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Peroxide Bond Strength of Antimalarial Drugs Containing an Endoperoxide Cycle. Relation with Biological Activity.

Supporting Informations

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Cartesian coordinates and total energies (ZPVE included) of all drugs studied. All data have been computed at the B3LYP/6-31+G(d) level.

Artemisinin (1), E= -960.551054

C	-1.073375000	1.207007000	0.922282000
C	0.005282000	0.279726000	0.296591000
C	1.409022000	0.923203000	0.293858000
C	1.375296000	2.325605000	-0.340749000
C	0.331080000	3.227621000	0.331495000
C	-1.090414000	2.630665000	0.292845000
C	0.076918000	-1.040269000	1.081293000
O	1.184289000	-1.885904000	0.717305000
C	2.302458000	-1.478987000	0.057847000
C	2.427549000	-0.017656000	-0.380380000
C	-2.472459000	0.537469000	1.001720000
C	-2.831585000	-0.481482000	-0.097423000
C	-1.797649000	-1.617792000	-0.266579000
O	-1.083030000	-1.809579000	0.974327000
C	-1.725825000	2.752079000	-1.104453000
O	-0.853216000	-1.328457000	-1.282859000
O	-0.349202000	0.031299000	-1.092030000
C	3.887015000	0.440087000	-0.207462000
C	-2.397571000	-2.958309000	-0.657658000
O	3.155614000	-2.305159000	-0.172285000
H	-0.743651000	1.370201000	1.960258000
H	1.693497000	1.042512000	1.352940000
H	1.166773000	2.230299000	-1.414580000
H	2.363341000	2.790709000	-0.255627000
H	0.330975000	4.216402000	-0.145520000
H	0.625444000	3.388734000	1.379758000
H	-1.714504000	3.233756000	0.969689000
H	0.204034000	-0.817344000	2.145496000
H	2.200091000	-0.039046000	-1.455391000
H	-3.239208000	1.322730000	1.007743000
H	-2.559901000	0.022873000	1.964479000
H	-2.965269000	-0.003884000	-1.072951000
H	-3.793097000	-0.935248000	0.171828000
H	-1.768694000	3.809597000	-1.394333000
H	-2.753240000	2.372021000	-1.113566000
H	-1.168456000	2.209571000	-1.871979000
H	4.564521000	-0.293760000	-0.649298000
H	4.145235000	0.542753000	0.854208000
H	4.056941000	1.404381000	-0.695398000
H	-1.601976000	-3.670887000	-0.891401000
H	-3.053505000	-2.843105000	-1.525995000
H	-2.979438000	-3.344671000	0.184627000

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Artemisinin (1T), E= -960.512084

C	0.489315000	1.547945000	-0.763252000
C	-0.202860000	0.314439000	-0.122487000
C	-1.757221000	0.321777000	-0.376174000
C	-2.357773000	1.642215000	0.135685000
C	-1.650797000	2.864812000	-0.470216000
C	-0.125930000	2.871203000	-0.223491000
C	0.269282000	-0.998230000	-0.884941000
O	-0.303445000	-2.175283000	-0.326986000
C	-1.554205000	-2.201729000	0.217056000
C	-2.405188000	-0.924150000	0.253519000
C	2.046804000	1.514656000	-0.704481000
C	2.702202000	0.657375000	0.385082000
C	2.531296000	-0.923013000	0.139831000
O	1.633490000	-1.154547000	-0.990217000
C	0.217805000	3.210667000	1.237940000
O	2.122242000	-1.418654000	1.300882000
O	0.020178000	0.157534000	1.203897000
C	-3.790123000	-1.233669000	-0.349566000
C	3.855018000	-1.568032000	-0.321204000
O	-1.961994000	-3.251754000	0.653971000
H	0.220020000	1.523210000	-1.830001000
H	-1.891988000	0.286919000	-1.468721000
H	-2.291002000	1.665759000	1.231030000
H	-3.425581000	1.678050000	-0.113017000
H	-2.094550000	3.784875000	-0.067755000
H	-1.836965000	2.880181000	-1.554722000
H	0.299057000	3.674564000	-0.844669000
H	-0.081649000	-0.895702000	-1.918274000
H	-2.535640000	-0.736465000	1.326873000
H	2.410063000	2.540944000	-0.554485000
H	2.436375000	1.196523000	-1.677268000
H	2.311544000	0.900577000	1.372959000
H	3.782325000	0.835724000	0.400362000
H	-0.192185000	4.195713000	1.494089000
H	1.300969000	3.257091000	1.398489000
H	-0.183231000	2.479919000	1.946028000
H	-4.224685000	-2.111259000	0.135226000
H	-3.717921000	-1.438276000	-1.425200000
H	-4.471330000	-0.387949000	-0.209862000
H	3.701478000	-2.638108000	-0.482363000
H	4.615927000	-1.419241000	0.448793000
H	4.179457000	-1.109012000	-1.259701000

6,6′-dimethyltrioxane (2), E= -691.277595

C	-2.547519000	1.114958000	0.509897000
C	-1.316464000	1.455605000	-0.352623000
C	-0.274792000	0.334017000	-0.315589000
C	-0.889740000	-0.999900000	-0.773886000
C	-2.110344000	-1.386661000	0.083216000
C	-3.126028000	-0.256906000	0.190659000
O	0.225612000	0.279476000	1.019203000
C	1.404195000	-0.512755000	1.175396000
C	2.481908000	-0.135101000	0.144216000
O	1.845064000	-0.204070000	-1.160749000
O	0.757780000	0.774937000	-1.193580000
O	-4.322926000	-0.442018000	0.051537000
C	3.562114000	-1.213872000	0.066887000
C	3.081150000	1.251671000	0.390695000
H	-3.333297000	1.866223000	0.388876000
H	-2.249002000	1.106953000	1.567739000
H	-0.850163000	2.381587000	-0.001840000

H	-1.614409000	1.607319000	-1.396562000
H	-0.143962000	-1.798194000	-0.757531000
H	-1.186844000	-0.876078000	-1.822198000
H	-1.777226000	-1.621296000	1.104912000
H	-2.612147000	-2.273455000	-0.315091000
H	1.161540000	-1.580958000	1.080228000
H	1.750605000	-0.326042000	2.196255000
H	4.311907000	-0.950158000	-0.685964000
H	3.132733000	-2.186143000	-0.197076000
H	4.066402000	-1.307403000	1.035846000
H	3.755463000	1.517782000	-0.430016000
H	3.654093000	1.252153000	1.325706000
H	2.303179000	2.014773000	0.462220000

6,6′-dimethyltrioxane (2T), E= -691.240227

C	1.826428000	1.269444000	0.626031000
C	0.972408000	0.206936000	1.332433000
C	0.478708000	-0.914751000	0.338151000
C	1.746464000	-1.551805000	-0.356844000
C	2.591080000	-0.495626000	-1.083181000
C	2.965087000	0.681134000	-0.193239000
O	-0.276600000	-0.265542000	-0.721947000
C	-1.630964000	-0.594676000	-0.856236000
C	-2.639648000	0.358453000	-0.050751000
O	-2.331967000	0.159904000	1.261878000
O	-0.156145000	-1.853984000	1.002787000
O	4.094467000	1.137648000	-0.162505000
C	-4.067728000	-0.113604000	-0.391031000
C	-2.396211000	1.823740000	-0.471563000
H	2.247108000	1.965865000	1.358911000
H	1.193074000	1.846696000	-0.061502000
H	0.080315000	0.646510000	1.783967000
H	1.544453000	-0.299284000	2.116302000
H	1.393206000	-2.316224000	-1.055064000
H	2.323557000	-2.047429000	0.429560000
H	2.021493000	-0.100337000	-1.934949000
H	3.510729000	-0.946607000	-1.470623000
H	-1.826972000	-1.624999000	-0.551128000
H	-1.884804000	-0.447237000	-1.911236000
H	-4.792374000	0.494597000	0.161237000
H	-4.206683000	-1.158295000	-0.093686000
H	-4.285645000	-0.014230000	-1.461390000
H	-3.056176000	2.483696000	0.101987000
H	-2.612714000	1.963980000	-1.537296000
H	-1.360350000	2.113629000	-0.279417000

