

Supplementary Data 1. Cartesian Coordinates of All Calculated Species (In

Angstrom)

a1

| | | | |
|---|-------------|-------------|-------------|
| C | -0.00247900 | 0.04553900 | 0.36251800 |
| H | 0.00796200 | 0.08774300 | 1.46843000 |
| O | 0.10251500 | 1.35882900 | -0.16547900 |
| H | 0.95629900 | 1.72144300 | 0.10524000 |
| C | -1.34241300 | -0.50341600 | -0.08815700 |
| H | -1.37574800 | -0.55844100 | -1.18739700 |
| H | -1.51084300 | -1.51031200 | 0.31846600 |
| H | -2.15924500 | 0.15084900 | 0.24938200 |
| C | 1.15959700 | -0.81805600 | -0.10180500 |
| H | 2.11855700 | -0.39148300 | 0.23108200 |
| H | 1.08378300 | -1.83735800 | 0.30447700 |
| H | 1.17088600 | -0.87746900 | -1.20118400 |

a1...(*i*PrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -2.21519000 | -0.21035900 | -0.31804200 |
| H | -2.48150600 | -0.59468500 | -1.31897600 |
| O | -1.20736900 | 0.79180200 | -0.45989100 |
| H | -1.55223300 | 1.51168700 | -1.00738100 |
| C | -1.59860200 | -1.33327600 | 0.49258400 |
| H | -1.33377700 | -0.97326600 | 1.49919200 |
| H | -2.30433700 | -2.16896000 | 0.59679800 |
| H | -0.68741800 | -1.70035900 | -0.00134700 |
| C | -3.45346000 | 0.37653900 | 0.33522600 |
| H | -3.86217900 | 1.19994900 | -0.27012400 |
| H | -4.23716800 | -0.38751000 | 0.44113600 |
| H | -3.20565600 | 0.76733900 | 1.33397000 |
| C | 1.94939200 | -0.09920400 | 0.21917700 |
| H | 1.40244100 | -0.61480100 | 1.03392400 |
| O | 1.27268500 | -0.30198900 | -1.00794900 |
| H | 0.39397100 | 0.11615700 | -0.92419000 |
| C | 3.32311700 | -0.73011000 | 0.09092500 |
| H | 3.89184000 | -0.23298800 | -0.71061700 |
| H | 3.88800300 | -0.63904500 | 1.02956000 |
| H | 3.23515600 | -1.79726700 | -0.16049300 |
| C | 2.02757700 | 1.38267200 | 0.55943700 |
| H | 1.01640100 | 1.80799600 | 0.64482800 |
| H | 2.55000000 | 1.54485300 | 1.51390400 |
| H | 2.56693400 | 1.92482900 | -0.23330100 |

a1... (2 ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.17784200 | 2.52625500 | 0.05235200 |
| H | -0.56281200 | 3.33126200 | -0.09629600 |
| O | -0.08622400 | 1.48973300 | -0.90497800 |
| H | 0.04636300 | 1.84045500 | -1.79924600 |
| C | -0.02481400 | 1.90496500 | 1.41893000 |
| H | 0.69975400 | 1.08934400 | 1.56711400 |
| H | 0.12164100 | 2.65409800 | 2.20926300 |
| H | -1.04432000 | 1.50084800 | 1.50365800 |
| C | 1.57618200 | 3.08195700 | -0.14505100 |
| H | 1.69203700 | 3.49717200 | -1.15795100 |
| H | 1.77371200 | 3.88788500 | 0.57624100 |
| H | 2.32343600 | 2.28703500 | -0.00248400 |
| C | -2.43604900 | -0.73977300 | 0.09822500 |
| H | -1.82344800 | -0.69976400 | 1.02147400 |
| O | -2.67285700 | 0.57753800 | -0.36534000 |
| H | -1.81214000 | 0.94104400 | -0.64305600 |
| C | -3.78021600 | -1.35150000 | 0.44568300 |
| H | -4.41352000 | -1.40716300 | -0.45359700 |
| H | -3.65847000 | -2.36559900 | 0.85219500 |
| H | -4.29943500 | -0.73640000 | 1.19516100 |
| C | -1.68179800 | -1.55326000 | -0.94459300 |
| H | -0.72062900 | -1.07154000 | -1.18488300 |
| H | -1.47583000 | -2.57260700 | -0.58466000 |
| H | -2.27391600 | -1.62055800 | -1.87124900 |
| C | 2.01510300 | -1.61264000 | -0.18282900 |
| H | 1.46406900 | -2.11255700 | -1.00289600 |
| O | 2.13476400 | -0.22940000 | -0.46451300 |
| H | 1.25358000 | 0.15973100 | -0.60591400 |
| C | 3.42087600 | -2.18196800 | -0.13330900 |
| H | 3.99583300 | -1.69040000 | 0.66709300 |
| H | 3.40173400 | -3.26303100 | 0.06486100 |
| H | 3.94073300 | -2.01063000 | -1.08708900 |
| C | 1.26019600 | -1.84615800 | 1.11734900 |
| H | 0.26506200 | -1.37787600 | 1.07884300 |
| H | 1.12198600 | -2.92109000 | 1.30843100 |
| H | 1.81518000 | -1.40989500 | 1.96308700 |

b1

| | | | |
|---|-------------|-------------|-------------|
| C | 0.00001100 | 0.17022500 | 0.33186600 |
| H | 0.00004100 | 0.10396000 | 1.47389000 |
| O | 0.00007500 | 1.42188500 | -0.14766700 |
| C | -1.25456900 | -0.63374700 | -0.08638800 |
| H | -1.28726800 | -0.70194900 | -1.18833000 |

| | | | |
|---|-------------|-------------|-------------|
| H | -1.29457900 | -1.65504200 | 0.33101200 |
| H | -2.15861200 | -0.09021200 | 0.23380100 |
| C | 1.25450000 | -0.63385800 | -0.08639500 |
| H | 2.15855300 | -0.09004900 | 0.23329500 |
| H | 1.29473600 | -1.65495000 | 0.33147600 |
| H | 1.28688800 | -0.70255800 | -1.18831100 |

b1...(*i*PrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | 1.82895600 | 0.09134200 | 0.17301900 |
| H | 1.34295300 | 0.53521600 | 1.08342500 |
| O | 1.02307400 | 0.19685700 | -0.93936900 |
| C | 2.13030300 | -1.37154700 | 0.52726500 |
| H | 2.63163700 | -1.86212400 | -0.32419700 |
| H | 2.77299700 | -1.47117200 | 1.41734600 |
| H | 1.18867700 | -1.90800100 | 0.71997600 |
| C | 3.13454500 | 0.86293900 | -0.03607300 |
| H | 2.91708700 | 1.91913900 | -0.25999400 |
| H | 3.79970500 | 0.82345100 | 0.84157100 |
| H | 3.67248900 | 0.44340900 | -0.90289100 |
| C | -2.04533400 | 0.14309800 | -0.31508800 |
| H | -2.18633300 | 0.54550800 | -1.34633400 |
| O | -1.07067600 | -0.85254900 | -0.30121800 |
| H | -0.11256500 | -0.39176300 | -0.62721700 |
| C | -3.37889300 | -0.45162000 | 0.12092500 |
| H | -3.29541000 | -0.83808800 | 1.15002100 |
| H | -4.19132600 | 0.29059500 | 0.09153500 |
| H | -3.65134200 | -1.29344700 | -0.53392300 |
| C | -1.65057300 | 1.32623200 | 0.56918000 |
| H | -0.68636100 | 1.72760800 | 0.22461100 |
| H | -2.40099800 | 2.13208500 | 0.54223400 |
| H | -1.53440900 | 0.99045600 | 1.61316100 |

