

Main interactions of dopamine and risperidone with dopamine D2 receptor

Supporting Information Available

Ana Martínez^{*†} Ponciano García-Gutiérrez[‡] Rafael Zubillaga [‡] Jorge Garza[‡]
Rubicelia Vargas^{‡§}

Abstract

Psychosis is one of the psychiatric disorders that is controlled by dopaminergic drugs such as antipsychotics that have affinity for dopamine D2 receptor (DRD2). In this investigation we perform quantum chemical calculations of two molecules [dopamine and risperidone] within a large cavity of DRD2 that represents the binding site of the receptor. Dopamine is an endogenous neurotransmitter and risperidone is a second-generation antipsychotic. Non-covalent interactions of dopamine and risperidone with DRD2 are analyzed using the Quantum Theory of Atoms in Molecules (QTAIM) and the Non-Covalent Interaction Index (NCI). The QTAIM results show that these molecules strongly interact with the receptor. There are 22 non-covalent interactions for dopamine and 54 for risperidone. The electron density evaluated at each critical binding points is small in both systems but it is higher for dopamine than for risperidone, indicating that the interactions of DRD2 with the first are stronger than with the second molecule. However, the binding energy is higher for risperidone (-72.6 kcal / mol) than for dopamine (-22.8 kcal / mol). Thus, the strength of the binding energy is due to the number of contacts rather than the strength of the interactions themselves. This could be related to the ability of risperidone to block DRD2 and may explain the efficacy of this drug for controlling the symptoms of schizophrenia, but likewise its secondary effects.

^{*}Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Circuito Exterior S. N., Ciudad Universitaria, CP 04510, CDMX, México.

[†]martina@unam.mx

[‡]Universidad Autónoma Metropolitana-Iztapalapa. Departamento de Química, División de Ciencias Básicas e Ingeniería. Universidad Autónoma Metropolitana-Iztapalapa. San Rafael Atlixco 186, Col. Vicentina. Iztapalapa. C. P. 09340. México City. México

[§]Email: ruvf@xanum.uam.mx

1 Cartesian coordinates in Angstroms

1.1 Dopamine in complex

22

TE= -516.2146917854

C -4.6470000000 -4.5840000000 6.5800000000
C -4.9990000000 -3.2320000000 6.7820000000
C -4.0080000000 -2.2210000000 6.7330000000
C -2.6630000000 -2.5400000000 6.4800000000
C -2.3140000000 -3.8830000000 6.2780000000
C -3.2930000000 -4.8990000000 6.3250000000
O -6.2830000000 -2.8850000000 7.0610000000
C -2.9090000000 -6.2430000000 6.2300000000
C -2.6670000000 -6.9000000000 7.5960000000
N -2.4900000000 -8.3510000000 7.5050000000
O -4.3880000000 -0.9360000000 6.9280000000
H -5.4080197322 -5.3546423075 6.6238424402
H -1.9583893495 -1.7194321843 6.4274618288
H -1.3020522059 -4.1743086458 6.0626200401
H -6.7627557099 -2.7333819568 6.2362593307
H -1.9729391327 -6.3426384339 5.6706556719
H -3.6279111032 -6.8323754282 5.6508751296
H -3.5661545307 -6.7097076983 8.2090462823
H -1.8712944269 -6.3305129715 8.0614952182
H -1.6951633191 -8.5742744614 6.9249363545
H -2.1924424260 -8.6598825780 8.4130372567
H -5.3485768159 -0.8958229445 6.8568910657

1.2 Receptor in dopamine-DRD2 complex

339

TE= -8426.4356282336

C 5.9930000000 -6.9810000000 6.5090000000
C 4.5820000000 -7.2570000000 6.1040000000
O 4.3090000000 -7.1500000000 5.0000000000
H 6.2152156050 -5.9397646089 6.2615828508
H 6.6507007818 -7.6062141566 5.9027359034
H 6.2215961723 -7.1404067911 7.5662588719
N 3.6790000000 -7.5860000000 7.1370000000
C 2.2050000000 -7.7820000000 6.9860000000
C 1.5020000000 -6.6690000000 6.1530000000
O 0.7180000000 -7.0500000000 5.3100000000
C 1.5750000000 -7.8270000000 8.3820000000
C 0.1080000000 -8.2000000000 8.3440000000
O -0.1850000000 -9.2630000000 7.7630000000
O -0.7780000000 -7.4620000000 8.8730000000
H 4.0501782740 -7.7074044477 8.0641386243
H 1.9707077673 -8.7041916538 6.4550222114
H 2.0878750494 -8.6023786943 8.9647417552
H 1.7113569202 -6.8678343795 8.8944210536
N 1.8090000000 -5.3760000000 6.3860000000

C 1.2820000000 -4.1690000000 5.7440000000
C 2.0250000000 -3.8680000000 4.4450000000
O 1.3620000000 -3.3760000000 3.5290000000
C 1.2980000000 -2.9880000000 6.7540000000
C 0.7250000000 -1.6830000000 6.1620000000
C 0.4630000000 -3.4340000000 7.9640000000
H 2.4429667343 -5.2266399504 7.1584279025
H 0.2687289492 -4.3778291922 5.4097439388
H 2.3432495741 -2.8319071159 7.0547527732
H -0.1665900363 -1.8884397934 5.5710667507
H 0.4597453339 -0.9829478250 6.9558109573
H 1.4367192987 -1.1935237735 5.4930484365
H 0.6074380102 -4.4793130783 8.2411944031
H 0.7173301504 -2.8207205217 8.8357316176
H -0.5991180502 -3.2947636996 7.7838947925
N 3.3560000000 -4.1320000000 4.3470000000
C 4.1700000000 -3.8380000000 3.1240000000
H 3.7209336508 -4.8316890110 4.9757118682
H 3.5793525462 -3.1685520737 2.5002477066
H 5.1002299771 -3.3512661251 3.4218069806
H 4.3855801520 -4.7581126650 2.5794951032
C 3.7530000000 -7.1830000000 1.2770000000
C 2.3850000000 -7.2260000000 0.5460000000
O 2.3980000000 -7.3270000000 -0.6680000000
H 4.2714167369 -6.2961204099 0.9073967828
H 4.3201889137 -8.0591497637 0.9607035876
H 3.6946800690 -7.1584192546 2.3684390915
N 1.2470000000 -7.1400000000 1.2760000000
C -0.0120000000 -6.8660000000 0.6480000000
C -0.0500000000 -5.4820000000 -0.0530000000
O -0.8030000000 -5.3200000000 -1.0590000000
C -1.2610000000 -7.0940000000 1.6350000000
S -1.2640000000 -5.8890000000 3.0500000000
H 1.3244471222 -6.9674663426 2.2693455498
H -0.1409771701 -7.5572051629 -0.1887551968
H -2.1701308421 -6.9179385401 1.0626406698
H -1.2575799653 -8.1153154681 2.0095166264
H -0.5011989247 -6.5874461300 3.9174240163
N 0.6480000000 -4.4650000000 0.3360000000
C 0.6320000000 -3.1870000000 -0.3980000000
H 1.0698177705 -4.4598698469 1.2561751159
H -0.3778618320 -2.7712907706 -0.4197765081
H 0.9554715809 -3.3579170714 -1.4258411767
H 1.3090722393 -2.5018130873 0.1117703691
C -5.4740000000 5.8270000000 13.4510000000
C -4.5610000000 5.5370000000 12.3080000000
O -5.0610000000 5.6990000000 11.1700000000
H -6.3118005130 5.1270137687 13.4098009148
H -5.8802781160 6.8292731620 13.3112822955
H -5.0122132356 5.7595876885 14.4400762945
N -3.3080000000 5.1540000000 12.5520000000
C -2.3840000000 4.7970000000 11.4580000000

C -2.904000000 3.506000000 10.686000000
O -2.552000000 3.418000000 9.490000000
C -0.981000000 4.526000000 11.938000000
C 0.045000000 4.438000000 10.810000000
C 0.570000000 5.621000000 10.261000000
C 0.493000000 3.224000000 10.270000000
C 1.534000000 5.588000000 9.278000000
C 1.467000000 3.212000000 9.243000000
C 2.029000000 4.363000000 8.757000000
H -2.9849422734 5.1109979389 13.5056882301
H -2.4102940171 5.5839333177 10.7042541007
H -0.6764349174 5.3422373473 12.6048619622
H -0.9601530414 3.6045677819 12.5304573876
H 0.2307585137 6.5828389806 10.6380085924
H 0.0920159775 2.2822626494 10.6295385839
H 1.9300720686 6.5246920000 8.8974920784
H 1.7765117544 2.2481901401 8.8503977618
H 2.7846846086 4.3506873774 7.9817094408
N -3.710000000 2.616000000 11.203000000
C -4.352000000 1.542000000 10.413000000
C -5.356000000 2.129000000 9.396000000
O -5.356000000 1.603000000 8.297000000
C -5.061000000 0.477000000 11.262000000
C -5.774000000 -0.717000000 10.528000000
C -3.943000000 -0.171000000 12.180000000
H -3.9757572660 2.7020951712 12.1742142711
H -3.5848566857 1.0811576909 9.7888916779
H -5.7996322451 0.9784399259 11.9029604858
H -5.0769947276 -1.2172897513 9.8528376617
H -6.1232522899 -1.4267561403 11.2777350053
H -6.6301985228 -0.3837659354 9.9362936841
H -3.2272100605 -0.7000800328 11.5451337043
H -3.3964491996 0.5703564152 12.7697108360
H -4.3907846907 -0.8944679217 12.8637682457
N -6.190000000 3.093000000 9.757000000
C -7.316000000 3.584000000 8.905000000
C -6.658000000 4.375000000 7.762000000
O -6.951000000 4.089000000 6.609000000
C -8.425000000 4.412000000 9.585000000
C -9.539000000 4.787000000 8.643000000
C -8.987000000 3.422000000 10.639000000
H -6.0063603024 3.5898863853 10.6178406098
H -7.7620088537 2.7106054708 8.4262785947
H -7.9891794674 5.2935217347 10.0675431470
H -9.9631045139 3.8946836162 8.1726347021
H -10.3356708298 5.2864789657 9.1995060742
H -9.2099286991 5.4574177114 7.8442729973
H -9.8114312166 3.8643198504 11.2061717613
H -9.3708472605 2.5308129420 10.1354989005
H -8.2272414306 3.0990903129 11.3543921910
N -5.778000000 5.365000000 8.116000000
C -4.909000000 6.056000000 7.212000000

C -4.0390000000 5.1270000000 6.2900000000
O -3.9190000000 5.4420000000 5.0980000000
C -3.9370000000 7.0040000000 8.0440000000
C -2.8700000000 7.7410000000 7.2490000000
C -1.5120000000 7.4170000000 7.4430000000
C -0.5080000000 8.0910000000 6.7290000000
C -0.8590000000 9.1100000000 5.8150000000
O 0.1170000000 9.7840000000 5.1410000000
C -2.2230000000 9.4340000000 5.6130000000
C -3.2230000000 8.7490000000 6.3300000000
H -5.5548995692 5.4383407054 9.1031469100
H -5.4812123073 6.6494638327 6.4956379069
H -3.4485231248 6.3718584946 8.7919132606
H -4.5661901516 7.7148312614 8.5922867053
H -1.2381173323 6.6124066431 8.1182740234
H -4.2672261507 8.9895514003 6.1622273958
H 0.5383802792 7.8387437451 6.8570748076
H -2.4935324390 10.2091485812 4.9008167218
H -0.3069475620 10.3572277380 4.4996168881
N -3.5300000000 4.0330000000 6.8500000000
C -2.8530000000 2.9580000000 6.0330000000
C -3.8690000000 2.2760000000 5.0240000000
O -3.4800000000 2.0170000000 3.8600000000
C -2.1320000000 1.7800000000 6.7900000000
O -1.4320000000 0.8520000000 5.9540000000
H -3.5454077024 3.9026883131 7.8532527742
H -2.1411591592 3.4481633754 5.3671913488
H -1.3958937320 2.2023503635 7.4776900988
H -2.8890117840 1.2448632311 7.3758262295
H -1.9387429390 0.7586462332 5.1364425740
N -5.0380000000 2.0100000000 5.4120000000
C -6.0950000000 1.4970000000 4.4840000000
C -6.5320000000 2.5400000000 3.4690000000
O -6.2900000000 2.3140000000 2.2860000000
C -7.4220000000 1.0370000000 5.1270000000
O -7.2340000000 0.0100000000 6.0960000000
H -5.3085203085 2.2200413154 6.3648346907
H -5.6444666223 0.7057297403 3.8872076113
H -7.9455187098 1.8899365041 5.5685811549
H -8.0358735531 0.6247291569 4.3237486924
H -6.9335921323 0.4395625984 6.9048478847
N -7.1450000000 3.6800000000 3.8220000000
C -7.7760000000 4.6070000000 2.8270000000
H -7.1427600569 3.9638540503 4.7921391235
H -7.8855363699 4.0534266716 1.8958716580
H -8.7463618527 4.9268058371 3.2118075651
H -7.1352024165 5.4754320481 2.6529695999
C -9.0150000000 -11.6400000000 -1.9410000000
C -8.3990000000 -10.5220000000 -1.1260000000
O -7.2330000000 -10.7040000000 -0.7160000000
H -9.9539092610 -11.3819263515 -2.4433829498
H -8.2808914587 -11.9422020351 -2.6884252772

