Supporting Information

THE EFFECTS OF TYPE II BINDING ON METABOLIC STABILITY AND BINDING AFFINITY IN CYTOCHROME P450 CYP3A4

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Table S1. DFT Energies for Different Basis Sets

No Ligand	OPBE	B3LYP	TPSS
Sextet	-1510.578919	-1510.73344361	-1510.91694
Doublet	-1510.56713522	-1510.72283315	-1510.92401887
delta	-7.394321950055	-6.65806364997025	4.44199092499161
Ligand/Heme			
pyridine reduced Heme	ND	ND	-1759.4275243
pyridine	-1758.78101922	-1759.04162094	-1759.2999094
water	-1586.973379	-1587.17171669	-1587.3789680
oxygen	ND		
Ligand only			
pyridine	-248.211402938	-248.3042282930	-248.353987
water	-76.4048721	-76.4169106417	-76.4415112070
oxygen	ND	ND	-150.370708894
Binding Energy versus doublet			
heme-pyridine	-1.556866405001	-9.13608436746017	-13.7444650749484
heme-water	-0.860729200092	-20.0629936832217	-8.43229668240951

Basis Set for All Calculations with Effective Core potentials-

```
H  0
S   3  1.00
     13.01000000      0.01968500
      1.96200000      0.13797700
      0.44460000      0.47814800
S   1  1.00
      0.12200000      1.00000000
P   1  1.00
      0.72700000      1.00000000
****
S  0
S  11  1.00
 110800.00000000      0.00024800
  16610.00000000      0.00192000
   3781.00000000      0.00996200
   1071.00000000      0.04029700
    349.80000000      0.12860400
    126.30000000      0.30348000
     49.26000000      0.42143200
     20.16000000      0.23078100
      5.72000000      0.01789700
      2.18200000     -0.00297500
      0.43270000      0.00085000
S  11  1.00
 110800.00000000     -0.00006900
  16610.00000000     -0.00052800
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```
   3781.00000000     -0.00279700
   1071.00000000     -0.01126500
    349.80000000     -0.03888300
    126.30000000     -0.09950200
     49.26000000     -0.19974000
     20.16000000     -0.12336000
      5.72000000      0.51319400
      2.18200000      0.60712000
      0.43270000      0.03967500
S  11  1.00
 110800.00000000      0.00002000
  16610.00000000      0.00015300
   3781.00000000      0.00081000
   1071.00000000      0.00329000
    349.80000000      0.01129700
    126.30000000      0.02963900
     49.26000000      0.05998500
     20.16000000      0.04132500
      5.72000000     -0.20747400
      2.18200000     -0.39288900
      0.43270000      0.63284000
S   1  1.00
      0.15700000      1.00000000
P   7  1.00
    399.70000000      0.00447500
     94.19000000      0.03417100
     29.75000000      0.14425000
     10.77000000      0.35392800
      4.11900000      0.45908500
      1.62500000      0.20638300
      0.47260000      0.01021400
P   7  1.00
    399.70000000     -0.00116300
     94.19000000     -0.00865700
     29.75000000     -0.03908900
     10.77000000     -0.09346300
      4.11900000     -0.14799400
      1.62500000      0.03019000
      0.47260000      0.56157300
P   1  1.00
      0.14070000      1.00000000
D   1  1.00
      0.47900000      1.00000000
S   1  1.00
      0.05070000      1.00000000
P   1  1.00
      0.03990000      1.00000000
****
O  0
S   8  1.00
  11720.00000000      0.00071000
   1759.00000000      0.00547000
    400.80000000      0.02783700
    113.70000000      0.10480000
     37.03000000      0.28306200
     13.27000000      0.44871900
      5.02500000      0.27095200
      1.01300000      0.01545800
S   8  1.00
```

```
  11720.00000000     -0.00016000
   1759.00000000     -0.00126300
    400.80000000     -0.00626700
    113.70000000     -0.02571600
     37.03000000     -0.07092400
     13.27000000     -0.16541100
      5.02500000     -0.11695500
      1.01300000      0.55736800
S   1  1.00
      0.30230000      1.00000000
P   3  1.00
     17.70000000      0.04301800
      3.85400000      0.22891300
      1.04600000      0.50872800
P   1  1.00
      0.27530000      1.00000000
D   1  1.00
      1.18500000      1.00000000
S   1  1.00
      0.07896000      1.00000000
P   1  1.00
      0.06856000      1.00000000
****
C  0
S   8  1.00
   6665.00000000      0.00069200
   1000.00000000      0.00532900
    228.00000000      0.02707700
     64.71000000      0.10171800
     21.06000000      0.27474000
