

## Supporting Information

# Are Heme Dependent Enzymes Always Using a Redox Mechanism? A Theoretical Study of the Kemp Elimination Catalysed by a Promiscuous Aldoxime Dehydratase.

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**Table S1.** Cartesian coordinates of the QM subset of atoms for the different states localized and optimized at B3LYP(Lan12DZ )/MM level along the two reaction mechanism in the three different electronic states

<sup>1</sup>RC:

C	-21.6937571030	-6.4771177046	5.1102338156
H	-20.7519163091	-6.9671311093	5.3750844636
H	-21.9137419694	-5.7064560587	5.8597908794
O	-22.7785323955	-7.4438873401	5.0547739439
H	-22.5157487781	-8.2592342673	5.5366932475
C	-24.6392768470	-7.7067672784	13.7977686319
H	-24.6072372091	-6.6137518968	13.7154250632
H	-24.2445826596	-7.9737386514	14.7857425886
N	-22.9666214290	-9.4050254092	12.9135135904
H	-22.6553313463	-9.7421463985	13.8331308465
C	-23.8578104207	-8.3541427365	12.6973259363
C	-22.4634296999	-9.8064726325	11.7056979573
H	-21.7395935061	-10.5925481825	11.5821460268
N	-22.9975584428	-9.0639075035	10.7251661667
C	-23.8724372957	-8.1607387131	11.3261005023
H	-24.4443344404	-7.4586731525	10.7433115449
C	-18.2143496516	-8.3004617914	4.8551980867
H	-17.6702951915	-7.3493720009	4.8768496338
H	-19.0795421960	-8.2200341466	5.5196826112
N	-17.7900819210	-10.5369888099	6.0309296170
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C	-16.7327095244	-11.3737212882	6.1400514602
H	-16.7217749393	-12.3253907822	6.6506248632
N	-15.6427415540	-10.8615297282	5.4896497936
H	-14.6785857100	-11.2659705946	5.4088179079
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H	-15.3375167074	-9.0842240890	4.3123465330
Fe	-22.4989623103	-9.1443862471	8.8536757358
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C	-22.1638815048	-4.8368941620	8.9197471777
C	-21.6684838621	-6.1986451733	9.1873521840
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C	-18.5227954469	-8.2291903820	10.0634192884
C	-18.3748147934	-9.5736094863	9.8292010329
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C	-19.9953659786	-11.4363057059	9.3231344860
H	-19.1818264210	-12.1503882762	9.4110444699
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H	-19.78612220020	-10.6129976170	6.1596673563
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H	-25.0582812609	-8.0668723065	2.8680844354
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<sup>1</sup>TS:

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H	-22.8084914291	-8.4418270210	5.3176313523
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H	-16.8247067793	-12.4320192542	6.7024921587
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C	-19.9703065655	-11.5497684672	9.4117536287
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H	-25.4390549219	-12.6288467348	8.2413520910
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C	-24.0077841106	-12.4021097835	4.8589720763
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C	-21.0487328679	-10.4854497636	6.0027556092
H	-20.1831991447	-13.0348365617	5.4410180865
H	-25.0701330691	-12.2135770791	4.7589732122
H	-24.1049709361	-14.5130744375	4.4370658961
H	-18.6447377692	-10.5629969411	6.4505772450
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H	-25.3034935772	-7.9050107924	3.1367018210
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<sup>1</sup>TS<sub>1</sub>:

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O	-22.6762219377	-7.4144235252	4.9852070084
H	-22.4878799547	-8.2603981133	5.4524044344
C	-24.4453911452	-7.6179402635	13.6027167319
H	-24.4446279909	-6.5267629490	13.5031004954
H	-24.0053804903	-7.8580602282	14.5783058454
N	-22.8117983748	-9.3375490262	12.6920822752
H	-22.5197389939	-9.6997830964	13.6061975350
C	-23.6929206771	-8.2713172928	12.4843669247
C	-22.3601252334	-9.7704739819	11.4770414524
H	-21.6666122597	-10.5810014707	11.3475425795
N	-22.9040547353	-9.0307245340	10.4965882796
C	-23.7374134204	-8.0932305953	11.1101945328
H	-24.3136712477	-7.3855910605	10.5384560708
C	-18.1232971703	-8.2679992533	5.2515731747
H	-17.5524296903	-7.3326337541	5.2834097587
H	-18.9688743576	-8.1863856385	5.9435998738
N	-17.7307089786	-10.6326610181	6.1682388929
C	-17.2489910588	-9.4359551287	5.6055845866
C	-16.6595019833	-11.4574139225	6.2353254458
H	-16.6653396870	-12.4685093740	6.6133316743
N	-15.5342672943	-10.8422933424	5.7453540342
H	-14.5642683386	-11.2231151081	5.6467266630
C	-15.8933893487	-9.5665967631	5.3474486876
H	-15.2072306261	-8.9010933311	4.8586230192
Fe	-22.4501895880	-9.2389431673	8.5524871970
N	-22.4155786116	-11.2285624183	8.8533208133
N	-24.3866900718	-9.3205939583	8.0617848442
N	-22.5275911025	-7.2050728287	8.3397114260
N	-20.5471014924	-9.0985619814	9.1441709649
C	-21.2876300814	-12.0107947461	9.0743002406
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C	-25.2077081802	-10.4334087290	8.0948058513
C	-26.4845718377	-10.1192039640	7.4613438398
C	-26.3760879768	-8.8648826333	6.9182544834
C	-25.0871817784	-8.3591767592	7.3482401570
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C	-19.8731718447	-7.9281077292	9.4687044877
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C	-19.6635777310	-10.1538432726	9.3164187802

