Fig. 4a

C 9.943537000 9.957975000 12.674605000

C 11.017279000 9.997738000 13.775253000

C 9.577023000 12.294149000 11.985680000

C 10.311201000 10.780675000 14.882375000

C 9.868038000 13.389927000 11.254988000

C 8.873887000 10.260009000 14.736487000

C 10.683131000 13.297713000 9.984061000

C 7.793512000 11.173267000 15.273541000

C 11.407230000 11.974770000 9.939947000

C 11.083445000 10.951383000 10.735717000

C 9.372032000 14.725927000 11.636294000

N 10.076737000 11.045427000 11.704266000

N 8.701091000 14.860071000 12.826333000

O 11.261804000 8.708198000 14.311599000

O 10.882733000 10.593961000 16.146523000

O 8.700675000 10.056414000 13.329365000

O 7.966917000 12.492011000 14.774293000

O 9.541861000 15.699111000 10.899439000

H 9.997583000 9.015383000 12.119173000

H 11.944460000 10.458981000 13.430770000

H 8.901557000 12.320183000 12.832541000

H 10.332603000 11.850424000 14.661930000

H 8.786944000 9.295672000 15.255921000

H 10.035774000 13.411139000 9.099764000

H 7.861380000 11.162451000 16.369993000

H 6.814810000 10.773424000 14.984393000

H 12.201046000 11.834851000 9.213210000

H 11.585328000 9.990350000 10.682681000

H 8.830823000 14.191235000 13.573254000

H 12.027921000 8.328039000 13.866577000

H 11.199764000 9.675535000 16.146920000

H 11.389313000 14.133370000 9.921697000

C 11.966506000 15.365789000 13.725290000

C 12.018227000 14.294379000 14.617537000

C 12.679169000 13.107263000 14.286809000

C 13.260957000 13.035603000 13.034519000

C 13.220029000 14.112905000 12.149441000

C 12.580077000 15.293472000 12.471264000

C 14.000501000 11.917608000 12.392946000

N 14.474051000 12.466692000 11.198321000

C 13.940773000 13.738750000 10.904898000

O 14.076910000 14.321371000 9.861047000

O 14.207978000 10.786255000 12.767958000

O 14.967378000 11.680685000 10.195694000

C 16.349716000 11.536038000 10.172481000

O 16.786020000 10.902206000 9.255700000

C 17.158981000 12.157875000 11.289915000

C 17.113191000 13.674123000 11.307411000

C 16.728201000 14.359645000 12.460730000

C 16.661462000 15.749850000 12.467190000

C 16.983943000 16.468889000 11.318879000

C 17.378201000 15.791104000 10.168008000

C 17.443294000 14.400800000 10.162481000

H 11.437790000 16.269661000 14.008033000

H 11.535122000 14.381842000 15.585282000

H 12.719610000 12.275508000 14.983559000

H 12.537631000 16.119509000 11.770805000

H 18.179761000 11.801215000 11.132826000

H 16.810321000 11.751697000 12.244838000

H 16.465442000 13.802696000 13.356788000

H 16.352073000 16.269217000 13.368945000

H 16.927098000 17.553016000 11.320555000

H 17.630639000 16.344781000 9.269025000

H 17.744221000 13.877286000 9.258489000

H 8.535055000 15.813359000 13.114699000

H 7.132388000 12.964675000 14.876906000

Supplementary Fig. 20d

C 13.860872000 8.970961000 9.229587000

H 13.312802000 9.733523000 8.656121000

H 13.951897000 9.324595000 10.266759000

O 15.109361000 8.662392000 8.650209000

H 15.665315000 9.452824000 8.719560000

C 20.776570000 13.651907000 11.753739000

H 21.440757000 14.515603000 11.669020000

H 20.115914000 13.641868000 10.880314000

C 19.929617000 13.707298000 13.000230000

O 19.582394000 12.672369000 13.585525000

N 19.578593000 14.932033000 13.436437000

H 18.856053000 15.000102000 14.142493000

H 19.708168000 15.739080000 12.845000000

C 14.556749000 10.781340000 15.671063000

C 15.693506000 10.393794000 14.966255000

H 15.704185000 9.451351000 14.426749000

C 16.822068000 11.207132000 14.933074000

H 17.709738000 10.900766000 14.386245000

C 16.815968000 12.436292000 15.605867000

O 17.885133000 13.265474000 15.594427000

H 18.550663000 12.934408000 14.941928000

C 15.677458000 12.829412000 16.315644000

H 15.683709000 13.784221000 16.832784000

C 14.560130000 11.999520000 16.348071000

H 13.676305000 12.309767000 16.898864000

C 10.041207000 9.958729000 12.897891000

C 11.140360000 10.141437000 13.961105000

C 9.532865000 12.211956000 12.035357000

C 10.416069000 10.956722000 15.032670000

C 9.734713000 13.253779000 11.202462000

C 9.005827000 10.352814000 14.962303000

C 10.509402000 13.099801000 9.912196000

C 7.894638000 11.250022000 15.461940000

C 11.261283000 11.792371000 9.920746000

C 11.023826000 10.826466000 10.813382000

C 9.171452000 14.588382000 11.484575000

N 10.085122000 10.968945000 11.840215000

N 8.533720000 14.789304000 12.682952000

O 11.477867000 8.910778000 14.581940000

O 11.022232000 10.896811000 16.294217000

O 8.810710000 10.042165000 13.578480000

O 7.993136000 12.533197000 14.860573000

O 9.256231000 15.498029000 10.657932000

H 10.134534000 8.979393000 12.415914000

H 12.029965000 10.625002000 13.552518000

H 8.889672000 12.277916000 12.904883000

H 10.366995000 12.008320000 14.742057000

H 8.979369000 9.424983000 15.550262000

H 9.831354000 13.147572000 9.045521000

H 7.991091000 11.323198000 16.553865000

H 6.929351000 10.784147000 15.229812000

H 12.005305000 11.613976000 9.150937000

H 11.550271000 9.877724000 10.799345000

H 8.722395000 14.194934000 13.478123000

H 12.214540000 8.514021000 14.101957000

H 11.346478000 9.985807000 16.382819000

H 11.193348000 13.946371000 9.774857000

C 11.819703000 15.676817000 13.294977000