H -9.1861523822 -12.4940795381 -1.2824242949
N -9.0890000000 -9.4610000000 -0.9000000000
C -8.5600000000 -8.3500000000 -0.1260000000
C -9.5180000000 -7.2000000000 0.0290000000
O -9.2980000000 -6.5000000000 1.0180000000
C -7.2700000000 -7.7950000000 -0.7910000000
C -6.1260000000 -8.7520000000 -0.8140000000
C -5.6140000000 -9.5220000000 -1.7690000000
C -5.3240000000 -8.9790000000 0.3840000000
C -4.2600000000 -9.8640000000 -0.0010000000
C -5.4470000000 -8.5020000000 1.7150000000
N -4.4640000000 -10.1400000000 -1.3820000000
C -3.3260000000 -10.2620000000 0.9050000000
C -4.4620000000 -8.9380000000 2.6060000000
C -3.4460000000 -9.8180000000 2.2290000000
H -10.0924184442 -9.5546487767 -0.9550033117
H -8.3195160703 -8.6901842177 0.8847806101
H -7.5320410002 -7.4726182657 -1.8071273498
H -6.9797961519 -6.9024831421 -0.2286491421
H -5.9591638254 -9.6452574345 -2.7873157155
H -4.0464071263 -10.9210101172 -1.8552875704
H -6.2493740784 -7.8429878293 2.0233505092
H -2.5381346478 -10.9596022462 0.6400947842
H -4.5095815149 -8.6201286246 3.6430967449
H -2.7222181376 -10.1407503471 2.9692658764
N -10.4450000000 -7.1000000000 -0.8980000000
C -11.4500000000 -6.0130000000 -0.8620000000
H -10.3306844979 -7.6428632687 -1.7391825803
H -11.2742839011 -5.2919444982 -1.6631680560
H -12.4562794598 -6.4270064558 -0.9499938689
H -11.3295597258 -5.5113661614 0.0971824281
C -12.4650000000 -8.8090000000 1.5090000000
C -11.4670000000 -8.9840000000 2.6350000000
O -11.0050000000 -10.1320000000 2.8010000000
H -12.8462366813 -7.7904532663 1.3848426520
H -11.9845177221 -9.1230805450 0.5821681400
H -13.3003978742 -9.4847491410 1.6970514596
N -11.1500000000 -7.9640000000 3.3510000000
C -10.1690000000 -8.0630000000 4.4820000000
C -9.8850000000 -6.7610000000 5.2530000000
O -9.8850000000 -6.7080000000 6.4980000000
C -8.8220000000 -8.5820000000 3.8530000000
C -7.6380000000 -8.9560000000 4.7690000000
C -6.8420000000 -7.9670000000 5.2420000000
C -7.4200000000 -10.3220000000 5.0130000000
C -5.7700000000 -8.3200000000 6.1400000000
C -6.3860000000 -10.6880000000 5.8730000000
C -5.5740000000 -9.6760000000 6.5060000000
H -11.5098462380 -7.0550965449 3.1139617536
H -10.5479705004 -8.7749731795 5.2149593677
H -9.0924992409 -9.4586802008 3.2699337306
H -8.5044272657 -7.8092047736 3.1435011194

H -7.0044933011 -6.9269608124 4.9808861213
H -8.0622687897 -11.0622295845 4.5485850573
H -5.1203585208 -7.5774651154 6.5789593853
H -6.1952315951 -11.7336841759 6.0947520821
H -4.7394101305 -9.9130095917 7.1567105225
N -9.6560000000 -5.6340000000 4.5390000000
C -9.4820000000 -4.2750000000 5.0490000000
C -10.7650000000 -3.7550000000 5.6320000000
O -10.6570000000 -3.1620000000 6.7200000000
C -8.8980000000 -3.2480000000 4.0370000000
C -7.4040000000 -3.5400000000 3.6250000000
C -6.5090000000 -2.4460000000 3.6830000000
C -6.8190000000 -4.7700000000 3.2020000000
C -5.1230000000 -2.6510000000 3.5120000000
C -5.4440000000 -4.9540000000 2.9740000000
C -4.5700000000 -3.8680000000 3.1760000000
H -9.5070479142 -5.7586494511 3.5428359445
H -8.8024791847 -4.3296571445 5.9032559704
H -9.5375613542 -3.2009609756 3.1458245023
H -8.9265145957 -2.2737713898 4.5276613651
H -6.8620699236 -1.4595252441 3.9629871170
H -7.4587397144 -5.6333289012 3.0471991877
H -4.4690570449 -1.7934965522 3.6431235086
H -5.0683358509 -5.9273080077 2.6819996055
H -3.4988511057 -3.9937773580 3.0777496102
N -11.9130000000 -3.9730000000 4.9600000000
C -13.1920000000 -3.3480000000 5.4590000000
H -11.8692219229 -4.3922762827 4.0473595307
H -13.2724709060 -2.3120477877 5.1224428548
H -13.1602628205 -3.3774886727 6.5462377339
H -14.0346047211 -3.9339328334 5.0933264674
C -13.7210000000 -5.9990000000 8.1830000000
C -12.6700000000 -5.6000000000 9.1780000000
O -12.9400000000 -5.5270000000 10.3250000000
H -14.4987055279 -5.2304904584 8.1757937451
H -14.1784911168 -6.9274028961 8.5277228667
H -13.3444076915 -6.1344309134 7.1654649296
N -11.3860000000 -5.3460000000 8.7400000000
C -10.3180000000 -4.8900000000 9.7010000000
C -10.5790000000 -3.5100000000 10.3940000000
O -10.3840000000 -3.4820000000 11.5910000000
C -8.9320000000 -5.0210000000 9.0540000000
C -7.7590000000 -4.7360000000 10.0060000000
C -7.6150000000 -4.8910000000 11.3190000000
N -6.5360000000 -4.2040000000 9.5780000000
C -5.8060000000 -4.0720000000 10.6740000000
N -6.4210000000 -4.4530000000 11.7770000000
H -11.0808153008 -5.6250395681 7.8170693397
H -10.3709622619 -5.5641849492 10.5590688495
H -8.8461121790 -6.0271572978 8.6336473262
H -8.8686821819 -4.3262027426 8.2091885918
H -6.3433130921 -3.8651312971 8.6456818362

H -8.3734345988 -5.2417555028 12.0043209222
H -4.7926480516 -3.6949718307 10.6353974928
N -11.0040000000 -2.5530000000 9.6350000000
C -11.5300000000 -1.2610000000 10.1690000000
C -12.7440000000 -1.4130000000 11.1100000000
O -12.7370000000 -0.7890000000 12.1940000000
C -11.7020000000 -0.0180000000 9.2680000000
C -12.8460000000 -0.1850000000 8.1840000000
C -10.3800000000 0.1580000000 8.5530000000
C -13.0390000000 0.9920000000 7.1780000000
H -11.0914596414 -2.7520014707 8.6430411762
H -10.7686875711 -0.9586160039 10.8965879388
H -11.9286149342 0.8089326176 9.9459235688
H -12.6129638666 -1.0925299417 7.6138643268
H -13.7926533339 -0.3680507708 8.7013347770
H -10.1973769190 -0.6637823110 7.8551128543
H -10.3387572051 1.0891056550 7.9774377439
H -9.5451033826 0.1691987094 9.2619211854
H -13.8958980941 0.7906743233 6.5298732276
H -13.2287169556 1.9320856175 7.7054645038
H -12.1596928758 1.1279052695 6.5437099070
N -13.7040000000 -2.2040000000 10.6810000000
C -14.9230000000 -2.4350000000 11.4890000000
H -13.4692686631 -2.8775916901 9.9688068517
H -15.8135995723 -2.1757414361 10.9108904737
H -14.9699746124 -3.4819911029 11.7958035828
H -14.8418852576 -1.7937629991 12.3651082151
C -5.2400000000 -12.7210000000 2.7120000000
C -4.1540000000 -13.7010000000 2.3360000000
O -3.5470000000 -13.6630000000 1.3070000000
H -4.8409034386 -11.9414967061 3.3669151890
H -5.5992901305 -12.2297515094 1.8080259794
H -6.0694084877 -13.2081766684 3.2312955991
N -3.9150000000 -14.6790000000 3.2820000000
C -3.0140000000 -15.8050000000 3.1170000000
C -3.4970000000 -16.8210000000 2.0450000000
O -2.7120000000 -17.4610000000 1.4300000000
C -2.8050000000 -16.6980000000 4.3490000000
C -2.3530000000 -15.9330000000 5.6070000000
C -1.3890000000 -14.9150000000 5.5950000000
C -2.9780000000 -16.2310000000 6.8220000000
C -1.1890000000 -14.1720000000 6.7560000000
C -2.7240000000 -15.4280000000 8.0020000000
C -1.8390000000 -14.3320000000 7.9140000000
O -1.6730000000 -13.4490000000 9.0330000000
H -4.3040165452 -14.5374949189 4.2024232821
H -2.0494296836 -15.4529364390 2.7404906713
H -3.7363376685 -17.2241005028 4.5821509774
H -2.0695009588 -17.4494517054 4.0492716293
H -0.8516752243 -14.6545034075 4.6908620596
H -3.7077157465 -17.0313756323 6.8872992089
H -0.4739219338 -13.3514933211 6.6868543896

H -3.2527390377 -15.6311586147 8.9261293725
H -1.2767669929 -12.6395393608 8.6922173710
N -4.8000000000 -16.9070000000 1.8850000000
C -5.3900000000 -17.8370000000 0.8950000000
H -5.3840279771 -16.2309514994 2.3499577830
H -5.8148068013 -17.2860131847 0.0516257259
H -4.5780621877 -18.4697244122 0.5405322448
H -6.1657207649 -18.4468325200 1.3636746348

1.3 Dopamine-DRD2 complex

361

TE= -8942.6866759851473034
C 5.9930000000 -6.9810000000 6.5090000000
C 4.5820000000 -7.2570000000 6.1040000000
O 4.3090000000 -7.1500000000 5.0000000000
H 6.2152156050 -5.9397646089 6.2615828508
H 6.6507007818 -7.6062141566 5.9027359034
H 6.2215961723 -7.1404067911 7.5662588719
N 3.6790000000 -7.5860000000 7.1370000000
C 2.2050000000 -7.7820000000 6.9860000000
C 1.5020000000 -6.6690000000 6.1530000000
O 0.7180000000 -7.0500000000 5.3100000000
C 1.5750000000 -7.8270000000 8.3820000000
C 0.1080000000 -8.2000000000 8.3440000000
O -0.1850000000 -9.2630000000 7.7630000000
O -0.7780000000 -7.4620000000 8.8730000000
H 4.0501782740 -7.7074044477 8.0641386243
H 1.9707077673 -8.7041916538 6.4550222114
H 2.0878750494 -8.6023786943 8.9647417552
H 1.7113569202 -6.8678343795 8.8944210536
N 1.8090000000 -5.3760000000 6.3860000000
C 1.2820000000 -4.1690000000 5.7440000000
C 2.0250000000 -3.8680000000 4.4450000000
O 1.3620000000 -3.3760000000 3.5290000000
C 1.2980000000 -2.9880000000 6.7540000000
C 0.7250000000 -1.6830000000 6.1620000000
C 0.4630000000 -3.4340000000 7.9640000000
H 2.4429667343 -5.2266399504 7.1584279025
H 0.2687289492 -4.3778291922 5.4097439388
H 2.3432495741 -2.8319071159 7.0547527732
H -0.1665900363 -1.8884397934 5.5710667507
H 0.4597453339 -0.9829478250 6.9558109573
H 1.4367192987 -1.1935237735 5.4930484365
H 0.6074380102 -4.4793130783 8.2411944031
H 0.7173301504 -2.8207205217 8.8357316176
H -0.5991180502 -3.2947636996 7.7838947925
N 3.3560000000 -4.1320000000 4.3470000000
C 4.1700000000 -3.8380000000 3.1240000000
H 3.7209336508 -4.8316890110 4.9757118682
H 3.5793525462 -3.1685520737 2.5002477066

H 5.1002299771 -3.3512661251 3.4218069806
H 4.3855801520 -4.7581126650 2.5794951032
C 3.7530000000 -7.1830000000 1.2770000000
C 2.3850000000 -7.2260000000 0.5460000000
O 2.3980000000 -7.3270000000 -0.6680000000
H 4.2714167369 -6.2961204099 0.9073967828
H 4.3201889137 -8.0591497637 0.9607035876
H 3.6946800690 -7.1584192546 2.3684390915
N 1.2470000000 -7.1400000000 1.2760000000
C -0.0120000000 -6.8660000000 0.6480000000
C -0.0500000000 -5.4820000000 -0.0530000000
O -0.8030000000 -5.3200000000 -1.0590000000
C -1.2610000000 -7.0940000000 1.6350000000
S -1.2640000000 -5.8890000000 3.0500000000
H 1.3244471222 -6.9674663426 2.2693455498
H -0.1409771701 -7.5572051629 -0.1887551968
H -2.1701308421 -6.9179385401 1.0626406698
H -1.2575799653 -8.1153154681 2.0095166264
H -0.5011989247 -6.5874461300 3.9174240163
N 0.6480000000 -4.4650000000 0.3360000000
C 0.6320000000 -3.1870000000 -0.3980000000
H 1.0698177705 -4.4598698469 1.2561751159
H -0.3778618320 -2.7712907706 -0.4197765081
H 0.9554715809 -3.3579170714 -1.4258411767
H 1.3090722393 -2.5018130873 0.1117703691
C -5.4740000000 5.8270000000 13.4510000000
C -4.5610000000 5.5370000000 12.3080000000
O -5.0610000000 5.6990000000 11.1700000000
H -6.3118005130 5.1270137687 13.4098009148
H -5.8802781160 6.8292731620 13.3112822955
H -5.0122132356 5.7595876885 14.4400762945
N -3.3080000000 5.1540000000 12.5520000000
C -2.3840000000 4.7970000000 11.4580000000
C -2.9040000000 3.5060000000 10.6860000000
O -2.5520000000 3.4180000000 9.4900000000
C -0.9810000000 4.5260000000 11.9380000000
C 0.0450000000 4.4380000000 10.8100000000
C 0.5700000000 5.6210000000 10.2610000000
C 0.4930000000 3.2240000000 10.2700000000
C 1.5340000000 5.5880000000 9.2780000000
C 1.4670000000 3.2120000000 9.2430000000
C 2.0290000000 4.3630000000 8.7570000000
H -2.9849422734 5.1109979389 13.5056882301
H -2.4102940171 5.5839333177 10.7042541007
H -0.6764349174 5.3422373473 12.6048619622
H -0.9601530414 3.6045677819 12.5304573876
H 0.2307585137 6.5828389806 10.6380085924
H 0.0920159775 2.2822626494 10.6295385839
H 1.9300720686 6.5246920000 8.8974920784
H 1.7765117544 2.2481901401 8.8503977618
H 2.7846846086 4.3506873774 7.9817094408
N -3.7100000000 2.6160000000 11.2030000000

