.63598500
O	-3.25137700	-2.61841700	2.37217700
C	-3.90147900	-0.08985800	-2.88219500
O	2.70780400	-1.96876500	-2.29888900
C	1.67025600	-2.05028900	-3.25466400
O	4.65435900	-2.01009400	-0.46129000
O	4.42287200	-0.66141400	1.83062400
C	-1.33193000	3.12176700	0.09320800
C	-0.73067800	4.43317400	-0.39777100
O	0.61857400	4.31486500	-0.48568000

C	1.03465500	3.00685000	-0.06409900
O	-1.30057700	5.45091500	-0.66420900
C	-1.73403800	3.26758600	1.56276500
H	2.04264000	0.58048100	2.20540800
H	0.46344200	-0.63388300	-1.57410100
H	-0.07903000	1.14844500	1.68330500
H	-0.27158600	1.84456700	-1.26286900
H	-1.94500500	0.59758400	-1.44744500
H	-1.05952400	-0.90367300	2.49056500
H	-5.06796200	-3.59149200	2.25242600
H	-3.70930500	-4.33475700	1.31528400
H	-4.69019500	-0.29461900	-3.60360300
H	-2.92931900	-0.25521400	-3.35927400
H	-3.97481200	0.95310600	-2.55669800
H	2.06316500	-2.65476400	-4.07031200
H	1.39711500	-1.06173500	-3.64033900
H	0.78081600	-2.53764700	-2.84206700
H	-2.22875100	2.92074300	-0.49346900
H	1.86787300	2.69969400	-0.69328100
H	1.38240600	3.06675600	0.97244100
H	-2.22201800	2.35916400	1.91915800
H	-2.43409800	4.09747300	1.67148100
H	-0.87407200	3.47235000	2.20584500
C	5.64239400	-1.33084300	-1.22750800
C	4.30562100	-0.03474400	3.09114200
H	6.47855300	-2.02112800	-1.33445000
H	5.98554800	-0.42754600	-0.71287000
H	5.26218600	-1.06961700	-2.21961400
H	4.15061000	1.04561500	2.99438200
H	5.24997100	-0.21408100	3.60205400
H	3.49093100	-0.46667500	3.68217900

Atomic coordinates - (2*R*,3*S*,5*S*)-**3**

B3PW91/TZVP opt

Total energy = –937089.0170 kcal/mol

Conf 1

C	-2.88360700	-0.81760600	-1.12220300
C	-3.24930700	-1.75611000	-0.15167400
C	-1.80929200	0.04631600	-0.90058700
C	-1.09063900	-0.01934100	0.28890100
C	-1.45682300	-0.94616000	1.26119700
C	-2.52797800	-1.81145200	1.04745100
C	0.11626500	0.86675800	0.56143200
C	0.01829000	2.25920000	-0.07170200
C	1.41724700	0.17751600	0.17242400
C	2.39790300	-0.02098000	1.13305600
C	3.62879200	-0.64057700	0.85319200
C	3.82279100	-1.05418600	-0.45299400
C	2.83254900	-0.85923300	-1.40995400
C	1.63101500	-0.25358400	-1.14677900
O	4.50300900	-0.73693100	1.88241300
O	4.93114300	-1.61228300	-1.05662400
C	4.43988600	-2.08086700	-2.30795700
O	3.28713100	-1.31025000	-2.62198400
C	5.58514100	-1.65519700	1.78348100
O	-2.95425600	-2.73539600	1.94212500
C	-2.23788600	-2.87416600	3.15206800
O	-4.25239100	-2.64644800	-0.39446600
O	-3.64231500	-0.81767300	-2.24561800
C	-1.15545700	3.15352300	0.35834900

C	-0.60401700	4.54982100	0.09685300
O	0.75010200	4.50185100	0.02020500
C	1.21712000	3.16048900	0.23310500
O	-1.21309000	5.57393400	-0.01321700
C	-1.58231800	3.04696100	1.82423400
H	-1.54169500	0.76834200	-1.65912500
H	-0.89083800	-0.99518100	2.18244200
H	0.15917900	1.00932100	1.64545200
H	-0.02664500	2.15370600	-1.16087900
H	2.23474300	0.29322100	2.15773100
H	0.88156300	-0.14282600	-1.91876400
H	5.19976000	-1.93242900	-3.07343700
H	4.15606300	-3.13894600	-2.21694200
H	6.07731800	-1.63242700	2.75427300
H	6.29338500	-1.36304000	1.00656500
H	5.22475600	-2.66806200	1.58249400
H	-2.73078100	-3.67544600	3.69989100
H	-2.27169900	-1.95700800	3.75046300
H	-1.19370400	-3.15106800	2.97240600
H	-2.03342300	3.01062200	-0.27221400
H	2.07025300	2.99419500	-0.42208900
H	1.55041800	3.06545600	1.27179300
H	-2.02365100	2.06941600	2.02448500
H	-2.32722900	3.81268400	2.04650700
H	-0.74181900	3.19301600	2.50785600
C	-5.54612200	-2.20451200	0.00005800
C	-3.29756600	0.06798000	-3.29068300
H	-6.23730000	-3.00811100	-0.25230600
H	-5.83516400	-1.29841500	-0.54143900
H	-5.58715500	-2.02034800	1.07821300
H	-3.37539900	1.11546500	-2.97913700
H	-4.01451100	-0.11886200	-4.08822400
H	-2.28701700	-0.12526200	-3.66628900

B3PW91/TZVP opt

Total energy = –937089.0132 kcal/mol

Conf 2

C	2.97448600	-0.60099900	1.05197300
C	3.36954700	-1.51696700	0.07179600
C	1.82230200	0.16848400	0.87594200
C	1.05608000	0.03162800	-0.27681300
C	1.45278300	-0.87051800	-1.26081800
C	2.59951900	-1.64320800	-1.09138900
C	-0.23585500	0.80619600	-0.49297500
C	-0.25766200	2.18408100	0.17978300
C	-1.45573800	-0.01277700	-0.08759600
C	-2.47793500	-0.21778000	-1.01556800
C	-3.63970000	-0.93966400	-0.69902800
C	-3.71872700	-1.44786200	0.58516900
C	-2.70269700	-1.24213000	1.49978700
C	-1.56046400	-0.53310700	1.20709100
O	-4.67767700	-1.17427900	-1.53524700
O	-4.74570300	-2.13962800	1.17061100
C	-4.18006900	-2.63197900	2.38174600
O	-3.05722800	-1.80938900	2.69510200
C	-4.61478700	-0.63274800	-2.83976500
O	3.05716600	-2.54119800	-1.99727900
C	2.28865600	-2.76825800	-3.16069900
O	4.44839800	-2.32402000	0.27652700
O	3.78115400	-0.52746000	2.13843800
C	0.80685700	3.20577600	-0.25166800
C	0.12392400	4.53171800	0.06104500
O	-1.21558200	4.34293200	0.17404100
C	-1.54975100	2.96714100	-0.06357400
O	0.62826400	5.61010300	0.18036400
C	1.20778300	3.18022000	-1.72847700
H	1.52987700	0.87193200	1.64235200
H	0.84992800	-0.97710400	-2.15346600

H	-0.32208000	0.97440100	-1.57117500
H	-0.17152900	2.05031600	1.26348700
H	-2.36308300	0.18716000	-2.01301900
H	-0.77331100	-0.41213800	1.93922200
H	-4.91593200	-2.56340400	3.18154900
H	-3.83944500	-3.66561400	2.23158800
H	-5.54160200	-0.92627800	-3.32895700
H	-3.76752900	-1.03743400	-3.40381700
H	-4.54993200	0.46033200	-2.81901600
H	2.81776600	-3.53617300	-3.72235300
H	2.20830200	-1.86542600	-3.77635700
H	1.28470700	-3.13027000	-2.91509700
H	1.71020700	3.13741000	0.35486200
H	-2.36062000	2.69710800	0.61036100
H	-1.90365000	2.86590200	-1.09492300
H	1.73677200	2.25594200	-1.96566500
H	1.87036700	4.02016200	-1.94328700
H	0.34229900	3.26351900	-2.39129700
C	5.68067600	-1.80624200	-0.21131500
C	3.40940100	0.33190800	3.19635700
H	6.44073600	-2.55302800	0.01623100
H	5.93848500	-0.86725100	0.28842300
H	5.64170800	-1.65128600	-1.29401200
H	3.38302400	1.38032000	2.87932500
H	4.17519500	0.21186900	3.96060900
H	2.43721700	0.05507200	3.61796300