C 11.855660000 14.627633000 14.213293000

C 12.491966000 13.421551000 13.907756000

C 13.066625000 13.305860000 12.656985000

C 13.068303000 14.371448000 11.756767000

C 12.444817000 15.568056000 12.049167000

C 13.797258000 12.167234000 12.047058000

N 14.343394000 12.709325000 10.881111000

C 13.862553000 13.992211000 10.558095000

O 14.093543000 14.585506000 9.536985000

O 13.964098000 11.027149000 12.416524000

O 14.980115000 11.936303000 9.955201000

C 16.302801000 11.642683000 10.233995000

O 16.829990000 10.883769000 9.464273000

C 16.955506000 12.228504000 11.463923000

C 16.905323000 13.737172000 11.587044000

C 16.347337000 14.333768000 12.719285000

C 16.307493000 15.718803000 12.841656000

C 16.837661000 16.524077000 11.835608000

C 17.400963000 15.935826000 10.705602000

C 17.431256000 14.548871000 10.580936000

H 11.306570000 16.596136000 13.555228000

H 11.383602000 14.749248000 15.182723000

H 12.553931000 12.617943000 14.632767000

H 12.438442000 16.386693000 11.338374000

H 17.988632000 11.873285000 11.440050000

H 16.487253000 11.761989000 12.338745000

H 15.927433000 13.712052000 13.505332000

H 15.858523000 16.166043000 13.723454000

H 16.806217000 17.605437000 11.928535000

H 17.809993000 16.555986000 9.913917000

H 17.860860000 14.096977000 9.689632000

H 8.321835000 15.753610000 12.895578000

H 7.183558000 13.020289000 15.058234000

H 13.263014000 8.054980000 9.229585000

H 21.361473000 12.731541000 11.756867000

H 13.672574000 10.152012000 15.680084000

Supplementary Fig. 27-RC

C -2.457435000 -1.288318000 0.165149000

C -1.622238000 -0.795693000 1.153793000

C -1.173128000 0.555725000 1.131250000

C -1.619599000 1.375232000 0.054495000

C -2.455194000 0.872151000 -0.928009000

C -2.881113000 -0.462312000 -0.883878000

H -2.782347000 -2.324058000 0.201878000

H -1.285371000 -1.443363000 1.957627000

H -1.276914000 2.404608000 0.008310000

H -2.779912000 1.515926000 -1.740456000

H -3.534997000 -0.852866000 -1.657144000

C -0.306663000 1.055163000 2.116368000

H 0.053479000 2.076809000 2.079451000

H 0.048062000 0.424591000 2.923433000

C 1.920623000 2.165295000 -0.792804000

H 2.526036000 2.797748000 -0.152796000

H 1.378096000 2.641535000 -1.601906000

C 1.848096000 0.778235000 -0.587354000

C 1.044085000 -0.051995000 -1.420618000

C 2.548048000 0.150031000 0.483308000

C 0.941071000 -1.411905000 -1.187054000

H 0.489041000 0.404676000 -2.233410000

C 2.439605000 -1.212151000 0.705463000

H 3.164420000 0.762903000 1.134683000

C 1.635311000 -2.004545000 -0.124228000

H 0.305653000 -2.019194000 -1.823676000

H 2.978873000 -1.667998000 1.530714000

H 1.547068000 -3.070802000 0.058003000

Supplementary Fig. 27-IC

C 2.104355000 -1.509455000 -0.971608000

C 1.284002000 -0.393267000 -1.140846000

C 1.492199000 0.772234000 -0.392191000

C 2.544052000 0.790938000 0.533749000

C 3.366959000 -0.322291000 0.707014000

C 3.148705000 -1.478099000 -0.046014000

H 1.926213000 -2.403793000 -1.561726000

H 0.467201000 -0.425708000 -1.856122000

H 2.718686000 1.688469000 1.122068000

H 4.179812000 -0.286766000 1.426769000

H 3.788830000 -2.345346000 0.086060000

C 0.569079000 1.958764000 -0.526784000

H 1.139424000 2.887573000 -0.414497000

H 0.122417000 1.971246000 -1.526719000

C -0.568942000 1.958715000 0.526886000

H -1.139295000 2.887533000 0.414695000

H -0.122293000 1.971069000 1.526822000

C -1.492110000 0.772231000 0.392210000

C -1.284147000 -0.393238000 1.140953000

C -2.543848000 0.790982000 -0.533879000

C -2.104612000 -1.509354000 0.971692000

H -0.467439000 -0.425741000 1.856336000

C -3.366852000 -0.322156000 -0.707176000

H -2.718297000 1.688494000 -1.122285000

C -3.148833000 -1.477945000 0.045971000

H -1.926628000 -2.403663000 1.561901000

H -4.179606000 -0.286601000 -1.427041000

H -3.789061000 -2.345113000 -0.086123000

Supplementary Fig. 28-RC

O -2.312670000 -0.354615000 1.706647000

O -4.000564000 -1.570939000 -0.126000000

O -1.279607000 -2.239465000 -1.145178000

O 4.227565000 0.594481000 -0.707167000

N 0.297427000 -1.664169000 0.522072000

N 3.088484000 -0.376556000 -2.420254000

C -1.136094000 -1.858835000 0.195818000

C -1.908207000 -0.535207000 0.369161000

C 1.137429000 -1.137894000 -0.424688000

C -3.017631000 -0.699327000 -0.673453000

C 2.430347000 -0.830466000 -0.126554000

C -2.224709000 -1.341942000 -1.803323000

C 2.978359000 -1.054801000 1.240814000

C 1.974107000 -1.568595000 2.198811000

C 0.698473000 -1.848431000 1.821194000

C 3.324837000 -0.152848000 -1.113777000

C 1.610238000 2.143366000 1.373535000

C 0.413703000 2.344455000 0.664613000

C -0.806705000 2.655081000 1.339636000

C -1.978512000 2.877857000 0.630305000

C -1.989774000 2.791041000 -0.771580000

C -0.806447000 2.475456000 -1.456219000

C 0.373465000 2.255472000 -0.759907000

H -1.502864000 -2.634206000 0.872205000

H -1.260787000 0.279391000 0.040891000

H 0.685827000 -0.976424000 -1.393424000

H -3.448421000 0.263520000 -0.968383000

H -2.839326000 -1.947189000 -2.472126000

H 3.837591000 -1.749811000 1.195187000

H 2.265760000 -1.735805000 3.229047000

H -0.053878000 -2.230139000 2.498676000

H 2.455896000 -1.097575000 -2.741253000

H -2.197816000 0.589766000 1.909460000