C -4.352000000 1.542000000 10.413000000
C -5.356000000 2.129000000 9.396000000
O -5.356000000 1.603000000 8.297000000
C -5.061000000 0.477000000 11.262000000
C -5.774000000 -0.717000000 10.528000000
C -3.943000000 -0.171000000 12.180000000
H -3.9757572660 2.7020951712 12.1742142711
H -3.5848566857 1.0811576909 9.7888916779
H -5.7996322451 0.9784399259 11.9029604858
H -5.0769947276 -1.2172897513 9.8528376617
H -6.1232522899 -1.4267561403 11.2777350053
H -6.6301985228 -0.3837659354 9.9362936841
H -3.2272100605 -0.7000800328 11.5451337043
H -3.3964491996 0.5703564152 12.7697108360
H -4.3907846907 -0.8944679217 12.8637682457
N -6.190000000 3.093000000 9.757000000
C -7.316000000 3.584000000 8.905000000
C -6.658000000 4.375000000 7.762000000
O -6.951000000 4.089000000 6.609000000
C -8.425000000 4.412000000 9.585000000
C -9.539000000 4.787000000 8.643000000
C -8.987000000 3.422000000 10.639000000
H -6.0063603024 3.5898863853 10.6178406098
H -7.7620088537 2.7106054708 8.4262785947
H -7.9891794674 5.2935217347 10.0675431470
H -9.9631045139 3.8946836162 8.1726347021
H -10.3356708298 5.2864789657 9.1995060742
H -9.2099286991 5.4574177114 7.8442729973
H -9.8114312166 3.8643198504 11.2061717613
H -9.3708472605 2.5308129420 10.1354989005
H -8.2272414306 3.0990903129 11.3543921910
N -5.778000000 5.365000000 8.116000000
C -4.909000000 6.056000000 7.212000000
C -4.039000000 5.127000000 6.290000000
O -3.919000000 5.442000000 5.098000000
C -3.937000000 7.004000000 8.044000000
C -2.870000000 7.741000000 7.249000000
C -1.512000000 7.417000000 7.443000000
C -0.508000000 8.091000000 6.729000000
C -0.859000000 9.110000000 5.815000000
O 0.117000000 9.784000000 5.141000000
C -2.223000000 9.434000000 5.613000000
C -3.223000000 8.749000000 6.330000000
H -5.5548995692 5.4383407054 9.1031469100
H -5.4812123073 6.6494638327 6.4956379069
H -3.4485231248 6.3718584946 8.7919132606
H -4.5661901516 7.7148312614 8.5922867053
H -1.2381173323 6.6124066431 8.1182740234
H -4.2672261507 8.9895514003 6.1622273958
H 0.5383802792 7.8387437451 6.8570748076
H -2.4935324390 10.2091485812 4.9008167218
H -0.3069475620 10.3572277380 4.4996168881

N -3.530000000 4.033000000 6.850000000
C -2.853000000 2.958000000 6.033000000
C -3.869000000 2.276000000 5.024000000
O -3.480000000 2.017000000 3.860000000
C -2.132000000 1.780000000 6.790000000
O -1.432000000 0.852000000 5.954000000
H -3.5454077024 3.9026883131 7.8532527742
H -2.1411591592 3.4481633754 5.3671913488
H -1.3958937320 2.2023503635 7.4776900988
H -2.8890117840 1.2448632311 7.3758262295
H -1.9387429390 0.7586462332 5.1364425740
N -5.038000000 2.010000000 5.412000000
C -6.095000000 1.497000000 4.484000000
C -6.532000000 2.540000000 3.469000000
O -6.290000000 2.314000000 2.286000000
C -7.422000000 1.037000000 5.127000000
O -7.234000000 0.010000000 6.096000000
H -5.3085203085 2.2200413154 6.3648346907
H -5.6444666223 0.7057297403 3.8872076113
H -7.9455187098 1.8899365041 5.5685811549
H -8.0358735531 0.6247291569 4.3237486924
H -6.9335921323 0.4395625984 6.9048478847
N -7.145000000 3.680000000 3.822000000
C -7.776000000 4.607000000 2.827000000
H -7.1427600569 3.9638540503 4.7921391235
H -7.8855363699 4.0534266716 1.8958716580
H -8.7463618527 4.9268058371 3.2118075651
H -7.1352024165 5.4754320481 2.6529695999
C -9.015000000 -11.640000000 -1.941000000
C -8.399000000 -10.522000000 -1.126000000
O -7.233000000 -10.704000000 -0.716000000
H -9.9539092610 -11.3819263515 -2.4433829498
H -8.2808914587 -11.9422020351 -2.6884252772
H -9.1861523822 -12.4940795381 -1.2824242949
N -9.089000000 -9.461000000 -0.900000000
C -8.560000000 -8.350000000 -0.126000000
C -9.518000000 -7.200000000 0.029000000
O -9.298000000 -6.500000000 1.018000000
C -7.270000000 -7.795000000 -0.791000000
C -6.126000000 -8.752000000 -0.814000000
C -5.614000000 -9.522000000 -1.769000000
C -5.324000000 -8.979000000 0.384000000
C -4.260000000 -9.864000000 -0.001000000
C -5.447000000 -8.502000000 1.715000000
N -4.464000000 -10.140000000 -1.382000000
C -3.326000000 -10.262000000 0.905000000
C -4.462000000 -8.938000000 2.606000000
C -3.446000000 -9.818000000 2.229000000
H -10.0924184442 -9.5546487767 -0.9550033117
H -8.3195160703 -8.6901842177 0.8847806101
H -7.5320410002 -7.4726182657 -1.8071273498
H -6.9797961519 -6.9024831421 -0.2286491421

H -5.9591638254 -9.6452574345 -2.7873157155
H -4.0464071263 -10.9210101172 -1.8552875704
H -6.2493740784 -7.8429878293 2.0233505092
H -2.5381346478 -10.9596022462 0.6400947842
H -4.5095815149 -8.6201286246 3.6430967449
H -2.7222181376 -10.1407503471 2.9692658764
N -10.4450000000 -7.1000000000 -0.8980000000
C -11.4500000000 -6.0130000000 -0.8620000000
H -10.3306844979 -7.6428632687 -1.7391825803
H -11.2742839011 -5.2919444982 -1.6631680560
H -12.4562794598 -6.4270064558 -0.9499938689
H -11.3295597258 -5.5113661614 0.0971824281
C -12.4650000000 -8.8090000000 1.5090000000
C -11.4670000000 -8.9840000000 2.6350000000
O -11.0050000000 -10.1320000000 2.8010000000
H -12.8462366813 -7.7904532663 1.3848426520
H -11.9845177221 -9.1230805450 0.5821681400
H -13.3003978742 -9.4847491410 1.6970514596
N -11.1500000000 -7.9640000000 3.3510000000
C -10.1690000000 -8.0630000000 4.4820000000
C -9.8850000000 -6.7610000000 5.2530000000
O -9.8850000000 -6.7080000000 6.4980000000
C -8.8220000000 -8.5820000000 3.8530000000
C -7.6380000000 -8.9560000000 4.7690000000
C -6.8420000000 -7.9670000000 5.2420000000
C -7.4200000000 -10.3220000000 5.0130000000
C -5.7700000000 -8.3200000000 6.1400000000
C -6.3860000000 -10.6880000000 5.8730000000
C -5.5740000000 -9.6760000000 6.5060000000
H -11.5098462380 -7.0550965449 3.1139617536
H -10.5479705004 -8.7749731795 5.2149593677
H -9.0924992409 -9.4586802008 3.2699337306
H -8.5044272657 -7.8092047736 3.1435011194
H -7.0044933011 -6.9269608124 4.9808861213
H -8.0622687897 -11.0622295845 4.5485850573
H -5.1203585208 -7.5774651154 6.5789593853
H -6.1952315951 -11.7336841759 6.0947520821
H -4.7394101305 -9.9130095917 7.1567105225
N -9.6560000000 -5.6340000000 4.5390000000
C -9.4820000000 -4.2750000000 5.0490000000
C -10.7650000000 -3.7550000000 5.6320000000
O -10.6570000000 -3.1620000000 6.7200000000
C -8.8980000000 -3.2480000000 4.0370000000
C -7.4040000000 -3.5400000000 3.6250000000
C -6.5090000000 -2.4460000000 3.6830000000
C -6.8190000000 -4.7700000000 3.2020000000
C -5.1230000000 -2.6510000000 3.5120000000
C -5.4440000000 -4.9540000000 2.9740000000
C -4.5700000000 -3.8680000000 3.1760000000
H -9.5070479142 -5.7586494511 3.5428359445
H -8.8024791847 -4.3296571445 5.9032559704
H -9.5375613542 -3.2009609756 3.1458245023

H -8.9265145957 -2.2737713898 4.5276613651
H -6.8620699236 -1.4595252441 3.9629871170
H -7.4587397144 -5.6333289012 3.0471991877
H -4.4690570449 -1.7934965522 3.6431235086
H -5.0683358509 -5.9273080077 2.6819996055
H -3.4988511057 -3.9937773580 3.0777496102
N -11.9130000000 -3.9730000000 4.9600000000
C -13.1920000000 -3.3480000000 5.4590000000
H -11.8692219229 -4.3922762827 4.0473595307
H -13.2724709060 -2.3120477877 5.1224428548
H -13.1602628205 -3.3774886727 6.5462377339
H -14.0346047211 -3.9339328334 5.0933264674
C -13.7210000000 -5.9990000000 8.1830000000
C -12.6700000000 -5.6000000000 9.1780000000
O -12.9400000000 -5.5270000000 10.3250000000
H -14.4987055279 -5.2304904584 8.1757937451
H -14.1784911168 -6.9274028961 8.5277228667
H -13.3444076915 -6.1344309134 7.1654649296
N -11.3860000000 -5.3460000000 8.7400000000
C -10.3180000000 -4.8900000000 9.7010000000
C -10.5790000000 -3.5100000000 10.3940000000
O -10.3840000000 -3.4820000000 11.5910000000
C -8.9320000000 -5.0210000000 9.0540000000
C -7.7590000000 -4.7360000000 10.0060000000
C -7.6150000000 -4.8910000000 11.3190000000
N -6.5360000000 -4.2040000000 9.5780000000
C -5.8060000000 -4.0720000000 10.6740000000
N -6.4210000000 -4.4530000000 11.7770000000
H -11.0808153008 -5.6250395681 7.8170693397
H -10.3709622619 -5.5641849492 10.5590688495
H -8.8461121790 -6.0271572978 8.6336473262
H -8.8686821819 -4.3262027426 8.2091885918
H -6.3433130921 -3.8651312971 8.6456818362
H -8.3734345988 -5.2417555028 12.0043209222
H -4.7926480516 -3.6949718307 10.6353974928
N -11.0040000000 -2.5530000000 9.6350000000
C -11.5300000000 -1.2610000000 10.1690000000
C -12.7440000000 -1.4130000000 11.1100000000
O -12.7370000000 -0.7890000000 12.1940000000
C -11.7020000000 -0.0180000000 9.2680000000
C -12.8460000000 -0.1850000000 8.1840000000
C -10.3800000000 0.1580000000 8.5530000000
C -13.0390000000 0.9920000000 7.1780000000
H -11.0914596414 -2.7520014707 8.6430411762
H -10.7686875711 -0.9586160039 10.8965879388
H -11.9286149342 0.8089326176 9.9459235688
H -12.6129638666 -1.0925299417 7.6138643268
H -13.7926533339 -0.3680507708 8.7013347770
H -10.1973769190 -0.6637823110 7.8551128543
H -10.3387572051 1.0891056550 7.9774377439
H -9.5451033826 0.1691987094 9.2619211854
H -13.8958980941 0.7906743233 6.5298732276

H -13.2287169556 1.9320856175 7.7054645038
H -12.1596928758 1.1279052695 6.5437099070
N -13.7040000000 -2.2040000000 10.6810000000
C -14.9230000000 -2.4350000000 11.4890000000
H -13.4692686631 -2.8775916901 9.9688068517
H -15.8135995723 -2.1757414361 10.9108904737
H -14.9699746124 -3.4819911029 11.7958035828
H -14.8418852576 -1.7937629991 12.3651082151
C -5.2400000000 -12.7210000000 2.7120000000
C -4.1540000000 -13.7010000000 2.3360000000
O -3.5470000000 -13.6630000000 1.3070000000
H -4.8409034386 -11.9414967061 3.3669151890
H -5.5992901305 -12.2297515094 1.8080259794
H -6.0694084877 -13.2081766684 3.2312955991
N -3.9150000000 -14.6790000000 3.2820000000
C -3.0140000000 -15.8050000000 3.1170000000
C -3.4970000000 -16.8210000000 2.0450000000
O -2.7120000000 -17.4610000000 1.4300000000
C -2.8050000000 -16.6980000000 4.3490000000
C -2.3530000000 -15.9330000000 5.6070000000
C -1.3890000000 -14.9150000000 5.5950000000
C -2.9780000000 -16.2310000000 6.8220000000
C -1.1890000000 -14.1720000000 6.7560000000
C -2.7240000000 -15.4280000000 8.0020000000
C -1.8390000000 -14.3320000000 7.9140000000
O -1.6730000000 -13.4490000000 9.0330000000
H -4.3040165452 -14.5374949189 4.2024232821
H -2.0494296836 -15.4529364390 2.7404906713
H -3.7363376685 -17.2241005028 4.5821509774
H -2.0695009588 -17.4494517054 4.0492716293
H -0.8516752243 -14.6545034075 4.6908620596
H -3.7077157465 -17.0313756323 6.8872992089
H -0.4739219338 -13.3514933211 6.6868543896
H -3.2527390377 -15.6311586147 8.9261293725
H -1.2767669929 -12.6395393608 8.6922173710
N -4.8000000000 -16.9070000000 1.8850000000
C -5.3900000000 -17.8370000000 0.8950000000
H -5.3840279771 -16.2309514994 2.3499577830
H -5.8148068013 -17.2860131847 0.0516257259
H -4.5780621877 -18.4697244122 0.5405322448
H -6.1657207649 -18.4468325200 1.3636746348
C -4.6470000000 -4.5840000000 6.5800000000
C -4.9990000000 -3.2320000000 6.7820000000
C -4.0080000000 -2.2210000000 6.7330000000
C -2.6630000000 -2.5400000000 6.4800000000
C -2.3140000000 -3.8830000000 6.2780000000
C -3.2930000000 -4.8990000000 6.3250000000
O -6.2830000000 -2.8850000000 7.0610000000
C -2.9090000000 -6.2430000000 6.2300000000
C -2.6670000000 -6.9000000000 7.5960000000
N -2.4900000000 -8.3510000000 7.5050000000
O -4.3880000000 -0.9360000000 6.9280000000

H -5.4080197322 -5.3546423075 6.6238424402
H -1.9583893495 -1.7194321843 6.4274618288
H -1.3020522059 -4.1743086458 6.0626200401
H -6.7627557099 -2.7333819568 6.2362593307
H -1.9729391327 -6.3426384339 5.6706556719
H -3.6279111032 -6.8323754282 5.6508751296
H -3.5661545307 -6.7097076983 8.2090462823
H -1.8712944269 -6.3305129715 8.0614952182
H -1.6951633191 -8.5742744614 6.9249363545
H -2.1924424260 -8.6598825780 8.4130372567
H -5.3485768159 -0.8958229445 6.8568910657