      7.49500000      0.44856400
      2.79700000      0.28507400
      0.52150000      0.01520400
S   8  1.00
   6665.00000000     -0.00014600
   1000.00000000     -0.00115400
    228.00000000     -0.00572500
     64.71000000     -0.02331200
     21.06000000     -0.06395500
      7.49500000     -0.14998100
      2.79700000     -0.12726200
      0.52150000      0.54452900
S   1  1.00
      0.15960000      1.00000000
P   3  1.00
      9.43900000      0.03810900
      2.00200000      0.20948000
      0.54560000      0.50855700
P   1  1.00
      0.15170000      1.00000000
D   1  1.00
      0.55000000      1.00000000
****
N  0
S   8  1.00
   9046.00000000      0.00070000
   1357.00000000      0.00538900
    309.30000000      0.02740600
     87.73000000      0.10320700
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```
     28.56000000      0.27872300
     10.21000000      0.44854000
      3.83800000      0.27823800
      0.74660000      0.01544000
S   8  1.00
   9046.00000000     -0.00015300
   1357.00000000     -0.00120800
    309.30000000     -0.00599200
     87.73000000     -0.02454400
     28.56000000     -0.06745900
     10.21000000     -0.15807800
      3.83800000     -0.12183100
      0.74660000      0.54900300
S   1  1.00
      0.22480000      1.00000000
P   3  1.00
     13.55000000      0.03991900
      2.91700000      0.21716900
      0.79730000      0.51031900
P   1  1.00
      0.21850000      1.00000000
D   1  1.00
      0.81700000      1.00000000
S   1  1.00
      0.06124000      1.00000000
P   1  1.00
      0.05611000      1.00000000
****
FE  0
S   7  1.00
    2473.84000000       0.00013600
     359.74200000       0.00087200
      24.48800000       0.05282000
       8.38751000      -0.39713800
       1.72801000       0.74367300
       0.72177500       0.45615900
       0.11761200       0.01647500
S   7  1.00
    2473.84000000      -0.00003100
     359.74200000      -0.00023700
      24.48800000      -0.01229200
       8.38751000       0.10023900
       1.72801000      -0.23426200
       0.72177500      -0.25124500
       0.11761200       0.55814300
S   7  1.00
    2473.84000000       0.00008100
     359.74200000       0.00043700
      24.48800000       0.02995000
       8.38751000      -0.23868800
       1.72801000       0.91993700
       0.72177500      -0.37908000
       0.11761200      -1.65503900
S   1  1.00
       0.04234500       1.00000000
P   6  1.00
      64.89790000       0.00341300
      12.47620000      -0.06656400
       3.24634000       0.34921700
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      1.45250000        0.50902000
      0.62102400        0.25794700
      0.16219100        0.01950900
P   6  1.00
     64.89790000       -0.00070700
     12.47620000        0.01518800
      3.24634000       -0.09188400
      1.45250000       -0.15848800
      0.62102400       -0.01210600
      0.16219100        0.53486500
P   6  1.00
     64.89790000       -0.00096400
     12.47620000        0.02147200
      3.24634000       -0.13033700
      1.45250000       -0.24593200
      0.62102400        0.03583900
      0.16219100        0.82279400
P   1  1.00
      0.05045400        1.00000000
D   5  1.00
     38.83200000        0.02115200
     12.16880000        0.11299100
      4.35712000        0.29456800
      1.59467000        0.42403200
      0.54388300        0.37571200
D   5  1.00
     38.83200000       -0.02336100
     12.16880000       -0.12793700
      4.35712000       -0.33745000
      1.59467000       -0.30119800
      0.54388300        0.36307300
D   1  1.00
      0.15752500        1.00000000
F   1  1.00
      1.62120000        1.00000000
****

Fe  0
FE-ECP   4   10
G POTENTIAL
 1
2         1.00000000        0.00000000
S-G POTENTIAL
 2
2        22.14297277      239.74474466
2         9.28465503       46.15501318
P-G POTENTIAL
 4
2        22.28449301       43.75598234
2        22.16423924       74.60461922
2         9.38245156       11.35204140
2         9.46218842       25.97902224
D-G POTENTIAL
 4
2        26.69705846       -8.78327657
2        26.89933437      -13.18404835
2         8.97801127       -0.51002419
2         8.94834948       -0.72953808
F-G POTENTIAL
```

