

Mechanism of N-Hydroxylation Catalyzed by Flavin-dependent Monooxygenases

Somayesadat Badieyan^{1*}, Robert D. Bach², Pablo Sobrado^{1,3*}

¹Department of Biochemistry, Virginia Tech, Blacksburg, VA, 24061

²Departments of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716

³Virginia Tech Center for Drug Discovery, Virginia Tech, Blacksburg, VA, 24061

* Emails: badieyan@vt.edu (SB) psobrado@vt.edu (PS)

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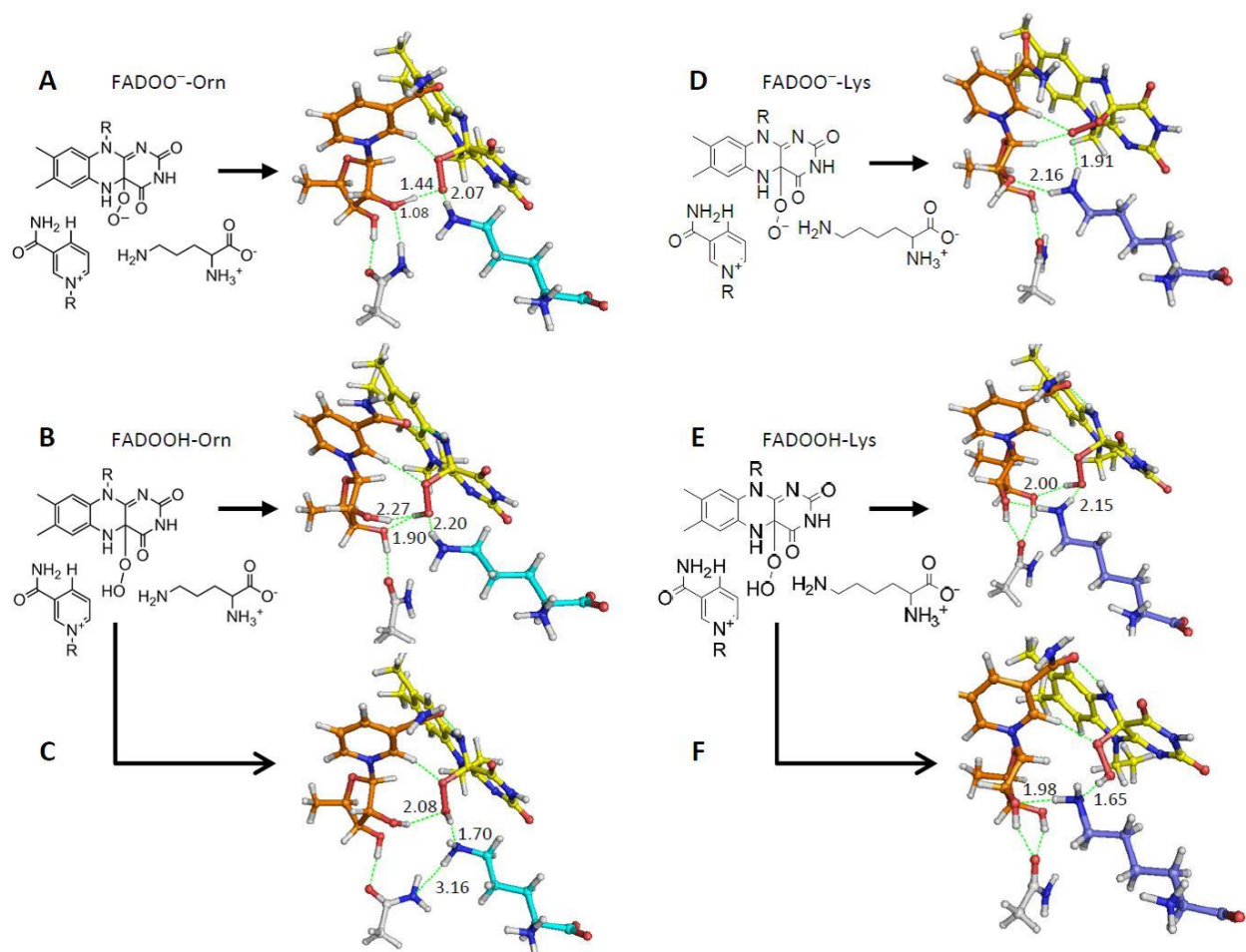


Figure S1. Ground state pre-reaction liganded complexes of ornithine hydroxylase (SidA) optimized at the B3LYP/6-31+G(d) theory level, stating different protonation states of ornithine/lysine and oxygenated flavin intermediates. Peroxyflavin and hydroperoxy-flavin are abbreviated as FAD_{OO-} and FAD_{OOH}, respectively. Similarly, the neutral ligands are referred to Orn or Lys.

XYZ Coordinates of optimized geometries for each Orn/Lys complexes (core of reactions at B3LYP/ 6-31+G(d)):

Orn complex: Reactant

N	39.934	36.820	50.336
N	38.185	35.923	49.104
N	38.486	39.396	48.267
N	40.622	39.110	50.051
N	40.705	40.303	44.280
N	36.039	39.779	43.711
N	38.418	29.431	45.451
N	40.029	34.692	45.830
C	39.154	35.723	50.094
C	38.001	37.031	48.317
C	39.067	38.113	48.427
C	39.263	40.515	48.593
C	38.969	41.771	48.055
C	39.692	42.915	48.401
C	39.332	44.251	47.795
C	40.754	42.793	49.320
C	41.568	43.996	49.736
C	41.052	41.536	49.856
C	40.329	40.383	49.511
C	39.840	38.035	49.673
C	41.754	38.935	50.976
C	41.407	39.222	52.440
C	45.130	40.610	43.940
C	44.212	39.870	44.900
C	41.886	39.690	44.964
C	40.885	41.129	43.221
C	39.473	39.951	44.702
C	38.344	40.409	44.039
C	38.507	41.235	42.922
C	39.792	41.607	42.523
C	36.988	40.083	44.618
C	42.372	38.416	44.228
C	43.879	38.393	44.598
C	38.782	31.261	47.127
C	38.987	29.776	46.796
C	38.338	28.861	47.855
C	39.451	32.237	46.148
C	39.405	33.670	46.689
O	39.267	34.652	50.688
O	37.068	37.136	47.526
O	39.936	37.957	47.219
O	40.815	36.805	47.302
O	42.938	40.597	44.923
O	36.797	40.170	45.835
O	41.654	37.265	44.557
O	44.083	37.599	45.753
O	37.377	28.136	47.517
O	38.841	28.924	49.021
H	37.526	35.160	48.986
H	37.833	39.493	47.490
H	38.152	41.839	47.342
H	38.482	44.158	47.112
H	39.064	44.987	48.564
H	40.169	44.680	47.230
H	42.340	43.720	50.461
H	40.941	44.772	50.196
H	42.067	44.465	48.879
H	41.862	41.473	50.572
H	42.562	39.585	50.636
H	42.137	37.918	50.853
H	41.049	40.248	52.563
H	35.125	39.539	44.077
H	36.323	39.335	42.830
H	44.646	36.836	45.469
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.622	39.905	45.915
H	41.553	39.462	45.983
H	41.910	41.380	42.986
H	39.430	39.286	45.557
H	37.639	41.606	42.388
H	39.950	42.267	41.679
H	42.259	38.574	43.151
H	44.471	38.008	43.762
H	38.606	28.425	45.202
H	38.848	30.004	44.720
H	37.379	29.605	45.425
H	40.358	36.099	46.723
H	40.954	34.381	45.528
H	39.192	31.416	48.131
H	37.707	31.475	47.189
H	40.057	29.550	46.753
H	40.498	31.944	45.984
H	38.949	32.216	45.171
H	39.902	33.707	47.666
H	38.364	33.970	46.847
H	42.299	39.091	53.062
H	44.698	40.670	42.963
H	41.829	37.075	45.502
H	40.629	38.546	52.811
H	39.489	34.823	44.976

