

## Supporting Information

Table 1. Cartesian coordinates (Optimized at B3LYP/6-31G\* level, in vacuo) of conformers used in the calculation

### 1. Conformer 1 of atRAL dimer E (low energy conformer)

C	1.63741600	3.34350000	-0.66272100
C	1.34027800	4.67733800	-0.95186600
C	0.01944000	5.11797900	-1.06782500
C	-1.09577900	4.34624900	-0.71529900
C	2.98251800	2.92494000	-0.54943200
C	3.42541500	1.63478800	-0.31633100
C	4.79298200	1.29179400	-0.23800500
C	5.33185300	0.03443700	-0.01183800
C	6.76575800	-0.08242900	0.02090400
C	7.45508500	-1.25064800	0.18009500
C	8.89839200	-1.45718500	0.20394500
C	4.48406800	-1.19578500	0.19573500
C	9.35905300	-2.78428400	-0.45482300
C	10.88174700	-2.76025900	-0.72214400
C	11.68647000	-2.26093400	0.47332900
C	11.26481400	-0.83317300	0.82062200
C	9.76859500	-0.59601100	0.81084000
C	9.36253200	0.65859100	1.54775800
C	8.65855600	-2.98455000	-1.81914400
C	9.00461400	-3.97614800	0.46756900
C	-2.34350200	4.96127400	-0.85702300
N	-3.53596800	4.46017200	-0.54593700
C	-4.80399400	5.16209000	-0.71433700
C	-5.41970000	5.58003500	0.62470700
O	-6.65041200	6.19296700	0.29913400
H	2.14994200	5.37985000	-1.12724700
H	-0.14997300	6.13472600	-1.41904700
H	3.73817000	3.70064400	-0.66984800
H	2.68775900	0.84779700	-0.19100000
H	5.49958300	2.10957100	-0.37515300
H	7.31853500	0.83940500	-0.13608000
H	6.86557000	-2.16415700	0.22887800
H	4.70521700	-1.94976800	-0.56902700
H	4.69732100	-1.65259500	1.16878900
H	3.41435800	-0.98945300	0.15349800
H	11.20253700	-3.76724200	-1.01687500
H	11.08110800	-2.10580500	-1.58262100
H	12.76007800	-2.29124600	0.25570600
H	11.52676100	-2.91402200	1.34000900
H	11.66696000	-0.54134200	1.79926400
H	11.71665500	-0.12701500	0.10351600
H	9.99054100	0.78961300	2.43636200
H	9.52168500	1.55183800	0.92605100
H	8.31847700	0.65562900	1.86615300
H	9.05773700	-3.87815700	-2.31291900
H	7.57624400	-3.12335300	-1.72190800
H	8.83040300	-2.12894200	-2.48202000
H	9.52014200	-3.91323600	1.43090800

H	7.92944300	-4.02964900	0.67437300
H	9.28944800	-4.92075600	-0.01091300
H	-2.37066700	5.96799900	-1.27141300
H	-3.55815200	3.49642800	-0.21297500
H	-5.50804000	4.51266400	-1.24492500
H	-4.63839500	6.04844200	-1.33322200
H	-4.73249100	6.26597500	1.14502300
H	-5.55228000	4.69139500	1.26355300
H	-7.08344500	6.48091400	1.11678200
C	-0.85892500	2.97461200	-0.05480600
C	0.47244200	2.37827500	-0.60969600
H	0.30220600	2.02535400	-1.63814000
H	0.70804900	1.48988700	-0.01778800
C	-0.72631800	3.19981000	1.46908800
H	-0.49383400	2.26097500	1.98374700
H	0.07826000	3.90904100	1.68378600
H	-1.65075000	3.60302200	1.89569400
C	-1.94550700	1.97140900	-0.40856500
C	-2.67740400	1.21601900	0.44396800
H	-2.08396500	1.81704600	-1.48101500
C	-3.63859000	0.22485100	0.01353000
H	-2.53676800	1.35043400	1.51349700
C	-4.42235900	-0.57308400	0.79677700
H	-3.72882100	0.10169400	-1.06620100
C	-5.30857200	-1.52444100	0.13955000
C	-4.41473800	-0.52579100	2.30602700
C	-6.16047500	-2.37569100	0.75872800
H	-5.27324200	-1.52304600	-0.94835600
H	-3.72901000	0.22210900	2.70779800
H	-5.41630300	-0.29841200	2.69101000
H	-4.12876200	-1.49863500	2.72307600
C	-7.05870700	-3.33975800	0.10045900
H	-6.23624100	-2.31710400	1.84231300
C	-6.64584100	-4.14351600	-0.91413500
C	-8.50464000	-3.37229500	0.65539200
C	-7.58537500	-5.07394300	-1.65347400
C	-5.21796200	-4.26137100	-1.39545200
C	-9.29123500	-4.57784800	0.08954900
C	-8.50591100	-3.51154100	2.19701300
C	-9.22107000	-2.05140000	0.28561700
C	-9.06432800	-4.78499500	-1.40565000
H	-7.35537800	-5.02179400	-2.72777700
H	-7.35136100	-6.11106000	-1.36183800
H	-4.97317700	-5.31957500	-1.55888900
H	-5.07916600	-3.76401800	-2.36617200
H	-4.49083500	-3.84412300	-0.69649600
H	-10.35716500	-4.43944700	0.31066400
H	-8.97791600	-5.48842600	0.62026500
H	-8.14887800	-2.60927000	2.70489900
H	-9.52934900	-3.68986500	2.54719500
H	-7.88950200	-4.35764000	2.52272300
H	-8.66586400	-1.18390200	0.66017100
H	-10.22638500	-2.02373100	0.72370300
H	-9.31994200	-1.93446800	-0.79893900
H	-9.68043800	-5.61107600	-1.77955700
H	-9.36820500	-3.89053400	-1.96436800

