**Supplementary Information for:**

The ins and outs of vanillyl alcohol oxidase: Identification of ligand migration paths

By: Gudrun Gygli, Maria Fátima Lucas, Victor Guallar and Willem J.H. van Berkel

Below template files for all substrate molecules used in this work as well as the FAD molecule and the covalently bound histidine. Partial charges are shown in the highlighted column.

\* LIGAND DATABASE FILE (OPLS2005)

\*

COD 19 19 31 41 82

 1 0 M CA \_C1\_ 1 4.015790 106.814730 -169.999760

 2 1 M CA \_C2\_ 2 1.392050 157.200990 167.214080

 3 1 M CA \_C6\_ 6 1.404820 55.798050 -114.441900

 4 1 M CT \_C7\_ 7 1.506470 69.313010 42.572980

 5 2 M CA \_C3\_ 3 1.396290 121.473090 65.341050

 6 2 M HA \_H1\_ 11 1.093070 119.007610 -114.658950

 7 5 M CA \_C4\_ 4 1.420090 123.555240 0.000000

 8 5 M HA \_H2\_ 12 1.091460 119.649850 -180.000000

 9 7 M CA \_C5\_ 5 1.439550 113.473990 0.000000

 10 7 M OM \_O1\_ 8 1.294310 124.046860 -180.000000

 11 3 M HA \_H3\_ 13 1.089830 118.069920 25.201290

 12 4 M HC \_H7\_ 17 1.097160 111.429780 -22.112930

 13 4 M HC \_H8\_ 18 1.099260 112.540740 97.918590

 14 4 M HC \_H9\_ 19 1.099260 112.540740 -142.144440

 15 9 S OS \_O2\_ 9 1.381090 114.247320 -180.000000

 16 15 S CT \_C8\_ 10 1.409010 116.858470 180.000000

 17 16 S HC \_H4\_ 14 1.093080 107.128750 180.000000

 18 16 S HC \_H5\_ 15 1.100640 111.964490 -60.751220

 19 16 S HC \_H6\_ 16 1.100640 111.964490 60.751220

 13 12 12 7 6 2 6 2 7 1 1 2 1 1 4 3 2

 1 1

 2 5 7 9 3 4 15 6 8 11 12 13 14

 5 7 9 3 4 10 6 8 11 12 13 14

 6 4 12 13 14 5 7 10 9 15 16 11

 6 11 12 13 14 5 9

 6 7 9 10 15 8

 8 7

 8 9 10 15 16 11

 10 9

 10 15 16 11 17 18 19

 15

 15

 13 14

 14

 0

 16 17 18 19

 17 18 19

 18 19

 19

 0

NBON

 1 3.5500 0.0700 0.154520 2.5000 1.7750 0.001000000 -0.843144165

 2 3.5500 0.0700 -0.305300 2.0020 1.7750 0.001000000 -0.843144165

 3 3.5500 0.0700 -0.433860 2.0020 1.7750 0.001000000 -0.843144165

 4 3.5000 0.0660 -0.343120 1.9750 1.7500 0.005000000 -0.741685710

 5 3.5500 0.0700 -0.359950 2.0020 1.7750 0.001000000 -0.843144165

 6 2.4200 0.0300 0.156930 1.3810 1.2100 0.030040813 0.268726247

 7 3.5500 0.0700 0.348960 2.5000 1.7750 0.001000000 -0.843144165

 8 2.4200 0.0300 0.141080 1.3810 1.2100 0.030040813 0.268726247

 9 3.5500 0.0700 0.235260 2.5000 1.7750 0.001000000 -0.843144165

 10 3.1500 0.2500 -0.863740 1.7825 1.5750 0.001000000 -0.126889456

 11 2.4200 0.0300 0.178320 1.3810 1.2100 0.030040813 0.268726247

 12 2.5000 0.0300 0.094890 1.4250 1.2500 0.008598240 0.268726247

 13 2.5000 0.0300 0.093800 1.4250 1.2500 0.008598240 0.268726247

 14 2.5000 0.0300 0.093800 1.4250 1.2500 0.008598240 0.268726247

 15 2.9000 0.1400 -0.401180 1.7660 1.5600 0.020110767 -0.896042159

 16 3.5000 0.0660 0.021640 1.9750 1.7500 0.005000000 -0.741685710

 17 2.5000 0.0300 0.083170 1.4250 1.2500 0.008598240 0.268726247

 18 2.5000 0.0300 0.052400 1.4250 1.2500 0.008598240 0.268726247

 19 2.5000 0.0300 0.052400 1.4250 1.2500 0.008598240 0.268726247

BOND

 1 2 469.000 1.400

 1 3 469.000 1.400

 1 4 317.000 1.510

 2 5 469.000 1.400

 2 6 367.000 1.080

 5 7 469.000 1.400

 5 8 367.000 1.080

 7 9 469.000 1.400

 7 10 450.000 1.364

 9 3 469.000 1.400

 9 15 450.000 1.364

 3 11 367.000 1.080

 4 12 340.000 1.090

 4 13 340.000 1.090

 4 14 340.000 1.090

 15 16 320.000 1.410

 16 17 340.000 1.090

 16 18 340.000 1.090

 16 19 340.000 1.090

THET

 1 2 5 63.00000 120.00000

 1 2 6 35.00000 120.00000

 1 3 9 63.00000 120.00000

 1 3 11 35.00000 120.00000

 1 4 12 35.00000 109.50000

 1 4 13 35.00000 109.50000

 1 4 14 35.00000 109.50000

 2 5 7 63.00000 120.00000

 2 5 8 35.00000 120.00000

 5 7 9 63.00000 120.00000

 5 7 10 70.00000 120.00000

 7 9 3 63.00000 120.00000

 7 9 15 70.00000 120.00000

 9 3 11 35.00000 120.00000

 9 15 16 75.00000 111.00000

 3 1 2 63.00000 120.00000

 4 1 2 70.00000 120.00000

 4 1 3 70.00000 120.00000

 10 7 9 70.00000 120.00000

 15 9 3 70.00000 120.00000

 15 16 17 35.00000 109.50000

 15 16 18 35.00000 109.50000

 15 16 19 35.00000 109.50000

 6 2 5 35.00000 120.00000

 8 5 7 35.00000 120.00000

 18 16 17 33.00000 107.80000

 19 16 17 33.00000 107.80000

 19 16 18 33.00000 107.80000

 13 4 12 33.00000 107.80000

 14 4 12 33.00000 107.80000

 14 4 13 33.00000 107.80000

PHI

 1 2 5 7 3.62500 -1.0 2.0

 1 2 5 8 3.62500 -1.0 2.0

 2 1 3 9 3.62500 -1.0 2.0

 2 1 3 11 3.62500 -1.0 2.0

 2 1 4 12 0.00000 1.0 1.0

 2 1 4 13 0.00000 1.0 1.0

 2 1 4 14 0.00000 1.0 1.0

 2 5 -7 9 3.62500 -1.0 2.0

 2 5 7 10 3.62500 -1.0 2.0

 5 7 9 3 3.62500 -1.0 2.0

 5 7 9 15 3.62500 -1.0 2.0

 7 9 -3 1 3.62500 -1.0 2.0

 7 9 3 11 3.62500 -1.0 2.0

 7 9 15 16 1.95800 -1.0 2.0

 9 15 16 17 0.08050 1.0 3.0

 9 15 16 18 0.08050 1.0 3.0

 9 15 16 19 0.08050 1.0 3.0

 3 1 -2 5 3.62500 -1.0 2.0

 3 1 2 6 3.62500 -1.0 2.0

 3 1 4 12 0.00000 1.0 1.0

 3 1 4 13 0.00000 1.0 1.0

 3 1 4 14 0.00000 1.0 1.0

 3 9 15 16 1.95800 -1.0 2.0

 4 1 2 5 3.62500 -1.0 2.0

 4 1 2 6 3.62500 -1.0 2.0

 4 1 3 9 3.62500 -1.0 2.0

 4 1 3 11 3.62500 -1.0 2.0

 10 7 9 3 3.62500 -1.0 2.0

 10 7 9 15 3.62500 -1.0 2.0

 15 9 3 1 3.62500 -1.0 2.0

 15 9 3 11 3.62500 -1.0 2.0

 6 2 5 7 3.62500 -1.0 2.0

 6 2 5 8 3.62500 -1.0 2.0

 8 5 7 9 3.62500 -1.0 2.0

 8 5 7 10 3.62500 -1.0 2.0

IPHI

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 5 6 2 1 1.10000 -1.0 2.0

 7 8 5 2 1.10000 -1.0 2.0

 9 10 7 5 4.00000 -1.0 2.0

 3 15 9 7 4.00000 -1.0 2.0

 9 11 3 1 1.10000 -1.0 2.0

END

\* LIGAND DATABASE FILE (OPLS2005)