Orn complex: TS_{OT}

N	39.820	37.147	49.447
N	37.588	36.473	48.867
N	38.046	39.835	47.891
N	40.594	39.212	48.764
N	40.708	40.168	43.806
N	36.063	39.898	42.950
N	38.537	29.460	45.484
N	40.073	34.683	45.832
C	38.845	36.185	49.461
C	37.299	37.554	48.092
C	38.492	38.463	47.772
C	39.050	40.797	47.747
C	38.789	42.068	47.222
C	39.788	43.033	47.094
C	39.457	44.391	46.522
C	41.104	42.712	47.490
C	42.228	43.711	47.345
C	41.364	41.445	48.018
C	40.356	40.482	48.168
C	39.648	38.243	48.747
C	41.887	38.957	49.427
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.127	39.887	44.832
C	41.793	39.660	44.715
C	41.036	40.709	42.607
C	39.421	40.036	44.193
C	38.388	40.418	43.345
C	38.705	40.945	42.090
C	40.045	41.104	41.730
C	36.969	40.315	43.863
C	42.339	38.273	44.281
C	43.879	38.394	44.548
C	38.859	31.287	47.178
C	39.069	29.801	46.846
C	38.383	28.882	47.879
C	39.638	32.258	46.278
C	39.370	33.716	46.677
O	38.983	35.094	50.005
O	36.190	37.764	47.610
O	38.912	38.201	46.474
O	39.414	36.433	46.268
O	42.849	40.566	44.645
O	36.702	40.648	45.018
O	41.798	37.204	45.023
O	44.217	37.626	45.691
O	37.427	28.168	47.509
O	38.855	28.931	49.059
H	36.865	35.772	48.996
H	37.227	39.999	47.308
H	37.781	42.284	46.881
H	38.398	44.462	46.259
H	39.681	45.194	47.236
H	40.044	44.604	45.619
H	43.171	43.302	47.720
H	42.022	44.638	47.896
H	42.383	43.996	46.296
H	42.379	41.219	48.321
H	42.673	39.209	48.708
H	41.937	37.885	49.606
H	41.739	40.767	50.601
H	35.114	39.779	43.286
H	36.369	39.277	42.192
H	44.742	36.842	45.367
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.401	39.972	45.889
H	41.339	39.601	45.710
H	42.092	40.819	42.404
H	39.236	39.572	45.160
H	37.916	41.249	41.411
H	40.324	41.534	40.776
H	42.133	38.107	43.220
H	44.441	38.045	43.678
H	38.702	28.447	45.247
H	39.001	30.014	44.761
H	37.504	29.656	45.427
H	40.183	36.824	45.792
H	41.085	34.655	45.940
H	39.171	31.428	48.218
H	37.787	31.518	47.134
H	40.138	29.567	46.837
H	40.713	32.045	46.343
H	39.349	32.135	45.226
H	39.667	33.903	47.712
H	38.302	33.934	46.594
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	42.496	37.031	45.701
H	41.515	39.323	51.537
H	39.840	34.595	44.846

Orn complex: Productor

N	40.165	36.841	49.462
N	38.087	35.829	48.811
N	38.099	39.195	47.738
N	40.654	38.987	48.757
N	40.710	40.199	43.928
N	36.071	39.796	42.921
N	38.645	29.506	45.340
N	40.732	34.582	45.615
C	39.346	35.745	49.469
C	37.657	36.854	48.023
C	38.726	37.914	47.719
C	38.940	40.307	47.651
C	38.498	41.532	47.140
C	39.340	42.642	47.057
C	38.820	43.942	46.493
C	40.680	42.520	47.487
C	41.640	43.682	47.385
C	41.113	41.304	48.017
C	40.257	40.198	48.128
C	39.864	37.890	48.734
C	41.960	38.923	49.439
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.175	39.844	44.853
C	41.851	39.576	44.679
C	40.964	41.091	42.939
C	39.451	39.810	44.224
C	38.372	40.298	43.493
C	38.619	41.194	42.448
C	39.928	41.599	42.181
C	36.968	39.941	43.929
C	42.470	38.385	43.909
C	43.901	38.367	44.504
C	39.120	31.342	47.001
C	39.184	29.835	46.702
C	38.403	28.997	47.743
C	39.893	32.225	46.002
C	40.016	33.646	46.550
O	39.620	34.698	50.043
O	36.540	36.900	47.524
O	39.261	37.620	46.424
O	41.127	35.760	46.250
O	42.866	40.522	44.818
O	36.678	39.877	45.125
O	41.745	37.198	43.984
O	43.930	37.580	45.682
O	37.439	28.306	47.347
O	38.818	29.068	48.942
H	37.457	35.045	48.954
H	37.279	39.235	47.136
H	37.478	41.599	46.776
H	37.763	43.860	46.223
H	38.920	44.763	47.214
H	39.375	44.243	45.595
H	42.624	43.417	47.781
H	41.279	44.557	47.941
H	41.774	44.005	46.344
H	42.140	41.231	48.353
H	42.710	39.254	48.714
H	42.147	37.872	49.644
H	41.739	40.767	50.601
H	35.136	39.542	43.221
H	36.395	39.329	42.068
H	44.504	36.806	45.470
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.522	39.879	45.890
H	41.428	39.257	45.637
H	42.000	41.371	42.810
H	39.335	39.092	45.032
H	37.794	41.595	41.869
H	40.147	42.312	41.395
H	42.527	38.666	42.851
H	44.618	37.984	43.771
H	38.740	28.478	45.135
H	39.161	30.003	44.609
H	37.631	29.776	45.261
H	39.916	36.841	46.424
H	41.575	34.120	45.242
H	39.537	31.474	48.004
H	38.075	31.670	47.046
H	40.227	29.504	46.713
H	40.895	31.810	45.832
H	39.375	32.251	45.035
H	40.599	33.678	47.472
H	39.037	34.092	46.735
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	41.791	36.815	44.899
H	41.515	39.323	51.537
H	40.135	34.788	44.802