b1...(*2*^{*i*}PrOH)

| | | | |
|---|-------------|------------|-------------|
| C | 0.42893000 | 2.34060000 | -0.37410400 |
| H | -0.09647800 | 2.99694100 | -1.11092000 |
| O | 0.04941400 | 1.01813900 | -0.54020300 |
| C | 0.03576200 | 2.84999900 | 1.01609700 |
| H | 0.59336000 | 2.29898200 | 1.79239900 |
| H | 0.23491800 | 3.92604100 | 1.14514600 |
| H | -1.03795700 | 2.67037600 | 1.18109900 |
| C | 1.92689600 | 2.52726900 | -0.61944500 |
| H | 2.19887900 | 2.15416000 | -1.61910200 |
| H | 2.22596500 | 3.58563300 | -0.55441500 |
| H | 2.51074800 | 1.95846000 | 0.12238600 |

| | | | |
|---|-------------|-------------|-------------|
| C | -2.45337900 | -0.60497900 | 0.21079500 |
| H | -1.80769700 | -0.64680900 | 1.11521000 |
| O | -2.41605500 | 0.68233600 | -0.34670500 |
| H | -1.40630600 | 0.87283400 | -0.48588300 |
| C | -3.87988900 | -0.91481200 | 0.63578400 |
| H | -4.54548900 | -0.88826100 | -0.24221600 |
| H | -3.95845900 | -1.90845600 | 1.10141200 |
| H | -4.23832000 | -0.16331500 | 1.35535000 |
| C | -1.92599300 | -1.63881500 | -0.78281400 |
| H | -0.89401700 | -1.39255200 | -1.07779500 |
| H | -1.93333300 | -2.65633200 | -0.36088900 |
| H | -2.55159100 | -1.63432400 | -1.69061700 |
| C | 1.68657300 | -1.60346400 | 0.23537100 |
| H | 0.66157300 | -1.86405600 | 0.57714900 |
| O | 1.62506700 | -0.88521900 | -0.96962000 |
| H | 1.01984600 | -0.06592800 | -0.81463400 |
| C | 2.43431300 | -2.90232700 | -0.02194300 |
| H | 3.45615400 | -2.68158900 | -0.37036600 |
| H | 2.50107900 | -3.51959900 | 0.88606600 |
| H | 1.92772400 | -3.48650000 | -0.80489200 |
| C | 2.34032300 | -0.78227900 | 1.34280100 |
| H | 1.76583700 | 0.14228600 | 1.50113300 |
| H | 2.37511900 | -1.33757200 | 2.29286600 |
| H | 3.36981800 | -0.50961900 | 1.05848700 |

b1...(³iPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.41097600 | -0.20216100 | 2.38163700 |
| H | 0.27430000 | 0.53144300 | 2.86495300 |
| O | -0.15160600 | -0.25755100 | 1.00802400 |
| C | -1.84169800 | 0.27030800 | 2.63903200 |
| H | -2.55345800 | -0.42974900 | 2.17103000 |
| H | -2.06812600 | 0.33082000 | 3.71505100 |
| H | -1.99551500 | 1.26577600 | 2.19581300 |
| C | -0.15489500 | -1.56301400 | 3.02762400 |
| H | 0.87323800 | -1.89652300 | 2.81912500 |
| H | -0.29629800 | -1.53539400 | 4.11946900 |
| H | -0.84666800 | -2.31251500 | 2.60771700 |
| C | 0.46837600 | 2.64619400 | -0.52934500 |
| H | 0.69184900 | 2.11023900 | -1.47718700 |
| O | -0.67092500 | 2.08920700 | 0.08066700 |
| H | -0.44696600 | 1.15655300 | 0.40971800 |
| C | 0.15642400 | 4.09279100 | -0.87549800 |
| H | -0.04619000 | 4.66361700 | 0.04491300 |
| H | 0.99466800 | 4.56928900 | -1.40458400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -0.73705100 | 4.14877400 | -1.51524800 |
| C | 1.69155200 | 2.52642200 | 0.37305500 |
| H | 1.90742400 | 1.47027500 | 0.59399600 |
| H | 2.58228000 | 2.96773600 | -0.10062400 |
| H | 1.50821200 | 3.05120000 | 1.32510900 |
| C | 2.36483400 | -1.18937800 | -0.76522300 |
| H | 1.96352200 | -0.32079200 | -1.33197300 |
| O | 2.27586900 | -0.93721100 | 0.61707700 |
| H | 1.30639800 | -0.68292600 | 0.79985400 |
| C | 3.83142200 | -1.35090700 | -1.12837500 |
| H | 4.26374800 | -2.19351800 | -0.56529100 |
| H | 3.95996500 | -1.54832000 | -2.20276400 |
| H | 4.39695300 | -0.44260700 | -0.87140600 |
| C | 1.54707800 | -2.41951000 | -1.14651500 |
| H | 0.49091200 | -2.28598800 | -0.86670700 |
| H | 1.59464800 | -2.61771000 | -2.22872300 |
| H | 1.93487400 | -3.30305700 | -0.61358300 |
| C | -2.36588300 | -0.63779200 | -1.20294200 |
| H | -2.64133500 | 0.29002900 | -0.66077800 |
| C | -3.60556700 | -1.17571400 | -1.89631000 |
| H | -4.01277500 | -0.44641100 | -2.61198600 |
| H | -3.36000900 | -2.09998000 | -2.44362200 |
| H | -4.38634700 | -1.41325300 | -1.15860500 |
| C | -1.26854800 | -0.27235000 | -2.19731300 |
| H | -1.58318500 | 0.54852100 | -2.86091400 |
| H | -0.36640600 | 0.05135400 | -1.65623600 |
| H | -1.00776800 | -1.14382600 | -2.82016200 |
| O | -1.91259000 | -1.60544900 | -0.28305400 |
| H | -1.19358600 | -1.14436100 | 0.26297400 |

c1

| | | | |
|---|-------------|-------------|-------------|
| C | -0.98276800 | -0.08862600 | 0.02587200 |
| C | -0.64250300 | 1.23929800 | 0.03005000 |
| C | 0.78005800 | 1.27520500 | 0.01650900 |
| C | 1.19565800 | -0.03088900 | 0.00523700 |
| O | 0.11366500 | -0.85838400 | 0.01074300 |
| H | -1.33601000 | 2.07519300 | 0.04020700 |
| H | 1.43002200 | 2.14745200 | 0.01429400 |
| C | 2.51565600 | -0.64065000 | -0.01729100 |
| H | 2.51485300 | -1.75303200 | -0.02615800 |
| O | 3.54526600 | -0.00027300 | -0.02651000 |
| C | -2.30396800 | -0.77766700 | 0.04219100 |
| H | -2.32498700 | -1.51740700 | -0.77921100 |
| H | -2.39744100 | -1.34313000 | 0.98764900 |

| | | | |
|---|-------------|-------------|-------------|
| O | -3.29665700 | 0.20318700 | -0.09053000 |
| H | -4.15742600 | -0.22535100 | -0.00182000 |