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H	-25.5383777533	-12.5214817088	8.3649375152
C	-24.6914114642	-7.0465165446	7.1688263946
H	-25.3254975160	-6.3858173450	6.5919544774
C	-20.3780927011	-6.6207238754	9.3655832494
H	-19.6865626425	-5.8267629664	9.6252193590
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O	-20.0243344840	-15.3463491756	4.4618412325
O	-22.0896729467	-16.2472407062	4.3315047347
N	-21.8315007987	-9.6264814613	6.7831767360
N	-21.2993956092	-15.2404505513	4.4678730391
C	-21.7062062700	-11.6709681705	5.5254579178
C	-23.1318438298	-11.4837382728	5.3359566627
C	-21.0794435217	-12.8811996850	5.1638793299
C	-21.8881509475	-13.9304569511	4.7052373298
C	-23.9090149393	-12.5930504901	4.8659560707
C	-23.2978419202	-13.7939388466	4.5557384506
C	-21.1022190012	-10.5765170950	6.2601936623
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H	-24.9817960864	-12.4622858467	4.7811992145
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H	-20.0018635949	-10.5795785097	6.4128232923
O	-25.1113794114	-7.5492629703	3.9119175557
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H	-24.1904630470	-7.4844519409	4.2843318886

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H	-22.5060000000	-8.2630000000	5.4580000000
C	-24.4480000000	-7.6080000000	13.5940000000
H	-24.4550000000	-6.5190000000	13.4770000000
H	-24.0030000000	-7.8310000000	14.5710000000
N	-22.8160000000	-9.3370000000	12.6930000000
H	-22.5250000000	-9.6980000000	13.6080000000
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C	-22.3630000000	-9.7740000000	11.4800000000
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C	-23.7390000000	-8.0970000000	11.1070000000
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H	-17.5220000000	-7.3290000000	5.2610000000
H	-18.9450000000	-8.1520000000	5.9460000000
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H	-16.6690000000	-12.4660000000	6.6110000000
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C	-25.2060000000	-10.4350000000	8.0960000000
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C	-23.5470000000	-6.5040000000	7.7430000000
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C	-21.0860000000	-12.8780000000	5.1650000000
C	-21.8930000000	-13.9290000000	4.7090000000
C	-23.9150000000	-12.5930000000	4.8700000000
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H	-24.1920000000	-7.4840000000	4.2810000000

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H	-22.9396954723	-8.4582053687	5.1863348258
C	-24.5953920765	-7.7181866575	13.6129140782
H	-24.5768467752	-6.6289665789	13.4960847482
H	-24.1663035993	-7.9506040623	14.5952714050
N	-22.9621149901	-9.4590272895	12.7450355919
H	-22.6578514570	-9.7927736983	13.6658296097
C	-23.8399847429	-8.3957927598	12.5111622926
C	-22.4827861827	-9.8987979514	11.5440298172
H	-21.7793891608	-10.7039319068	11.4373111699
N	-23.0031620465	-9.1650285088	10.5468687314
C	-23.8571597112	-8.2289273259	11.1348653287
H	-24.4220055068	-7.5246028089	10.5484235293
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H	-17.4627989704	-7.3436512910	5.0401144795
H	-18.9913324355	-7.9540326631	5.7066045551
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C	-17.4190293879	-9.4252906228	5.5427672289
C	-17.1004642018	-11.5132924990	6.2363202215
H	-17.2354950108	-12.5077516522	6.6327067360
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H	-14.9669260468	-11.4808344368	5.7525698012
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H	-15.2711072010	-9.1388116827	4.9716298331
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N	-20.5273155433	-9.1574267508	9.3858663132
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C	-21.5824638152	-13.4894977201	9.0687098696
C	-22.9039289666	-13.5388123150	8.6992213425
C	-23.3861842417	-12.1732439971	8.6253363305

