Supplementary Materials

Table S1. The absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for reaction species involved in 2′/5′-hydroxylation of (*R*)/(*S*)-NNN on doublet states.

Species	BSI	BSII/BSI + ZPE + G	ZPE	G	BSII/BSI + ZPE + G
	AE	AE	AE	AE	RE
2-R-RC	-2174.909905	-2174.46881	0.485766	0.419933	1.80
2-R-TS1	-2174.888941	-2174.45315	0.479129	0.415421	11.62
2-R-IC	-2174.924462	-2174.47308	0.482966	0.417769	-10.70
2-R-PCOH	-2174.991339	-2174.54369	0.487365	0.422796	-45.19
2-S-RC	-2174.906852	-2174.47168	0.485428	0.418655	0.00
2-S-TS1	-2174.878811	-2174.45822	0.478378	0.412522	8.44
2-S-IC	-2174.935672	-2174.48954	0.483843	0.417873	-11.21
2-S-PCOH	-2174.998594	-2174.55263	0.488565	0.423542	-50.80
5-R-RC	-2174.910152	-2174.46832	0.485884	0.420006	2.11
5-R-TS1	-2174.873639	-2174.45558	0.478575	0.413441	10.10
5-R-IC	-2174.932561	-2174.47925	0.481973	0.416366	-4.75
5-R-PCOH	-2175.000425	-2174.55196	0.489439	0.425538	-50.38
5-S-RC	-2174.903567	-2174.47441	0.485548	0.41808	-3.82
5-S-TS1	-2174.873772	-2174.45977	0.47875	0.412345	5.37
5-S-IC	-2174.926746	-2174.47849	0.481967	0.416072	-6.38
5-S-PCOH	-2174.988325	-2174.54667	0.48814	0.423397	-49.17
2-R-^{4}RC	-2174.871610	-2174.468318	0.486614	0.419885	2.42
2-R-^{4}TS1	-2174.886438	-2174.455538	0.478547	0.413413	10.44
2-S-^{4}RC	-2174.906848	-2174.472181	0.485458	0.418115	0.00
2-S-^{4}TS1	-2174.876754	-2174.458697	0.478092	0.412206	8.46
5-R-^{4}RC	-2174.909909	-2174.468745	0.485898	0.419352	-0.27
5-R-^{4}TS1	-2174.874891	-2174.455807	0.479092	0.413018	7.85
5-S-^{4}RC	-2174.903468	-2174.474703	0.485571	0.417574	-1.58
5-S-^{4}TS1	-2174.868000	-2174.458214	0.480343	0.414295	8.77

ZPE: Zero-point energy; G: Gibbs free energy correction; RC = reactant complex in low-spin state, TS1 = transition state of H-abstraction in low-spin state, IC = intermediate complex with H abstracted by Cpd I in low-spin state, PCOH = hydroxylation product +Fe (Por SH) in low-spin state; ^{4}RC=reactant complex in high-spin state; ^{4}TS1=transition state of H-abstraction in high-spin state.

Table S2. The calculated spin densities for the reaction species involved in 2′/5′-hydroxylation of (*R*)/(*S*)-NNN on doublet states at UB3LYP-D3/B1 level.

Species	Cpd I				Substrate			
	Fe	O	Por	SH	H	C	N	Rest
2-R-RC	1.25	0.83	-0.54	-0.54	0.00	0.00	0.00	0.00
2-R-TS1	1.07	0.58	-0.55	-0.42	-0.06	0.27	-0.03	0.14
2-R-IC	1.31	0.07	-0.27	-0.06	-0.04	0.01	0.00	-0.02
2-R-PC	1.11	0.00	-0.10	-0.01	0.00	0.00	0.00	0.00
2-S-RC	1.25	0.83	-0.54	-0.54	0.00	0.00	0.00	0.00
2-S-TS1	1.04	0.57	-0.54	-0.44	-0.06	0.31	-0.01	0.13
2-S-IC	1.45	0.02	-0.44	-0.06	-0.01	0.00	-0.01	0.05
2-S-PC	1.09	0.00	-0.08	0.00	0.00	0.00	0.00	0.00
5-R-RC	1.25	0.83	-0.52	-0.56	0.00	0.00	0.00	0.00
5-R-TS1	1.06	0.54	-0.52	-0.38	-0.05	0.28	-0.03	0.11
5-R-IC	1.21	0.07	-0.21	-0.04	-0.01	0.00	0.00	-0.01
5-R-PC	1.09	0.00	-0.09	0.00	0.00	0.00	0.00	0.00
5-S-RC	1.23	0.85	-0.53	-0.56	0.00	0.00	0.00	0.00
5-S-TS1	1.35	0.36	-0.44	-0.23	-0.03	0.02	0.05	0.03
5-S-IC	1.16	0.07	-0.18	-0.03	-0.02	0.00	0.00	0.00
5-S-PC	1.10	0.00	-0.09	-0.01	0.00	0.00	0.00	0.00

2-R-^{4}RC	1.14	0.88	0.50	0.47	0.00	0.00	0.00	0.00
2-R-^{4}TS1	0.96	0.66	0.55	0.40	-0.06	0.34	-0.02	0.17
2-S-^{4}RC	1.14	0.88	0.48	0.49	0.00	0.00	0.00	0.00
2-S-^{4}TS1	0.94	0.66	0.53	0.44	-0.06	0.36	0.01	0.15
5-R-^{4}RC	1.14	0.88	0.45	0.52	0.00	0.00	0.00	0.00
5-R-^{4}TS1	1.21	0.66	0.25	0.41	-0.04	0.35	0.00	0.14
5-S-^{4}RC	1.12	0.89	0.46	0.51	0.00	0.00	0.00	0.00
5-S-^{4}TS1	1.36	0.70	0.01	0.45	-0.03	0.32	0.03	0.14

Table S3. The absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for reaction species involved in nonenzymatic decomposition of four α-hydroxyNNNs in the aqueous medium.

Species	BSIII	BSIV/BSIII+ZPE+G	ZPE	G	BSII/BSI+ZPE+G
	AE	AE	AE	AE	RE
2-R-PC$_{OH}$'	-664.2542336	-664.2575942	0.199242	0.160076	-0.02
2-R-TS2	-664.2221708	-664.2186251	0.196511	0.158565	18.02
2-R-PC	-664.2603075	-664.2476555	0.197222	0.154613	-8.96
2-S-PC$_{OH}$'	-664.2544469	-664.0785881	0.199647	0.160924	0.00
2-S-TS2	-664.2225143	-664.0498716	0.19651	0.158562	18.02
2-S-PC	-664.2603075	-664.0864213	0.197334	0.155391	-4.92
5-R-PC$_{OH}$'	-664.2589800	-664.0796655	0.200435	0.161567	-0.68
5-R-TS2	-664.2193652	-664.0504504	0.196928	0.158307	17.65
5-R-PC	-664.2453873	-664.0781517	0.196533	0.154627	0.27
5-S-PC$_{OH}$'	-664.2575942	-664.0782284	0.200454	0.16148	0.23
5-S-TS2	-664.2186251	-664.0471018	0.196504	0.157764	19.76
5-S-PC	-664.2476555	-664.0821310	0.196589	0.153709	-2.22

ZPE: Zero-point energy; G: Gibbs free energy correction; PCOH' = hydroxylation product, TS2 = transition state of decomposition, PC = decomposition products.

Table S4. The absolute energies (AE: a.u.) and relative energies (RE: kcal/mol) for reaction species involved in alkylation of 2′-hydroxylation diazonium ion with ten DNA base site.