cis-[5-6]-terpentrioxane (Cis-3m), E= -905.906115

C	-0.668508000	0.321317000	-0.883492000
C	-2.008621000	-0.331360000	-1.093021000
C	-3.026426000	-0.284936000	-0.218200000
C	-4.333589000	-1.008914000	-0.511936000
C	-0.697199000	1.386600000	0.233877000
C	-1.246963000	2.719389000	-0.280367000
C	-1.465965000	0.854716000	1.448212000
C	-2.914262000	0.492390000	1.078852000
C	-4.530286000	-2.231707000	0.409083000
C	-5.555481000	-0.072004000	-0.443372000
H	-0.341589000	0.802119000	-1.817954000
H	-2.112673000	-0.903181000	-2.014714000
H	-4.264171000	-1.386807000	-1.541276000
H	-2.269373000	2.598201000	-0.649960000

H	-0.628779000	3.100176000	-1.100258000
H	-1.249828000	3.463298000	0.523455000
H	-0.949376000	-0.034566000	1.820801000
H	-1.447326000	1.604905000	2.247825000
H	-3.523297000	1.406064000	1.000542000
H	-3.363775000	-0.082630000	1.898796000
H	-5.434870000	-2.782221000	0.121984000
H	-4.646165000	-1.936465000	1.459198000
H	-3.678406000	-2.917826000	0.342541000
H	-5.433794000	0.793219000	-1.106246000
H	-5.722680000	0.301312000	0.574516000
H	-6.462737000	-0.606619000	-0.749892000
O	0.260808000	-0.740661000	-0.569984000
C	1.544433000	-0.324318000	-0.121601000
O	1.379697000	0.535544000	1.011166000
O	0.669896000	1.733373000	0.575124000
C	2.236121000	-1.572399000	0.436362000
C	3.691770000	-1.321225000	0.855200000
C	4.519708000	-0.690450000	-0.272882000
C	3.828744000	0.589026000	-0.784946000
C	2.380390000	0.332985000	-1.233114000
N	5.903055000	-0.502256000	0.185765000
H	2.191194000	-2.331437000	-0.355095000
H	1.641944000	-1.949517000	1.275749000
H	3.712054000	-0.653808000	1.728444000
H	4.158622000	-2.263679000	1.163611000
H	4.566770000	-1.410392000	-1.104856000
H	3.835590000	1.342967000	0.014725000
H	4.401173000	1.009286000	-1.623671000
H	1.917831000	1.270370000	-1.552613000
H	2.364653000	-0.350336000	-2.092805000
H	6.479860000	-0.115341000	-0.560262000
H	5.931365000	0.167984000	0.954685000

cis-[5-6]-terpentrioxane (Cis-3m-T), E= -905.860190

C	-0.615433000	0.404814000	-0.631809000
C	-1.813868000	-0.469990000	-0.912869000
C	-2.961275000	-0.451655000	-0.215750000
C	-4.082525000	-1.428645000	-0.546376000
C	-1.009725000	1.666891000	0.188718000
C	-1.729903000	2.687721000	-0.752467000
C	-1.907514000	1.253568000	1.370535000
C	-3.189360000	0.545097000	0.903754000
C	-4.273150000	-2.482341000	0.564849000
C	-5.414980000	-0.718009000	-0.855619000
H	-0.166878000	0.733917000	-1.579512000
H	-1.678149000	-1.203364000	-1.707559000
H	-3.777734000	-1.967082000	-1.454450000
H	-2.599934000	2.211194000	-1.213097000
H	-1.050555000	3.020612000	-1.542901000
H	-2.052756000	3.558934000	-0.175738000
H	-1.316929000	0.581677000	2.003666000
H	-2.147597000	2.140206000	1.968324000
H	-3.927249000	1.289776000	0.567772000
H	-3.658788000	0.044618000	1.761142000
H	-5.022973000	-3.223054000	0.260312000
H	-4.622366000	-2.028511000	1.500389000
H	-3.336367000	-3.011158000	0.773621000
H	-5.298237000	0.022262000	-1.656450000
H	-5.812968000	-0.202813000	0.027232000
H	-6.168880000	-1.446823000	-1.177379000
O	0.311926000	-0.463990000	0.047952000

C	1.681231000	-0.100684000	0.265904000
O	1.864074000	0.768844000	1.270785000
O	0.088537000	2.392892000	0.600552000
C	2.361199000	-1.457417000	0.687823000
C	3.880318000	-1.354072000	0.816067000
C	4.538892000	-0.829679000	-0.466632000
C	3.906239000	0.515818000	-0.875892000
C	2.382907000	0.436976000	-1.026305000
N	5.995789000	-0.793254000	-0.287706000
H	2.075261000	-2.178760000	-0.086826000
H	1.897148000	-1.780511000	1.624535000
H	4.137270000	-0.689759000	1.652371000
H	4.294499000	-2.341829000	1.052255000
H	4.345303000	-1.557801000	-1.269715000
H	4.161078000	1.275602000	-0.125212000
H	4.338870000	0.850809000	-1.829527000
H	1.971928000	1.423091000	-1.258256000
H	2.107315000	-0.252186000	-1.835857000
H	6.457643000	-0.485595000	-1.142532000
H	6.246891000	-0.123004000	0.439444000

Trans-[5-6]-terpentrioxane (Trans-3m), E= -905.904811

C	0.476493000	0.357545000	-0.736460000
C	0.868957000	1.769480000	-0.253645000
H	0.066683000	0.438076000	-1.754774000
C	1.744509000	1.676237000	1.000207000
H	1.162945000	1.195871000	1.792380000
H	1.995110000	2.686722000	1.344932000
C	3.019854000	0.862074000	0.730449000
H	3.504079000	0.616238000	1.685060000
H	3.757485000	1.473995000	0.186210000
C	-1.638151000	0.621593000	0.433407000
C	-2.399500000	-0.059808000	1.575673000
C	-2.563186000	0.882430000	-0.768748000
C	-3.103526000	-1.340470000	1.101302000
H	-3.133040000	0.657689000	1.964853000
H	-1.690816000	-0.280457000	2.380392000
C	-3.267587000	-0.404034000	-1.226819000
H	-3.301339000	1.630377000	-0.451307000
H	-2.005456000	1.331941000	-1.594128000
C	-4.043505000	-1.068303000	-0.081125000
H	-3.668353000	-1.771150000	1.940177000
H	-2.361271000	-2.086646000	0.794614000
H	-3.950391000	-0.168997000	-2.055700000
H	-2.534249000	-1.124777000	-1.610115000
H	-4.817817000	-0.353119000	0.259893000
O	-1.145910000	1.834011000	1.006653000
O	-0.346191000	2.521428000	-0.004423000
O	-0.535433000	-0.221196000	0.117597000
C	1.523804000	2.580274000	-1.375058000
H	0.836230000	2.694224000	-2.219821000
H	1.792872000	3.578175000	-1.012776000
H	2.428790000	2.081409000	-1.734372000
C	1.635310000	-0.604501000	-0.735087000
C	2.780545000	-0.407993000	-0.062997000
H	1.476926000	-1.517978000	-1.303229000
C	3.923905000	-1.416640000	-0.045719000
H	4.857906000	-0.831904000	-0.048444000
C	3.968067000	-2.356904000	-1.259762000
H	4.876330000	-2.970503000	-1.227799000
H	3.112977000	-3.043592000	-1.272073000
H	3.967596000	-1.798328000	-2.202829000