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C	-26.3285172016	-8.9079496114	6.9874613659
C	-25.0204082626	-8.4212004393	7.3868664722
C	-23.4819275242	-6.5761450388	7.8377379300
C	-23.2423031707	-5.1607123732	7.9349247410
C	-22.1165260091	-4.9717488051	8.6990021554
C	-21.5978296038	-6.3236238393	8.9934215732
C	-19.8519436482	-7.9831186454	9.6821676699
C	-18.4803125606	-8.3275453963	10.0444909756
C	-18.3376244557	-9.6891347428	9.8897513442
C	-19.6366757253	-10.2112863269	9.5224464156
C	-19.9513495969	-11.5725760772	9.4055288309
H	-19.1471006068	-12.2902490672	9.5322886405
C	-24.7032231815	-11.8171218896	8.3389402353
H	-25.4289946838	-12.6179092032	8.2326534483
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H	-25.2533560175	-6.4395958858	6.6734198105
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O	-22.2956821575	-16.0749011878	4.9390188991
N	-21.4786480378	-9.5854643499	6.9925337061
N	-21.4492194278	-15.1032402717	4.7808660715
C	-21.5924427461	-11.4590355266	5.5081186501
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C	-21.0717537583	-12.7303288822	5.2392313635
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C	-23.8423624161	-12.2608243898	4.8443943017
C	-23.3407110643	-13.5325474169	4.6631025397
C	-20.8660861471	-10.4478642617	6.3074271893
H	-20.0281636915	-12.9671606075	5.4189591161
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H	-23.9779895816	-14.3626040033	4.3753647415
H	-19.4905283567	-10.5386855263	6.2761933404
O	-25.3288870210	-7.3905991023	3.9714757873
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O	-22.5240866581	-6.8772861102	5.1454806043
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C	-25.0014336435	-7.2625577476	14.2565391708
H	-25.1319490844	-6.1799803327	14.1428467380
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N	-23.1907452191	-8.8419338203	13.4499736705
H	-22.8839878000	-9.2037743077	14.3572039924
C	-24.1080771222	-7.8225266119	13.1995954497
C	-22.6531126154	-9.2422124921	12.2554030919
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N	-23.1878026935	-8.5398567936	11.2518546210
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C	-18.1545740295	-8.5885713086	6.7926021038
H	-17.7140295404	-7.6515986970	7.1521565891
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C	-17.1491472132	-9.7044371333	6.8087593730
C	-16.3976097532	-11.7084555628	6.3152965622
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C	-23.0442624554	-13.1681277671	9.6018812891
C	-23.5525916556	-11.8234441215	9.4097228348
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C	-26.5386313726	-10.0727390758	7.8228011821
C	-26.4751249415	-8.8313219560	7.2385546408
C	-25.2107336323	-8.2565841723	7.6665006141
C	-23.7018069550	-6.3432956167	7.9404440328
C	-23.4485705155	-4.9233639682	7.8603087377
C	-22.3418259231	-4.6500849279	8.6246450864
C	-21.8236625359	-5.9587963357	9.0730049036
C	-20.0178217347	-7.5214086811	9.8192010738
C	-18.6209979713	-7.8135690355	10.1335736311
C	-18.4749862528	-9.1790452588	10.1435858884
C	-19.7903308992	-9.7442334657	9.9092649889
C	-20.0932744070	-11.1077537121	9.9811425075
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C	-24.8658157495	-11.5222601279	9.0345009339
H	-25.5789143146	-12.3424087079	9.0238891241
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C	-20.5584843567	-6.2396587321	9.6127045820
H	-19.87554468721	-5.4103232004	9.7638344415
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O	-20.8339391897	-16.5276629030	4.9078336907
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N	-21.3968527097	-10.4304381163	6.7627096000
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C	-21.4501416319	-12.6105894584	6.0295658292
C	-22.7781425560	-12.1231836373	6.0092755660
C	-21.1794646651	-13.9213384574	5.6105255802
C	-22.2858181487	-14.7054841928	5.2605177288
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H	-24.8864801964	-12.4962798923	5.6490799562
H	-24.4250471006	-14.8882731478	4.9637535123
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H	-22.1230090610	-7.6890784851	4.8038250285
C	-25.0340203486	-7.2386379971	14.2668789617
H	-25.1800999646	-6.1582520125	14.1513252824
H	-24.6382603319	-7.4241704051	15.2727292595
N	-23.2172872611	-8.8084072381	13.4639553175
H	-22.9112470717	-9.1716803945	14.3700657028
C	-24.1339526377	-7.7887080542	13.2127429028
C	-22.6898595441	-9.2169618742	12.2678062945
H	-21.9456254368	-9.9885838944	12.1727823747
N	-23.2296473244	-8.5184119965	11.2651567409
C	-24.1280099041	-7.6211562359	11.8369992023
H	-24.7169961997	-6.9495329629	11.2329490651
C	-18.2390776202	-8.5921484002	6.7377945058
H	-17.7721641784	-7.6777576163	7.1177953619
H	-19.1577419519	-8.7930386876	7.2904654754
N	-17.6537121791	-11.0740814166	6.5506666334
C	-17.2617723923	-9.7335955209	6.7594769180
C	-16.5401247241	-11.7729240812	6.2170754691
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N	-15.4601471837	-10.9541470442	6.2546502176

H	-14.4758055626	-11.1954565751	5.9602075928
C	-15.8860490511	-9.6790958806	6.6044080367
H	-15.2142376410	-8.8376805007	6.6155201205
Fe	-22.6920698084	-8.9029858303	9.2190755228
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C	-23.0767502602	-13.1669482523	9.6087482077
C	-23.5938831858	-11.8199780475	9.4244085060
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C	-19.8310761687	-9.7327146445	9.9240080122
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H	-25.5169669630	-6.3292155987	6.7995348253
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H	-19.8995048351	-5.4021597254	9.7454371339
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H	-20.1628114117	-14.3754505964	5.5200668872
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H	-18.8375862300	-11.4202130136	6.5736757631
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**<sup>3</sup>PC:**

C	-21.6482589783	-5.7292766530	4.9832490493
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H	-22.1329966787	-4.8816031666	5.4656125770
O	-22.5310324245	-6.8799631314	5.1378389269
H	-22.0796586014	-7.6841927890	4.7728127388
C	-24.9938176733	-7.2760383386	14.2457263389
H	-25.1139528630	-6.1925106811	14.1292791385
H	-24.5965720168	-7.4656442961	15.2503159978
N	-23.1895045436	-8.8644423843	13.4372670275
H	-22.8840953017	-9.2260794282	14.3449923409
C	-24.1072914857	-7.8448146544	13.1874506079
C	-22.6493256924	-9.2618850315	12.2424347379
H	-21.9008776636	-10.0299501847	12.1484810419
N	-23.1825943019	-8.5572072016	11.2396651269
C	-24.0897420378	-7.6682746045	11.8121906271
H	-24.6746315439	-6.9932538654	11.2081330465
C	-17.9681902705	-8.3402443920	6.8076879966
H	-17.5432617695	-7.3577709002	7.0278521551

