**Supplementary material 1**

**Quantum chemical calculations**

The electron correlation effects are included by employing density functional theory (DFT)[[1](#_ENREF_1)] at the M06-2X-D3 level[[2](#_ENREF_2)], which include the London-dispersion correction[[3](#_ENREF_3)]. The ultrafine grid (99,590), having 99 radial shells and 590 angular points per shell, is used to evaluate the numerical integration accuracy. Geometry optimizations are performed with the double-zeta basis set 6-31G(d,p) in water medium (373.15 K) while using SMD solvation model[[4](#_ENREF_4)]. Based on the optimized structures, the electronic energy (*E*electron) and solvation free energy (Δ*G*solv) are calculated at the same theoretical level. The harmonic vibrational frequencies are analyzed after the geometry optimizations to characterize the nature of the stationary point as a minimum with all positive frequencies or as a transition state with only one imaginary frequency, and to provide the zero-point energy (*E*ZPE) and the thermal correction to Gibbs free energy (*G*corr) at the same theoretical level. Then, the intrinsic reaction coordinate (IRC)[[5](#_ENREF_5)] calculations are carried out to verify the transition state (TS) associated with the correct reactant complexes (RC), intermediate (IM) and product complexes (PC) at the same level of theory. The Gibbs free energy of free reactant (*G*aconitine) are defined as reference-point. All calculations were carried out with Gaussian 16 program[[6](#_ENREF_6)].

*G* = *E*electron + Δ*G*solv + *E*ZPE + *G*corr (1)

Δ*G* = *G* – *G*aconitine (2)

**Results**

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**Figure 1.** DFT-computed relative energy profiles (in kcal/mol) for the hydrolysis reaction of aconitine along two pathways at the M06-2X-D3/6-31G(d,p)/SMD(Water) level.