B3PW91/TZVP opt

Total energy = –937088.5545 kcal/mol

Conf 3

C	-2.73006000	-1.51161800	1.19804500
C	-3.49922200	-1.38800100	0.03373600
C	-1.57375100	-0.75229200	1.35914500
C	-1.16550200	0.13316300	0.36479200
C	-1.92392600	0.25950100	-0.79418800
C	-3.08341800	-0.50083600	-0.96421900
C	0.13247900	0.89758500	0.57850200
C	0.18303100	2.25888500	-0.12493200
C	1.34409700	0.05352200	0.20375900
C	2.35728700	-0.14156800	1.13098100
C	3.52192800	-0.87614000	0.84664200
C	3.62171500	-1.39527300	-0.43231800
C	2.60465700	-1.19203900	-1.35896400
C	1.45935200	-0.48942400	-1.08597900
O	4.40482900	-1.02725000	1.86201000
O	4.57734800	-2.22349400	-0.98475000
C	4.28671900	-2.19883600	-2.37785200
O	2.91189600	-1.86310000	-2.51424100
C	5.74534600	-1.39452200	1.55767900
O	-3.87517700	-0.44682900	-2.06264500
C	-3.53565100	0.45764400	-3.09287500
O	-4.67498700	-2.06432600	-0.09885100
O	-3.19755400	-2.39568800	2.11300300
C	-0.87319000	3.30530400	0.26670400
C	-0.16626300	4.61363900	-0.06581600
O	1.17206500	4.40332000	-0.15405000
C	1.48232200	3.02905700	0.12195900
O	-0.65261400	5.69601000	-0.21896500
C	-1.29806900	3.31819200	1.73702100
H	-0.97440900	-0.85268600	2.25480600
H	-1.61945900	0.94717400	-1.57027800
H	0.21086100	1.08839200	1.65322200
H	0.11134400	2.10180400	-1.20669200
H	2.27873300	0.27847900	2.12733800
H	0.67519100	-0.38794800	-1.82433100
H	4.89940700	-1.42746800	-2.86598300
H	4.46737200	-3.18474900	-2.80289000
H	6.28459700	-1.34206200	2.50192700

H	6.19224900	-0.69527400	0.84516200
H	5.80574600	-2.40716300	1.15611900
H	-4.30453400	0.34322200	-3.85493000
H	-2.55930600	0.22504000	-3.53247300
H	-3.53661700	1.49391200	-2.73811700
H	-1.76785500	3.23658300	-0.35254900
H	2.29997500	2.73198300	-0.53223300
H	1.81818000	2.94680300	1.16079300
H	-1.84955900	2.40975300	1.98370200
H	-1.94758400	4.17490000	1.92350700
H	-0.44191800	3.39784800	2.41216600
C	-4.54550800	-3.39096300	-0.59709000
C	-2.48291800	-2.54600600	3.32297300
H	-5.55445000	-3.79818600	-0.65527500
H	-3.94587100	-4.00930200	0.07743200
H	-4.09878500	-3.39292000	-1.59651800
H	-2.44151500	-1.60669500	3.88459900
H	-1.46451700	-2.90990200	3.14916000
H	-3.03247200	-3.28451800	3.90403200

B3PW91/TZVP opt

Total energy = –937088.5206 kcal/mol

Conf 4

C	3.08878000	-0.34022600	0.93746100
C	3.54546100	-1.17624800	-0.08654600
C	1.87170000	0.33346800	0.80845200
C	1.09712000	0.17104100	-0.33519200
C	1.54628000	-0.66436600	-1.35496000
C	2.75977100	-1.33729400	-1.23494200
C	-0.25672100	0.84334300	-0.50580700
C	-0.37701800	2.19444100	0.21014700
C	-1.40071000	-0.08133300	-0.10622000
C	-2.44025400	-0.31036800	-1.00908900
C	-3.54361400	-1.11647700	-0.68773500
C	-3.55808400	-1.66387200	0.58276600
C	-2.52346200	-1.43742100	1.47127000
C	-1.42876300	-0.66125500	1.16706300
O	-4.57891100	-1.40572800	-1.50974700
O	-4.46818300	-2.52827700	1.13134400
C	-4.11938500	-2.56099600	2.51162900
O	-2.75776200	-2.14804100	2.61883900
C	-4.56356900	-0.86176400	-2.81480700
O	3.26991400	-2.16773100	-2.17708300
C	2.53922400	-2.35159600	-3.37212800
O	4.77039700	-1.76628300	0.00569000
O	3.90021900	-0.24658000	2.01829700
C	0.59838800	3.30970300	-0.20043400
C	-0.18085100	4.56710800	0.16425600
O	-1.49995600	4.27050400	0.28845600
C	-1.72958800	2.88141700	0.00825100
O	0.23904500	5.67742700	0.31322400
C	0.98012600	3.36258300	-1.68166900
H	1.53551500	0.98224400	1.60470000
H	0.93494000	-0.79356400	-2.23883700
H	-0.37519400	1.03676200	-1.57663100
H	-0.26524700	2.03393500	1.28785000
H	-2.38967000	0.14962600	-1.98779700
H	-0.61925600	-0.53119800	1.87287500
H	-4.75485900	-1.85619100	3.06552100
H	-4.22243500	-3.57708900	2.88944100
H	-5.46782000	-1.22511600	-3.29931200
H	-3.69032100	-1.20103100	-3.38210900
H	-4.58254600	0.23320900	-2.79520100
H	3.12889800	-3.03533100	-3.98029500
H	2.41182100	-1.40869900	-3.91476200
H	1.55646100	-2.79625100	-3.18123600
H	1.51304800	3.29397400	0.39285800
H	-2.50723500	2.52671800	0.68216900

H	-2.08916200	2.78745300	-1.02181800
H	1.58294100	2.49454600	-1.95252900
H	1.56661300	4.26168500	-1.87726700
H	0.10215200	3.39155500	-2.33258700
C	4.75073100	-3.10211100	0.49605100
C	3.51557200	0.60540400	3.07732000
H	5.78707800	-3.43770200	0.51827100
H	4.17421900	-3.75640800	-0.16464400
H	4.33777200	-3.14209800	1.50902300
H	3.42973100	1.64660800	2.74837700
H	4.30775600	0.53277200	3.82035000
H	2.56990200	0.28816800	3.53062400

B3PW91/TZVP opt

Total energy = –937088.3361kcal/mol

Conf 5

C	-2.78482100	-0.87251400	-1.12126200
C	-3.20993900	-1.75095300	-0.11904100
C	-1.72573700	0.00682600	-0.88838900
C	-1.07820600	0.01365900	0.34287100
C	-1.50394300	-0.85250300	1.34637600
C	-2.56224800	-1.73123400	1.12252300
C	0.11431800	0.91383500	0.62940500
C	0.06197700	2.26511500	-0.09096400
C	1.43509800	0.20324800	0.35632800
C	1.72480600	-0.29189500	-0.90798600
C	2.93187100	-0.93687500	-1.21382400
C	3.83927000	-1.07313300	-0.17409600
C	3.54071700	-0.58811600	1.09095100
C	2.36565100	0.05618700	1.39547700
O	3.10233800	-1.33014200	-2.49787600
O	5.12441500	-1.57649100	-0.17439000
C	5.43660000	-1.71427400	1.20731700
O	4.61468800	-0.79589900	1.91776900
C	4.05781200	-2.34482100	-2.78520300
O	-3.04314500	-2.59847100	2.04584900
C	-2.40526900	-2.65446600	3.30501800
O	-4.19706500	-2.65861300	-0.36326500
O	-3.47260500	-0.94431600	-2.28751600
C	-1.13344000	3.18551200	0.20420300
C	-0.55937900	4.56283400	-0.10437100
O	0.79677600	4.50926200	-0.08803700
C	1.24167600	3.18341000	0.23765100
O	-1.15482200	5.57882100	-0.31648500
C	-1.65777700	3.16778100	1.64218200
H	-1.41104200	0.68083800	-1.67257500
H	-0.99509000	-0.84340100	2.30160600
H	0.09508700	1.12213900	1.70356100
H	0.09057600	2.09159400	-1.17182300
H	0.99773000	-0.22076900	-1.70752800
H	2.17454000	0.42722000	2.39455000
H	5.20375700	-2.73762800	1.53476300
H	6.48486400	-1.46836800	1.36838500
H	3.93027700	-2.57588800	-3.84135400
H	3.86655500	-3.24353500	-2.19184400
H	5.07792100	-2.00236800	-2.60502600
H	-2.93293700	-3.41897000	3.87266000
H	-2.47594600	-1.69953300	3.83757400
H	-1.35205600	-2.93972000	3.21106000
H	-1.96840500	3.00527500	-0.47355400
H	2.13603000	2.97609300	-0.34698300
H	1.50227500	3.15320000	1.30095700
H	-2.11649100	2.20440500	1.86988000
H	-2.41226500	3.94603000	1.76782900
H	-0.86453600	3.35420900	2.37111500

C	-5.51666200	-2.17493700	-0.14120600
C	-3.06118400	-0.12490300	-3.36251200
H	-6.19073500	-2.99860300	-0.37445100
H	-5.74221500	-1.32864300	-0.79705100
H	-5.65657800	-1.88107900	0.90400800
H	-3.15748400	0.93966300	-3.12247600
H	-3.72651200	-0.36335100	-4.19043000
H	-2.02911100	-0.33871300	-3.65994400