C	3.905559000	-2.237689000	1.263779000
H	4.785394000	-2.890508000	1.320609000
H	3.908568000	-1.597092000	2.152774000
H	3.008835000	-2.867441000	1.306934000
N	-4.629203000	-2.332991000	-0.547842000
H	-5.164818000	-2.777862000	0.196588000
H	-5.275780000	-2.167118000	-1.318149000

Trans-[5-6]-terpentrioxane (Trans-3m-T), E= -905.858322

N	5.862074000	-0.723219000	0.272793000
H	6.304985000	-0.379840000	1.124029000
H	6.284076000	-1.626866000	0.062724000
C	4.411087000	-0.857013000	0.458229000
H	4.159889000	-1.551714000	1.284508000
C	3.804682000	0.511183000	0.795753000
H	4.242904000	0.895286000	1.728278000
H	4.067863000	1.218405000	0.000752000
C	2.280327000	0.442747000	0.954538000
H	2.013988000	-0.206495000	1.799818000
H	1.885085000	1.443274000	1.156178000
C	3.775147000	-1.407380000	-0.824761000
H	4.067356000	-0.765610000	-1.663779000
H	4.167516000	-2.413258000	-1.034736000
C	2.251224000	-1.486274000	-0.713935000
H	1.944351000	-2.189705000	0.070359000
H	1.794852000	-1.820229000	-1.650540000
C	1.587879000	-0.118677000	-0.314457000
O	1.753097000	0.681060000	-1.389878000
O	0.190416000	2.413020000	-0.378941000
O	0.201589000	-0.460037000	-0.093039000
C	-0.954516000	1.786637000	0.018294000
C	-1.733716000	2.709858000	0.981191000
H	-1.113021000	2.935954000	1.855793000
H	-2.663921000	2.255908000	1.333373000
H	-1.960905000	3.654349000	0.476221000
C	-0.675566000	0.380942000	0.661052000
H	-0.242309000	0.564833000	1.655376000
C	-1.947836000	-0.418035000	0.809319000
H	-1.915451000	-1.204767000	1.559140000
C	-3.036130000	-0.252146000	0.043631000
C	-3.100539000	0.848670000	-0.995278000
H	-3.831448000	1.600686000	-0.659208000
H	-3.508743000	0.450263000	-1.935077000
C	-1.756835000	1.517043000	-1.311214000
H	-1.132034000	0.871862000	-1.933283000
H	-1.904996000	2.465854000	-1.836053000
C	-4.287325000	-1.115312000	0.158300000
H	-5.147756000	-0.445477000	-0.001488000
C	-4.477566000	-1.785113000	1.527651000
C	-4.324370000	-2.177026000	-0.964460000
H	-4.227469000	-1.729279000	-1.959860000
H	-3.505089000	-2.895244000	-0.839438000
H	-5.271319000	-2.730311000	-0.939326000
H	-3.705418000	-2.539787000	1.720466000
H	-5.447205000	-2.295652000	1.565312000
H	-4.446813000	-1.052866000	2.342669000

Yingzhaosu fragment (4m), E= -580.090624

C	-0.994216000	-1.014393000	0.714049000
H	-1.355375000	-1.948948000	1.164195000
O	-0.111655000	-1.533397000	-0.300120000

O	0.493229000	-0.435301000	-1.061653000
C	1.300357000	0.426779000	-0.226185000
C	0.427609000	0.987835000	0.939997000
H	1.093539000	1.564309000	1.597246000
C	-0.740525000	1.900449000	0.500424000
H	-1.218271000	2.270595000	1.419645000
H	-0.371987000	2.789764000	-0.024434000
C	-1.793699000	1.179830000	-0.367081000
H	-2.692812000	1.807481000	-0.440834000
H	-1.411228000	1.058656000	-1.385133000
C	-2.197948000	-0.211518000	0.175588000
H	-2.834887000	-0.050443000	1.061380000
C	-0.164167000	-0.203895000	1.711307000
H	-0.796213000	0.150353000	2.536128000
H	0.621198000	-0.838054000	2.136045000
C	-3.009520000	-1.005580000	-0.854610000
H	-3.887831000	-0.434614000	-1.180620000
H	-3.363819000	-1.957269000	-0.438205000
H	-2.401626000	-1.231471000	-1.737295000
C	1.751607000	1.514987000	-1.216406000
H	2.366628000	1.068009000	-2.002917000
H	2.353942000	2.265883000	-0.691953000
H	0.897350000	2.014815000	-1.680854000
C	2.536331000	-0.273560000	0.312089000
H	3.113966000	0.321555000	1.022153000
C	2.971391000	-1.484828000	-0.038929000
H	2.417628000	-2.109416000	-0.733244000
H	3.893882000	-1.888266000	0.371435000

Yingzhaosu fragment (4m-T), E= -580.049610

C	-1.296024000	-1.062631000	0.618021000
H	-1.881771000	-1.823003000	1.169726000
O	-0.777181000	-1.599227000	-0.517290000
O	0.984224000	0.016875000	-1.374103000
C	1.567999000	0.367418000	-0.175960000
C	0.504325000	0.777806000	0.917760000
H	1.100462000	1.228565000	1.725102000
C	-0.533630000	1.827071000	0.458859000
H	-0.986379000	2.254367000	1.366781000
H	-0.046441000	2.663219000	-0.054242000
C	-1.653701000	1.262802000	-0.432652000
H	-2.407739000	2.046271000	-0.596898000
H	-1.246552000	0.991771000	-1.410654000
C	-2.359080000	0.047615000	0.181032000
H	-2.806003000	0.339799000	1.144171000
C	-0.234308000	-0.424130000	1.538099000
H	-0.752672000	-0.086770000	2.447499000
H	0.472221000	-1.202667000	1.844369000
C	-3.454953000	-0.525862000	-0.718971000
H	-4.242122000	0.222833000	-0.873725000
H	-3.919259000	-1.412801000	-0.271101000
H	-3.057374000	-0.811175000	-1.698040000
C	2.450672000	1.606321000	-0.551708000
H	3.199422000	1.310927000	-1.291176000
H	2.965593000	1.961733000	0.348501000
H	1.846104000	2.416652000	-0.965473000
C	2.505624000	-0.705245000	0.369210000
H	3.013339000	-0.453435000	1.302690000
C	2.739777000	-1.878413000	-0.222351000
H	2.238829000	-2.145472000	-1.148642000
H	3.433786000	-2.598510000	0.204226000

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Arteflene (5), E= -1559.214944