2
2 13.46316084 -2.77838720
2 16.56769645 -5.89469136

OPBE Water Coordinates Energy -76.4048721826

O 0.00000 0.124352 0.00000
H 0.781337 -0.497604 0.00000
H -0.781337 -0.497215 0.00000

OPBE Pyridine Energy -248.2114029380

C -7.40000e-05 1.39115 1.70000e-05
C -1.20681 0.677053 5.90000e-05
C -1.15606 -0.723596 -0.000292000
N -5.00000e-06 -1.43510 7.10000e-05
C 1.15610 -0.723301 4.80000e-05
C 1.20686 0.676873 -8.00000e-05
H -8.50000e-05 2.48109 0.000135000
H -2.16544 1.19452 0.000201000
H -2.07836 -1.30672 0.000547000
H 2.07832 -1.30658 0.000158000
H 2.16553 1.19427 -5.00000e-05

OPBE Doublet Heme-Pyridine Ligand Energy -1758.7810192200

N -1.39555 1.40764 -0.409839
C -1.22144 2.77925 -0.250637
C -2.49976 3.46273 -0.343424
C -3.44703 2.50479 -0.594222
C -2.75999 1.22531 -0.623762
C -3.39718 0.000811000 -0.756806
C -2.75925 -1.22372 -0.621479
N -1.39317 -1.40506 -0.410412
C -1.21973 -2.77705 -0.238452
C 1.22184 -2.77614 -0.238403
N 1.39423 -1.40402 -0.410329
C 2.76018 -1.22163 -0.621410
C -3.44545 -2.50233 -0.581939
C -2.49791 -3.45955 -0.325046
C -0.00131500 3.42423 -0.121546
C 1.21929 2.78017 -0.250643
N 1.39444 1.40870 -0.409840
C 2.75903 1.22740 -0.623723
C 3.44509 2.50741 -0.594195
C 2.49710 3.46462 -0.343401
C 3.39716 0.00339200 -0.756729
C 3.44734 -2.49972 -0.581884
C 2.50053 -3.45766 -0.325015
H -2.63256 4.53441 -0.251164
H -4.51318 2.63411 -0.741310
H -4.51214 -2.63250 -0.724728
H -2.63209 -4.53022 -0.222773
H 4.51115 2.63753 -0.741268
H 2.62909 4.53641 -0.251136
H 4.51413 -2.62908 -0.724684
H 2.63552 -4.52823 -0.222774
Fe -1.60000e-05 0.00109800 -0.422407

S 0.000191000 0.0454660 -2.65553
H -0.000262000 -1.31321 -2.90764
C 0.00128800 -3.42055 -0.105202
H 0.00168500 -4.50191 0.0199130
H 4.47370 0.00363500 -0.919707
H -0.00172500 4.50673 -0.00723300
H -4.47372 0.000222000 -0.919796
N -1.70000e-05 0.00589000 1.59954
C -1.16820 0.00597400 2.29913
H -2.08039 0.00694700 1.71480
C 1.16816 0.00626500 2.29913
H 2.08035 0.00742500 1.71481
C 1.20288 0.00503000 3.69558
C -1.20291 0.00474000 3.69558
H 2.16515 0.00517100 4.20441
C -2.10000e-05 0.00402600 4.41354
H -2.16519 0.00464200 4.20441
H -1.40000e-05 0.00298900 5.50294

OPBE Heme-Water complex Energy -1586.9733790300

N -1.41992 1.40047 -0.113101
C -2.80266 1.22571 -0.125015
C -3.47736 2.51144 -0.109429
C -2.50158 3.47078 -0.0755420
C -1.22515 2.77802 -0.0752980
C -0.00123300 3.42303 -0.0512030
C 1.22225 2.77618 -0.0719220
N 1.41579 1.39726 -0.107073
C 2.80003 1.22214 -0.132079
C 2.80563 -1.21863 -0.125107
N 1.41691 -1.38996 -0.115748
C 1.22048 -2.77303 -0.0561900
C 2.49882 3.46706 -0.0793870
C 3.47459 2.50715 -0.119956
C -3.46173 0.00798300 -0.131277
C -2.81131 -1.21414 -0.110516
N -1.42468 -1.38875 -0.113734
C -1.23086 -2.77092 -0.0521360
C -2.50742 -3.45864 -0.0294340
C -3.48371 -2.49738 -0.0677250
C -0.00599000 -3.41670 -0.0275800
C 2.49518 -3.46225 -0.0444720
C 3.47425 -2.50293 -0.0894410
H -4.55318 2.64106 -0.118685
H -2.61516 4.54835 -0.0526080
H 2.61330 4.54464 -0.0594350
H 4.55033 2.63692 -0.138812
H -2.62401 -4.53533 0.0156720
H -4.55955 -2.62774 -0.0606810
H 2.61007 -4.53933 -0.00354600
H 4.54975 -2.63664 -0.0932190
Fe -0.00155700 0.0147770 -0.0480240
S -0.0422600 0.0340350 2.17263
H 1.31714 0.0590620 2.42043
C 3.45767 0.00321200 -0.145932
H 4.54605 0.00574400 -0.155657
H -0.00666000 -4.50454 0.0195310
H -4.55005 0.0119180 -0.130007

H -0.000286000 4.51132 -0.0230600
O -0.00872200 -0.0531970 -2.12566
H -0.824416 -0.588992 -2.33017
H 0.776931 -0.631368 -2.33255

OPBE Heme No Ligand Doublet Energy -1510.5671352200

N 1.41729 -1.39909 -0.220421
C 2.79560 -1.23200 -0.301362
C 3.47331 -2.50635 -0.286020
C 2.50317 -3.46522 -0.172202
C 1.23593 -2.77409 -0.134796
C 0.00274700 -3.41444 -0.0731020
C -1.22935 -2.77186 -0.140080
N -1.40855 -1.39620 -0.226587
C -2.78684 -1.22722 -0.315435
C -2.78457 1.23222 -0.315987
N -1.40601 1.39874 -0.226729
C -1.22434 2.77412 -0.140646
C -2.49721 -3.46073 -0.184577
C -3.46589 -2.50052 -0.303621
C 3.44451 -0.00305700 -0.355568
C 2.79783 1.22704 -0.300746
N 1.41979 1.39659 -0.220227
C 1.24092 2.77189 -0.134180
C 2.50943 3.46072 -0.170810
C 3.47786 2.50014 -0.284580
C 0.00887800 3.41447 -0.0730830
C -2.49093 3.46525 -0.185893
C -3.46131 2.50676 -0.304996
H 4.55485 -2.63168 -0.351581
H 2.61639 -4.54928 -0.127218
H -2.61213 -4.54468 -0.141094
H -4.54717 -2.62480 -0.375809
H 2.62460 4.54455 -0.125448
H 4.55966 2.62353 -0.349736
H -2.60389 4.54943 -0.142793
H -4.54232 2.63296 -0.377601
Fe 0.00297400 -1.00000e-05 -0.0247650
S 0.0199970 -0.000178000 2.16676
H -1.32646 0.00153500 2.40149
C -3.43326 0.00308900 -0.373299
H -4.52494 0.00409100 -0.438701
H 0.00956000 4.50630 -0.00924400
H 4.53654 -0.00403600 -0.413548
H 0.00147900 -4.50628 -0.00925600