## 2.. Conformer 2 of atRAL dimer E (high energy conformer)

C	1.63686900	1.65983400	-0.61243800
C	1.68243500	3.02236200	-0.92004500
C	0.50803200	3.76802200	-1.04302000
C	-0.76620700	3.30158700	-0.68870800
C	2.76584800	0.82100300	-0.44410700
C	4.09368200	1.21107000	-0.49215900
C	5.16915600	0.31422300	-0.32631900
C	6.52398700	0.61324900	-0.35645300
C	7.45112400	-0.47288500	-0.18495200
C	8.81097400	-0.34712300	-0.14813200
C	9.81293600	-1.39101800	0.02780900
C	7.05039700	2.01117300	-0.56534200
C	11.04680000	-0.95251900	0.85895600
C	11.86357700	-2.18525200	1.31118800
C	12.10608400	-3.18454200	0.18467800
C	10.76871600	-3.69605800	-0.35237200
C	9.71368500	-2.62716700	-0.54657400
C	8.57943600	-3.07013700	-1.44053200
C	10.60066100	-0.20525500	2.13791900
C	11.93729300	-0.00897900	0.01479300
C	-1.82017900	4.20567500	-0.84261700
N	-3.10112700	4.02110900	-0.53113100
C	-4.15551300	5.01006500	-0.72651500
C	-4.67350000	5.57965600	0.59768200
O	-5.70263900	6.48120000	0.24371700
H	2.62922300	3.51824800	-1.10602600
H	0.59393100	4.79221000	-1.40336300
H	2.56306400	-0.23241100	-0.25738400
H	4.31733300	2.26002200	-0.66523600
H	4.90154600	-0.72918300	-0.16331800
H	7.00816500	-1.45415600	-0.04081000
H	9.21040300	0.66430200	-0.18980200
H	7.69309200	2.30906000	0.27132300
H	7.66047800	2.06380100	-1.47439200
H	6.25970200	2.75668300	-0.65153300
H	12.81350300	-1.84029800	1.73824900
H	11.32307100	-2.69100100	2.12405800
H	12.71231200	-4.02550300	0.53981700
H	12.67406100	-2.71418100	-0.62740100
H	10.91429900	-4.23080900	-1.29980100
H	10.35283500	-4.44841700	0.33907200
H	8.96597200	-3.69831000	-2.25114800
H	7.85979900	-3.69187400	-0.88803200
H	8.02910600	-2.23971300	-1.88638500
H	11.47401600	0.01497700	2.76270600
H	10.10906000	0.74946100	1.92020600
H	9.90805000	-0.81337700	2.73076500
H	12.32447500	-0.50657300	-0.87961900
H	11.39153000	0.88212400	-0.31639400
H	12.79079900	0.33708500	0.60971500
H	-1.59611000	5.18227600	-1.26928900
H	-3.36383500	3.09725200	-0.18856700
H	-4.98811500	4.54902200	-1.26821500
H	-3.76687900	5.82351100	-1.34573400