C	3.621134000	-0.975828000	-1.319672000
C	4.474248000	0.220776000	-0.886346000
C	3.729313000	0.921307000	0.262934000
C	2.290352000	1.303084000	-0.205778000
O	1.636119000	0.076415000	-0.609893000
O	2.336423000	-0.496476000	-1.759215000
C	3.503746000	-2.042140000	-0.209438000
C	3.095159000	-1.413815000	1.130040000
C	3.687837000	-0.046039000	1.467466000
C	2.628580000	-3.235150000	-0.599787000
O	2.386658000	-2.005095000	1.927413000
C	2.277645000	2.334888000	-1.350713000
C	1.491787000	1.885894000	0.943143000
C	0.223401000	1.717344000	1.341697000
C	-0.813689000	0.760116000	0.864958000
C	-2.000186000	1.192823000	0.233795000
C	-2.990241000	0.277927000	-0.136002000
C	-2.820455000	-1.079033000	0.132880000
C	-1.659988000	-1.523020000	0.772838000
C	-0.673482000	-0.610680000	1.133831000
C	-2.222223000	2.655307000	-0.073659000
F	-2.189510000	3.427536000	1.047697000
F	-3.420253000	2.884919000	-0.661057000
F	-1.278179000	3.158052000	-0.912961000
C	-3.877621000	-2.081345000	-0.246913000
F	-4.936552000	-1.515281000	-0.871963000
F	-4.363361000	-2.737309000	0.841198000
F	-3.389785000	-3.038671000	-1.080001000
H	4.007924000	-1.439140000	-2.235530000
H	4.636904000	0.889672000	-1.736860000
H	5.462529000	-0.116542000	-0.547572000
H	4.255163000	1.839512000	0.554564000
H	4.536259000	-2.397648000	-0.046453000
H	3.130320000	0.359892000	2.316400000
H	4.719618000	-0.216171000	1.811160000
H	2.614585000	-3.981243000	0.198786000
H	3.012866000	-3.705916000	-1.512296000
H	1.599383000	-2.916951000	-0.787238000
H	1.244474000	2.573649000	-1.615109000
H	2.781250000	1.955110000	-2.241505000
H	2.774683000	3.258508000	-1.032853000
H	2.061102000	2.652308000	1.471210000
H	-0.112733000	2.374947000	2.143124000
H	-3.888685000	0.625082000	-0.630193000
H	-1.524197000	-2.577964000	0.992560000
H	0.221817000	-0.963557000	1.633520000

Arteflene (5T), E= -1559.171682

C	4.287757000	0.638153000	1.096116000
C	4.505991000	-0.781177000	0.521525000
C	3.422099000	-1.212879000	-0.487312000
C	2.001728000	-1.489166000	0.118816000
O	1.421957000	-0.365346000	0.651263000
O	3.315652000	0.696013000	2.060441000
C	4.149280000	1.721142000	-0.022722000
C	3.157464000	1.264079000	-1.094819000
C	3.342146000	-0.157113000	-1.615980000
C	3.841595000	3.112707000	0.526825000
O	2.303425000	2.003955000	-1.552704000
C	2.078240000	-2.467830000	1.352496000

C	1.114710000	-2.177462000	-0.919081000
C	-0.153257000	-1.925961000	-1.270111000
C	-1.046425000	-0.822219000	-0.826933000
C	-2.275491000	-1.069653000	-0.175651000
C	-3.117534000	-0.016198000	0.187333000
C	-2.754540000	1.300104000	-0.100397000
C	-1.549695000	1.562831000	-0.755553000
C	-0.713716000	0.509780000	-1.117891000
C	-2.693787000	-2.479735000	0.167916000
F	-2.815854000	-3.263740000	-0.940283000
F	-3.887775000	-2.527196000	0.802513000
F	-1.797719000	-3.101851000	0.979446000
C	-3.678906000	2.437484000	0.245181000
F	-4.585420000	2.100282000	1.193837000
F	-4.387521000	2.857332000	-0.839659000
F	-3.003287000	3.520710000	0.702406000
H	5.199830000	0.901995000	1.677657000
H	4.594926000	-1.488226000	1.351695000
H	5.470462000	-0.791302000	-0.005115000
H	3.752498000	-2.159818000	-0.935826000
H	5.126678000	1.738271000	-0.535220000
H	2.541386000	-0.376375000	-2.328060000
H	4.290621000	-0.176919000	-2.173530000
H	3.820044000	3.851284000	-0.279423000
H	4.605709000	3.412514000	1.253835000
H	2.870337000	3.125022000	1.027408000
H	1.068394000	-2.755778000	1.649343000
H	2.580078000	-1.983530000	2.191829000
H	2.638873000	-3.359155000	1.047696000
H	1.598506000	-3.036109000	-1.386103000
H	-0.603900000	-2.623357000	-1.975459000
H	-4.049459000	-0.221957000	0.699228000
H	-1.255687000	2.582832000	-0.982656000
H	0.214658000	0.732490000	-1.632182000

10-deoxo-13-carbaartemisinin (6), E= -850.561864

O	-0.539313000	-0.618732000	-1.390670000
O	-1.743167000	-1.357452000	-1.019375000
C	-2.523309000	-0.604123000	-0.065367000
C	-2.712827000	0.851526000	-0.547003000
C	-1.657707000	1.857687000	-0.059109000
C	-0.180645000	1.526513000	-0.367444000
C	0.785762000	2.439136000	0.433348000
C	2.240557000	2.143511000	0.040423000
C	2.596680000	0.665881000	0.208277000
C	1.658461000	-0.257782000	-0.594337000
C	1.979435000	-1.763851000	-0.439924000
C	1.557908000	-2.241753000	0.949466000
O	0.172777000	-2.014272000	1.179261000
C	-0.253397000	-0.654849000	1.075706000
C	0.158096000	0.002641000	-0.268257000
C	-1.781968000	-0.695470000	1.281571000
C	-3.853348000	-1.359344000	-0.039090000
C	0.480473000	3.934928000	0.246290000
C	3.440620000	-2.123484000	-0.740202000
H	-3.692529000	1.204021000	-0.196742000
H	-2.756524000	0.834252000	-1.642402000
H	-1.895129000	2.829027000	-0.507902000
H	-1.776411000	2.002233000	1.024153000
H	-0.013611000	1.750410000	-1.432641000
H	0.670467000	2.208911000	1.505425000
H	2.919844000	2.761781000	0.643177000

H	2.394419000	2.443238000	-1.008005000
H	3.629120000	0.500274000	-0.120961000
H	2.572350000	0.411988000	1.276673000
H	1.779573000	0.001524000	-1.657691000
H	1.343190000	-2.294819000	-1.158252000
H	2.157617000	-1.757083000	1.739828000
H	1.691717000	-3.323949000	1.048710000
H	0.223922000	-0.076674000	1.882977000
H	-2.112867000	0.094485000	1.964377000
H	-2.003764000	-1.653444000	1.761783000
H	-4.474983000	-0.987487000	0.783915000
H	-3.682671000	-2.430297000	0.113287000
H	-4.397770000	-1.221655000	-0.979597000
H	1.241266000	4.544045000	0.750048000
H	-0.492548000	4.221403000	0.658124000
H	0.489745000	4.207240000	-0.818047000
H	3.754133000	-1.722584000	-1.712372000
H	3.567636000	-3.212507000	-0.776177000
H	4.132707000	-1.737693000	0.018492000

10-deoxo-13-carbaartemisinin (6T), E= -850.515038

C	0.124121000	1.327837000	-0.910166000
C	-0.339798000	-0.000886000	-0.133596000
C	-1.904691000	-0.102449000	-0.237106000
C	-2.566444000	1.150897000	0.348685000
C	-2.106376000	2.418476000	-0.383596000
C	-0.575211000	2.604271000	-0.377611000
C	0.304988000	-1.264796000	-0.796696000
O	-0.191325000	-2.434432000	-0.146137000
C	-2.371380000	-1.430268000	0.402073000
C	1.656362000	1.487133000	-1.080595000
C	2.580695000	0.984610000	0.041581000
C	2.655052000	-0.567284000	0.248378000
C	1.841334000	-1.381087000	-0.793875000
C	-0.055100000	3.131278000	0.969666000
O	2.319935000	-0.918237000	1.543519000
O	0.045102000	0.131519000	1.163385000
C	-3.881192000	-1.675892000	0.268326000
C	4.142684000	-1.030337000	0.144799000
H	-0.295708000	1.152034000	-1.911555000
H	-2.150875000	-0.149208000	-1.312170000
H	-2.333431000	1.215997000	1.418753000
H	-3.656493000	1.069748000	0.265825000
H	-2.584992000	3.304017000	0.055023000
H	-2.452260000	2.364373000	-1.427242000
H	-0.347003000	3.378827000	-1.127879000
H	-0.046859000	-1.281447000	-1.845215000
H	-2.106787000	-1.404375000	1.469207000
H	1.853745000	2.558747000	-1.222404000
H	1.957723000	1.016302000	-2.024410000
H	2.283085000	1.410445000	1.003087000
H	3.586445000	1.369649000	-0.173430000
H	2.219142000	-1.133086000	-1.793026000
H	2.058554000	-2.440921000	-0.628531000
H	-0.584983000	4.054584000	1.235840000
H	1.012901000	3.370826000	0.925705000
H	-0.199580000	2.406729000	1.777107000
H	-4.146263000	-2.671071000	0.647316000
H	-4.202433000	-1.623463000	-0.781056000
H	-4.468131000	-0.946289000	0.834908000
H	4.230509000	-2.102866000	0.341004000
H	4.758472000	-0.485554000	0.866856000