H	-18.7961651499	-8.5390818069	7.4887612258
N	-17.2356517195	-10.7547584468	6.7687429140
C	-16.9075309074	-9.3955431546	6.8417441860
C	-16.1434613643	-11.4552498225	6.4009407571
H	-16.0874128878	-12.5149664306	6.2100917945
N	-15.1164028401	-10.5943989922	6.3053354244
H	-14.1504968192	-10.8999327635	6.0026784856
C	-15.5552701617	-9.3083785754	6.5760438907
H	-14.9202701507	-8.4478044497	6.4893216015
Fe	-22.6474293755	-8.9060091388	9.1788093300
N	-22.5056998812	-10.9021999098	9.4858790568
N	-24.4931056262	-9.1421046091	8.4425687497
N	-22.7161740133	-6.9553515050	8.6711970330
N	-20.6970791782	-8.7146208843	9.6387392347
C	-21.3673288486	-11.6408517310	9.8011884535
C	-21.7000924580	-13.0550411094	9.8679752071
C	-23.0426446872	-13.1540226891	9.5923331490
C	-23.5455683249	-11.8104719727	9.3780300929
C	-25.2808112088	-10.2768338298	8.5312566962
C	-26.5437103585	-10.0577928094	7.8351188284
C	-26.4776404613	-8.8249349058	7.2387427769
C	-25.2089981809	-8.2516169370	7.6588908741
C	-23.7000894924	-6.3389074975	7.9239146494
C	-23.4496077362	-4.9181523353	7.8489620534
C	-22.3438775886	-4.6450303879	8.6163983681
C	-21.8226947930	-5.9528116039	9.0594254692
C	-20.0112989047	-7.5127526165	9.7941251418
C	-18.6193476494	-7.8055196285	10.1192175267
C	-18.4745206135	-9.1750006333	10.1297595869
C	-19.7861286709	-9.7385429522	9.8880850218
C	-20.0945731866	-11.0991503579	9.9762644021
H	-19.2794959753	-11.7825066623	10.1972495840
C	-24.8638690837	-11.5074379261	9.0276264927
H	-25.5719842758	-12.3312758800	9.02139575960
C	-24.8230410171	-6.9487710455	7.3813460897
H	-25.4464452700	-6.3530905179	6.7263144623
C	-20.5563535864	-6.2302331333	9.5958051577
H	-19.8776204305	-5.3993681347	9.7565961836
O	-23.3885166984	-10.9036609522	6.1301513389
O	-20.9842341682	-16.5989007918	4.9497540720
O	-23.1728694530	-17.0776292929	4.6530588732
N	-19.7176861517	-11.5154620198	6.8710464315
N	-22.2300074681	-16.2490208358	4.9176793218
C	-21.8124446988	-12.7192080592	5.9779364762
C	-23.1615678178	-12.1491597008	5.9301465851
C	-21.5240660876	-14.0356416648	5.5879231505
C	-22.5638568845	-14.8884197609	5.2302882238
C	-24.2004449215	-13.1269176305	5.6267336083
C	-23.9179620109	-14.4260863842	5.2528190232
C	-20.7215856337	-11.9778093934	6.4580932003
H	-20.5079790951	-14.4151694982	5.5862992421
H	-25.2216512312	-12.7587186027	5.6151787449
H	-24.7069106297	-15.1008260812	4.9497478963
H	-18.2365114468	-11.1083837010	6.8810186048
O	-25.1055169586	-7.2979039307	4.1882677470
H	-25.0477215589	-7.7240914495	3.3034755419
H	-24.2079979008	-7.1441902129	4.5745579132

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<sup>3</sup>TS<sub>1</sub>:

C	-21.5541323402	-6.4063329663	5.0424213923
H	-20.6030024476	-6.9110195256	5.2366519744
H	-21.7124462777	-5.6395657445	5.8115890598
O	-22.6553154945	-7.3518962440	5.0325071107
H	-22.4365997907	-8.1937391667	5.5068630512
C	-24.4751169657	-7.6249036779	13.7064769162
H	-24.4670576026	-6.5323324201	13.6226851898
H	-24.0786103835	-7.8847954049	14.6953944339
N	-22.8174068099	-9.3325818733	12.8090773341
H	-22.5150022833	-9.6912715353	13.7226014095
C	-23.6914211553	-8.2635249861	12.6036317925
C	-22.3655149556	-9.7601408997	11.5875314024

H	-21.6752042230	-10.5743226385	11.4537487478
N	-22.9094526875	-9.0193721804	10.6118958350
C	-23.7364010245	-8.0835380272	11.2299111632
H	-24.3159501887	-7.3753742395	10.6605803883
C	-18.1363649297	-8.2715643849	5.2536671766
H	-17.5745833536	-7.3314018401	5.2951804310
H	-18.9857604769	-8.2034036852	5.9423513414
N	-17.7190317102	-10.6254268426	6.1945091972
C	-17.2514421850	-9.4324842099	5.6119831665
C	-16.6407231135	-11.4387921397	6.2681386404
H	-16.6396492306	-12.4461504053	6.6571353145
N	-15.5204391893	-10.8205842081	5.7667541695
H	-14.5506303331	-11.1994281224	5.6651553014
C	-15.8947753800	-9.5538290736	5.3523019016
H	-15.2170881796	-8.8870431736	4.8529431857
Fe	-22.4522831279	-9.2007262045	8.5640962073
N	-22.4175360944	-11.8752938616	8.8235970230
N	-24.4033135817	-9.3010156663	8.0393235236
N	-22.5379934885	-7.1826295825	8.3488731690
N	-20.5360844202	-9.0700207899	9.0806370691
C	-21.2882177416	-11.9899637773	9.0451832663
C	-21.6611084479	-13.3944133204	9.0304782950
C	-23.0052714445	-13.4427149510	8.7461956155
C	-23.4855141060	-12.0726593911	8.6634817201
C	-25.2197025743	-10.4155751647	8.0712873956
C	-26.4948799763	-10.1026266004	7.4308950523
C	-26.3896122102	-8.8472650090	6.8870396714
C	-25.1015973941	-8.3402489646	7.3258183985
C	-23.5635385752	-6.4824712565	7.7486896557
C	-23.3259170416	-5.0668133017	7.8632488597
C	-22.1678596477	-4.8867710638	8.5826390470
C	-21.6329117988	-6.2371990735	8.8379181996
C	-19.8673228420	-7.9050556393	9.4370611943
C	-18.5147717000	-8.2644814405	9.8552879170
C	-18.3724756813	-9.6207918214	9.6883094361
C	-19.6599387462	-10.1312787345	9.2645612423
C	-19.9950318842	-11.4903476229	9.2137356628
H	-19.1911689189	-12.2081049339	9.3353547824
C	-24.8106375068	-11.7044817179	8.4128077672
H	-25.5419163587	-12.5054861794	8.3499960723
C	-24.7050089963	-7.0240938122	7.1689958711
H	-25.3385240613	-6.3567644573	6.5999096421
C	-20.3782899659	-6.5995759869	9.3539071829
H	-19.6856560154	-5.8083621045	9.6174954201
O	-23.5614894534	-10.3841486238	5.6225230296
O	-20.0434069509	-15.4397807365	4.4292007249
O	-22.1125242788	-16.3360563023	4.3119219018
N	-21.9794043390	-9.6625409139	6.5042741645
N	-21.3185192500	-15.3349097404	4.4420872282
C	-21.6791880259	-11.7515826222	5.4383422908
C	-23.0963691129	-11.5729603211	5.2770198770
C	-21.0664602650	-12.9733971932	5.1066839429
C	-21.8997954802	-14.0180814882	4.6811832336
C	-23.9089219671	-12.6649554675	4.8677746240
C	-23.3082156186	-13.8775946085	4.5578767386
C	-21.1374177638	-10.6162976905	6.1639302864
H	-19.9972019302	-13.1296860013	5.2047879651
H	-24.9819768316	-12.5283222767	4.8053623270
H	-23.8922654482	-14.7270566914	4.2220285849
H	-20.0885837383	-10.6113459220	6.4950658201
O	-25.0789244183	-7.5327690876	3.9265567433
H	-25.0426756580	-7.9361567290	3.0295343039
H	-24.1596567203	-7.4518377057	4.3030254175