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COP 20 20 32 43 86

 1 0 M CA \_C1\_ 1 2.849650 106.090450 174.217510

 2 1 M CA \_C2\_ 2 1.397800 73.456300 -109.250200

 3 1 M CA \_C6\_ 6 1.403990 148.956230 132.727090

 4 1 M CT \_C7\_ 7 1.512320 56.106510 38.390060

 5 2 M CA \_C3\_ 3 1.396180 121.223510 -148.821460

 6 2 M HA \_H1\_ 8 1.086890 119.590990 31.178540

 7 5 M CA \_C4\_ 4 1.390230 120.122620 0.000000

 8 5 M HA \_H2\_ 9 1.085180 121.387030 -180.000000

 9 7 M CA \_C5\_ 5 1.406420 119.245400 -0.000000

 10 3 M HA \_H3\_ 12 1.084850 119.321290 -74.226970

 11 4 M HC \_H8\_ 18 1.093900 111.498350 143.282700

 12 4 M HC \_H9\_ 19 1.096260 111.484180 -96.486200

 13 4 M HC \_H10 20 1.096260 111.484180 23.051590

 14 7 S OH \_O1\_ 10 1.364420 120.288820 180.000000

 15 14 S HO \_H4\_ 13 0.969600 106.810550 -180.000000

 16 9 S OS \_O2\_ 11 1.377110 113.608660 -180.000000

 17 16 S CT \_C8\_ 14 1.418310 118.234020 -180.000000

 18 17 S HC \_H5\_ 15 1.091120 106.265420 -180.000000

 19 17 S HC \_H6\_ 16 1.097260 111.405400 -61.043720

 20 17 S HC \_H7\_ 17 1.097260 111.405400 61.043720

 13 12 12 7 7 2 7 2 8 1 2 1 1 2 1 4 3

 2 1 1

 2 5 7 9 3 4 6 8 16 10 11 12 13

 5 7 9 3 4 6 8 14 10 11 12 13

 6 4 11 12 13 5 7 9 14 16 10 17

 6 10 11 12 13 5 9

 6 7 9 8 14 16 15

 8 7

 8 9 14 16 10 15 17

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 14 16 10 15 17 18 19 20

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 13

 0

 16 15

 0

 17 18 19 20

 18 19 20

 19 20

 20

 0

NBON

 1 3.5500 0.0700 -0.115000 2.5000 1.7750 0.001000000 -0.843144165

 2 3.5500 0.0700 -0.115000 2.0020 1.7750 0.001000000 -0.843144165

 3 3.5500 0.0700 -0.115000 2.0020 1.7750 0.001000000 -0.843144165

 4 3.5000 0.0660 -0.065000 1.9750 1.7500 0.005000000 -0.741685710

 5 3.5500 0.0700 -0.115000 2.0020 1.7750 0.001000000 -0.843144165

 6 2.4200 0.0300 0.115000 1.3810 1.2100 0.030040813 0.268726247

 7 3.5500 0.0700 0.150000 2.0020 1.7750 0.001000000 -0.843144165

 8 2.4200 0.0300 0.115000 1.3810 1.2100 0.030040813 0.268726247

 9 3.5500 0.0700 0.085000 2.5000 1.7750 0.001000000 -0.843144165

 10 2.4200 0.0300 0.115000 1.3810 1.2100 0.030040813 0.268726247

 11 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 12 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 13 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 14 3.0700 0.1700 -0.585000 1.7660 1.5600 0.021068034 -0.322181743

 15 0.5000 0.0300 0.435000 0.9960 0.8600 0.030040813 -0.651083722

 16 2.9000 0.1400 -0.285000 1.7660 1.5600 0.020110767 -0.896042159

 17 3.5000 0.0660 0.110000 1.9750 1.7500 0.005000000 -0.741685710

 18 2.5000 0.0300 0.030000 1.4250 1.2500 0.008598240 0.268726247

 19 2.5000 0.0300 0.030000 1.4250 1.2500 0.008598240 0.268726247

 20 2.5000 0.0300 0.030000 1.4250 1.2500 0.008598240 0.268726247

BOND

 1 2 469.000 1.400

 1 3 469.000 1.400

 1 4 317.000 1.510

 2 5 469.000 1.400

 2 6 367.000 1.080

 5 7 469.000 1.400

 5 8 367.000 1.080

 7 9 469.000 1.400

 7 14 450.000 1.364

 9 3 469.000 1.400

 9 16 450.000 1.364

 3 10 367.000 1.080

 4 11 340.000 1.090

 4 12 340.000 1.090

 4 13 340.000 1.090

 14 15 553.000 0.945

 16 17 320.000 1.410

 17 18 340.000 1.090

 17 19 340.000 1.090

 17 20 340.000 1.090

THET

 1 2 5 63.00000 120.00000

 1 2 6 35.00000 120.00000

 1 3 9 63.00000 120.00000

 1 3 10 35.00000 120.00000

 1 4 11 35.00000 109.50000

 1 4 12 35.00000 109.50000

 1 4 13 35.00000 109.50000

 2 5 7 63.00000 120.00000

 2 5 8 35.00000 120.00000

 5 7 9 63.00000 120.00000

 5 7 14 70.00000 120.00000

 7 9 3 63.00000 120.00000

 7 9 16 70.00000 120.00000

 7 14 15 35.00000 113.00000

 9 3 10 35.00000 120.00000

 9 16 17 75.00000 111.00000

 3 1 2 63.00000 120.00000

 4 1 2 70.00000 120.00000

 4 1 3 70.00000 120.00000

 6 2 5 35.00000 120.00000

 8 5 7 35.00000 120.00000

 14 7 9 70.00000 120.00000

 16 9 3 70.00000 120.00000

 16 17 18 35.00000 109.50000

 16 17 19 35.00000 109.50000

 16 17 20 35.00000 109.50000

 19 17 18 33.00000 107.80000

 20 17 18 33.00000 107.80000

 20 17 19 33.00000 107.80000

 12 4 11 33.00000 107.80000

 13 4 11 33.00000 107.80000

 13 4 12 33.00000 107.80000

PHI

 1 2 5 7 3.62500 -1.0 2.0

 1 2 5 8 3.62500 -1.0 2.0

 2 1 3 9 3.62500 -1.0 2.0

 2 1 3 10 3.62500 -1.0 2.0

 2 1 4 11 0.00000 1.0 1.0

 2 1 4 12 0.00000 1.0 1.0

 2 1 4 13 0.00000 1.0 1.0

 2 5 -7 9 3.62500 -1.0 2.0

 2 5 7 14 3.62500 -1.0 2.0

 5 7 9 3 3.62500 -1.0 2.0

 5 7 9 16 3.62500 -1.0 2.0

 5 7 14 15 0.84100 -1.0 2.0

 7 9 -3 1 3.62500 -1.0 2.0

 7 9 3 10 3.62500 -1.0 2.0

 7 9 16 17 1.95800 -1.0 2.0

 9 7 14 15 0.84100 -1.0 2.0

 9 16 17 18 0.08050 1.0 3.0

 9 16 17 19 0.08050 1.0 3.0

 9 16 17 20 0.08050 1.0 3.0

 3 1 -2 5 3.62500 -1.0 2.0

 3 1 2 6 3.62500 -1.0 2.0

 3 1 4 11 0.00000 1.0 1.0

 3 1 4 12 0.00000 1.0 1.0

 3 1 4 13 0.00000 1.0 1.0

 3 9 16 17 1.95800 -1.0 2.0

 4 1 2 5 3.62500 -1.0 2.0

 4 1 2 6 3.62500 -1.0 2.0

 4 1 3 9 3.62500 -1.0 2.0

 4 1 3 10 3.62500 -1.0 2.0

 6 2 5 7 3.62500 -1.0 2.0

 6 2 5 8 3.62500 -1.0 2.0

 8 5 7 9 3.62500 -1.0 2.0

 8 5 7 14 3.62500 -1.0 2.0

 14 7 9 3 3.62500 -1.0 2.0

 14 7 9 16 3.62500 -1.0 2.0

 16 9 3 1 3.62500 -1.0 2.0

 16 9 3 10 3.62500 -1.0 2.0

IPHI

 3 4 1 2 4.00000 -1.0 2.0

 5 6 2 1 1.10000 -1.0 2.0

 7 8 5 2 1.10000 -1.0 2.0

 9 14 7 5 4.00000 -1.0 2.0

 3 16 9 7 4.00000 -1.0 2.0

 9 10 3 1 1.10000 -1.0 2.0

END

\* LIGAND DATABASE FILE (OPLS2005)