1.4 Risperidone in complex

57

TE= -1360.7952667038
C 5.7980000000 4.5200000000 -12.8980000000
C 7.1440000000 4.0330000000 -13.3650000000
C 8.2620000000 4.6000000000 -12.9090000000
C 8.2060000000 5.7460000000 -11.8970000000
C 8.7980000000 5.2360000000 -10.5560000000
C 9.8570000000 7.3230000000 -9.9030000000
C 10.0850000000 8.3470000000 -8.7770000000
C 10.5980000000 7.5820000000 -7.5530000000
C 9.5690000000 6.5280000000 -7.1200000000
C 9.3630000000 5.5650000000 -8.2800000000
C 10.9780000000 8.5130000000 -6.4340000000
C 11.6040000000 9.3870000000 -4.5610000000
C 11.3460000000 8.1840000000 -5.1480000000
C 11.4800000000 6.9760000000 -4.4820000000
C 11.8930000000 7.0420000000 -3.1520000000
C 12.1580000000 8.2710000000 -2.5380000000
C 12.0170000000 9.4710000000 -3.2390000000
C 9.5440000000 4.0890000000 -13.3910000000
C 10.8280000000 2.5500000000 -14.8120000000
C 10.6590000000 1.6890000000 -16.0720000000
C 9.6330000000 0.6130000000 -15.7710000000
C 8.2570000000 1.2840000000 -15.6410000000
C 8.3110000000 2.4650000000 -14.7030000000
F 12.5550000000 8.2900000000 -1.2570000000
N 8.8820000000 6.2720000000 -9.4860000000
N 11.0470000000 9.8420000000 -6.5210000000
N 9.5520000000 3.0330000000 -14.3060000000
N 7.2090000000 2.9460000000 -14.2700000000
O 11.4040000000 10.3280000000 -5.4310000000
O 10.7140000000 4.6530000000 -12.9830000000
H 5.0125471848 3.8903668493 -13.3174055842
H 5.6194371037 5.5477200558 -13.2215405832
H 5.7334846977 4.5008236175 -11.8063470601
H 7.1956600416 6.1111270214 -11.7379484381
H 8.8234662205 6.5615637784 -12.2838303278

H 9.7808133817 4.7861034891 -10.7554995655
H 8.1245822321 4.4643796548 -10.1727395520
H 10.8251583459 6.8717382283 -10.2017547790
H 9.4374762032 7.8348284110 -10.7710632693
H 9.1281077075 8.8239687957 -8.5540173074
H 10.8083306340 9.1054930883 -9.0959105871
H 11.5195536303 7.0458697860 -7.8333968909
H 8.6143438256 7.0108903104 -6.8876724228
H 9.8899149803 5.9740875837 -6.2436384643
H 8.6003810138 4.8249444028 -8.0211957053
H 10.3084359875 5.0241367544 -8.4828140355
H 11.2972446844 6.0142545484 -4.9407313716
H 12.0105593131 6.1298971772 -2.5737994381
H 12.2306544234 10.3979768387 -2.7220531702
H 11.4613474340 3.4233776496 -14.9757619914
H 11.3057664683 1.9548549399 -14.0278466894
H 11.6391811187 1.2676960952 -16.3103092182
H 10.3390938228 2.3031801066 -16.9215195110
H 9.8970383620 0.1141956432 -14.8305463485
H 9.6049121778 -0.1514383613 -16.5553824404
H 7.4784139439 0.6199732066 -15.2608984846
H 7.9255818468 1.6459448167 -16.6214062198

1.5 Receptor in DRD2-risperidone system

515

TE= -12506.8940346149
C -3.6000000000 1.5980000000 -15.1060000000
C -2.4770000000 1.3790000000 -16.1110000000
O -2.7060000000 0.8780000000 -17.2190000000
H -4.0702039840 0.6335126897 -14.9046883898
H -3.2745478051 2.0452062504 -14.1634925861
H -4.3520252574 2.2398131423 -15.5682273145
N -1.2500000000 1.7240000000 -15.7220000000
C -0.0900000000 1.5900000000 -16.5920000000
C 0.1870000000 0.1430000000 -16.9840000000
O 0.8060000000 -0.0960000000 -18.0270000000
C 1.1310000000 2.1920000000 -15.8930000000
C 2.3620000000 2.4810000000 -16.7450000000
C 1.9520000000 3.2410000000 -17.9870000000
C 3.3660000000 3.2770000000 -15.9310000000
H -1.1205543986 2.1785306353 -14.8324107506
H -0.2983360363 2.1013728624 -17.5335974754
H 1.4017707717 1.5550339565 -15.0401890360
H 0.8083389034 3.1554441970 -15.4684908204
H 2.8085891620 1.5273630099 -17.0504712608
H 1.3560213051 2.6308800220 -18.6659319592
H 1.3637643772 4.1277749141 -17.7165567625
H 2.8273742843 3.5932048274 -18.5346241993
H 2.9944174933 4.2872433655 -15.7267242443
H 3.5846830413 2.7965356578 -14.9716096890

H 4.3094249395 3.3828664384 -16.4630895807
N -0.2440000000 -0.8270000000 -16.1750000000
C -0.0070000000 -2.2280000000 -16.5050000000
H -0.8456650685 -0.5861135701 -15.4063449803
H 0.9476210540 -2.2970816312 -17.0251004254
H 0.0224272227 -2.8173966008 -15.5871835478
H -0.7887775348 -2.6179953500 -17.1647442059
C 1.6090000000 1.9380000000 -22.3780000000
C 1.2590000000 3.1510000000 -21.5290000000
O 0.2530000000 3.1630000000 -20.8150000000
H 2.5550573898 2.0375376306 -22.9145042223
H 1.6500154568 1.0680118756 -21.7191926583
H 0.8002080017 1.7722498407 -23.0927356227
N 2.1100000000 4.1740000000 -21.6140000000
C 1.8710000000 5.4460000000 -20.9320000000
C 0.8920000000 6.3020000000 -21.7420000000
O 1.2170000000 7.3820000000 -22.2360000000
C 3.1880000000 6.1770000000 -20.7020000000
C 4.1480000000 5.4710000000 -19.7840000000
C 4.7310000000 4.2520000000 -19.9830000000
C 4.6550000000 5.9580000000 -18.5340000000
N 5.5580000000 3.9440000000 -18.9280000000
C 5.5300000000 4.9750000000 -18.0270000000
C 4.4490000000 7.1250000000 -17.7920000000
C 6.1980000000 5.1250000000 -16.8110000000
C 5.1140000000 7.2730000000 -16.5830000000
C 5.9770000000 6.2790000000 -16.1070000000
H 2.8134092477 4.1642423196 -22.3349051155
H 1.4075947669 5.1873439250 -19.9754838889
H 2.9470796453 7.1626616036 -20.2996535897
H 3.6452665967 6.3826336149 -21.6770199972
H 4.6126031077 3.5515790026 -20.7947409174
H 6.0715002414 3.0883465861 -18.8199744588
H 3.7819760483 7.9010257118 -18.1537378273
H 6.8448080975 4.3487639175 -16.4176413807
H 4.9649271836 8.1718112024 -15.9941105884
H 6.4882307234 6.4261692504 -15.1625595456
N -0.3290000000 5.7910000000 -21.8770000000
C -1.3650000000 6.4460000000 -22.6780000000
H -0.5265341041 4.9058983349 -21.4205936860
H -0.9521622899 6.7495494079 -23.6420517395
H -1.7462402121 7.3398881599 -22.1758256735
H -2.1813494616 5.7401335821 -22.8296227801
C 2.5330000000 13.1950000000 -7.2140000000
C 3.3480000000 11.9750000000 -6.7990000000
O 3.5730000000 11.7520000000 -5.6040000000
H 3.0854643441 14.0959311525 -6.9359931228
H 2.3082961366 13.2333026585 -8.2823426775
H 1.6024107627 13.1896102563 -6.6450818845
N 3.7940000000 11.1740000000 -7.7680000000
C 4.5980000000 9.9990000000 -7.4450000000
C 5.8850000000 10.3920000000 -6.7340000000

O 6.262000000 9.778000000 -5.730000000
C 4.901000000 9.208000000 -8.720000000
C 5.951000000 8.133000000 -8.509000000
O 5.746000000 7.255000000 -7.648000000
O 6.981000000 8.161000000 -9.214000000
H 3.5325079861 11.3313800345 -8.7275519210
H 4.0752852324 9.3633220338 -6.7290639702
H 5.2662732459 9.8815656750 -9.5033412411
H 3.9714490737 8.7402682536 -9.0636023634
N 6.568000000 11.421000000 -7.235000000
C 7.809000000 11.865000000 -6.610000000
C 7.535000000 12.461000000 -5.234000000
O 8.282000000 12.220000000 -4.279000000
C 8.536000000 12.862000000 -7.531000000
C 9.683000000 13.529000000 -6.804000000
C 9.043000000 12.156000000 -8.778000000
H 6.3133156007 11.7948270565 -8.1353059934
H 8.4558063229 10.9998354431 -6.4341065883
H 7.8013204988 13.6324982563 -7.8133749834
H 9.3558278141 14.1380864450 -5.9572680612
H 10.3935071497 12.7928317712 -6.4180030382
H 10.2297340361 14.1887009087 -7.4835756666
H 9.8304649102 11.4492678648 -8.4989040472
H 8.2675140173 11.5816338352 -9.2935567503
H 9.4573581097 12.8818166922 -9.4837738826
N 6.454000000 13.232000000 -5.103000000
C 6.164000000 13.889000000 -3.832000000
H 5.7198192997 13.1258437234 -5.7863493813
H 6.9987412278 14.5342169547 -3.5529514621
H 6.0020730689 13.1544178545 -3.0399654584
H 5.2618024802 14.4875904079 -3.9485270830
C 4.373000000 11.084000000 -1.977000000
C 5.457000000 10.093000000 -1.578000000
O 5.388000000 9.526000000 -0.482000000
H 4.5760599372 12.0378814677 -1.4798315934
H 3.4244459170 10.7077211411 -1.5961887302
H 4.2985402453 11.2488538892 -3.0556824996
N 6.449000000 9.867000000 -2.434000000
C 7.576000000 9.023000000 -2.062000000
C 8.689000000 9.813000000 -1.387000000
O 9.435000000 9.249000000 -0.578000000
C 8.121000000 8.295000000 -3.295000000
S 6.974000000 7.093000000 -4.021000000
H 6.3251494791 10.0815580974 -3.4181505471
H 7.2345690025 8.3090059738 -1.3110954966
H 9.0656336694 7.8106807757 -3.0434291976
H 8.3174944185 9.0136185915 -4.0959528333
H 7.1248913707 6.1797849323 -3.0404547654
N 8.819000000 11.105000000 -1.703000000
C 9.769000000 11.947000000 -0.985000000
C 9.300000000 12.212000000 0.440000000
O 10.125000000 12.295000000 1.357000000

C 9.9810000000 13.2710000000 -1.7280000000
O 10.2680000000 13.0090000000 -3.1050000000
C 11.1480000000 14.0450000000 -1.1290000000
H 8.2609873210 11.4849375640 -2.4578888725
H 10.7212672366 11.4189536385 -0.9001180153
H 9.0560244270 13.8656027926 -1.6619602806
H 10.9458282064 14.3162176968 -0.0921241002
H 12.0499039560 13.4275041677 -1.1462922302
H 11.3295010308 14.9469935300 -1.7157482401
H 9.5019294672 12.6642731223 -3.5951884734
N 7.9870000000 12.3430000000 0.6420000000
C 7.4570000000 12.4860000000 1.9920000000
H 7.3682150683 12.0702454143 -0.1051208589
H 7.1993392256 13.5270397408 2.2074091109
H 8.2203991608 12.1564265897 2.6958850207
H 6.5687697550 11.8610900103 2.0981156087
C 8.2080000000 8.8890000000 2.9980000000
C 9.6620000000 9.0030000000 3.4310000000
O 10.0140000000 8.6430000000 4.5610000000
H 7.6087939134 9.5364980127 3.6424672523
H 7.8802403613 7.8622656594 3.1695081625
H 8.0360988415 9.1525801709 1.9515906822
N 10.5220000000 9.5000000000 2.5440000000
C 11.9320000000 9.6320000000 2.8820000000
C 12.1440000000 10.7310000000 3.9110000000
O 12.8700000000 10.5440000000 4.8930000000
C 12.7460000000 9.9050000000 1.6210000000
H 10.2313323649 9.6582244316 1.5883191022
H 12.2620756551 8.7179248282 3.3801813350
H 12.6490872083 9.0830469019 0.9117173104
H 12.4136008033 10.8232918503 1.1306924902
H 13.8008460559 10.0224584211 1.8757418722
N 11.5110000000 11.8860000000 3.7070000000
C 11.6610000000 12.9820000000 4.6540000000
H 10.9483414784 12.0200084046 2.8782275844
H 12.6956119709 13.3376923974 4.6878014680
H 11.0080523450 13.7990684826 4.3422052051
H 11.3882636235 12.6541695156 5.6607085692
C 8.7820000000 15.5050000000 -17.2430000000
C 9.6310000000 14.2530000000 -17.0700000000
O 10.8560000000 14.3490000000 -16.9440000000
H 9.1292447099 16.0260462364 -18.1374054856
H 8.9632852708 16.1596434848 -16.3892060678
H 7.7097166026 15.3108798182 -17.3313091623
N 9.0200000000 13.0660000000 -17.0780000000
C 9.8080000000 11.8480000000 -16.9450000000
C 10.6490000000 11.6030000000 -18.1870000000
O 11.5890000000 10.8020000000 -18.1480000000
C 8.9070000000 10.6360000000 -16.6450000000
C 9.6940000000 9.5740000000 -15.8760000000
C 8.3460000000 10.0520000000 -17.9320000000
C 8.8610000000 8.3830000000 -15.4560000000