Orn complex: TS_{1PT}

N	40.023	36.954	49.449
N	37.868	36.081	48.843
N	38.071	39.460	47.803
N	40.629	39.076	48.759
N	40.685	40.379	43.958
N	36.070	39.867	42.992
N	38.600	29.480	45.391
N	40.803	34.454	45.720
C	39.139	35.908	49.458
C	37.476	37.156	48.107
C	38.604	38.143	47.775
C	38.984	40.511	47.689
C	38.616	41.760	47.178
C	39.531	42.808	47.070
C	39.090	44.138	46.508
C	40.867	42.597	47.476
C	41.903	43.689	47.346
C	41.227	41.357	48.005
C	40.301	40.313	48.139
C	39.771	38.033	48.746
C	41.933	38.933	49.436
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.150	39.860	44.838
C	41.819	39.705	44.668
C	40.939	41.282	42.979
C	39.425	39.999	44.261
C	38.344	40.499	43.543
C	38.589	41.403	42.505
C	39.899	41.807	42.236
C	36.942	40.144	43.991
C	42.376	38.517	43.852
C	43.804	38.409	44.441
C	39.039	31.332	47.034
C	39.132	29.824	46.752
C	38.373	28.972	47.795
C	39.938	32.194	46.132
C	39.873	33.672	46.536
O	39.370	34.834	50.000
O	36.345	37.308	47.663
O	39.072	37.809	46.452
O	40.990	35.872	46.257
O	42.874	40.604	44.817
O	36.638	40.195	45.183
O	41.593	37.363	43.907
O	43.780	37.579	45.587
O	37.422	28.259	47.409
O	38.796	29.054	48.992
H	37.199	35.331	48.986
H	37.231	39.555	47.235
H	37.597	41.893	46.831
H	38.027	44.126	46.252
H	39.254	44.952	47.227
H	39.653	44.401	45.603
H	42.873	43.360	47.730
H	41.613	44.592	47.898
H	42.042	43.990	46.300
H	42.253	41.217	48.323
H	42.698	39.229	48.713
H	42.062	37.871	49.633
H	41.739	40.767	50.601
H	35.138	39.608	43.299
H	36.418	39.361	42.171
H	44.328	36.792	45.354
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.494	39.850	45.876
H	41.405	39.372	45.626
H	41.976	41.552	42.841
H	39.308	39.276	45.062
H	37.763	41.808	41.931
H	40.116	42.528	41.458
H	42.434	38.824	42.802
H	44.504	38.016	43.698
H	38.735	28.458	45.174
H	39.090	30.006	44.663
H	37.576	29.708	45.320
H	39.671	37.015	46.455
H	41.791	34.971	46.130
H	39.334	31.477	48.079
H	37.996	31.659	46.949
H	40.182	29.512	46.768
H	40.976	31.849	46.204
H	39.639	32.103	45.079
H	40.181	33.804	47.576
H	38.859	34.073	46.419
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	41.673	36.958	44.801
H	41.515	39.323	51.537
H	40.547	34.541	44.736

Orn complex: Product_{1PT}

N	39.899	37.055	49.494
N	37.666	36.321	48.992
N	38.051	39.635	47.816
N	40.596	39.139	48.773
N	40.703	40.322	43.943
N	36.081	39.860	43.013
N	38.624	29.487	45.462
N	41.002	34.421	46.305
C	38.937	36.081	49.580
C	37.331	37.379	48.204
C	38.509	38.293	47.835
C	39.018	40.632	47.677
C	38.712	41.885	47.133
C	39.676	42.885	47.003
C	39.302	44.219	46.405
C	40.999	42.621	47.423
C	42.086	43.659	47.272
C	41.298	41.378	47.982
C	40.324	40.381	48.132
C	39.684	38.145	48.790
C	41.902	38.940	49.437
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.160	39.852	44.844
C	41.827	39.673	44.696
C	40.975	41.169	42.919
C	39.435	39.988	44.266
C	38.365	40.478	43.526
C	38.628	41.320	42.442
C	39.946	41.678	42.150
C	36.955	40.183	43.994
C	42.380	38.434	43.953
C	43.840	38.384	44.475
C	39.002	31.299	47.167
C	39.132	29.802	46.840
C	38.380	28.913	47.852
C	40.007	32.195	46.427
C	39.865	33.662	46.849
O	39.105	35.021	50.168
O	36.211	37.569	47.748
O	38.951	37.886	46.518
O	40.850	35.829	46.653
O	42.879	40.577	44.804
O	36.653	40.316	45.181
O	41.636	37.271	44.174
O	43.890	37.553	45.624
O	37.421	28.218	47.453
O	38.818	28.955	49.046
H	36.954	35.619	49.173
H	37.218	39.757	47.242
H	37.701	42.057	46.779
H	38.242	44.250	46.138
H	39.498	45.042	47.104
H	39.884	44.431	45.499
H	43.035	43.298	47.677
H	41.832	44.592	47.791
H	42.249	43.919	46.218
H	42.315	41.200	48.308
H	42.670	39.206	48.706
H	41.991	37.874	49.632
H	41.739	40.767	50.601
H	35.142	39.638	43.326
H	36.423	39.324	42.207
H	44.523	36.818	45.416
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.504	39.864	45.883
H	41.401	39.395	45.666
H	42.017	41.412	42.768
H	39.302	39.308	45.102
H	37.810	41.714	41.848
H	40.179	42.352	41.335
H	42.372	38.637	42.877
H	44.516	38.005	43.703
H	38.764	28.472	45.222
H	39.120	30.036	44.755
H	37.598	29.710	45.381
H	39.485	37.058	46.560
H	39.166	31.403	48.244
H	37.975	31.629	46.968
H	40.187	29.509	46.861
H	41.026	31.858	46.651
H	39.876	32.121	45.338
H	39.911	33.743	47.940
H	38.899	34.070	46.518
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	41.655	37.106	45.140
H	41.515	39.323	51.537
H	40.911	34.461	45.289
H	41.366	35.921	47.473

Orn complex: TS_{FR}

N	40.432	36.674	49.774
N	38.385	35.459	49.561
N	38.040	38.515	47.559
N	40.603	38.776	48.840
N	40.857	40.460	43.838
N	36.567	40.158	41.773
N	38.605	29.480	45.369
N	41.071	34.420	45.752
C	39.724	35.529	50.014
C	37.777	36.334	48.697
C	38.736	37.367	48.082
C	38.749	39.706	47.553
C	38.186	40.823	46.902
C	38.840	42.046	46.787
C	38.169	43.203	46.085
C	40.135	42.185	47.340
C	40.895	43.486	47.233
C	40.702	41.094	47.998
C	40.034	39.865	48.123
C	39.949	37.598	48.966
C	41.951	38.914	49.437
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.214	39.844	44.883
C	41.875	39.699	44.652
C	41.200	41.615	43.222
C	39.618	39.936	43.718
C	38.658	40.564	42.935
C	38.996	41.755	42.284
C	40.278	42.283	42.435
C	37.272	39.962	42.910
C	42.469	38.511	43.851
C	43.879	38.405	44.477
C	39.151	31.313	47.014
C	39.165	29.804	46.722
C	38.388	28.980	47.778
C	40.074	32.139	46.095
C	40.243	33.549	46.660
O	40.172	34.574	50.645
O	36.603	36.215	48.370
O	39.110	36.776	46.798
O	41.349	35.683	46.313
O	42.924	40.549	44.976
O	36.833	39.373	43.897
O	41.718	37.336	43.950
O	43.796	37.570	45.621
O	37.435	28.268	47.396
O	38.804	29.076	48.975
H	37.848	34.656	49.872
H	38.405	37.744	46.489
H	37.201	40.691	46.463
H	37.189	42.912	45.694
H	38.021	44.055	46.762
H	38.770	43.573	45.245
H	41.872	43.414	47.721
H	40.350	44.318	47.698
H	41.067	43.773	46.186
H	41.692	41.218	48.420
H	42.592	39.341	48.659
H	42.296	37.900	49.626
H	41.739	40.767	50.601
H	35.645	39.746	41.707
H	36.999	40.454	40.909
H	44.381	36.798	45.436
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.629	39.831	45.894
H	41.329	39.352	45.537
H	42.207	41.963	43.402
H	39.419	39.008	44.238
H	38.262	42.286	41.688
H	40.565	43.211	41.957
H	42.535	38.791	42.795
H	44.601	38.005	43.759
H	38.739	28.458	45.145
H	39.083	30.008	44.633
H	37.575	29.696	45.309
H	40.425	36.145	46.494
H	42.012	34.020	45.580
H	39.474	31.430	48.053
H	38.125	31.697	46.953
H	40.200	29.447	46.725
H	41.055	31.653	46.021
H	39.657	32.197	45.082
H	40.767	33.549	47.617
H	39.290	34.072	46.770
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	41.971	36.929	44.808
H	41.515	39.323	51.537
H	40.615	34.544	44.838