Species	BSIII	BSIV/BSIII+ZPE+G	ZPE	G	BSII/BSI+ZPE+G
	AE	AE	AE	AE	RE
N1A-R	-1134.179980	-1133.925416	0.351251	0.289941	0
N1A-TS	-1134.175372	-1133.921559	0.349479	0.288645	2.42
N1A-P	-1134.259980	-1134.017051	0.347382	0.292816	-57.50
N3A-R	-1134.182703	-1133.927191	0.350565	0.291143	0
N3A-TS	-1134.172331	-1133.925721	0.348854	0.287419	0.92
N3A-P	-1134.271204	-1134.015472	0.346092	0.293083	-55.40
N7A-R	-1134.181048	-1133.926850	0.351073	0.289243	0
N7A-TS	-1134.173762	-1133.920706	0.349250	0.288492	3.85
N7A-P	-1134.268722	-1134.020627	0.345028	0.290729	-58.85
N3G-R	-1209.411945	-1209.192458	0.35519	0.292878	0
N3G-TS	-1209.398974	-1209.191091	0.352842	0.289695	0.86
N3G-P	-1209.485015	-1209.270923	0.355568	0.289030	-49.24
O^{6}G-R	-1170.131922	-1169.931381	0.327037	0.267783	0
O^{6}G-TS	-1170.123654	-1169.927631	0.325129	0.265411	2.35
O^{6}G-P	-1170.223654	-1170.01579	0.308123	0.254258	-52.97
N7G-R	-1170.131368	-1169.931997	0.326962	0.267178	0
N7G-TS	-1170.120256	-1169.924483	0.324704	0.263876	4.72
N7G-P	-1170.20868	-1170.025414	0.321295	0.267564	-58.62
N3C-R	-1022.496133	-1022.291101	0.308500	0.250217	0
N3C-TS	-1022.487422	-1022.283081	0.307300	0.250117	5.03
N3C-P	-1022.572632	-1022.377067	0.304397	0.254682	-53.94
O^{2}C-R	-1022.491368	-1022.289422	0.308531	0.251184	0
O^{2}C-TS	-1022.489631	-1022.286689	0.307511	0.250255	1.71
O^{2}C-P	-1022.568067	-1022.365364	0.304167	0.253511	-47.65

O^2T-R	-1081.680433	-1081.477794	0.324679	0.262497	0
O^2T-TS	-1081.672038	-1081.471710	0.322451	0.261252	3.82
O^2T-P	-1081.762038	-1081.572970	0.315834	0.262043	-59.72
O^4T-R	-1081.685124	-1081.476827	0.324951	0.263820	0
O^4T-TS	-1081.676775	-1081.472373	0.322565	0.260928	2.79
O^4T-P	-1081.754737	-1081.547165	0.314665	0.259372	-44.14

N1A = N1 position of adenine, N3A = N3 position of adenine, N7A = N7 position of adenine, N3G = N3 position of guanine, O^6G = O^6 position of guanine, N7G = N7 position of guanine, O^2C = O^2 position of cytosine, N3C = N3 position of cytosine, O^2T = O^2 position of thymine, O^4T = O^4 position of thymine.; R = reactant complex, TS = transition state of alkylation, P = alkylation products.

Table S5. Comparison of free energies and optimized structures calculated for diazonium ions derived from 2′-hydroxylation of NNN binding with the nucleophilic O^6 position of N9-methylguanine and 2'- deoxyguanosine at the BSV//BSIII level.

Complex	$\Delta G^{\ddagger}$	Frequency (*i* cm^{-1})	C-N distance (Å)	C-O distance (Å)
RC(N9-methylguanine)	0.00	-	-	-
TS(N9-methylguanine)	2.35	-355.23	1.746	2.577
RC(2′-deoxyguanosine)	0.00			
TS(2′-deoxyguanosine)	1.68	-342.84	1.738	2.570

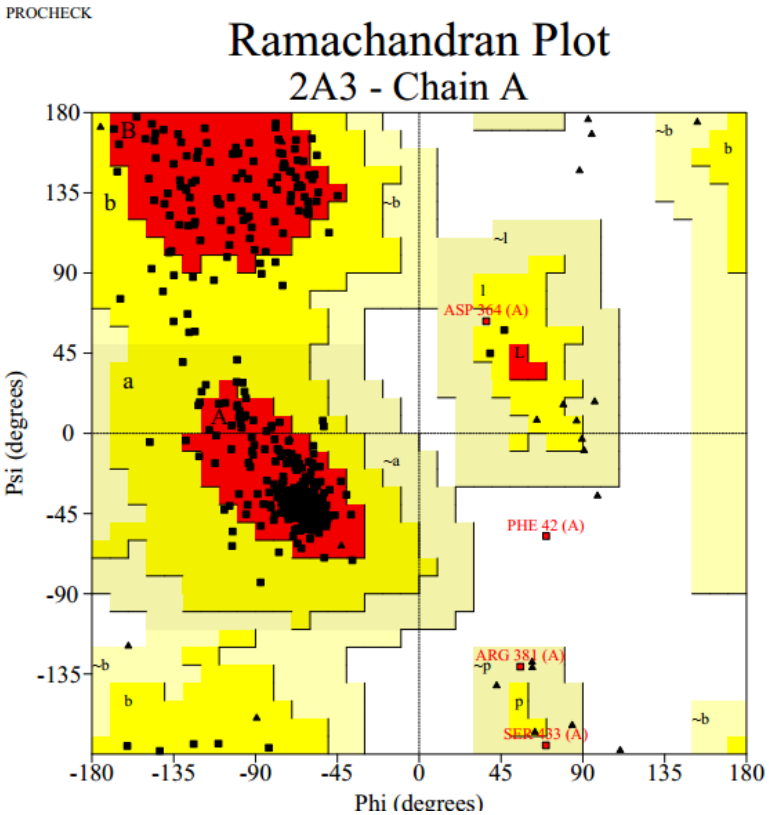

Figure S1. Ramachandran Plot and statistics of modeled rat 2A3 enzymes.

Plot statistics

Residues in most favoured regions [A,B,L] 353	**88.3%**
Residues in additional allowed regions [a,b,l,p] 43	10.8%
Residues in generously allowed regions [~a,~b,~l,~p] 3	0.8%
Residues in disallowed regions 1	0.3%

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SAVES validation

Vertify3D **98%** of residues had an averaged 3D-1D score ≥0.2.

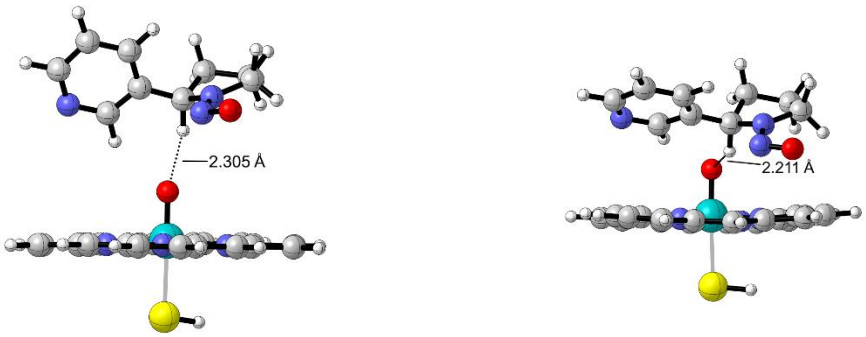

Figure S2. Optimized structures of 2-(*R*)-RC calculated by B3LYP and B3LYP-D3.