c1...(*i*PrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.53628300 | 1.21464800 | -0.02519400 |
| C | 0.65311200 | 1.10288800 | 1.33505000 |
| C | 1.74375900 | 0.21552900 | 1.55500800 |
| C | 2.20775600 | -0.13804700 | 0.31413000 |
| O | 1.46577800 | 0.47478100 | -0.64659300 |
| H | 0.02249100 | 1.58557900 | 2.07601800 |
| H | 2.14494700 | -0.12735900 | 2.50642100 |
| C | 3.29374700 | -1.01295700 | -0.09427000 |
| H | 3.84027200 | -1.47809500 | 0.75425100 |
| O | 3.59441500 | -1.23123500 | -1.24832400 |
| C | -0.42310300 | 1.96619200 | -0.88322700 |
| H | 0.04907900 | 2.89874400 | -1.23900200 |
| H | -0.65949400 | 1.35337400 | -1.77091700 |
| O | -1.56307000 | 2.24003400 | -0.10239300 |
| H | -2.16381100 | 2.80328500 | -0.60997800 |
| H | -2.15865700 | 0.67814800 | 0.76444400 |
| O | -2.28723400 | -0.23959700 | 1.06027100 |
| C | -1.98645100 | -1.07674500 | -0.04150800 |
| H | -0.93770600 | -0.90950900 | -0.36272800 |
| C | -2.11193500 | -2.51283300 | 0.43048800 |
| C | -2.90497700 | -0.77023800 | -1.21610000 |
| H | -3.14155400 | -2.70969500 | 0.76799600 |
| H | -1.86744600 | -3.21634000 | -0.37785200 |
| H | -1.43038100 | -2.69924600 | 1.27344200 |
| H | -2.82426700 | 0.29151300 | -1.49682100 |
| H | -2.64981500 | -1.38027500 | -2.09514800 |
| H | -3.95191200 | -0.97261500 | -0.94007100 |

c1...(2 *i*PrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.79745400 | -0.44837100 | 0.40714600 |
| C | -2.29294300 | 0.18027300 | 1.51931100 |
| C | -3.70503700 | 0.22368800 | 1.33894600 |
| C | -3.95658600 | -0.37949900 | 0.13470100 |
| O | -2.78815900 | -0.79002400 | -0.42841300 |
| H | -1.71376200 | 0.56510800 | 2.35446800 |
| H | -4.45097900 | 0.64753100 | 2.00793800 |
| C | -5.19954900 | -0.62009300 | -0.57995100 |
| H | -6.10357800 | -0.25497300 | -0.04661200 |
| O | -5.26735800 | -1.16599400 | -1.66003600 |
| C | -0.40514400 | -0.78722700 | -0.01343700 |

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|---|-------------|-------------|-------------|
| H | -0.34364800 | -1.85635500 | -0.27601600 |
| H | -0.14239200 | -0.21255600 | -0.91550900 |
| O | 0.52259700 | -0.44059700 | 0.99069600 |
| H | 0.36019300 | 1.47496300 | 0.93155000 |
| O | 0.29218500 | 2.27132700 | 0.38216800 |
| C | 1.47234000 | 2.32756800 | -0.40453900 |
| H | 1.53682100 | 1.42328600 | -1.04119000 |
| C | 1.35795300 | 3.54383600 | -1.30304500 |
| C | 2.71061800 | 2.37581300 | 0.47858800 |
| H | 1.28815900 | 4.45877200 | -0.69388800 |
| H | 2.23337100 | 3.62853000 | -1.96225600 |
| H | 0.45547300 | 3.47663500 | -1.92782400 |
| H | 2.74852900 | 1.49804600 | 1.14247800 |
| H | 3.62962500 | 2.37919900 | -0.12605100 |
| H | 2.69556300 | 3.28233600 | 1.10416800 |
| H | 0.40712100 | -1.02280400 | 1.75779400 |
| H | 2.14247900 | -0.51168500 | 0.04797800 |
| O | 2.82714500 | -0.71860800 | -0.60989500 |
| C | 3.45068100 | -1.92752300 | -0.20985400 |
| H | 2.71240400 | -2.75324300 | -0.23969600 |
| C | 4.54801700 | -2.22445300 | -1.21367600 |
| C | 3.98577900 | -1.80856600 | 1.20942600 |
| H | 5.30089100 | -1.42101100 | -1.19595800 |
| H | 5.04642700 | -3.17648000 | -0.98293900 |
| H | 4.13306600 | -2.28620900 | -2.23022500 |
| H | 3.16981600 | -1.57485800 | 1.91130000 |
| H | 4.45935800 | -2.74555300 | 1.53781300 |
| H | 4.73173000 | -1.00018900 | 1.26482300 |

d1

| | | | |
|---|-------------|-------------|-------------|
| C | -0.96176600 | -0.07139600 | 0.00002400 |
| C | -0.83965500 | 1.29773400 | -0.00005800 |
| C | 0.55249000 | 1.57343400 | 0.00006100 |
| C | 1.18630300 | 0.35357100 | -0.00003800 |
| O | 0.25666000 | -0.64427400 | 0.00003000 |
| H | -1.67408900 | 1.99189900 | -0.00011200 |
| H | 1.04763900 | 2.54285000 | 0.00008700 |
| C | 2.59146300 | 0.01602100 | -0.00010400 |
| H | 3.26275700 | 0.90338500 | 0.00001000 |
| O | 3.03486200 | -1.11639600 | 0.00009500 |
| C | -2.21848300 | -0.91795200 | 0.00000400 |
| H | -2.05968500 | -1.62403600 | -0.87703400 |
| H | -2.05974500 | -1.62401300 | 0.87706900 |
| O | -3.33889600 | -0.20165000 | -0.00004400 |

d1...(ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | 1.10149500 | -0.47806700 | 0.26844500 |
| C | 1.51678500 | -1.51172300 | -0.53519200 |
| C | 2.87193700 | -1.23677700 | -0.86194400 |
| C | 3.18731200 | -0.05663500 | -0.23386900 |
| O | 2.10299300 | 0.39944000 | 0.45386400 |
| H | 0.90119700 | -2.35297200 | -0.83836900 |
| H | 3.54672400 | -1.82485100 | -1.48125900 |
| C | 4.41600800 | 0.70745600 | -0.19828500 |
| H | 5.24257600 | 0.25355300 | -0.78797400 |
| O | 4.56401700 | 1.74943900 | 0.40885200 |
| C | -0.22796700 | -0.22877200 | 0.92759800 |
| H | -0.00958900 | -0.13420800 | 2.02122000 |
| H | -0.52338800 | 0.80872500 | 0.62292000 |
| O | -1.14671900 | -1.18191600 | 0.62016400 |
| H | -2.01738900 | -0.53947200 | -0.28457900 |
| O | -2.66929000 | 0.05168400 | -0.87209300 |
| C | -3.64252300 | 0.54450500 | 0.00488400 |
| H | -3.16477500 | 1.11041300 | 0.83650600 |
| C | -4.54225900 | 1.50908100 | -0.75357200 |
| C | -4.44304300 | -0.59276700 | 0.63611500 |
| H | -5.04653100 | 0.97914500 | -1.57794900 |
| H | -5.31050100 | 1.95028800 | -0.10091700 |
| H | -3.94563300 | 2.32415800 | -1.19023900 |
| H | -3.75373500 | -1.27086500 | 1.16011000 |
| H | -5.18950600 | -0.22408300 | 1.35676900 |
| H | -4.96392900 | -1.16681100 | -0.14762200 |