H -4.667649000 -1.723493000 -0.816052000

H 3.700786000 0.057844000 -3.100336000

H 1.633125000 2.202909000 2.456913000

H 3.434379000 -0.127016000 1.621305000

H 2.539763000 1.947200000 0.850873000

H -0.799206000 2.730741000 2.423780000

H -2.892922000 3.121598000 1.163762000

H -2.909315000 2.965548000 -1.321052000

H -0.812876000 2.402628000 -2.540037000

H 1.287950000 2.015901000 -1.294625000

H -1.672454000 -0.592303000 -2.380275000

Supplementary Fig. 28-TS

O -2.534083000 0.810991000 1.313110000

O -4.439956000 -0.604996000 0.006947000

O -1.991966000 -2.236071000 -0.502675000

O 4.001706000 -0.654433000 -0.927854000

N -0.266110000 -1.458124000 0.907883000

N 2.662174000 -2.061819000 -2.108394000

C -1.701828000 -1.411954000 0.601892000

C -2.148349000 0.020072000 0.212444000

C 0.653472000 -1.516530000 -0.123642000

C -3.287846000 -0.266949000 -0.758365000

C 1.983194000 -1.343210000 0.107798000

C -2.711979000 -1.464739000 -1.504055000

C 2.449036000 -0.964758000 1.441795000

C 1.463823000 -1.050829000 2.498114000

C 0.146482000 -1.245990000 2.218533000

C 2.964444000 -1.333134000 -1.013984000

C 2.562103000 1.808573000 1.017681000

C 1.411885000 2.209498000 0.263754000

C 0.285966000 2.810567000 0.902265000

C -0.806464000 3.223012000 0.161980000

C -0.833092000 3.017477000 -1.230465000

C 0.254786000 2.397841000 -1.876579000

C 1.356525000 1.996414000 -1.147877000

H -2.229465000 -1.754350000 1.496157000

H -1.336220000 0.491625000 -0.350250000

H 0.227688000 -1.699322000 -1.099968000

H -3.480452000 0.581069000 -1.426174000

H -3.482271000 -2.110460000 -1.930855000

H 3.495886000 -1.123861000 1.684606000

H 1.762438000 -0.900707000 3.529474000

H -0.634218000 -1.260036000 2.967089000

H 1.911032000 -2.738559000 -2.112642000

H -1.724359000 1.196597000 1.689049000

H -5.133479000 -0.867824000 -0.620864000

H 3.329539000 -2.083798000 -2.869606000

H 2.646544000 2.207888000 2.028677000

H 2.459431000 0.520061000 1.257121000

H 3.503511000 1.748796000 0.468636000

H 0.315879000 2.962781000 1.977039000

H -1.649435000 3.698117000 0.652465000

H -1.698063000 3.330025000 -1.806407000

H 0.223537000 2.237502000 -2.949482000

H 2.200135000 1.515804000 -1.633270000

H -2.018653000 -1.147821000 -2.291189000

Supplementary Fig. 28-IC

O -2.277756000 -0.357284000 1.754937000

O -4.055709000 -1.451819000 -0.084734000

O -1.371289000 -2.168403000 -1.178852000

O 4.218113000 0.531558000 -0.666484000

N 0.259093000 -1.697802000 0.481680000

N 3.134621000 -0.479404000 -2.394642000

C -1.199969000 -1.839698000 0.169909000

C -1.918480000 -0.502463000 0.399153000

C 1.085415000 -1.162482000 -0.440927000

C -3.055026000 -0.594051000 -0.622608000

C 2.407269000 -0.901623000 -0.121620000

C -2.305516000 -1.224358000 -1.789349000

C 2.859726000 -1.181869000 1.171884000

C 1.988210000 -1.741046000 2.100985000

C 0.677517000 -1.984424000 1.734048000

C 3.336709000 -0.227364000 -1.090396000

C 1.607119000 2.064784000 1.650877000

C 0.434760000 2.319591000 0.738095000

C -0.811894000 2.693264000 1.266815000

C -1.904625000 2.930438000 0.431172000

C -1.772999000 2.791180000 -0.954684000

C -0.539952000 2.420456000 -1.492533000

C 0.553740000 2.191129000 -0.651607000

H -1.568330000 -2.630003000 0.826995000

H -1.250121000 0.300616000 0.081624000

H 0.641898000 -0.947743000 -1.403357000

H -3.460004000 0.390577000 -0.878823000

H -2.951580000 -1.792325000 -2.461051000

H 3.886194000 -0.957053000 1.437088000

H 2.309532000 -1.980247000 3.106904000

H -0.060401000 -2.403727000 2.405284000

H 2.507569000 -1.206282000 -2.714380000

H -2.260021000 0.594915000 1.952148000

H -4.737549000 -1.562418000 -0.768346000

H 3.756579000 -0.053566000 -3.071573000

H 1.808551000 2.935861000 2.285798000

H 1.406835000 1.219106000 2.319212000

H 2.513282000 1.837888000 1.083252000

H -0.921020000 2.805445000 2.343171000

H -2.858992000 3.221696000 0.860708000

H -2.623261000 2.972201000 -1.605356000

H -0.423847000 2.311693000 -2.567218000

H 1.513519000 1.916975000 -1.079543000

H -1.743746000 -0.474378000 -2.356007000

Supplementary Fig. 39a-RC

C 5.561657000 -2.397893000 -3.241571000

H 6.227836000 -2.383189000 -2.365992000

H 5.763123000 -1.502316000 -3.847212000

O 4.193592000 -2.495400000 -2.873067000

H 3.966038000 -1.718895000 -2.323404000

C 4.813046000 4.849708000 -1.045486000

H 4.003256000 5.463987000 -0.629696000

H 5.015828000 5.221009000 -2.055754000

C 4.432644000 3.391061000 -1.055166000

C 4.802353000 2.537707000 -0.010270000

H 5.409509000 2.922856000 0.804565000

C 4.403236000 1.200855000 0.017570000

H 4.701719000 0.558286000 0.840282000

C 3.613549000 0.700326000 -1.017915000

O 3.197593000 -0.614197000 -1.055177000

H 3.257047000 -1.029192000 -0.159483000

C 3.228204000 1.529924000 -2.072586000

H 2.593066000 1.131931000 -2.857206000

C 3.644423000 2.858871000 -2.085128000

H 3.341618000 3.499594000 -2.909533000

C -6.266745000 -1.962243000 -1.399135000

H -6.315948000 -2.806335000 -0.701957000

H -5.392698000 -2.093839000 -2.042619000

C -6.221426000 -0.640796000 -0.672127000

C -5.369180000 0.386537000 -1.101499000

H -4.708877000 0.207100000 -1.944248000

C -5.352537000 1.625022000 -0.452996000