<sup>3</sup>IC:

C	-21.5369389114	-6.4093614209	5.0568174238
H	-20.5788654574	-6.8982953183	5.2519443490
H	-21.7013747640	-5.6359030758	5.8189201305
O	-22.6252633899	-7.3692538531	5.0630289060
H	-22.3834164729	-8.2177902832	5.5140568214
C	-24.4541859059	-7.6453197453	13.6452562058

H	-24.4384048307	-6.5527925278	13.5614705624
H	-24.0329829521	-7.9071058156	14.6234582005
N	-22.8070653274	-9.3495354347	12.7286957020
H	-22.5037416108	-9.7086853659	13.6417534410
C	-23.6982965418	-8.2931063379	12.5266184252
C	-22.3577355711	-9.7798072691	11.5113555158
H	-21.6561400534	-10.5830623825	11.3790020418
N	-22.9183299351	-9.0466472963	10.5351459820
C	-23.7558024405	-8.1170646326	11.1521648089
H	-24.3426015557	-7.4153100698	10.5844696637
C	-18.1148027293	-8.2566228813	5.2737181730
H	-17.5503328798	-7.3171417458	5.2985808478
H	-18.9610762675	-8.1820925645	5.9652489030
N	-17.6973909269	-10.6066517862	6.2187605453
C	-17.2297271546	-9.4160748533	5.6324294612
C	-16.6212235052	-11.4234026477	6.2869716308
H	-16.6235964578	-12.4327580284	6.6702315133
N	-15.5026835899	-10.8088379761	5.7785063358
H	-14.5356177851	-11.1921555456	5.6711832086
C	-15.8754625835	-9.5420572403	5.3645663146
H	-15.2007660800	-8.8798175098	4.8564502257
Fe	-22.4433738627	-9.2223309540	8.6004987252
N	-22.4107463569	-11.2042270561	8.8438492592
N	-24.3711904231	-9.3191737292	8.0459139831
N	-22.5328615172	-7.2045315375	8.3900584875
N	-20.5461625759	-9.0800048136	9.1563964114
C	-21.2767395080	-11.9864817056	9.0475588362
C	-21.6529312875	-13.3882944117	9.0336029107
C	-22.9960701285	-13.4349484689	8.7586088748
C	-23.4785751442	-12.0702477852	8.6851924608
C	-25.2024941807	-10.4231056567	8.0932928771
C	-26.4768667472	-10.1038718765	7.4609853175
C	-26.3569575891	-8.8603105838	6.9014714268
C	-25.0602342758	-8.3629942807	7.3172214171
C	-23.5401046387	-6.5083723107	7.7562855509
C	-23.3073818440	-5.0941743508	7.8717660561
C	-22.1618507750	-4.9084630919	8.6062862336
C	-21.6327529223	-6.2542848702	8.8823094853
C	-19.8741060879	-7.9135332534	9.4955728045
C	-18.5136492343	-8.2688286146	9.8806497909
C	-18.3673229307	-9.6231985130	9.6989868054
C	-19.6564614366	-10.1359232735	9.2923658302
C	-19.9840951407	-11.4930707669	9.2140875985
H	-19.1778587869	-12.2123951233	9.3065685615
C	-24.8033080690	-11.7093934373	8.4403116591
H	-25.5321810377	-12.5101752054	8.3658362916
C	-24.6647060027	-7.0509057994	7.1506670799
H	-25.2857042373	-6.3903009087	6.5603435968
C	-20.3816092912	-6.6086416194	9.4055838571
H	-19.6837848189	-5.8157885002	9.6449925138
O	-23.8606331520	-10.4198052713	5.5174827240
O	-20.0224003561	-15.3355432013	4.4558107307
O	-22.0596922751	-16.3092535677	4.3947586964
N	-21.7425609089	-9.5468789949	6.6938007125
N	-21.3021637351	-15.2699078061	4.4979395525
C	-21.8248940037	-11.6875724667	5.5111238572
C	-23.2730625026	-11.5432811083	5.3113621075
C	-21.1687098096	-12.8927212464	5.1558072969
C	-21.9325469931	-13.9862811218	4.7332883618
C	-24.0003590792	-12.7312304990	4.9046587920
C	-23.3557514969	-13.9113524423	4.6153293788
C	-21.1463966701	-10.6018725037	6.1781466425
H	-20.0901262108	-12.9958388327	5.2472842124
H	-25.0783976015	-12.6432082561	4.8175375310
H	-23.8957097002	-14.7936895578	4.2884968370
H	-20.0447212071	-10.6725650367	6.2849780228
O	-25.0565924963	-7.4973637453	3.9501643814
H	-25.0394796041	-7.9457749307	3.0748745343
H	-24.1364222314	-7.4609628409	4.3297803359