B3PW91/TZVP opt

Total energy = –937088.2388 kcal/mol

Conf 6

C	-2.92127600	-0.48502700	-0.98223200
C	-3.32954400	-1.44538600	-0.05176600
C	-1.76630800	0.26926600	-0.75803000
C	-1.01736400	0.08118000	0.39862500
C	-1.42962500	-0.86397600	1.33533400
C	-2.57147900	-1.62897100	1.11281500
C	0.27441400	0.83716400	0.66979100
C	0.36516300	2.20013800	-0.02756100
C	1.49894200	-0.01345800	0.34875200
C	1.61784200	-0.62839300	-0.89904900
C	2.74541100	-1.38065500	-1.25077100
C	3.75340100	-1.46917700	-0.30295100
C	3.62799500	-0.86696500	0.93210200
C	2.51786500	-0.13575400	1.29882800
O	2.92888200	-2.02997000	-2.42226400
O	4.92093400	-2.18462300	-0.36042200
C	5.66002500	-1.71819400	0.76328100
O	4.72456100	-1.17445800	1.69449900
C	1.88340200	-1.98578700	-3.37520400
O	-3.03539800	-2.57536700	1.96478000
C	-2.27677100	-2.86363300	3.12233800
O	-4.40801300	-2.23509100	-0.31607900
O	-3.71358000	-0.35596700	-2.07443000
C	-0.69278200	3.25826800	0.32796900
C	0.03780700	4.55884200	0.01722300
O	1.37538100	4.33480800	-0.02692300
C	1.66238500	2.95829200	0.26431900
O	-0.43350900	5.64517700	-0.15453700
C	-1.16611600	3.27605300	1.78329800
H	-1.46248000	1.00457600	-1.48901800
H	-0.83712800	-1.01333500	2.22888000
H	0.30656400	1.02670400	1.74756600
H	0.33198100	2.04320500	-1.11120600
H	0.79711900	-0.54228900	-1.59885500
H	2.44333300	0.31484600	2.28064200
H	6.18922400	-2.55126600	1.22323100
H	6.35088200	-0.92586700	0.44287500
H	2.22393200	-2.58495900	-4.21745500
H	1.69433100	-0.96211800	-3.71571900
H	0.95849700	-2.41454600	-2.97643800
H	-2.80606000	-3.66589300	3.63341100
H	-2.20960900	-1.99686500	3.78885600
H	-1.26804500	-3.20392600	2.86665100
H	-1.56744800	3.20028700	-0.32024000
H	2.50040700	2.65106700	-0.35839100
H	1.95911600	2.87798600	1.31500300
H	-1.73791700	2.37503300	2.01085300
H	-1.80923700	4.14173600	1.94958300
H	-0.33168900	3.34276500	2.48639100
C	-5.61516400	-1.83510100	0.32298600
C	-3.35217400	0.58845900	-3.05989600
H	-6.37745800	-2.55022300	0.01549000
H	-5.91381800	-0.83164300	0.00291800
H	-5.51418500	-1.86228900	1.41172400
H	-3.34077000	1.60872700	-2.66090300
H	-4.11468600	0.51820400	-3.83361700

H	-2.37520500	0.36090800	-3.50042500

B3PW91/TZVP opt

Total energy = –937088.2137 kcal/mol

Conf 7

C	-2.66204000	-1.53176400	1.22598900
C	-3.35036600	-1.53009300	0.00632700
C	-1.56212500	-0.69703100	1.41131000
C	-1.12818400	0.13922000	0.38596800
C	-1.80608700	0.14334500	-0.82860100
C	-2.90947400	-0.69045000	-1.02185100
C	0.10890100	0.99051900	0.63060100
C	0.11197800	2.32290300	-0.12485300
C	1.38928100	0.20938700	0.35604200
C	1.63729900	-0.32007300	-0.90318700
C	2.80731200	-1.02795800	-1.21400600
C	3.72079200	-1.19240600	-0.18349600
C	3.46341500	-0.67178000	1.07656600
C	2.32555900	0.03432800	1.38546200
O	2.93771500	-1.44953800	-2.49373900
O	4.98043000	-1.75752900	-0.19087000
C	5.30467100	-1.88579600	1.18888200
O	4.53723100	-0.91702300	1.89306000
C	3.87490700	-2.47800300	-2.79018200
O	-3.62342500	-0.75441700	-2.17195800
C	-3.26112200	0.10004400	-3.23701500
O	-4.47870300	-2.27811400	-0.15296800
O	-3.14682600	-2.37763300	2.16774600
C	-1.03042100	3.31060600	0.16289800
C	-0.39071300	4.64926000	-0.18546900
O	0.96116700	4.52576400	-0.18848700
C	1.34224000	3.18716700	0.16297200
O	-0.93607300	5.68984000	-0.41200700
C	-1.53784500	3.35346600	1.60645500
H	-1.02683800	-0.70002800	2.35200100
H	-1.48099900	0.79104500	-1.63051900
H	0.11638200	1.22796100	1.69891400
H	0.11473300	2.12003100	-1.20096600
H	0.90429000	-0.22460500	-1.69487500
H	2.16717200	0.43215200	2.37989900
H	5.02813200	-2.89101800	1.53792800
H	6.36557700	-1.68746100	1.33189400
H	3.72328300	-2.71709000	-3.84136700
H	3.68624800	-3.36901100	-2.18461100
H	4.90240100	-2.14576000	-2.63426900
H	-3.96749900	-0.10767700	-4.03880200
H	-2.24534400	-0.10325500	-3.59359900
H	-3.34275800	1.15500400	-2.95432200
H	-1.88209900	3.15894800	-0.50085200
H	2.21525000	2.91974600	-0.42957800
H	1.61813700	3.16861800	1.22271000
H	-2.04992000	2.42394000	1.85981800
H	-2.24421400	4.17690400	1.72300000
H	-0.72628400	3.50831900	2.32252600
C	-4.25221300	-3.60322700	-0.61840900
C	-2.52225900	-2.39509400	3.43482100
H	-5.23186300	-4.07302000	-0.70109800
H	-3.63980400	-4.17028300	0.08942600
H	-3.77188900	-3.59776100	-1.60200400
H	-1.47427600	-2.70684800	3.36607100
H	-3.07312200	-3.12224300	4.02889200
H	-2.57786800	-1.41680900	3.92421200

B3PW91/TZVP opt

Total energy = –937088.0989 kcal/mol

Conf 8

C	-2.99283900	-0.31575900	-0.87503800
C	-3.46350200	-1.16414500	0.13194100
C	-1.78611100	0.37027600	-0.71350400
C	-1.03741000	0.21110300	0.44783400
C	-1.50223600	-0.63465200	1.45211400
C	-2.70435900	-1.32058500	1.29941900
C	0.30363300	0.89730900	0.65757500
C	0.44974100	2.22791500	-0.09061900
C	1.47042900	-0.03248000	0.34250900
C	1.53841800	-0.68388000	-0.89070400
C	2.61363600	-1.51345000	-1.23266900
C	3.62255400	-1.64339300	-0.29083400
C	3.54795000	-1.00352500	0.92923700
C	2.48993700	-0.19431000	1.28594900
O	2.74554300	-2.20091600	-2.38980100
O	4.74192200	-2.43240700	-0.34032900
C	5.52000500	-1.98748800	0.76593300
O	4.63057400	-1.36040100	1.68981700
C	1.70245800	-2.10318000	-3.34052600
O	-3.22874700	-2.15927300	2.22578000
C	-2.53085000	-2.33212500	3.44281900
O	-4.68032900	-1.76454300	0.00565900
O	-3.77948600	-0.22299400	-1.97489900
C	-0.54440600	3.35091800	0.24851400
C	0.24371000	4.59916600	-0.12843400
O	1.56742400	4.30514700	-0.19025100
C	1.79067800	2.92698600	0.14522100
O	-0.17482700	5.70108800	-0.33358500
C	-0.98000600	3.44884900	1.71249900
H	-1.44009300	1.02895100	-1.49733300
H	-0.91151100	-0.76022300	2.35045000
H	0.37373100	1.12307700	1.72636900
H	0.38274900	2.03617400	-1.16703800
H	0.71868100	-0.56255500	-1.58649900
H	2.45419800	0.28579100	2.25584800
H	5.99749000	-2.84185900	1.24314400
H	6.25851200	-1.25077300	0.42032500
H	1.99692400	-2.74130700	-4.17149600
H	1.58319300	-1.07584700	-3.70108800
H	0.75137800	-2.45839500	-2.93078700
H	-3.12933900	-3.02276200	4.03422700
H	-2.43227200	-1.38677400	3.98677900
H	-1.53723600	-2.76374100	3.28157800
H	-1.43668400	3.31274700	-0.37685900
H	2.59670600	2.55451200	-0.48424200
H	2.10815400	2.86850500	1.19137500
H	-1.58936300	2.58721100	1.98951600
H	-1.57634800	4.35095100	1.85796900
H	-0.12643300	3.50217000	2.39344500
C	-4.63556600	-3.11476600	-0.44114400
C	-3.40169300	0.67274300	-2.99910200
H	-5.66870800	-3.45699200	-0.49185500
H	-4.08123400	-3.74510400	0.26019800
H	-4.18521100	-3.18311900	-1.43676700
H	-3.34873500	1.70442000	-2.63530100
H	-4.17956900	0.60333000	-3.75744700
H	-2.44058200	0.39685000	-3.44758400