H -4.680815000 2.401071000 -0.806243000

C -6.191098000 1.859176000 0.638768000

H -6.195357000 2.827200000 1.131438000

C -7.042554000 0.839716000 1.082245000

H -7.703050000 1.012608000 1.927170000

C -7.048079000 -0.398597000 0.438653000

H -7.722657000 -1.180186000 0.780454000

C 1.637927000 -3.718913000 0.799347000

C 1.877786000 -2.506255000 1.718743000

C -0.325135000 -2.914405000 -0.426236000

C 1.854755000 -3.186028000 3.097841000

C -0.932093000 -2.362288000 -1.508546000

C 0.722511000 -4.193417000 2.886703000

C -0.208737000 -2.225112000 -2.803980000

C 1.171103000 -2.752195000 -2.762920000

C 1.719789000 -3.252441000 -1.618067000

C -2.335806000 -1.838233000 -1.457451000

N 0.987310000 -3.321871000 -0.467368000

N -2.878420000 -1.672778000 -0.225650000

O 3.056724000 -1.838855000 1.377299000

O 3.113860000 -3.798435000 3.274678000

O 0.781502000 -4.578599000 1.495099000

O -2.925418000 -1.592125000 -2.509651000

H 2.584817000 -4.199133000 0.536667000

H 0.999409000 -1.845748000 1.657035000

H -0.815709000 -3.071650000 0.523000000

H 1.624822000 -2.470235000 3.898932000

H 0.834952000 -5.096313000 3.492556000

H -0.802810000 -2.666458000 -3.621823000

H 1.810873000 -2.695436000 -3.635748000

H 2.756236000 -3.564303000 -1.574601000

H -2.304546000 -1.603514000 0.608116000

H 3.208206000 -1.148955000 2.088079000

H 3.111839000 -4.279453000 4.116986000

H -3.774181000 -1.201356000 -0.180823000

H -0.181216000 -1.149984000 -3.081140000

C 0.253732000 4.216676000 -0.910809000

C 0.465856000 4.113446000 0.474942000

C -0.366967000 4.791461000 1.413897000

C -0.180620000 4.635969000 2.777217000

C 0.848485000 3.813762000 3.264815000

C 1.693299000 3.149996000 2.360336000

C 1.502602000 3.285914000 0.993538000

H 0.887398000 3.684574000 -1.611124000

H -0.533130000 4.845913000 -1.314574000

H -1.159983000 5.435034000 1.041880000

H -0.827720000 5.161194000 3.473909000

H 1.005564000 3.714893000 4.335238000

H 2.499124000 2.518910000 2.724135000

H 2.147549000 2.761401000 0.300976000

C 0.292496000 0.467754000 -0.034730000

C -0.835806000 1.082471000 -0.410973000

C -1.844401000 1.643337000 0.548189000

C -1.093947000 1.204134000 -1.872624000

C -2.670083000 1.781342000 -3.523990000

O -2.303218000 1.730880000 -2.131862000

O -0.323441000 0.852470000 -2.754620000

H -2.806450000 1.137272000 0.437107000

H -1.499978000 1.533737000 1.579005000

H -2.014502000 2.706695000 0.362706000

H -2.731824000 0.767877000 -3.926837000

H -3.645645000 2.266695000 -3.551732000

H -1.938223000 2.361159000 -4.090765000

H 0.545927000 0.366535000 1.014302000

H 0.999313000 0.089805000 -0.762512000

O 0.383965000 0.444360000 3.490418000

H 0.255059000 1.375307000 3.237203000

H -0.375629000 -0.062092000 3.123799000

O 3.042457000 0.019529000 3.229519000

H 3.427855000 -0.136499000 4.104466000

H 2.071003000 0.163325000 3.371399000

O -1.697113000 -1.198744000 2.543542000

H -2.579199000 -0.745073000 2.498280000

H -1.805539000 -1.837233000 3.266606000

O -4.202171000 -0.214606000 2.241201000

H -4.451724000 0.655257000 1.885361000

H -5.003450000 -0.746681000 2.111235000

H 5.803399000 -3.279707000 -3.841644000

H 5.704423000 5.029457000 -0.436086000

H -0.260881000 -3.751317000 3.095007000

H -7.159387000 -2.021363000 -2.034632000

Supplementary Fig. 39a-TS

C 5.225846000 -2.488759000 -3.262127000

H 5.918351000 -2.381756000 -2.413809000

H 5.301827000 -1.587285000 -3.887389000

O 3.892370000 -2.731929000 -2.837432000

H 3.606485000 -1.969426000 -2.296767000

C 5.566707000 4.190211000 -2.027914000

H 4.864779000 4.958802000 -2.371243000

H 6.332444000 4.082944000 -2.806939000

C 4.866584000 2.881617000 -1.760316000

C 5.107518000 2.151634000 -0.592270000

H 5.806910000 2.538295000 0.144431000

C 4.472476000 0.932162000 -0.346628000

H 4.671607000 0.387161000 0.571461000

C 3.569715000 0.431184000 -1.284066000

O 2.902012000 -0.759387000 -1.101527000

H 3.024612000 -1.100033000 -0.178606000

C 3.306546000 1.141146000 -2.457894000

H 2.571682000 0.754917000 -3.156641000

C 3.954104000 2.351581000 -2.685050000

H 3.737416000 2.903160000 -3.596385000

C -6.466516000 -1.943581000 -1.206447000

H -6.484207000 -2.689875000 -0.404287000

H -5.610614000 -2.150124000 -1.854749000

C -6.415280000 -0.538790000 -0.658728000

C -5.609262000 0.437373000 -1.262223000

H -4.991369000 0.160676000 -2.110894000

C -5.584259000 1.748685000 -0.778651000

H -4.947890000 2.482220000 -1.263756000

C -6.369367000 2.109057000 0.318620000

H -6.368464000 3.132310000 0.683002000

C -7.176031000 1.143570000 0.933133000

H -7.795956000 1.414431000 1.783125000

C -7.188532000 -0.167610000 0.454579000

H -7.828113000 -0.908185000 0.929184000

C 1.343117000 -3.594358000 0.974069000

C 1.667840000 -2.303622000 1.753877000

C -0.570042000 -2.788719000 -0.322747000

C 1.530260000 -2.789252000 3.207558000

C -1.151175000 -2.306865000 -1.449255000

C 0.343914000 -3.744949000 3.071256000

C -0.426700000 -2.319729000 -2.749874000

C 0.905895000 -2.952896000 -2.670242000

C 1.430821000 -3.385595000 -1.485501000

C -2.544411000 -1.754354000 -1.440774000

N 0.713682000 -3.286114000 -0.329233000

N -3.034984000 -1.383972000 -0.232630000