OPBE Heme Sextet No Ligand Energy -1510.5789197200

N 1.40762 -1.39184 -0.211375
C 2.77617 -1.22549 -0.293937
C 3.45789 -2.49128 -0.285793
C 2.49188 -3.44930 -0.174899
C 1.23163 -2.75844 -0.132068
C 0.00396800 -3.40091 -0.0713870
C -1.22334 -2.75731 -0.135204
N -1.39930 -1.39013 -0.215090
C -2.76817 -1.22416 -0.306138
C -2.76753 1.22557 -0.306367

N	-1.39857	1.39085	-0.215167
C	-1.22193	2.75794	-0.135446
C	-2.48318	-3.44762	-0.184837
C	-3.44927	-2.48981	-0.301515
C	3.42479	-0.000865000	-0.349789
C	2.77681	1.22409	-0.293696
N	1.40834	1.39114	-0.211308
C	1.23304	2.75781	-0.131836
C	2.49365	3.44803	-0.174359
C	3.45918	2.48952	-0.285220
C	0.00569500	3.40091	-0.0713930
C	-2.48141	3.44890	-0.185353
C	-3.44796	2.49158	-0.302070
H	4.53924	-2.61559	-0.356045
H	2.60760	-4.53338	-0.136143
H	-2.59889	-4.53178	-0.147733
H	-4.53007	-2.61474	-0.378833
H	2.60993	4.53205	-0.135430
H	4.54061	2.61328	-0.355273
H	-2.59656	4.53312	-0.148408
H	-4.52869	2.61706	-0.379578
Fe	0.00161500	-9.00000e-06	-0.0187240
S	0.0313150	-4.80000e-05	2.11859
H	-1.30594	0.000657000	2.38876
C	-3.41602	0.000871000	-0.365448
H	-4.50635	0.00115500	-0.434770
H	0.00550000	4.49193	-0.0121190
H	4.51550	-0.00114600	-0.411744
H	0.00321900	-4.49192	-0.0121170

B3LYP Water Energy -76.4169106417

O	0.00000	0.00000	0.00000
H	-0.922641	0.652406	0.00000
H	0.922641	0.652406	0.00000

B3LYP Pyridine Energy -248.3042282930

C	0.00000	1.38700	0.00000
C	1.20000	0.674000	0.00000
C	1.14600	-0.722000	0.00000
N	0.00000	-1.42300	0.00000
C	-1.14600	-0.722000	0.00000
C	-1.20000	0.674000	0.00000
H	0.00100000	2.47000	0.00000
H	2.15500	1.18400	0.00000
H	2.06000	-1.30900	0.00000
H	-2.06100	-1.30700	0.00000
H	-2.15600	1.18200	0.00000

B3LYP Heme-Pyridine Energy -1759.0416209400

N	-1.43409	1.40878	-0.401520
C	-1.26316	2.78458	-0.338530
C	-2.55537	3.44188	-0.409080
C	-3.49709	2.46616	-0.535220
C	-2.79998	1.19236	-0.531160
C	-3.41927	-0.0432800	-0.599270
C	-2.76553	-1.26196	-0.533620

N	-1.39304	-1.44105	-0.410100
C	-1.18478	-2.81309	-0.341680
C	1.26355	-2.77893	-0.343420
N	1.43318	-1.40149	-0.411490
C	2.80015	-1.18406	-0.535780
C	-3.42691	-2.55371	-0.532650
C	-2.45850	-3.50406	-0.406880
C	-0.0482700	3.44261	-0.278200
C	1.18451	2.81866	-0.336780
N	1.39408	1.44819	-0.400000
C	2.76546	1.27022	-0.529410
C	3.42657	2.56305	-0.532550
C	2.45782	3.51193	-0.406450
C	3.41931	0.0526500	-0.599700
C	3.49741	-2.45682	-0.536040
C	2.55605	-3.43394	-0.409980
H	-2.69966	4.50993	-0.379740
H	-4.56568	2.57709	-0.627020
H	-4.49248	-2.69402	-0.619550
H	-2.57481	-4.57543	-0.372840
H	4.49165	2.70393	-0.624010
H	2.57211	4.58359	-0.376750
H	4.56644	-2.56722	-0.623690
H	2.70232	-4.50166	-0.376440
Fe	-2.00000e-05	0.00212000	-0.445380
S	-0.00289000	0.0616500	-2.72059
H	0.0342800	-1.29354	-2.97424
C	0.0483600	-3.43712	-0.282770
H	0.0635100	-4.51999	-0.239330
H	4.49891	0.0681000	-0.695530
H	-0.0633700	4.52559	-0.239730
H	-4.49890	-0.0584800	-0.694840
N	5.00000e-05	-0.00155000	1.66851
C	-1.16576	-0.00992000	2.36076
H	-2.07312	-0.0100800	1.77764
C	1.16603	-0.000310000	2.36052
H	2.07325	0.00604000	1.77722
C	1.20069	-0.00689000	3.75164
C	-1.20006	-0.0171100	3.75190
H	2.15479	-0.00522000	4.26205
C	0.000400000	-0.0155200	4.46270
H	-2.15404	-0.0236100	4.26251
H	0.000550000	-0.0208000	5.54598