H 8.0147006954 13.0035089891 -17.0865226582
H 10.5290062892 11.9985577647 -16.1376845779
H 8.0875942492 10.9910143781 -16.0033111460
H 10.1280359292 10.0437029973 -14.9847154952
H 10.5406135692 9.2624173237 -16.4958462766
H 7.8954828059 10.8165002612 -18.5742761548
H 9.1422028342 9.5665562024 -18.5025702355
H 7.5737372279 9.3065004392 -17.7283286501
H 8.0027473263 8.6904490646 -14.8473626130
H 8.4740314697 7.8232244122 -16.3109125104
H 9.4531579152 7.6863656142 -14.8553992246
N 10.3350000000 12.2790000000 -19.2910000000
C 11.1620000000 12.2340000000 -20.4870000000
H 9.6107985507 12.9731278903 -19.2280669372
H 11.8315095647 11.3810368709 -20.3834542825
H 10.5400131738 12.1099378634 -21.3766986963
H 11.7592970993 13.1460124208 -20.5837264561
C 17.0080000000 15.2090000000 -9.7860000000
C 16.3860000000 14.3230000000 -8.7140000000
O 16.7430000000 14.4070000000 -7.5340000000
H 18.0932823814 15.1290235392 -9.7106711814
H 16.7356900495 16.2443136791 -9.5701385629
H 16.6906926580 14.9587118809 -10.8006445973
N 15.4570000000 13.4490000000 -9.1140000000
C 14.7150000000 12.6540000000 -8.1390000000
C 15.6150000000 11.6810000000 -7.3860000000
O 15.2940000000 11.2860000000 -6.2600000000
C 13.5800000000 11.8970000000 -8.8300000000
O 14.0750000000 10.9340000000 -9.7410000000
H 15.1863018066 13.3922694336 -10.0829227572
H 14.2747820948 13.3117212116 -7.3844503434
H 12.9404038454 12.6330913291 -9.3408833552
H 12.9816678935 11.4288510514 -8.0396148873
H 13.3803921996 10.2903108367 -9.8879136361
N 16.7390000000 11.2830000000 -7.9800000000
C 17.6640000000 10.4070000000 -7.2710000000
H 16.9605958004 11.6299028067 -8.8969428791
H 17.0923162548 9.8009834499 -6.5693790937
H 18.1718672096 9.7560481443 -7.9845317292
H 18.4100931234 10.9902729801 -6.7199181342
C 17.3320000000 15.4630000000 -4.1050000000
C 16.3430000000 14.6560000000 -3.2690000000
O 16.2680000000 14.8140000000 -2.0460000000
H 18.3340326600 15.2809287531 -3.7112399343
H 17.3040514073 15.2297464452 -5.1721894253
H 17.1073349534 16.5208968959 -3.9550059006
N 15.5710000000 13.7780000000 -3.9110000000
C 14.5050000000 13.0730000000 -3.2110000000
C 14.9860000000 11.8390000000 -2.4600000000
O 14.3040000000 11.4010000000 -1.5280000000
C 13.4010000000 12.6680000000 -4.1910000000
O 12.4160000000 13.6770000000 -4.2970000000

H 15.5923850063 13.7350176567 -4.9195183426
H 14.0978911222 13.7319553586 -2.4441940740
H 12.9603024522 11.7354540750 -3.8451721145
H 13.8406359491 12.4590290235 -5.1671479236
H 11.6234326048 13.3998091430 -3.8045225064
N 16.1340000000 11.2650000000 -2.8240000000
C 16.5630000000 10.0060000000 -2.2250000000
C 17.9510000000 10.0800000000 -1.5970000000
O 18.0760000000 9.8530000000 -0.3910000000
C 16.5180000000 8.8870000000 -3.2690000000
C 16.8360000000 7.5250000000 -2.7140000000
C 15.8890000000 6.8220000000 -1.9860000000
C 18.0740000000 6.9440000000 -2.9270000000
C 16.1730000000 5.5660000000 -1.4810000000
C 18.3650000000 5.6870000000 -2.4230000000
C 17.4120000000 4.9970000000 -1.7000000000
H 16.5960462004 11.6301020671 -3.6433977253
H 15.8740004819 9.8097825864 -1.4053104901
H 17.2001107545 9.1163969342 -4.0964898767
H 15.5132836273 8.8821227096 -3.7035227837
H 14.9132760795 7.2661671063 -1.8108126436
H 18.8217795564 7.4776659744 -3.5068949425
H 15.4135252474 5.0320240299 -0.9187521274
H 19.3411567595 5.2467074509 -2.6021067742
H 17.6343396167 4.0086894779 -1.3070595354
N 18.9960000000 10.3800000000 -2.3730000000
C 20.3560000000 10.2300000000 -1.8610000000
H 18.8675926702 10.4042759746 -3.3711058154
H 21.0334658033 10.8634834784 -2.4357137203
H 20.6914960078 9.1881273836 -1.9118771207
H 20.3545132507 10.5391354911 -0.8170766807
C 13.7580000000 -1.9180000000 5.0570000000
C 13.4120000000 -0.9780000000 3.9100000000
O 13.3110000000 -1.3970000000 2.7510000000
H 14.7762936910 -2.2815543513 4.9012931361
H 13.6911034973 -1.4556074275 6.0447949398
H 13.0882116201 -2.7772546931 5.0101362208
N 13.2310000000 0.3080000000 4.2140000000
C 13.0140000000 1.2980000000 3.1660000000
C 14.1650000000 1.2940000000 2.1710000000
O 13.9530000000 1.1860000000 0.9580000000
C 12.8440000000 2.6790000000 3.7960000000
C 12.5140000000 3.7670000000 2.8150000000
C 11.2030000000 4.0130000000 2.4520000000
C 13.5130000000 4.5600000000 2.2760000000
C 10.8950000000 5.0210000000 1.5570000000
C 13.2110000000 5.5660000000 1.3800000000
C 11.9000000000 5.7970000000 1.0210000000
H 13.2358327400 0.6114998894 5.1743371520
H 12.1326585540 1.0293535883 2.5791067623
H 13.7578998795 2.9431685268 4.3413896787
H 12.0403343419 2.6111970177 4.5388734844

H 10.4050390267 3.4149095536 2.8844366173
H 14.5458563276 4.3933008544 2.5707628870
H 9.8607630480 5.2187644691 1.2955214259
H 14.0009165808 6.1932349152 0.9796108359
H 11.6564970053 6.6020414818 0.3364921696
N 15.3990000000 1.3950000000 2.6720000000
C 16.5640000000 1.4050000000 1.7920000000
H 15.5273084101 1.3755743587 3.6693278660
H 16.4215045749 2.1510786293 1.0079499602
H 16.7066981824 0.4268178572 1.3232221780
H 17.4467942897 1.6611814863 2.3773768705
C 13.2140000000 -1.7440000000 -1.1060000000
C 13.4830000000 -0.8070000000 -2.2810000000
O 13.1990000000 -1.1600000000 -3.4320000000
H 13.8092785674 -2.6478344094 -1.2519329087
H 13.4290753789 -1.3090802741 -0.1275511387
H 12.1618410013 -2.0294994154 -1.1495333643
N 14.0180000000 0.3840000000 -2.0240000000
C 14.2130000000 1.3500000000 -3.0950000000
C 15.6180000000 1.3460000000 -3.6770000000
O 15.8120000000 1.8740000000 -4.7760000000
C 13.8850000000 2.7670000000 -2.6120000000
C 12.4150000000 3.0710000000 -2.5650000000
C 11.6480000000 3.2360000000 -1.4480000000
C 11.5340000000 3.2440000000 -3.6840000000
N 10.3480000000 3.5020000000 -1.8010000000
C 10.2510000000 3.5120000000 -3.1680000000
C 11.7060000000 3.2000000000 -5.0720000000
C 9.1460000000 3.7360000000 -3.9880000000
C 10.6060000000 3.4210000000 -5.8850000000
C 9.3430000000 3.6840000000 -5.3400000000
H 14.0108169306 0.7223600133 -1.0650753911
H 13.5529415615 1.0656975384 -3.9184842161
H 14.3870722387 3.4684140480 -3.2833412515
H 14.3241368180 2.9155341250 -1.6196484668
H 11.9340634910 3.1578407318 -0.4087136444
H 9.5605265197 3.4353699873 -1.1796856407
H 12.6778741268 2.9959399753 -5.5093117149
H 8.1622897930 3.9091171408 -3.5685715537
H 10.7235898873 3.3714572118 -6.9614569494
H 8.4953286683 3.8251079379 -6.0014243737
N 16.5990000000 0.7790000000 -2.9860000000
C 17.9630000000 0.9080000000 -3.4860000000
H 16.3813945873 0.3398488689 -2.1048851108
H 18.3391718717 1.9250719655 -3.3395522317
H 17.9825104118 0.6859402854 -4.5529616004
H 18.6092880335 0.2045875209 -2.9610484665
C 17.7850000000 -1.7800000000 -6.2230000000
C 17.1900000000 -0.9670000000 -7.3560000000
O 17.6700000000 -1.0540000000 -8.4930000000
H 17.1799712352 -1.7761117228 -5.3129141091
H 18.7768966038 -1.3814637210 -5.9925044625

N 16.1570000000 -0.1680000000 -7.0770000000
C 15.5880000000 0.6990000000 -8.1030000000
C 16.5810000000 1.7760000000 -8.5240000000
O 16.7910000000 2.0090000000 -9.7190000000
C 14.2870000000 1.3230000000 -7.5920000000
C 13.6700000000 2.3190000000 -8.5360000000
C 12.9470000000 1.8970000000 -9.6380000000
C 13.7950000000 3.6770000000 -8.3090000000
C 12.3740000000 2.8120000000 -10.5010000000
C 13.2210000000 4.5930000000 -9.1690000000
C 12.5080000000 4.1600000000 -10.2630000000
H 15.7777679819 -0.1084450689 -6.1439124329
H 15.4168610939 0.1140303215 -9.0086853672
H 14.4951307678 1.8135396205 -6.6370402482
H 13.5746174115 0.5131418307 -7.3925736512
H 12.8409496173 0.8323638082 -9.8317122452
H 14.3522182098 4.0291875182 -7.4457220633
H 11.9091056525 2.5302497691 -11.4389414489
H 13.3195432382 5.6538289149 -8.9562792610
H 12.0433736801 4.8553663970 -10.9560442868
N 17.2110000000 2.4380000000 -7.5530000000
C 18.1540000000 3.5030000000 -7.8650000000
C 19.5200000000 2.9770000000 -8.2850000000
O 20.2660000000 3.6990000000 -8.9550000000
C 18.2900000000 4.4410000000 -6.6660000000
C 17.0460000000 5.2290000000 -6.3840000000
C 16.7700000000 6.3840000000 -7.0950000000
C 16.1460000000 4.8100000000 -5.4230000000
C 15.6240000000 7.1100000000 -6.8480000000
C 14.9950000000 5.5330000000 -5.1710000000
C 14.7350000000 6.6850000000 -5.8840000000
H 16.9037807101 2.3127194114 -6.5926539669
H 17.7781879241 4.0518522296 -8.7319261421
H 19.1223285211 5.1162761058 -6.8836543825
H 18.5744297612 3.8552594217 -5.7845294062
H 17.4722408931 6.7241228438 -7.8531863231
H 16.3493738450 3.9153035250 -4.8505042494
H 15.4236115787 8.0197104057 -7.4065959399
H 14.2939808172 5.2089094017 -4.4104258875
H 13.8383845391 7.2586631107 -5.6775072235
N 19.8650000000 1.7440000000 -7.9050000000
C 21.0440000000 1.1000000000 -8.4770000000
H 19.1009463137 1.1411656841 -7.6329074799
H 21.9544104972 1.4762315104 -8.0050612351
H 21.1021750721 1.2984220488 -9.5495822039
H 20.9628706235 0.0265028073 -8.3113851438
C 19.3470000000 0.3410000000 -11.8010000000
C 19.5100000000 1.6220000000 -12.6110000000
O 19.9720000000 1.5850000000 -13.7590000000
H 20.3444089789 -0.0173081205 -11.5320392739
H 18.7443932871 0.4588263800 -10.8971295667
H 18.8896838199 -0.4125307125 -12.4430569082

N 19.1870000000 2.7420000000 -12.0310000000
C 19.3630000000 3.9570000000 -12.7380000000
C 20.8090000000 4.1810000000 -13.0330000000
O 21.1450000000 4.6510000000 -14.0710000000
C 18.8630000000 5.0740000000 -11.8930000000
C 17.4120000000 5.3340000000 -12.0640000000
N 16.8150000000 5.3550000000 -13.2960000000
C 16.4400000000 5.5910000000 -11.1680000000
C 15.5360000000 5.6220000000 -13.1550000000
N 15.2820000000 5.7620000000 -11.8720000000
H 18.5932780616 2.7213437732 -11.2102818764
H 18.8579082062 3.9477550676 -13.7055789801
H 19.3981645506 5.9859005400 -12.1880404407
H 19.1122544113 4.9012005375 -10.8406851232
H 16.4341336444 5.6372864387 -10.0889451039
H 14.3741486357 5.8669640633 -11.4466780761
H 14.7949250278 5.6593338117 -13.9361725714
N 21.6750000000 3.8690000000 -12.0940000000
C 23.1030000000 4.0650000000 -12.3040000000
H 21.3452297198 3.5694342124 -11.1872572325
H 23.3577741110 5.1279633185 -12.3705809817
H 23.4039907108 3.5878777869 -13.2390216146
H 23.6449242097 3.6151627123 -11.4711066731
C 13.5920000000 -6.2960000000 -14.0890000000
C 13.3900000000 -4.8380000000 -13.6980000000
O 13.2000000000 -4.5330000000 -12.5160000000
H 12.6436965744 -6.8218045152 -13.9490347915
H 14.3214064831 -6.7384897293 -13.4104327515
H 13.9198071623 -6.4340084657 -15.1222702978
N 13.3700000000 -3.9560000000 -14.6500000000
C 13.1430000000 -2.5990000000 -14.2990000000
C 11.7640000000 -2.4930000000 -13.7130000000
O 11.5780000000 -1.7950000000 -12.7660000000
C 13.2630000000 -1.7460000000 -15.5210000000
C 13.9090000000 -0.4440000000 -15.2740000000
C 13.6940000000 0.2270000000 -14.1290000000
C 14.7250000000 0.1220000000 -16.1990000000
C 14.2870000000 1.4340000000 -13.9040000000
C 15.3230000000 1.3310000000 -15.9730000000
C 15.0860000000 1.9740000000 -14.8140000000
O 15.6400000000 3.1780000000 -14.5330000000
H 13.6690512118 -4.1960503196 -15.5811859578
H 13.8332715487 -2.2906841926 -13.5123338478
H 12.2749345735 -1.6078285795 -15.9827023226
H 13.8570689057 -2.2780436044 -16.2752014847
H 13.0488968645 -0.1790718375 -13.3550249616
H 14.9277302259 -0.3981307292 -17.1332588382
H 14.1376332120 1.9564748067 -12.9640174804
H 15.9903678161 1.7596898793 -16.7148284052
H 16.4332021871 3.3614407364 -15.0421161528
N 10.7810000000 -3.1730000000 -14.2780000000
C 9.4310000000 -3.1190000000 -13.7270000000