Orn complex: Product_{FR}

N	40.386	36.717	50.002
N	38.516	35.304	49.509
N	37.940	38.462	47.930
N	40.503	38.808	48.993
N	40.846	40.133	43.573
N	36.334	39.772	42.175
N	38.434	29.486	45.307
N	40.594	34.532	45.353
C	39.742	35.523	50.191
C	37.886	36.169	48.652
C	38.534	37.507	48.595
C	38.572	39.664	47.824
C	37.917	40.728	47.166
C	38.524	41.954	46.979
C	37.797	43.076	46.282
C	39.861	42.130	47.450
C	40.568	43.445	47.250
C	40.523	41.092	48.097
C	39.894	39.856	48.321
C	39.826	37.637	49.243
C	41.906	38.925	49.447
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.181	39.818	44.839
C	41.877	39.480	44.453
C	41.257	40.978	42.597
C	39.538	39.835	43.746
C	38.578	40.376	42.895
C	38.992	41.209	41.852
C	40.346	41.520	41.713
C	37.104	40.199	43.205
C	42.620	38.326	43.731
C	43.976	38.337	44.477
C	38.966	31.366	46.909
C	39.030	29.854	46.636
C	38.322	29.015	47.729
C	39.654	32.234	45.834
C	39.979	33.622	46.385
O	40.174	34.625	50.905
O	36.901	35.850	47.989
O	39.087	37.111	45.247
O	41.233	35.626	45.937
O	42.843	40.435	44.777
O	36.673	40.532	44.307
O	41.941	37.111	43.692
O	43.891	37.554	45.654
O	37.381	28.267	47.385
O	38.771	29.139	48.911
H	38.114	34.377	49.610
H	38.411	37.131	45.943
H	36.920	40.539	46.785
H	36.828	42.736	45.912
H	37.634	43.926	46.957
H	38.370	43.455	45.428
H	41.570	43.431	47.684
H	40.006	44.268	47.709
H	40.660	43.685	46.184
H	41.535	41.265	48.441
H	42.474	39.359	48.621
H	42.257	37.907	49.599
H	41.739	40.767	50.601
H	35.352	39.657	42.401
H	36.713	39.079	41.517
H	44.477	36.774	45.494
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.501	39.871	45.884
H	41.327	39.120	45.328
H	42.315	41.198	42.572
H	39.297	39.126	44.535
H	38.260	41.631	41.172
H	40.695	42.187	40.934
H	42.783	38.636	42.691
H	44.775	37.964	43.827
H	38.597	28.467	45.099
H	38.873	30.014	44.548
H	37.398	29.675	45.280
H	39.901	36.731	45.676
H	41.267	34.004	44.779
H	39.455	31.518	47.877
H	37.924	31.685	47.026
H	40.078	29.540	46.600
H	40.587	31.756	45.507
H	39.003	32.330	44.956
H	40.717	33.574	47.187
H	39.091	34.141	46.752
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	41.910	36.699	44.593
H	41.515	39.323	51.537
H	39.861	34.867	44.709

Orn complex: TS_{PS}

N	40.337	36.758	50.071
N	38.373	35.422	49.776
N	37.794	38.581	48.194
N	40.450	38.838	49.042
N	40.759	40.063	43.929
N	36.151	39.783	42.681
N	38.267	29.496	45.413
N	40.332	34.607	45.704
C	39.664	35.593	50.335
C	37.688	36.314	48.986
C	38.404	37.608	48.816
C	38.472	39.744	47.995
C	37.811	40.819	47.357
C	38.452	42.010	47.084
C	37.721	43.140	46.404
C	39.828	42.142	47.448
C	40.571	43.417	47.147
C	40.492	41.097	48.082
C	39.834	39.892	48.385
C	39.753	37.691	49.348
C	41.871	38.930	49.448
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.225	39.791	44.861
C	41.912	39.417	44.640
C	40.993	41.137	43.135
C	39.518	39.541	44.085
C	38.441	40.118	43.415
C	38.667	41.215	42.576
C	39.958	41.726	42.437
C	37.041	39.630	43.706
C	42.615	38.334	43.786
C	44.007	38.323	44.452
C	38.856	31.316	47.069
C	38.943	29.823	46.714
C	38.323	28.926	47.813
C	39.450	32.278	46.016
C	39.911	33.573	46.692
O	40.125	34.686	51.019
O	36.606	36.048	48.472
O	39.255	36.806	45.517
O	41.203	35.568	46.295
O	42.879	40.391	44.904
O	36.737	39.217	44.822
O	41.970	37.095	43.765
O	43.942	37.488	45.598
O	37.376	28.172	47.498
O	38.836	29.019	48.971
H	37.929	34.526	49.953
H	38.538	36.923	46.160
H	36.779	40.660	47.067
H	36.680	42.869	46.209
H	37.726	44.049	47.017
H	38.187	43.401	45.445
H	41.606	43.368	47.494
H	40.089	44.278	47.625
H	40.582	43.620	46.069
H	41.531	41.239	48.350
H	42.421	39.358	48.607
H	42.210	37.906	49.586
H	41.739	40.767	50.601
H	35.220	39.439	42.892
H	36.480	39.503	41.758
H	44.604	36.764	45.452
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.607	39.808	45.885
H	41.485	38.986	45.552
H	42.013	41.493	43.112
H	39.416	38.648	44.716
H	37.836	41.682	42.059
H	40.161	42.585	41.809
H	42.685	38.692	42.753
H	44.778	37.970	43.760
H	38.442	28.494	45.149
H	38.633	30.074	44.652
H	37.224	29.654	45.473
H	40.520	36.383	46.187
H	40.818	34.195	44.903
H	39.396	31.427	48.015
H	37.814	31.593	47.270
H	39.993	29.540	46.596
H	40.315	31.817	45.519
H	38.703	32.502	45.245
H	40.773	33.386	47.336
H	39.118	34.024	47.292
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	42.138	36.683	44.637
H	41.515	39.323	51.537
H	39.528	35.351	45.398

Orn complex: Product_{ps}

N	40.433	36.694	49.903
N	38.591	35.257	49.389
N	38.023	38.385	47.746
N	40.526	38.803	48.937
N	40.939	40.505	43.783
N	36.620	40.446	41.740
N	38.486	29.459	45.368
N	40.489	34.463	45.398
C	39.814	35.483	50.067
C	37.952	36.113	48.528
C	38.604	37.449	48.445
C	38.635	39.599	47.659
C	37.989	40.639	46.953
C	38.563	41.886	46.805
C	37.838	42.986	46.070
C	39.860	42.108	47.361
C	40.531	43.448	47.206
C	40.516	41.092	48.048
C	39.918	39.833	48.233
C	39.872	37.608	49.139
C	41.917	38.940	49.431
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.240	39.815	44.886
C	41.905	39.681	44.599
C	41.349	41.636	43.162
C	39.674	40.054	43.668
C	38.752	40.726	42.875
C	39.156	41.893	42.218
C	40.466	42.350	42.372
C	37.349	40.163	42.841
C	42.530	38.529	43.764
C	43.910	38.384	44.443
C	39.022	31.306	46.986
C	39.076	29.797	46.706
C	38.353	28.957	47.782
C	39.793	32.168	45.971
C	39.920	33.615	46.454
O	40.265	34.581	50.765
O	36.946	35.790	47.903
O	38.860	37.367	44.955
O	40.782	35.760	45.985
O	42.943	40.496	45.029
O	36.921	39.506	43.792
O	41.769	37.361	43.719
O	43.785	37.520	45.559
O	37.396	28.231	47.433
O	38.805	29.056	48.967
H	38.191	34.330	49.499
H	38.024	37.661	45.353
H	37.021	40.415	46.516
H	36.878	42.631	45.687
H	37.645	43.844	46.725
H	38.426	43.359	45.222
H	41.510	43.462	47.691
H	39.921	44.248	47.643
H	40.670	43.700	46.148
H	41.497	41.299	48.455
H	42.493	39.396	48.622
H	42.280	37.924	49.571
H	41.739	40.767	50.601
H	35.690	40.051	41.672
H	37.026	40.819	40.894
H	44.425	36.783	45.401
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.678	39.784	45.887
H	41.310	39.290	45.431
H	42.372	41.933	43.343
H	39.419	39.148	44.216
H	38.458	42.464	41.615
H	40.804	43.259	41.891
H	42.656	38.877	42.733
H	44.653	37.997	43.739
H	38.646	28.444	45.134
H	38.927	30.009	44.627
H	37.451	29.651	45.342
H	40.029	36.315	45.661
H	41.425	34.114	45.182
H	39.445	31.453	47.985
H	37.977	31.637	47.033
H	40.121	29.472	46.674
H	40.795	31.745	45.809
H	39.284	32.174	44.998
H	40.521	33.654	47.376
H	38.927	34.014	46.689
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	41.840	36.912	44.590
H	41.515	39.323	51.537
H	38.659	37.133	44.009