O 2.923744000 -1.813012000 1.383993000

O 2.736548000 -3.444982000 3.538420000

O 0.437986000 -4.322224000 1.751762000

O -3.174199000 -1.683152000 -2.495649000

H 2.255194000 -4.160286000 0.765388000

H 0.869568000 -1.568227000 1.567898000

H -1.067992000 -2.835248000 0.634336000

H 1.308189000 -1.958647000 3.890873000

H 0.364976000 -4.561268000 3.797934000

H -1.060595000 -2.761243000 -3.535968000

H 1.537612000 -3.022437000 -3.547868000

H 2.439802000 -3.772638000 -1.415683000

H -2.428828000 -1.206987000 0.561002000

H 3.161123000 -1.101168000 2.051793000

H 2.652345000 -3.820515000 4.428864000

H -3.928986000 -0.907194000 -0.223271000

H -0.310183000 -1.266807000 -3.090225000

C 1.316988000 3.118778000 -0.104162000

C 1.370841000 3.462047000 1.285515000

C 0.282176000 4.101901000 1.927941000

C 0.301482000 4.345482000 3.296221000

C 1.413036000 3.971951000 4.064989000

C 2.503713000 3.351856000 3.444095000

C 2.482346000 3.092057000 2.079329000

H 2.209578000 2.757112000 -0.599098000

H 0.596952000 3.617854000 -0.742995000

H -0.576729000 4.403249000 1.335248000

H -0.542500000 4.839497000 3.769129000

H 1.429487000 4.170354000 5.132244000

H 3.368924000 3.058164000 4.030529000

H 3.318524000 2.588333000 1.607619000

C 0.246049000 1.102186000 -0.112974000

C -1.003043000 1.383458000 -0.606798000

C -2.085557000 1.995051000 0.233583000

C -1.225883000 1.200982000 -2.047006000

C -2.787089000 1.362967000 -3.812658000

O -2.467096000 1.579215000 -2.426708000

O -0.405825000 0.745216000 -2.840333000

H -3.029062000 1.457297000 0.118032000

H -1.800606000 2.003430000 1.289145000

H -2.285891000 3.032085000 -0.067384000

H -2.829209000 0.292158000 -4.023303000

H -3.766975000 1.818002000 -3.960652000

H -2.045096000 1.840488000 -4.456608000

H 0.409626000 1.044389000 0.955955000

H 0.969598000 0.605776000 -0.747801000

O 0.502773000 0.701643000 3.433667000

H 0.382937000 1.665544000 3.472205000

H -0.312570000 0.331400000 3.028855000

O 3.167647000 0.122186000 3.122249000

H 3.462706000 -0.143896000 4.006062000

H 2.223429000 0.401056000 3.224411000

O -1.768551000 -0.669865000 2.468981000

H -2.637866000 -0.199230000 2.386999000

H -1.900377000 -1.250443000 3.235652000

O -4.292838000 0.272780000 2.120917000

H -4.574858000 1.091519000 1.678996000

H -5.081565000 -0.290560000 2.068914000

H 5.543332000 -3.349484000 -3.857590000

H 6.063764000 4.569630000 -1.129794000

H -0.614700000 -3.217078000 3.165830000

H -7.376864000 -2.092222000 -1.800973000

Supplementary Fig. 39b-RC

C -2.608072000 4.106679000 3.137310000

H -3.658167000 4.258120000 2.844320000

H -1.975494000 4.768572000 2.527035000

O -2.211271000 2.746832000 3.036367000

H -2.280719000 2.489459000 2.093715000

C -1.214335000 5.345845000 -4.072651000

H -0.382111000 4.996464000 -4.691478000

H -0.978217000 6.364194000 -3.742699000

C -1.454100000 4.426805000 -2.901312000

C -0.784884000 3.205474000 -2.778018000

H -0.066676000 2.909846000 -3.538774000

C -1.010029000 2.349651000 -1.699245000

H -0.472237000 1.412726000 -1.631157000

C -1.935027000 2.703601000 -0.708606000

O -2.216604000 1.901086000 0.358747000

H -1.705513000 1.042931000 0.290612000

C -2.616290000 3.922957000 -0.814898000

H -3.332895000 4.194793000 -0.045907000

C -2.371359000 4.765676000 -1.895203000

H -2.908383000 5.708594000 -1.959871000

C 7.066052000 -4.129025000 0.070462000

H 6.270982000 -4.856257000 0.269173000

H 7.545603000 -3.884262000 1.023125000

C 6.533980000 -2.896191000 -0.615662000

C 6.999953000 -1.620941000 -0.280517000

H 7.746672000 -1.517159000 0.502588000

C 6.525031000 -0.481960000 -0.937959000

H 6.906982000 0.497038000 -0.662082000

C 5.563740000 -0.598521000 -1.939839000

H 5.172428000 0.275899000 -2.446820000

C 5.095666000 -1.867410000 -2.294529000

H 4.353882000 -1.956905000 -3.082378000

C 5.576456000 -3.002942000 -1.639189000

H 5.227917000 -3.991045000 -1.934912000

C -4.922978000 -2.346138000 0.932390000

C -4.971161000 -1.508342000 -0.363280000

C -2.569906000 -2.584295000 1.632968000

C -5.789487000 -2.466310000 -1.250872000

C -1.442208000 -2.100305000 2.228399000

C -5.144106000 -3.799044000 -0.863670000

C -1.503311000 -0.911243000 3.123812000

C -2.832586000 -0.253950000 3.147994000

C -3.888798000 -0.764179000 2.468043000

C -0.077579000 -2.655485000 1.956543000

N -3.765987000 -1.937358000 1.754505000

N 0.057820000 -3.438227000 0.856369000

O -5.465709000 -0.242794000 -0.125200000

O -7.133638000 -2.376529000 -0.829102000

O -4.798092000 -3.678523000 0.542720000

O 0.854575000 -2.363883000 2.706935000

H -5.820973000 -2.174713000 1.535020000

H -3.947821000 -1.481224000 -0.767463000

H -2.599556000 -3.469107000 1.013710000

H -5.668360000 -2.236053000 -2.317981000

H -5.818916000 -4.652466000 -0.965675000

H -1.176911000 -1.188171000 4.142363000

H -2.935699000 0.696159000 3.662279000

H -4.858244000 -0.288171000 2.410726000

H -0.614394000 -3.409250000 0.092489000

H -5.076829000 0.346065000 -0.827120000

H -7.676547000 -2.945748000 -1.395661000

H 1.012560000 -3.643218000 0.577169000

H -0.739634000 -0.178994000 2.817753000

C 0.984697000 4.949769000 0.064820000

C 2.109006000 4.174747000 0.396860000