B3LYP Heme-Water Energy -1587.1717166900

N	-1.43326	1.41603	-0.125510
C	-2.80979	1.23230	-0.113950
C	-3.47697	2.52136	-0.0920900
C	-2.50644	3.47528	-0.0819200
C	-1.22720	2.78749	-0.0980000
C	-0.000630000	3.42324	-0.0875900
C	1.22574	2.78586	-0.0982400
N	1.43046	1.41336	-0.120450
C	2.80852	1.22856	-0.119340
C	2.81414	-1.21778	-0.118350
N	1.43140	-1.39952	-0.143420
C	1.22357	-2.77697	-0.0887400
C	2.50523	3.47163	-0.0908100

C 3.47569 2.51674 -0.104330
C -3.45945 0.0119800 -0.111310
C -2.81922 -1.21320 -0.112950
N -1.43874 -1.39817 -0.148560
C -1.23355 -2.77503 -0.0884000
C -2.51238 -3.45576 -0.0450100
C -3.48332 -2.49883 -0.0602900
C -0.00580000 -3.41119 -0.0722800
C 2.50079 -3.45965 -0.0542900
C 3.47453 -2.50470 -0.0728800
H -4.54664 2.65490 -0.0820000
H -2.62241 4.54688 -0.0619900
H 2.62247 4.54321 -0.0756200
H 4.54546 2.65036 -0.102680
H -2.63233 -4.52629 0.000520000
H -4.55262 -2.63306 -0.0303000
H 2.61892 -4.53062 -0.0138300
H 4.54367 -2.64232 -0.0515900
Fe -0.000550000 0.0177800 -0.0431300
S -0.0537100 0.00111000 2.21552
H 1.30224 -0.000710000 2.46715
C 3.45646 0.00684000 -0.119750
H 4.54003 0.00946000 -0.105260
H -0.00651000 -4.49429 -0.0271700
H -4.54276 0.0163000 -0.0871600
H 0.000210000 4.50688 -0.0673200
O -0.00246000 -0.0590700 -2.09351
H -0.807380 -0.609630 -2.29660
H 0.802490 -0.609480 -2.29639

B3LYP Heme No Ligand Doublet Energy -1510.7228331500

N 1.42050 -1.40375 -0.222233
C 2.78823 -1.22814 -0.302464
C 3.46721 -2.50068 -0.294025
C 2.50258 -3.45835 -0.188550
C 1.23516 -2.76978 -0.147533
C 0.00463300 -3.40896 -0.0908400
C -1.22619 -2.76977 -0.150701
N -1.41228 -1.40351 -0.224872
C -2.78029 -1.22851 -0.313508
C -2.78039 1.22827 -0.313613
N -1.41240 1.40339 -0.224895
C -1.22644 2.76967 -0.150815
C -2.49286 -3.45854 -0.198367
C -3.45796 -2.50131 -0.308700
C 3.43238 0.000156000 -0.352205
C 2.78812 1.22839 -0.302351
N 1.42038 1.40388 -0.222215
C 1.23491 2.76988 -0.147426
C 2.50228 3.45857 -0.188288
C 3.46700 2.50099 -0.293739
C 0.00432800 3.40896 -0.0908440
C -2.49316 3.45833 -0.198609
C -3.45817 2.50101 -0.308976
H 4.54624 -2.62604 -0.356626
H 2.61982 -4.53944 -0.149412
H -2.60965 -4.53976 -0.161100
H -4.53648 -2.62778 -0.378090

H 2.61942 4.53967 -0.149061
H 4.54602 2.62645 -0.356231
H -2.61004 4.53955 -0.161420
H -4.53669 2.62738 -0.378468
Fe 0.00141100 -8.00000e-06 -0.00775800
S 0.0359490 -3.20000e-05 2.20482
H -1.30323 0.000231000 2.44628
C -3.42432 -0.000148000 -0.367589
H -4.51321 -0.000195000 -0.433445
H 0.00403400 4.49854 -0.0367260
H 4.52168 0.000204000 -0.409962
H 0.00443400 -4.49853 -0.0367250