Lys complex: Reactant

N	38.431	29.397	45.448
N	40.221	35.562	44.705
N	39.408	37.916	49.778
N	37.486	37.159	48.713
N	38.542	40.206	47.141
N	40.703	39.734	48.883
N	41.004	39.748	43.234
N	36.333	39.913	42.541
C	39.075	29.712	46.767
C	38.358	28.895	47.862
C	39.075	31.229	47.006
C	40.051	31.982	46.085
C	39.730	33.474	45.954
C	40.667	34.180	44.972
C	38.383	37.013	49.781
C	37.555	38.039	47.666
C	38.826	38.878	47.573
C	39.602	41.127	47.209
C	39.589	42.287	46.427
C	40.617	43.232	46.478
C	40.552	44.469	45.613
C	41.707	43.003	47.343
C	42.848	43.990	47.438
C	41.722	41.846	48.126
C	40.690	40.897	48.083
C	39.586	38.920	48.838
C	41.945	39.261	49.518
C	42.145	39.785	50.940
C	45.130	40.610	43.940
C	44.199	39.794	44.836
C	42.046	39.180	44.148
C	41.360	40.345	42.070
C	39.716	39.712	43.636
C	38.709	40.241	42.839
C	39.053	40.803	41.607
C	40.396	40.867	41.231
C	37.302	40.300	43.392
C	43.039	38.201	43.499
C	44.168	38.288	44.547
O	42.819	40.249	44.628
O	37.108	40.747	44.527
O	42.466	36.935	43.272
O	43.814	37.614	45.742
O	37.393	28.167	47.534
O	38.829	29.002	49.037
O	38.223	36.154	50.646
O	36.684	38.113	46.804
O	39.628	38.281	46.495
O	40.148	36.995	46.936
H	35.386	39.919	42.903
H	36.560	39.208	41.829
H	43.810	36.654	45.527
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.431	39.945	45.894
H	41.492	38.679	44.946
H	42.416	40.386	41.845
H	39.521	39.236	44.590
H	38.284	41.213	40.961
H	40.699	41.326	40.298
H	43.412	38.617	42.553
H	45.122	37.924	44.146
H	44.698	40.670	42.963
H	43.125	36.233	43.462
H	36.687	36.534	48.738
H	37.938	40.278	46.322
H	38.754	42.433	45.748
H	39.643	44.476	45.004
H	40.558	45.387	46.215
H	41.411	44.535	44.933
H	43.601	43.655	48.158
H	42.502	44.983	47.753
H	43.349	44.126	46.471
H	42.559	41.695	48.799
H	42.782	39.549	48.875
H	41.919	38.167	49.509
H	42.294	40.869	50.943
H	43.022	39.310	51.392
H	41.273	39.569	51.566
H	40.076	36.450	46.085
H	40.106	29.347	46.709
H	39.337	31.410	48.052
H	38.054	31.608	46.866
H	41.076	31.839	46.451
H	40.037	31.554	45.072
H	39.781	33.969	46.933
H	38.695	33.579	45.604
H	41.680	34.234	45.383
H	40.732	33.594	44.042
H	40.936	36.060	44.168
H	39.388	35.548	44.118
H	38.587	28.390	45.175
H	38.837	29.968	44.703
H	37.400	29.598	45.475

Lys complex: TS_{OT}

N	39.627	37.446	48.938
N	37.444	37.150	47.967
N	38.495	40.481	47.414
N	40.751	39.446	48.602
N	41.097	39.645	42.856
N	36.461	39.806	42.058
N	38.293	29.429	45.464
N	40.321	35.486	44.633
C	38.550	36.633	48.688
C	37.425	38.329	47.286
C	38.760	39.075	47.255
C	39.640	41.284	47.449
C	39.656	42.586	46.944
C	40.804	43.379	46.990
C	40.776	44.782	46.433
C	41.983	42.840	47.547
C	43.259	43.648	47.600
C	41.962	41.538	48.056
C	40.804	40.751	48.033
C	39.707	38.621	48.357
C	41.890	38.969	49.413
C	42.080	39.740	50.730
C	45.130	40.610	43.940
C	44.128	39.814	44.786
C	42.056	39.154	43.902
C	41.506	39.955	41.601
C	39.803	39.783	43.220
C	38.842	40.170	42.295
C	39.236	40.429	40.981
C	40.590	40.346	40.644
C	37.431	40.378	42.803
C	43.104	38.141	43.421
C	44.127	38.293	44.567
C	38.875	31.279	47.032
C	38.934	29.763	46.782
C	38.271	28.905	47.878
C	39.938	32.045	46.225
C	39.623	33.533	46.028
C	40.748	34.229	45.257
O	38.475	35.478	49.097
O	36.455	38.741	46.656
O	39.378	38.845	46.022
O	39.688	37.112	45.529
O	42.774	40.250	44.408
O	37.248	41.066	43.807
O	42.540	36.863	43.227
O	43.662	37.661	45.749
O	37.337	28.137	47.559
O	38.761	29.023	49.045
H	36.665	36.510	47.810
H	37.762	40.792	46.780
H	38.748	42.978	46.491
H	39.785	45.033	46.043
H	41.035	45.525	47.199
H	41.500	44.907	45.618
H	44.068	43.080	48.068
H	43.127	44.576	48.173
H	43.594	43.944	46.597
H	42.876	41.145	48.485
H	42.781	39.054	48.784
H	41.717	37.910	49.593
H	41.739	40.767	50.601
H	35.516	39.898	42.413
H	36.657	38.981	41.476
H	43.744	36.695	45.587
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.243	40.015	45.855
H	41.420	38.695	44.660
H	42.562	39.873	41.389
H	39.552	39.559	44.256
H	38.503	40.718	40.235
H	40.937	40.575	39.644
H	43.580	38.486	42.494
H	45.117	37.919	44.279
H	38.483	28.432	45.186
H	38.671	30.020	44.718
H	37.253	29.587	45.503
H	41.601	34.447	45.906
H	39.020	31.457	48.102
H	37.867	31.639	46.787
H	39.979	29.443	46.713
H	40.911	31.925	46.719
H	40.054	31.597	45.228
H	39.450	34.033	46.988
H	38.688	33.615	45.455
H	43.110	39.630	50.999
H	44.698	40.670	42.963
H	43.212	36.176	43.432
H	41.515	39.323	51.537
H	41.117	33.560	44.463
H	41.068	35.951	44.108
H	39.514	35.367	44.026
H	40.510	37.115	46.053