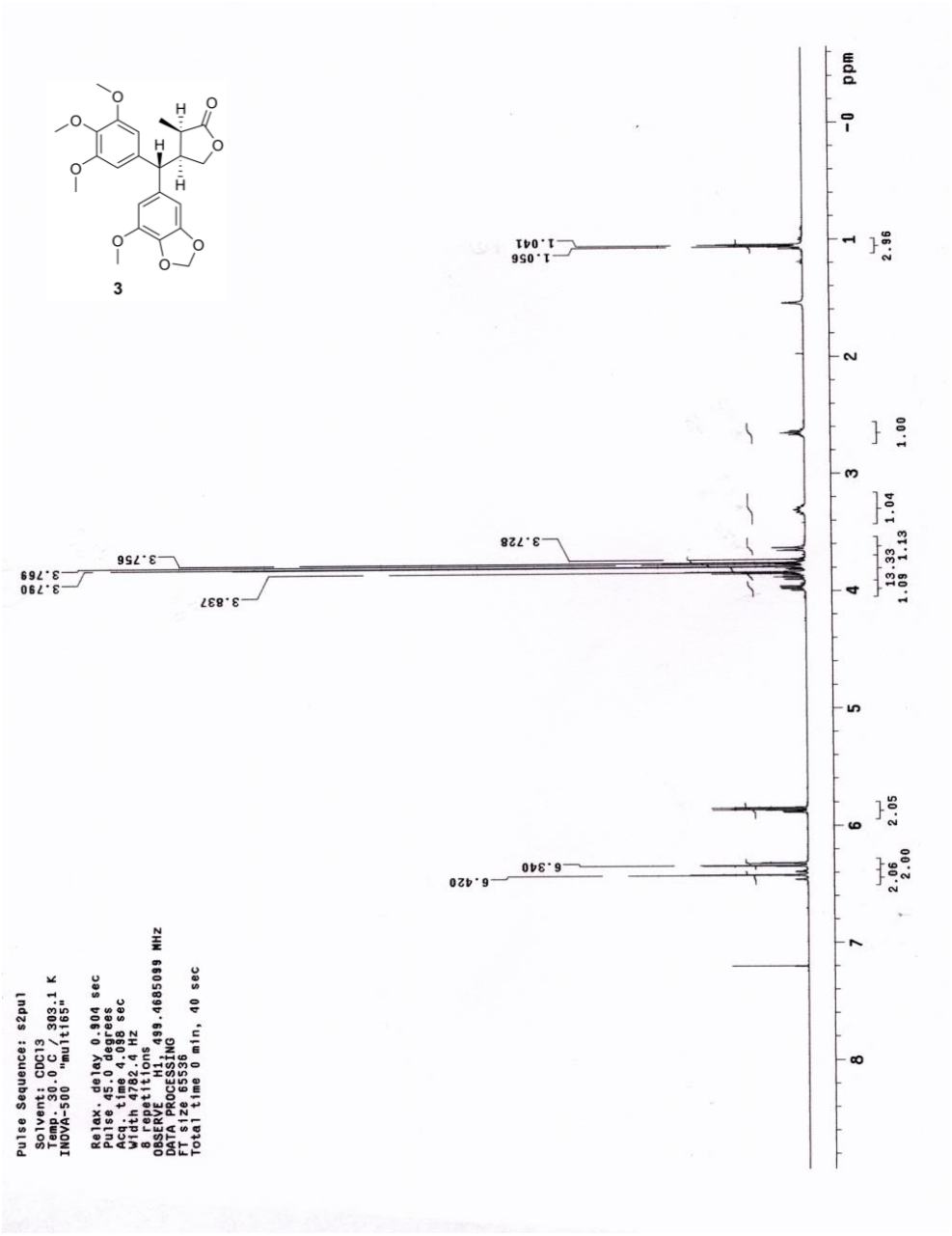

Figure 6 ^{1}H NMR spectrum of **3** in $CDCl_3$

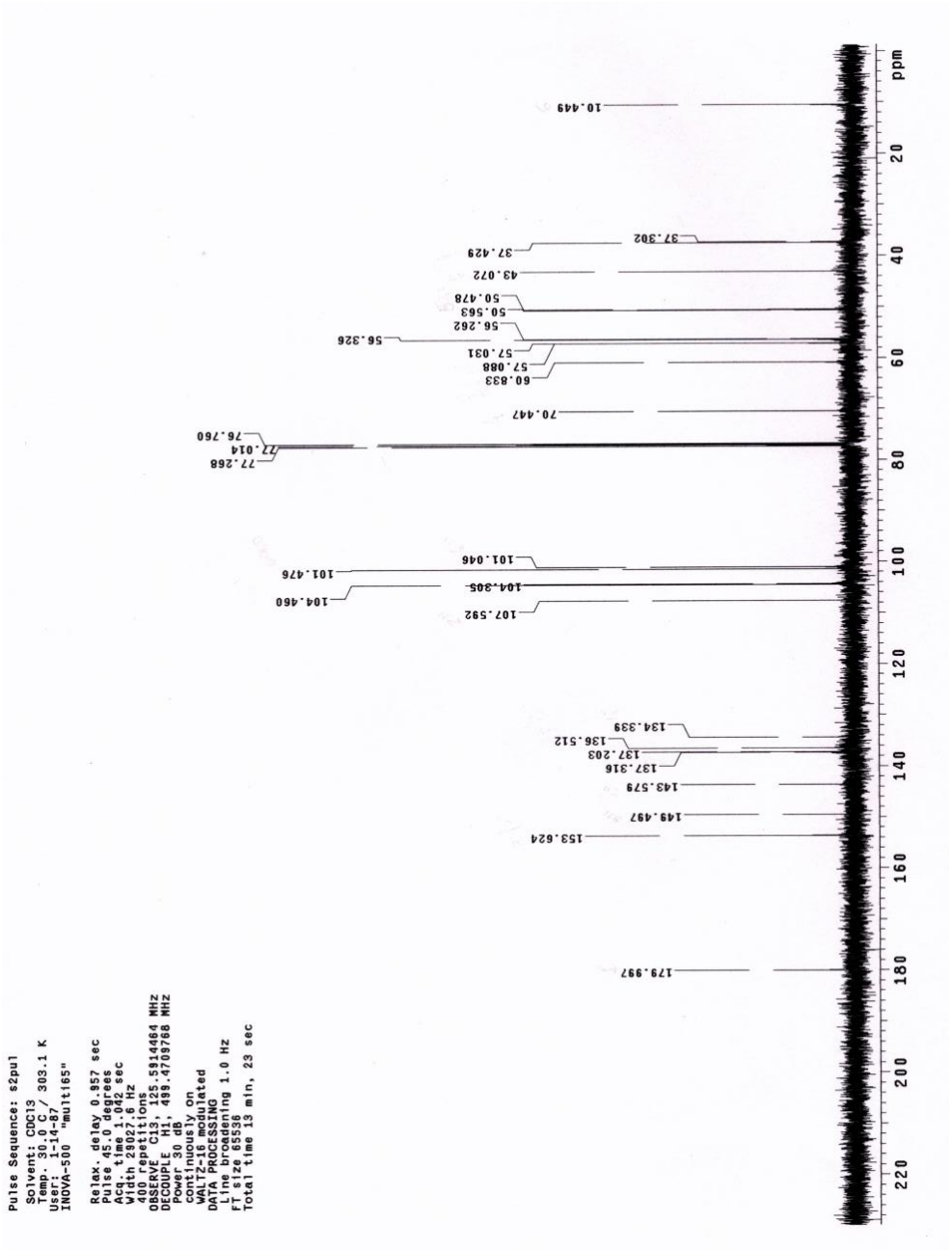

Figure 7 ^{13}C NMR spectrum of **3** in $CDCl_3$

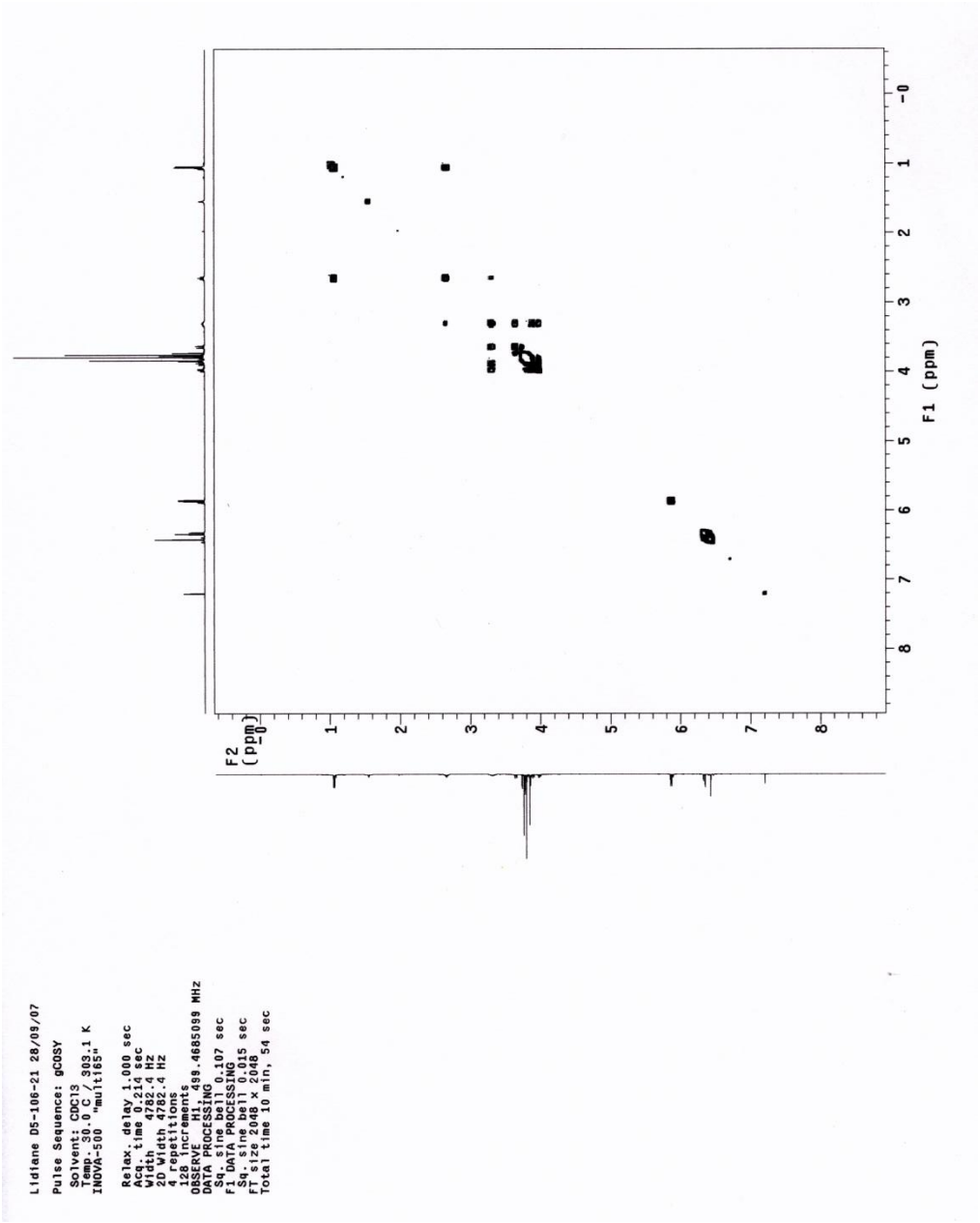