H	-3.84651400	6.07414400	1.13168200
H	-5.04000400	4.75871700	1.23572800
H	-6.07313700	6.86688300	1.05176100
C	-0.88126700	1.91844500	-0.01869000
C	0.26534900	1.01811300	-0.56893200
H	0.01891200	0.72486700	-1.60162400
H	0.28966300	0.09054100	0.01247000
C	-0.70469300	2.11077300	1.50483100
H	-0.71271400	1.14652100	2.02470100
H	0.24862100	2.60133300	1.72182400
H	-1.50385200	2.73106200	1.92409500
C	-2.18037800	1.21470500	-0.37687300
C	-3.07664700	0.66132700	0.47345600
H	-2.35071800	1.10241200	-1.44995400
C	-4.25592900	-0.05580900	0.04191500
H	-2.90702300	0.75295400	1.54315400
C	-5.20676700	-0.64398300	0.82561700
H	-4.38377100	-0.13656500	-1.03798100
C	-6.31512500	-1.32462600	0.16884100
C	-5.16912300	-0.62921700	2.33521000
C	-7.35146000	-1.93604900	0.78981600
H	-6.29518800	-1.31087400	-0.91938600
H	-4.30471800	-0.09828500	2.73759900
H	-6.07017700	-0.15340100	2.74110300
H	-5.14488200	-1.65142300	2.73075100
C	-8.48316000	-2.61314100	0.13367100
H	-7.39403800	-1.88208100	1.87541700
C	-8.31587300	-3.47263100	-0.90488500
C	-9.87604200	-2.27383900	0.72083400
C	-9.48138900	-4.09932700	-1.64201700
C	-6.97858600	-3.95293000	-1.42015500
C	-10.96801900	-3.20430500	0.14193400
C	-9.89143600	-2.45611800	2.25791100
C	-10.21724400	-0.79822800	0.40228700
C	-10.82292500	-3.42570700	-1.36139900
H	-9.26031800	-4.08768800	-2.71935100
H	-9.53297300	-5.16718800	-1.37292600
H	-7.02623800	-5.03366700	-1.61025200
H	-6.72829300	-3.48570600	-2.38349500
H	-6.15548300	-3.76150700	-0.72943200
H	-11.95302800	-2.78588300	0.38515600
H	-10.91067800	-4.17960800	0.64637200
H	-9.29694400	-1.69939300	2.78080700
H	-10.91994300	-2.36354200	2.62583000
H	-9.52050400	-3.44642800	2.54687200
H	-9.44111000	-0.12340400	0.78092800
H	-11.16857100	-0.51459100	0.86902900
H	-10.30406100	-0.62688300	-0.67610300
H	-11.64530100	-4.04209800	-1.74297700
H	-10.87636400	-2.46744200	-1.89374400