B3LYP Heme No Ligand Sextet Energy -1510.7334436100

N 1.56267 -1.24205 -0.213860
C 2.90450 -0.917540 -0.268540
C 3.71712 -2.11740 -0.256440
C 2.85933 -3.17173 -0.183610
C 1.51821 -2.62094 -0.159690
C 0.368580 -3.38808 -0.131310
C -0.916680 -2.88056 -0.185240
N -1.25249 -1.54127 -0.234370
C -2.63347 -1.50908 -0.302300
C -2.89598 0.920260 -0.278430
N -1.55333 1.24391 -0.212340
C -1.50860 2.62341 -0.160630
C -2.10910 -3.70235 -0.232500
C -3.17120 -2.85366 -0.310420
C 3.41526 0.366280 -0.311790
C 2.64162 1.51173 -0.288900
N 1.26097 1.54485 -0.230940
C 0.926100 2.88392 -0.179970
C 2.11953 3.70558 -0.218510
C 3.18097 2.85628 -0.291170
C -0.358910 3.39119 -0.129300
C -2.84888 3.17437 -0.193430
C -3.70724 2.12034 -0.271750
H 4.79538 -2.12660 -0.298120
H 3.08785 -4.22605 -0.155490
H -2.10892 -4.78137 -0.214220
H -4.22216 -3.09200 -0.367240
H 2.11994 4.78453 -0.197020
H 4.23258 3.09343 -0.339560
H -3.07701 4.22888 -0.168790
H -4.78513 2.13070 -0.322560
Fe 0.00248000 0.000780000 -0.00969000
S 0.0309200 -0.0122600 2.19642
H -1.30864 -0.0517600 2.41216
C -3.40704 -0.363410 -0.327940
H -4.48386 -0.479400 -0.374520
H -0.473850 4.46858 -0.0918200
H 4.49238 0.482660 -0.348310
H 0.482740 -4.46554 -0.0934800

B3LYP Heme-Pyridine Energy -1759.0416209400

N -1.43409 1.40878 -0.401520
C -1.26316 2.78458 -0.338530

C -2.55537 3.44188 -0.409080
C -3.49709 2.46616 -0.535220
C -2.79998 1.19236 -0.531160
C -3.41927 -0.0432800 -0.599270
C -2.76553 -1.26196 -0.533620
N -1.39304 -1.44105 -0.410100
C -1.18478 -2.81309 -0.341680
C 1.26355 -2.77893 -0.343420
N 1.43318 -1.40149 -0.411490
C 2.80015 -1.18406 -0.535780
C -3.42691 -2.55371 -0.532650
C -2.45850 -3.50406 -0.406880
C -0.0482700 3.44261 -0.278200
C 1.18451 2.81866 -0.336780
N 1.39408 1.44819 -0.400000
C 2.76546 1.27022 -0.529410
C 3.42657 2.56305 -0.532550
C 2.45782 3.51193 -0.406450
C 3.41931 0.0526500 -0.599700
C 3.49741 -2.45682 -0.536040
C 2.55605 -3.43394 -0.409980
H -2.69966 4.50993 -0.379740
H -4.56568 2.57709 -0.627020
H -4.49248 -2.69402 -0.619550
H -2.57481 -4.57543 -0.372840
H 4.49165 2.70393 -0.624010
H 2.57211 4.58359 -0.376750
H 4.56644 -2.56722 -0.623690
H 2.70232 -4.50166 -0.376440
Fe -2.00000e-05 0.00212000 -0.445380
S -0.00289000 0.0616500 -2.72059
H 0.0342800 -1.29354 -2.97424
C 0.0483600 -3.43712 -0.282770
H 0.0635100 -4.51999 -0.239330
H 4.49891 0.0681000 -0.695530
H -0.0633700 4.52559 -0.239730
H -4.49890 -0.0584800 -0.694840
N 5.00000e-05 -0.00155000 1.66851
C -1.16576 -0.00992000 2.36076
H -2.07312 -0.0100800 1.77764
C 1.16603 -0.000310000 2.36052
H 2.07325 0.00604000 1.77722
C 1.20069 -0.00689000 3.75164
C -1.20006 -0.0171100 3.75190
H 2.15479 -0.00522000 4.26205
C 0.000400000 -0.0155200 4.46270
H -2.15404 -0.0236100 4.26251
H 0.000550000 -0.0208000 5.54598

TPSS Triplet Molecular Oxygen Energy -150.3707088940
O 0.00000 0.00000 0.00000
O 1.46000 0.00000 0.00000

TPSS Water Energy -76.4415112070
O 0.00000 0.00000 0.00000
H 0.922641 0.652406 0.00000

H -0.922641 0.652406 0.00000

TPSS Pyridine Energy -248.3539872730

C 0.00000 1.38700 0.00000
C 1.20000 0.674000 0.00000
C 1.14600 -0.722000 0.00000
N 0.00000 -1.42300 0.00000
C -1.14600 -0.722000 0.00000
C -1.20000 0.674000 0.00000
H 0.00100000 2.47000 0.00000
H 2.15500 1.18400 0.00000
H 2.06000 -1.30900 0.00000
H -2.06100 -1.30700 0.00000
H -2.15600 1.18200 0.00000