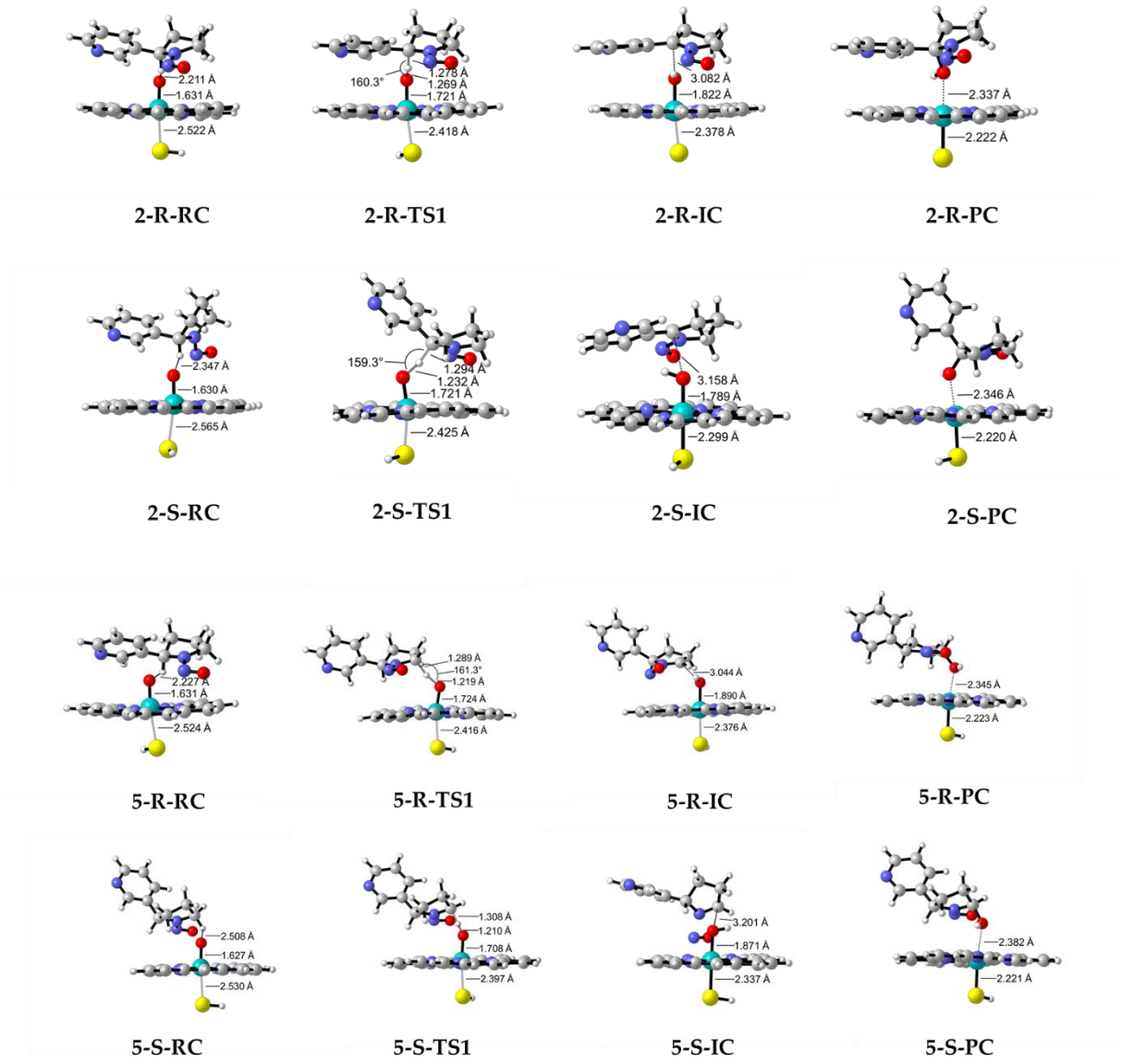

Figure S3. Optimized geometries for 2'- and 5'-hydroxylation of *(R)*- and *(S)*-NNN catalyzed by Cpd I on low spin states. Bond lengths are given in angstroms.

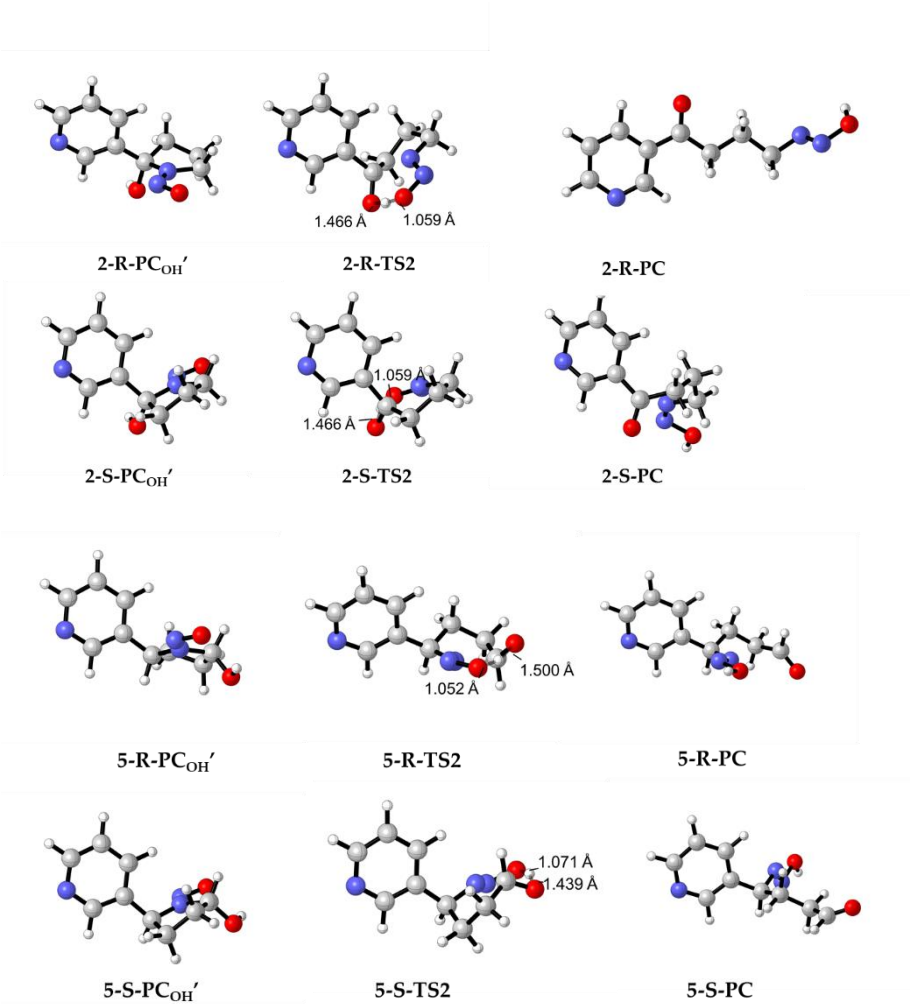

Figure S4. Optimized geometries for the decomposition of the hydroxylation products of *(R)*- and *(S)*-NNN. Bond lengths are given in angstroms.

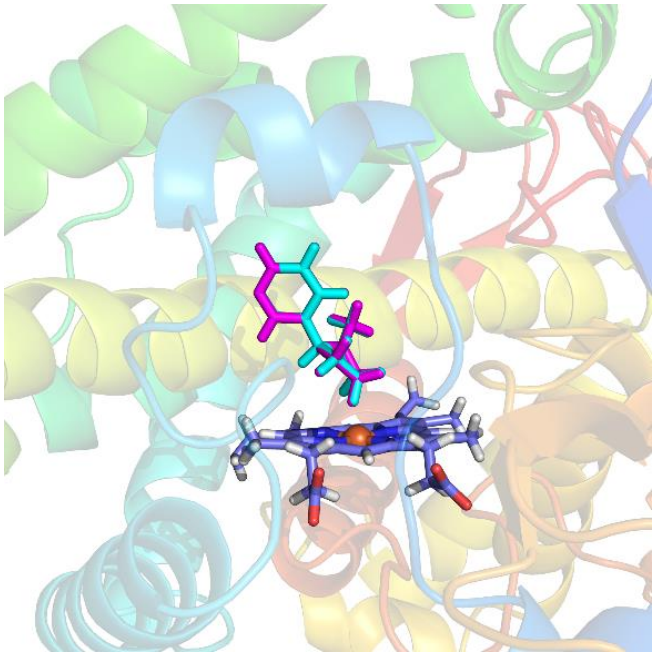

Figure S5. Self-docking structure of nicotine and CYP450 2A13, in which the brilliant blue nicotine is the native structure in the crystal complex and the pink nicotine is the redocked structure.