C 9.3630000000 -3.7500000000 -12.3410000000
O 8.5430000000 -3.3360000000 -11.5130000000
C 8.4470000000 -3.8110000000 -14.6720000000
O 8.4930000000 -3.2390000000 -15.9670000000
H 10.9041680326 -3.6188462710 -15.1738986403
H 9.1375410900 -2.0740208074 -13.5816907177
H 7.4486892903 -3.7625476634 -14.2240668894
H 8.7193854384 -4.8631903868 -14.7920867693
H 8.1781973235 -2.3341641956 -15.8979711179
N 10.2160000000 -4.7400000000 -12.0690000000
C 10.1960000000 -5.4050000000 -10.7690000000
H 11.0727152982 -4.8030003125 -12.6000588577
H 9.3400187726 -6.0799565671 -10.6972018676
H 10.1270324572 -4.6690033259 -9.9650498798
H 11.1212900318 -5.9688917645 -10.6624599755
C 12.4460000000 -2.9770000000 -8.8830000000
C 11.5930000000 -1.7450000000 -8.6140000000
O 11.6580000000 -1.1790000000 -7.5160000000
H 12.0342637384 -3.8013308601 -8.2950172427
H 13.4535550745 -2.7795416195 -8.5154858077
H 12.4867847918 -3.2664356261 -9.9361171175
N 10.7990000000 -1.3100000000 -9.5960000000
C 9.8540000000 -0.2250000000 -9.3530000000
C 8.7120000000 -0.6930000000 -8.4590000000
O 8.3350000000 -0.0050000000 -7.5030000000
C 9.3100000000 0.3150000000 -10.6770000000
O 10.3970000000 0.6240000000 -11.5570000000
C 8.4910000000 1.5780000000 -10.4360000000
H 10.9564778424 -1.5975682995 -10.5548643372
H 10.3512987522 0.5732188697 -8.7946682365
H 8.7278074921 -0.4623873242 -11.1818549813
H 7.6635746488 1.4142114817 -9.7437308433
H 9.1303435981 2.3471671659 -9.9935210535
H 8.0992277534 1.9574023527 -11.3821617978
H 10.7985888989 1.4126621433 -11.1836938956
N 8.1480000000 -1.8660000000 -8.7580000000
C 7.0780000000 -2.4060000000 -7.9270000000
H 8.4428293569 -2.3808704681 -9.5788253873
H 6.1659920141 -1.8079995247 -8.0135525835
H 6.8710983958 -3.4265735912 -8.2496482365
H 7.3853251435 -2.4056992893 -6.8788017663
C 9.7450000000 0.1790000000 -4.0810000000
C 8.3570000000 0.5810000000 -3.6180000000
O 8.1800000000 1.0430000000 -2.4880000000
H 10.0683054205 -0.6929338923 -3.5059788334
H 9.8059332431 -0.0540146389 -5.1460044255
H 10.4326315781 0.9907286926 -3.8504596748
N 7.3550000000 0.4230000000 -4.4850000000
C 5.9780000000 0.6950000000 -4.0890000000
C 5.4940000000 -0.2880000000 -3.0300000000
O 4.6290000000 0.0580000000 -2.2150000000
C 5.0650000000 0.6460000000 -5.3120000000

C 5.2570000000 1.8000000000 -6.2660000000
C 5.3340000000 3.1070000000 -5.8020000000
C 5.3620000000 1.5840000000 -7.6330000000
C 5.5050000000 4.1660000000 -6.6750000000
C 5.5370000000 2.6370000000 -8.5130000000
C 5.6080000000 3.9250000000 -8.0300000000
O 5.7810000000 4.9740000000 -8.9060000000
H 17.9136766655 -2.8042934516 -6.5732670840
H 7.5694240846 0.2688693537 -5.4665359669
H 5.9202423994 1.6672530112 -3.5965356116
H 4.0352270610 0.6336287071 -4.9357946259
H 5.2212181155 -0.3026956256 -5.8382188045
H 5.2496596274 3.3125488090 -4.7387366985
H 5.3256234472 0.5679187723 -8.0154466195
H 5.5552791826 5.1910411147 -6.3207897855
H 5.6115303863 2.4717419603 -9.5824877229
H 5.8734911639 5.8326800373 -8.3959950123
N 6.0360000000 -1.5100000000 -3.0310000000
C 5.6820000000 -2.5030000000 -2.0190000000
H 6.8348749432 -1.6598306501 -3.6263966773
H 4.7742477643 -2.1480229650 -1.5325727912
H 5.5016543210 -3.4748407350 -2.4858308535
H 6.4729933136 -2.6008165265 -1.2685453420

1.6 DRD2-risperidone system

572

TE= -13867.8050602696439455
C -3.6000000000 1.5980000000 -15.1060000000
C -2.4770000000 1.3790000000 -16.1110000000
O -2.7060000000 0.8780000000 -17.2190000000
H -4.0702039840 0.6335126897 -14.9046883898
H -3.2745478051 2.0452062504 -14.1634925861
H -4.3520252574 2.2398131423 -15.5682273145
N -1.2500000000 1.7240000000 -15.7220000000
C -0.0900000000 1.5900000000 -16.5920000000
C 0.1870000000 0.1430000000 -16.9840000000
O 0.8060000000 -0.0960000000 -18.0270000000
C 1.1310000000 2.1920000000 -15.8930000000
C 2.3620000000 2.4810000000 -16.7450000000
C 1.9520000000 3.2410000000 -17.9870000000
C 3.3660000000 3.2770000000 -15.9310000000
H -1.1205543986 2.1785306353 -14.8324107506
H -0.2983360363 2.1013728624 -17.5335974754
H 1.4017707717 1.5550339565 -15.0401890360
H 0.8083389034 3.1554441970 -15.4684908204
H 2.8085891620 1.5273630099 -17.0504712608
H 1.3560213051 2.6308800220 -18.6659319592
H 1.3637643772 4.1277749141 -17.7165567625
H 2.8273742843 3.5932048274 -18.5346241993
H 2.9944174933 4.2872433655 -15.7267242443

H 3.5846830413 2.7965356578 -14.9716096890
H 4.3094249395 3.3828664384 -16.4630895807
N -0.2440000000 -0.8270000000 -16.1750000000
C -0.0070000000 -2.2280000000 -16.5050000000
H -0.8456650685 -0.5861135701 -15.4063449803
H 0.9476210540 -2.2970816312 -17.0251004254
H 0.0224272227 -2.8173966008 -15.5871835478
H -0.7887775348 -2.6179953500 -17.1647442059
C 1.6090000000 1.9380000000 -22.3780000000
C 1.2590000000 3.1510000000 -21.5290000000
O 0.2530000000 3.1630000000 -20.8150000000
H 2.5550573898 2.0375376306 -22.9145042223
H 1.6500154568 1.0680118756 -21.7191926583
H 0.8002080017 1.7722498407 -23.0927356227
N 2.1100000000 4.1740000000 -21.6140000000
C 1.8710000000 5.4460000000 -20.9320000000
C 0.8920000000 6.3020000000 -21.7420000000
O 1.2170000000 7.3820000000 -22.2360000000
C 3.1880000000 6.1770000000 -20.7020000000
C 4.1480000000 5.4710000000 -19.7840000000
C 4.7310000000 4.2520000000 -19.9830000000
C 4.6550000000 5.9580000000 -18.5340000000
N 5.5580000000 3.9440000000 -18.9280000000
C 5.5300000000 4.9750000000 -18.0270000000
C 4.4490000000 7.1250000000 -17.7920000000
C 6.1980000000 5.1250000000 -16.8110000000
C 5.1140000000 7.2730000000 -16.5830000000
C 5.9770000000 6.2790000000 -16.1070000000
H 2.8134092477 4.1642423196 -22.3349051155
H 1.4075947669 5.1873439250 -19.9754838889
H 2.9470796453 7.1626616036 -20.2996535897
H 3.6452665967 6.3826336149 -21.6770199972
H 4.6126031077 3.5515790026 -20.7947409174
H 6.0715002414 3.0883465861 -18.8199744588
H 3.7819760483 7.9010257118 -18.1537378273
H 6.8448080975 4.3487639175 -16.4176413807
H 4.9649271836 8.1718112024 -15.9941105884
H 6.4882307234 6.4261692504 -15.1625595456
N -0.3290000000 5.7910000000 -21.8770000000
C -1.3650000000 6.4460000000 -22.6780000000
H -0.5265341041 4.9058983349 -21.4205936860
H -0.9521622899 6.7495494079 -23.6420517395
H -1.7462402121 7.3398881599 -22.1758256735
H -2.1813494616 5.7401335821 -22.8296227801
C 2.5330000000 13.1950000000 -7.2140000000
C 3.3480000000 11.9750000000 -6.7990000000
O 3.5730000000 11.7520000000 -5.6040000000
H 3.0854643441 14.0959311525 -6.9359931228
H 2.3082961366 13.2333026585 -8.2823426775
H 1.6024107627 13.1896102563 -6.6450818845
N 3.7940000000 11.1740000000 -7.7680000000
C 4.5980000000 9.9990000000 -7.4450000000

C 5.885000000 10.392000000 -6.734000000
O 6.262000000 9.778000000 -5.730000000
C 4.901000000 9.208000000 -8.720000000
C 5.951000000 8.133000000 -8.509000000
O 5.746000000 7.255000000 -7.648000000
O 6.981000000 8.161000000 -9.214000000
H 3.5325079861 11.3313800345 -8.7275519210
H 4.0752852324 9.3633220338 -6.7290639702
H 5.2662732459 9.8815656750 -9.5033412411
H 3.9714490737 8.7402682536 -9.0636023634
N 6.568000000 11.421000000 -7.235000000
C 7.809000000 11.865000000 -6.610000000
C 7.535000000 12.461000000 -5.234000000
O 8.282000000 12.220000000 -4.279000000
C 8.536000000 12.862000000 -7.531000000
C 9.683000000 13.529000000 -6.804000000
C 9.043000000 12.156000000 -8.778000000
H 6.3133156007 11.7948270565 -8.1353059934
H 8.4558063229 10.9998354431 -6.4341065883
H 7.8013204988 13.6324982563 -7.8133749834
H 9.3558278141 14.1380864450 -5.9572680612
H 10.3935071497 12.7928317712 -6.4180030382
H 10.2297340361 14.1887009087 -7.4835756666
H 9.8304649102 11.4492678648 -8.4989040472
H 8.2675140173 11.5816338352 -9.2935567503
H 9.4573581097 12.8818166922 -9.4837738826
N 6.454000000 13.232000000 -5.103000000
C 6.164000000 13.889000000 -3.832000000
H 5.7198192997 13.1258437234 -5.7863493813
H 6.9987412278 14.5342169547 -3.5529514621
H 6.0020730689 13.1544178545 -3.0399654584
H 5.2618024802 14.4875904079 -3.9485270830
C 4.373000000 11.084000000 -1.977000000
C 5.457000000 10.093000000 -1.578000000
O 5.388000000 9.526000000 -0.482000000
H 4.5760599372 12.0378814677 -1.4798315934
H 3.4244459170 10.7077211411 -1.5961887302
H 4.2985402453 11.2488538892 -3.0556824996
N 6.449000000 9.867000000 -2.434000000
C 7.576000000 9.023000000 -2.062000000
C 8.689000000 9.813000000 -1.387000000
O 9.435000000 9.249000000 -0.578000000
C 8.121000000 8.295000000 -3.295000000
S 6.974000000 7.093000000 -4.021000000
H 6.3251494791 10.0815580974 -3.4181505471
H 7.2345690025 8.3090059738 -1.3110954966
H 9.0656336694 7.8106807757 -3.0434291976
H 8.3174944185 9.0136185915 -4.0959528333
H 7.1248913707 6.1797849323 -3.0404547654
N 8.819000000 11.105000000 -1.703000000
C 9.769000000 11.947000000 -0.985000000
C 9.300000000 12.212000000 0.440000000

O 10.1250000000 12.2950000000 1.3570000000
C 9.9810000000 13.2710000000 -1.7280000000
O 10.2680000000 13.0090000000 -3.1050000000
C 11.1480000000 14.0450000000 -1.1290000000
H 8.2609873210 11.4849375640 -2.4578888725
H 10.7212672366 11.4189536385 -0.9001180153
H 9.0560244270 13.8656027926 -1.6619602806
H 10.9458282064 14.3162176968 -0.0921241002
H 12.0499039560 13.4275041677 -1.1462922302
H 11.3295010308 14.9469935300 -1.7157482401
H 9.5019294672 12.6642731223 -3.5951884734
N 7.9870000000 12.3430000000 0.6420000000
C 7.4570000000 12.4860000000 1.9920000000
H 7.3682150683 12.0702454143 -0.1051208589
H 7.1993392256 13.5270397408 2.2074091109
H 8.2203991608 12.1564265897 2.6958850207
H 6.5687697550 11.8610900103 2.0981156087
C 8.2080000000 8.8890000000 2.9980000000
C 9.6620000000 9.0030000000 3.4310000000
O 10.0140000000 8.6430000000 4.5610000000
H 7.6087939134 9.5364980127 3.6424672523
H 7.8802403613 7.8622656594 3.1695081625
H 8.0360988415 9.1525801709 1.9515906822
N 10.5220000000 9.5000000000 2.5440000000
C 11.9320000000 9.6320000000 2.8820000000
C 12.1440000000 10.7310000000 3.9110000000
O 12.8700000000 10.5440000000 4.8930000000
C 12.7460000000 9.9050000000 1.6210000000
H 10.2313323649 9.6582244316 1.5883191022
H 12.2620756551 8.7179248282 3.3801813350
H 12.6490872083 9.0830469019 0.9117173104
H 12.4136008033 10.8232918503 1.1306924902
H 13.8008460559 10.0224584211 1.8757418722
N 11.5110000000 11.8860000000 3.7070000000
C 11.6610000000 12.9820000000 4.6540000000
H 10.9483414784 12.0200084046 2.8782275844
H 12.6956119709 13.3376923974 4.6878014680
H 11.0080523450 13.7990684826 4.3422052051
H 11.3882636235 12.6541695156 5.6607085692
C 8.7820000000 15.5050000000 -17.2430000000
C 9.6310000000 14.2530000000 -17.0700000000
O 10.8560000000 14.3490000000 -16.9440000000
H 9.1292447099 16.0260462364 -18.1374054856
H 8.9632852708 16.1596434848 -16.3892060678
H 7.7097166026 15.3108798182 -17.3313091623
N 9.0200000000 13.0660000000 -17.0780000000
C 9.8080000000 11.8480000000 -16.9450000000
C 10.6490000000 11.6030000000 -18.1870000000
O 11.5890000000 10.8020000000 -18.1480000000
C 8.9070000000 10.6360000000 -16.6450000000
C 9.6940000000 9.5740000000 -15.8760000000
C 8.3460000000 10.0520000000 -17.9320000000