\*

VAD 20 20 32 44 87

 1 0 M CA \_C2\_ 2 2.900133 102.726631 -179.105004

 2 1 M CA \_C1\_ 1 1.394220 86.328799 -122.749318

 3 2 M CA \_C6\_ 6 1.398280 119.034327 -150.748894

 4 1 M CA \_C3\_ 3 1.393340 141.212691 99.224453

 5 1 M HA \_H1\_ 8 1.090610 43.465564 19.090134

 6 4 M CA \_C4\_ 4 1.387770 120.041970 128.882547

 7 4 M HA \_H2\_ 9 1.089140 121.119380 -51.117453

 8 6 M CA \_C5\_ 5 1.403260 119.390170 0.000000

 9 6 M OM \_O1\_ 10 1.363330 119.955390 -180.000000

 10 3 M HA \_H3\_ 12 1.086630 119.314680 -180.000000

 11 2 S CT \_C7\_ 7 1.509610 118.469191 29.251117

 12 11 S OH \_O3\_ 17 1.413970 111.711330 -180.000000

 13 11 S HC \_H8\_ 19 1.103650 108.676400 -57.335850

 14 11 S HC \_H9\_ 20 1.103650 108.676400 57.335840

 15 12 S HO \_H7\_ 18 0.970490 107.596400 -180.000000

 16 8 S OS \_O2\_ 11 1.362980 113.778650 180.000000

 17 16 S CT \_C8\_ 13 1.416370 118.236170 -180.000000

 18 17 S HC \_H4\_ 14 1.092670 106.412710 -180.000000

 19 17 S HC \_H5\_ 15 1.098260 111.237870 -61.041590

 20 17 S HC \_H6\_ 16 1.098260 111.237870 61.041590

 13 13 12 7 3 6 2 8 1 2 4 3 2 1 1 4 3

 2 1 1

 2 4 6 8 3 11 5 7 9 10 12 13 14

 4 6 8 3 11 5 7 16 10 12 15 13 14

 5 11 13 14 4 12 6 9 8 16 10 17

 5 11 6 8 7 9 16

 7 11 6

 7 8 9 16 10 17

 9 8

 11 9 16 10 17 18 19 20

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 11 16

 12 15 13 14

 13 14 15

 14 15

 15

 0

 17 18 19 20

 18 19 20

 19 20

 20

 0

NBON

 1 3.5500 0.0700 -0.325440 2.0020 1.7750 0.001000000 -0.843144165

 2 3.5500 0.0700 0.087160 2.5000 1.7750 0.001000000 -0.843144165

 3 3.5500 0.0700 -0.298210 2.0020 1.7750 0.001000000 -0.843144165

 4 3.5500 0.0700 -0.184850 2.0020 1.7750 0.001000000 -0.843144165

 5 2.4200 0.0300 0.166260 1.3810 1.2100 0.030040813 0.268726247

 6 3.5500 0.0700 0.192690 2.5000 1.7750 0.001000000 -0.843144165

 7 2.4200 0.0300 0.174580 1.3810 1.2100 0.030040813 0.268726247

 8 3.5500 0.0700 0.198920 2.5000 1.7750 0.001000000 -0.843144165

 9 3.1500 0.2500 -0.597340 1.7825 1.5750 0.001000000 -0.126889456

 10 2.4200 0.0300 0.167800 1.3810 1.2100 0.030040813 0.268726247

 11 3.5000 0.0660 0.257980 1.9750 1.7500 0.005000000 -0.741685710

 12 3.1200 0.1700 -0.718950 1.7660 1.5600 0.021068034 -0.322181743

 13 2.5000 0.0300 0.017500 1.4250 1.2500 0.008598240 0.268726247

 14 2.5000 0.0300 0.017500 1.4250 1.2500 0.008598240 0.268726247

 15 0.5000 0.0300 0.472940 0.9960 0.8600 0.030040813 -0.651083722

 16 2.9000 0.1400 -0.273610 1.7660 1.5600 0.020110767 -0.896042159

 17 3.5000 0.0660 -0.164910 1.9750 1.7500 0.005000000 -0.741685710

 18 2.5000 0.0300 0.136180 1.4250 1.2500 0.008598240 0.268726247

 19 2.5000 0.0300 0.114830 1.4250 1.2500 0.008598240 0.268726247

 20 2.5000 0.0300 0.114830 1.4250 1.2500 0.008598240 0.268726247

BOND

 2 1 469.000 1.400

 2 3 469.000 1.400

 2 11 317.000 1.510

 1 4 469.000 1.400

 1 5 367.000 1.080

 4 6 469.000 1.400

 4 7 367.000 1.080

 6 8 469.000 1.400

 6 9 450.000 1.364

 8 3 469.000 1.400

 8 16 450.000 1.364

 3 10 367.000 1.080

 11 12 320.000 1.410

 11 13 340.000 1.090

 11 14 340.000 1.090

 16 17 320.000 1.410

 17 18 340.000 1.090

 17 19 340.000 1.090

 17 20 340.000 1.090

 12 15 553.000 0.945

THET

 2 1 4 63.00000 120.00000

 2 1 5 35.00000 120.00000

 2 3 8 63.00000 120.00000

 2 3 10 35.00000 120.00000

 2 11 12 90.00000 112.51600

 2 11 13 35.00000 109.50000

 2 11 14 35.00000 109.50000

 1 4 6 63.00000 120.00000

 1 4 7 35.00000 120.00000

 4 6 8 63.00000 120.00000

 4 6 9 70.00000 120.00000

 6 8 3 63.00000 120.00000

 6 8 16 70.00000 120.00000

 8 3 10 35.00000 120.00000

 8 16 17 75.00000 111.00000

 3 2 1 63.00000 120.00000

 11 2 1 70.00000 120.00000

 11 2 3 70.00000 120.00000

 11 12 15 55.00000 108.50000

 5 1 4 35.00000 120.00000

 7 4 6 35.00000 120.00000

 9 6 8 70.00000 120.00000

 16 8 3 70.00000 120.00000

 16 17 18 35.00000 109.50000

 16 17 19 35.00000 109.50000

 16 17 20 35.00000 109.50000

 19 17 18 33.00000 107.80000

 20 17 18 33.00000 107.80000

 20 17 19 33.00000 107.80000

 13 11 12 35.00000 109.50000

 14 11 12 35.00000 109.50000

 14 11 13 33.00000 107.80000

PHI

 2 1 4 6 3.62500 -1.0 2.0

 2 1 4 7 3.62500 -1.0 2.0

 2 11 12 15 0.31900 1.0 1.0

 2 11 12 15 -0.11800 -1.0 2.0

 2 11 12 15 0.38750 1.0 3.0

 1 2 3 8 3.62500 -1.0 2.0

 1 2 3 10 3.62500 -1.0 2.0

 1 2 11 12 0.14300 -1.0 2.0

 1 2 11 12 0.00300 1.0 3.0

 1 2 11 13 0.00000 1.0 1.0

 1 2 11 14 0.00000 1.0 1.0

 1 4 -6 8 3.62500 -1.0 2.0

 1 4 6 9 3.62500 -1.0 2.0

 4 6 8 3 3.62500 -1.0 2.0

 4 6 8 16 3.62500 -1.0 2.0

 6 8 -3 2 3.62500 -1.0 2.0

 6 8 3 10 3.62500 -1.0 2.0

 6 8 16 17 1.95800 -1.0 2.0

 8 16 17 18 0.08050 1.0 3.0

 8 16 17 19 0.08050 1.0 3.0

 8 16 17 20 0.08050 1.0 3.0

 3 2 -1 4 3.62500 -1.0 2.0

 3 2 1 5 3.62500 -1.0 2.0

 3 2 11 12 0.14300 -1.0 2.0

 3 2 11 12 0.00300 1.0 3.0

 3 2 11 13 0.00000 1.0 1.0

 3 2 11 14 0.00000 1.0 1.0

 3 8 16 17 1.95800 -1.0 2.0

 11 2 1 4 3.62500 -1.0 2.0

 11 2 1 5 3.62500 -1.0 2.0

 11 2 3 8 3.62500 -1.0 2.0

 11 2 3 10 3.62500 -1.0 2.0

 5 1 4 6 3.62500 -1.0 2.0

 5 1 4 7 3.62500 -1.0 2.0

 7 4 6 8 3.62500 -1.0 2.0

 7 4 6 9 3.62500 -1.0 2.0

 9 6 8 3 3.62500 -1.0 2.0

 9 6 8 16 3.62500 -1.0 2.0

 16 8 3 2 3.62500 -1.0 2.0

 16 8 3 10 3.62500 -1.0 2.0

 13 11 12 15 0.19450 1.0 3.0

 14 11 12 15 0.19450 1.0 3.0

IPHI

 3 11 2 1 4.00000 -1.0 2.0

 4 5 1 2 1.10000 -1.0 2.0

 6 7 4 1 1.10000 -1.0 2.0

 8 9 6 4 4.00000 -1.0 2.0

 3 16 8 6 4.00000 -1.0 2.0

 8 10 3 2 1.10000 -1.0 2.0

END

\* LIGAND DATABASE FILE (OPLS2005)