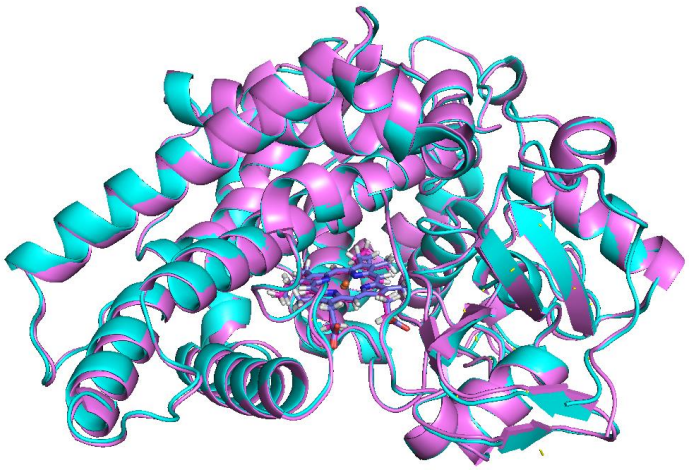

Figure S6. Overlap of the rat 2A3 and the human 2A13 protein crystal structures.

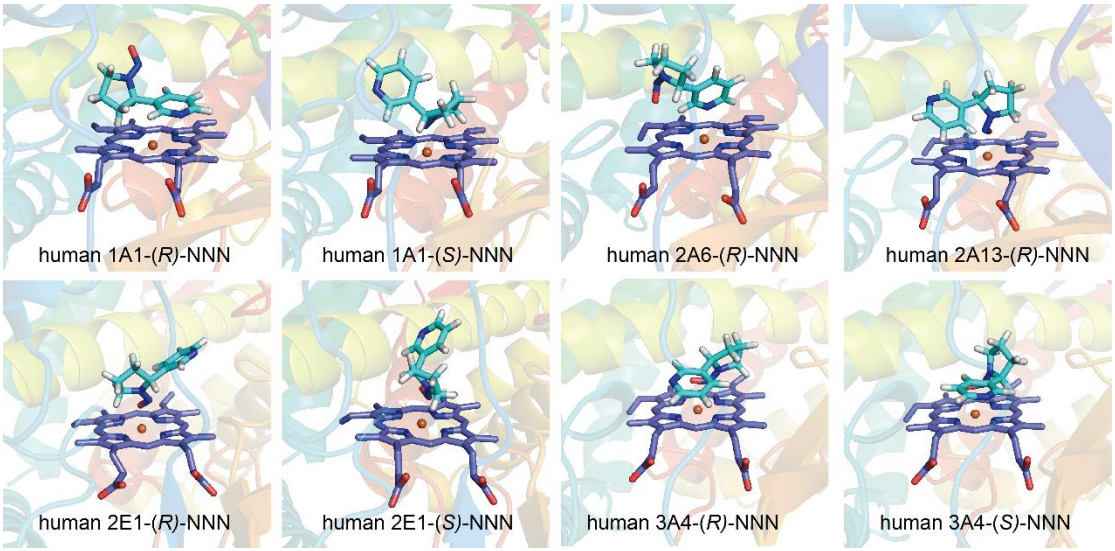

Figure S7. Detailed docking results of human CYP450 enzymes with NNN.

Cartesian coordinates of TS structures discussed in this work.

2-R-TS1

Fe	-1.10898	0.19663	0.42756
O	-0.35248	0.04937	-1.11102
C	0.12539	-2.32299	1.61681
C	-0.0072	-3.75876	1.61536
C	-1.09748	-4.0487	0.8512
C	-1.63765	-2.78881	0.39733
N	-0.87196	-1.75043	0.86896
H	0.67041	-4.43618	2.116
H	-1.51576	-5.01779	0.61341
C	1.1468	1.84659	1.57397
C	2.36645	1.7452	2.33953
C	2.49777	0.4378	2.69308
C	1.36662	-0.25743	2.12941
N	0.5608	0.61382	1.44391
H	3.02129	2.57632	2.56266
H	3.28505	-0.03502	3.26399
C	-2.49974	2.73521	-0.53589
C	-2.30517	4.16141	-0.64435
C	-1.10171	4.43578	-0.06889
C	-0.57418	3.17872	0.40362
N	-1.44105	2.15895	0.11425
H	-3.00105	4.84395	-1.11374
H	-0.60296	5.38992	0.03505
C	-3.37295	-1.46596	-0.76473
C	-4.61462	-1.35972	-1.49667
C	-4.85924	-0.03202	-1.66479
C	-3.7586	0.67398	-1.05052
N	-2.87367	-0.21769	-0.49552
H	-5.2096	-2.20217	-1.82356
H	-5.6937	0.4431	-2.16322
C	-2.78335	-2.66144	-0.37784
C	-3.59412	2.05063	-1.05712
C	0.63599	3.03597	1.07179
C	1.15568	-1.62626	2.23233
H	-4.3649	2.64244	-1.54083
H	1.23009	3.93126	1.21889
H	1.89511	-2.20706	2.77152
H	-3.28408	-3.57868	-0.67179
S	-2.52894	0.19803	2.38515
H	-3.35595	1.18033	1.97326
C	2.34058	1.77718	-1.51278

C	2.878	0.50493	-1.23085
C	4.179	0.45927	-0.71509
C	4.87073	1.65463	-0.52856
C	4.24372	2.85669	-0.85381
N	2.99478	2.9278	-1.33633
H	4.63274	-0.48739	-0.45205
H	1.31415	1.85153	-1.86472
H	5.88165	1.65275	-0.13262
H	4.76117	3.80484	-0.71696
C	2.01539	-0.67572	-1.51743
C	1.65579	-0.98339	-2.97804
H	0.85299	-0.3481	-1.09985
C	0.94817	-2.34368	-2.85613
H	2.57474	-1.05568	-3.57546
H	1.02021	-0.20501	-3.40228
C	1.73432	-3.07382	-1.75608
H	-0.08005	-2.17536	-2.52468
H	0.93115	-2.90627	-3.79243
H	1.12113	-3.68045	-1.08569
H	2.54166	-3.70909	-2.13625
N	2.34202	-1.96805	-0.99032
N	3.05906	-2.17736	0.10941
O	3.17185	-3.37364	0.40759

2-S-TS1

Fe	1.24448	-0.2065	0.31905
O	0.07266	0.57348	-0.67029
C	1.859	2.59233	1.34783
C	2.65766	3.7671	1.0779
C	3.44362	3.47142	0.00854
C	3.11502	2.12119	-0.38792
N	2.16048	1.59964	0.45377
H	2.60952	4.68629	1.64637
H	4.17205	4.09826	-0.48826
C	-0.55672	-0.70672	2.72229
C	-1.13899	-0.03693	3.85945
C	-0.66979	1.23893	3.84162
C	0.21238	1.34544	2.70249
N	0.26064	0.15007	2.02895
H	-1.83758	-0.49408	4.54622
H	-0.88583	2.04728	4.52724
C	0.65903	-2.99832	-0.70058
C	-0.05936	-4.20744	-0.37871
C	-0.68083	-3.98628	0.8145