**Cartesian coordinate for theoretical calculation**

**RC**

C -3.51584500 -2.84095000 -1.05021100

C -4.58747600 -1.80914400 -0.74100700

C -4.05391500 -0.33212400 -0.67163800

C -2.63534400 -0.25299100 -1.30272000

C -1.67764400 -1.17286100 -0.46797800

C -2.17751500 -2.64184100 -0.35652500

C -1.94600600 1.12744300 -1.11512200

C -1.22665000 1.02190400 0.25305900

C 0.28402500 1.06036400 0.00720700

C 0.64310900 0.03225100 -1.09549800

C -0.20905600 -1.26422300 -0.98668200

C 2.06573200 -0.50592200 -0.95219800

C 1.92873500 -1.39382000 0.28929800

C 0.65306300 -2.17437300 -0.06034200

C 1.78569600 -0.48984000 1.53946000

C 1.14062800 0.89902600 1.29857800

O 2.97074700 0.60978500 -0.81280700

O 3.11135400 -0.30368900 2.01993900

O 0.58245900 2.34222900 -0.64423700

C -1.63618200 -0.35572600 0.83231100

C -3.98587100 0.22606800 0.76141200

C -5.08868400 0.50073300 -1.43675300

N -2.91062100 -0.36706200 1.54173800

C -2.82132100 0.23204700 2.87207700

C -2.05885600 -0.63830800 3.86351800

C 3.19035800 0.20164700 3.34591700

O 0.42897200 1.22385300 2.47728100

O -2.74573500 2.29696100 -1.15686000

C -2.93501600 2.76717900 -2.48090500

O -6.35976600 0.22372900 -0.86103000

C -7.40104300 0.88600900 -1.55115900

O -2.18473100 -3.07518800 1.00224800

H -3.91315800 -3.83874700 -0.83709400

H -3.32236500 -2.80720100 -2.12754800

H -5.29546800 -1.84549900 -1.57897700

H -2.67864700 -0.53723200 -2.36054700

H -1.45570000 -3.27661700 -0.89085900

H -1.21514300 1.23688900 -1.91955300

H -1.52378200 1.84710400 0.90409900

H 0.52560000 0.51716800 -2.06362900

H -0.24250700 -1.70895800 -1.98676200

H 2.33354600 -1.11328600 -1.81940300

H 0.97031400 -3.07498800 -0.59233400

H 0.12674600 -2.49350900 0.84257800

H 1.20176600 -1.02415800 2.30430100

H 1.98411000 1.58603900 1.17458900

H -0.88295900 -0.74225400 1.52049300

H -3.87957600 1.32224300 0.69113000

H -4.92815600 0.03787000 1.28134500

H -5.09223100 0.21042900 -2.50018600

H -4.89257700 1.57528600 -1.36736500

H -2.37782800 1.24339900 2.83787000

H -3.84751500 0.35911500 3.23343200

H -2.10118500 -0.19017700 4.86010100

H -2.50267100 -1.63647300 3.91426000

H -1.00337300 -0.74435400 3.59848300

H 4.23939400 0.14366700 3.64021000

H 2.58349300 -0.40800000 4.02599100

H 2.85640600 1.24178500 3.39626300

H 0.20938900 2.16756900 2.39426700

H -3.58071900 3.64553900 -2.42650300

H -3.41334400 2.01115400 -3.11627200

H -1.97439300 3.04888600 -2.93167800

H -8.33797800 0.64638900 -1.04574800

H -7.45697400 0.55103900 -2.59513600

H -7.25223300 1.97346100 -1.53944500

C -1.96973300 -4.46794600 1.12347100

H -1.99713700 -4.70764800 2.18816200

H -2.74474100 -5.05110500 0.61109200

H -0.98970000 -4.75194600 0.71546100

O -5.28561600 -2.20167500 0.43516300

H -6.04966800 -1.60941600 0.49493100

C 0.36012600 3.50871500 -0.02384800

O 0.17707800 3.61891500 1.17525800

C 0.31619300 4.65527700 -0.98533100

H 0.64086200 5.56606500 -0.48381400

H 0.91994400 4.45757300 -1.86987100

H -0.72917900 4.77303700 -1.29139900

C 4.28502500 0.47287200 -0.56612200

O 4.85153400 1.37165100 0.02990100

C 5.02238300 -0.71191900 -1.07747700

C 4.81131000 -1.20109200 -2.36819300

C 5.99898600 -1.27585000 -0.25265300

C 5.57292500 -2.27226900 -2.82573200

H 4.08109400 -0.72993700 -3.01867600

C 6.73780200 -2.36164200 -0.70737200

H 6.15531600 -0.87036600 0.74251900

C 6.52449400 -2.85881000 -1.99325300

H 5.42336200 -2.64780200 -3.83222700

H 7.48300800 -2.81634900 -0.06364700

H 7.10715200 -3.70190900 -2.34985200

O 2.97070700 -2.32430700 0.48532100

H 3.60319000 -1.91976100 1.10080000

O 3.20583600 3.59695200 -0.88032100

H 2.61161200 2.85430600 -1.06894200

H 4.04967900 3.15362900 -0.70259500

O 3.46311900 3.26333400 1.93883000

H 3.96281100 2.48410300 1.65054900

H 3.13218900 3.60370800 1.08993800

**TS1**

C -3.33889400 -2.91499000 -1.21428500

C -4.44312400 -1.96181200 -0.79092800

C -3.97499000 -0.46840300 -0.63176400

C -2.58143800 -0.28244600 -1.29952400

C -1.56444600 -1.20982800 -0.55837700

C -1.99312200 -2.70446500 -0.54002100

C -1.93990500 1.10836400 -1.03868600

C -1.17319400 0.94600400 0.29923700

C 0.33998300 1.10252600 0.03472600

C 0.69283000 0.15013500 -1.15482900

C -0.11438500 -1.18510600 -1.12035400

C 2.12699900 -0.38845600 -1.11237100

C 2.06443400 -1.34847300 0.08431000

C 0.79718900 -2.12976500 -0.28186500

C 1.95410200 -0.53209100 1.39388200

C 1.24934400 0.84041200 1.27644900

O 2.99774800 0.74991400 -1.01508900

O 3.30613400 -0.32058300 1.79543700

O 0.58974100 2.45857700 -0.40912500

C -1.50837300 -0.48119900 0.79127000

C -3.88320900 -0.00742100 0.83457100

C -5.07818700 0.36167000 -1.29912500

N -2.75618800 -0.59666800 1.54241000

C -2.64432400 -0.06034100 2.89740900

C -1.80258700 -0.93835800 3.81556500

C 3.45300900 0.20147100 3.10627300

O 0.58872200 1.10967400 2.49472000

O -2.81683800 2.22325900 -0.98419800

C -3.08816100 2.75110000 -2.27053000

O -6.31177300 -0.01930800 -0.70016900

C -7.40821700 0.64361600 -1.29752600

O -1.95209400 -3.22755400 0.78595800

H -3.68470700 -3.94388400 -1.07043600

H -3.18063500 -2.78785200 -2.29031500

H -5.18299800 -1.97230400 -1.60158700

H -2.64825100 -0.49963400 -2.37215800

H -1.25776500 -3.26941200 -1.13123700

H -1.24299700 1.31525900 -1.85500100

H -1.50064100 1.70838500 1.00012400

H 0.53992600 0.69737800 -2.08571000

H -0.15362100 -1.55689800 -2.15015000

H 2.34965700 -0.94745700 -2.02507400

H 1.12140300 -2.98521200 -0.88014500

H 0.30751500 -2.52197700 0.61230100

H 1.44418500 -1.13878600 2.15854100

H 2.08074900 1.54915000 1.13815000

H -0.71675700 -0.88088900 1.42748300

H -3.83007100 1.09475700 0.83442800

H -4.79830400 -0.27557200 1.36827000

H -5.10949400 0.14612500 -2.37990000

H -4.93482900 1.43719700 -1.15958700

H -2.25091700 0.97286500 2.89947000

H -3.66053500 -0.00201900 3.30260700

H -1.83749300 -0.54844000 4.83670300

H -2.18821700 -1.96172900 3.82308200

H -0.75224700 -0.96845500 3.51417400

H 4.51728000 0.16268400 3.34363300

H 2.89261100 -0.40468600 3.82828100

H 3.10664200 1.23837100 3.16793700

H 0.20290300 2.02269000 2.34906100

H -3.80174700 3.56802700 -2.14584100

H -3.52396000 1.99547900 -2.93644700

H -2.17052400 3.13924200 -2.73218100

H -8.31268800 0.32179900 -0.77875000