TPSS Heme Doublet No Ligand Energy -1510.9240188700

N 1.56267 -1.24205 -0.213860
C 2.90450 -0.917540 -0.268540
C 3.71712 -2.11740 -0.256440
C 2.85933 -3.17173 -0.183610
C 1.51821 -2.62094 -0.159690
C 0.368580 -3.38808 -0.131310
C -0.916680 -2.88056 -0.185240
N -1.25249 -1.54127 -0.234370
C -2.63347 -1.50908 -0.302300
C -2.89598 0.920260 -0.278430
N -1.55333 1.24391 -0.212340
C -1.50860 2.62341 -0.160630
C -2.10910 -3.70235 -0.232500
C -3.17120 -2.85366 -0.310420
C 3.41526 0.366280 -0.311790
C 2.64162 1.51173 -0.288900
N 1.26097 1.54485 -0.230940
C 0.926100 2.88392 -0.179970
C 2.11953 3.70558 -0.218510
C 3.18097 2.85628 -0.291170
C -0.358910 3.39119 -0.129300
C -2.84888 3.17437 -0.193430
C -3.70724 2.12034 -0.271750
H 4.79538 -2.12660 -0.298120
H 3.08785 -4.22605 -0.155490
H -2.10892 -4.78137 -0.214220
H -4.22216 -3.09200 -0.367240
H 2.11994 4.78453 -0.197020
H 4.23258 3.09343 -0.339560
H -3.07701 4.22888 -0.168790
H -4.78513 2.13070 -0.322560
Fe 0.00248000 0.000780000 -0.00969000
S 0.0309200 -0.0122600 2.19642
H -1.30864 -0.0517600 2.41216
C -3.40704 -0.363410 -0.327940
H -4.48386 -0.479400 -0.374520
H -0.473850 4.46858 -0.0918200
H 4.49238 0.482660 -0.348310
H 0.482740 -4.46554 -0.0934800

TPSS Heme Sextet No Ligand Energy -1510.9169410200

N	1.56267	-1.24205	-0.213860
C	2.90450	-0.917540	-0.268540
C	3.71712	-2.11740	-0.256440
C	2.85933	-3.17173	-0.183610
C	1.51821	-2.62094	-0.159690
C	0.368580	-3.38808	-0.131310
C	-0.916680	-2.88056	-0.185240
N	-1.25249	-1.54127	-0.234370
C	-2.63347	-1.50908	-0.302300
C	-2.89598	0.920260	-0.278430
N	-1.55333	1.24391	-0.212340
C	-1.50860	2.62341	-0.160630
C	-2.10910	-3.70235	-0.232500
C	-3.17120	-2.85366	-0.310420
C	3.41526	0.366280	-0.311790
C	2.64162	1.51173	-0.288900
N	1.26097	1.54485	-0.230940
C	0.926100	2.88392	-0.179970
C	2.11953	3.70558	-0.218510
C	3.18097	2.85628	-0.291170
C	-0.358910	3.39119	-0.129300
C	-2.84888	3.17437	-0.193430
C	-3.70724	2.12034	-0.271750
H	4.79538	-2.12660	-0.298120
H	3.08785	-4.22605	-0.155490
H	-2.10892	-4.78137	-0.214220
H	-4.22216	-3.09200	-0.367240
H	2.11994	4.78453	-0.197020
H	4.23258	3.09343	-0.339560
H	-3.07701	4.22888	-0.168790
H	-4.78513	2.13070	-0.322560
Fe	0.00248000	0.000780000	-0.00969000
S	0.0309200	-0.0122600	2.19642
H	-1.30864	-0.0517600	2.41216
C	-3.40704	-0.363410	-0.327940
H	-4.48386	-0.479400	-0.374520
H	-0.473850	4.46858	-0.0918200
H	4.49238	0.482660	-0.348310
H	0.482740	-4.46554	-0.0934800

TPSS Heme-Water Energy -1587.3789680300

N	-1.43299	1.42118	-0.115410
C	-2.79802	1.24482	-0.121520
C	-3.47198	2.52333	-0.106180
C	-2.49870	3.47769	-0.0809200
C	-1.23161	2.78104	-0.0834200
C	0.00554000	3.41487	-0.0663200
C	1.23991	2.77484	-0.0837300
N	1.43520	1.41371	-0.112780
C	2.80003	1.23104	-0.127140
C	2.79848	-1.23390	-0.125730
N	1.43016	-1.40941	-0.127890
C	1.22730	-2.77252	-0.0762300
C	2.51003	3.46525	-0.0875400
C	3.47933	2.50639	-0.116340
C	-3.44860	0.0156900	-0.127320
C	-2.80911	-1.21957	-0.117600

N -1.44250 -1.40256 -0.128080
C -1.24714 -2.76634 -0.0734800
C -2.51722 -3.45364 -0.0484000
C -3.48685 -2.49344 -0.0778300
C -0.0117000 -3.40526 -0.0526600
C 2.49352 -3.46640 -0.0589100
C 3.46881 -2.51146 -0.0918700
H -4.55240 2.65377 -0.111380
H -2.60927 4.56021 -0.0617800
H 2.62565 4.54731 -0.0713900
H 4.56025 2.63246 -0.128190
H -2.63483 -4.53493 -0.00907000
H -4.56775 -2.61986 -0.0672700
H 2.60539 -4.54844 -0.0230900
H 4.54900 -2.64443 -0.0885100
Fe 0.000110000 0.0143700 0.00203000
S -0.0509400 0.00256000 2.22489
H 1.28660 0.00765000 2.47223
C 3.44430 -0.00164000 -0.137090
H 4.53539 -0.00232000 -0.138060
H -0.0142800 -4.49566 -0.0107800
H -4.53957 0.0206300 -0.120680
H 0.00838000 4.50575 -0.0429400
O -0.00382000 -0.0229500 -2.22430
H -0.778600 -0.563800 -2.45001
H 0.761750 -0.574510 -2.45519