C	-0.35617	-2.63601	1.20485
N	0.45325	-2.0486	0.26755
H	-0.05945	-5.10419	-0.98405
H	-1.30215	-4.65982	1.38962
C	3.28068	0.19188	-1.9198
C	3.79429	-0.4371	-3.1133
C	3.16744	-1.64147	-3.21988
C	2.28233	-1.74753	-2.08478
N	2.37126	-0.62356	-1.30501
H	4.5305	0.00238	-3.7731
H	3.28519	-2.39935	-3.98299
C	3.64844	1.46352	-1.48305
C	1.48118	-2.84881	-1.81263
C	-0.82578	-2.01609	2.35711
C	0.93263	2.48625	2.37598
H	1.52925	-3.68096	-2.50816
H	-1.50148	-2.58037	2.98993
H	0.78703	3.35919	3.00419
H	4.39015	1.99453	-2.07134
S	3.05238	-0.82268	1.81315
H	4.05579	-0.50667	0.96937
C	-4.03154	1.87353	-0.77188
C	-2.84184	1.35942	-1.30139
C	-2.09791	2.1994	-2.1545
C	-3.62155	3.89574	-1.9984
H	-1.14659	1.84751	-2.54694
H	-4.63607	1.27988	-0.09569
H	-3.90697	4.90279	-2.29747
C	-2.12187	-0.9712	-2.19863
C	-3.29537	-1.96318	-2.07158
H	-1.16524	-1.49003	-2.08737
H	-2.10749	-0.4394	-3.15164
C	-3.49007	-2.10948	-0.55779
H	-4.19818	-1.5381	-2.52303
H	-3.09258	-2.92242	-2.55452
H	-4.5202	-2.28217	-0.238
H	-2.86306	-2.89372	-0.12286
N	-3.0456	-0.79726	-0.05629
N	-3.24656	-0.38017	1.19015
O	-3.85459	-1.19042	1.89754
C	-2.31805	-0.0091	-1.014
H	-1.10875	0.2277	-0.62039
N	-2.46959	3.43196	-2.50554
C	-4.42855	3.16004	-1.13061

H	-5.34998	3.5852	-0.7446

5-R-TS1

Fe	1.564	-0.03725	0.26818
O	1.01823	-0.05628	-1.36655
C	3.48359	2.11592	-0.68998
C	4.77209	2.3159	-1.31547
C	5.32725	1.08462	-1.4728
C	4.37146	0.12917	-0.95975
N	3.26603	0.78208	-0.47172
H	5.18136	3.28049	-1.58474
H	6.28545	0.82554	-1.90319
C	-0.27205	2.09578	1.43458
C	-0.43033	3.52734	1.51738
C	0.60494	4.07461	0.82883
C	1.40956	2.97803	0.34152
N	0.85215	1.7797	0.71116
H	-1.24742	4.02548	2.02065
H	0.82534	5.11975	0.65859
C	-0.30827	-2.19745	1.27334
C	-1.5005	-2.40167	2.05977
C	-1.93843	-1.16486	2.4346
C	-1.02507	-0.21073	1.85521
N	-0.04406	-0.85386	1.14856
H	-1.91957	-3.36853	2.30521
H	-2.79637	-0.90534	3.04015
C	3.57653	-2.17747	-0.58493
C	3.72391	-3.60749	-0.71879
C	2.57473	-4.16368	-0.24479
C	1.7365	-3.07098	0.18913
N	2.36611	-1.8744	-0.02354
H	4.59467	-4.1015	-1.129
H	2.3076	-5.21008	-0.17891
C	4.52653	-1.24688	-0.99874
C	0.48914	-3.22448	0.78414
C	-1.14412	1.17103	1.98322
C	2.60954	3.13562	-0.33825
H	0.13177	-4.23943	0.92903
H	-1.99068	1.55047	2.54518
H	2.91518	4.15109	-0.56958
H	5.44946	-1.63315	-1.41977
S	2.75776	0.20264	2.3547
H	3.7769	-0.62212	2.03988
C	-5.11744	-0.93038	0.59143

C	-4.54325	-0.32742	-0.5321
C	-5.35471	0.51441	-1.30046
C	-6.67699	0.70934	-0.91535
C	-7.14626	0.05113	0.22544
N	-6.38902	-0.7585	0.97395
H	-4.9491	1.0176	-2.17309
H	-4.51172	-1.58682	1.21422
H	-7.33484	1.36091	-1.48189
H	-8.17608	0.18459	0.55217
C	-3.12094	-0.65129	-0.91015
C	-2.96859	-1.55531	-2.15222
H	-2.62204	-1.1233	-0.05867
C	-1.53833	-1.2564	-2.64858
H	-3.70985	-1.25771	-2.90229
H	-3.13739	-2.60657	-1.90684
C	-1.28656	0.19114	-2.23292
H	-0.81051	-1.90232	-2.14493
H	-1.42142	-1.40461	-3.72496
H	-0.14053	0.20303	-1.64406
H	-1.12775	0.96224	-2.98726
N	-2.31909	0.51831	-1.32267
N	-2.52907	1.73548	-0.80171
O	-1.7414	2.58871	-1.21615

5-S-TS1

Fe	1.57043	0.07094	0.25033
O	0.70386	0.15685	-1.22469
C	4.11108	0.07559	-1.44038
C	5.02721	-0.81274	-2.1178
C	4.59705	-2.08034	-1.87512
C	3.42398	-1.96626	-1.03946
N	3.15088	-0.65021	-0.78342
H	5.87834	-0.4877	-2.70234
H	5.02215	-3.01625	-2.21438
C	1.55603	3.12168	0.19828
C	2.2595	4.26105	-0.34389
C	3.33462	3.77033	-1.01893
C	3.27972	2.33227	-0.89764
N	2.1927	1.96253	-0.15033
H	1.96008	5.29221	-0.20623
H	4.10076	4.31342	-1.55721
C	-0.75633	0.0972	2.21398
C	-1.65273	0.99053	2.90792
C	-1.33886	2.2534	2.49883

C	-0.23951	2.12879	1.57252
N	0.08561	0.80379	1.40128
H	-2.41478	0.67557	3.60919
H	-1.78405	3.19208	2.8032
C	1.62172	-2.94758	0.32866
C	0.98658	-4.0824	0.95393
C	0.0374	-3.58915	1.793
C	0.07889	-2.15336	1.67148
N	1.04743	-1.7779	0.76846
H	1.24958	-5.11467	0.7628
H	-0.65606	-4.12933	2.42331
C	2.7024	-3.04088	-0.53705
C	-0.76762	-1.2885	2.3435
C	0.41747	3.20392	0.99205
C	4.18453	1.45934	-1.48595
H	-1.49732	-1.7245	3.01724
H	0.03404	4.19624	1.20958
H	5.00344	1.896	-2.0494
H	3.03884	-4.03757	-0.80553
S	3.08613	0.20605	2.09203
H	3.2327	-1.12851	2.24886
H	-0.29615	-0.49278	-1.39237
C	-5.16658	-0.53967	-1.4721
C	-4.53327	0.30372	-0.55526
C	-5.34606	1.14401	0.21647
C	-7.26322	0.39295	-0.77018
H	-4.8887	1.80352	0.95484
H	-4.58607	-1.23176	-2.07534
H	-8.34847	0.45244	-0.83174
C	-2.35611	1.35956	-1.41629
C	-1.91028	0.44314	-2.57187
H	-1.47139	1.80444	-0.95368
H	-3.03817	2.15506	-1.7249
C	-1.5004	-0.81279	-1.82574
H	-2.74284	0.22702	-3.25667
H	-1.08425	0.86405	-3.14885
H	-1.34802	-1.76514	-2.32972
N	-2.35444	-0.88169	-0.71586
N	-2.62783	-1.98492	0.01564
O	-2.03356	-2.9908	-0.36774
C	-3.02895	0.39249	-0.40152
H	-2.78851	0.677	0.62399
C	-6.55503	-0.49451	-1.58297
N	-6.67793	1.20232	0.12198

H	-7.08082	-1.1386	-2.28153

2-R-TS2

C	-1.91165	0.6438	0.94747
C	-0.8573	0.04058	0.24237
C	-1.18998	-0.70544	-0.89318
C	-2.53012	-0.81983	-1.26433
C	-3.49894	-0.18838	-0.48378
N	-3.20301	0.53528	0.60718
H	-0.42632	-1.17416	-1.50431
H	-1.69016	1.24401	1.82527
H	-2.8177	-1.38123	-2.1472
H	-4.55189	-0.25805	-0.74607
C	0.54455	0.23525	0.81764
C	1.14755	-0.98711	1.53521
C	1.60203	-2.03118	0.49916
H	0.40789	-1.4038	2.22588
H	1.99794	-0.62195	2.12021
C	2.32469	-1.26012	-0.62214
H	2.265	-2.77396	0.94834
H	0.74027	-2.56914	0.09363
H	3.38767	-1.11744	-0.40942
H	2.22054	-1.72833	-1.60495
N	1.65349	0.05066	-0.62471
N	2.19628	1.02856	-1.17993
O	1.5803	2.19129	-0.92309
O	0.80274	1.41417	1.28577
H	1.09018	2.07351	0.00869