d1...(2 ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | 1.39496500 | -0.74192500 | 0.52001000 |
| C | 1.90899100 | -0.13728600 | 1.64094200 |
| C | 3.31428300 | -0.06812200 | 1.43909700 |
| C | 3.55505400 | -0.63394000 | 0.21157400 |
| O | 2.37995400 | -1.04263100 | -0.34266200 |
| H | 1.32912300 | 0.20883900 | 2.49126600 |
| H | 4.06882400 | 0.34605500 | 2.10507400 |
| C | 4.78667200 | -0.83210000 | -0.52531400 |
| H | 5.69084500 | -0.46190700 | 0.00578100 |
| O | 4.85718400 | -1.35097800 | -1.62096600 |
| C | -0.01923700 | -1.06495000 | 0.14171900 |
| H | -0.12707200 | -0.78089800 | -0.93266500 |
| H | -0.12058800 | -2.17468700 | 0.14774600 |
| O | -0.91680500 | -0.44159100 | 0.97208700 |

| | | | |
|---|-------------|-------------|-------------|
| H | -2.15161700 | -1.31180300 | 0.89786200 |
| O | -2.95789600 | -1.88979200 | 0.65790400 |
| C | -3.65357000 | -1.17194900 | -0.33116400 |
| H | -2.93544600 | -0.74709100 | -1.06398300 |
| C | -4.57393700 | -2.13241000 | -1.06715300 |
| C | -4.42529500 | -0.00591100 | 0.28033300 |
| H | -5.30468700 | -2.56431000 | -0.36439200 |
| H | -5.12501700 | -1.62780500 | -1.87442600 |
| H | -3.99291800 | -2.95828000 | -1.50370800 |
| H | -3.73217400 | 0.68869600 | 0.77784600 |
| H | -4.97927100 | 0.56014500 | -0.48469400 |
| H | -5.14281200 | -0.38059900 | 1.02820300 |
| H | -1.28754900 | 0.78411300 | 0.21273100 |
| O | -1.46808700 | 1.62926300 | -0.34336400 |
| C | -0.44591200 | 2.54760100 | -0.04378100 |
| H | -0.05624500 | 2.34779800 | 0.97568500 |
| C | 0.71659700 | 2.41383000 | -1.02455700 |
| C | -1.02286400 | 3.95605200 | -0.06402200 |
| H | 0.36369900 | 2.60990700 | -2.05014300 |
| H | 1.52714400 | 3.12248600 | -0.79380900 |
| H | 1.13753300 | 1.39658500 | -1.00052400 |
| H | -1.84380500 | 4.04424300 | 0.66278500 |
| H | -0.25995500 | 4.71100600 | 0.17758600 |
| H | -1.42729300 | 4.18000400 | -1.06430200 |

d1... (3 ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.76095500 | 0.38987100 | -0.76826800 |
| C | -1.93044900 | 1.13663900 | 0.37327600 |
| C | -3.32903600 | 1.14954700 | 0.62780700 |
| C | -3.91085200 | 0.41496900 | -0.37518900 |
| O | -2.95006900 | -0.04310100 | -1.22251700 |
| H | -1.13093800 | 1.59273900 | 0.95240400 |
| H | -3.85565600 | 1.63487500 | 1.44720400 |
| C | -5.29592200 | 0.07718800 | -0.63785900 |
| H | -6.00887900 | 0.49094500 | 0.10839200 |
| O | -5.67235000 | -0.59392400 | -1.57695300 |
| C | -0.53737600 | -0.01162400 | -1.54067600 |
| H | -0.74805700 | -1.02149400 | -1.95539900 |
| H | -0.47536300 | 0.65811100 | -2.42683700 |
| O | 0.60878700 | 0.02319000 | -0.77513700 |
| H | 1.99355000 | -0.20673400 | -1.54598200 |
| O | 2.89556600 | -0.43796700 | -1.91774400 |
| C | 3.44362000 | -1.40673300 | -1.04902500 |
| H | 2.73129100 | -2.24755200 | -0.93077900 |

| | | | |
|---|-------------|-------------|-------------|
| C | 4.71394400 | -1.94344000 | -1.68534200 |
| C | 3.70737400 | -0.82548600 | 0.33619000 |
| H | 5.44117800 | -1.12673400 | -1.81944000 |
| H | 5.17590600 | -2.72156400 | -1.06028900 |
| H | 4.49655600 | -2.37338000 | -2.67438500 |
| H | 2.79990100 | -0.35011100 | 0.73903900 |
| H | 4.02705700 | -1.60842300 | 1.04139700 |
| H | 4.49976300 | -0.06077700 | 0.28472600 |
| H | 0.62216900 | -1.31602700 | 0.03135000 |
| O | 0.57622100 | -2.14832400 | 0.59852100 |
| C | -0.23070100 | -1.84508300 | 1.71428200 |
| H | -0.23710200 | -0.74783400 | 1.87218400 |
| C | -1.66600100 | -2.30652100 | 1.47861100 |
| C | 0.36793100 | -2.49877700 | 2.95108500 |
| H | -1.69180400 | -3.40264800 | 1.36583000 |
| H | -2.32765600 | -2.02761100 | 2.31348200 |
| H | -2.07095000 | -1.86430800 | 0.55488000 |
| H | 1.39042700 | -2.13020800 | 3.12134900 |
| H | -0.23290000 | -2.29071100 | 3.84891000 |
| H | 0.41647500 | -3.59080000 | 2.81203700 |
| H | 0.90442100 | 1.02167400 | 0.41514100 |
| O | 1.14827200 | 1.69312800 | 1.12172200 |
| C | 1.50459400 | 2.87359700 | 0.43259000 |
| H | 0.74988000 | 3.07982300 | -0.35464300 |
| C | 1.49184800 | 4.02573300 | 1.42255500 |
| C | 2.86195400 | 2.71916500 | -0.24298100 |
| H | 2.20174800 | 3.82214200 | 2.24008700 |
| H | 1.78030500 | 4.97060400 | 0.93952600 |
| H | 0.49142400 | 4.15212200 | 1.86288000 |
| H | 2.86156700 | 1.84452400 | -0.91084800 |
| H | 3.11828600 | 3.61134500 | -0.83483700 |
| H | 3.64615800 | 2.56973800 | 0.51712900 |

e1

| | | | |
|---|-------------|-------------|-------------|
| C | 0.81136700 | -1.03342400 | 0.00016600 |
| C | -0.55994200 | -1.28859500 | 0.00002600 |
| C | -1.47158300 | -0.23092000 | -0.00005100 |
| C | -1.00546200 | 1.09291000 | -0.00007800 |
| C | 0.35749300 | 1.34429500 | -0.00006700 |
| C | 1.27837800 | 0.28254100 | 0.00008500 |
| H | 1.52771000 | -1.85433400 | 0.00028100 |
| H | -0.92794500 | -2.31791600 | 0.00002400 |
| H | -1.72893000 | 1.91056800 | -0.00018700 |
| H | 0.72475700 | 2.37368300 | -0.00010800 |

| | | | |
|---|-------------|-------------|-------------|
| C | -2.92233300 | -0.51307500 | -0.00002600 |
| H | -3.19392300 | -1.59349600 | 0.00000600 |
| C | 2.75264300 | 0.59109300 | 0.00023500 |
| H | 2.97737400 | 1.21346200 | -0.88566800 |
| H | 2.97748900 | 1.21238000 | 0.88685300 |
| O | 3.50085400 | -0.59675600 | -0.00039900 |
| H | 4.43699800 | -0.36053700 | 0.00016600 |
| O | -3.78046600 | 0.34016000 | 0.00001000 |