\*

VAP 21 21 33 46 91

 1 0 M CA \_C2\_ 2 2.900133 102.726631 -179.105004

 2 1 M CA \_C1\_ 1 1.394220 86.328799 -122.749318

 3 2 M CA \_C6\_ 6 1.398280 119.034327 -150.748894

 4 1 M CA \_C3\_ 3 1.393340 141.212691 99.224453

 5 1 M HA \_H1\_ 8 1.090610 43.465564 19.090134

 6 4 M CA \_C4\_ 4 1.387770 120.041970 128.882547

 7 4 M HA \_H2\_ 9 1.089140 121.119380 -51.117453

 8 6 M CA \_C5\_ 5 1.403260 119.390170 0.000000

 9 3 M HA \_H3\_ 12 1.086630 119.314680 -180.000000

 10 2 S CT \_C7\_ 7 1.509610 118.469191 29.251117

 11 10 S OH \_O3\_ 18 1.413970 111.711330 -180.000000

 12 10 S HC \_H9\_ 20 1.103650 108.676400 -57.335850

 13 10 S HC \_H10 21 1.103650 108.676400 57.335840

 14 11 S HO \_H8\_ 19 0.970490 107.596400 -180.000000

 15 6 S OH \_O1\_ 10 1.363330 119.955390 -180.000000

 16 15 S HO \_H4\_ 13 0.973660 109.241500 180.000000

 17 8 S OS \_O2\_ 11 1.362980 113.778650 180.000000

 18 17 S CT \_C8\_ 14 1.416370 118.236170 -180.000000

 19 18 S HC \_H5\_ 15 1.092670 106.412710 -180.000000

 20 18 S HC \_H6\_ 16 1.098260 111.237870 -61.041590

 21 18 S HC \_H7\_ 17 1.098260 111.237870 61.041590

 13 13 12 8 3 7 2 9 2 4 3 2 1 1 2 1 4

 3 2 1 1

 2 4 6 8 3 10 5 7 15 9 11 12 13

 4 6 8 3 10 5 7 17 9 11 14 12 13

 5 10 12 13 4 11 6 8 15 17 9 18

 5 10 6 8 7 15 17 16

 7 10 6

 7 8 15 17 9 16 18

 15 8

 10 15 17 9 16 18 19 20 21

 10 17

 11 14 12 13

 12 13 14

 13 14

 14

 0

 17 16

 0

 18 19 20 21

 19 20 21

 20 21

 21

 0

NBON

 1 3.5500 0.0700 -0.325440 2.0020 1.7750 0.001000000 -0.843144165

 2 3.5500 0.0700 0.087160 2.5000 1.7750 0.001000000 -0.843144165

 3 3.5500 0.0700 -0.298210 2.0020 1.7750 0.001000000 -0.843144165

 4 3.5500 0.0700 -0.184850 2.0020 1.7750 0.001000000 -0.843144165

 5 2.4200 0.0300 0.166260 1.3810 1.2100 0.030040813 0.268726247

 6 3.5500 0.0700 0.192690 2.0020 1.7750 0.001000000 -0.843144165

 7 2.4200 0.0300 0.174580 1.3810 1.2100 0.030040813 0.268726247

 8 3.5500 0.0700 0.198920 2.5000 1.7750 0.001000000 -0.843144165

 9 2.4200 0.0300 0.167800 1.3810 1.2100 0.030040813 0.268726247

 10 3.5000 0.0660 0.257980 1.9750 1.7500 0.005000000 -0.741685710

 11 3.1200 0.1700 -0.718950 1.7660 1.5600 0.021068034 -0.322181743

 12 2.5000 0.0300 0.017500 1.4250 1.2500 0.008598240 0.268726247

 13 2.5000 0.0300 0.017500 1.4250 1.2500 0.008598240 0.268726247

 14 0.5000 0.0300 0.472940 0.9960 0.8600 0.030040813 -0.651083722

 15 3.0700 0.1700 -0.597340 1.7660 1.5600 0.021068034 -0.322181743

 16 0.5000 0.0300 0.444150 0.9960 0.8600 0.030040813 -0.651083722

 17 2.9000 0.1400 -0.273610 1.7660 1.5600 0.020110767 -0.896042159

 18 3.5000 0.0660 -0.164910 1.9750 1.7500 0.005000000 -0.741685710

 19 2.5000 0.0300 0.136180 1.4250 1.2500 0.008598240 0.268726247

 20 2.5000 0.0300 0.114830 1.4250 1.2500 0.008598240 0.268726247

 21 2.5000 0.0300 0.114830 1.4250 1.2500 0.008598240 0.268726247

BOND

 2 1 469.000 1.400

 2 3 469.000 1.400

 2 10 317.000 1.510

 1 4 469.000 1.400

 1 5 367.000 1.080

 4 6 469.000 1.400

 4 7 367.000 1.080

 6 8 469.000 1.400

 6 15 450.000 1.364

 8 3 469.000 1.400

 8 17 450.000 1.364

 3 9 367.000 1.080

 10 11 320.000 1.410

 10 12 340.000 1.090

 10 13 340.000 1.090

 15 16 553.000 0.945

 17 18 320.000 1.410

 18 19 340.000 1.090

 18 20 340.000 1.090

 18 21 340.000 1.090

 11 14 553.000 0.945

THET

 2 1 4 63.00000 120.00000

 2 1 5 35.00000 120.00000

 2 3 8 63.00000 120.00000

 2 3 9 35.00000 120.00000

 2 10 11 90.00000 112.51600

 2 10 12 35.00000 109.50000

 2 10 13 35.00000 109.50000

 1 4 6 63.00000 120.00000

 1 4 7 35.00000 120.00000

 4 6 8 63.00000 120.00000

 4 6 15 70.00000 120.00000

 6 8 3 63.00000 120.00000

 6 8 17 70.00000 120.00000

 6 15 16 35.00000 113.00000

 8 3 9 35.00000 120.00000

 8 17 18 75.00000 111.00000

 3 2 1 63.00000 120.00000

 10 2 1 70.00000 120.00000

 10 2 3 70.00000 120.00000

 10 11 14 55.00000 108.50000

 5 1 4 35.00000 120.00000

 7 4 6 35.00000 120.00000

 15 6 8 70.00000 120.00000

 17 8 3 70.00000 120.00000

 17 18 19 35.00000 109.50000

 17 18 20 35.00000 109.50000

 17 18 21 35.00000 109.50000

 20 18 19 33.00000 107.80000

 21 18 19 33.00000 107.80000

 21 18 20 33.00000 107.80000

 12 10 11 35.00000 109.50000

 13 10 11 35.00000 109.50000

 13 10 12 33.00000 107.80000

PHI

 2 1 4 6 3.62500 -1.0 2.0

 2 1 4 7 3.62500 -1.0 2.0

 2 10 11 14 0.31900 1.0 1.0

 2 10 11 14 -0.11800 -1.0 2.0

 2 10 11 14 0.38750 1.0 3.0

 1 2 3 8 3.62500 -1.0 2.0

 1 2 3 9 3.62500 -1.0 2.0

 1 2 10 11 0.14300 -1.0 2.0

 1 2 10 11 0.00300 1.0 3.0

 1 2 10 12 0.00000 1.0 1.0

 1 2 10 13 0.00000 1.0 1.0

 1 4 -6 8 3.62500 -1.0 2.0

 1 4 6 15 3.62500 -1.0 2.0

 4 6 8 3 3.62500 -1.0 2.0

 4 6 8 17 3.62500 -1.0 2.0

 4 6 15 16 0.84100 -1.0 2.0

 6 8 -3 2 3.62500 -1.0 2.0

 6 8 3 9 3.62500 -1.0 2.0

 6 8 17 18 1.95800 -1.0 2.0

 8 6 15 16 0.84100 -1.0 2.0

 8 17 18 19 0.08050 1.0 3.0

 8 17 18 20 0.08050 1.0 3.0

 8 17 18 21 0.08050 1.0 3.0

 3 2 -1 4 3.62500 -1.0 2.0

 3 2 1 5 3.62500 -1.0 2.0

 3 2 10 11 0.14300 -1.0 2.0

 3 2 10 11 0.00300 1.0 3.0

 3 2 10 12 0.00000 1.0 1.0

 3 2 10 13 0.00000 1.0 1.0

 3 8 17 18 1.95800 -1.0 2.0

 10 2 1 4 3.62500 -1.0 2.0

 10 2 1 5 3.62500 -1.0 2.0

 10 2 3 8 3.62500 -1.0 2.0

 10 2 3 9 3.62500 -1.0 2.0

 5 1 4 6 3.62500 -1.0 2.0

 5 1 4 7 3.62500 -1.0 2.0

 7 4 6 8 3.62500 -1.0 2.0

 7 4 6 15 3.62500 -1.0 2.0

 15 6 8 3 3.62500 -1.0 2.0

 15 6 8 17 3.62500 -1.0 2.0

 17 8 3 2 3.62500 -1.0 2.0

 17 8 3 9 3.62500 -1.0 2.0

 12 10 11 14 0.19450 1.0 3.0

 13 10 11 14 0.19450 1.0 3.0

IPHI

 3 10 2 1 4.00000 -1.0 2.0

 4 5 1 2 1.10000 -1.0 2.0

 6 7 4 1 1.10000 -1.0 2.0

 8 15 6 4 4.00000 -1.0 2.0

 3 17 8 6 4.00000 -1.0 2.0

 8 9 3 2 1.10000 -1.0 2.0

END

\* LIGAND DATABASE FILE (OPLS2005)