Figure 8 *g*COSY spectrum of **3** in $CDCl_3$

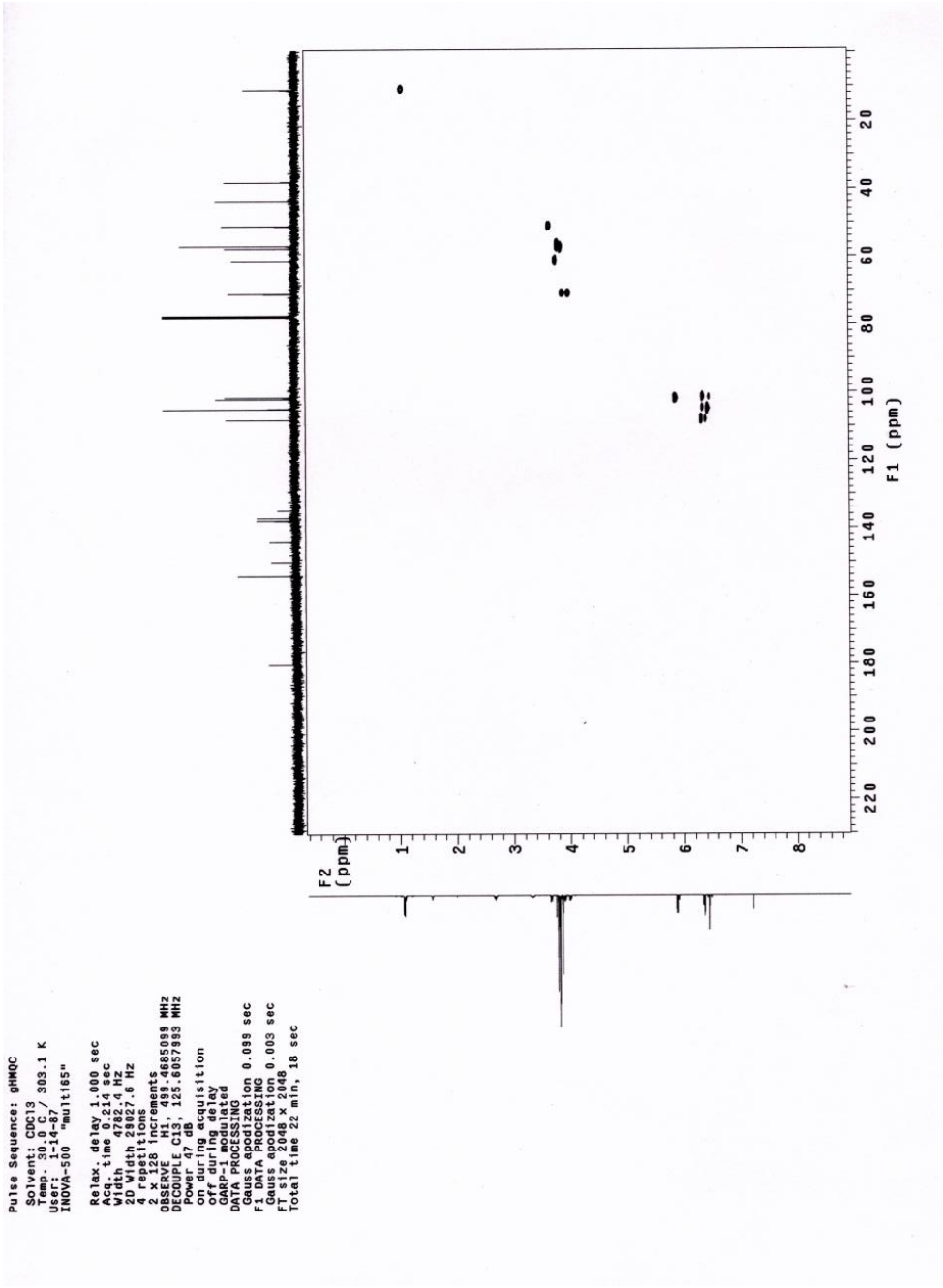

Figure 9 *g*HMQC spectrum of **3** in $CDCl_3$

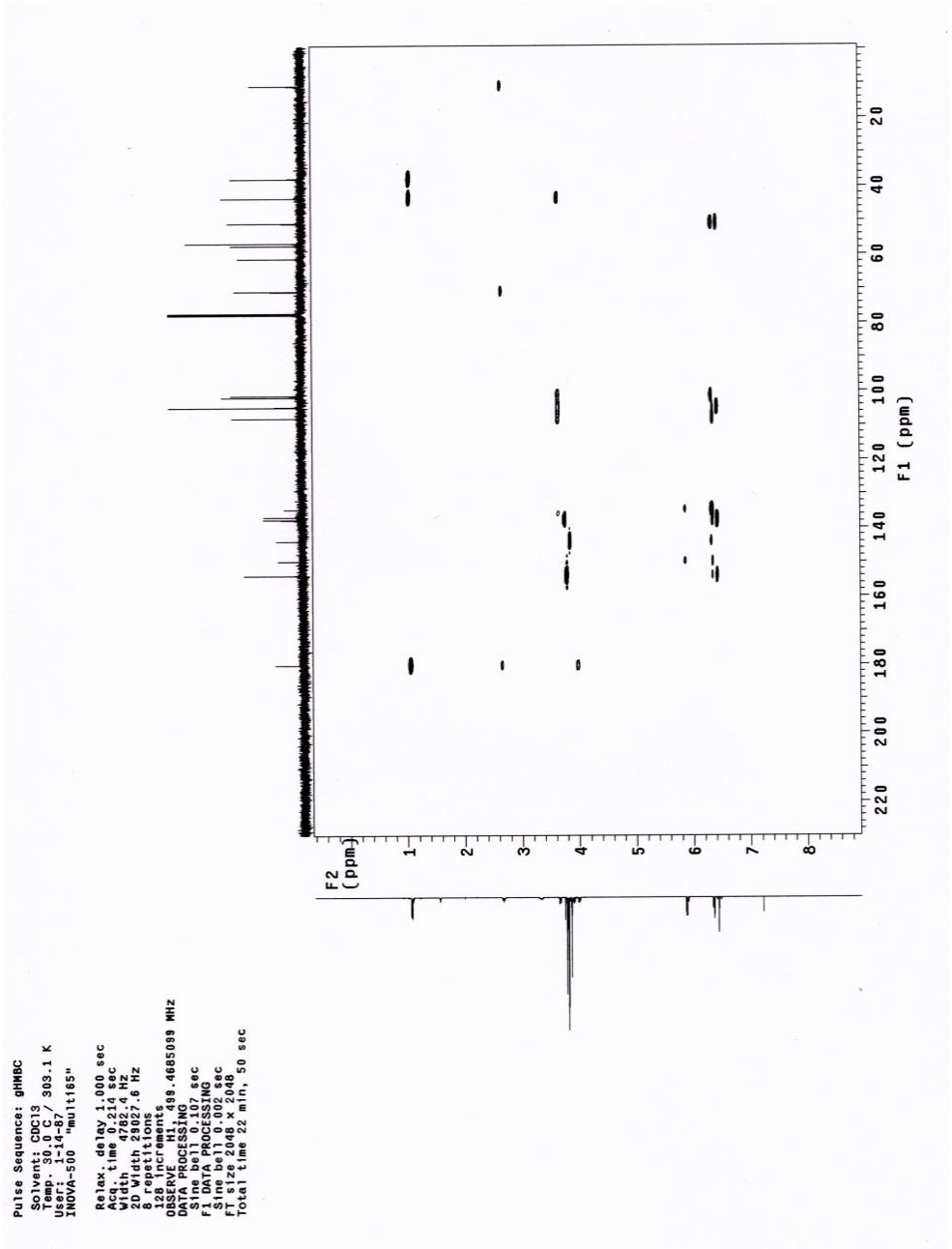

Figure 10 *g*HMBC spectrum of **3** in $CDCl_3$