<sup>3</sup>TS<sub>2</sub>:

C	-21.6805697807	-6.7579614320	5.0775046243
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H	-21.6601328376	-6.0639649006	5.9282619517
O	-22.9407062135	-7.4565911122	5.0384484379
H	-22.9017950683	-8.4490052017	5.2207191721
C	-24.5986216916	-7.7368450009	13.6720222122
H	-24.5661798756	-6.6457415080	13.5814724288
H	-24.1877178140	-7.9992387589	14.6538208214
N	-22.9591091684	-9.4608553752	12.7810603961
H	-22.6362752161	-9.7924123071	13.6980724409
C	-23.8469630391	-8.4021068929	12.5630621082
C	-22.5037098228	-9.9017298254	11.5728441559
H	-21.7943040197	-10.7011757885	11.4519440208
N	-23.0560868726	-9.1765139281	10.5853968546
C	-23.8996762855	-8.2418974629	11.1873733123
H	-24.4804357068	-7.5412601499	10.6117692494
C	-18.0978207737	-8.2211053230	5.0718251882
H	-17.4491370591	-7.3403288798	5.0430259748
H	-18.9433968813	-8.0185034662	5.7340663391
N	-17.9337182803	-10.6082323490	5.9766654842
C	-17.3272244365	-9.4309990243	5.4997108433
C	-16.9463235831	-11.5348870865	6.1075048508
H	-17.0566112101	-12.5472194302	6.4644970572
N	-15.7482482591	-10.9890905893	5.7322510566
H	-14.8011604861	-11.4147332382	5.6591254253
C	-15.9734318453	-9.6719971464	5.3541112449
H	-15.1879757914	-9.0529741942	4.9582477378
Fe	-22.4228615197	-9.2996876186	8.6578126291
N	-22.3689221792	-11.2892875663	8.8225283185
N	-24.3302703250	-9.4049149373	8.0039096822
N	-22.5402011862	-7.2744907316	8.4830828730
N	-20.5736818559	-9.1662225100	9.4077686789
C	-21.2527322622	-12.0695853173	9.1096370664
C	-21.6111182203	-13.4722887545	9.0420713061
C	-22.9314552705	-13.5288122217	8.6713210569
C	-23.4165371487	-12.1657853106	8.5858906695
C	-25.1501025864	-10.5176704103	8.0176659741
C	-26.4512792839	-10.1834196566	7.4514145820
C	-26.3704655167	-8.9027547136	6.9649107554
C	-25.0640716921	-8.4152821047	7.3668516040
C	-23.5342092343	-6.5705363984	7.8372565090
C	-23.2836858634	-5.1566507422	7.9318994353
C	-22.1535748260	-4.9789405086	8.6937019980
C	-21.6448534138	-6.3313729372	8.9909656794
C	-19.8986873244	-7.9896266773	9.6876946777
C	-18.5216858857	-8.3278508353	10.0372457199
C	-18.3765054431	-9.6876860726	9.8814840629
C	-19.6743128036	-10.2121359294	9.5261697043
C	-19.9814134623	-11.5700300242	9.3889484510
H	-19.1767819942	-12.2875220546	9.5108731187
C	-24.7351793713	-11.8139929491	8.3066757500
H	-25.4579765695	-12.6180794910	8.2040044963
C	-24.6679388846	-7.0983165266	7.2330334923
H	-25.2963213515	-6.4242535923	6.6665292240
C	-20.4069347567	-6.6847302036	9.5552537912
H	-19.7147191877	-5.8853827457	9.7948510649
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C	-21.5502201548	-11.4872446726	5.5490678966
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C	-21.0779606339	-12.7752403663	5.2803378562
C	-21.9846829150	-13.7834464866	4.8989104552
C	-23.8290991760	-12.2280905664	4.9006520442
C	-23.3699315125	-13.5164039060	4.7206543891
C	-20.7268224527	-10.4637707467	6.2193215759
H	-20.0367268587	-13.0371913956	5.4364055408
H	-24.8751167375	-11.9712768197	4.7678600168

H	-24.0302530085	-14.3269497333	4.4292594514
H	-19.3497036279	-10.6013723170	6.1257837278
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H	-25.3066257090	-7.8888829254	3.1344878960
H	-24.3893112874	-7.3281410923	4.3439896397

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<sup>5</sup>RC:

C	-21.6467994071	-5.7395069251	4.9951722554
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H	-22.3543421601	-8.2637933446	5.3793850669
C	-24.4718369960	-7.6479447295	13.7284123162
H	-24.4446296969	-6.5547500485	13.6503970992
H	-24.0869842521	-7.9191698579	14.7185742268
N	-22.8415690278	-9.3814073352	12.8259637235
H	-22.5323277528	-9.7362892502	13.7393464507
C	-23.6968761708	-8.2964558839	12.6263110912
C	-22.4098814643	-9.8215650844	11.6031165064
H	-21.7342329148	-10.6471060558	11.4631029336
N	-22.9482092499	-9.0721781364	10.6308298372
C	-23.7511344515	-8.1180913655	11.2531939909
H	-24.3234376713	-7.4001507195	10.6885504505
C	-18.1261838940	-8.2524705702	5.2486409738
H	-17.5685185517	-7.3092839831	5.2757023850
H	-18.9767275077	-8.1844163706	5.9355556599
N	-17.6923967517	-10.6068877483	6.1798592771
C	-17.2324625726	-9.4055877869	5.6102801316
C	-16.6109141137	-11.4130686341	6.2574192715
H	-16.6103728274	-12.4240779261	6.6356956804
N	-15.4924230928	-10.7827735357	5.7708923702
H	-14.5236605484	-11.1631300384	5.6685748994
C	-15.8725654478	-9.5152339081	5.3617533067
H	-15.2005616009	-8.8402164730	4.8686683228
Fe	-22.4562691913	-9.1900653845	8.4865311842
N	-22.4122510498	-11.2019683581	8.7428742726
N	-24.3668163887	-9.2965482839	7.9507708788
N	-22.5487432916	-7.1771803082	8.3335325988
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C	-21.2857549004	-11.9801852257	8.9949326090
C	-21.6587886769	-13.3844381714	8.9991289157
C	-22.9979777136	-13.4391174976	8.7007289863
C	-23.4731482813	-12.0746992548	8.5785666329
C	-25.1865616878	-10.4174628006	7.9827474461
C	-26.4736631386	-10.0920689487	7.3932956950
C	-26.3764246935	-8.8327935796	6.8560693414
C	-25.0833574660	-8.3267392959	7.2674803152