Lys complex: Productor

N	39.818	37.578	49.369
N	37.637	37.054	48.511
N	38.478	40.319	47.478
N	40.808	39.585	48.788
N	40.943	39.916	43.342
N	36.298	40.059	42.676
N	38.607	29.385	45.545
N	40.045	35.549	45.018
C	38.788	36.682	49.258
C	37.543	38.109	47.658
C	38.831	38.934	47.517
C	39.555	41.212	47.476
C	39.469	42.464	46.860
C	40.524	43.377	46.896
C	40.387	44.718	46.215
C	41.714	43.020	47.568
C	42.886	43.972	47.634
C	41.801	41.766	48.176
C	40.741	40.850	48.143
C	39.809	38.681	48.658
C	42.018	39.195	49.540
C	42.146	39.785	50.942
C	45.130	40.610	43.940
C	44.185	39.821	44.843
C	41.961	39.324	44.272
C	41.317	40.448	42.151
C	39.657	39.948	43.747
C	38.665	40.464	42.924
C	39.021	40.959	41.669
C	40.368	40.968	41.293
C	37.264	40.535	43.490
C	42.837	38.221	43.656
C	44.080	38.312	44.569
C	39.123	31.155	47.210
C	39.186	29.652	46.903
C	38.440	28.791	47.940
C	40.161	31.993	46.440
C	39.660	33.426	46.240
C	40.707	34.341	45.614
O	38.779	35.589	49.811
O	36.547	38.360	46.988
O	39.496	38.527	46.335
O	39.109	36.078	45.906
O	42.834	40.353	44.649
O	37.075	41.039	44.599
O	42.167	36.975	43.659
O	43.855	37.643	45.798
O	37.452	28.118	47.576
O	38.913	28.829	49.121
H	36.865	36.395	48.538
H	37.763	40.509	46.775
H	38.557	42.710	46.323
H	39.407	44.821	45.740
H	40.504	45.545	46.927
H	41.152	44.859	45.442
H	43.714	43.539	48.203
H	42.611	44.921	48.113
H	43.262	44.222	46.634
H	42.719	41.513	48.692
H	42.881	39.463	48.925
H	41.986	38.109	49.606
H	42.294	40.869	50.943
H	35.356	40.043	43.053
H	36.543	39.330	41.997
H	43.817	36.684	45.581
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.441	39.958	45.897
H	41.391	38.936	45.120
H	42.373	40.443	41.921
H	39.443	39.526	44.727
H	38.264	41.357	41.000
H	40.684	41.377	40.342
H	43.124	38.490	42.631
H	44.974	37.925	44.064
H	38.747	28.380	45.255
H	39.065	29.965	44.837
H	37.580	29.609	45.525
H	41.421	34.713	46.353
H	39.264	31.298	48.284
H	38.109	31.508	46.981
H	40.228	29.315	46.879
H	41.113	31.979	46.985
H	40.373	31.557	45.454
H	39.337	33.853	47.194
H	38.771	33.393	45.599
H	43.022	39.310	51.392
H	44.698	40.670	42.963
H	42.833	36.255	43.636
H	41.273	39.569	51.566
H	41.264	33.857	44.805
H	40.774	36.220	44.710
H	39.550	35.269	44.159
H	39.389	37.510	46.146

Lys complex: TS_{1PT}

N	40.381	36.936	49.578
N	38.657	35.613	48.664
N	38.473	38.929	47.319
N	40.795	39.119	48.832
N	40.884	39.895	43.563
N	36.138	40.020	42.830
N	39.089	29.573	45.348
N	40.209	35.144	43.700
C	39.690	35.710	49.582
C	38.264	36.561	47.744
C	39.230	37.743	47.558
C	39.122	40.156	47.407
C	38.588	41.308	46.812
C	39.222	42.543	46.909
C	38.611	43.753	46.248
C	40.440	42.647	47.626
C	41.162	43.967	47.749
C	40.964	41.509	48.231
C	40.316	40.269	48.137
C	40.137	37.977	48.754
C	42.105	39.176	49.537
C	42.148	39.783	50.942
C	45.130	40.610	43.940
C	44.210	39.795	44.850
C	41.964	39.299	44.332
C	41.157	40.718	42.446
C	39.589	39.639	43.908
C	38.519	40.128	43.203
C	38.772	40.960	42.041
C	40.107	41.227	41.715
C	37.177	39.744	43.680
C	42.859	38.299	43.582
C	44.103	38.305	44.488
C	39.187	31.420	47.061
C	39.340	29.913	46.793
C	38.392	29.070	47.668
C	40.218	32.320	46.332
C	39.593	33.321	45.347
C	40.679	34.132	44.640
O	39.976	34.835	50.367
O	37.272	36.424	47.053
O	40.212	37.386	46.584
O	39.502	36.322	44.334
O	42.856	40.323	44.764
O	36.954	39.242	44.803
O	42.207	37.050	43.426
O	43.880	37.571	45.684
O	37.447	28.466	47.120
O	38.671	29.061	48.911
H	38.101	34.764	48.724
H	37.786	38.857	46.562
H	37.664	41.210	46.252
H	37.673	43.500	45.748
H	38.404	44.545	46.978
H	39.288	44.185	45.500
H	42.074	43.863	48.344
H	40.533	44.728	48.226
H	41.447	44.363	46.766
H	41.881	41.605	48.798
H	42.773	39.712	48.862
H	42.481	38.153	49.553
H	42.294	40.869	50.943
H	35.243	39.634	43.107
H	36.322	39.984	41.835
H	43.775	36.629	45.418
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.536	39.872	45.893
H	41.506	38.788	45.183
H	42.197	40.941	42.261
H	39.448	38.997	44.763
H	37.963	41.414	41.483
H	40.342	41.867	40.869
H	43.124	38.707	42.596
H	44.998	37.943	43.964
H	39.048	28.535	45.193
H	39.846	29.931	44.758
H	38.201	30.002	44.993
H	41.320	34.647	45.361
H	39.284	31.546	48.142
H	38.163	31.723	46.807
H	40.365	29.602	47.011
H	40.800	32.873	47.078
H	40.952	31.701	45.796
H	38.916	33.995	45.883
H	38.983	32.787	44.607
H	43.022	39.310	51.392
H	44.698	40.670	42.963
H	42.853	36.318	43.467
H	41.273	39.569	51.566
H	41.330	33.470	44.054
H	40.581	36.309	43.705
H	39.565	34.822	42.973
H	39.836	36.842	45.788