\*

VND 18 18 28 40 76

 1 0 M CA \_C2\_ 2 3.064368 116.227442 142.323089

 2 1 M CA \_C1\_ 1 1.405080 77.217801 83.574396

 3 2 M CA \_C6\_ 6 1.418560 118.414709 151.755930

 4 1 M CA \_C3\_ 3 1.379200 148.232770 -146.797288

 5 1 M HA \_H1\_ 8 1.092380 49.699899 -63.469015

 6 4 M CA \_C4\_ 4 1.431000 122.603550 -118.765641

 7 4 M HA \_H2\_ 9 1.089810 120.908130 61.234359

 8 6 M CA \_C5\_ 5 1.456220 114.909680 -0.000000

 9 6 M OM \_O1\_ 10 1.270190 123.474750 -180.000000

 10 3 M HA \_H3\_ 12 1.088040 117.378450 -180.000000

 11 2 S CO4 \_C7\_ 7 1.434090 120.449883 -28.244062

 12 11 S O \_O3\_ 17 1.237290 126.682500 -180.000000

 13 11 S HC \_H7\_ 18 1.115380 113.836570 0.000000

 14 8 S OS \_O2\_ 11 1.370380 113.528550 -180.000000

 15 14 S CT \_C8\_ 13 1.411200 116.547750 180.000000

 16 15 S HC \_H4\_ 14 1.092350 106.989600 -180.000000

 17 15 S HC \_H5\_ 15 1.099930 111.661320 -60.706860

 18 15 S HC \_H6\_ 16 1.099930 111.661320 60.706860

 12 11 11 7 3 6 2 8 1 2 2 1 1 4 3 2 1

 1

 2 4 6 8 3 11 5 7 9 10 12 13

 4 6 8 3 11 5 7 14 10 12 13

 5 11 12 13 4 6 9 8 14 10 15

 5 11 6 8 7 9 14

 7 11 6

 7 8 9 14 10 15

 9 8

 11 9 14 10 15 16 17 18

 14

 11 14

 12 13

 13

 0

 15 16 17 18

 16 17 18

 17 18

 18

 0

NBON

 1 3.5500 0.0700 -0.185410 2.0020 1.7750 0.001000000 -0.843144165

 2 3.5500 0.0700 -0.202540 2.5000 1.7750 0.001000000 -0.843144165

 3 3.5500 0.0700 -0.199980 2.0020 1.7750 0.001000000 -0.843144165

 4 3.5500 0.0700 -0.352040 2.0020 1.7750 0.001000000 -0.843144165

 5 2.4200 0.0300 0.159200 1.3810 1.2100 0.030040813 0.268726247

 6 3.5500 0.0700 0.463890 2.5000 1.7750 0.001000000 -0.843144165

 7 2.4200 0.0300 0.141020 1.3810 1.2100 0.030040813 0.268726247

 8 3.5500 0.0700 0.167460 2.5000 1.7750 0.001000000 -0.843144165

 9 3.1500 0.2500 -0.787180 1.7825 1.5750 0.001000000 -0.126889456

 10 2.4200 0.0300 0.137730 1.3810 1.2100 0.030040813 0.268726247

 11 3.7500 0.1050 0.475400 2.1120 1.8750 0.001000000 -0.126889456

 12 2.9600 0.2100 -0.623400 1.6780 1.4800 0.001000000 -0.126889456

 13 2.4200 0.0150 -0.030880 1.3810 1.2100 0.008598240 0.268726247

 14 2.9000 0.1400 -0.384990 1.7660 1.5600 0.020110767 -0.896042159

 15 3.5000 0.0660 0.013050 1.9750 1.7500 0.005000000 -0.741685710

 16 2.5000 0.0300 0.091700 1.4250 1.2500 0.008598240 0.268726247

 17 2.5000 0.0300 0.058480 1.4250 1.2500 0.008598240 0.268726247

 18 2.5000 0.0300 0.058480 1.4250 1.2500 0.008598240 0.268726247

BOND

 2 1 469.000 1.400

 2 3 469.000 1.400

 2 11 310.000 1.470

 1 4 469.000 1.400

 1 5 367.000 1.080

 4 6 469.000 1.400

 4 7 367.000 1.080

 6 8 469.000 1.400

 6 9 450.000 1.364

 8 3 469.000 1.400

 8 14 450.000 1.364

 3 10 367.000 1.080

 11 12 570.000 1.229

 11 13 340.000 1.090

 14 15 320.000 1.410

 15 16 340.000 1.090

 15 17 340.000 1.090

 15 18 340.000 1.090

THET

 2 1 4 63.00000 120.00000

 2 1 5 35.00000 120.00000

 2 3 8 63.00000 120.00000

 2 3 10 35.00000 120.00000

 2 11 12 75.00000 123.78400

 2 11 13 35.00000 115.00000

 1 4 6 63.00000 120.00000

 1 4 7 35.00000 120.00000

 4 6 8 63.00000 120.00000

 4 6 9 70.00000 120.00000

 6 8 3 63.00000 120.00000

 6 8 14 70.00000 120.00000

 8 3 10 35.00000 120.00000

 8 14 15 75.00000 111.00000

 3 2 1 63.00000 120.00000

 11 2 1 60.00000 119.52600

 11 2 3 60.00000 119.52600

 5 1 4 35.00000 120.00000

 7 4 6 35.00000 120.00000

 9 6 8 70.00000 120.00000

 14 8 3 70.00000 120.00000

 14 15 16 35.00000 109.50000

 14 15 17 35.00000 109.50000

 14 15 18 35.00000 109.50000

 17 15 16 33.00000 107.80000

 18 15 16 33.00000 107.80000

 18 15 17 33.00000 107.80000

 13 11 12 35.00000 123.00000

PHI

 2 1 4 6 3.62500 -1.0 2.0

 2 1 4 7 3.62500 -1.0 2.0

 1 2 3 8 3.62500 -1.0 2.0

 1 2 3 10 3.62500 -1.0 2.0

 1 2 11 12 1.05000 -1.0 2.0

 1 2 11 13 1.00000 -1.0 2.0

 1 4 -6 8 3.62500 -1.0 2.0

 1 4 6 9 3.62500 -1.0 2.0

 4 6 8 3 3.62500 -1.0 2.0

 4 6 8 14 3.62500 -1.0 2.0

 6 8 -3 2 3.62500 -1.0 2.0

 6 8 3 10 3.62500 -1.0 2.0

 6 8 14 15 1.95800 -1.0 2.0

 8 14 15 16 0.08050 1.0 3.0

 8 14 15 17 0.08050 1.0 3.0

 8 14 15 18 0.08050 1.0 3.0

 3 2 -1 4 3.62500 -1.0 2.0

 3 2 1 5 3.62500 -1.0 2.0

 3 2 11 12 1.05000 -1.0 2.0

 3 2 11 13 1.00000 -1.0 2.0

 3 8 14 15 1.95800 -1.0 2.0

 11 2 1 4 3.62500 -1.0 2.0

 11 2 1 5 3.62500 -1.0 2.0

 11 2 3 8 3.62500 -1.0 2.0

 11 2 3 10 3.62500 -1.0 2.0

 5 1 4 6 3.62500 -1.0 2.0

 5 1 4 7 3.62500 -1.0 2.0

 7 4 6 8 3.62500 -1.0 2.0

 7 4 6 9 3.62500 -1.0 2.0

 9 6 8 3 3.62500 -1.0 2.0

 9 6 8 14 3.62500 -1.0 2.0

 14 8 3 2 3.62500 -1.0 2.0

 14 8 3 10 3.62500 -1.0 2.0

IPHI

 3 11 2 1 4.00000 -1.0 2.0

 4 5 1 2 1.10000 -1.0 2.0

 6 7 4 1 1.10000 -1.0 2.0

 8 9 6 4 4.00000 -1.0 2.0

 3 14 8 6 4.00000 -1.0 2.0

 8 10 3 2 1.10000 -1.0 2.0

 2 13 11 12 10.50000 -1.0 2.0

END

\* LIGAND DATABASE FILE (OPLS2005)