H -7.49133600 0.38768900 -2.36194600

H -7.30767800 1.73285600 -1.20601500

C -1.67908600 -4.61502900 0.80877700

H -1.66344700 -4.92437400 1.85565400

H -2.44627800 -5.19560400 0.28180000

H -0.70194400 -4.83162700 0.35487400

O -5.07272800 -2.47420400 0.37819300

H -5.86337800 -1.93055100 0.50826900

C 0.24994100 3.68991000 0.55312800

O -0.35065900 3.35903400 1.64177500

C -0.46794000 4.62507300 -0.40125800

H -0.64601700 5.57412400 0.11006100

H 0.12249100 4.80700500 -1.30246000

H -1.42356400 4.17454600 -0.67290700

C 4.30888300 0.75852800 -0.79137400

O 4.79584400 1.83786400 -0.47769700

C 5.13534300 -0.45985500 -0.96807400

C 5.03414400 -1.23825200 -2.12254700

C 6.05107800 -0.78086700 0.03684100

C 5.84161400 -2.36301900 -2.25645800

H 4.34904400 -0.95696500 -2.91569300

C 6.83295600 -1.92374300 -0.09338200

H 6.12366400 -0.15068100 0.91805400

C 6.72568100 -2.71411300 -1.23745200

H 5.77712500 -2.96801100 -3.15430300

H 7.52871000 -2.19435100 0.69342600

H 7.33986800 -3.60287200 -1.33842900

O 3.10825800 -2.29174800 0.19514000

H 3.81406200 -1.88167500 0.71894100

O 2.71694800 3.43429800 -1.18473200

H 1.87112200 2.80864600 -1.00955000

H 3.53027200 2.92765600 -0.91478700

O 1.54317700 4.28232600 0.81767900

H 1.87097400 3.84918200 1.62289800

H 2.50262400 4.05041700 -0.40787100

**IM1**

C -3.34507900 -3.13437600 -0.76851900

C -4.44239500 -2.11060200 -0.53568300

C -3.95804800 -0.61847700 -0.64791800

C -2.55701700 -0.56329600 -1.32069400

C -1.55268600 -1.35629800 -0.41585300

C -2.00264800 -2.81800600 -0.13021500

C -1.91022400 0.85100700 -1.30108200

C -1.14566400 0.91296800 0.04498800

C 0.35630700 0.98799300 -0.25662200

C 0.71322100 -0.16575600 -1.24033000

C -0.09555000 -1.46280800 -0.96312800

C 2.15698300 -0.64263900 -1.07708200

C 2.07641000 -1.38834000 0.26384200

C 0.81197100 -2.23109200 0.04195900

C 1.95436500 -0.34951900 1.40545100

C 1.24081500 0.97439300 1.03344000

O 3.00066200 0.53207000 -1.11190500

O 3.30134100 -0.07673700 1.78018400

O 0.52209400 2.24493500 -0.90413400

C -1.50542500 -0.39556000 0.78336000

C -3.87791700 0.10046100 0.71097700

C -5.03934700 0.08527800 -1.47549800

N -2.76329200 -0.36100800 1.52592700

C -2.65967100 0.40636200 2.76562800

C -1.86163600 -0.31727200 3.84335600

C 3.44842900 0.74500000 2.92600200

O 0.55045000 1.39443400 2.19885900

O -2.76358400 1.97693200 -1.43646300

C -2.99229600 2.31753600 -2.79244200

O -6.28605400 -0.16208800 -0.83601600

C -7.36794600 0.36023700 -1.58110700

O -1.97860600 -3.09445400 1.26887500

H -3.70206100 -4.11759700 -0.44445100

H -3.17674700 -3.20438700 -1.84836600

H -5.17649000 -2.26192200 -1.33742500

H -2.61486500 -0.96405900 -2.33959900

H -1.26959100 -3.48909200 -0.60106700

H -1.20697100 0.90465200 -2.13493300

H -1.44299200 1.80904200 0.59494400

H 0.56086000 0.20593600 -2.25397500

H -0.14041200 -2.02799900 -1.90060900

H 2.43563800 -1.33465900 -1.87536500

H 1.14193200 -3.18216500 -0.38411400

H 0.31741400 -2.45148900 0.99131500

H 1.43132300 -0.80608400 2.26050500

H 2.05125400 1.68484400 0.81587100

H -0.72572400 -0.68244900 1.49067700

H -3.81481700 1.18400500 0.51351300

H -4.80098500 -0.06027400 1.27341500

H -5.05809100 -0.32959200 -2.49680500

H -4.88020200 1.16581500 -1.53942300

H -2.23634300 1.41278700 2.59192700

H -3.68027800 0.56257200 3.13169800

H -1.87963600 0.26089900 4.77150000

H -2.29500100 -1.30164200 4.04105700

H -0.81354900 -0.45390600 3.56412700

H 4.50953800 0.74250100 3.17968700

H 2.86770800 0.34562100 3.76611400

H 3.12980200 1.77473400 2.72938500

H 0.13256900 2.25684600 2.03004000

H -3.69206200 3.15541400 -2.80580900

H -3.42704600 1.48114000 -3.35449400

H -2.05535000 2.62024800 -3.27757300

H -8.28377300 0.15377500 -1.02484300

H -7.43067200 -0.11371300 -2.56948300

H -7.26559300 1.44448000 -1.71859600

C -1.72097300 -4.45757300 1.54259600

H -1.72547800 -4.57639800 2.62786300

H -2.48585600 -5.11634300 1.11321400

H -0.73915200 -4.75911000 1.15164300

O -5.08679300 -2.39472300 0.70124200

H -5.87094700 -1.82677000 0.72322600

C 0.07143100 4.44533400 0.75479000

O -0.69580100 3.88973000 1.52278700

C -0.32131500 5.09405000 -0.53068900

H -0.54968900 6.14514000 -0.33046200

H 0.49591700 5.04131300 -1.25033400

H -1.21050200 4.59770700 -0.91888200

C 4.29872200 0.55008200 -0.77782000

O 4.77092000 1.60175400 -0.38098100

C 5.13783900 -0.66252200 -0.95847400

C 5.04116600 -1.44894400 -2.10801400

C 6.07574300 -0.96069000 0.03348200

C 5.87474600 -2.55392700 -2.25086600

H 4.34233800 -1.18387300 -2.89499300

C 6.88577500 -2.08211600 -0.10434500

H 6.14468000 -0.32526900 0.91154900

C 6.78347200 -2.87842200 -1.24503400

H 5.81343000 -3.16237600 -3.14665600

H 7.59962900 -2.33213600 0.67308000

H 7.42027900 -3.75024200 -1.35356400

O 3.12865000 -2.28855400 0.54118600

H 3.80997800 -1.79976700 1.02815700

O 2.92887000 3.57870100 -1.18812600

H 1.46617200 2.42911800 -1.08638800

H 3.60449100 2.97947200 -0.82286600

O 1.37548200 4.56994700 1.03980800

H 1.55748400 4.15000800 1.90033100

H 2.59108200 4.06192200 -0.41852300

**IM2**

C -3.20796000 -2.80908100 -0.87007200

C -4.32588400 -1.82327100 -0.58777700

C -3.88549700 -0.31385000 -0.67286500

C -2.49161300 -0.20171100 -1.36188800

C -1.45720300 -0.99601300 -0.49488500

C -1.86802700 -2.47558500 -0.23830400

C -1.88976500 1.22755600 -1.32084400

C -1.08589700 1.28008200 0.01324400

C 0.41388700 1.35690400 -0.29057700

C 0.76284200 0.25128000 -1.32352900

C -0.01273300 -1.06549900 -1.07725800

C 2.22385800 -0.17955200 -1.19638500

C 2.18288900 -0.98804500 0.11354600

C 0.93615300 -1.85420600 -0.12798300

C 2.03340600 -0.02059900 1.31325000

C 1.30348100 1.30602300 0.99933200

O 2.99793000 1.04257400 -1.21094500

O 3.36915400 0.25578100 1.71837300

O 0.62622300 2.63901800 -0.90587500

C -1.41229900 -0.06040000 0.72493600

C -3.80423500 0.37213800 0.70302900

C -5.00560500 0.36584900 -1.47094500

N -2.65931300 -0.07556100 1.48315100

C -2.55822100 0.64340000 2.75080700

C -1.73927700 -0.11078000 3.79150700

C 3.49253600 1.01277400 2.91058200

O 0.61326600 1.70098500 2.16999500

O -2.86169100 2.24931900 -1.45421600

C -2.29817600 3.52405500 -1.69613800

O -6.23068200 0.06708600 -0.80970300

C -7.34381000 0.56385600 -1.52526500