TPSS Heme FE+2-Pyridine Energy -1759.4275243000

N -1.41924 1.41634 -0.414576
C -1.23950 2.78903 -0.357458
C -2.51195 3.47851 -0.416391
C -3.47721 2.51226 -0.529431
C -2.78850 1.23763 -0.525370
C -3.42831 -0.00125900 -0.589678
C -2.78712 -1.23875 -0.509183
N -1.41736 -1.41569 -0.396985
C -1.23715 -2.78802 -0.325990
C 1.23904 -2.78734 -0.326258
N 1.41801 -1.41494 -0.397114
C 2.78756 -1.23645 -0.509877
C -3.47503 -2.51359 -0.498536
C -2.50922 -3.47854 -0.376448
C -0.00196700 3.43154 -0.304281
C 1.23633 2.79055 -0.357496
N 1.41729 1.41815 -0.414797
C 2.78672 1.24033 -0.525224
C 3.47436 2.51555 -0.528985
C 2.50827 3.48103 -0.416097
C 3.42739 0.00183300 -0.589989
C 3.47664 -2.51067 -0.499695
C 2.51180 -3.47657 -0.377337
H -2.63016 4.56416 -0.390383
H -4.55987 2.63180 -0.611574
H -4.55778 -2.63437 -0.577693
H -2.62715 -4.56388 -0.338007
H 4.55693 2.63607 -0.610884
H 2.62564 4.56676 -0.389961
H 4.55947 -2.63050 -0.579290

H 2.63083 -4.56181 -0.339093
Fe 0.000661000 -0.000586000 -0.406057
S 0.000715000 0.0205320 -2.77142
H 0.00181900 -1.32750 -2.98131
C 0.00114000 -3.42906 -0.268586
H 0.00141600 -4.52355 -0.222610
H 4.51892 0.00150600 -0.680553
H -0.00267700 4.52636 -0.269283
H -4.51983 -0.00260700 -0.680154
N 0.000582000 0.0165050 1.61274
C -1.15976 0.0188780 2.32352
H -2.07429 0.0176530 1.72595
C 1.16089 0.0190780 2.32357
H 2.07547 0.0180020 1.72607
C 1.20094 0.0226420 3.72012
C -1.19986 0.0224210 3.72006
H 2.17228 0.0244910 4.22557
C 0.000526000 0.0241100 4.44540
H -2.17123 0.0240780 4.22548
H 0.000504000 0.0267010 5.54086

TPSS Heme Pyridine Ligand Fe3+ Energy -1759.2999094200

N 1.29744 -1.22356 -0.608358
C 1.00462 -2.57158 -0.717060
C 2.21698 -3.34244 -0.888382
C 3.25306 -2.44706 -0.909819
C 2.67359 -1.13281 -0.730129
C 3.41278 0.0480720 -0.641231
C 2.88309 1.31124 -0.370405
N 1.53873 1.59137 -0.190313
C 1.47955 2.94221 0.108317
C -0.982290 3.14957 0.135256
N -1.27318 1.82895 -0.162638
C -2.64748 1.78085 -0.325603
C 3.67828 2.50476 -0.177850
C 2.80728 3.51554 0.132600
C -0.281515 -3.11155 -0.729896
C -1.45678 -2.36061 -0.711395
N -1.51603 -0.982245 -0.599021
C -2.85806 -0.659612 -0.706801
C -3.65319 -1.85610 -0.884277
C -2.78371 -2.91416 -0.873464
C -3.38581 0.628238 -0.600709
C -3.22734 3.09006 -0.116500
C -2.19395 3.93805 0.183214
H 2.25081 -4.42765 -0.994691
H 4.31966 -2.64176 -1.03183
H 4.76491 2.54520 -0.267762
H 3.02589 4.56287 0.346096
H -4.73847 -1.86692 -0.995996
H -3.00211 -3.97763 -0.980598
H -4.29279 3.31354 -0.189630
H -2.22947 5.00615 0.402608
Fe 0.0128480 0.312135 -0.437322
S 0.0306530 0.610872 -2.64494
H 0.163808 1.96911 -2.69209
C 0.302896 3.66774 0.297248
H 0.395059 4.73316 0.527177

H	-4.46919	0.738188	-0.705101
H	-0.374938	-4.19712	-0.825966
H	4.49780	-0.0276340	-0.758053
N	-0.000664000	-0.00595500	1.65557
C	1.15785	-0.104865	2.34973
H	2.06955	-0.156525	1.74962
C	-1.15764	0.0422740	2.35752
H	-2.07238	0.105814	1.76327
C	-1.19526	0.0420430	3.75532
C	1.20455	-0.112050	3.74715
H	-2.16032	0.0970300	4.26708
C	0.00743200	-0.0296580	4.46915
H	2.17224	-0.181352	4.25221
H	0.0116480	-0.0230070	5.56378