\*

VNP 19 19 29 42 80

 1 0 M CA \_C2\_ 2 99.411233 59.252189 -41.951782

 2 1 M CA \_C1\_ 1 1.404880 136.359926 -113.464201

 3 2 M CA \_C6\_ 6 1.418380 118.430472 -125.552603

 4 1 M CA \_C3\_ 3 1.379460 88.275489 110.774546

 5 1 M HA \_H1\_ 12 1.092460 45.589870 -26.382699

 6 4 M CA \_C4\_ 4 1.431500 122.566160 145.781207

 7 4 M HA \_H2\_ 13 1.088760 120.941770 -34.164753

 8 6 M CA \_C5\_ 5 1.455980 114.903230 0.048460

 9 3 M HA \_H3\_ 14 1.088570 117.398300 179.991961

 10 2 S CO4 \_C7\_ 7 1.433960 120.455547 54.534365

 11 10 S O \_O3\_ 11 1.237760 126.711700 179.994797

 12 10 S HC \_H7\_ 18 1.115900 113.823060 -0.036503

 13 6 S OH \_O1\_ 8 1.269700 123.472920 -179.972020

 14 13 S HO \_H8\_ 19 0.959830 109.503320 180.000000

 15 8 S OS \_O2\_ 9 1.371050 113.536380 180.000000

 16 15 S CT \_C8\_ 10 1.411270 116.557250 179.951540

 17 16 S HC \_H4\_ 15 1.092290 106.938890 179.955770

 18 16 S HC \_H5\_ 16 1.099240 111.633170 -60.701140

 19 16 S HC \_H6\_ 17 1.100100 111.619120 60.729110

 12 11 11 8 3 7 2 9 2 2 1 1 2 1 4 3 2

 1 1

 2 4 6 8 3 10 13 11 5 7 9 12

 4 6 8 3 10 15 11 5 7 9 12

 10 11 5 12 4 6 8 13 15 16 9

 10 5 6 8 13 15 7 14

 10 7 6

 7 8 13 15 16 9 14

 8 13

 10 13 15 16 9 17 18 19 14

 10 15

 11 12

 12

 0

 15 14

 0

 16 17 18 19

 17 18 19

 18 19

 19

 0

NBON

 1 3.5500 0.0700 -0.115000 2.0020 1.7750 0.001000000 -0.843144165

 2 3.5500 0.0700 -0.115000 2.5000 1.7750 0.001000000 -0.843144165

 3 3.5500 0.0700 -0.115000 2.0020 1.7750 0.001000000 -0.843144165

 4 3.5500 0.0700 -0.115000 2.0020 1.7750 0.001000000 -0.843144165

 5 2.4200 0.0300 0.115000 1.3810 1.2100 0.030040813 0.268726247

 6 3.5500 0.0700 0.150000 2.0020 1.7750 0.001000000 -0.843144165

 7 2.4200 0.0300 0.115000 1.3810 1.2100 0.030040813 0.268726247

 8 3.5500 0.0700 0.085000 2.5000 1.7750 0.001000000 -0.843144165

 9 2.4200 0.0300 0.115000 1.3810 1.2100 0.030040813 0.268726247

 10 3.7500 0.1050 0.565000 2.1120 1.8750 0.001000000 -0.126889456

 11 2.9600 0.2100 -0.450000 1.6780 1.4800 0.001000000 -0.126889456

 12 2.4200 0.0150 0.000000 1.3810 1.2100 0.008598240 0.268726247

 13 3.0700 0.1700 -0.585000 1.7660 1.5600 0.021068034 -0.322181743

 14 0.5000 0.0300 0.435000 0.9960 0.8600 0.030040813 -0.651083722

 15 2.9000 0.1400 -0.285000 1.7660 1.5600 0.020110767 -0.896042159

 16 3.5000 0.0660 0.110000 1.9750 1.7500 0.005000000 -0.741685710

 17 2.5000 0.0300 0.030000 1.4250 1.2500 0.008598240 0.268726247

 18 2.5000 0.0300 0.030000 1.4250 1.2500 0.008598240 0.268726247

 19 2.5000 0.0300 0.030000 1.4250 1.2500 0.008598240 0.268726247

BOND

 2 1 469.000 1.400

 2 3 469.000 1.400

 2 10 310.000 1.470

 1 4 469.000 1.400

 1 5 367.000 1.080

 4 6 469.000 1.400

 4 7 367.000 1.080

 6 8 469.000 1.400

 6 13 450.000 1.364

 8 3 469.000 1.400

 8 15 450.000 1.364

 3 9 367.000 1.080

 10 11 570.000 1.229

 10 12 340.000 1.090

 13 14 553.000 0.945

 15 16 320.000 1.410

 16 17 340.000 1.090

 16 18 340.000 1.090

 16 19 340.000 1.090

THET

 2 1 4 63.00000 120.00000

 2 1 5 35.00000 120.00000

 2 3 8 63.00000 120.00000

 2 3 9 35.00000 120.00000

 2 10 11 75.00000 123.78400

 2 10 12 35.00000 115.00000

 1 4 6 63.00000 120.00000

 1 4 7 35.00000 120.00000

 4 6 8 63.00000 120.00000

 4 6 13 70.00000 120.00000

 6 8 3 63.00000 120.00000

 6 8 15 70.00000 120.00000

 6 13 14 35.00000 113.00000

 8 3 9 35.00000 120.00000

 8 15 16 75.00000 111.00000

 3 2 1 63.00000 120.00000

 10 2 1 60.00000 119.52600

 10 2 3 60.00000 119.52600

 13 6 8 70.00000 120.00000

 15 8 3 70.00000 120.00000

 15 16 17 35.00000 109.50000

 15 16 18 35.00000 109.50000

 15 16 19 35.00000 109.50000

 5 1 4 35.00000 120.00000

 7 4 6 35.00000 120.00000

 18 16 17 33.00000 107.80000

 19 16 17 33.00000 107.80000

 19 16 18 33.00000 107.80000

 12 10 11 35.00000 123.00000

PHI

 2 1 4 6 3.62500 -1.0 2.0

 2 1 4 7 3.62500 -1.0 2.0

 1 2 3 8 3.62500 -1.0 2.0

 1 2 3 9 3.62500 -1.0 2.0

 1 2 10 11 1.05000 -1.0 2.0

 1 2 10 12 1.00000 -1.0 2.0

 1 4 -6 8 3.62500 -1.0 2.0

 1 4 6 13 3.62500 -1.0 2.0

 4 6 8 3 3.62500 -1.0 2.0

 4 6 8 15 3.62500 -1.0 2.0

 4 6 13 14 0.84100 -1.0 2.0

 6 8 -3 2 3.62500 -1.0 2.0

 6 8 3 9 3.62500 -1.0 2.0

 6 8 15 16 1.95800 -1.0 2.0

 8 6 13 14 0.84100 -1.0 2.0

 8 15 16 17 0.08050 1.0 3.0

 8 15 16 18 0.08050 1.0 3.0

 8 15 16 19 0.08050 1.0 3.0

 3 2 -1 4 3.62500 -1.0 2.0

 3 2 1 5 3.62500 -1.0 2.0

 3 2 10 11 1.05000 -1.0 2.0

 3 2 10 12 1.00000 -1.0 2.0

 3 8 15 16 1.95800 -1.0 2.0

 10 2 1 4 3.62500 -1.0 2.0

 10 2 1 5 3.62500 -1.0 2.0

 10 2 3 8 3.62500 -1.0 2.0

 10 2 3 9 3.62500 -1.0 2.0

 13 6 8 3 3.62500 -1.0 2.0

 13 6 8 15 3.62500 -1.0 2.0

 15 8 3 2 3.62500 -1.0 2.0

 15 8 3 9 3.62500 -1.0 2.0