### 3. Conformer 1 of dihydro-A2E (low energy conformer)

C	1.56794700	2.75224300	-0.34849700
C	0.33108300	3.47248700	0.22150100
N	0.28631100	4.88154400	-0.31549800

C	1.43597000	5.53025600	-0.45989700
C	2.69830800	4.94407900	-0.31958700
C	2.84405100	3.56024100	-0.23057000
C	-0.98870300	5.60021400	-0.44456400
C	-1.53554200	5.58910500	-1.87550800
O	-2.70978500	6.37444900	-1.83068400
C	4.12292100	2.96996200	-0.14664500
C	-0.91238900	2.68999100	-0.07099400
C	4.39403300	1.61293300	-0.09886300
C	5.70336900	1.09204800	-0.03853500
C	6.07605200	-0.24380900	0.01333900
C	7.48177600	-0.54011700	0.07049600
C	8.02230500	-1.79525500	0.07589400
C	5.07831500	-1.37490000	0.01156700
C	9.42876800	-2.17334500	0.11588100
C	10.35872500	-1.51741600	0.87357800
C	11.81697300	-1.92579000	0.89606300
C	12.10160100	-3.32136300	0.33892400
C	11.29733900	-3.54304700	-0.93815100
C	9.77091500	-3.43603100	-0.71704200
C	10.05812000	-0.34425500	1.77613700
C	9.11022500	-3.36079500	-2.11383400
C	9.25139100	-4.69899400	0.01161400
C	-1.87177900	2.28357900	0.80300900
C	-2.96537400	1.46839900	0.29771600
C	-4.01601300	0.99427200	1.02081700
C	-5.06698300	0.19709200	0.45389700
C	-6.16895500	-0.31153200	1.08690500
C	-7.11043700	-1.09179900	0.29947100
C	-6.45727300	-0.10097000	2.55325500
C	-8.26724100	-1.63458900	0.74973000
C	-9.24692400	-2.40452900	-0.03428500
C	-1.87150600	2.63141700	2.27510900
C	-10.72117300	-2.00477000	0.22395700
C	-11.64172100	-2.56603300	-0.88406900
C	-11.35963300	-4.03106300	-1.20512800
C	-9.91725900	-4.18683900	-1.68866900
C	-8.89705500	-3.41287600	-0.87483000
C	-7.48095900	-3.89388500	-1.09429300
C	-10.87262900	-0.46627300	0.21588000
C	-11.17348900	-2.53922500	1.60507200
H	1.64258800	1.79139100	0.16601000
H	1.39986100	2.52425800	-1.41206600
H	0.47246900	3.59114300	1.30310700
H	1.35639000	6.59099300	-0.68615800
H	3.56705000	5.59247700	-0.35321500
H	-1.71815000	5.14037800	0.22310100
H	-0.84414100	6.63805500	-0.12972300
H	-0.77956600	6.00885500	-2.55985500
H	-1.73604500	4.55409600	-2.18974500
H	-3.13536600	6.35150300	-2.70089900
H	4.96982300	3.65466000	-0.12827800
H	-1.01150100	2.37581400	-1.11036100
H	3.56007600	0.91699500	-0.10929000
H	6.50929100	1.82481800	-0.03389900
H	8.14592400	0.31934200	0.06841900
H	7.32961300	-2.62783000	-0.03182400

H	4.04396100	-1.03320800	-0.03399900
H	5.24620200	-2.03421200	-0.84816600
H	5.18775600	-1.98770400	0.91335200
H	12.19757500	-1.83604800	1.92163300
H	12.37749600	-1.17269900	0.31653400
H	13.17389700	-3.43323300	0.14306000
H	11.84327900	-4.07878700	1.08906400
H	11.52137500	-4.52458100	-1.37399900
H	11.60116400	-2.79460200	-1.68374900
H	10.34697700	0.60446500	1.30059000
H	9.00591000	-0.27072200	2.05634100
H	10.65151500	-0.41745200	2.69458600
H	8.01626000	-3.39333500	-2.06518800
H	9.43287400	-4.21305100	-2.72309900
H	9.39759900	-2.44359800	-2.64031200
H	9.45441400	-5.59208300	-0.59113100
H	8.16849300	-4.66033400	0.17793400
H	9.72713300	-4.83138200	0.98813500
H	-2.92555700	1.22760100	-0.76471600
H	-4.07111500	1.22869000	2.08039700
H	-4.96608400	-0.01957300	-0.60987300
H	-6.85242900	-1.21537400	-0.75055300
H	-7.41091700	0.42392600	2.68900300
H	-5.68604900	0.48095300	3.06025300
H	-6.54589500	-1.06245300	3.07279100
H	-8.55261800	-1.43418900	1.78183900
H	-1.02365800	3.25068100	2.57437500
H	-1.85155400	1.72177800	2.88622800
H	-2.78604700	3.17412800	2.54091100
H	-12.68754400	-2.42600800	-0.58115800
H	-11.49955800	-1.97052100	-1.79739500
H	-11.52021200	-4.65215000	-0.31490800
H	-12.05510000	-4.39887800	-1.96890300
H	-9.63354100	-5.24783800	-1.70301800
H	-9.83975300	-3.85521600	-2.73786000
H	-7.45344700	-4.99115500	-1.08517100
H	-6.78059500	-3.52759800	-0.34212800
H	-7.10488000	-3.58759300	-2.08165700
H	-11.92974000	-0.19340000	0.32084800
H	-10.32548500	0.01109200	1.03576700
H	-10.50561000	-0.03859400	-0.72420800
H	-10.54515900	-2.15516500	2.41671200
H	-12.20316500	-2.22463100	1.81483400
H	-11.13528700	-3.63219200	1.64953200