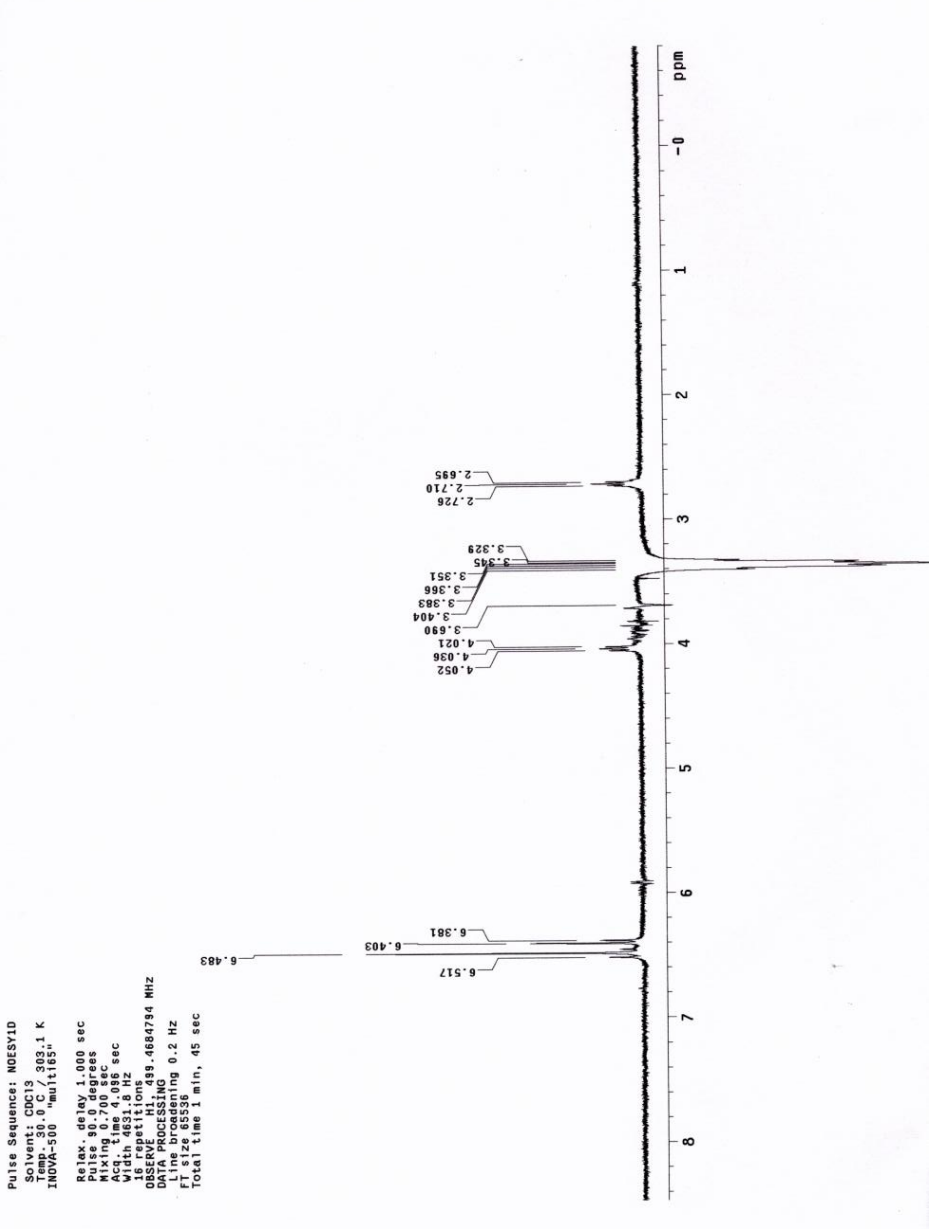

Figure 11 1D NOESY spectrum of **3** in $CDCl_3$

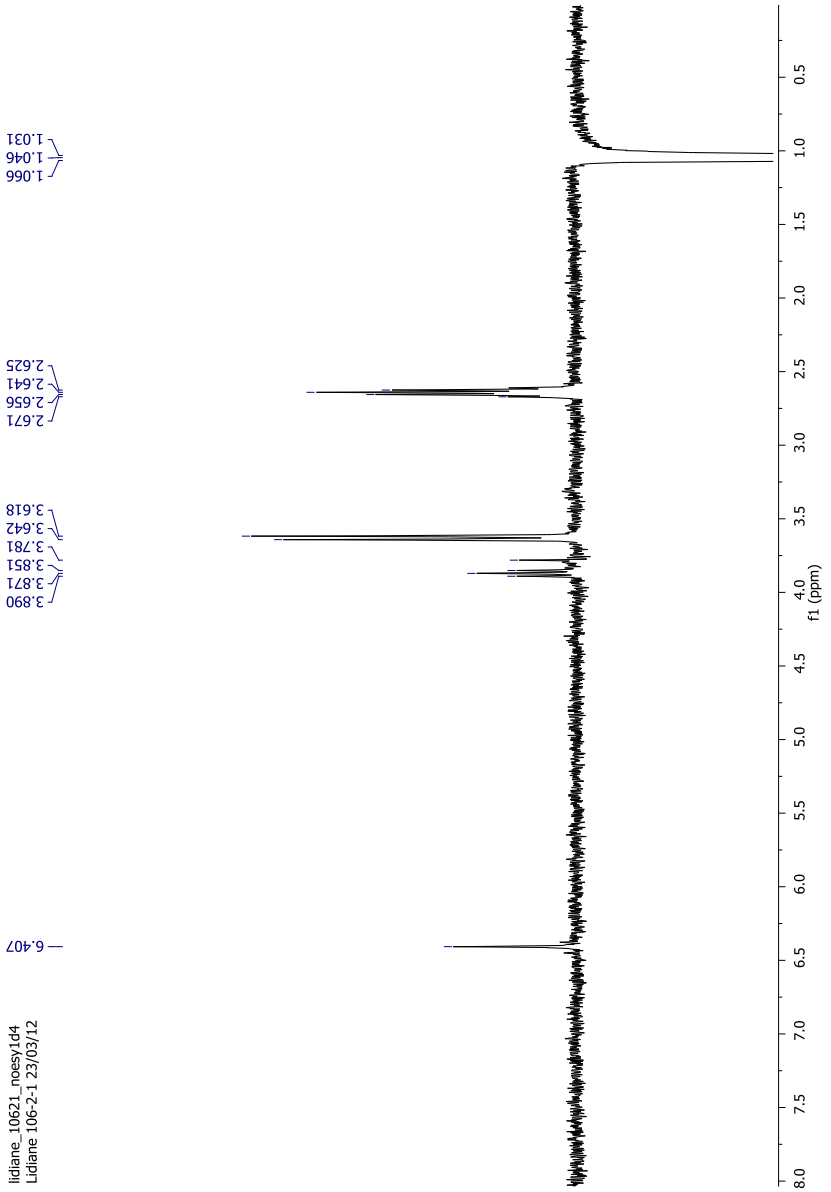

Figure 12 1D NOESY spectrum of **3** in $CDCl_3$

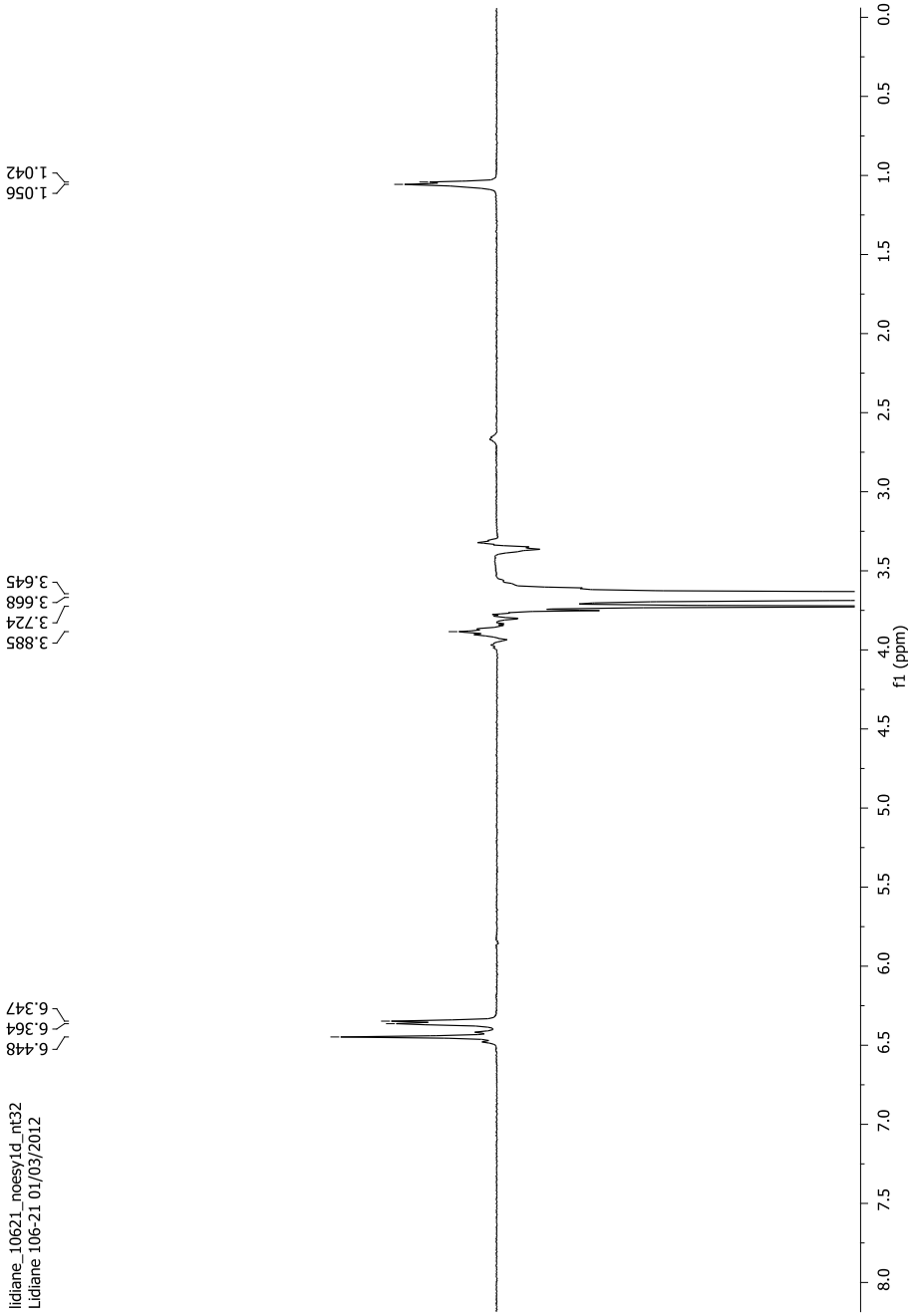