 5 1 4 6 3.62500 -1.0 2.0

 5 1 4 7 3.62500 -1.0 2.0

 7 4 6 8 3.62500 -1.0 2.0

 7 4 6 13 3.62500 -1.0 2.0

IPHI

 3 10 2 1 4.00000 -1.0 2.0

 4 5 1 2 1.10000 -1.0 2.0

 6 7 4 1 1.10000 -1.0 2.0

 8 13 6 4 4.00000 -1.0 2.0

 3 15 8 6 4.00000 -1.0 2.0

 8 9 3 2 1.10000 -1.0 2.0

 2 12 10 11 10.50000 -1.0 2.0

END

\* LIGAND DATABASE FILE (OPLS2005)

\*

FAD 84 89 153 243 444

 1 0 S P1 \_PA\_ 1 128.29359 72.10143 -30.64046

 2 1 S O2Z \_O1A 2 1.48818 153.08600 109.99841

 3 1 S OS \_O2A 3 1.49001 54.44365 -163.11388

 4 3 S HO HO2A 54 0.96000 109.50003 31.42609

 5 1 S OS \_O5B 4 1.59683 60.15034 41.85886

 6 1 S OS \_O3P 53 1.62055 96.91510 -54.03036

 7 5 S CT \_C5B 5 1.30538 130.61222 -40.30041

 8 6 S P2 \_P\_\_ 50 1.62402 130.25431 -142.45319

 9 8 S O2Z \_O1P 51 1.48700 107.62731 149.66378

 10 8 S O2Z \_O2P 52 1.49421 108.99963 18.24207

 11 7 S HC H5B1 55 1.08999 109.41314 53.60794

 12 7 S HC H5B2 56 1.09000 109.41290 -70.15510

 13 7 S CT \_C4B 6 1.50749 106.42524 171.72675

 14 13 S HC \_H4B 57 1.09000 111.53793 73.96642

 15 8 S OS \_O5' 49 1.61410 101.54991 -96.35270

 16 13 S OS \_O4B 7 1.45264 102.11602 -166.79932

 17 13 S CT \_C3B 8 1.53258 113.69829 -53.20877

 18 17 S HC \_H3B 58 1.09000 112.07712 -5.61213

 19 15 S CT \_C5' 48 1.42020 112.70859 -84.31735

 20 19 S HC H5'1 83 1.09000 109.44072 23.15812

 21 19 S HC H5'2 84 1.09000 109.44111 140.91196

 22 17 S OH \_O3B 9 1.43527 110.55829 120.21223

 23 22 S HO HO3B 59 0.96000 109.50041 67.92137

 24 17 S CT \_C2B 10 1.53138 102.88590 -126.20048

 25 24 S HC \_H2B 60 1.09000 111.49937 151.83926

 26 19 S CT \_C4' 46 1.52436 111.34349 -97.96468

 27 26 S HC \_H4' 81 1.09000 108.66714 -17.39737

 28 24 S OH \_O2B 11 1.41359 112.21276 -82.26419

 29 28 S HO HO2B 61 0.96000 109.50022 -180.00000

 30 16 S CO \_C1B 12 1.40854 109.45067 108.45788

 31 30 S HC \_H1B 62 1.09000 108.89794 148.42607

 32 26 S CT \_C3' 44 1.52707 111.68414 -137.25919

 33 32 S HC \_H3' 79 1.08999 108.57269 -162.89345

 34 26 S OH \_O4' 47 1.42391 109.88567 101.38362

 35 34 S HO HO4' 82 0.96000 109.49982 -35.43880

 36 30 S N\* \_N9A 13 1.46651 113.19136 -90.30268

 37 32 S CT \_C2' 42 1.52534 109.48554 78.72676

 38 37 S HC \_H2' 77 1.09000 107.93121 -55.19416

 39 32 S OH \_O3' 45 1.43016 110.36522 -44.00304

 40 39 S HO HO3' 80 0.96000 109.49946 167.68897

 41 36 S CRAB \_C8A 14 1.36748 129.05612 36.44547

 42 41 S HA \_H8A 63 1.08000 120.00015 -0.85707

 43 37 S CT \_C1' 41 1.52805 113.43006 -174.72567

 44 43 S HC H1'1 75 1.09001 109.36145 49.76354

 45 43 S HC H1'2 76 1.09000 109.36121 164.18719

 46 37 S OH \_O2' 43 1.42375 108.61162 61.57705

 47 46 S HO HO2' 78 0.96000 109.49946 -105.68774

 48 41 S NNA \_N7A 15 1.31118 113.49783 179.14271

 49 43 S NE \_N10 39 1.48300 114.04111 -73.02441

 50 48 S C56B \_C5A 16 1.38591 103.98851 -0.54858

 51 49 S CA \_C9A 38 1.37300 120.26651 -92.91675

 52 49 S CDX \_C10 40 1.37243 120.09761 91.51859

 53 50 S CA \_C6A 17 1.41037 132.88213 -179.82086

 54 52 S NI \_N1\_ 23 1.35038 120.01719 -8.03544

 55 53 S NND \_N6A 18 1.33719 123.55292 -0.03956

 56 53 S NB \_N1A 19 1.34969 117.81953 -180.00000

 57 54 S C \_C2\_ 24 1.32424 120.81712 -174.15434

 58 57 S O \_O2\_ 25 1.22990 119.82087 -179.42223

 59 55 S H H6A1 64 1.01000 120.00021 -180.00000

 60 55 S H H6A2 65 1.01001 119.99980 -0.00000

 61 56 S CQ \_C2A 20 1.33777 118.86545 0.02798

 62 61 S HA \_H2A 66 1.07999 120.00001 179.82086

 63 57 S N \_N3\_ 26 1.39036 121.65002 0.75666

 64 63 S H \_HN3 67 1.01000 119.99991 -179.81655

 65 61 S NB \_N3A 21 1.33217 128.64903 -0.18023

 66 63 S C \_C4\_ 27 1.38902 121.52793 0.18345

 67 66 S O \_O4\_ 28 1.23013 120.33953 178.86771

 68 36 S C56A \_C4A 22 1.37164 124.88888 -145.45261

 69 52 S CD \_C4X 29 1.42611 118.97942 178.24654

 70 69 S NI \_N5\_ 30 1.35061 122.15426 -1.78761

 71 70 S CA \_C5X 31 1.34913 118.09812 0.90590

 72 71 S CA \_C6\_ 32 1.40025 117.56966 -178.38723

 73 72 S HA \_H6\_ 68 1.08000 120.00010 -3.65848

 74 72 S CA \_C7\_ 33 1.40107 120.38206 176.34189

 75 74 S CT \_C7M 34 1.50778 120.41451 -180.00000

 76 75 S HC H7M1 69 1.09000 109.50006 180.00000

 77 75 S HC H7M2 70 1.09000 109.50008 -59.99991

 78 75 S HC H7M3 71 1.09000 109.49969 60.00001

 79 74 S CA \_C8\_ 35 1.42619 119.66170 -0.51244

 80 79 S CM \_C8M 36 1.51295 120.30648 179.82754

 81 80 S H H8M1 72 1.09000 109.21423 -124.20875

 82 80 S H H8M2 73 1.09000 109.21425 -13.14448

 83 79 S CA \_C9\_ 37 1.40177 119.51283 0.86048

 84 83 S HA \_H9\_ 74 1.08000 120.00022 -179.51382

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NBON

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 2 2.9800 0.2000 -0.666100 1.6890 1.4900 0.001000000 -0.126889456