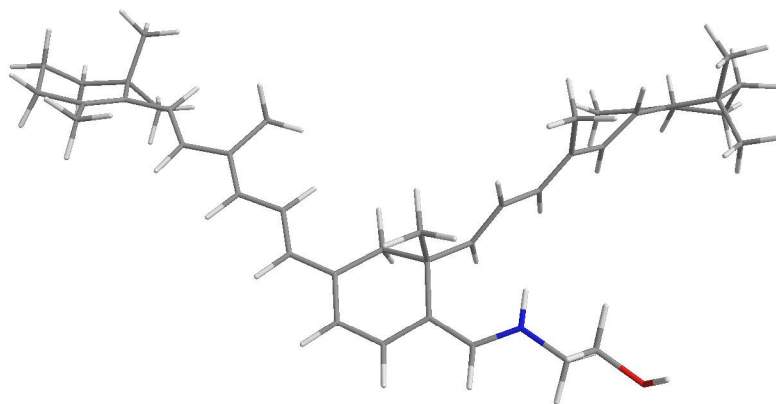
#### 4. Conformer 2 of dihydro-A2E (high energy conformer)

C	1.54921400	2.68845100	-0.45494600
C	0.31254400	3.42097900	0.09805500
N	0.26616900	4.81960800	-0.47138800
C	1.41657700	5.46516900	-0.61136200
C	2.67777500	4.87604800	-0.45323100
C	2.82461700	3.49543000	-0.34113000
C	-1.04418600	5.48280200	-0.54329500
C	-1.04344600	6.87391200	-1.17483700
O	-2.41203600	7.22036500	-1.25574800

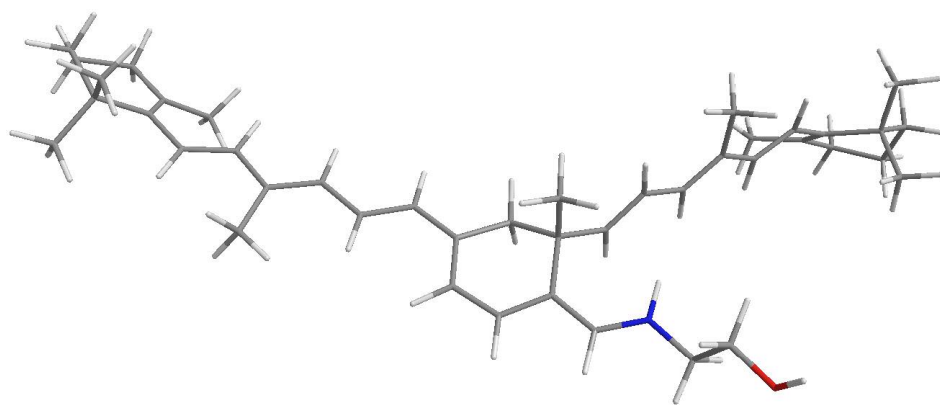
C	4.10343100	2.90573300	-0.23792900
C	-0.93100000	2.63477900	-0.18272800
C	4.37230500	1.55005500	-0.16843500
C	5.68077600	1.02744700	-0.08886700
C	6.05031700	-0.30762700	-0.01655300
C	7.45541600	-0.60625300	0.05734100
C	7.99340300	-1.86171500	0.08264600
C	5.05088800	-1.43723800	-0.01383800
C	9.39960000	-2.24082900	0.13966000
C	10.32216300	-1.58022300	0.90158800
C	11.77981400	-1.98979600	0.94297000
C	12.06907500	-3.38932900	0.39805000
C	11.27755100	-3.61908100	-0.88551400
C	9.74901300	-3.50955400	-0.68063200
C	10.01345500	-0.39928300	1.79130400
C	9.10252500	-3.44380800	-2.08451200
C	9.22131300	-4.76701000	0.05169500
C	-1.88726300	2.23682600	0.69802600
C	-2.98320100	1.41816200	0.20397100
C	-4.03073200	0.95130300	0.93640600
C	-5.08508700	0.14931200	0.38290400
C	-6.18275600	-0.35351400	1.02800100
C	-7.12877400	-1.14268400	0.25499800
C	-6.46177500	-0.12829200	2.49404900
C	-8.28190900	-1.68155400	0.71908000
C	-9.26596000	-2.46201500	-0.04900800
C	-1.88295800	2.59927800	2.16640400
C	-10.73881800	-2.05928300	0.21257400
C	-11.66608700	-2.63750500	-0.88103900
C	-11.38436400	-4.10664600	-1.18317300
C	-9.94522100	-4.26726700	-1.67463700
C	-8.92055000	-3.48135900	-0.87803900
C	-7.50538800	-3.96386900	-1.10008300
C	-10.89097000	-0.52113700	0.18229900
C	-11.18223900	-2.57284600	1.60447600
H	1.61731900	1.73458300	0.07344400
H	1.38464200	2.44651400	-1.51578000
H	0.45055900	3.56435500	1.17724900
H	1.35952200	6.52114500	-0.85203200
H	3.54650100	5.52404100	-0.49597800
H	-1.71463100	4.84537800	-1.12432200
H	-1.46696200	5.54580800	0.46694400
H	-0.48363200	7.59045000	-0.55286400
H	-0.56616000	6.83949700	-2.16787100
H	-2.48408400	8.12246700	-1.60264700
H	4.95048300	3.59036100	-0.22313900
H	-1.03482400	2.31483600	-1.22021800
H	3.53746200	0.85512500	-0.17666700
H	6.48781900	1.75903500	-0.08632200
H	8.12126600	0.25196200	0.05154200
H	7.30065000	-2.69480300	-0.02090600
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H	5.22405500	-2.10565500	-0.86548700
H	5.15277300	-2.04092400	0.89495900
H	12.14869200	-1.89399200	1.97231600
H	12.34796800	-1.24109300	0.36522000
H	13.14322500	-3.50329500	0.21372100