C 8.8610000000 8.3830000000 -15.4560000000
H 8.0147006954 13.0035089891 -17.0865226582
H 10.5290062892 11.9985577647 -16.1376845779
H 8.0875942492 10.9910143781 -16.0033111460
H 10.1280359292 10.0437029973 -14.9847154952
H 10.5406135692 9.2624173237 -16.4958462766
H 7.8954828059 10.8165002612 -18.5742761548
H 9.1422028342 9.5665562024 -18.5025702355
H 7.5737372279 9.3065004392 -17.7283286501
H 8.0027473263 8.6904490646 -14.8473626130
H 8.4740314697 7.8232244122 -16.3109125104
H 9.4531579152 7.6863656142 -14.8553992246
N 10.3350000000 12.2790000000 -19.2910000000
C 11.1620000000 12.2340000000 -20.4870000000
H 9.6107985507 12.9731278903 -19.2280669372
H 11.8315095647 11.3810368709 -20.3834542825
H 10.5400131738 12.1099378634 -21.3766986963
H 11.7592970993 13.1460124208 -20.5837264561
C 17.0080000000 15.2090000000 -9.7860000000
C 16.3860000000 14.3230000000 -8.7140000000
O 16.7430000000 14.4070000000 -7.5340000000
H 18.0932823814 15.1290235392 -9.7106711814
H 16.7356900495 16.2443136791 -9.5701385629
H 16.6906926580 14.9587118809 -10.8006445973
N 15.4570000000 13.4490000000 -9.1140000000
C 14.7150000000 12.6540000000 -8.1390000000
C 15.6150000000 11.6810000000 -7.3860000000
O 15.2940000000 11.2860000000 -6.2600000000
C 13.5800000000 11.8970000000 -8.8300000000
O 14.0750000000 10.9340000000 -9.7410000000
H 15.1863018066 13.3922694336 -10.0829227572
H 14.2747820948 13.3117212116 -7.3844503434
H 12.9404038454 12.6330913291 -9.3408833552
H 12.9816678935 11.4288510514 -8.0396148873
H 13.3803921996 10.2903108367 -9.8879136361
N 16.7390000000 11.2830000000 -7.9800000000
C 17.6640000000 10.4070000000 -7.2710000000
H 16.9605958004 11.6299028067 -8.8969428791
H 17.0923162548 9.8009834499 -6.5693790937
H 18.1718672096 9.7560481443 -7.9845317292
H 18.4100931234 10.9902729801 -6.7199181342
C 17.3320000000 15.4630000000 -4.1050000000
C 16.3430000000 14.6560000000 -3.2690000000
O 16.2680000000 14.8140000000 -2.0460000000
H 18.3340326600 15.2809287531 -3.7112399343
H 17.3040514073 15.2297464452 -5.1721894253
H 17.1073349534 16.5208968959 -3.9550059006
N 15.5710000000 13.7780000000 -3.9110000000
C 14.5050000000 13.0730000000 -3.2110000000
C 14.9860000000 11.8390000000 -2.4600000000
O 14.3040000000 11.4010000000 -1.5280000000
C 13.4010000000 12.6680000000 -4.1910000000

O 12.416000000 13.677000000 -4.297000000
H 15.5923850063 13.7350176567 -4.9195183426
H 14.0978911222 13.7319553586 -2.4441940740
H 12.9603024522 11.7354540750 -3.8451721145
H 13.8406359491 12.4590290235 -5.1671479236
H 11.6234326048 13.3998091430 -3.8045225064
N 16.1340000000 11.2650000000 -2.8240000000
C 16.5630000000 10.0060000000 -2.2250000000
C 17.9510000000 10.0800000000 -1.5970000000
O 18.0760000000 9.8530000000 -0.3910000000
C 16.5180000000 8.8870000000 -3.2690000000
C 16.8360000000 7.5250000000 -2.7140000000
C 15.8890000000 6.8220000000 -1.9860000000
C 18.0740000000 6.9440000000 -2.9270000000
C 16.1730000000 5.5660000000 -1.4810000000
C 18.3650000000 5.6870000000 -2.4230000000
C 17.4120000000 4.9970000000 -1.7000000000
H 16.5960462004 11.6301020671 -3.6433977253
H 15.8740004819 9.8097825864 -1.4053104901
H 17.2001107545 9.1163969342 -4.0964898767
H 15.5132836273 8.8821227096 -3.7035227837
H 14.9132760795 7.2661671063 -1.8108126436
H 18.8217795564 7.4776659744 -3.5068949425
H 15.4135252474 5.0320240299 -0.9187521274
H 19.3411567595 5.2467074509 -2.6021067742
H 17.6343396167 4.0086894779 -1.3070595354
N 18.9960000000 10.3800000000 -2.3730000000
C 20.3560000000 10.2300000000 -1.8610000000
H 18.8675926702 10.4042759746 -3.3711058154
H 21.0334658033 10.8634834784 -2.4357137203
H 20.6914960078 9.1881273836 -1.9118771207
H 20.3545132507 10.5391354911 -0.8170766807
C 13.7580000000 -1.9180000000 5.0570000000
C 13.4120000000 -0.9780000000 3.9100000000
O 13.3110000000 -1.3970000000 2.7510000000
H 14.7762936910 -2.2815543513 4.9012931361
H 13.6911034973 -1.4556074275 6.0447949398
H 13.0882116201 -2.7772546931 5.0101362208
N 13.2310000000 0.3080000000 4.2140000000
C 13.0140000000 1.2980000000 3.1660000000
C 14.1650000000 1.2940000000 2.1710000000
O 13.9530000000 1.1860000000 0.9580000000
C 12.8440000000 2.6790000000 3.7960000000
C 12.5140000000 3.7670000000 2.8150000000
C 11.2030000000 4.0130000000 2.4520000000
C 13.5130000000 4.5600000000 2.2760000000
C 10.8950000000 5.0210000000 1.5570000000
C 13.2110000000 5.5660000000 1.3800000000
C 11.9000000000 5.7970000000 1.0210000000
H 13.2358327400 0.6114998894 5.1743371520
H 12.1326585540 1.0293535883 2.5791067623
H 13.7578998795 2.9431685268 4.3413896787

H 12.0403343419 2.6111970177 4.5388734844
H 10.4050390267 3.4149095536 2.8844366173
H 14.5458563276 4.3933008544 2.5707628870
H 9.8607630480 5.2187644691 1.2955214259
H 14.0009165808 6.1932349152 0.9796108359
H 11.6564970053 6.6020414818 0.3364921696
N 15.3990000000 1.3950000000 2.6720000000
C 16.5640000000 1.4050000000 1.7920000000
H 15.5273084101 1.3755743587 3.6693278660
H 16.4215045749 2.1510786293 1.0079499602
H 16.7066981824 0.4268178572 1.3232221780
H 17.4467942897 1.6611814863 2.3773768705
C 13.2140000000 -1.7440000000 -1.1060000000
C 13.4830000000 -0.8070000000 -2.2810000000
O 13.1990000000 -1.1600000000 -3.4320000000
H 13.8092785674 -2.6478344094 -1.2519329087
H 13.4290753789 -1.3090802741 -0.1275511387
H 12.1618410013 -2.0294994154 -1.1495333643
N 14.0180000000 0.3840000000 -2.0240000000
C 14.2130000000 1.3500000000 -3.0950000000
C 15.6180000000 1.3460000000 -3.6770000000
O 15.8120000000 1.8740000000 -4.7760000000
C 13.8850000000 2.7670000000 -2.6120000000
C 12.4150000000 3.0710000000 -2.5650000000
C 11.6480000000 3.2360000000 -1.4480000000
C 11.5340000000 3.2440000000 -3.6840000000
N 10.3480000000 3.5020000000 -1.8010000000
C 10.2510000000 3.5120000000 -3.1680000000
C 11.7060000000 3.2000000000 -5.0720000000
C 9.1460000000 3.7360000000 -3.9880000000
C 10.6060000000 3.4210000000 -5.8850000000
C 9.3430000000 3.6840000000 -5.3400000000
H 14.0108169306 0.7223600133 -1.0650753911
H 13.5529415615 1.0656975384 -3.9184842161
H 14.3870722387 3.4684140480 -3.2833412515
H 14.3241368180 2.9155341250 -1.6196484668
H 11.9340634910 3.1578407318 -0.4087136444
H 9.5605265197 3.4353699873 -1.1796856407
H 12.6778741268 2.9959399753 -5.5093117149
H 8.1622897930 3.9091171408 -3.5685715537
H 10.7235898873 3.3714572118 -6.9614569494
H 8.4953286683 3.8251079379 -6.0014243737
N 16.5990000000 0.7790000000 -2.9860000000
C 17.9630000000 0.9080000000 -3.4860000000
H 16.3813945873 0.3398488689 -2.1048851108
H 18.3391718717 1.9250719655 -3.3395522317
H 17.9825104118 0.6859402854 -4.5529616004
H 18.6092880335 0.2045875209 -2.9610484665
C 17.7850000000 -1.7800000000 -6.2230000000
C 17.1900000000 -0.9670000000 -7.3560000000
O 17.6700000000 -1.0540000000 -8.4930000000
H 17.1799712352 -1.7761117228 -5.3129141091

H 18.7768966038 -1.3814637210 -5.9925044625
N 16.1570000000 -0.1680000000 -7.0770000000
C 15.5880000000 0.6990000000 -8.1030000000
C 16.5810000000 1.7760000000 -8.5240000000
O 16.7910000000 2.0090000000 -9.7190000000
C 14.2870000000 1.3230000000 -7.5920000000
C 13.6700000000 2.3190000000 -8.5360000000
C 12.9470000000 1.8970000000 -9.6380000000
C 13.7950000000 3.6770000000 -8.3090000000
C 12.3740000000 2.8120000000 -10.5010000000
C 13.2210000000 4.5930000000 -9.1690000000
C 12.5080000000 4.1600000000 -10.2630000000
H 15.7777679819 -0.1084450689 -6.1439124329
H 15.4168610939 0.1140303215 -9.0086853672
H 14.4951307678 1.8135396205 -6.6370402482
H 13.5746174115 0.5131418307 -7.3925736512
H 12.8409496173 0.8323638082 -9.8317122452
H 14.3522182098 4.0291875182 -7.4457220633
H 11.9091056525 2.5302497691 -11.4389414489
H 13.3195432382 5.6538289149 -8.9562792610
H 12.0433736801 4.8553663970 -10.9560442868
N 17.2110000000 2.4380000000 -7.5530000000
C 18.1540000000 3.5030000000 -7.8650000000
C 19.5200000000 2.9770000000 -8.2850000000
O 20.2660000000 3.6990000000 -8.9550000000
C 18.2900000000 4.4410000000 -6.6660000000
C 17.0460000000 5.2290000000 -6.3840000000
C 16.7700000000 6.3840000000 -7.0950000000
C 16.1460000000 4.8100000000 -5.4230000000
C 15.6240000000 7.1100000000 -6.8480000000
C 14.9950000000 5.5330000000 -5.1710000000
C 14.7350000000 6.6850000000 -5.8840000000
H 16.9037807101 2.3127194114 -6.5926539669
H 17.7781879241 4.0518522296 -8.7319261421
H 19.1223285211 5.1162761058 -6.8836543825
H 18.5744297612 3.8552594217 -5.7845294062
H 17.4722408931 6.7241228438 -7.8531863231
H 16.3493738450 3.9153035250 -4.8505042494
H 15.4236115787 8.0197104057 -7.4065959399
H 14.2939808172 5.2089094017 -4.4104258875
H 13.8383845391 7.2586631107 -5.6775072235
N 19.8650000000 1.7440000000 -7.9050000000
C 21.0440000000 1.1000000000 -8.4770000000
H 19.1009463137 1.1411656841 -7.6329074799
H 21.9544104972 1.4762315104 -8.0050612351
H 21.1021750721 1.2984220488 -9.5495822039
H 20.9628706235 0.0265028073 -8.3113851438
C 19.3470000000 0.3410000000 -11.8010000000
C 19.5100000000 1.6220000000 -12.6110000000
O 19.9720000000 1.5850000000 -13.7590000000
H 20.3444089789 -0.0173081205 -11.5320392739
H 18.7443932871 0.4588263800 -10.8971295667

H 18.8896838199 -0.4125307125 -12.4430569082
N 19.1870000000 2.7420000000 -12.0310000000
C 19.3630000000 3.9570000000 -12.7380000000
C 20.8090000000 4.1810000000 -13.0330000000
O 21.1450000000 4.6510000000 -14.0710000000
C 18.8630000000 5.0740000000 -11.8930000000
C 17.4120000000 5.3340000000 -12.0640000000
N 16.8150000000 5.3550000000 -13.2960000000
C 16.4400000000 5.5910000000 -11.1680000000
C 15.5360000000 5.6220000000 -13.1550000000
N 15.2820000000 5.7620000000 -11.8720000000
H 18.5932780616 2.7213437732 -11.2102818764
H 18.8579082062 3.9477550676 -13.7055789801
H 19.3981645506 5.9859005400 -12.1880404407
H 19.1122544113 4.9012005375 -10.8406851232
H 16.4341336444 5.6372864387 -10.0889451039
H 14.3741486357 5.8669640633 -11.4466780761
H 14.7949250278 5.6593338117 -13.9361725714
N 21.6750000000 3.8690000000 -12.0940000000
C 23.1030000000 4.0650000000 -12.3040000000
H 21.3452297198 3.5694342124 -11.1872572325
H 23.3577741110 5.1279633185 -12.3705809817
H 23.4039907108 3.5878777869 -13.2390216146
H 23.6449242097 3.6151627123 -11.4711066731
C 13.5920000000 -6.2960000000 -14.0890000000
C 13.3900000000 -4.8380000000 -13.6980000000
O 13.2000000000 -4.5330000000 -12.5160000000
H 12.6436965744 -6.8218045152 -13.9490347915
H 14.3214064831 -6.7384897293 -13.4104327515
H 13.9198071623 -6.4340084657 -15.1222702978
N 13.3700000000 -3.9560000000 -14.6500000000
C 13.1430000000 -2.5990000000 -14.2990000000
C 11.7640000000 -2.4930000000 -13.7130000000
O 11.5780000000 -1.7950000000 -12.7660000000
C 13.2630000000 -1.7460000000 -15.5210000000
C 13.9090000000 -0.4440000000 -15.2740000000
C 13.6940000000 0.2270000000 -14.1290000000
C 14.7250000000 0.1220000000 -16.1990000000
C 14.2870000000 1.4340000000 -13.9040000000
C 15.3230000000 1.3310000000 -15.9730000000
C 15.0860000000 1.9740000000 -14.8140000000
O 15.6400000000 3.1780000000 -14.5330000000
H 13.6690512118 -4.1960503196 -15.5811859578
H 13.8332715487 -2.2906841926 -13.5123338478
H 12.2749345735 -1.6078285795 -15.9827023226
H 13.8570689057 -2.2780436044 -16.2752014847
H 13.0488968645 -0.1790718375 -13.3550249616
H 14.9277302259 -0.3981307292 -17.1332588382
H 14.1376332120 1.9564748067 -12.9640174804
H 15.9903678161 1.7596898793 -16.7148284052
H 16.4332021871 3.3614407364 -15.0421161528
N 10.7810000000 -3.1730000000 -14.2780000000