e1...(ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.81364000 | 0.09355800 | -0.73287900 |
| C | 1.92576600 | -0.73343600 | -0.61143900 |
| C | 3.03341300 | -0.31574800 | 0.13406400 |
| C | 3.01855500 | 0.93543700 | 0.76250900 |
| C | 1.90594500 | 1.75950800 | 0.64311300 |
| C | 0.79586900 | 1.34622800 | -0.10569100 |
| H | -0.05486500 | -0.23680900 | -1.30263900 |
| H | 1.94747600 | -1.71272300 | -1.09370000 |
| H | 3.88476900 | 1.25656400 | 1.34643800 |
| H | 1.89193000 | 2.73502400 | 1.13485800 |
| C | 4.22067800 | -1.18739000 | 0.26670600 |
| H | 5.04675400 | -0.76941900 | 0.88628700 |
| C | -0.38205000 | 2.27636000 | -0.23668100 |
| H | -0.67521000 | 2.63206000 | 0.76620300 |
| H | -0.06897700 | 3.16237100 | -0.81633300 |
| O | -1.45218500 | 1.61795400 | -0.87735800 |
| H | -2.17255800 | 2.24879800 | -1.01185700 |
| O | 4.32350900 | -2.27868600 | -0.24540100 |
| H | -1.94499200 | 0.08182500 | 0.00081200 |
| O | -2.29922100 | -0.77566900 | 0.29681400 |
| C | -3.65430600 | -0.81687100 | -0.11274400 |
| H | -3.71573500 | -0.67070700 | -1.20921100 |
| C | -4.19037700 | -2.19627200 | 0.21959800 |
| C | -4.45313500 | 0.28763900 | 0.56594900 |
| H | -4.13814900 | -2.36839300 | 1.30623000 |
| H | -5.23657200 | -2.30196500 | -0.10049000 |
| H | -3.59204800 | -2.97197200 | -0.28017400 |
| H | -4.02238600 | 1.27329200 | 0.33083100 |
| H | -5.50267700 | 0.28497300 | 0.23640200 |
| H | -4.42756800 | 0.15420500 | 1.65886800 |

e1...(2 ⁱPrOH)

| | | | |
|---|------------|-------------|------------|
| C | 0.49059300 | -0.95859200 | 0.87042200 |
| C | 1.47829800 | -1.52579700 | 0.07621400 |

| | | | |
|---|-------------|-------------|-------------|
| C | 2.77800100 | -1.00065300 | 0.09628800 |
| C | 3.07957900 | 0.09207200 | 0.91308400 |
| C | 2.08357400 | 0.66744400 | 1.70007000 |
| C | 0.78639700 | 0.14740800 | 1.68354700 |
| H | -0.52161900 | -1.36951600 | 0.86699800 |
| H | 1.25980600 | -2.38233500 | -0.56470700 |
| H | 4.09486600 | 0.49655900 | 0.92149100 |
| H | 2.31133000 | 1.53390100 | 2.32477900 |
| C | 3.84019600 | -1.59488600 | -0.74568500 |
| H | 4.83921400 | -1.11079700 | -0.65506000 |
| C | -0.29640000 | 0.77173300 | 2.52304000 |
| H | -0.50798100 | 0.13343500 | 3.39840200 |
| H | 0.03727000 | 1.75291700 | 2.89291100 |
| O | -1.47073000 | 0.90941400 | 1.73111000 |
| H | -2.11297200 | 1.45652500 | 2.20810800 |
| O | 3.67207100 | -2.53568600 | -1.48649100 |
| H | -2.45950700 | -0.63910200 | 1.35160200 |
| O | -2.88561800 | -1.42084400 | 0.95902800 |
| C | -3.04680300 | -1.15290800 | -0.42712400 |
| H | -2.05847800 | -0.93851200 | -0.87509300 |
| C | -3.61694500 | -2.40467800 | -1.06552800 |
| C | -3.93605800 | 0.06289000 | -0.64363500 |
| H | -4.59512000 | -2.64397200 | -0.61941600 |
| H | -3.75088500 | -2.26720000 | -2.14775000 |
| H | -2.94628400 | -3.26129900 | -0.90416200 |
| H | -3.50851300 | 0.94951300 | -0.15063600 |
| H | -4.03762900 | 0.29121700 | -1.71503200 |
| H | -4.93894300 | -0.11781500 | -0.22518000 |
| H | -1.13503200 | 1.20013000 | -0.12153100 |
| O | -0.98352300 | 1.33943200 | -1.07274100 |
| C | 0.30421300 | 1.90563800 | -1.24809500 |
| H | 1.07705100 | 1.16957800 | -0.95166300 |
| C | 0.46796900 | 2.20341900 | -2.72640100 |
| C | 0.46611200 | 3.14949500 | -0.38653300 |
| H | -0.29059500 | 2.93232200 | -3.05213700 |
| H | 1.46465000 | 2.61747500 | -2.93505700 |
| H | 0.34146800 | 1.28568200 | -3.31886600 |
| H | 0.28489900 | 2.91111300 | 0.67365500 |
| H | 1.48115100 | 3.56502900 | -0.47419600 |
| H | -0.25809300 | 3.92112300 | -0.69269000 |

f1

| | | | |
|---|-------------|-------------|------------|
| C | -0.85669800 | -1.03399700 | 0.00020800 |
| C | 0.51325900 | -1.28899300 | 0.00025100 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.42296800 | -0.22605300 | 0.00004300 |
| C | 0.94729400 | 1.09792700 | -0.00000900 |
| C | -0.41719600 | 1.34120800 | -0.00002600 |
| C | -1.33731200 | 0.27665400 | 0.00001500 |
| H | -1.60332600 | -1.82959200 | 0.00012000 |
| H | 0.88955200 | -2.31627100 | 0.00011500 |
| H | 1.66883000 | 1.91803400 | -0.00004600 |
| H | -0.78966800 | 2.37065800 | 0.00020600 |
| C | 2.86826800 | -0.50470600 | -0.00010100 |
| H | 3.13795700 | -1.58646800 | -0.00057500 |
| C | -2.85687100 | 0.50300300 | 0.00010400 |
| H | -3.00555700 | 1.21289500 | 0.87755400 |
| H | -3.00512100 | 1.21351200 | -0.87669100 |
| O | -3.60922100 | -0.59004700 | -0.00037600 |
| O | 3.73485400 | 0.34341900 | -0.00007300 |

f1...(^tPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.98168300 | 0.21884500 | -1.01526900 |
| C | -2.22090600 | -0.40525900 | -0.92392800 |
| C | -3.04257400 | -0.16922200 | 0.18619600 |
| C | -2.60960700 | 0.69775800 | 1.19977100 |
| C | -1.37027900 | 1.31860500 | 1.10120900 |
| C | -0.54116700 | 1.08521400 | -0.00630900 |
| H | -0.31781500 | 0.05328600 | -1.86493500 |
| H | -2.57133500 | -1.08270800 | -1.70611900 |
| H | -3.25409800 | 0.87724100 | 2.06477500 |
| H | -1.03171400 | 1.99388000 | 1.89233300 |
| C | -4.35701300 | -0.82650000 | 0.30048700 |
| H | -4.93022400 | -0.57717600 | 1.22350500 |
| C | 0.81213700 | 1.77397000 | -0.13574600 |
| H | 0.57406200 | 2.87075200 | -0.14937400 |
| H | 1.31513400 | 1.63281900 | 0.85649100 |
| O | 1.57271500 | 1.36566300 | -1.18329400 |
| O | -4.81810900 | -1.58706400 | -0.52238800 |
| H | 2.76220900 | 0.93583400 | -0.57943200 |
| O | 3.61183600 | 0.57901100 | -0.05043700 |
| C | 3.58996600 | -0.81673600 | -0.13957600 |
| H | 3.54124000 | -1.13812100 | -1.20443000 |
| C | 4.88285400 | -1.36398700 | 0.44741700 |
| C | 2.36719300 | -1.40121800 | 0.56505300 |
| H | 4.96204200 | -1.07282600 | 1.50742000 |
| H | 4.92998400 | -2.46149600 | 0.38331400 |
| H | 5.75070400 | -0.94537200 | -0.08413200 |
| H | 1.45225700 | -0.97960800 | 0.12251700 |