H	11.80269800	-4.14162100	1.15056100
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H	11.58939100	-2.87578600	-1.63296400
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H	9.43090500	-4.30036400	-2.68463900
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H	9.43048700	-5.66467400	-0.54211100
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H	-12.08468900	-4.48606100	-1.93678400
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H	-9.87547300	-3.94952100	-2.72864100
H	-7.47640900	-5.06088900	-1.07544300
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H	-10.54996800	-2.17511900	2.40640500
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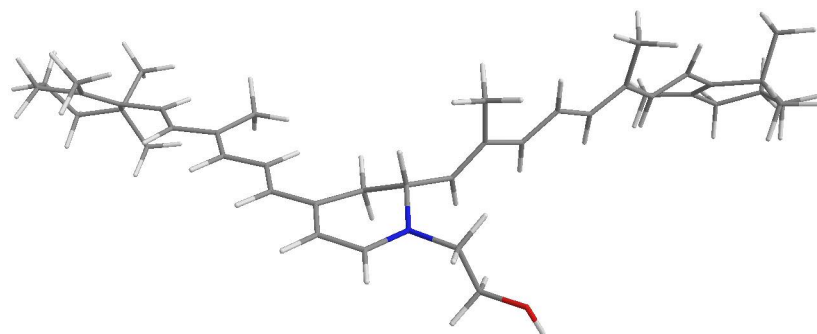


**A**

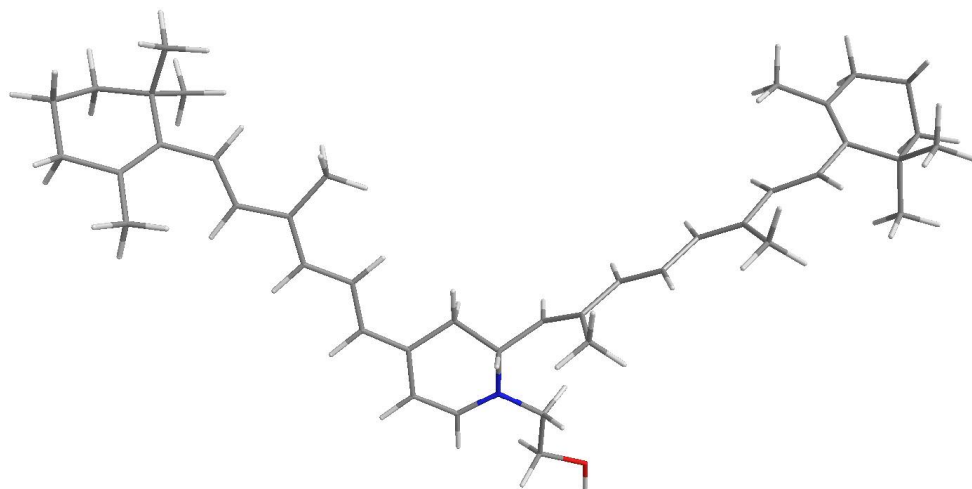


**B**

Figure 1: Stick models of atRAL dimer E used to calculate UV-visible absorbance spectra. (A) conformer 1. (B) conformer 2.



**A.**



**B**

Figure 2: Stick models of dihydro-A2E used to calculate UV-visible absorbance spectra. (A) conformer 1. (B) conformer 2.