H	4.512031000	-0.819341000	-0.865875000
C	-1.600064000	-2.588698000	-0.239229000
H	-1.825021000	-3.535381000	0.262297000
H	-1.891376000	-2.686906000	-1.302504000

13-carbaartemisinin (7), E= -924.614673

C	-0.959328000	1.231219000	0.977868000
C	0.041138000	0.240707000	0.309535000
C	1.474535000	0.828693000	0.258586000
C	1.492881000	2.232500000	-0.371139000
C	0.530443000	3.183393000	0.350408000
C	-0.919404000	2.663191000	0.363354000
C	0.081653000	-1.085818000	1.091135000
O	1.191814000	-1.952253000	0.747718000
C	2.340263000	-1.567919000	0.133660000
C	2.427131000	-0.158502000	-0.445870000
C	-2.398602000	0.664736000	1.092728000
C	-2.887712000	-0.279821000	-0.023750000
C	-1.993196000	-1.510869000	-0.299467000
C	-1.187291000	-1.951798000	0.932834000
C	-1.603119000	2.844526000	-1.004874000
O	-1.018702000	-1.224596000	-1.331959000
O	-0.364737000	0.055318000	-1.073145000
C	3.893477000	0.302143000	-0.476668000
C	-2.797927000	-2.663835000	-0.901315000
O	3.226310000	-2.387453000	0.033046000
H	-0.590694000	1.366619000	2.006813000
H	1.799497000	0.933635000	1.307660000
H	1.236140000	2.157074000	-1.435879000
H	2.507673000	2.641276000	-0.322053000
H	0.564334000	4.176848000	-0.115766000
H	0.875689000	3.314619000	1.387452000
H	-1.481955000	3.289065000	1.073116000
H	0.232890000	-0.823972000	2.144849000
H	2.075851000	-0.267112000	-1.482304000
H	-3.099432000	1.506933000	1.160767000
H	-2.495000000	0.138087000	2.050455000
H	-3.015666000	0.252354000	-0.971739000
H	-3.881292000	-0.644232000	0.269655000
H	-1.802130000	-1.916248000	1.838471000
H	-0.854895000	-2.986048000	0.806923000
H	-1.581533000	3.905946000	-1.282969000
H	-2.655440000	2.541603000	-0.973483000
H	-1.119377000	2.271147000	-1.799082000
H	4.525340000	-0.488792000	-0.886370000
H	4.258324000	0.533646000	0.532201000
H	4.012441000	1.194691000	-1.097569000
H	-2.129028000	-3.449275000	-1.268312000
H	-3.416818000	-2.313569000	-1.734188000
H	-3.452065000	-3.097694000	-0.136084000

13-carbaartemisinin (7T), E= -924.569886

C	0.549011000	1.468244000	-0.862747000
C	-0.212001000	0.232977000	-0.170538000
C	-1.756819000	0.445162000	-0.309152000
C	-2.189449000	1.803657000	0.257652000
C	-1.446706000	2.962958000	-0.417179000
C	0.086308000	2.839496000	-0.314495000
C	0.159571000	-1.075847000	-0.914587000
O	-0.605155000	-2.198220000	-0.401293000
C	-1.892900000	-2.114020000	0.018391000

C	-2.480207000	-0.741094000	0.367315000
C	2.092445000	1.318212000	-0.933885000
C	2.806409000	0.538677000	0.183991000
C	2.555714000	-1.009732000	0.230247000
C	1.630334000	-1.531368000	-0.902282000
C	0.615767000	3.206584000	1.082162000
O	2.108958000	-1.408392000	1.475486000
O	0.138679000	0.211692000	1.142161000
C	-3.998491000	-0.749867000	0.130554000
C	3.919673000	-1.759771000	0.100264000
O	-2.507855000	-3.144766000	0.178501000
H	0.164293000	1.412019000	-1.892006000
H	-1.986430000	0.427951000	-1.387078000
H	-2.013912000	1.813591000	1.340633000
H	-3.267070000	1.936520000	0.111410000
H	-1.768745000	3.918073000	0.017142000
H	-1.730708000	2.993643000	-1.480100000
H	0.511617000	3.574691000	-1.016612000
H	-0.152814000	-0.952288000	-1.960498000
H	-2.300722000	-0.649701000	1.450840000
H	2.513694000	2.332126000	-0.953931000
H	2.362314000	0.880175000	-1.902546000
H	2.520711000	0.931945000	1.163701000
H	3.882562000	0.725959000	0.075243000
H	2.083617000	-1.273991000	-1.866380000
H	1.612663000	-2.623781000	-0.845086000
H	0.278473000	4.214454000	1.353969000
H	1.710913000	3.212070000	1.110422000
H	0.269758000	2.508412000	1.850212000
H	-4.443455000	-1.642956000	0.574602000
H	-4.228228000	-0.758718000	-0.942680000
H	-4.472080000	0.130592000	0.574632000
H	3.778104000	-2.841296000	0.179483000
H	4.605207000	-1.431875000	0.887180000
H	4.361266000	-1.525742000	-0.875649000

OZ277 fragment (8m), E= -849.412360

H	5.729557000	-0.075851000	-0.292259000
C	4.757558000	0.055106000	0.200757000
H	4.968922000	0.298898000	1.253484000
C	3.990822000	1.219139000	-0.446727000
H	3.888460000	1.035533000	-1.524974000
H	4.551499000	2.156442000	-0.338974000
C	2.593886000	1.389110000	0.175409000
H	2.017671000	2.168002000	-0.335701000
H	2.686323000	1.688226000	1.227904000
C	1.786134000	0.090873000	0.155579000
C	2.554281000	-1.088361000	0.762712000
H	1.956814000	-1.997220000	0.636286000
H	2.644253000	-0.903745000	1.841805000
C	3.947360000	-1.249020000	0.131071000
H	4.486062000	-2.061909000	0.634583000
H	3.831892000	-1.550202000	-0.919009000
O	0.528490000	0.266156000	0.815697000
O	1.420266000	-0.167397000	-1.212501000
O	0.212115000	-0.966098000	-1.043085000
C	-0.504037000	-0.198226000	-0.063201000
C	-1.475844000	-1.142053000	0.663808000
H	-0.891884000	-1.963760000	1.094713000
C	-2.517478000	-1.680291000	-0.343982000
H	-3.202928000	-2.360610000	0.180751000
H	-2.023122000	-2.265943000	-1.129061000

C	-3.301421000	-0.503191000	-0.963198000
H	-4.039060000	-0.891347000	-1.678546000
C	-4.020594000	0.281748000	0.154544000
H	-4.739807000	-0.370250000	0.671144000
H	-4.596339000	1.111898000	-0.279484000
C	-2.983173000	0.826973000	1.159376000
H	-3.494835000	1.383335000	1.956450000
C	-1.994980000	1.761702000	0.428550000
H	-1.263561000	2.170014000	1.136595000
H	-2.532095000	2.614033000	-0.010562000
C	-1.273685000	0.981167000	-0.692434000
H	-0.554383000	1.627212000	-1.208153000
C	-2.196023000	-0.348307000	1.777979000
H	-1.466277000	0.020588000	2.508771000
H	-2.877494000	-1.025230000	2.311963000
C	-2.313609000	0.431121000	-1.694053000
H	-2.854315000	1.271777000	-2.150681000
H	-1.807502000	-0.106114000	-2.505071000