C 2.769820000 4.326046000 1.652267000

C 3.849711000 3.530113000 1.995280000

C 4.318897000 2.550003000 1.109459000

C 3.697931000 2.389584000 -0.137446000

C 2.616612000 3.179826000 -0.491798000

H 0.476009000 4.831375000 -0.884325000

H 0.603705000 5.700738000 0.749552000

H 2.405098000 5.079164000 2.345580000

H 4.333856000 3.664997000 2.958469000

H 5.161228000 1.922866000 1.385397000

H 4.057188000 1.638586000 -0.832861000

H 2.136520000 3.039269000 -1.455786000

C 0.616184000 1.843534000 1.847033000

C 1.446938000 1.001752000 2.476570000

C 1.703924000 1.031892000 3.957819000

C 2.185492000 0.012155000 1.664467000

C 4.039488000 -1.465600000 1.629616000

O 3.251563000 -0.454792000 2.284425000

O 1.851238000 -0.350879000 0.519921000

H 2.725628000 1.364115000 4.170726000

H 1.009169000 1.719832000 4.447109000

H 1.590448000 0.035432000 4.397387000

H 3.459393000 -2.387038000 1.564185000

H 4.357509000 -1.119482000 0.645944000

H 4.906414000 -1.609447000 2.272560000

H 0.030895000 2.573413000 2.393754000

H 0.503863000 1.829164000 0.772772000

O 0.910070000 -2.847940000 -2.998650000

H 1.535234000 -2.727160000 -2.212036000

H 1.344146000 -3.487984000 -3.584791000

O -2.038652000 -0.882811000 -2.326107000

H -1.367099000 -0.639236000 -3.011780000

H -2.069061000 -1.864723000 -2.308224000

O -1.417460000 -3.501614000 -1.760775000

H -0.558338000 -3.393032000 -2.248789000

H -1.751054000 -4.377243000 -2.010799000

O 2.384672000 -2.715976000 -0.828679000

H 3.336785000 -2.700578000 -1.047065000

H 2.235639000 -1.840475000 -0.398255000

O -0.926347000 -0.375980000 0.074762000

H 0.052967000 -0.342190000 0.116805000

H -1.208121000 -0.629584000 -0.840162000

O 2.437187000 0.159465000 -2.267567000

H 1.631186000 0.328675000 -2.787580000

H 2.210363000 0.370403000 -1.347720000

O -4.197631000 0.934382000 -2.169713000

H -3.793177000 1.799384000 -1.994332000

H -3.439202000 0.329235000 -2.314896000

H 7.815416000 -4.634286000 -0.552166000

H -4.230744000 -3.991759000 -1.441094000

H -2.099476000 5.414323000 -4.717577000

H -2.502305000 4.403365000 4.184760000

O 0.144635000 -0.381485000 -3.826048000

H 0.551861000 -1.273656000 -3.681719000

H 0.154035000 -0.219321000 -4.782058000

Supplementary Fig. 39b-TS

C 3.017076000 4.006493000 -2.978727000

H 4.092801000 3.900460000 -2.772748000

H 2.601188000 4.758413000 -2.292346000

O 2.328777000 2.766454000 -2.895674000

H 2.447717000 2.413901000 -1.988687000

C 1.291861000 5.443815000 3.835224000

H 0.438022000 5.139721000 4.448453000

H 1.063104000 6.429896000 3.413612000

C 1.581912000 4.434030000 2.753502000

C 0.871031000 3.234385000 2.660044000

H 0.089121000 3.017513000 3.383801000

C 1.138797000 2.296857000 1.660693000

H 0.576369000 1.371936000 1.622234000

C 2.141214000 2.552380000 0.715448000

O 2.442033000 1.688218000 -0.299416000

H 1.849409000 0.882373000 -0.254677000

C 2.875413000 3.741981000 0.803379000

H 3.662167000 3.930195000 0.079354000

C 2.592300000 4.662536000 1.807779000

H 3.170737000 5.581620000 1.858059000

C -5.189934000 -5.062954000 0.424268000

H -4.147504000 -5.027243000 0.081498000

H -5.781526000 -5.522301000 -0.372804000

C -5.692683000 -3.682320000 0.763261000

C -6.564800000 -2.995450000 -0.090011000

H -6.911129000 -3.479982000 -0.999048000

C -7.007748000 -1.708868000 0.221987000

H -7.697760000 -1.202130000 -0.446895000

C -6.566948000 -1.073853000 1.383543000

H -6.914243000 -0.075033000 1.628465000

C -5.689962000 -1.738777000 2.241414000

H -5.326820000 -1.250288000 3.138774000

C -5.270790000 -3.035691000 1.936836000

H -4.625168000 -3.567555000 2.633950000

C 4.760550000 -2.453697000 -1.136753000

C 4.826999000 -1.683644000 0.198943000

C 2.393404000 -2.628012000 -1.801134000

C 5.647164000 -2.690767000 1.028815000

C 1.259493000 -2.096803000 -2.341790000

C 4.990162000 -3.998152000 0.579989000

C 1.316747000 -0.866823000 -3.179854000

C 2.661851000 -0.244106000 -3.227133000

C 3.725114000 -0.801178000 -2.596909000

C -0.106111000 -2.640036000 -2.056002000

N 3.597339000 -1.997076000 -1.923792000

N -0.218271000 -3.493126000 -1.004369000

O 5.329143000 -0.411954000 0.017373000

O 6.988211000 -2.587513000 0.599677000

O 4.631711000 -3.803859000 -0.814724000

O -1.056259000 -2.284202000 -2.752488000

H 5.653210000 -2.256461000 -1.739293000

H 3.807418000 -1.669872000 0.614241000

H 2.421956000 -3.539971000 -1.222724000

H 5.537529000 -2.514575000 2.107347000

H 5.660647000 -4.859490000 0.631852000

H 0.939373000 -1.083642000 -4.195032000

H 2.775448000 0.721320000 -3.708866000

H 4.705464000 -0.346954000 -2.550606000

H 0.472474000 -3.503331000 -0.256782000

H 4.987415000 0.133492000 0.775964000

H 7.532164000 -3.187949000 1.131956000

H -1.170593000 -3.684645000 -0.708208000

H 0.586315000 -0.130931000 -2.804950000

C -1.698086000 3.883341000 -0.782361000

C -3.013743000 3.359719000 -0.577903000

C -3.985692000 3.427554000 -1.603064000

C -5.219751000 2.807486000 -1.458646000

C -5.516549000 2.096274000 -0.291882000

C -4.571795000 2.020933000 0.737350000

C -3.339204000 2.646324000 0.598289000

H -1.027258000 4.007007000 0.062370000

H -1.511059000 4.524583000 -1.637863000

H -3.752720000 3.971446000 -2.514404000