 3 2.8500 0.1400 -0.568200 1.7660 1.5600 0.021068034 -0.322181743

 4 0.5000 0.0300 0.380000 0.9960 0.8600 0.030040813 -0.651083722

 5 2.8500 0.1400 -0.461100 1.7660 1.5600 0.020110767 -0.896042159

 6 2.8500 0.1400 -0.500700 1.5900 1.4000 0.020110767 -0.896042159

 7 3.5000 0.0660 0.152900 1.9750 1.7500 0.005000000 -0.741685710

 8 3.7400 0.2000 1.662500 2.1070 1.8700 0.005000000 0.000000000

 9 2.9800 0.2000 -0.970000 1.6890 1.4900 0.001000000 -0.126889456

 10 2.9800 0.2000 -0.970000 1.6890 1.4900 0.001000000 -0.126889456

 11 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 12 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 13 3.5000 0.0660 0.170000 1.9750 1.7500 0.005000000 -0.741685710

 14 2.5000 0.0300 0.030000 1.4250 1.2500 0.008598240 0.268726247

 15 2.8500 0.1400 -0.610000 1.5900 1.4000 0.020110767 -0.896042159

 16 2.9000 0.1400 -0.400000 1.7660 1.5600 0.020110767 -0.896042159

 17 3.5000 0.0660 0.205000 1.9750 1.7500 0.005000000 -0.741685710

 18 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 19 3.5000 0.0660 0.080000 1.9750 1.7500 0.005000000 -0.741685710

 20 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

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 22 3.1200 0.1700 -0.683000 1.7660 1.5600 0.021068034 -0.322181743

 23 0.5000 0.0300 0.418000 0.9960 0.8600 0.030040813 -0.651083722

 24 3.5000 0.0660 0.205000 1.9750 1.7500 0.005000000 -0.741685710

 25 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 26 3.5000 0.0660 0.205000 1.9750 1.7500 0.005000000 -0.741685710

 27 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 28 3.1200 0.1700 -0.683000 1.7660 1.5600 0.021068034 -0.322181743

 29 0.5000 0.0300 0.418000 0.9960 0.8600 0.030040813 -0.651083722

 30 3.5000 0.0660 0.450000 1.9750 1.7500 0.005000000 -0.741685710

 31 2.5000 0.0500 0.100000 1.4250 1.2500 0.008598240 0.268726247

 32 3.5000 0.0660 0.205000 1.9750 1.7500 0.005000000 -0.741685710

 33 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 34 3.1200 0.1700 -0.683000 1.7660 1.5600 0.021068034 -0.322181743

 35 0.5000 0.0300 0.418000 0.9960 0.8600 0.030040813 -0.651083722

 36 3.2500 0.1700 -0.500000 1.8000 1.6000 0.001000000 -0.511443539

 37 3.5000 0.0660 0.205000 1.9750 1.7500 0.005000000 -0.741685710

 38 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

 39 3.1200 0.1700 -0.683000 1.7660 1.5600 0.021068034 -0.322181743

 40 0.5000 0.0300 0.418000 0.9960 0.8600 0.030040813 -0.651083722

 41 3.5000 0.0800 0.200000 2.0020 1.7750 0.001000000 -0.843144165

 42 2.5000 0.0500 0.200000 1.3810 1.2100 0.030040813 0.268726247

 43 3.5000 0.0660 0.002500 1.9750 1.7500 0.005000000 -0.741685710

 44 2.5000 0.0150 0.060000 1.4250 1.2500 0.008598240 0.268726247

 45 2.5000 0.0150 0.060000 1.4250 1.2500 0.008598240 0.268726247

 46 3.1200 0.1700 -0.683000 1.7660 1.5600 0.021068034 -0.322181743

 47 0.5000 0.0300 0.418000 0.9960 0.8600 0.030040813 -0.651083722

 48 3.2500 0.1700 -0.490000 1.8000 1.6000 0.001000000 -0.511443539

 49 3.2500 0.1700 -0.197700 1.9050 1.6860 0.051222218 -2.220205820

 50 3.5000 0.0800 0.150000 2.5000 1.7750 0.001000000 -0.843144165

 51 3.5500 0.0700 0.100200 2.5000 1.7750 0.001000000 -0.843144165

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 53 3.5000 0.0800 0.440000 2.0020 1.7750 0.001000000 -0.843144165

 54 3.2800 0.1700 -0.481500 1.8540 1.6400 0.005000000 0.000000000

 55 3.2500 0.1700 -0.810000 1.8650 1.6500 0.051222218 -2.220205820

 56 3.2500 0.1700 -0.530000 1.8000 1.6000 0.001000000 -0.511443539

 57 3.7500 0.1050 0.753000 1.9250 1.7000 0.001000000 -0.126889456

 58 2.9600 0.2100 -0.508000 1.5250 1.4250 0.001000000 -1.480495490

 59 0.5000 0.0300 0.370000 0.9960 0.8600 0.030040813 -0.651083722

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 62 2.5000 0.0500 0.200000 1.3810 1.2100 0.030040813 0.268726247

 63 3.2500 0.1700 -0.536200 1.8100 1.6000 0.054801302 -1.445846770

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 65 3.2500 0.1700 -0.550000 1.8000 1.6000 0.001000000 -0.511443539

 66 3.7500 0.1050 0.630500 1.9250 1.7000 0.001000000 -0.126889456

 67 2.9600 0.2100 -0.508000 1.5250 1.4250 0.001000000 -1.480495490

 68 3.5000 0.0800 0.380000 2.5000 1.7750 0.001000000 -0.843144165

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 70 3.2800 0.1700 -0.468500 1.8540 1.6400 0.005000000 0.000000000

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 73 2.4200 0.0300 0.115000 1.3810 1.2100 0.030040813 0.268726247

 74 3.5500 0.0700 -0.115000 2.5000 1.7750 0.001000000 -0.843144165

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 76 2.5000 0.0300 0.060000 1.4250 1.2500 0.008598240 0.268726247

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 79 3.5500 0.0700 0.000000 2.5000 1.7750 0.001000000 -0.843144165

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 83 3.5500 0.0700 -0.115000 2.0020 1.7750 0.001000000 -0.843144165

 84 2.4200 0.0300 0.115000 1.3810 1.2100 0.030040813 0.268726247

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 1 6 405.000 1.623

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 7 12 340.000 1.090

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 17 22 320.000 1.410

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 17 18 340.000 1.090

 22 23 553.000 0.945

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 24 25 340.000 1.090

 28 29 553.000 0.945

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 36 68 436.000 1.374

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 80 81 380.000 1.080

 80 82 380.000 1.080

 83 51 469.000 1.400

 83 84 367.000 1.080

 51 49 481.000 1.393

 49 52 445.000 1.380

 49 43 382.000 1.448

 43 37 268.000 1.529

 43 44 340.000 1.090

 43 45 340.000 1.090

 37 46 320.000 1.410

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 37 38 340.000 1.090

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 84 83 51 35.00000 120.00000

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 45 43 37 37.50000 110.70000

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 21 19 20 33.00000 107.80000

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 3 1 6 8 0.16450 -1.0 2.0

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\* LIGAND DATABASE FILE (OPLS2005)

\*

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 3 1 M CT1 \_CA\_ 2 1.44126 118.43521 -179.94405

 4 3 S HC \_HA\_ 15 1.09026 105.09173 5.88783

 5 3 M C \_C\_\_ 3 1.50445 111.47958 -107.43472

 6 5 S O \_O\_\_ 4 1.23381 120.25866 -28.32038

 7 3 S CT \_CB\_ 5 1.54182 112.46574 119.70006

 8 7 S HC \_HB2 11 1.09044 109.23908 -166.53273

 9 7 S HC \_HB3 16 1.09021 109.22708 -55.00168

 10 7 S CA5 \_CG\_ 6 1.50095 116.36422 69.22096

 11 10 S N5B \_ND1 7 1.37689 124.23761 -32.92503

 12 10 S CA5 \_CD2 8 1.35510 129.73426 154.69055

 13 12 S HA \_HD2 12 1.08036 120.02487 -4.01610

 14 11 S CA5 \_CE1 9 1.32338 109.45786 -176.74418

 15 14 S HA \_HE1 13 1.08025 119.96810 -177.99904

 16 12 S NB \_NE2 10 1.37223 107.68894 175.99337

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 12 3.5500 0.0700 -0.261000 2.0020 1.7750 0.001000000 -0.843144165

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 3 7 268.000 1.529

 3 4 340.000 1.090

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 10 12 360.000 1.432

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 14 15 385.000 1.083

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