O -1.81760300 -2.78753500 1.15240300

H -3.53448800 -3.81194300 -0.57583500

H -3.05189100 -2.83730300 -1.95376800

H -5.07324900 -1.97521000 -1.37660800

H -2.55505300 -0.56955200 -2.39229100

H -1.12479100 -3.11564600 -0.73516800

H -1.21166300 1.33957200 -2.17274900

H -1.37580400 2.15118700 0.60913200

H 0.58053900 0.65858400 -2.31862800

H -0.07416900 -1.59524100 -2.03415600

H 2.52413200 -0.82783300 -2.02385500

H 1.28063400 -2.77544900 -0.60496200

H 0.46663400 -2.13041700 0.81978300

H 1.51044900 -0.53420000 2.13536200

H 2.10917400 2.02586600 0.80452600

H -0.61790200 -0.34936700 1.41491500

H -3.78007600 1.46137300 0.53478700

H -4.70948100 0.16374700 1.27850200

H -5.02859300 -0.04108500 -2.49522400

H -4.88462700 1.44921100 -1.53201700

H -2.15228900 1.66229500 2.61456800

H -3.57798000 0.76789800 3.13091200

H -1.74985100 0.43278000 4.74044700

H -2.16082100 -1.10596300 3.95805100

H -0.69384300 -0.22697800 3.49321000

H 4.54932800 0.99965100 3.18191500

H 2.90033100 0.56361300 3.71689800

H 3.17138600 2.04965300 2.76659000

H 0.37566800 2.64475100 2.05167300

H -3.12783000 4.20893500 -1.88053000

H -1.63998400 3.50585400 -2.57445200

H -1.72101600 3.88490800 -0.83622600

H -8.24113900 0.32002400 -0.95408000

H -7.41164900 0.10210700 -2.51915200

H -7.27982200 1.65267700 -1.64926000

C -1.53705900 -4.15347000 1.38718200

H -1.51572900 -4.29794100 2.46907900

H -2.30313400 -4.81164300 0.95921100

H -0.56058500 -4.43277300 0.96735300

O -4.93526600 -2.15607900 0.65468000

H -5.73720600 -1.61535900 0.70389600

C 4.26601200 1.18425700 -0.77113700

O 4.58688000 2.26399000 -0.32020300

C 5.22030900 0.05541100 -0.92127400

C 5.21920500 -0.75662200 -2.05717900

C 6.15951700 -0.14233500 0.09446200

C 6.15018400 -1.78528300 -2.16327600

H 4.51260600 -0.57259700 -2.85996900

C 7.07063100 -1.18754400 -0.00714800

H 6.15189600 0.51043400 0.96224000

C 7.06385800 -2.00902800 -1.13464900

H 6.16047500 -2.41355800 -3.04739500

H 7.78778300 -1.35930800 0.78830400

H 7.77807400 -2.82208200 -1.21455200

O 3.26459800 -1.86900900 0.33097000

H 3.94124600 -1.38059800 0.82547400

H 1.55964400 2.67640000 -1.17062000

O 0.05808000 4.26939400 1.28974900

H -0.90527700 4.33979600 1.33072600

H 0.23496700 3.89119800 0.40507300

**TS2**

C 3.19943600 2.76139400 -0.80730900

C 4.34356900 1.77876800 -0.65029400

C 3.91065300 0.26702000 -0.75600200

C 2.46364700 0.15862700 -1.32828800

C 1.49945800 0.92159100 -0.35657900

C 1.92076500 2.39321800 -0.07618500

C 1.87973600 -1.28400300 -1.27948500

C 1.16290400 -1.37435400 0.09848600

C -0.35153000 -1.31611700 -0.04075500

C -0.75767400 -0.29955800 -1.10606400

C 0.02235200 1.01390000 -0.84245800

C -2.20851900 0.14551400 -0.96211800

C -2.15357800 0.89185600 0.38007900

C -0.88723800 1.74632400 0.18838200

C -2.01178300 -0.13734500 1.51473900

C -1.13662900 -1.33088100 1.18566400

O -3.03630400 -1.03242300 -1.01906800

O -3.36650200 -0.50098100 1.84653800

O -0.63146900 -2.84932000 -0.86249400

C 1.56140100 -0.05275900 0.83435500

C 3.95094000 -0.46528400 0.59682700

C 4.96539400 -0.36908600 -1.66997400

N 2.86743600 -0.05690700 1.47841800

C 2.87936600 -0.80730400 2.73164200

C 2.14424900 -0.09110900 3.85858700

C -3.46686300 -1.27851800 3.02358800

O -0.38146000 -1.74661300 2.33272800

O 2.85608100 -2.28757500 -1.49108900

C 2.30019500 -3.56089000 -1.75879100

O 6.23789300 -0.08866300 -1.09630100

C 7.29256800 -0.54876000 -1.91720400

O 1.98093600 2.64666600 1.32576700

H 3.54214200 3.75815300 -0.51062500

H 2.95069900 2.82064300 -1.87243500

H 5.02720100 1.96718000 -1.48743300

H 2.43656100 0.55446500 -2.34994200

H 1.13557100 3.04650500 -0.48216600

H 1.15653000 -1.39276700 -2.09393900

H 1.46054200 -2.26786000 0.65186600

H -0.57498200 -0.67879200 -2.11154400

H 0.02696200 1.58051000 -1.78022800

H -2.47270700 0.83928700 -1.76390000

H -1.20805800 2.71679800 -0.19893700

H -0.38730300 1.92359800 1.14512900

H -1.59001400 0.37516800 2.39681800

H -2.04819400 -2.48182700 0.94008500

H 0.82699000 0.20228800 1.59892300

H 3.92631100 -1.54849900 0.39660500

H 4.89637800 -0.26079000 1.10495200

H 4.90403000 0.08160500 -2.67414900

H 4.84448600 -1.44975200 -1.76784900

H 2.47370600 -1.82685800 2.60372300

H 3.92885600 -0.92862700 3.02096500

H 2.26499900 -0.64630600 4.79309600

H 2.55131900 0.91412800 3.99897700

H 1.07188400 -0.00540100 3.66616000

H -4.52910800 -1.38223000 3.25282700

H -2.96004700 -0.78480200 3.86292700

H -3.03546500 -2.27694000 2.88687700

H -0.69551200 -2.62338800 2.58767800

H 3.13113600 -4.22342600 -2.00783600

H 1.60422300 -3.51745600 -2.60711500

H 1.76645400 -3.96410500 -0.89118300

H 8.23143900 -0.32219900 -1.40914300

H 7.27983900 -0.04690200 -2.89370800

H 7.22276900 -1.63211700 -2.07987700

C 1.70835800 3.99873600 1.63822500

H 1.76789500 4.09809500 2.72379300

H 2.43493300 4.68235000 1.18207200

H 0.70081400 4.28444400 1.30532600

O 5.04152700 2.07598700 0.55406700

H 5.85265700 1.54797500 0.52351100

C -4.36577600 -1.02824200 -0.81158900

O -4.89192900 -2.06304100 -0.45819200

C -5.15983100 0.20534800 -1.07220600

C -4.98829300 0.96019500 -2.23381400

C -6.14486100 0.54797900 -0.14258100

C -5.79351900 2.07450500 -2.45180500

H -4.25112800 0.66502800 -2.97384800

C -6.92805400 1.67720000 -0.35387500

H -6.27322800 -0.06175400 0.74702800

C -6.75146400 2.44037700 -1.50792900

H -5.67187400 2.65701900 -3.35874000

H -7.67929600 1.95871800 0.37624200

H -7.36737000 3.31787800 -1.67558000

O -3.23323600 1.76667700 0.63687000

H -3.89903600 1.25290500 1.12066900

H -0.95327500 -2.68060400 -1.76241500

O -2.44303000 -3.50251100 0.60735400

H -2.10545500 -4.12190800 1.27152600

H -1.44366400 -3.29674000 -0.31514700

**IM3**

C -3.32953100 -2.43671500 -1.42642300

C -4.43987800 -1.45844300 -1.09244600

C -3.93985500 -0.00024700 -0.76616200

C -2.45993600 0.18074100 -1.21491800

C -1.58258600 -0.87228000 -0.44358200

C -2.08896300 -2.33916500 -0.55590900

C -1.82233600 1.53357200 -0.75641500

C -1.13440600 1.21280200 0.60139000

C 0.34972200 0.95364600 0.45440900

C 0.70459500 0.37330700 -0.89302600

C -0.10135900 -0.93594500 -0.94293000

C 2.14482600 -0.09596300 -0.95989800

C 2.15830800 -1.13855300 0.17248200

C 0.81668300 -1.87958300 -0.09520000