2-S-TS2

C	-1.18998	0.70523	-0.89335
C	-0.85727	-0.04059	0.24232
C	-1.9116	-0.64367	0.94757
C	-3.49894	0.18838	-0.48372
H	-1.69007	-1.24377	1.82544
H	-0.42629	1.17375	-1.5046
H	-4.5519	0.25808	-0.74594
C	1.14753	0.9872	1.53515
C	1.60209	2.03125	0.49912
H	1.9979	0.62201	2.12015
H	0.40785	1.40386	2.22581
C	2.32458	1.26011	-0.62224
H	0.74039	2.56935	0.09364
H	2.26519	2.77392	0.94828

H	2.22029	1.72828	-1.60505
H	3.38759	1.11744	-0.4097
N	1.65339	-0.05068	-0.62472
N	2.19624	-1.02862	-1.17981
O	1.5803	-2.19134	-0.92295
C	0.54461	-0.23519	0.81752
O	0.80279	-1.41406	1.28586
H	1.09012	-2.07352	0.00879
N	-3.20296	-0.53513	0.60735
C	-2.53014	0.81963	-1.26443
H	-2.81775	1.38088	-2.14739

5-R-TS2

C	1.64571	0.043	1.07243
C	1.27789	-0.23986	-0.25169
C	2.28348	-0.21329	-1.22208
C	3.59232	0.0807	-0.83795
C	3.84806	0.34751	0.50739
N	2.89537	0.33401	1.45425
H	2.0471	-0.41841	-2.2626
H	0.89646	0.04322	1.86172
H	4.39665	0.10845	-1.56556
H	4.85521	0.58349	0.84205
C	-0.14979	-0.58379	-0.62184
C	-0.69882	-1.90151	-0.01935
H	-0.23856	-0.6153	-1.71278
C	-2.23249	-1.78284	-0.00092
H	-0.31732	-2.02652	0.99971
H	-0.35683	-2.75852	-0.6036
C	-2.59483	-0.42488	0.59883
H	-2.65454	-1.8435	-1.00983
H	-2.68232	-2.57362	0.60873
H	-2.27527	-0.32861	1.65274
N	-1.13896	0.40512	-0.12783
N	-1.15974	1.56417	-0.58284
O	-2.21487	2.27953	-0.15539
O	-3.62594	0.23997	0.21678
H	-2.94994	1.60002	0.14428

5-S-TS2

C	2.34673	0.61401	-0.95952
C	1.42864	-0.85194	0.69464
C	2.73436	-1.09418	1.12538
C	3.78593	-0.45053	0.47376
N	3.60368	0.39026	-0.55791
H	0.59482	-1.35001	1.17907
H	2.22981	1.29287	-1.80272
H	2.93232	-1.77226	1.94894
H	4.81453	-0.61704	0.78387
C	-0.66745	1.7888	-0.49881
C	-1.23026	1.66534	0.93462
H	-1.46421	2.08305	-1.18922
H	0.12818	2.53486	-0.56158
C	-2.02949	0.36465	1.07021
H	-0.41319	1.65701	1.66298
H	-1.88933	2.50589	1.16874
H	-1.66403	-0.31039	1.85972
N	-1.21077	-0.47052	-0.35098
N	-1.85884	-1.21247	-1.12436
O	-2.97749	-1.6938	-0.57178
O	-3.28807	0.32276	0.78777
H	-3.29121	-0.96779	0.15094
C	-0.1566	0.3827	-0.91842
H	-0.15846	0.27722	-2.00755
C	1.21593	0.02848	-0.36991

N1A-TS

N	0.01965	3.66847	-0.62144
N	-0.30225	4.65497	-1.0324
N	2.41125	0.20551	0.34488
C	2.47147	-0.62023	-0.74748
N	3.53659	-1.28721	-1.20355
C	4.64588	-1.08281	-0.45517
C	4.71449	-0.27708	0.6934
C	3.53587	0.37438	1.10041
N	5.90954	-1.60882	-0.61973
C	6.67947	-1.10226	0.42578
N	5.99532	-0.30015	1.23662
N	3.49851	1.15921	2.20845
C	6.33155	-2.52144	-1.68687
H	1.54758	-0.7465	-1.29972
H	7.72103	-1.35546	0.53973
H	4.33739	1.26345	2.76028

H	2.61867	1.43371	2.61244
H	6.72471	-3.44746	-1.26075
H	5.45667	-2.74872	-2.29722
H	7.09557	-2.05229	-2.31184
C	-6.40375	-1.9785	1.50715
C	-7.43883	-2.07683	0.57043
N	-7.39649	-1.47133	-0.64038
C	-6.30594	-0.74518	-0.94657
C	-5.21193	-0.58783	-0.07065
C	-5.2747	-1.22442	1.1826
C	-4.06276	0.23547	-0.51303
C	-2.85548	0.409	0.41204
C	-1.74597	1.2158	-0.27744
C	-0.5666	1.52828	0.65847
O	-4.0563	0.79829	-1.6279
C	0.60305	2.19961	-0.0298
H	-6.48367	-2.48092	2.46401
H	-8.33252	-2.65297	0.78227
H	-6.29011	-0.26813	-1.9193
H	-4.46328	-1.13739	1.89727
H	-3.18505	0.91088	1.33419
H	-2.4822	-0.57854	0.71621
H	-1.39226	0.65873	-1.15418
H	-2.18772	2.14065	-0.66948
H	-0.88494	2.11371	1.52941
H	-0.11609	0.60261	1.04178
H	1.42432	2.57184	0.58022
H	0.94262	1.76608	-0.96899

N3A-TS

N	-0.30947	3.76993	-0.62937
N	0.00646	4.82621	-0.68116
N	-4.18444	-0.84567	-2.06695
C	-3.17251	-0.0776	-1.67599
N	-2.78768	0.25428	-0.42848
C	-3.58762	-0.31444	0.50045
C	-4.68406	-1.14185	0.23656
C	-4.97568	-1.40195	-1.12179
N	-3.52166	-0.23492	1.87362
C	-4.57162	-1.00792	2.34634
N	-5.28623	-1.56456	1.40216
N	-6.00111	-2.17564	-1.50505
C	-2.55921	0.50123	2.6733
H	-2.5718	0.33681	-2.48593

H	-4.74473	-1.11432	3.40936
H	-6.60176	-2.60173	-0.81682
H	-6.16432	-2.33096	-2.48766
H	-2.71549	0.26071	3.72561
H	-1.53866	0.21534	2.40302
H	-2.68717	1.58143	2.54618
C	6.04379	-2.25738	-1.06453
C	7.08847	-2.08673	-0.15285
N	7.0653	-1.19493	0.84822
C	5.97598	-0.43602	0.96603
C	4.86416	-0.51983	0.10765
C	4.91221	-1.46003	-0.93148
C	3.71164	0.38848	0.3508
C	2.49268	0.30984	-0.57794
C	1.4182	1.30985	-0.14628
C	0.18751	1.29491	-1.0594
O	3.71097	1.19569	1.26909
C	-0.93503	2.1832	-0.59246
H	6.12098	-2.9963	-1.85484
H	7.98728	-2.69473	-0.2295
H	5.96083	0.2858	1.77807
H	4.08675	-1.57301	-1.62752
H	2.81628	0.50252	-1.60949
H	2.09794	-0.71444	-0.57039
H	1.12106	1.09121	0.88529
H	1.86631	2.31002	-0.11986
H	0.43805	1.52255	-2.10112
H	-0.28948	0.30657	-1.05777
H	-1.79073	2.34909	-1.24158
H	-1.20065	2.15245	0.46071