H -5.952616000 2.871623000 -2.257559000

H -6.478050000 1.603853000 -0.186114000

H -4.779165000 1.456743000 1.640023000

H -2.603204000 2.569046000 1.393632000

C -0.521008000 2.081401000 -1.559651000

C -1.380086000 1.289195000 -2.277387000

C -1.677544000 1.529325000 -3.730183000

C -2.155092000 0.279079000 -1.561527000

C -4.087600000 -1.102341000 -1.639191000

O -3.241022000 -0.094961000 -2.218022000

O -1.842872000 -0.195696000 -0.441508000

H -2.664765000 1.989656000 -3.861040000

H -0.926799000 2.194600000 -4.166231000

H -1.691703000 0.591828000 -4.296046000

H -3.570036000 -2.062560000 -1.650663000

H -4.385270000 -0.816257000 -0.629841000

H -4.963408000 -1.138643000 -2.285006000

H 0.184324000 2.726859000 -2.071363000

H -0.298852000 1.837760000 -0.531906000

O -1.001091000 -3.041863000 2.801023000

H -1.611520000 -2.843035000 2.015451000

H -1.475565000 -3.686969000 3.348835000

O 1.974381000 -1.081681000 2.326112000

H 1.268019000 -0.853706000 2.980565000

H 1.980342000 -2.061645000 2.252708000

O 1.333611000 -3.660909000 1.582940000

H 0.467364000 -3.572207000 2.062466000

H 1.663486000 -4.545890000 1.803266000

O -2.469796000 -2.677035000 0.665652000

H -3.395614000 -2.580208000 0.967232000

H -2.261838000 -1.800584000 0.260504000

O 0.919736000 -0.459964000 -0.075929000

H -0.054973000 -0.335737000 -0.101096000

H 1.183840000 -0.747590000 0.833468000

O -2.774185000 -0.130040000 2.331214000

H -1.937662000 0.017445000 2.809103000

H -2.588609000 0.149102000 1.418901000

O 4.212379000 0.635635000 2.223476000

H 3.842785000 1.526688000 2.115010000

H 3.430682000 0.057648000 2.357648000

H -5.224000000 -5.728300000 1.294225000

H 4.081195000 -4.214700000 1.155585000

H 2.150984000 5.573113000 4.505176000

H 2.901995000 4.376970000 -4.001349000

O -0.303410000 -0.597348000 3.708549000

H -0.669174000 -1.504803000 3.544208000

H -0.344252000 -0.450718000 4.666582000

Supplementary Fig. 44-RC

C -2.005279000 -1.794164000 0.969817000

H -2.710426000 -2.356582000 0.351445000

H -2.339893000 -1.860017000 2.012498000

C -1.934776000 -0.383232000 0.499094000

N -1.109229000 0.564454000 1.074228000

H -0.392867000 0.377415000 1.765453000

C -1.256647000 1.725775000 0.379460000

H -0.701265000 2.618578000 0.626843000

N -2.152996000 1.608337000 -0.585348000

C -2.574775000 0.288443000 -0.515447000

H -3.318018000 -0.106198000 -1.195163000

C 0.361335000 -1.361270000 -2.008410000

C 1.123721000 -0.696190000 -1.031644000

C 1.556433000 -1.364547000 0.152146000

C 2.262763000 -0.689931000 1.136141000

C 2.580206000 0.668719000 0.979548000

C 2.184727000 1.341945000 -0.185323000

C 1.470884000 0.679695000 -1.172923000

H 0.023191000 -0.843570000 -2.900257000

H 0.085827000 -2.404060000 -1.887814000

H 1.314074000 -2.416505000 0.275751000

H 2.574575000 -1.217852000 2.033201000

H 3.133412000 1.192854000 1.752930000

H 2.431355000 2.392463000 -0.312333000

H 1.151713000 1.209199000 -2.066353000

H -1.027663000 -2.286723000 0.906882000

Supplementary Fig. 44-TS

C 4.524146000 -0.006968000 0.603789000

H 4.988196000 0.978726000 0.695838000

H 5.193617000 -0.648156000 0.016734000

C 3.187655000 0.118159000 -0.037658000

N 2.387288000 -0.958124000 -0.336149000

H 2.554151000 -1.906889000 -0.024893000

C 1.159216000 -0.471906000 -0.782353000

H 0.537005000 -1.100613000 -1.408051000

N 1.258136000 0.871630000 -0.987296000

C 2.468189000 1.223777000 -0.466895000

H 2.795389000 2.255326000 -0.427967000

C -0.078800000 -0.724928000 0.903667000

C -1.422657000 -0.342304000 0.548770000

C -2.327696000 -1.284328000 0.004327000

C -3.605673000 -0.905414000 -0.394478000

C -4.021670000 0.425250000 -0.267211000

C -3.138710000 1.372981000 0.264558000

C -1.859783000 0.998716000 0.663684000

H 0.491734000 -0.060376000 1.548019000

H 0.114004000 -1.785087000 1.051588000

H -2.011237000 -2.319757000 -0.096294000

H -4.284014000 -1.648745000 -0.804964000

H -5.020176000 0.719522000 -0.576933000

H -3.453140000 2.408162000 0.368335000

H -1.179135000 1.739902000 1.074040000

H 4.450331000 -0.444758000 1.607471000

Supplementary Fig. 44-IC

C 4.581472000 0.122152000 0.384781000

H 5.038483000 1.098625000 0.202481000

H 5.182653000 -0.642217000 -0.125716000

C 3.173980000 0.111682000 -0.088504000

N 2.357960000 -0.999273000 0.008461000

H 2.456991000 -1.611004000 0.813627000

C 1.000605000 -0.568352000 -0.380276000

H 0.592002000 -1.255442000 -1.132880000

N 1.155882000 0.761288000 -0.959142000

C 2.422268000 1.107586000 -0.716298000

H 2.810077000 2.078746000 -1.007675000

C 0.049681000 -0.577025000 0.838585000

C -1.376798000 -0.255669000 0.472733000

C -2.184938000 -1.223537000 -0.140794000

C -3.496786000 -0.928436000 -0.513306000

C -4.023775000 0.343587000 -0.274860000

C -3.228755000 1.314953000 0.337139000

C -1.915400000 1.016021000 0.705092000

H 0.434026000 0.140022000 1.571879000

H 0.104324000 -1.577184000 1.285467000

H -1.781039000 -2.216708000 -0.322342000

H -4.109108000 -1.692003000 -0.985115000

H -5.046141000 0.574015000 -0.560675000

H -3.630475000 2.306069000 0.529223000

H -1.299230000 1.775309000 1.179523000

H 4.641232000 -0.090109000 1.461220000

Supplementary Fig. 45-RC