C	-23.5720045574	-6.4700099250	7.7307241171
C	-23.3295613879	-5.0596647936	7.8542476880
C	-22.1704859590	-4.8844851530	8.5735617678
C	-21.6356392372	-6.2326911361	8.8208065222
C	-19.8746094963	-7.8948766192	9.4303088038
C	-18.5255164703	-8.2561020619	9.8443563447
C	-18.3874702555	-9.6147212855	9.6782096765
C	-19.6742078317	-10.1211320176	9.2612742428
C	-19.9991790415	-11.4801207224	9.1872015636
H	-19.1936528466	-12.1965628067	9.3096091953
C	-24.7933900643	-11.7080251637	8.3178041124
H	-25.5274575098	-12.5048093654	8.2442885472
C	-24.7030382604	-7.0041951236	7.1312560575
H	-25.3377081472	-6.3358231059	6.5648181576
C	-20.3824097209	-6.5880056815	9.3368278873
H	-19.6864005746	-5.7956404154	9.5859748387
O	-23.6394188068	-10.3775317269	5.5008611065
O	-20.1068792155	-15.5080638551	4.5024364887
O	-22.1875170492	-16.3723579393	4.3268605671
N	-21.4848622654	-9.5748707777	6.4695119264
N	-21.3840362873	-15.3775308005	4.4849810349
C	-21.6852040882	-11.7637902864	5.4377556733
C	-23.1223637616	-11.5405036542	5.2774816378
C	-21.1126621571	-13.0114061350	5.1101814223
C	-21.9498047645	-14.0632589588	4.7147846269
C	-23.9294965908	-12.6775969316	4.8947270266
C	-23.3638798878	-13.8999742943	4.6047205706
C	-20.9308584716	-10.6661066903	6.0148514409
H	-20.0427230313	-13.1863812209	5.1874571742
H	-24.9997548791	-12.5130336585	4.8221183042
H	-23.9653072725	-14.7438383519	4.2820035898
H	-19.8277436991	-10.7628922545	6.1047936053
O	-25.0691175925	-7.5176384998	3.9353368110
H	-25.0443334933	-7.9464422862	3.0498885228
H	-24.1493023605	-7.4730567455	4.3169473029

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<sup>5</sup>TS<sub>2F</sub>:

C	-21.7064624906	-6.6964991876	5.0721677292
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H	-21.7354974594	-5.9720364050	5.8961122620
O	-22.9485398712	-7.4333285607	5.0279933313
H	-22.8731953111	-8.4158999324	5.1925667916
C	-24.6302878870	-7.7140795471	13.7116295318
H	-24.5991051632	-6.6228996881	13.6110160063
H	-24.2458208940	-7.9659617006	14.7073834408
N	-22.9829712642	-9.4519749211	12.8572458934
H	-22.6548014089	-9.7698211877	13.7768680717
C	-23.8535875176	-8.3859457308	12.6252504907
C	-22.5316355688	-9.9101632794	11.6486498890
H	-21.8344949487	-10.7217482104	11.5369911960
N	-23.0704923632	-9.1922851423	10.6542476483
C	-23.9000334485	-8.2415146210	11.2476393455
H	-24.4769804738	-7.5441791775	10.6625573295
C	-18.1413227603	-8.2418054542	5.0806052134
H	-17.5007135102	-7.3539692374	5.0821226235
H	-18.9995014903	-8.0544141789	5.7306632821
N	-17.9491111473	-10.6246388588	6.0221926328
C	-17.3645794424	-9.4482204010	5.5120763636
C	-16.9435252175	-11.5299729218	6.1643343912
H	-17.0347061604	-12.5347019986	6.5470315312
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H	-14.8039466851	-11.3860991551	5.6889088898
C	-16.0081180630	-9.6705696907	5.3605461198
H	-15.2368927417	-9.0450283869	4.9479481528
Fe	-22.3800227745	-9.2654427764	8.5718629403
N	-22.3582698684	-11.3308873756	8.8395346821
N	-24.3685688081	-9.3898067391	7.9865875750
N	-22.5158153950	-7.1988711293	8.4759234001
N	-20.4907771149	-9.1276097672	9.4012281427
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C	-23.4065953836	-12.1919718883	8.5890413747
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C	-26.4702449314	-10.1833867339	7.4351941196
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C	-23.5383632340	-6.5145811655	7.8584429146
C	-23.2783212755	-5.1017666245	7.9474774749
C	-22.1279267270	-4.9205571831	8.6912920867
C	-21.6046179380	-6.2727265279	8.9755243221
C	-19.8250726160	-7.9522416029	9.6812158916
C	-18.4511610694	-8.3057453983	10.0590521167
C	-18.3198250748	-9.6733165799	9.9248616379
C	-19.6248005086	-10.1935438499	9.5510175934
C	-19.9657629697	-11.5559217238	9.4263161666
H	-19.1654250461	-12.2758164302	9.5730498935
C	-24.7252630194	-11.8149620672	8.2842571889
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O	-22.3755814206	-16.1473314180	4.9055676386
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C	-21.0552730169	-12.8417693118	5.2199733340
C	-21.9737223346	-13.8349592990	4.8432011704
C	-23.8159453485	-12.2717042927	4.8658350900
C	-23.3589966405	-13.5597873079	4.6739084665
C	-20.7479871337	-10.5302596250	6.1989762914
H	-20.0164992123	-13.1123260007	5.3742422598
H	-24.8631950029	-12.0134594903	4.7565097835
H	-24.0279050490	-14.3657682645	4.3892338358
H	-19.4331395193	-10.6500192137	6.2040305536
O	-25.3321291233	-7.3606087470	3.9637354897
H	-25.3029040462	-7.8486496890	3.1114844979
H	-24.4092684847	-7.2952161235	4.3418708869