| | | | |
|---|------------|-------------|------------|
| H | 2.32491500 | -2.49795900 | 0.47542900 |
| H | 2.38757300 | -1.13824400 | 1.63576200 |

f1...(2^i PrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | 0.74925300 | -0.72142200 | -0.45560200 |
| C | 1.92367800 | -1.39403800 | -0.77342300 |
| C | 2.88153800 | -1.64239000 | 0.21851200 |
| C | 2.65049100 | -1.21032300 | 1.53104700 |
| C | 1.47416700 | -0.53837700 | 1.84320100 |
| C | 0.50982600 | -0.28827100 | 0.85617600 |
| H | -0.00071900 | -0.51563500 | -1.22028100 |
| H | 2.11701800 | -1.73490800 | -1.79284600 |
| H | 3.40221200 | -1.40237700 | 2.30145500 |
| H | 1.29487100 | -0.19708600 | 2.86655000 |
| C | 4.13220100 | -2.35391300 | -0.10444600 |
| H | 4.82483500 | -2.50117900 | 0.75637100 |
| C | -0.78620000 | 0.42853000 | 1.21116400 |
| H | -1.36190600 | -0.28835700 | 1.84569300 |
| H | -0.50998300 | 1.25222100 | 1.91054000 |
| O | -1.51947700 | 0.86642500 | 0.13840200 |
| O | 4.42393600 | -2.76536300 | -1.20577800 |
| H | -2.19253800 | -0.38272500 | -0.36912800 |
| O | -2.63057400 | -1.27447800 | -0.62173400 |
| C | -4.02114200 | -1.11724800 | -0.49680700 |
| H | -4.38808800 | -0.35176100 | -1.21432100 |
| C | -4.68561300 | -2.43865000 | -0.84682700 |
| C | -4.39468900 | -0.65031100 | 0.90674600 |
| H | -4.35638100 | -3.22002000 | -0.14329700 |
| H | -5.78223500 | -2.36529900 | -0.80040300 |
| H | -4.40038100 | -2.75319000 | -1.86194300 |
| H | -3.87423000 | 0.29188500 | 1.13372100 |
| H | -5.47827000 | -0.48406100 | 1.00641600 |
| H | -4.08765700 | -1.40550900 | 1.64858000 |
| H | -0.59711300 | 1.72924100 | -0.73688400 |
| O | 0.07807300 | 2.30774500 | -1.23565700 |
| C | 0.74396300 | 3.07524500 | -0.26507600 |
| H | 1.24401700 | 2.40932300 | 0.47234000 |
| C | 1.82167700 | 3.89361100 | -0.95666700 |
| C | -0.24053200 | 3.95886200 | 0.49524000 |
| H | 1.36260400 | 4.56383100 | -1.70115800 |
| H | 2.38756600 | 4.50524600 | -0.23855900 |
| H | 2.52618700 | 3.23218400 | -1.48257900 |
| H | -1.04251300 | 3.33788300 | 0.92239500 |
| H | 0.24952600 | 4.51416300 | 1.30960900 |

| | | | |
|---|-------------|------------|-------------|
| H | -0.70420000 | 4.68367900 | -0.19355400 |
|---|-------------|------------|-------------|

f1... (3 ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -2.13022800 | -0.01271300 | -0.47738700 |
| C | -3.51290100 | -0.07521600 | -0.61383400 |
| C | -4.32829700 | -0.15094900 | 0.52199000 |
| C | -3.74488000 | -0.16379200 | 1.79604700 |
| C | -2.36306300 | -0.10108000 | 1.92677800 |
| C | -1.54039100 | -0.02414400 | 0.79358600 |
| H | -1.48865100 | 0.04734700 | -1.35759100 |
| H | -3.97982200 | -0.06628000 | -1.60100000 |
| H | -4.38430400 | -0.22371900 | 2.68078600 |
| H | -1.90690500 | -0.11106100 | 2.92036300 |
| C | -5.79649800 | -0.21804800 | 0.39102300 |
| H | -6.35265100 | -0.27689900 | 1.35515700 |
| C | -0.03156900 | 0.05401100 | 0.96078700 |
| H | 0.16489300 | 0.95933800 | 1.57904800 |
| H | 0.26026600 | -0.80142700 | 1.61078700 |
| O | 0.66870000 | 0.07387900 | -0.22634100 |
| O | -6.39228000 | -0.21310800 | -0.66338500 |
| H | 0.29755400 | 1.45890000 | -0.89427600 |
| O | 0.05620300 | 2.37097000 | -1.24228300 |
| C | 1.18454200 | 3.20012000 | -1.08634300 |
| H | 2.06409100 | 2.74508500 | -1.58792300 |
| C | 0.88714400 | 4.52883100 | -1.76045900 |
| C | 1.53482300 | 3.37527100 | 0.38715400 |
| H | 0.02310700 | 5.01036300 | -1.27495000 |
| H | 1.74618200 | 5.21272900 | -1.70051200 |
| H | 0.63901900 | 4.37193200 | -2.82064800 |
| H | 1.78438400 | 2.40097600 | 0.83255900 |
| H | 2.40275700 | 4.03973100 | 0.51959200 |
| H | 0.67689100 | 3.80477700 | 0.92929200 |
| H | 0.35989600 | -1.34141900 | -0.86409100 |
| O | 0.14215400 | -2.28902200 | -1.12109800 |
| C | 1.23622600 | -3.08538600 | -0.73194800 |
| H | 1.43763600 | -2.94907600 | 0.35215200 |
| C | 0.86585600 | -4.54096200 | -0.96170300 |
| C | 2.49812100 | -2.69597800 | -1.49602100 |
| H | 0.66251100 | -4.70965300 | -2.03141500 |
| H | 1.67612200 | -5.21636100 | -0.65060900 |
| H | -0.04201800 | -4.80124700 | -0.39766100 |
| H | 2.73879900 | -1.63569700 | -1.32417300 |
| H | 3.36240400 | -3.30262200 | -1.18300100 |
| H | 2.34081700 | -2.84448700 | -2.57661900 |

| | | | |
|---|------------|-------------|-------------|
| H | 2.21484800 | 0.31533900 | -0.11900100 |
| O | 3.21820400 | 0.41565000 | -0.07519400 |
| C | 3.66925600 | -0.34861500 | 1.01944500 |
| H | 3.11573300 | -1.31048100 | 1.05322700 |
| C | 5.14362000 | -0.65531400 | 0.81266100 |
| C | 3.42676100 | 0.38252400 | 2.33589700 |
| H | 5.71135100 | 0.28536300 | 0.73187300 |
| H | 5.55477000 | -1.23898000 | 1.64922000 |
| H | 5.29346000 | -1.22439600 | -0.11698500 |
| H | 2.35637100 | 0.60455900 | 2.46541600 |
| H | 3.75730100 | -0.21749700 | 3.19758200 |
| H | 3.97819800 | 1.33654000 | 2.34376700 |