N7A-TS

N	0.3207	-0.13829	0.08359
N	0.3193	-0.16354	1.13786
N	0.56931	-3.09816	-6.40095
C	0.76615	-2.34349	-7.50559
N	0.9298	-1.01557	-7.58182
C	0.88209	-0.41875	-6.37753
C	0.68515	-1.10832	-5.19358
C	0.52555	-2.47496	-5.20547
N	1.01727	0.9237	-6.14526
C	0.90544	1.05747	-4.8424
N	0.70324	-0.14669	-4.22332
N	0.34426	-3.12374	-4.13357

C	1.23929	1.98523	-7.13762
H	0.79565	-2.88761	-8.46113
H	0.96688	2.02014	-4.31373
H	0.3135	-2.61912	-3.21328
H	0.22467	-4.16643	-4.16484
H	1.30445	2.96901	-6.6211
H	2.18953	1.78957	-7.68309
H	0.39244	2.00088	-7.85967
C	-7.52257	1.38046	-1.08955
C	-7.84419	2.71558	-0.90416
N	-6.93978	3.6706	-0.59603
C	-5.65608	3.26983	-0.4681
C	-5.23738	1.95931	-0.63418
C	-6.19213	0.99868	-0.95103
C	-3.93648	1.62364	-0.49211
C	-3.15162	1.12561	-1.68082
C	-1.72204	0.8195	-1.25404
C	-0.92989	0.31685	-2.45378
O	-3.40158	1.7222	0.58651
C	0.49968	0.01074	-2.02701
H	-8.29871	0.64218	-1.3396
H	-8.89688	3.01509	-1.01427
H	-4.89923	4.02773	-0.21757
H	-5.89812	-0.05207	-1.09064
H	-3.62629	0.20002	-2.07672
H	-3.14277	1.90718	-2.47319
H	-1.24737	1.7451	-0.85815
H	-1.73088	0.03793	-0.46168
H	-1.34719	-0.55599	-3.00404
H	-0.92106	1.09842	-3.24615
H	0.79568	-0.99917	-1.8337
H	1.20804	0.80558	-1.92048

N3G-TS

N	0.71365	3.11893	-1.41868
N	0.58916	3.93967	-2.16494
N	5.03853	0.64001	0.91956
C	3.73986	0.80845	1.31946
N	2.74773	0.00232	0.93462
C	3.17374	-1.0685	0.17456
C	4.46655	-1.3056	-0.30343
C	5.5345	-0.4121	0.04099
N	2.4036	-2.12329	-0.26856
C	3.26605	-2.94992	-1.00087
N	4.50304	-2.48379	-1.03895
C	0.99703	-2.37978	0.03121
H	2.92319	-3.86183	-1.46155
H	0.79697	-3.44548	-0.09146
H	0.78592	-2.10072	1.06592
H	0.3349	-1.82381	-0.64147
C	-6.60984	-0.54661	1.77238
C	-7.53779	-0.9873	0.82165
N	-7.26215	-1.04971	-0.50294
C	-6.03908	-0.6682	-0.91355
C	-5.03751	-0.20945	-0.03285
C	-5.34268	-0.1523	1.33981
C	-3.72605	0.18509	-0.59499
C	-2.62061	0.68405	0.33994
C	-1.36569	1.07361	-0.45462
C	-0.21119	1.54614	0.4442
O	-3.49336	0.11893	-1.82027
C	1.07478	1.82731	-0.28279
H	-6.87711	-0.51428	2.82207
H	-8.53295	-1.30199	1.11489
H	-5.83775	-0.72462	-1.97675
H	-4.61139	0.19253	2.06318
H	-2.99489	1.53991	0.91941
H	-2.38756	-0.10325	1.07185
H	-1.04859	0.21834	-1.06352
H	-1.6376	1.86052	-1.17012
H	-0.49924	2.40616	1.06033
H	0.08736	0.74744	1.14154
H	1.87567	2.33432	0.25681
H	1.41471	1.10145	-1.01928
O	6.73133	-0.41492	-0.26293
H	5.7729	1.25109	1.2604
N	3.43604	1.89602	2.10906

H	2.60924	1.82841	2.68376
H	4.16303	2.51318	2.43884

O6G-TS

N	5.01988	1.04344	0.73802
C	3.99034	1.96247	0.72616
H	4.1379	2.97398	1.07927
N	2.86238	1.47592	0.25577
C	3.16468	0.16313	-0.06012
C	2.3474	-0.86704	-0.60599
O	1.14953	-0.82678	-0.9317
N	3.07692	-2.06409	-0.7686
H	2.55023	-2.82176	-1.18985
C	4.40814	-2.24358	-0.44166
N	4.95377	-3.4593	-0.70554
H	4.38049	-4.2768	-0.84649
H	5.89441	-3.60983	-0.37006
N	5.15777	-1.28869	0.06983
C	4.50017	-0.1209	0.23224
C	-5.45911	-0.01058	-0.84754
C	-4.88984	-0.40425	0.37472
C	-5.7156	-1.07018	1.29657
C	-7.04287	-1.30366	0.96036
C	-7.50407	-0.86535	-0.2873
N	-6.73383	-0.23037	-1.18156
H	-5.30156	-1.38643	2.24841
H	-4.86833	0.50454	-1.60191
H	-7.71463	-1.81322	1.64317
H	-8.53736	-1.03101	-0.58253
C	-3.46639	-0.15067	0.72777
C	-2.57472	0.60407	-0.26782
H	-3.04927	1.56601	-0.50475
H	-2.53514	0.03777	-1.20739
C	-1.16792	0.80076	0.29964
H	-0.72306	-0.17537	0.53699
H	-1.18017	1.35124	1.24422
C	-0.16049	1.37383	-0.64393
O	-2.99172	-0.5291	1.78957
N	-0.64956	3.02455	-0.93709
N	-0.84957	4.10179	-1.07032
H	-0.1725	1.04423	-1.68023
H	0.8399	1.61948	-0.26177
C	6.39398	1.25179	1.18925
H	6.64008	0.53502	1.97529

H	7.08738	1.12209	0.35535
H	6.4825	2.26532	1.58166

N7G-TS

N	3.62182	0.15251	-1.597
C	4.26485	-1.02509	-1.26869
N	3.93212	-1.76096	-0.22823
C	2.91009	-1.24398	0.48464
C	2.19016	-0.07424	0.23905
C	2.54655	0.72942	-0.88521
N	1.21138	0.1082	1.20003
C	1.34502	-0.92869	1.99897
N	2.3573	-1.78352	1.6194
H	3.94118	0.70471	-2.38474
N	5.31072	-1.3982	-2.04831
O	2.05831	1.79836	-1.27228
H	0.74532	-1.12533	2.87739
H	5.42151	-1.03848	-2.98314
H	5.69807	-2.3106	-1.85908
C	-3.09899	-1.64604	-0.0807
C	-3.855	-0.4836	-0.29512
C	-5.20391	-0.63537	-0.65387
C	-5.72238	-1.91688	-0.77608
C	-4.87616	-3.00469	-0.53639
N	-3.58609	-2.88347	-0.19514
H	-5.80803	0.24907	-0.82627
H	-2.048	-1.58476	0.19585
H	-6.75904	-2.08018	-1.05043
H	-5.25212	-4.02172	-0.62283
C	-3.29656	0.88937	-0.16082
C	-1.8209	1.03057	0.24835
H	-1.18697	0.54671	-0.50166
H	-1.64163	0.49907	1.18681
C	-1.4718	2.53244	0.38099
H	-2.09776	2.97956	1.1562
H	-1.7042	3.01535	-0.5714
C	-0.02418	2.62886	0.69786
H	0.72558	2.38969	-0.07372
H	0.31402	2.48559	1.71982
O	-3.97137	1.88404	-0.36537
N	0.33585	4.45513	0.65936
N	0.58968	5.52078	0.52674
C	2.76585	-3.02478	2.27276
H	3.00262	-2.83836	3.3224