C 2.17957700 -0.39245400 1.51434600

C 1.08126600 0.64767000 1.53986800

O 2.94548400 1.09942900 -0.81714100

O 3.51635900 0.04775900 1.69396800

O 1.31357500 3.50767700 -1.63761100

C -1.66987100 -0.22633700 0.95930200

C -4.03643900 0.34892300 0.72812300

C -4.90064400 0.91734600 -1.53090900

N -3.00671200 -0.30268100 1.52654100

C -3.05806800 0.16840900 2.90920300

C -2.26365500 -0.69958800 3.87800300

C 3.72724700 0.89399600 2.81134500

O 0.61736300 1.04210400 2.77544200

O -2.73146400 2.61829200 -0.66622200

C -2.05087100 3.86048600 -0.64194900

O -6.21986200 0.58101400 -1.11641100

C -7.19415400 1.30944800 -1.83651300

O -2.24559600 -2.92415400 0.73340000

H -3.73533500 -3.45360600 -1.41493300

H -3.00706000 -2.24078900 -2.45501300

H -5.06301200 -1.38015400 -1.99228500

H -2.38596800 0.07147500 -2.30314000

H -1.30813800 -2.91867400 -1.06865500

H -1.08529700 1.83523500 -1.50342300

H -1.37666000 1.96088100 1.36001100

H 0.49971500 1.05393400 -1.71644100

H -0.13519600 -1.29930600 -1.97729000

H 2.35742900 -0.58030600 -1.91607300

H 1.05851200 -2.78724800 -0.65327300

H 0.35240000 -2.18857800 0.84695800

H 1.93105700 -1.10865700 2.31809500

H 3.23364800 3.19264000 0.61614000

H -0.99732900 -0.71077700 1.66735600

H -3.98084900 1.44430300 0.82331400

H -5.00988100 0.04887300 1.12401300

H -4.79597500 0.73964600 -2.61373600

H -4.71611900 1.97626600 -1.33473800

H -2.72820200 1.22042100 2.99349900

H -4.11254000 0.15422800 3.20602100

H -2.50595000 -0.41958400 4.90669700

H -2.51599800 -1.75499500 3.73903300

H -1.18455200 -0.58191700 3.75216500

H 4.80312400 1.06162000 2.88275700

H 3.37564300 0.41608600 3.73536700

H 3.22184800 1.85714900 2.68090600

H 1.07314300 0.55209100 3.47478700

H -2.80376600 4.63950100 -0.51193700

H -1.50913300 4.02959900 -1.58098400

H -1.33389600 3.91386400 0.18761000

H -8.17472600 1.01584700 -1.45818500

H -7.13923100 1.08617000 -2.91011400

H -7.06208400 2.39013800 -1.69653500

C -2.06500600 -4.32672400 0.71140000

H -2.19338300 -4.68524800 1.73453100

H -2.79927200 -4.82768200 0.06860700

H -1.05676400 -4.58910800 0.36196600

O -5.24207600 -2.01445100 -0.05582100

H -6.02345000 -1.44518600 0.00285400

C 4.26143700 1.14392700 -0.57411300

O 4.70945500 2.16159100 -0.07553500

C 5.13160500 0.00480100 -0.96687800

C 4.99508300 -0.62708200 -2.20448700

C 6.12737400 -0.39297900 -0.07022800

C 5.84532300 -1.67875200 -2.53269000

H 4.24805600 -0.28578700 -2.91394100

C 6.95564500 -1.46175800 -0.39475700

H 6.22714000 0.12211400 0.88039900

C 6.81214500 -2.10521900 -1.62411200

H 5.74960100 -2.16742300 -3.49623600

H 7.71483100 -1.78978600 0.30704900

H 7.46132200 -2.93705100 -1.87710600

O 3.20141700 -2.08866800 0.13171400

H 3.98823800 -1.68273900 0.52743100

H 1.89020800 2.75892100 -1.84156300

O 2.41547300 3.58926600 0.96955800

H 1.83369900 2.81901100 1.07123900

H 1.60643600 3.74675100 -0.73968900

**IM4**

C -3.26390500 -2.76793200 -0.20227000

C -4.40338000 -1.77298400 -0.31619100

C -3.95414500 -0.31484900 -0.70887000

C -2.49328000 -0.32352600 -1.24617100

C -1.55726600 -0.88640100 -0.11461900

C -2.01077900 -2.25115300 0.48170000

C -1.89751500 1.10425700 -1.48346400

C -1.15359600 1.45662700 -0.16317200

C 0.33273200 1.18180700 -0.23214900

C 0.67107100 0.05569100 -1.17686500

C -0.09193700 -1.14796200 -0.59770500

C 2.12827500 -0.36652200 -1.08602400

C 2.20140400 -0.77910400 0.38995200

C 0.88193500 -1.58643800 0.54574100

C 2.21772500 0.50179700 1.23938200

C 1.12847500 1.45376400 0.81224400

O 2.90463600 0.77831000 -1.49920500

O 3.53612500 1.06312500 1.23326000

O 3.07491000 3.79748700 1.37865700

C -1.62906800 0.33254200 0.83610400

C -4.02801900 0.67663500 0.46385000

C -4.97205700 0.12628000 -1.76719700

N -2.94871600 0.49892800 1.42592000

C -2.98887700 1.56020900 2.43034900

C -2.11242100 1.28444000 3.64613500

C 4.18265300 1.03221200 2.50462600

O 0.74389400 2.37822500 1.76488800

O -2.85293200 2.08165500 -1.86081400

C -2.23598800 3.22974100 -2.41343700

O -6.26503000 -0.01859700 -1.18944500

C -7.28824900 0.26317000 -2.12335100

O -2.12031200 -2.18481600 1.90131600

H -3.63111200 -3.67461300 0.28957100

H -2.97000900 -3.05984100 -1.21662200

H -5.04458000 -2.13166300 -1.13142200

H -2.44025500 -0.91761000 -2.16596800

H -1.22017100 -2.98314100 0.26539800

H -1.19780700 1.04517500 -2.31969800

H -1.39363900 2.46367500 0.18760300

H 0.42176800 0.28994400 -2.21091300

H -0.14827000 -1.94370200 -1.35063700

H 2.32708800 -1.22098800 -1.73716200

H 1.13813800 -2.64452600 0.45153800

H 0.45455200 -1.43983400 1.54335000

H 1.96538300 0.21806200 2.27157000

H -0.92138300 0.24289900 1.66127500

H -4.02361000 1.69495500 0.04557000

H -4.97517600 0.56180600 0.99689600

H -4.88755900 -0.52386600 -2.65321300

H -4.83008800 1.16212600 -2.08323600

H -2.72600700 2.54200300 1.99507600

H -4.03148500 1.64089700 2.75743100

H -2.35412300 1.99385600 4.44208700

H -2.28888500 0.27192900 4.02152100

H -1.04798000 1.39137700 3.42510400

H 5.15788800 1.50449800 2.37655800

H 4.31586300 0.00063100 2.84767400

H 3.60078100 1.59037600 3.24624700

H 1.51863800 2.96551000 1.90623500

H -3.03034400 3.93207100 -2.67087400

H -1.67039000 2.97346900 -3.31883900

H -1.55469900 3.70829400 -1.69911100

H -8.24512900 0.15003900 -1.61106600

H -7.24848300 -0.43139500 -2.97273500

H -7.20240100 1.28865900 -2.50524000

C -1.87325100 -3.43470400 2.51587100

H -1.97316900 -3.29036100 3.59336300

H -2.58967400 -4.20143800 2.19600700

H -0.85758400 -3.78978900 2.29283400

O -5.16600300 -1.81089300 0.88472200

H -5.96296000 -1.29113700 0.70332900

C 4.23697300 0.90922900 -1.39566500

O 4.70011500 2.03108600 -1.44015500

C 5.09977400 -0.29717900 -1.26150000

C 4.92740900 -1.42931500 -2.06048300

C 6.12947400 -0.24502700 -0.31650900

C 5.77478200 -2.52057300 -1.89311900

H 4.15353200 -1.45015600 -2.82104000

C 6.95453000 -1.35034800 -0.13613300

H 6.25874600 0.65224600 0.28144700

C 6.77469700 -2.48788400 -0.92275000

H 5.65107900 -3.39834700 -2.51821600

H 7.73978000 -1.32237900 0.61175700

H 7.42122200 -3.34823600 -0.78428000

O 3.27077700 -1.62430300 0.76085600

H 4.07951800 -1.09084000 0.78680600

H 2.74490500 4.25454700 0.59332300

H 3.42060900 2.95307600 1.03674600