Lys complex: Product_{1PT}

N	40.384	36.931	49.613
N	38.610	35.619	48.784
N	38.440	38.904	47.368
N	40.788	39.105	48.837
N	40.903	39.862	43.571
N	36.147	40.047	42.900
N	38.489	29.416	45.479
N	40.194	34.766	43.524
C	39.672	35.719	49.669
C	38.210	36.548	47.851
C	39.181	37.718	47.619
C	39.093	40.131	47.433
C	38.549	41.277	46.837
C	39.185	42.512	46.911
C	38.565	43.717	46.249
C	40.416	42.622	47.606
C	41.141	43.942	47.704
C	40.951	41.489	48.212
C	40.300	40.249	48.141
C	40.126	37.963	48.782
C	42.103	39.172	49.536
C	42.148	39.783	50.941
C	45.130	40.610	43.940
C	44.226	39.794	44.864
C	41.991	39.274	44.332
C	41.167	40.717	42.476
C	39.608	39.603	43.922
C	38.535	40.118	43.243
C	38.779	40.987	42.108
C	40.113	41.256	41.773
C	37.193	39.727	43.722
C	42.912	38.302	43.572
C	44.131	38.303	44.507
C	39.198	31.204	47.064
C	39.128	29.690	46.811
C	38.373	28.885	47.887
C	40.224	31.911	46.144
C	39.709	33.202	45.493
C	40.665	33.692	44.399
O	39.964	34.858	50.467
O	37.206	36.410	47.181
O	40.105	37.325	46.601
O	39.956	35.982	44.282
O	42.863	40.302	44.792
O	36.981	39.180	44.825
O	42.279	37.051	43.359
O	43.872	37.576	45.700
O	37.400	28.178	47.541
O	38.834	28.972	49.069
H	38.045	34.778	48.873
H	37.747	38.826	46.615
H	37.615	41.175	46.295
H	37.618	43.459	45.767
H	38.370	44.515	46.976
H	39.230	44.141	45.486
H	42.062	43.845	48.285
H	40.519	44.708	48.185
H	41.409	44.329	46.713
H	41.877	41.591	48.764
H	42.764	39.710	48.855
H	42.485	38.151	49.551
H	42.294	40.869	50.943
H	35.247	39.667	43.168
H	36.313	40.099	41.903
H	43.786	36.630	45.440
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.561	39.881	45.903
H	41.538	38.736	45.171
H	42.206	40.937	42.282
H	39.469	38.941	44.765
H	37.968	41.469	41.577
H	40.342	41.919	40.944
H	43.193	38.738	42.604
H	45.040	37.939	44.010
H	38.610	28.409	45.196
H	38.928	29.979	44.746
H	37.465	29.654	45.496
H	41.625	34.008	44.821
H	39.454	31.360	48.115
H	38.196	31.629	46.921
H	40.143	29.282	46.760
H	41.142	32.114	46.709
H	40.535	31.229	45.339
H	39.569	33.979	46.254
H	38.722	33.015	45.049
H	43.022	39.310	51.392
H	44.698	40.670	42.963
H	42.911	36.316	43.490
H	41.273	39.569	51.566
H	40.880	32.860	43.713
H	40.721	36.528	43.985
H	39.266	34.537	43.166
H	39.749	36.680	45.936

Lys complex: TS_{FR}

N	40.109	37.316	49.218
N	37.883	36.622	48.706
N	38.124	40.134	47.813
N	40.734	39.507	48.841
N	40.992	39.867	43.272
N	36.345	40.094	42.485
N	38.514	29.394	45.392
N	40.072	35.695	44.832
C	39.187	36.313	49.162
C	37.500	37.773	48.077
C	38.635	38.784	47.829
C	39.096	41.107	48.002
C	38.782	42.448	47.702
C	39.710	43.481	47.776
C	39.303	44.894	47.426
C	41.036	43.186	48.174
C	42.088	44.267	48.256
C	41.357	41.869	48.501
C	40.414	40.832	48.438
C	39.851	38.495	48.682
C	42.020	39.227	49.516
C	42.146	39.786	50.937
C	45.130	40.610	43.940
C	44.193	39.826	44.855
C	41.989	39.300	44.240
C	41.385	40.319	42.055
C	39.703	39.948	43.662
C	38.724	40.407	42.792
C	39.101	40.811	41.510
C	40.453	40.792	41.154
C	37.312	40.538	43.320
C	42.898	38.204	43.657
C	44.107	38.313	44.610
C	39.077	31.244	46.958
C	39.115	29.728	46.726
C	38.372	28.918	47.810
C	40.053	32.036	46.066
C	39.616	33.500	45.953
C	40.635	34.347	45.196
O	39.410	35.161	49.531
O	36.363	37.939	47.651
O	38.930	38.676	46.408
O	39.366	36.196	45.941
O	42.832	40.335	44.649
O	37.119	41.068	44.413
O	42.249	36.946	43.633
O	43.837	37.666	45.840
O	37.405	28.201	47.468
O	38.822	29.027	48.994
H	37.204	35.868	48.756
H	38.260	39.713	46.510
H	37.765	42.656	47.379
H	38.247	44.942	47.145
H	39.459	45.581	48.267
H	39.893	45.289	46.587
H	43.052	43.856	48.572
H	41.812	45.053	48.972
H	42.239	44.765	47.289
H	42.375	41.656	48.807
H	42.819	39.617	48.879
H	42.112	38.144	49.534
H	42.294	40.869	50.943
H	35.397	40.123	42.843
H	36.570	39.337	41.834
H	43.844	36.702	45.646
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.442	39.989	45.907
H	41.392	38.905	45.068
H	42.443	40.288	41.836
H	39.483	39.629	44.675
H	38.355	41.165	40.807
H	40.784	41.138	40.183
H	43.217	38.471	42.642
H	45.019	37.922	44.144
H	38.675	28.381	45.145
H	38.946	29.950	44.650
H	37.482	29.595	45.379
H	41.530	34.541	45.789
H	39.308	31.434	48.009
H	38.050	31.596	46.794
H	40.152	29.379	46.703
H	41.066	31.960	46.482
H	40.108	31.611	45.054
H	39.470	33.923	46.951
H	38.646	33.536	45.443
H	43.022	39.310	51.392
H	44.698	40.670	42.963
H	42.927	36.234	43.662
H	41.273	39.569	51.566
H	40.935	33.892	44.247
H	40.858	36.324	44.549
H	39.434	35.627	44.021
H	39.242	37.208	45.876

Lys complex: Product_{FR}

N	39.957	37.433	49.533
N	37.784	36.733	48.814
N	38.401	39.965	47.415
N	40.764	39.500	48.843
N	41.087	39.932	43.151
N	36.518	40.160	42.274
N	38.653	29.483	45.412
N	40.267	35.847	44.975
C	38.995	36.461	49.500
C	37.518	37.827	48.042
C	38.583	38.861	48.087
C	39.391	40.899	47.433
C	39.215	42.090	46.692
C	40.179	43.078	46.666
C	39.969	44.335	45.860
C	41.379	42.880	47.416
C	42.449	43.941	47.425
C	41.574	41.708	48.139
C	40.599	40.695	48.159
C	39.771	38.548	48.855
C	42.033	39.192	49.536
C	42.147	39.784	50.942
C	45.130	40.610	43.940
C	44.200	39.800	44.848
C	42.022	39.267	44.124
C	41.580	40.544	42.045
C	39.771	39.983	43.448
C	38.876	40.627	42.600
C	39.361	41.212	41.430
C	40.732	41.177	41.160
C	37.431	40.799	43.034
C	42.989	38.233	43.515
C	44.132	38.299	44.552
C	38.991	31.382	47.016
C	39.134	29.866	46.783
C	38.369	29.009	47.814
C	39.999	32.226	46.218
C	39.658	33.725	46.198
C	40.740	34.513	45.460
O	39.117	35.365	50.038
O	36.491	37.940	47.370
O	37.950	38.142	44.820
O	39.855	36.702	45.992
O	42.820	40.273	44.686
O	37.170	41.557	43.968
O	42.369	36.972	43.357
O	43.775	37.622	45.742
O	37.442	28.272	47.415
O	38.766	29.106	49.019
H	37.106	35.978	48.800
H	37.320	38.370	45.527
H	38.301	42.182	46.114
H	39.014	44.301	45.329
H	39.970	45.227	46.499
H	40.765	44.475	45.119
H	43.296	43.649	48.050
H	42.057	44.894	47.802
H	42.821	44.133	46.411
H	42.494	41.593	48.697
H	42.848	39.534	48.895
H	42.080	38.107	49.590
H	42.294	40.869	50.943
H	35.554	40.233	42.579
H	36.779	39.311	41.759
H	43.800	36.662	45.526
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.459	39.940	45.900
H	41.375	38.779	44.863
H	42.650	40.510	41.898
H	39.417	39.466	44.336
H	38.682	41.708	40.744
H	41.145	41.644	40.274
H	43.366	38.582	42.545
H	45.073	37.917	44.137
H	38.813	28.462	45.212
H	39.149	30.011	44.690
H	37.625	29.681	45.307
H	41.607	34.714	46.093
H	39.130	31.564	48.086
H	37.965	31.687	46.775
H	40.190	29.583	46.837
H	41.004	32.071	46.634
H	40.048	31.885	45.174
H	39.541	34.112	47.215
H	38.692	33.857	45.693
H	43.022	39.310	51.392
H	44.698	40.670	42.963
H	43.047	36.267	43.441
H	41.273	39.569	51.566
H	41.083	33.974	44.568
H	41.037	36.285	44.436
H	39.507	35.693	44.293
H	38.657	37.606	45.297