Figure 13 1D NOESY spectrum of **3** in $CDCl_3$

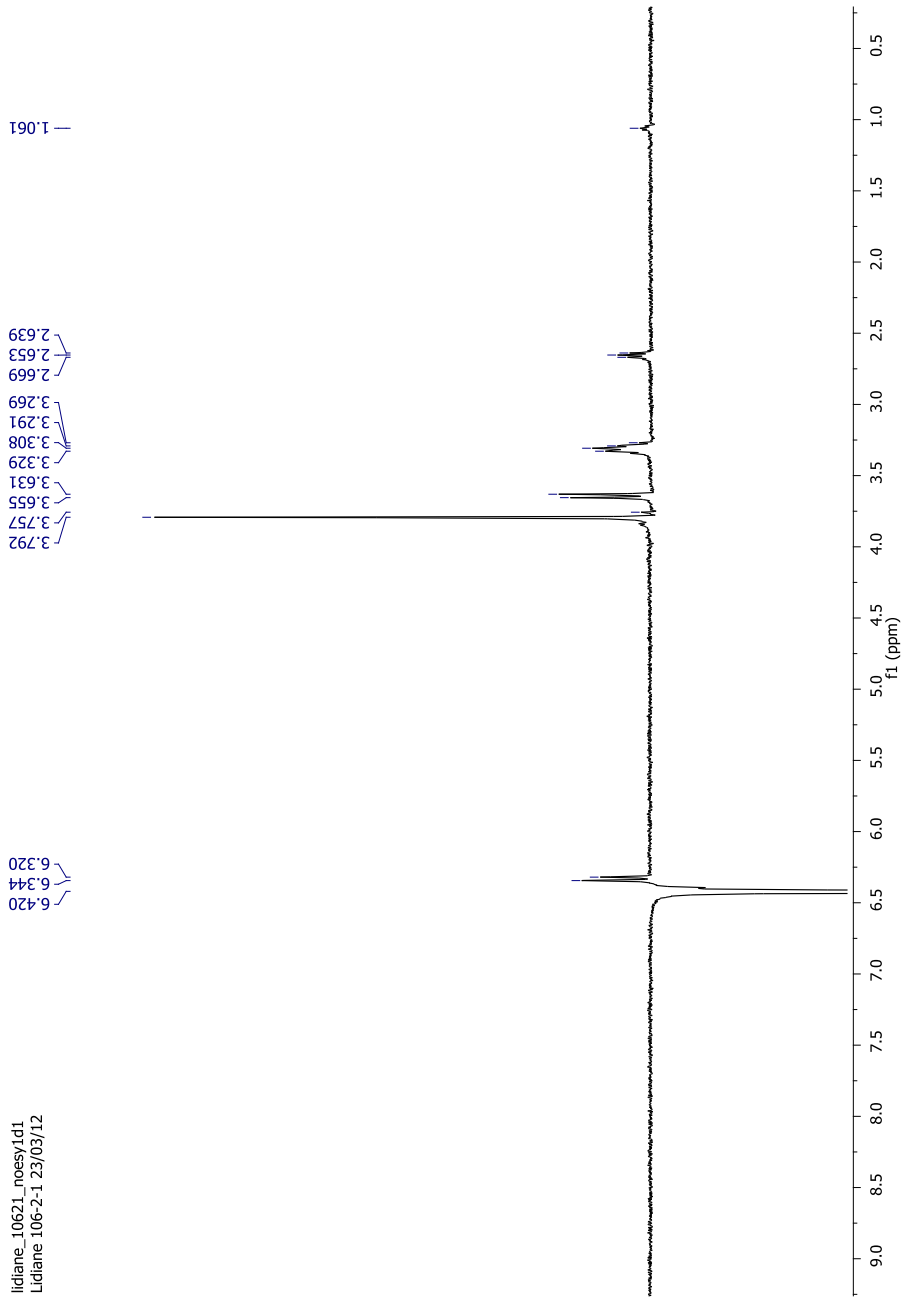

Figure 14 1D NOESY spectrum of **3** in $CDCl_3$

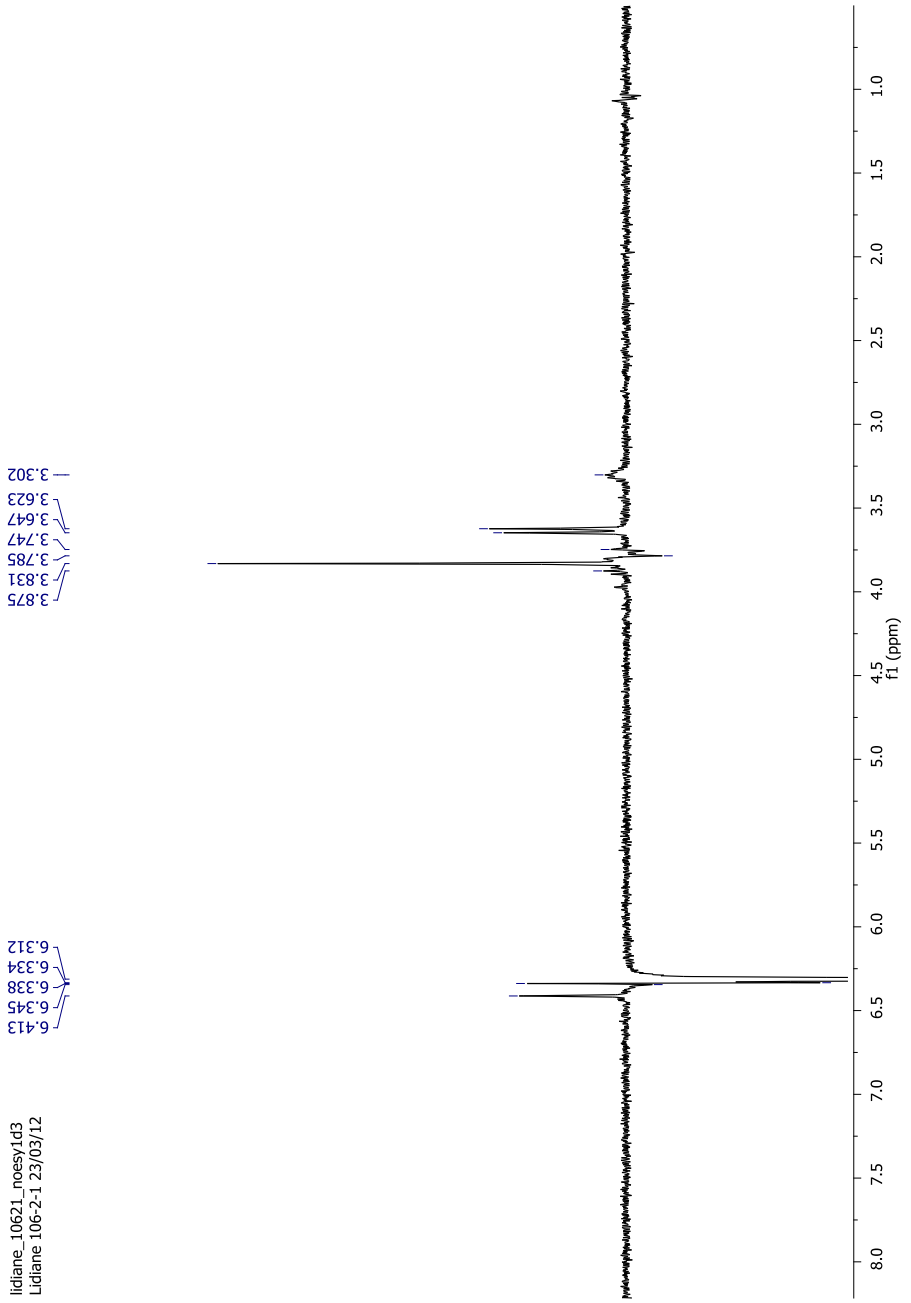

Figure 15 1D NOESY spectrum of **3** in $CDCl_3$

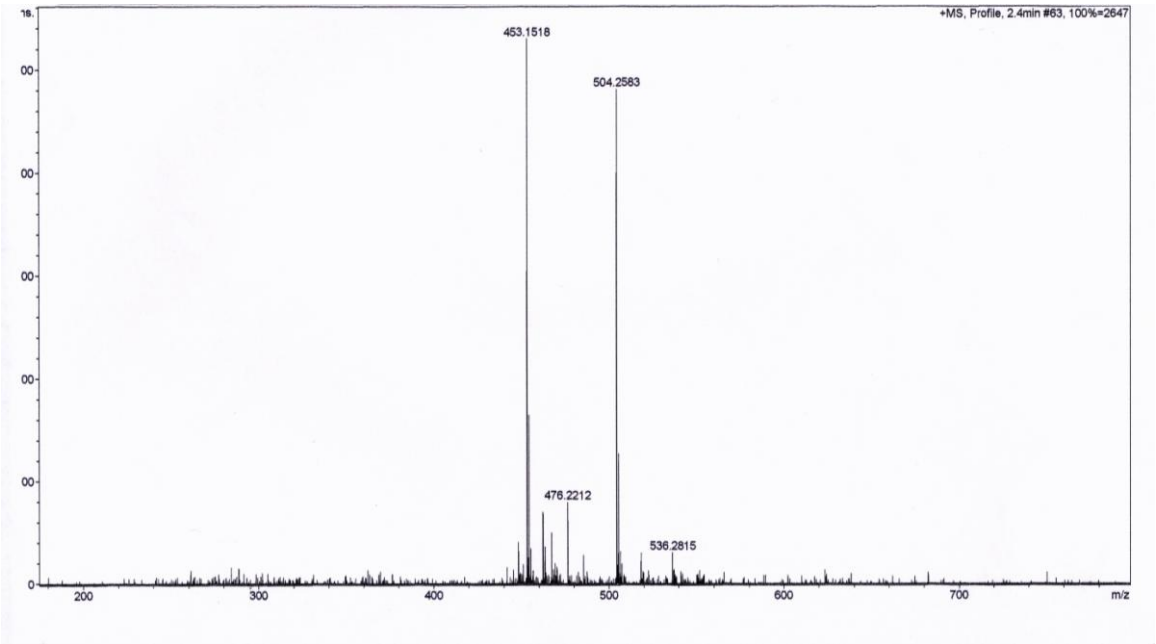