C 9.4310000000 -3.1190000000 -13.7270000000
C 9.3630000000 -3.7500000000 -12.3410000000
O 8.5430000000 -3.3360000000 -11.5130000000
C 8.4470000000 -3.8110000000 -14.6720000000
O 8.4930000000 -3.2390000000 -15.9670000000
H 10.9041680326 -3.6188462710 -15.1738986403
H 9.1375410900 -2.0740208074 -13.5816907177
H 7.4486892903 -3.7625476634 -14.2240668894
H 8.7193854384 -4.8631903868 -14.7920867693
H 8.1781973235 -2.3341641956 -15.8979711179
N 10.2160000000 -4.7400000000 -12.0690000000
C 10.1960000000 -5.4050000000 -10.7690000000
H 11.0727152982 -4.8030003125 -12.6000588577
H 9.3400187726 -6.0799565671 -10.6972018676
H 10.1270324572 -4.6690033259 -9.9650498798
H 11.1212900318 -5.9688917645 -10.6624599755
C 12.4460000000 -2.9770000000 -8.8830000000
C 11.5930000000 -1.7450000000 -8.6140000000
O 11.6580000000 -1.1790000000 -7.5160000000
H 12.0342637384 -3.8013308601 -8.2950172427
H 13.4535550745 -2.7795416195 -8.5154858077
H 12.4867847918 -3.2664356261 -9.9361171175
N 10.7990000000 -1.3100000000 -9.5960000000
C 9.8540000000 -0.2250000000 -9.3530000000
C 8.7120000000 -0.6930000000 -8.4590000000
O 8.3350000000 -0.0050000000 -7.5030000000
C 9.3100000000 0.3150000000 -10.6770000000
O 10.3970000000 0.6240000000 -11.5570000000
C 8.4910000000 1.5780000000 -10.4360000000
H 10.9564778424 -1.5975682995 -10.5548643372
H 10.3512987522 0.5732188697 -8.7946682365
H 8.7278074921 -0.4623873242 -11.1818549813
H 7.6635746488 1.4142114817 -9.7437308433
H 9.1303435981 2.3471671659 -9.9935210535
H 8.0992277534 1.9574023527 -11.3821617978
H 10.7985888989 1.4126621433 -11.1836938956
N 8.1480000000 -1.8660000000 -8.7580000000
C 7.0780000000 -2.4060000000 -7.9270000000
H 8.4428293569 -2.3808704681 -9.5788253873
H 6.1659920141 -1.8079995247 -8.0135525835
H 6.8710983958 -3.4265735912 -8.2496482365
H 7.3853251435 -2.4056992893 -6.8788017663
C 9.7450000000 0.1790000000 -4.0810000000
C 8.3570000000 0.5810000000 -3.6180000000
O 8.1800000000 1.0430000000 -2.4880000000
H 10.0683054205 -0.6929338923 -3.5059788334
H 9.8059332431 -0.0540146389 -5.1460044255
H 10.4326315781 0.9907286926 -3.8504596748
N 7.3550000000 0.4230000000 -4.4850000000
C 5.9780000000 0.6950000000 -4.0890000000
C 5.4940000000 -0.2880000000 -3.0300000000
O 4.6290000000 0.0580000000 -2.2150000000

C 5.0650000000 0.6460000000 -5.3120000000
C 5.2570000000 1.8000000000 -6.2660000000
C 5.3340000000 3.1070000000 -5.8020000000
C 5.3620000000 1.5840000000 -7.6330000000
C 5.5050000000 4.1660000000 -6.6750000000
C 5.5370000000 2.6370000000 -8.5130000000
C 5.6080000000 3.9250000000 -8.0300000000
O 5.7810000000 4.9740000000 -8.9060000000
H 17.9136766655 -2.8042934516 -6.5732670840
H 7.5694240846 0.2688693537 -5.4665359669
H 5.9202423994 1.6672530112 -3.5965356116
H 4.0352270610 0.6336287071 -4.9357946259
H 5.2212181155 -0.3026956256 -5.8382188045
H 5.2496596274 3.3125488090 -4.7387366985
H 5.3256234472 0.5679187723 -8.0154466195
H 5.5552791826 5.1910411147 -6.3207897855
H 5.6115303863 2.4717419603 -9.5824877229
H 5.8734911639 5.8326800373 -8.3959950123
N 6.0360000000 -1.5100000000 -3.0310000000
C 5.6820000000 -2.5030000000 -2.0190000000
H 6.8348749432 -1.6598306501 -3.6263966773
H 4.7742477643 -2.1480229650 -1.5325727912
H 5.5016543210 -3.4748407350 -2.4858308535
H 6.4729933136 -2.6008165265 -1.2685453420
C 5.7980000000 4.5200000000 -12.8980000000
C 7.1440000000 4.0330000000 -13.3650000000
C 8.2620000000 4.6000000000 -12.9090000000
C 8.2060000000 5.7460000000 -11.8970000000
C 8.7980000000 5.2360000000 -10.5560000000
C 9.8570000000 7.3230000000 -9.9030000000
C 10.0850000000 8.3470000000 -8.7770000000
C 10.5980000000 7.5820000000 -7.5530000000
C 9.5690000000 6.5280000000 -7.1200000000
C 9.3630000000 5.5650000000 -8.2800000000
C 10.9780000000 8.5130000000 -6.4340000000
C 11.6040000000 9.3870000000 -4.5610000000
C 11.3460000000 8.1840000000 -5.1480000000
C 11.4800000000 6.9760000000 -4.4820000000
C 11.8930000000 7.0420000000 -3.1520000000
C 12.1580000000 8.2710000000 -2.5380000000
C 12.0170000000 9.4710000000 -3.2390000000
C 9.5440000000 4.0890000000 -13.3910000000
C 10.8280000000 2.5500000000 -14.8120000000
C 10.6590000000 1.6890000000 -16.0720000000
C 9.6330000000 0.6130000000 -15.7710000000
C 8.2570000000 1.2840000000 -15.6410000000
C 8.3110000000 2.4650000000 -14.7030000000
F 12.5550000000 8.2900000000 -1.2570000000
N 8.8820000000 6.2720000000 -9.4860000000
N 11.0470000000 9.8420000000 -6.5210000000
N 9.5520000000 3.0330000000 -14.3060000000
N 7.2090000000 2.9460000000 -14.2700000000

O 11.404000000 10.328000000 -5.431000000
O 10.714000000 4.653000000 -12.983000000
H 5.0125471848 3.8903668493 -13.3174055842
H 5.6194371037 5.5477200558 -13.2215405832
H 5.7334846977 4.5008236175 -11.8063470601
H 7.1956600416 6.1111270214 -11.7379484381
H 8.8234662205 6.5615637784 -12.2838303278
H 9.7808133817 4.7861034891 -10.7554995655
H 8.1245822321 4.4643796548 -10.1727395520
H 10.8251583459 6.8717382283 -10.2017547790
H 9.4374762032 7.8348284110 -10.7710632693
H 9.1281077075 8.8239687957 -8.5540173074
H 10.8083306340 9.1054930883 -9.0959105871
H 11.5195536303 7.0458697860 -7.8333968909
H 8.6143438256 7.0108903104 -6.8876724228
H 9.8899149803 5.9740875837 -6.2436384643
H 8.6003810138 4.8249444028 -8.0211957053
H 10.3084359875 5.0241367544 -8.4828140355
H 11.2972446844 6.0142545484 -4.9407313716
H 12.0105593131 6.1298971772 -2.5737994381
H 12.2306544234 10.3979768387 -2.7220531702
H 11.4613474340 3.4233776496 -14.9757619914
H 11.3057664683 1.9548549399 -14.0278466894
H 11.6391811187 1.2676960952 -16.3103092182
H 10.3390938228 2.3031801066 -16.9215195110
H 9.8970383620 0.1141956432 -14.8305463485
H 9.6049121778 -0.1514383613 -16.5553824404
H 7.4784139439 0.6199732066 -15.2608984846
H 7.9255818468 1.6459448167 -16.6214062198

2 Hydrogen bond characterization

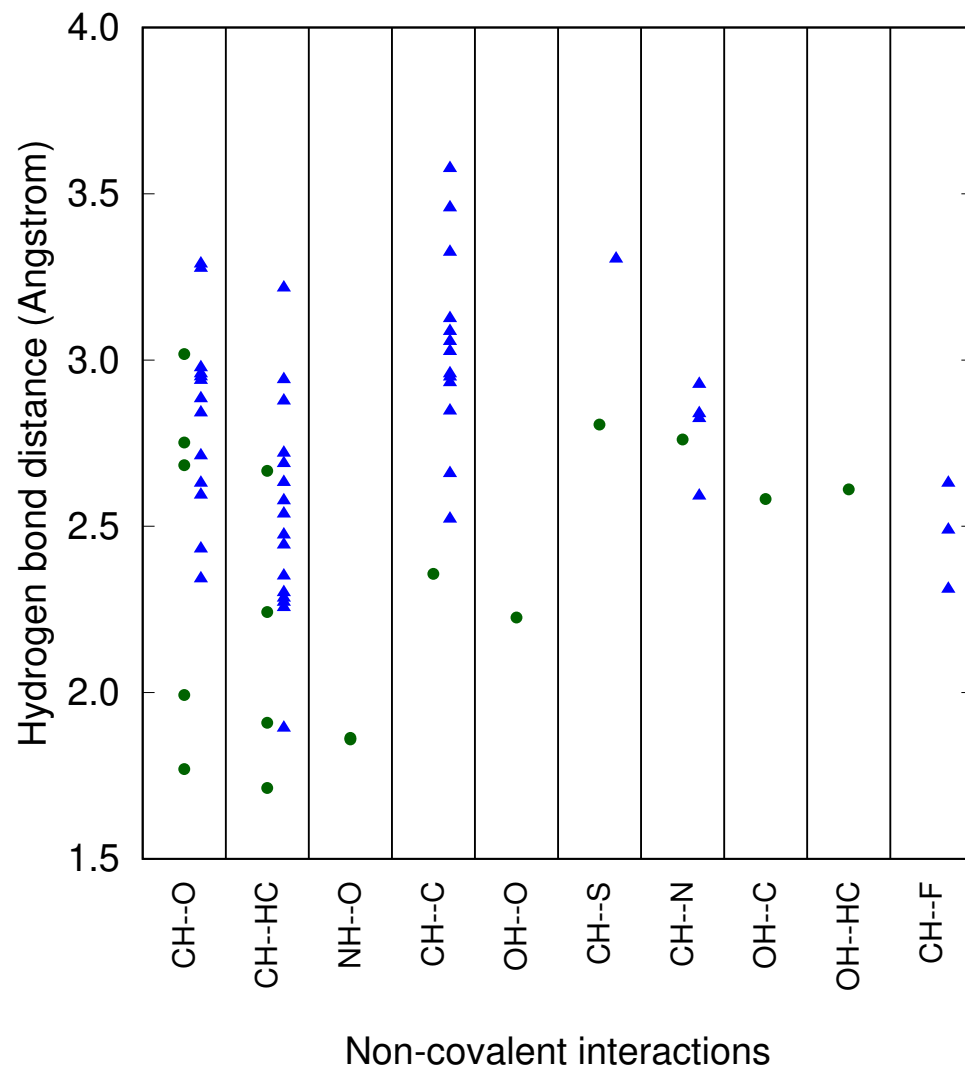


Figure S1. Hydrogen bond distance in dopamine-DRD2 (circles) and risperidone-DRD2 complexes (triangles).

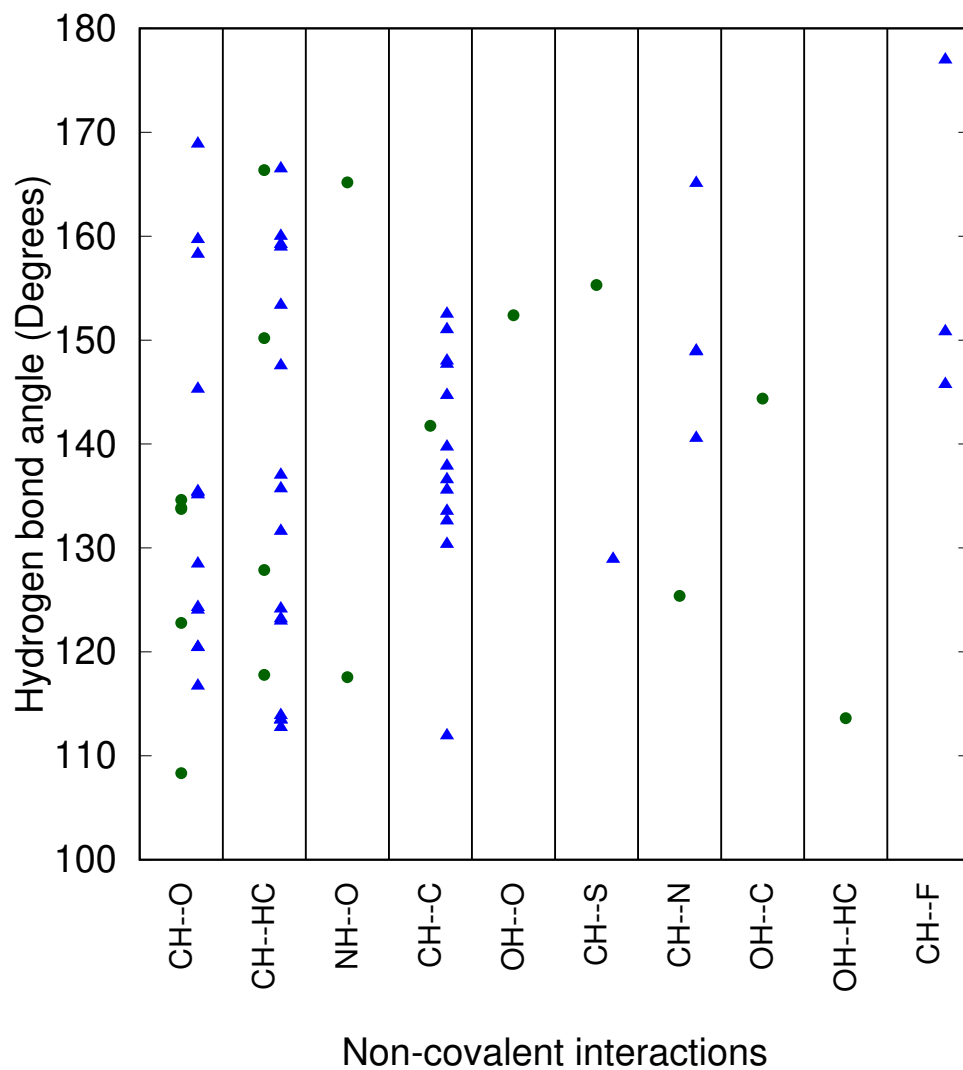


Figure S2. Hydrogen bond angle in dopamine-DRD2 (circles) and risperidone-DRD2 complexes (triangles).