Lys complex: TS_{ps}

N	39.964	37.387	49.605
N	37.787	36.598	49.008
N	38.048	40.002	47.931
N	40.604	39.530	48.983
N	40.950	39.834	43.422
N	36.304	39.905	42.603
N	38.410	29.418	45.440
N	40.640	35.777	45.388
C	39.050	36.367	49.606
C	37.376	37.738	48.369
C	38.368	38.846	48.439
C	38.994	40.982	47.919
C	38.666	42.234	47.351
C	39.581	43.267	47.284
C	39.204	44.591	46.669
C	40.893	43.049	47.806
C	41.920	44.150	47.756
C	41.234	41.821	48.364
C	40.304	40.769	48.434
C	39.654	38.537	49.039
C	41.952	39.240	49.526
C	42.144	39.786	50.942
C	45.130	40.610	43.940
C	44.221	39.788	44.854
C	42.006	39.223	44.292
C	41.329	40.558	42.338
C	39.650	39.706	43.777
C	38.663	40.303	42.995
C	39.030	41.000	41.843
C	40.383	41.137	41.520
C	37.234	40.310	43.499
C	42.941	38.222	43.588
C	44.153	38.288	44.538
C	38.917	31.281	47.037
C	39.000	29.768	46.775
C	38.303	28.914	47.854
C	39.829	32.093	46.109
C	39.710	33.612	46.292
C	40.689	34.300	45.347
O	39.269	35.261	50.090
O	36.301	37.817	47.778
O	39.010	37.588	45.708
O	40.929	36.296	46.684
O	42.837	40.263	44.735
O	36.992	40.745	44.623
O	42.340	36.951	43.433
O	43.892	37.595	45.745
O	37.357	28.169	47.515
O	38.773	29.018	49.031
H	37.158	35.801	48.983
H	38.072	37.534	45.939
H	37.666	42.343	46.946
H	38.168	44.578	46.319
H	39.306	45.413	47.389
H	39.847	44.836	45.815
H	42.869	43.831	48.194
H	41.573	45.038	48.298
H	42.110	44.467	46.723
H	42.236	41.694	48.752
H	42.686	39.646	48.827
H	42.043	38.157	49.519
H	42.294	40.869	50.943
H	35.347	39.881	42.938
H	36.565	39.210	41.894
H	43.839	36.639	45.514
H	45.268	41.605	44.362
H	46.101	40.116	43.894
H	44.511	39.909	45.902
H	41.467	38.739	45.112
H	42.392	40.660	42.168
H	39.413	39.069	44.649
H	38.270	41.458	41.218
H	40.704	41.699	40.651
H	43.231	38.615	42.604
H	45.068	37.926	44.053
H	38.587	28.409	45.195
H	38.836	29.977	44.697
H	37.375	29.604	45.426
H	41.722	34.014	45.566
H	39.208	31.450	48.078
H	37.876	31.613	46.937
H	40.051	29.461	46.743
H	40.870	31.785	46.276
H	39.607	31.867	45.057
H	39.929	33.896	47.327
H	38.684	33.932	46.072
H	43.022	39.310	51.392
H	44.698	40.670	42.963
H	43.038	36.262	43.425
H	41.273	39.569	51.566
H	40.482	34.038	44.303
H	41.336	36.177	44.734
H	39.685	36.308	45.207
H	40.124	36.990	46.676

Lys complex: Product_{ps}

N	39.896	37.491	49.549
N	37.759	36.781	48.732
N	38.350	40.080	47.495
N	40.731	39.551	48.870
N	41.300	40.024	42.894
N	37.204	41.008	43.608
N	38.655	29.493	45.464
N	40.163	35.803	45.007
C	38.932	36.524	49.493
C	37.524	37.876	47.956
C	38.547	38.940	48.100
C	39.328	41.021	47.565
C	39.127	42.263	46.918
C	40.093	43.249	46.917
C	39.853	44.564	46.219
C	41.328	42.992	47.591
C	42.408	44.041	47.612
C	41.543	41.777	48.232
C	40.558	40.774	48.240
C	39.727	38.611	48.874
C	42.009	39.211	49.533
C	42.146	39.785	50.943
C	45.134	40.605	43.947
C	44.202	39.790	44.848
C	42.084	39.284	43.958
C	41.906	40.488	41.775
C	40.010	40.328	43.162
C	39.267	41.121	42.295
C	39.882	41.589	41.130
C	41.210	41.261	40.866
C	37.840	41.564	42.558
C	43.075	38.220	43.446
C	44.152	38.289	44.555
C	38.966	31.368	47.103
C	39.132	29.859	46.841
C	38.380	28.976	47.858
C	39.965	32.246	46.332
C	39.619	33.744	46.353
C	40.676	34.570	45.605
O	39.022	35.437	50.054
O	36.559	37.963	47.188
O	38.135	38.558	44.888
O	40.056	36.814	46.056
O	42.820	40.242	44.666
O	37.341	42.423	41.829
O	42.428	36.980	43.270
O	43.732	37.618	45.727
O	37.450	28.245	47.454
O	38.787	29.052	49.061
H	37.102	36.010	48.663
H	37.372	38.412	45.485
H	38.181	42.405	46.406
H	38.862	44.585	45.757
H	39.919	45.406	46.918
H	40.597	44.743	45.434
H	43.287	43.699	48.163
H	42.049	44.968	48.077
H	42.723	44.303	46.594
H	42.487	41.623	48.739
H	42.816	39.551	48.881
H	42.040	38.124	49.569
H	42.294	40.869	50.943
H	36.241	41.284	43.751
H	37.540	40.184	44.114
H	43.741	36.659	45.507
H	45.272	41.600	44.369
H	46.105	40.111	43.901
H	44.440	39.942	45.904
H	41.328	38.807	44.588
H	42.944	40.230	41.631
H	39.612	39.922	44.083
H	39.308	42.214	40.456
H	41.714	41.610	39.973
H	43.539	38.535	42.502
H	45.116	37.907	44.197
H	38.820	28.477	45.248
H	39.149	30.037	44.752
H	37.625	29.686	45.359
H	41.546	34.761	46.254
H	39.093	31.530	48.178
H	37.936	31.662	46.861
H	40.192	29.591	46.890
H	40.972	32.082	46.740
H	40.014	31.936	45.277
H	39.512	34.097	47.386
H	38.649	33.890	45.862
H	43.022	39.310	51.392
H	44.702	40.665	42.970
H	43.074	36.257	43.414
H	41.273	39.569	51.566
H	41.045	33.990	44.748
H	40.913	36.172	44.417
H	38.003	38.039	44.048
H	39.354	37.398	45.695