g1

| | | | |
|---|-------------|-------------|-------------|
| C | -1.21529500 | 1.18506500 | -0.00006000 |
| C | 0.16557900 | 1.33744600 | -0.00004500 |
| C | 1.00476300 | 0.21725200 | -0.00002700 |
| C | 0.44098800 | -1.06904200 | -0.00007300 |
| C | -0.93336100 | -1.23302500 | -0.00006900 |
| C | -1.76944300 | -0.10249300 | 0.00001600 |
| H | -1.87731600 | 2.05385800 | -0.00010200 |
| H | 0.60223400 | 2.33952500 | -0.00005800 |
| H | 1.10320400 | -1.93727100 | -0.00011500 |
| H | -1.39042300 | -2.22368000 | -0.00008500 |
| C | 2.46581000 | 0.39534000 | 0.00004600 |
| H | 2.81027200 | 1.45511200 | -0.00006600 |
| O | 3.26709900 | -0.51370400 | 0.00009100 |
| O | -3.09599500 | -0.31176900 | 0.00005500 |
| H | -3.57105400 | 0.53297700 | 0.00053600 |

g1...(ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.35101800 | -0.29975100 | -0.73857900 |
| C | -1.54071700 | -0.99750000 | -0.58176200 |
| C | -2.66630600 | -0.37299500 | -0.02873000 |
| C | -2.58776100 | 0.96934400 | 0.36845200 |
| C | -1.40573700 | 1.67834200 | 0.21731200 |
| C | -0.28530700 | 1.04179500 | -0.33812200 |
| H | 0.53961200 | -0.76495300 | -1.16434400 |
| H | -1.60226900 | -2.04411800 | -0.89098000 |
| H | -3.46954900 | 1.44886800 | 0.79813500 |
| H | -1.33327500 | 2.72443700 | 0.52299200 |
| C | -3.92155100 | -1.12782100 | 0.13059200 |
| H | -3.88222000 | -2.18515700 | -0.21849200 |
| O | -4.94015600 | -0.67040400 | 0.60033700 |

| | | | |
|---|------------|-------------|-------------|
| O | 0.88838700 | 1.68515300 | -0.51132300 |
| H | 0.83954100 | 2.60080000 | -0.19579100 |
| H | 2.40012900 | 0.58074600 | -1.12271200 |
| O | 2.92625800 | -0.23091200 | -1.06002800 |
| C | 3.13463100 | -0.47664900 | 0.32264100 |
| H | 2.15387900 | -0.54712700 | 0.83375700 |
| C | 3.84036300 | -1.81383700 | 0.44046500 |
| C | 3.93158600 | 0.65526300 | 0.95383800 |
| H | 4.80866300 | -1.77481200 | -0.08260500 |
| H | 4.02252200 | -2.06999400 | 1.49365200 |
| H | 3.23579400 | -2.61270500 | -0.01306900 |
| H | 3.39506700 | 1.61033700 | 0.84575300 |
| H | 4.09644300 | 0.47591500 | 2.02642300 |
| H | 4.91065500 | 0.74992000 | 0.45875800 |

g1... (2 ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.47961500 | -0.79089400 | -0.40022800 |
| C | -1.64419600 | -1.08681200 | -1.09607300 |
| C | -2.87506700 | -1.15079600 | -0.43017700 |
| C | -2.93093000 | -0.91955100 | 0.95133300 |
| C | -1.77520400 | -0.62159300 | 1.65772000 |
| C | -0.55388400 | -0.55218400 | 0.97573700 |
| H | 0.49055800 | -0.74291400 | -0.89579000 |
| H | -1.60254400 | -1.27476400 | -2.17187900 |
| H | -3.89426800 | -0.97451300 | 1.46205600 |
| H | -1.80164800 | -0.43061700 | 2.73287900 |
| C | -4.10266100 | -1.46596400 | -1.18409200 |
| H | -3.95523800 | -1.63869700 | -2.27473000 |
| O | -5.20565700 | -1.54092400 | -0.68993000 |
| O | 0.60006900 | -0.22800400 | 1.61238800 |
| H | 0.46823000 | -0.16164400 | 2.57222000 |
| H | 2.11668800 | -1.17884000 | 0.79803300 |
| O | 2.67463500 | -1.79207600 | 0.29642300 |
| C | 3.93585600 | -1.18052200 | 0.07530000 |
| H | 4.33674200 | -0.80483100 | 1.03593600 |
| C | 4.86860300 | -2.25744800 | -0.44626600 |
| C | 3.81544000 | -0.01154200 | -0.89152600 |
| H | 4.48317100 | -2.66104300 | -1.39570800 |
| H | 5.87583200 | -1.85424800 | -0.62242400 |
| H | 4.94386900 | -3.08448800 | 0.27448300 |
| H | 3.10257000 | 0.74021700 | -0.52093800 |
| H | 4.78780100 | 0.48296500 | -1.03609000 |
| H | 3.45876900 | -0.36764700 | -1.87139700 |
| H | 1.05666700 | 1.47837300 | 0.66276100 |

| | | | |
|---|-------------|------------|-------------|
| O | 1.05138400 | 2.03801200 | -0.12826100 |
| C | 0.29875400 | 3.21049300 | 0.14162800 |
| H | 0.84424400 | 3.84010500 | 0.87067500 |
| C | 0.18234200 | 3.97315400 | -1.16369800 |
| C | -1.05939500 | 2.85852500 | 0.72849300 |
| H | -0.36341700 | 3.36853900 | -1.90468600 |
| H | -0.35550900 | 4.92052900 | -1.01851700 |
| H | 1.17996100 | 4.19753200 | -1.56833700 |
| H | -0.94266200 | 2.30029900 | 1.67093500 |
| H | -1.64213700 | 3.76645200 | 0.94348700 |
| H | -1.63139600 | 2.23397400 | 0.02315100 |

h1

| | | | |
|---|-------------|-------------|-------------|
| C | 1.25867500 | 1.19914700 | 0.00013600 |
| C | -0.11022800 | 1.33864600 | 0.00019900 |
| C | -0.96899500 | 0.21448500 | 0.00001000 |
| C | -0.37705000 | -1.07353100 | 0.00038500 |
| C | 0.98674100 | -1.23278800 | 0.00019100 |
| C | 1.89882500 | -0.10180400 | -0.00043200 |
| H | 1.91320600 | 2.07480400 | 0.00034700 |
| H | -0.55592800 | 2.33939700 | 0.00031000 |
| H | -1.03696900 | -1.94603800 | 0.00058400 |
| H | 1.43654700 | -2.22944800 | 0.00032100 |
| C | -2.40213500 | 0.38429200 | -0.00010100 |
| H | -2.74033400 | 1.44977800 | 0.00006900 |
| O | -3.23525000 | -0.51305400 | -0.00028600 |
| O | 3.14381000 | -0.24434300 | -0.00020700 |

h1...(ⁱPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -0.38683600 | -0.47687800 | -0.64084700 |
| C | -1.60628800 | -1.08880000 | -0.43806800 |
| C | -2.72885500 | -0.36200800 | 0.01003800 |
| C | -2.57716700 | 1.02261800 | 0.25093200 |
| C | -1.36793800 | 1.64972100 | 0.05522100 |
| C | -0.20609600 | 0.93109700 | -0.40373900 |
| H | 0.47808400 | -1.04358700 | -0.99286900 |
| H | -1.71388800 | -2.16165500 | -0.62892400 |
| H | -3.44611600 | 1.58840500 | 0.59802600 |
| H | -1.25088200 | 2.72014400 | 0.24145700 |
| C | -4.00127300 | -1.02728300 | 0.21248400 |
| H | -3.99304000 | -2.12153400 | -0.01202600 |
| O | -5.03244000 | -0.49563600 | 0.59377300 |
| O | 0.90750300 | 1.51882700 | -0.58804700 |
| H | 2.11869200 | 0.50243600 | -0.94215300 |