**TS3**

C -3.31686300 -2.56644100 -1.04680600

C -4.43435300 -1.56493300 -0.83031500

C -3.95147300 -0.06819600 -0.74572300

C -2.48934400 0.06392300 -1.26348400

C -1.56930900 -0.84660200 -0.36962600

C -2.05991600 -2.31879200 -0.23214200

C -1.86176800 1.48081000 -1.04147600

C -1.11057900 1.38617200 0.31878500

C 0.38438300 1.16116300 0.14330800

C 0.67555400 0.32417900 -1.08581800

C -0.11182200 -0.98262300 -0.92739400

C 2.12528900 -0.12862000 -1.12316800

C 2.17980600 -1.01033200 0.12828300

C 0.85090200 -1.80532800 -0.00885500

C 2.17795200 -0.10410500 1.36332800

C 1.14755700 1.01342500 1.28376400

O 2.90832100 1.09919400 -1.10311900

O 3.49996400 0.38147600 1.58717000

O 2.39612400 3.34540700 0.62650400

C -1.61099600 0.02272900 0.91164800

C -4.00675500 0.50550800 0.67884600

C -4.95576900 0.70667600 -1.60700500

N -2.93196800 0.02320000 1.53696600

C -2.96035500 0.76057800 2.79953200

C -1.97399300 0.24494900 3.83980200

C 3.95494900 0.23268000 2.92395200

O 1.03714300 1.73734600 2.35695500

O -2.79666200 2.54858800 -1.09869500

C -2.14917800 3.79790300 -1.24630600

O -6.25419700 0.41655700 -1.09988900

C -7.26722900 1.00323000 -1.89215000

O -2.18220800 -2.69968800 1.13630400

H -3.70393600 -3.57608200 -0.87448800

H -3.02240300 -2.52081500 -2.10120500

H -5.08706800 -1.63435300 -1.70990900

H -2.44701300 -0.21165500 -2.32410000

H -1.28335200 -2.96561400 -0.66416900

H -1.15802300 1.66960100 -1.85590500

H -1.34881200 2.23560700 0.96625300

H 0.44761400 0.85593700 -2.01128500

H -0.20039000 -1.49264500 -1.89615700

H 2.36053700 -0.70031700 -2.02379800

H 1.09350700 -2.76810800 -0.46648000

H 0.42382900 -2.01033700 0.97863900

H 1.87551800 -0.72029900 2.22416700

H -0.90615500 -0.33997300 1.66158400

H -3.98217900 1.60341300 0.59590000

H -4.95775600 0.25146400 1.15436900

H -4.88301000 0.36732100 -2.65329600

H -4.78845400 1.78590800 -1.58119100

H -2.79495800 1.84252100 2.64016200

H -3.97918000 0.66550400 3.19316800

H -2.22432600 0.65847900 4.82034300

H -2.01972100 -0.84673900 3.90494100

H -0.94624700 0.53751200 3.61124300

H 4.95745100 0.66202800 2.97320800

H 3.99923400 -0.82643400 3.20501400

H 3.29670700 0.76463600 3.61792900

H 2.22799800 3.01346500 1.54830900

H -2.92453600 4.56547200 -1.27241300

H -1.57240900 3.83388200 -2.18021400

H -1.47055000 4.00577800 -0.40949800

H -8.22817700 0.75917500 -1.43614600

H -7.24319800 0.61021300 -2.91709900

H -7.15415900 2.09431300 -1.93305700

C -1.99980700 -4.08905800 1.32460800

H -2.08607100 -4.28463500 2.39522300

H -2.75810600 -4.68127900 0.79762600

H -1.00584800 -4.40696600 0.98005400

O -5.19250500 -1.96684500 0.30565100

H -5.97858900 -1.40113700 0.30930500

C 4.18346800 1.24583800 -0.78515900

O 4.51181400 2.33032400 -0.29443900

C 5.17067400 0.18185300 -1.05990200

C 5.09268500 -0.59683000 -2.21703100

C 6.19772600 -0.01387400 -0.13150600

C 6.04448700 -1.58687900 -2.43640500

H 4.31413800 -0.41259400 -2.94991000

C 7.12999200 -1.02180600 -0.34732200

H 6.24122800 0.60896300 0.75656900

C 7.05150500 -1.80698600 -1.49786600

H 5.99866500 -2.18809300 -3.33777200

H 7.91829200 -1.19344600 0.37743600

H 7.78254000 -2.59106500 -1.66579100

O 3.25684700 -1.92336000 0.19456500

H 4.01094500 -1.44225400 0.57178500

H 1.70711800 2.80309400 0.13530900

H 3.32142000 2.98490100 0.27615600

**PC**

C -3.31455700 -2.57669900 -1.08963300

C -4.42498200 -1.60516300 -0.73708400

C -3.95901500 -0.10528800 -0.65021700

C -2.55522900 0.05970100 -1.30311200

C -1.54329900 -0.83760500 -0.51079500

C -1.98330900 -2.32733300 -0.40239200

C -1.93273600 1.46853200 -1.10877200

C -1.13195000 1.37041400 0.22527500

C 0.37243800 1.42622400 -0.09544300

C 0.70210500 0.43343400 -1.23094000

C -0.09643200 -0.88641000 -1.10150800

C 2.16163700 -0.01666000 -1.12186100

C 2.10263800 -0.96612300 0.08633900

C 0.83983300 -1.78146000 -0.23332200

C 1.97535000 -0.11375500 1.36808000

C 1.18572000 1.19240800 1.16295800

O 2.92866900 1.19363200 -0.92630400

O 3.28065600 0.23410600 1.79051400

O 2.40797100 4.13082300 0.28351300

C -1.49538400 -0.02478000 0.79633200

C -3.88768200 0.43068600 0.78974300

C -5.05204400 0.67924300 -1.38703000

N -2.74822300 -0.07915800 1.54456500

C -2.67239700 0.61152200 2.83277000

C -1.55371400 0.10719600 3.73580700

C 3.50191300 0.08373900 3.18905200

O 1.24825200 2.04687800 2.03126100

O -2.86706100 2.53091900 -1.13540700

C -2.22771100 3.79001700 -1.24618600

O -6.29272700 0.33954400 -0.77734100

C -7.38536900 0.92722800 -1.45496700

O -1.95911700 -2.76792100 0.95302500

H -3.66173100 -3.59785000 -0.90172800

H -3.13353300 -2.50271100 -2.16729800

H -5.15279600 -1.66024200 -1.55645700

H -2.60617500 -0.19806700 -2.36697200

H -1.24125300 -2.92976400 -0.94555800

H -1.24599800 1.64945800 -1.94256800

H -1.39567300 2.18281100 0.90986100

H 0.53811900 0.91890000 -2.19254400

H -0.17743000 -1.33043200 -2.09961600

H 2.49198000 -0.54993800 -2.01525800

H 1.16719100 -2.65684800 -0.80029800

H 0.36613100 -2.14337000 0.68335800

H 1.46621100 -0.70386400 2.14469000

H -0.71976800 -0.41225500 1.46190100

H -3.85946100 1.53152100 0.73054200

H -4.79771300 0.17119000 1.33646400

H -5.06681200 0.38204100 -2.44828600

H -4.90673700 1.76052400 -1.33293100

H -2.57525900 1.70492000 2.70178100

H -3.63610500 0.45071600 3.32947700

H -1.71015300 0.47312000 4.75366100

H -1.54223500 -0.98707900 3.76102100

H -0.56864400 0.45586000 3.41109200

H 4.53515500 0.37842100 3.37711600

H 3.35717900 -0.95995000 3.48939500

H 2.82775400 0.72771600 3.76076900

H 1.89087600 3.74754100 1.00556600

H -3.01150100 4.54667000 -1.30669100

H -1.60750700 3.83612900 -2.15109700

H -1.59485900 4.00300200 -0.37567100

H -8.29567000 0.64528800 -0.92322600

H -7.44571800 0.56831800 -2.49080400

H -7.29933900 2.02143500 -1.46786700

C -1.71301300 -4.15655600 1.06307100

H -1.70275200 -4.39949000 2.12725000

H -2.49132700 -4.75416500 0.57313800

H -0.74046200 -4.41958700 0.62418200

O -5.07125500 -2.05148100 0.44926400

H -5.86239600 -1.49989200 0.53805300

C 4.23845800 1.26175600 -0.64199100

O 4.65094400 2.29346900 -0.14584700

C 5.13793900 0.12157400 -0.95916500

C 5.09389300 -0.53041200 -2.19303900

C 6.06824200 -0.25452700 0.01388100

C 5.97302400 -1.57979300 -2.44207300