OZ277 fragment (8m-T), E= -849.381020

H	-5.841628000	0.117566000	-0.117428000
C	-4.794556000	0.169119000	-0.442308000
H	-4.809821000	0.375927000	-1.523619000
C	-4.074257000	1.314369000	0.284351000
H	-4.173173000	1.183685000	1.369240000
H	-4.544208000	2.275746000	0.035398000
C	-2.592188000	1.386806000	-0.086011000
H	-2.070048000	2.165282000	0.478887000
H	-2.455848000	1.597597000	-1.153379000
C	-1.831619000	0.024641000	0.172652000
C	-2.612268000	-1.125243000	-0.569543000
H	-2.098834000	-2.060854000	-0.337583000
H	-2.487658000	-0.920728000	-1.640429000
C	-4.094346000	-1.174457000	-0.191673000
H	-4.580154000	-1.967403000	-0.776614000
H	-4.193739000	-1.453789000	0.864875000
O	-0.541720000	0.213865000	-0.442003000
O	-1.809324000	-0.196540000	1.479981000
O	0.268032000	-1.784109000	0.425377000
C	0.567861000	-0.578535000	0.016632000
C	1.594796000	-0.647044000	-1.217021000
H	1.058272000	-1.178089000	-2.010561000
C	2.854128000	-1.416698000	-0.785658000
H	3.522674000	-1.501811000	-1.654726000
H	2.592880000	-2.433411000	-0.474205000
C	3.570361000	-0.667331000	0.357151000
H	4.474365000	-1.220340000	0.645162000
C	3.953884000	0.751522000	-0.115676000
H	4.648672000	0.691933000	-0.965890000
H	4.479351000	1.287607000	0.687744000
C	2.681591000	1.524612000	-0.524865000
H	2.950283000	2.534931000	-0.861179000
C	1.725732000	1.619622000	0.681552000
H	0.824411000	2.181730000	0.416005000
H	2.213722000	2.157934000	1.507757000
C	1.356083000	0.215265000	1.183577000
H	0.644452000	0.264927000	2.011744000
C	1.964904000	0.776173000	-1.666452000
H	1.071280000	1.321032000	-1.986914000
H	2.630183000	0.694971000	-2.538837000
C	2.619189000	-0.568334000	1.568453000
H	3.119402000	-0.040956000	2.393936000

H	2.353506000	-1.566133000	1.932816000

RKA216 fragment (9m), E= -924.544638

H	-5.671917000	0.732946000	0.871945000
C	-4.857911000	0.351267000	0.241351000
H	-5.314370000	0.050579000	-0.714565000
C	-4.203654000	-0.873402000	0.897039000
H	-3.807502000	-0.593351000	1.881463000
H	-4.939031000	-1.670448000	1.064319000
C	-3.056794000	-1.418387000	0.026602000
H	-2.549400000	-2.262145000	0.506789000
H	-3.449959000	-1.772513000	-0.934849000
C	-2.022981000	-0.333292000	-0.294864000
C	-2.658674000	0.927418000	-0.893431000
H	-3.030383000	0.654782000	-1.889482000
H	-1.894942000	1.695675000	-1.030371000
C	-3.813441000	1.447256000	-0.019067000
H	-4.276558000	2.313769000	-0.508006000
H	-3.408188000	1.801894000	0.937753000
C	0.679024000	0.217072000	-0.200121000
C	1.760728000	1.273628000	-0.509691000
H	1.267040000	2.153385000	-0.939588000
C	2.491233000	1.645437000	0.802608000
H	1.792086000	2.094307000	1.517283000
H	3.254073000	2.402389000	0.574336000
C	3.148147000	0.386271000	1.407134000
H	3.664782000	0.656762000	2.338197000
C	2.054475000	-0.660917000	1.707731000
H	2.505534000	-1.563045000	2.143366000
H	1.338810000	-0.270704000	2.440715000
C	1.323875000	-1.048614000	0.401949000
H	0.543744000	-1.784586000	0.610495000
C	2.338757000	-1.623284000	-0.611844000
H	1.826107000	-1.912544000	-1.536744000
H	2.785725000	-2.534239000	-0.190822000
C	3.434911000	-0.578069000	-0.908869000
H	4.156317000	-0.992727000	-1.626180000
C	2.775335000	0.678673000	-1.514418000
H	2.277543000	0.432061000	-2.459128000
H	3.533680000	1.441747000	-1.737124000
C	4.160563000	-0.201320000	0.400733000
H	4.646039000	-1.089099000	0.830677000
H	4.956533000	0.528804000	0.195175000
O	-1.093807000	-0.961740000	-1.183003000
O	-0.001200000	-0.019443000	-1.436181000
O	-0.251080000	0.855854000	0.683075000
O	-1.344827000	-0.081186000	0.943270000

RKA216 fragment (9m-T), E= -924.511339

H	-6.099561000	0.644430000	0.110239000
C	-5.132154000	0.311177000	-0.286728000
H	-5.289680000	0.085177000	-1.352637000
C	-4.676357000	-0.963006000	0.440314000
H	-4.648992000	-0.783531000	1.522188000
H	-5.395240000	-1.775525000	0.269617000
C	-3.297329000	-1.428493000	-0.036479000
H	-2.945109000	-2.297190000	0.528515000
H	-3.317136000	-1.703112000	-1.097861000
C	-2.212666000	-0.292798000	0.081600000
C	-2.705656000	0.994002000	-0.643107000
H	-2.721239000	0.760074000	-1.714926000

H	-1.962139000	1.776879000	-0.481721000
C	-4.090089000	1.431340000	-0.152825000
H	-4.405071000	2.311486000	-0.728961000
H	-4.020337000	1.747434000	0.895693000
C	0.833408000	0.449431000	0.057057000
C	2.009353000	1.213411000	-0.711604000
H	1.549788000	2.083248000	-1.193077000
C	3.068616000	1.646337000	0.318799000
H	2.631572000	2.326636000	1.057142000
H	3.858081000	2.199566000	-0.209443000
C	3.668282000	0.404641000	1.012374000
H	4.429252000	0.725171000	1.736322000
C	2.548645000	-0.361151000	1.747754000
H	2.967877000	-1.246294000	2.247072000
H	2.097076000	0.266009000	2.523503000
C	1.478547000	-0.827087000	0.744006000
H	0.662143000	-1.344756000	1.253585000
C	2.110486000	-1.723114000	-0.336055000
H	1.348201000	-2.063361000	-1.044535000
H	2.516769000	-2.617613000	0.158263000
C	3.238071000	-0.964920000	-1.065108000
H	3.691862000	-1.620256000	-1.820420000
C	2.636556000	0.273569000	-1.758144000
H	1.893684000	-0.022531000	-2.505121000
H	3.424674000	0.833068000	-2.283465000
C	4.309864000	-0.518075000	-0.046526000
H	4.756720000	-1.396633000	0.440353000
H	5.124986000	0.008444000	-0.563851000
O	-1.066959000	-0.890518000	-0.581043000
O	-0.086717000	0.102907000	-1.006541000
O	0.304062000	1.260675000	0.958844000
O	-2.009592000	-0.069115000	1.386434000