C 3.907871000 -2.162211000 -0.092446000

H 4.133464000 -3.101449000 -0.606856000

H 3.066838000 -2.338433000 0.583087000

C 3.577389000 -1.074511000 -1.113757000

H 4.392067000 -0.952035000 -1.834741000

H 2.689102000 -1.363098000 -1.691507000

C 3.266333000 0.261777000 -0.471787000

O 2.683821000 0.357058000 0.629851000

N 3.635953000 1.355739000 -1.153228000

H 3.387023000 2.271650000 -0.798733000

H 4.106786000 1.289634000 -2.045786000

C -3.863066000 -1.782665000 -1.517687000

H -4.589159000 -2.470876000 -1.072836000

H -3.663998000 -2.112508000 -2.543612000

C -2.596722000 -1.714994000 -0.701423000

C -1.412309000 -1.207100000 -1.251797000

H -1.400967000 -0.888659000 -2.291320000

C -0.249833000 -1.078987000 -0.495196000

H 0.644893000 -0.658239000 -0.938649000

C -0.249104000 -1.464593000 0.851414000

O 0.857365000 -1.350672000 1.653431000

H 1.550226000 -0.804106000 1.198448000

C -1.416840000 -1.987630000 1.415753000

H -1.411169000 -2.286807000 2.459776000

C -2.571630000 -2.107853000 0.642398000

H -3.474233000 -2.508276000 1.097843000

C 0.143677000 1.818401000 2.353112000

C -0.587301000 1.994439000 1.165673000

C 0.041256000 2.449994000 -0.032173000

C -0.683658000 2.602192000 -1.204058000

C -2.055973000 2.311723000 -1.236161000

C -2.697014000 1.863306000 -0.070961000

C -1.983713000 1.705789000 1.106819000

H -0.339423000 1.462352000 3.257453000

H 1.209189000 2.017475000 2.387698000

H 1.104424000 2.671476000 -0.013098000

H -0.183089000 2.946046000 -2.105147000

H -2.617929000 2.428733000 -2.157763000

H -3.757936000 1.629953000 -0.094010000

H -2.479783000 1.345791000 2.003901000

H -4.343057000 -0.796676000 -1.584862000

H 4.779409000 -1.885676000 0.510706000

Supplementary Fig. 45-TS

C 4.121400000 -1.557743000 0.713011000

H 4.316731000 -2.619140000 0.896316000

H 3.451168000 -1.195366000 1.498343000

C 3.503467000 -1.369005000 -0.667392000

H 4.163068000 -1.771934000 -1.446776000

H 2.561243000 -1.922666000 -0.748646000

C 3.231076000 0.087477000 -1.003771000

O 3.607880000 1.025299000 -0.282930000

N 2.582158000 0.304396000 -2.171084000

H 2.259988000 1.240840000 -2.383780000

H 2.159784000 -0.464365000 -2.675631000

C -4.315366000 -1.175676000 -1.431739000

H -5.105557000 -1.716556000 -0.902420000

H -4.265383000 -1.554103000 -2.459020000

C -2.989864000 -1.312677000 -0.730295000

C -1.797714000 -0.937072000 -1.374562000

H -1.839887000 -0.569072000 -2.396629000

C -0.573269000 -1.017395000 -0.726004000

H 0.340303000 -0.710175000 -1.222412000

C -0.503354000 -1.476089000 0.604965000

O 0.676013000 -1.527161000 1.256920000

H 0.928592000 -0.411661000 1.644663000

C -1.692571000 -1.862687000 1.254536000

H -1.636552000 -2.210821000 2.281636000

C -2.910574000 -1.790287000 0.587199000

H -3.821434000 -2.091751000 1.098046000

C 1.006936000 0.896342000 2.074733000

C 0.017448000 1.547003000 1.247718000

C 0.377835000 2.173726000 0.027498000

C -0.593406000 2.693332000 -0.817614000

C -1.949730000 2.595894000 -0.479216000

C -2.325670000 1.992258000 0.727626000

C -1.358439000 1.478269000 1.581143000

H 0.753194000 0.756276000 3.126500000

H 2.050695000 1.143901000 1.885836000

H 1.428765000 2.239018000 -0.235121000

H -0.300014000 3.170916000 -1.748092000

H -2.707606000 2.992586000 -1.148083000

H -3.375875000 1.920783000 0.994444000

H -1.648537000 1.001183000 2.512386000

H -4.616596000 -0.121505000 -1.493240000

H 5.068431000 -1.016283000 0.800337000

Supplementary Fig. 45-IC

C 3.204782000 -1.860979000 -1.642674000

H 2.830031000 -2.089411000 -2.645604000

H 2.605105000 -2.417238000 -0.917917000

C 3.119863000 -0.361490000 -1.376152000

H 3.686901000 0.207589000 -2.121318000

H 2.079251000 -0.020767000 -1.458058000

C 3.590724000 0.023393000 0.014686000

O 3.618115000 -0.780803000 0.958701000

N 3.985303000 1.310302000 0.162790000

H 4.125531000 1.666966000 1.100540000

H 3.826164000 1.983328000 -0.576077000

C -4.373846000 -0.852624000 -0.884566000

H -4.689159000 0.118059000 -0.478280000

H -5.114171000 -1.590352000 -0.554341000

C -3.006507000 -1.199589000 -0.384139000

C -1.880717000 -1.137493000 -1.240404000

H -2.030465000 -0.855027000 -2.278219000

C -0.617311000 -1.416353000 -0.777740000

H 0.246406000 -1.373829000 -1.432658000

C -0.400224000 -1.786229000 0.605246000

O 0.755810000 -2.053818000 1.049164000

H 1.262376000 0.353508000 1.833210000

C -1.565547000 -1.843317000 1.465459000

H -1.409036000 -2.117345000 2.504190000

C -2.815922000 -1.565316000 0.974153000

H -3.682333000 -1.612257000 1.628277000

C 0.803366000 1.327925000 2.033148000

C -0.154905000 1.713390000 0.934904000

C 0.315538000 2.035117000 -0.348776000

C -0.568247000 2.367981000 -1.375013000

C -1.945147000 2.392708000 -1.136113000

C -2.425093000 2.086566000 0.138417000

C -1.535950000 1.749770000 1.161439000

H 0.291586000 1.264306000 2.998427000

H 1.618774000 2.054774000 2.124669000

H 1.384886000 2.027834000 -0.538952000

H -0.182011000 2.609488000 -2.361534000

H -2.635450000 2.649708000 -1.934390000

H -3.492897000 2.105100000 0.337348000

H -1.918503000 1.503035000 2.148171000

H -4.399134000 -0.785783000 -1.975361000

H 4.238481000 -2.217585000 -1.575823000