H 4.39825600 -0.20465600 -2.95978800

C 6.92463900 -1.32202100 -0.23318000

H 6.09626400 0.27714400 0.96039200

C 6.87475200 -1.98474200 -1.45930800

H 5.95142500 -2.08318300 -3.40253000

H 7.63315500 -1.63332800 0.52679100

H 7.54681800 -2.81444000 -1.65240100

O 3.17759100 -1.86730100 0.22944600

H 3.87013100 -1.40954000 0.73251900

H 0.63425400 2.44211200 -0.41172600

H 3.14174600 3.50250000 0.17560600

2. Pathway-2

**Aconitine**

C -3.26559800 -2.76857500 -1.21532700

C -4.38106300 -1.81483700 -0.82928200

C -3.92688300 -0.31388100 -0.69481000

C -2.52189900 -0.12617800 -1.34385700

C -1.50684400 -1.03908600 -0.57913100

C -1.93193000 -2.53504800 -0.52735800

C -1.90873700 1.27692200 -1.10351700

C -1.12958200 1.14525800 0.24294700

C 0.38037300 1.23517800 -0.02081000

C 0.73916400 0.28912300 -1.19459300

C -0.05537700 -1.04047300 -1.14497500

C 2.19417800 -0.18173100 -1.11981200

C 2.12569700 -1.16653700 0.05910300

C 0.86914100 -1.96897200 -0.30552700

C 1.98421400 -0.36520700 1.37416000

C 1.26520100 1.00299400 1.25038000

O 3.00525200 0.99693700 -0.94730100

O 3.32020300 -0.15587900 1.81220700

O 0.69288300 2.55494400 -0.57584800

C -1.47210000 -0.28306300 0.75839500

C -3.85691500 0.17254700 0.76412300

C -5.03175300 0.48356600 -1.40104800

N -2.72921300 -0.39597800 1.48825700

C -2.64237700 0.12891300 2.84920200

C -1.84062700 -0.77389600 3.77919800

C 3.44784200 0.42223600 3.10071300

O 0.56274400 1.20084200 2.46061400

O -2.87268100 2.31223200 -1.12345300

C -2.30620300 3.60652400 -1.18408100

O -6.26802800 0.09907800 -0.80750500

C -7.36717600 0.71528100 -1.44793900

O -1.89859000 -3.02751500 0.81021700

H -3.60671100 -3.79685300 -1.05723900

H -3.09076100 -2.66085200 -2.29110600

H -5.10764500 -1.84789200 -1.65087400

H -2.57287600 -0.35021300 -2.41534100

H -1.18771300 -3.10940500 -1.09742900

H -1.21446500 1.49233900 -1.92213600

H -1.43635400 1.92241700 0.94841900

H 0.57232600 0.83165400 -2.12460700

H -0.10548000 -1.42468700 -2.16936500

H 2.47677100 -0.71412500 -2.03208200

H 1.20195800 -2.82305700 -0.90075900

H 0.38558300 -2.36235800 0.59221700

H 1.45304300 -0.97508300 2.12118600

H 2.07702600 1.73591100 1.16847200

H -0.68885400 -0.67001900 1.41214600

H -3.81637600 1.27448600 0.74854800

H -4.77217600 -0.10132900 1.29408300

H -5.04180500 0.23196500 -2.47416700

H -4.90612000 1.56337400 -1.29961900

H -2.23130500 1.15434100 2.86892700

H -3.66691500 0.20224300 3.22958800

H -1.86770900 -0.37705500 4.79792500

H -2.26470800 -1.78177700 3.78958000

H -0.79019100 -0.84632300 3.48486900

H 4.50637800 0.37536200 3.36072400

H 2.86238800 -0.14147900 3.83681900

H 3.12216300 1.46769000 3.10904000

H 0.28482200 2.13223400 2.44975300

H -3.12188800 4.30467000 -1.38053100

H -1.56721800 3.67745000 -1.99307300

H -1.83243600 3.88620600 -0.23448700

H -8.27368100 0.39682100 -0.93052100

H -7.42836700 0.41504200 -2.50226900

H -7.28955200 1.80916200 -1.39954300

C -1.62731300 -4.41466200 0.86570800

H -1.61279700 -4.69889400 1.91965800

H -2.39498100 -5.00637100 0.35218000

H -0.65019000 -4.64309600 0.41763800

O -5.02661700 -2.30501800 0.34016200

H -5.82357000 -1.76437600 0.44251200

C 0.65385800 3.65894400 0.17042900

O 0.33741200 3.68250000 1.34854900

C 1.05715500 4.86605600 -0.61879800

H 2.08427000 4.73085300 -0.96743200

H 0.41328100 4.96422900 -1.49601100

H 0.98530100 5.75361100 0.00656600

C 4.28990100 1.01452400 -0.54258800

O 4.67855300 1.99709600 0.05527700

C 5.18735400 -0.11794200 -0.89301200

C 5.14167100 -0.72606700 -2.14904500

C 6.11736100 -0.53149800 0.06442300

C 6.01792800 -1.76792800 -2.43698700

H 4.44457700 -0.37225600 -2.90199800

C 6.97214800 -1.59048700 -0.22116900

H 6.14631100 -0.03441000 1.02954400

C 6.92022000 -2.20901700 -1.47035800

H 5.99427000 -2.23726100 -3.41458200

H 7.68061700 -1.93072400 0.52644100

H 7.59044200 -3.03274600 -1.69338200

O 3.18999200 -2.08766800 0.16337100

H 3.87065900 -1.68584500 0.72508600

**TS4**

C -3.45845700 -2.57756800 -1.27528500

C -4.54360000 -1.56916900 -0.94948200

C -4.02089700 -0.09206500 -0.77100300

C -2.56178500 0.03098800 -1.30606000

C -1.66513600 -0.95973000 -0.48736800

C -2.17741000 -2.43088300 -0.47563900

C -1.89997700 1.41058000 -1.00003200

C -1.18267300 1.22664000 0.36235000

C 0.23677200 0.91720200 0.26950100

C 0.66650800 0.25081800 -0.98867700

C -0.18885100 -1.05926800 -0.96813900

C 2.09309000 -0.28034000 -0.93953400

C 1.99861600 -1.24222000 0.25975800

C 0.67891900 -1.98174900 -0.05785900

C 1.95188400 -0.39997800 1.55104000

C 1.06843500 0.86012600 1.42203600

O 2.96479300 0.85528400 -0.80982000

O 3.30059800 -0.10835600 1.86034200

O 0.92307100 3.24603200 -0.54868600

C -1.69711400 -0.24153500 0.87213300

C -4.04433100 0.38227500 0.69288000

C -5.02253700 0.76222200 -1.55920800

N -2.98512400 -0.21774600 1.49277800

C -2.97091400 0.28810200 2.86410600

C -2.24606200 -0.63460500 3.83570900

C 3.48417300 0.60199100 3.07494200

O 0.42877900 1.17860300 2.63766000

O -2.81528400 2.48381400 -0.99882100

C -2.18441800 3.75191500 -1.04440400

O -6.31624300 0.45560400 -1.05154300

C -7.33292100 1.10248800 -1.79131900

O -2.28472900 -2.91014800 0.86052300

H -3.86665100 -3.58742700 -1.16656700

H -3.19144300 -2.45895900 -2.33082500

H -5.22011800 -1.55746500 -1.81252100

H -2.53935500 -0.17394500 -2.38151700

H -1.42140600 -3.04966700 -0.97864600

H -1.17106400 1.62929300 -1.78580600

H -1.41779700 1.98379200 1.11237300

H 0.48903700 0.86855600 -1.86645000

H -0.19960200 -1.44640400 -1.99146900

H 2.31311400 -0.83984400 -1.85154100

H 0.95047500 -2.89654100 -0.58911100

H 0.16339600 -2.27728000 0.86110800

H 1.51052900 -1.00278300 2.36126800

H 1.78826700 1.83423000 1.17258600

H -0.99418400 -0.66702100 1.58742800

H -3.96895600 1.48018900 0.69985800

H -4.99782400 0.12603800 1.15830400

H -4.96916700 0.49693700 -2.62750400

H -4.83891400 1.83368900 -1.45818300

H -2.53917100 1.30372000 2.91150200

H -4.01626200 0.38062400 3.17450000

H -2.38637600 -0.27171500 4.85729800

H -2.64844000 -1.64918700 3.77020400

H -1.16984200 -0.67507700 3.65005700

H 4.55912400 0.64038800 3.25658700

H 2.98855000 0.08500500 3.90514400

H 3.09652400 1.62351500 3.00072000

H 0.61964700 2.10797800 2.83586200

H -2.97781500 4.49601800 -1.12912600