RKA216 fragment (9m-T2),E= -924.511193

H	-5.051074000	-2.043435000	0.377516000
C	-4.616300000	-1.039459000	0.291530000
H	-5.431070000	-0.325369000	0.486885000
C	-4.078552000	-0.823315000	-1.130418000
H	-3.364370000	-1.616237000	-1.381252000
H	-4.897681000	-0.883975000	-1.860143000
C	-3.398803000	0.542632000	-1.292581000
H	-2.940608000	0.647393000	-2.281256000
H	-4.118842000	1.358317000	-1.166840000
C	-2.272633000	0.768446000	-0.215186000
C	-2.838993000	0.523641000	1.214330000
H	-3.560161000	1.326919000	1.404499000
H	-2.015494000	0.638668000	1.922108000
C	-3.509694000	-0.848361000	1.339359000
H	-3.927221000	-0.940845000	2.350947000
H	-2.753240000	-1.635302000	1.232790000
C	0.798627000	0.397826000	0.456538000
C	1.881468000	-0.351232000	1.364690000
H	1.434560000	-0.454589000	2.359313000
C	2.191386000	-1.731902000	0.755398000
H	1.292524000	-2.355222000	0.732977000
H	2.921472000	-2.231077000	1.409539000
C	2.777546000	-1.565709000	-0.660973000
H	3.002619000	-2.555513000	-1.079957000
C	1.740314000	-0.852845000	-1.553064000
H	2.141628000	-0.729145000	-2.569486000
H	0.825457000	-1.448171000	-1.638899000
C	1.425957000	0.544735000	-0.990376000

H	0.675190000	1.052492000	-1.600722000
C	2.713949000	1.382632000	-0.894759000
H	2.491324000	2.382411000	-0.507000000
H	3.121773000	1.509419000	-1.907684000
C	3.747456000	0.668838000	0.001543000
H	4.664091000	1.271132000	0.055772000
C	3.160246000	0.504281000	1.419553000
H	2.949782000	1.481943000	1.865567000
H	3.886119000	-0.003519000	2.070501000
C	4.068223000	-0.721691000	-0.589091000
H	4.503707000	-0.612499000	-1.592632000
H	4.819346000	-1.232150000	0.030781000
O	-1.839153000	2.027466000	-0.350618000
O	0.527959000	1.578848000	0.988849000
O	-0.335419000	-0.507351000	0.478975000
O	-1.279764000	-0.223059000	-0.593741000

IRON-HEME COMPLEXES (high spin)

Fe(III)-heme-dioxane, E= -2558.331507

O	2.745717000	-0.427561000	1.672797000
C	2.768688000	0.257442000	2.850061000
C	1.994536000	-0.382154000	4.010190000
C	0.468044000	-0.255842000	3.929780000
C	-0.176646000	-0.818560000	2.658935000
O	0.115686000	-0.025535000	1.551725000
Fe	-0.220111000	0.046746000	-0.237121000
N	-2.281283000	-0.429403000	-0.308998000
C	-3.313606000	0.444054000	-0.073654000
C	-4.547162000	-0.292052000	0.096787000
C	-4.240474000	-1.616346000	-0.043174000
C	-2.818797000	-1.692014000	-0.299072000
C	-3.202758000	1.836267000	-0.033841000
C	-2.042349000	2.580937000	-0.260392000
C	-1.976489000	4.026441000	-0.273797000
C	-0.683417000	4.359813000	-0.562587000
C	0.041648000	3.118128000	-0.726084000
N	-0.805434000	2.057616000	-0.535098000
C	1.396323000	3.019744000	-1.055711000
C	2.107235000	1.838121000	-1.279372000
C	3.496171000	1.771578000	-1.681814000
C	3.801724000	0.448467000	-1.822934000
C	2.600862000	-0.293894000	-1.507011000
N	1.590554000	0.572544000	-1.183220000
H	-0.250440000	5.353796000	-0.668218000
H	-2.820614000	4.691226000	-0.094683000
H	-5.520630000	0.158039000	0.287578000
H	-4.911229000	-2.473024000	0.009614000
C	-2.108396000	-2.873461000	-0.527908000
C	-0.749819000	-2.971741000	-0.839180000
C	-0.055342000	-4.204153000	-1.142099000
C	1.237723000	-3.868612000	-1.429231000
C	1.336114000	-2.431103000	-1.302335000
N	0.118556000	-1.914115000	-0.937980000
H	-0.511696000	-5.193250000	-1.143452000
H	2.057773000	-4.526674000	-1.713730000
C	2.489734000	-1.684839000	-1.552624000
H	4.749756000	0.002553000	-2.120846000
H	4.141487000	2.634547000	-1.841296000
H	1.944627000	3.956562000	-1.174982000
H	-4.117605000	2.397620000	0.167278000
H	-2.674686000	-3.806258000	-0.487826000

H	3.386057000	-2.242244000	-1.832076000
H	0.169424000	-1.859891000	2.493681000
H	-1.275069000	-0.867819000	2.807919000
H	0.024332000	-0.772059000	4.799863000
H	0.173387000	0.805748000	4.012633000
H	2.339020000	0.074970000	4.955196000
H	2.281877000	-1.448069000	4.051211000
H	2.491540000	1.326066000	2.705524000
H	3.856325000	0.293709000	3.115051000

Fe(III)-heme-trioxane 1, E= -2594.227388

N	0.868529000	-1.384893000	-1.218552000
C	0.671366000	-2.743080000	-1.237413000
C	1.853102000	-3.401090000	-1.750510000
C	2.758046000	-2.419733000	-2.041296000
C	2.131348000	-1.159411000	-1.707830000
C	-0.501880000	-3.394433000	-0.847111000
C	-1.678571000	-2.783299000	-0.404856000
N	-1.860973000	-1.432004000	-0.254761000
C	-3.154082000	-1.248284000	0.165943000
C	-3.812818000	-2.530282000	0.292202000
C	-2.898518000	-3.481813000	-0.062284000
Fe	-0.339141000	0.031699000	-0.222204000
N	0.848742000	1.514406000	-1.145422000
C	0.632201000	2.867028000	-1.086242000
C	1.804779000	3.570839000	-1.559302000
C	2.724145000	2.620674000	-1.903890000
C	2.114246000	1.334545000	-1.642713000
C	-3.757826000	-0.011633000	0.407897000
C	-3.170345000	1.244687000	0.234489000
C	-3.845917000	2.508873000	0.433696000
C	-2.944813000	3.489973000	0.131382000
C	-1.717025000	2.826704000	-0.251932000
N	-1.882172000	1.467576000	-0.178297000
C	-0.549916000	3.478105000	-0.659644000
C	2.716625000	0.096801000	-1.888233000
O	0.270356000	-0.045769000	1.490363000
C	0.744273000	-0.985310000	2.395833000
C	1.302110000	-0.319460000	3.656289000
H	-3.089814000	4.569238000	0.154406000
H	-4.880910000	2.619300000	0.754612000
H	-4.847124000	-2.672026000	0.602984000
H	-3.030527000	-4.562337000	-0.100837000
H	1.962579000	-4.477477000	-1.876073000
H	3.760562000	-2.527771000	-2.453025000
H	3.724057000	2.765986000	-2.310720000
H	1.898025000	4.654123000	-1.624297000
H	-0.571253000	4.569786000	-0.666829000
H	-4.797859000	-0.027577000	0.740237000
H	-0.508054000	-4.484052000	-0.917807000
H	3.732798000	0.113222000	-2.287507000
H	1.527170000	-1.616261000	1.929715000
H	-0.060920000	-1.677870000	2.719977000
H	1.735762000	-1.109068000	4.299925000
H	0.484636000	0.166859000	4.210002000
O	2.245325000	0.712258000	3.414241000
C	3.245803000	0.458858000	2.475209000
H	3.950360000	1.323775000	2.538013000
O	3.883814000	-0.698912000	2.509609000
H	2.815351000	0.536193000	1.431942000