H	1.97357	-3.77387	2.20195
H	3.65509	-3.39265	1.76165

N3C-TS

N	0.	0.	0.
C	0.	0.	1.3639
H	0.97872	0.	1.83384
C	-1.16621	-0.01094	2.06536
H	-1.16603	-0.01044	3.14794
C	-2.37768	-0.04128	1.30788
N	-3.57231	-0.07481	1.93975
H	-4.4232	-0.04724	1.40009
H	-3.63719	-0.03836	2.94441
N	-2.38303	-0.04484	-0.02719
C	-1.20868	-0.0076	-0.71843
O	-1.17996	0.02428	-1.96542
C	-3.0112	3.3427	-6.02258
C	-3.437	4.08347	-4.90769
C	-3.47677	5.48305	-5.02906
C	-3.09865	6.06238	-6.23346
C	-2.69287	5.22514	-7.28031
N	-2.64636	3.88913	-7.18591
H	-3.80111	6.08012	-4.183
H	-2.95541	2.25694	-5.98721
H	-3.11519	7.13871	-6.36929
H	-2.39171	5.64495	-8.23706
C	-3.84288	3.45542	-3.62025
C	-3.82942	1.9256	-3.5016
H	-2.82525	1.55489	-3.74242
H	-4.50221	1.51701	-4.26906
C	-4.23867	1.47999	-2.09659
H	-5.20761	1.89609	-1.80723
H	-3.5203	1.85178	-1.35805
C	-4.20096	-0.00919	-1.86412
O	-4.19139	4.12934	-2.66079
N	-5.47374	-0.6514	-2.73949
N	-6.35619	-1.10107	-3.22782
H	-4.47533	-0.37548	-0.86789
H	-3.66348	-0.62618	-2.58061
C	1.2786	-0.03632	-0.7244
H	1.31998	-0.9168	-1.33099
H	1.36047	0.82996	-1.3471
H	2.08603	-0.04856	-0.0224

O2C-TS

N	3.62182	0.15251	-1.597
C	4.26485	-1.02509	-1.26869
N	3.93212	-1.76096	-0.22823
C	2.91009	-1.24398	0.48464
C	2.19016	-0.07424	0.23905
C	2.54655	0.72942	-0.88521
N	1.21138	0.1082	1.20003
C	1.34502	-0.92869	1.99897
N	2.3573	-1.78352	1.6194
H	3.94118	0.70471	-2.38474
N	5.31072	-1.3982	-2.04831
O	2.05831	1.79836	-1.27228
H	0.74532	-1.12533	2.87739
H	5.42151	-1.03848	-2.98314
H	5.69807	-2.3106	-1.85908
C	-3.09899	-1.64604	-0.0807
C	-3.855	-0.4836	-0.29512
C	-5.20391	-0.63537	-0.65387
C	-5.72238	-1.91688	-0.77608
C	-4.87616	-3.00469	-0.53639
N	-3.58609	-2.88347	-0.19514
H	-5.80803	0.24907	-0.82627
H	-2.048	-1.58476	0.19585
H	-6.75904	-2.08018	-1.05043
H	-5.25212	-4.02172	-0.62283
C	-3.29656	0.88937	-0.16082
C	-1.8209	1.03057	0.24835
H	-1.18697	0.54671	-0.50166
H	-1.64163	0.49907	1.18681
C	-1.4718	2.53244	0.38099
H	-2.09776	2.97956	1.1562
H	-1.7042	3.01535	-0.5714
C	-0.02418	2.62886	0.69786
H	0.72558	2.38969	-0.07372
H	0.31402	2.48559	1.71982
O	-3.97137	1.88404	-0.36537
N	0.33585	4.45513	0.65936
N	0.58968	5.52078	0.52674
C	2.76585	-3.02478	2.27276
H	3.00262	-2.83836	3.3224
H	1.97357	-3.77387	2.20195
H	3.65509	-3.39265	1.76165

O2T-TS

N	-3.60125	0.0466	1.38879
C	-4.78484	-0.68308	1.30698
H	-5.27053	-0.85538	2.26073
C	-5.31055	-1.15192	0.15107
C	-6.58726	-1.93755	0.07239
H	-7.02656	-2.07952	1.0628
H	-7.31568	-1.42716	-0.56581
H	-6.40864	-2.91943	-0.37742
C	-4.59006	-0.87547	-1.09214
O	-4.92024	-1.22097	-2.21394
N	-3.39969	-0.12848	-0.91073
H	-2.8784	0.06757	-1.75754
C	-2.87415	0.34655	0.26218
O	-1.81578	1.00161	0.30587
C	5.01035	-0.13967	0.6604
C	4.12958	-0.91855	-0.10918
C	4.54388	-2.21342	-0.46958
C	5.79415	-2.65423	-0.05696
C	6.59009	-1.7909	0.70711
N	6.21212	-0.55594	1.06606
H	3.8833	-2.83909	-1.06079
H	4.74307	0.86688	0.97514
H	6.15454	-3.64423	-0.31574
H	7.57428	-2.10412	1.04663
C	2.79346	-0.44025	-0.54143
C	2.35169	0.9916	-0.18224
H	3.16004	1.69947	-0.3967
H	2.17746	1.02696	0.90197
C	1.08074	1.35441	-0.95307
H	0.39112	0.49065	-0.9192
H	1.2715	1.5277	-2.01594
C	0.22347	2.40871	-0.37217
O	2.01916	-1.15471	-1.16342
N	1.17456	3.93985	-0.41191
N	1.77215	4.86511	-0.47942
H	-0.61154	2.78792	-0.95538
H	0.04148	2.41264	0.69967
C	-3.09407	0.52075	2.68193
H	-2.09733	0.11552	2.86904
H	-3.04488	1.61201	2.69497
H	-3.7725	0.1823	3.46416

O4T-TS

N	5.00502	-1.2497	-0.28152
C	4.03222	-1.67122	0.58919
H	4.22734	-2.62955	1.05849
C	2.89763	-0.97361	0.87065
C	1.85294	-1.4569	1.83686
H	2.11488	-2.43939	2.23645
H	1.74888	-0.76703	2.68149
H	0.86921	-1.53345	1.36248
C	2.70907	0.29912	0.20308
O	1.72568	1.04444	0.35397
N	3.73112	0.66621	-0.65914
H	3.64221	1.55239	-1.14121
C	4.89934	-0.03558	-0.95748
O	5.7375	0.37761	-1.7335
C	-4.76078	-0.18282	-0.94024
C	-3.90011	-0.85578	-0.05836
C	-4.25367	-2.15767	0.33535
C	-5.42858	-2.70853	-0.15473
C	-6.21099	-1.94343	-1.02713
N	-5.89024	-0.70395	-1.42141
H	-3.60359	-2.70056	1.01311
H	-4.53308	0.8237	-1.28625
H	-5.74141	-3.70828	0.12645
H	-7.13853	-2.3452	-1.42861
C	-2.64329	-0.2653	0.4605
C	-2.27379	1.17999	0.07369
H	-3.15168	1.83008	0.14615
H	-1.97567	1.17052	-0.98396
C	-1.13274	1.67896	0.96111
H	-0.42571	0.84521	1.12905
H	-1.47344	1.9817	1.95492
C	-0.20738	2.67318	0.37589
O	-1.8784	-0.89915	1.17372
N	-1.1265	4.16169	0.11327
N	-1.75126	5.0622	-0.01546
H	0.55635	3.10653	1.01668
H	0.12123	2.53824	-0.65121
C	6.21415	-2.03991	-0.54953
H	6.16137	-2.96494	0.02369
H	6.28073	-2.26692	-1.61489
H	7.10156	-1.47428	-0.2596