H -1.51697300 3.82739200 -1.91198200

H -1.60096900 3.94777800 -0.13775800

H -8.28972700 0.84529000 -1.33406000

H -7.33056800 0.76977700 -2.83751600

H -7.20382500 2.19223900 -1.76971000

C -2.10621500 -4.31144200 0.94539500

H -2.19633700 -4.58393800 1.99848300

H -2.86544700 -4.85813700 0.37312200

H -1.11192100 -4.60345900 0.58072800

O -5.27971700 -2.03400500 0.17525100

H -6.06739400 -1.47235100 0.22378600

C 2.03252400 3.53017800 -0.04881000

O 2.40802700 3.12441600 1.11003700

C 3.01958100 4.34655400 -0.85371900

H 3.48367400 3.68283700 -1.59051600

H 2.49992800 5.14053400 -1.39269700

H 3.80090900 4.76423300 -0.21850400

C 4.29209200 0.77354600 -0.58097900

O 4.84543400 1.72935800 -0.08175900

C 5.04015300 -0.44585500 -0.99493200

C 4.85293500 -1.03343300 -2.24751100

C 5.99356500 -0.95218000 -0.10757800

C 5.60672000 -2.14919800 -2.59923400

H 4.14554900 -0.60682800 -2.95188400

C 6.72359800 -2.08347200 -0.45525700

H 6.13740900 -0.46804100 0.85405300

C 6.52816100 -2.68234100 -1.69963300

H 5.47292900 -2.60307300 -3.57528200

H 7.44821800 -2.49400500 0.23974900

H 7.10215800 -3.56198700 -1.97200400

O 3.01321900 -2.21553900 0.35836000

H 3.75382200 -1.82276200 0.84551400

**IM5**

C -3.48656700 -2.34840500 -1.60788000

C -4.55870000 -1.34275300 -1.23282800

C -3.99996800 0.06159300 -0.78806900

C -2.50116600 0.19796700 -1.18095000

C -1.70079700 -0.95129700 -0.46484600

C -2.27998300 -2.37887800 -0.68694600

C -1.81177600 1.48234700 -0.61196100

C -1.16989400 1.02801200 0.73111200

C 0.30490100 0.70711600 0.58731100

C 0.64797500 0.20722300 -0.79799800

C -0.21612800 -1.05556700 -0.94564000

C 2.06601000 -0.32072200 -0.89210700

C 2.02293100 -1.44136000 0.16222700

C 0.64605200 -2.09507000 -0.15341800

C 2.07682600 -0.79067500 1.55063700

C 1.01561700 0.28369900 1.65007700

O 2.91645000 0.82067700 -0.66224300

O 3.42977200 -0.41598900 1.75977800

O 1.34260300 3.41080800 -1.18382100

C -1.79077400 -0.39868900 0.97777800

C -4.12320300 0.31175400 0.72398200

C -4.89052200 1.07769600 -1.51198100

N -3.14551000 -0.43479300 1.50655200

C -3.21563600 -0.03260700 2.91012700

C -2.45752300 -0.96017000 3.85179200

C 3.64854100 0.50497800 2.81460500

O 0.64851500 0.51308900 2.95060200

O -2.66852200 2.60067100 -0.45326800

C -1.92850700 3.80400900 -0.34176500

O -6.23595100 0.78312700 -1.15497000

C -7.15293900 1.59695300 -1.85871000

O -2.52651400 -3.02895000 0.55605600

H -3.94176600 -3.34073300 -1.68958900

H -3.11558600 -2.09123100 -2.60622800

H -5.15128800 -1.16980100 -2.14001900

H -2.39766400 0.16109800 -2.27150200

H -1.51072200 -2.97117300 -1.20242100

H -1.04473900 1.80256400 -1.31911300

H -1.40371200 1.74553700 1.52467700

H 0.48857800 0.95658400 -1.56988900

H -0.25176700 -1.34699500 -2.00259800

H 2.25599600 -0.74648300 -1.88061200

H 0.84240800 -2.97991800 -0.76344200

H 0.15882400 -2.43414300 0.76680400

H 1.79257800 -1.53996200 2.30742000

H 1.57497900 2.47389400 0.91101000

H -1.16505600 -0.96754900 1.66694700

H -4.02368400 1.39470700 0.89442300

H -5.11916300 0.03006200 1.07464700

H -4.76338500 0.96730000 -2.60130800

H -4.65833500 2.11014100 -1.23977500

H -2.86987500 1.00854800 3.05262700

H -4.27643300 -0.03994900 3.18385600

H -2.72696400 -0.73302400 4.88667900

H -2.71606800 -2.00383000 3.64910500

H -1.37421000 -0.84873500 3.76340300

H 4.72893900 0.63144100 2.90166400

H 3.24716300 0.12366000 3.76057100

H 3.19035400 1.47593200 2.59242800

H -0.11751800 1.10647800 2.98476600

H -2.64225200 4.60571100 -0.14607100

H -1.38560200 4.01767000 -1.27122900

H -1.20418100 3.75984700 0.48262000

H -8.15693400 1.33232700 -1.52285700

H -7.07798100 1.42924900 -2.94118700

H -6.97309000 2.66061800 -1.65592300

C -2.44278100 -4.43702400 0.45339300

H -2.62111700 -4.84424300 1.45050900

H -3.19366300 -4.84741700 -0.23290800

H -1.44653500 -4.74904600 0.11051200

O -5.41470900 -1.93122900 -0.26000800

H -6.17223600 -1.33305800 -0.18058300

C 2.09070200 3.82049400 -0.31488700

O 2.13706500 3.27898300 0.90602500

C 3.05694600 4.95207600 -0.47581700

H 4.07164300 4.54947700 -0.41118300

H 2.90744100 5.43474600 -1.43944100

H 2.92773800 5.66925700 0.33713900

C 4.24100600 0.78778000 -0.45990600

O 4.75985100 1.75547800 0.06078000

C 5.03446100 -0.38277800 -0.92721200

C 4.86065300 -0.92143100 -2.20346800

C 6.00311300 -0.90134800 -0.06338000

C 5.64106700 -2.00238000 -2.60306900

H 4.13770400 -0.48690800 -2.88651700

C 6.76043000 -1.99869200 -0.45962500

H 6.13635900 -0.45639600 0.91819800

C 6.57670300 -2.55022500 -1.72760000

H 5.51524000 -2.41874800 -3.59672400

H 7.49643400 -2.41985900 0.21683100

H 7.17056700 -3.40429300 -2.03629800

O 3.01596200 -2.43983200 0.05370600

H 3.83853800 -2.08622800 0.42575700

**IM6**

C -3.30472100 -2.88953400 -0.96029000

C -4.41572700 -1.86162400 -0.85920300

C -3.91503000 -0.36822800 -0.82125700

C -2.42656600 -0.28487400 -1.26584800

C -1.57185900 -1.16317600 -0.27864000

C -2.09207300 -2.61822600 -0.08836800

C -1.78940700 1.13324300 -1.08202000

C -1.11245900 1.09057100 0.31761200

C 0.36868000 0.78644500 0.23196200

C 0.72269700 -0.05792100 -0.96674100

C -0.08967800 -1.34406300 -0.74488900

C 2.16169700 -0.53081400 -0.92621100

C 2.16663400 -1.31764500 0.39613500

C 0.82151400 -2.09151100 0.28697600

C 2.19565200 -0.30332100 1.54843200

C 1.12198800 0.73456400 1.34341500

O 2.96258300 0.66684200 -1.01478600

O 3.54431300 0.14274900 1.64633800

O 0.62848200 3.85078800 1.17208900

C -1.66840600 -0.23756200 0.95776100

C -4.03551900 0.27792800 0.56870500

C -4.85877100 0.37692900 -1.77278600

N -3.01608400 -0.18001600 1.50471700

C -3.09283500 0.59541900 2.74160400

C -2.27161800 0.01063200 3.88382700

C 3.73559000 1.36545000 2.33686800

O 0.76065100 1.38591300 2.50141800

O -2.69837500 2.21005400 -1.23715300

C -2.02891100 3.45497500 -1.32430100

O -6.18659300 0.12825900 -1.32408900

C -7.14634800 0.69245600 -2.19540300

O -2.30076600 -2.91416500 1.28912000

H -3.71897000 -3.88245400 -0.75695800

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**TS5**

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**PC2**

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**Pyraconitine**

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