Figure 16 HRESIMS spectrum of **3**

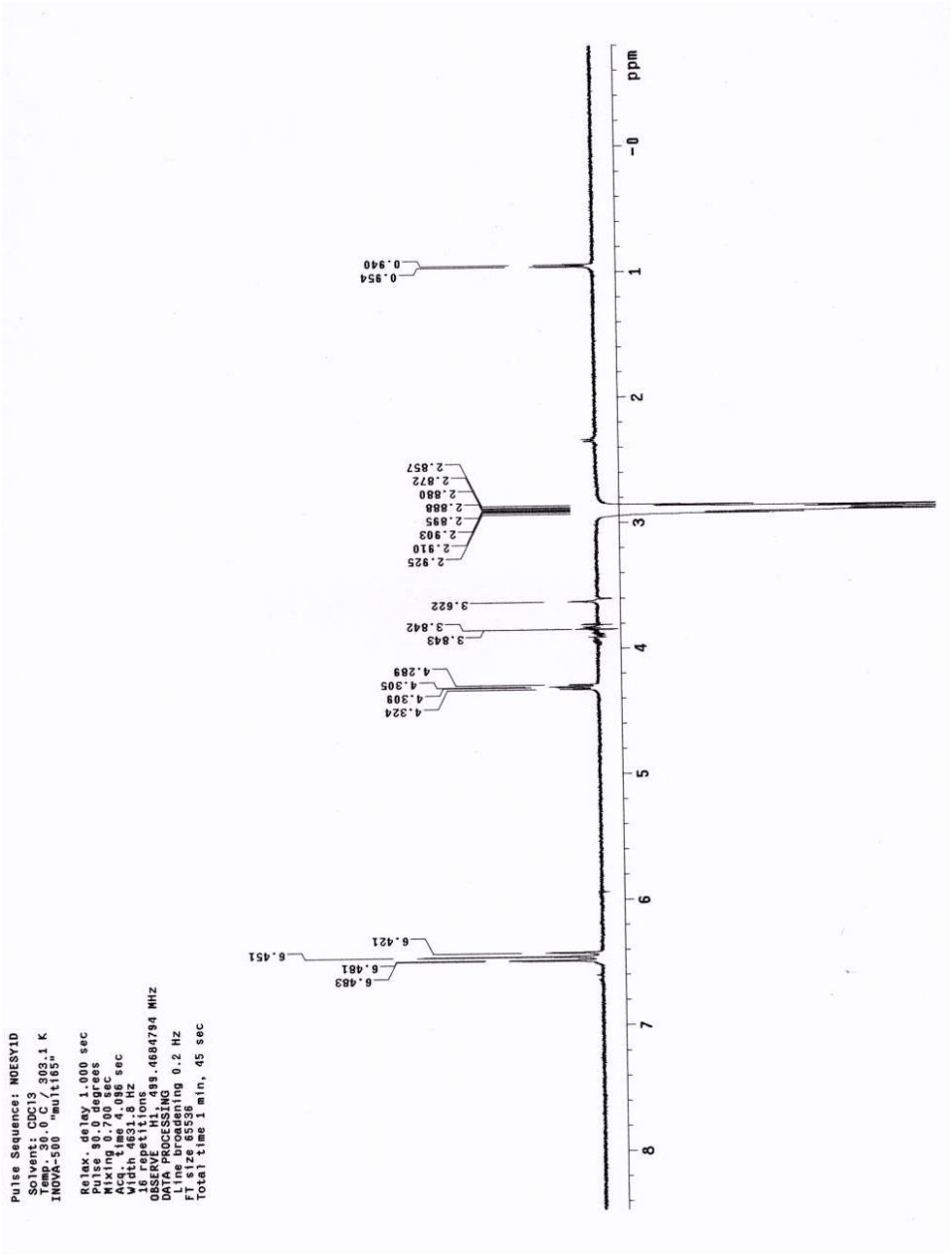

Figure 17 1D NOESY spectrum of **2** in $CDCl_3$

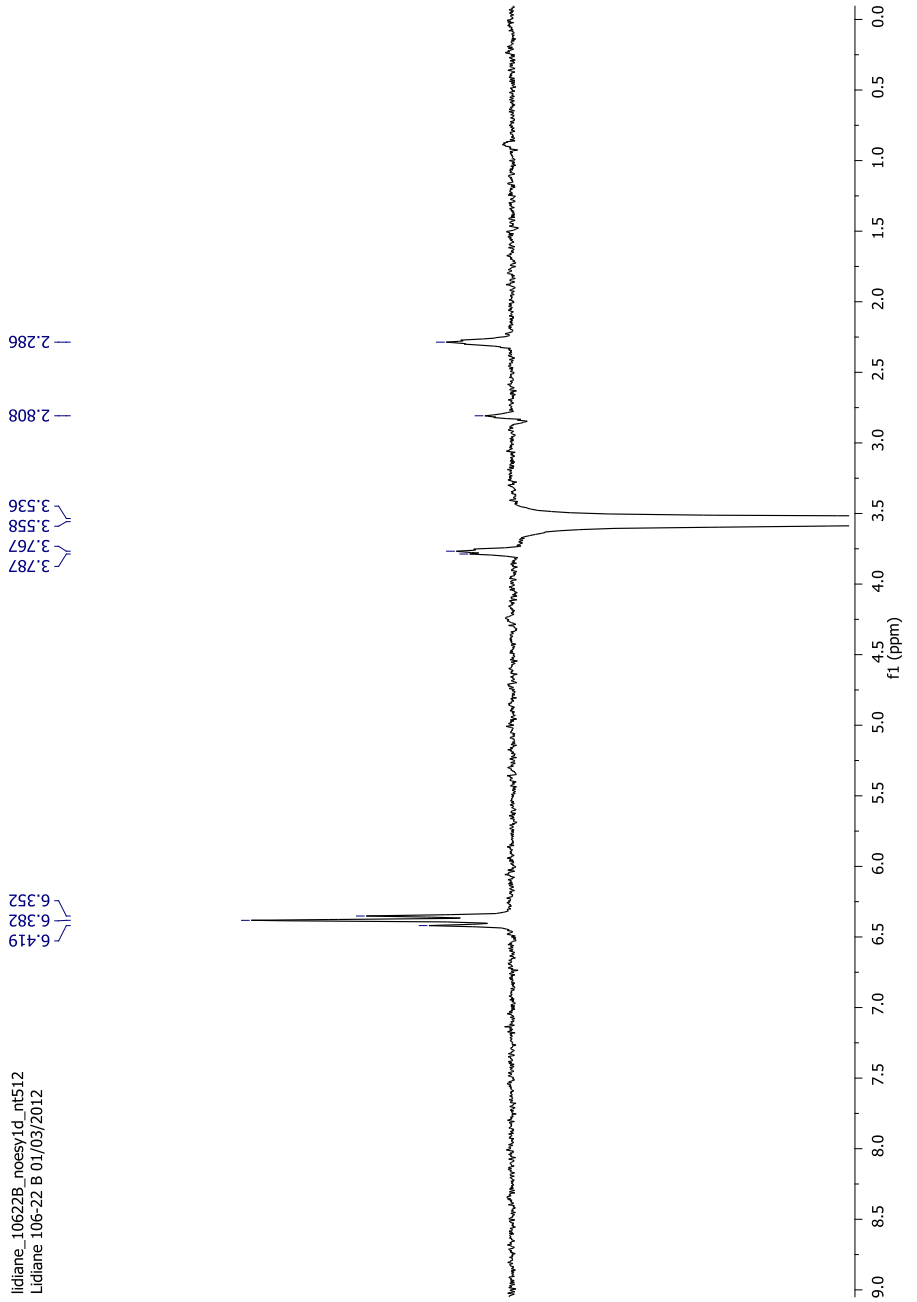

Figure 18 1D NOESY spectrum of **2** in $CDCl_3$