Fe(III)-heme-trioxane 2, E= -2594.223271

O	2.816895000	-0.294245000	1.700243000
C	2.722962000	0.232898000	2.951315000
C	1.843304000	-0.548495000	3.939772000
O	0.464021000	-0.294070000	3.824329000
C	-0.161645000	-0.787536000	2.668715000
O	0.133770000	-0.038371000	1.551778000
Fe	-0.220679000	0.052418000	-0.237989000
N	-2.306636000	-0.291136000	-0.296470000
C	-3.278700000	0.649514000	-0.061220000
C	-4.556427000	-0.003078000	0.120263000
C	-4.338143000	-1.345402000	-0.013623000
C	-2.926210000	-1.515840000	-0.276051000
C	-3.076964000	2.031631000	-0.031679000
C	-1.871873000	2.696807000	-0.270011000
C	-1.711420000	4.134454000	-0.294334000
C	-0.401012000	4.380376000	-0.592032000
C	0.240596000	3.093137000	-0.749512000
N	-0.673141000	2.091375000	-0.547191000
C	1.584667000	2.903884000	-1.081403000
C	2.216141000	1.676542000	-1.294445000
C	3.597762000	1.516050000	-1.693811000
C	3.817347000	0.174866000	-1.821714000
C	2.570779000	-0.485124000	-1.501162000
N	1.617446000	0.448182000	-1.188362000
H	0.095861000	5.342999000	-0.705970000
H	-2.509051000	4.854110000	-0.114521000
H	-5.496942000	0.511021000	0.314257000
H	-5.063164000	-2.155962000	0.048394000
C	-2.296057000	-2.742548000	-0.499373000
C	-0.947642000	-2.931445000	-0.811836000
C	-0.335747000	-4.208540000	-1.105469000
C	0.976812000	-3.961074000	-1.393891000
C	1.169723000	-2.532679000	-1.277807000
N	-0.011378000	-1.933211000	-0.917747000
H	-0.856300000	-5.165371000	-1.099942000
H	1.751741000	-4.673760000	-1.673174000
C	2.370047000	-1.866056000	-1.532665000
H	4.735134000	-0.334363000	-2.112614000
H	4.297984000	2.333911000	-1.858913000
H	2.193114000	3.801609000	-1.208784000
H	-3.951637000	2.652991000	0.171369000
H	-2.922203000	-3.635868000	-0.451777000
H	3.228150000	-2.483328000	-1.806191000
H	0.136075000	-1.848665000	2.507950000
H	-1.246279000	-0.751295000	2.887287000
H	2.115007000	-0.261020000	4.968961000
H	2.063423000	-1.628390000	3.808998000
H	2.442186000	1.308985000	2.943707000
H	3.773217000	0.202486000	3.338118000

Fe(III)-heme-tetraoxane, E= -2630.051387

N	-0.734177000	-1.961229000	-0.607011000
C	-1.892863000	-2.663147000	-0.384184000
C	-1.659236000	-4.073898000	-0.602002000
C	-0.349407000	-4.206586000	-0.967328000
C	0.221222000	-2.877626000	-0.971925000
C	-3.124675000	-2.101460000	-0.040379000
C	-3.401115000	-0.738455000	0.094412000
N	-2.491080000	0.274367000	-0.062169000
C	-3.169377000	1.450744000	0.130265000
C	-4.561111000	1.172758000	0.414993000

C	-4.704710000	-0.185076000	0.393535000
Fe	-0.386369000	0.051283000	-0.067730000
N	1.442115000	-0.126005000	-1.108863000
C	2.335082000	0.892365000	-1.326363000
C	3.599434000	0.348543000	-1.770095000
C	3.451229000	-1.009296000	-1.815217000
C	2.095741000	-1.295698000	-1.398256000
C	-2.611206000	2.727843000	0.048595000
C	-1.282751000	3.029620000	-0.264684000
C	-0.748369000	4.367463000	-0.397935000
C	0.567495000	4.234314000	-0.739066000
C	0.837853000	2.815480000	-0.816034000
N	-0.300041000	2.109073000	-0.518873000
C	2.063271000	2.255023000	-1.176847000
C	1.537388000	-2.573943000	-1.324494000
O	-0.013361000	-0.067469000	1.716507000
C	0.472830000	-0.943545000	2.639278000
O	1.786234000	-0.665327000	3.074063000
O	2.689364000	-1.032353000	1.994169000
C	3.674400000	-0.033108000	1.931133000
O	3.320560000	1.176847000	1.508710000
H	1.297406000	5.019167000	-0.932600000
H	-1.319225000	5.284021000	-0.255196000
H	-5.322985000	1.929171000	0.598889000
H	-5.608637000	-0.770827000	0.555585000
H	-2.412751000	-4.853649000	-0.498653000
H	0.190258000	-5.117327000	-1.223707000
H	4.182556000	-1.758878000	-2.115051000
H	4.477558000	0.941401000	-2.022631000
H	2.883379000	2.946294000	-1.379013000
H	-3.280558000	3.572011000	0.226371000
H	-3.957518000	-2.791723000	0.108693000
H	2.184430000	-3.412673000	-1.588967000
H	0.433811000	-1.990580000	2.273936000
H	-0.089954000	-0.869587000	3.592425000
H	4.148556000	0.100246000	2.938065000
H	4.452446000	-0.481349000	1.269227000

Fe(III)-heme-trioxolane, E= -2554.978412

O	-2.992895000	0.896348000	2.094936000
C	-2.732574000	-0.088226000	2.955447000
O	-1.993386000	-1.183935000	2.504779000
C	-0.584620000	-1.044911000	2.594000000
O	-0.071852000	-0.089326000	1.761507000
Fe	0.253700000	0.048714000	-0.043556000
N	-1.514778000	-0.605715000	-0.979699000
C	-2.621550000	0.167834000	-1.222067000
C	-3.745050000	-0.677811000	-1.558758000
C	-3.297434000	-1.967345000	-1.513187000
C	-1.898685000	-1.911528000	-1.149960000
C	-2.660231000	1.562071000	-1.177861000
C	-1.586685000	2.409277000	-0.897544000
C	-1.646064000	3.854080000	-0.918355000
C	-0.390105000	4.305716000	-0.626973000
C	0.438569000	3.136842000	-0.428343000
N	-0.313047000	2.001746000	-0.593733000
C	1.805832000	3.164566000	-0.143212000
C	2.642956000	2.054055000	-0.011420000
C	4.067978000	2.116494000	0.229122000
C	4.518787000	0.827443000	0.268563000
C	3.369818000	-0.024394000	0.052397000

N	2.246471000	0.744735000	-0.113758000
H	-0.042139000	5.335639000	-0.559200000
H	-2.539155000	4.437758000	-1.137385000
H	-4.743682000	-0.318266000	-1.803219000
H	-3.853271000	-2.882563000	-1.712644000
C	-1.062022000	-3.022504000	-1.024373000
C	0.303073000	-2.996237000	-0.728952000
C	1.162004000	-4.157851000	-0.670427000
C	2.419729000	-3.706350000	-0.383384000
C	2.332137000	-2.267945000	-0.265271000
N	1.036777000	-1.863861000	-0.475700000
H	0.835925000	-5.183246000	-0.839800000
H	3.334559000	-4.286548000	-0.269477000
C	3.410985000	-1.419678000	-0.005469000
H	5.537620000	0.473395000	0.420577000
H	4.641362000	3.035603000	0.342792000
H	2.269142000	4.147727000	-0.037987000
H	-3.619060000	2.036197000	-1.395968000
H	-1.512048000	-4.002397000	-1.195920000
H	4.384662000	-1.891223000	0.142828000
H	-0.317745000	-0.787431000	3.644764000
H	-0.190064000	-2.054024000	2.367782000
H	-3.721175000	-0.487974000	3.297286000
H	-2.265111000	0.356171000	3.874653000