| | | | |
|---|------------|-------------|-------------|
| O | 2.84809500 | -0.17864000 | -0.99084000 |
| C | 3.23060600 | -0.42622400 | 0.34437500 |
| H | 2.33975100 | -0.71392700 | 0.94128800 |
| C | 4.20261700 | -1.59291000 | 0.34705800 |
| C | 3.83580000 | 0.82271600 | 0.97463900 |
| H | 5.09347100 | -1.34003800 | -0.24971300 |
| H | 4.52584800 | -1.84163900 | 1.36830800 |
| H | 3.73640100 | -2.48486200 | -0.09715900 |
| H | 3.10925600 | 1.64806400 | 0.93837000 |
| H | 4.11358500 | 0.65080900 | 2.02556400 |
| H | 4.73615100 | 1.12867600 | 0.41818300 |

h1...(2^i PrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.42170500 | -1.49459600 | 0.02169200 |
| C | -2.76807400 | -1.53965400 | 0.32701700 |
| C | -3.60547500 | -0.43048100 | 0.09940600 |
| C | -3.03974400 | 0.74040700 | -0.44853800 |
| C | -1.69814300 | 0.80207600 | -0.75930700 |
| C | -0.83204200 | -0.31953800 | -0.54115500 |
| H | -0.76841800 | -2.35075300 | 0.20374800 |
| H | -3.19906700 | -2.45028900 | 0.75500800 |
| H | -3.68895200 | 1.60229300 | -0.62409500 |
| H | -1.25834400 | 1.70868800 | -1.18228800 |
| C | -5.02141500 | -0.50285100 | 0.42493000 |
| H | -5.34949100 | -1.47933000 | 0.85549900 |
| O | -5.83329700 | 0.39222600 | 0.26435400 |
| O | 0.41738200 | -0.26981000 | -0.83706900 |
| H | 1.26273700 | -1.68197100 | -0.70512900 |
| O | 1.84917800 | -2.44182400 | -0.45578400 |
| C | 2.89643400 | -1.87446600 | 0.30213700 |
| H | 2.47428100 | -1.28485700 | 1.14176100 |
| C | 3.72276200 | -3.00825000 | 0.88282100 |
| C | 3.73748500 | -0.93988700 | -0.56084300 |
| H | 4.16164300 | -3.60804700 | 0.06969500 |
| H | 4.53889300 | -2.62602600 | 1.51278900 |
| H | 3.09162100 | -3.67004400 | 1.49423900 |
| H | 3.12095500 | -0.11884100 | -0.95840700 |
| H | 4.56786100 | -0.49928800 | 0.01222100 |
| H | 4.15888700 | -1.49854000 | -1.41202100 |
| H | 1.16350000 | 1.18446400 | -0.99378500 |
| O | 1.67187400 | 2.03710500 | -0.99467800 |
| C | 2.06406600 | 2.29985500 | 0.33619800 |
| H | 2.66106600 | 1.44917000 | 0.72409100 |
| C | 2.95150000 | 3.53195800 | 0.32066800 |

| | | | |
|---|------------|------------|-------------|
| C | 0.85698500 | 2.47974100 | 1.24884600 |
| H | 2.38801100 | 4.39572600 | -0.06661100 |
| H | 3.31407000 | 3.77553300 | 1.32969400 |
| H | 3.82133300 | 3.36956500 | -0.33292100 |
| H | 0.24189400 | 1.56696000 | 1.26173000 |
| H | 1.16943900 | 2.69342700 | 2.28228100 |
| H | 0.23119100 | 3.31469900 | 0.89469000 |

h1... (3 ^tPrOH)

| | | | |
|---|-------------|-------------|-------------|
| C | -1.97534100 | -1.08132900 | -1.05975000 |
| C | -3.35318800 | -1.18561600 | -0.99001100 |
| C | -4.12739900 | -0.17564300 | -0.39229100 |
| C | -3.47438100 | 0.95684100 | 0.13359200 |
| C | -2.10042800 | 1.07361100 | 0.07146900 |
| C | -1.29888500 | 0.05224700 | -0.52364400 |
| H | -1.37707400 | -1.86307800 | -1.53362000 |
| H | -3.85520100 | -2.06418000 | -1.40665100 |
| H | -4.07795600 | 1.74462300 | 0.59142400 |
| H | -1.59225500 | 1.95494300 | 0.46953700 |
| C | -5.57905000 | -0.30539600 | -0.32909100 |
| H | -5.98351600 | -1.24195400 | -0.78172000 |
| O | -6.33733200 | 0.50892400 | 0.16458800 |
| O | -0.00796500 | 0.16168900 | -0.57848400 |
| H | 0.96385000 | -1.06452200 | -1.21947400 |
| O | 1.62619400 | -1.74233400 | -1.49459500 |
| C | 2.90672900 | -1.14806100 | -1.39975800 |
| H | 3.11456700 | -0.88464500 | -0.34336800 |
| C | 3.92595000 | -2.17986000 | -1.84844200 |
| C | 2.97980600 | 0.12644200 | -2.23159000 |
| H | 3.73682100 | -2.46294000 | -2.89615100 |
| H | 4.94994300 | -1.78676400 | -1.77174800 |
| H | 3.85533800 | -3.08829500 | -1.23164900 |
| H | 2.22440900 | 0.85489400 | -1.89975400 |
| H | 3.96970900 | 0.60070500 | -2.14491800 |
| H | 2.79362100 | -0.10337100 | -3.29317100 |
| H | 0.54387400 | 1.74341200 | -0.66776700 |
| O | 0.96966300 | 2.63468400 | -0.68811400 |
| C | 1.92253400 | 2.65431500 | 0.35680000 |
| H | 2.51320300 | 1.71647900 | 0.33556100 |
| C | 2.86044800 | 3.82173700 | 0.10605900 |
| C | 1.23898200 | 2.74822200 | 1.71541000 |
| H | 2.28969000 | 4.76402900 | 0.09076300 |
| H | 3.62820000 | 3.89174600 | 0.88995800 |
| H | 3.36386900 | 3.71022100 | -0.86589800 |

| | | | |
|---|-------------|-------------|------------|
| H | 0.56668900 | 1.89086000 | 1.86516900 |
| H | 1.97634400 | 2.74400200 | 2.53268100 |
| H | 0.64880100 | 3.67667400 | 1.77890400 |
| H | 0.98931700 | -0.27713700 | 0.81996800 |
| O | 1.51418000 | -0.47742800 | 1.62345900 |
| C | 1.50139800 | -1.87416600 | 1.85462000 |
| H | 2.23654200 | -2.36610600 | 1.18602000 |
| C | 1.93000000 | -2.10127400 | 3.29300600 |
| C | 0.13154900 | -2.46296500 | 1.55606500 |
| H | 1.20143300 | -1.64375300 | 3.98085700 |
| H | 2.00132500 | -3.17483700 | 3.51915700 |
| H | 2.91240000 | -1.64187200 | 3.47722700 |
| H | -0.10903400 | -2.32797500 | 0.49205600 |
| H | 0.10717000 | -3.54015300 | 1.77865000 |
| H | -0.64234100 | -1.95991100 | 2.15846500 |