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<sup>5</sup>TS<sub>1A</sub>:

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O	-22.6683879080	-7.3860206262	5.0043717527
H	-22.4227063462	-8.2680490997	5.3706509051
C	-24.4727734725	-7.6324796628	13.6828559152
H	-24.4581388339	-6.5403146916	13.5942421247
H	-24.0677529689	-7.8888545727	14.6689753217
N	-22.8348319759	-9.3581934073	12.7820331182
H	-22.5321716181	-9.7142058051	13.6960530697
C	-23.7021334828	-8.2825235974	12.5767533538
C	-22.3900719664	-9.7923867764	11.5604886498
H	-21.7059347198	-10.6115317472	11.4281454223
N	-22.9284571490	-9.0497029313	10.5837038582
C	-23.7471066762	-8.1057285570	11.2022563218
H	-24.3211860145	-7.3929409381	10.6335102013
C	-18.1335377414	-8.2676792544	5.2632603984
H	-17.5630285847	-7.3327975493	5.3020181304
H	-18.9852013392	-8.1897940887	5.9481695914
N	-17.7399614370	-10.6497943667	6.1373977023
C	-17.2573051268	-9.4340160645	5.6186959774
C	-16.6622391703	-11.4642677860	6.2174924417
H	-16.6677688555	-12.4843259052	6.5704712558
N	-15.5304679238	-10.8241890433	5.7787118871
H	-14.5581650544	-11.2013213988	5.6778564691
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Fe	-22.4263615741	-9.2045187807	8.4187773161

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N	-20.4914408058	-9.0607251489	9.1222315686
C	-21.2779756663	-12.0171715547	9.0415117389
C	-21.6528856331	-13.4249881506	9.0229410466
C	-22.9961423382	-13.4754406992	8.7182906148
C	-23.4768838035	-12.1074376503	8.6141468667
C	-25.2243205890	-10.4277769500	7.9984369021
C	-26.5116263805	-10.1067336029	7.3890889532
C	-26.4219884422	-8.8360179079	6.8690694550
C	-25.1335955801	-8.3207166219	7.3013117223
C	-23.5727405156	-6.4434837906	7.7309692343
C	-23.3281910843	-5.0297206773	7.8524416310
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C	-24.7271141208	-6.9970133315	7.1701639743
H	-25.3773306955	-6.3228084142	6.6249253885
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C	-23.1046341410	-11.5334881230	5.2734868864
C	-21.0813743826	-12.9790743412	5.1019957318
C	-21.9140270694	-14.0225703647	4.6849859862
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5IC<sub>A</sub>:

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H	-22.3442085569	-8.2548907337	5.3911059458
C	-24.4673964252	-7.6386975476	13.6876992768
H	-24.4471515468	-6.5457280979	13.6115900597
H	-24.0664182792	-7.9100725550	14.6710096032
N	-22.8321271836	-9.3608700360	12.7793039964
H	-22.5286848235	-9.7197531842	13.6925549924
C	-23.6971602142	-8.2830578663	12.5773381279
C	-22.3890179438	-9.7927895632	11.5565815522
H	-21.7075965822	-10.6137915230	11.4196363982
N	-22.9268075946	-9.0463447762	10.5820400239
C	-23.7434541908	-8.1015385630	11.2040629300
H	-24.3159880567	-7.3853424099	10.6373615214
C	-18.1769959077	-8.2857159210	5.2790267006
H	-17.6541551952	-7.3259190049	5.3582889933
H	-19.0489240884	-8.2694377999	5.9412102520
N	-17.7322882047	-10.6519625024	6.1468050276
C	-17.2690557988	-9.4301987120	5.6246839709
C	-16.6438595233	-11.4506127724	6.2275571116

H	-16.6342575698	-12.4659755771	6.5945384711
N	-15.5217398330	-10.7977295490	5.7837329072
H	-14.5471469341	-11.1698447574	5.6828905426
C	-15.9030464334	-9.5211367743	5.4035434620
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Fe	-22.4267528575	-9.2054024660	8.4192996161
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C	-21.6540307296	-13.4258660234	9.0214120002
C	-22.9971600520	-13.4770818798	8.7176576066
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C	-25.2259968776	-10.4297514822	7.9987462704
C	-26.5135539240	-10.1096029149	7.3887852862
C	-26.4234028899	-8.8386519574	6.8689747061
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C	-23.5737203639	-6.4449888363	7.7304986207
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C	-22.1600023093	-4.8536071529	8.5604950097
C	-21.6139319739	-6.2050567557	8.8009478914
C	-19.8296629997	-7.8904652174	9.4462326360
C	-18.4744846049	-8.2523179566	9.8719623311
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C	-19.6327604075	-10.1296301745	9.3030997627
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C	-21.0088991713	-10.6499723838	6.0915636912
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H	-23.9317298037	-14.7239754452	4.2706165474
H	-19.9037519049	-10.6918207149	6.2387250014
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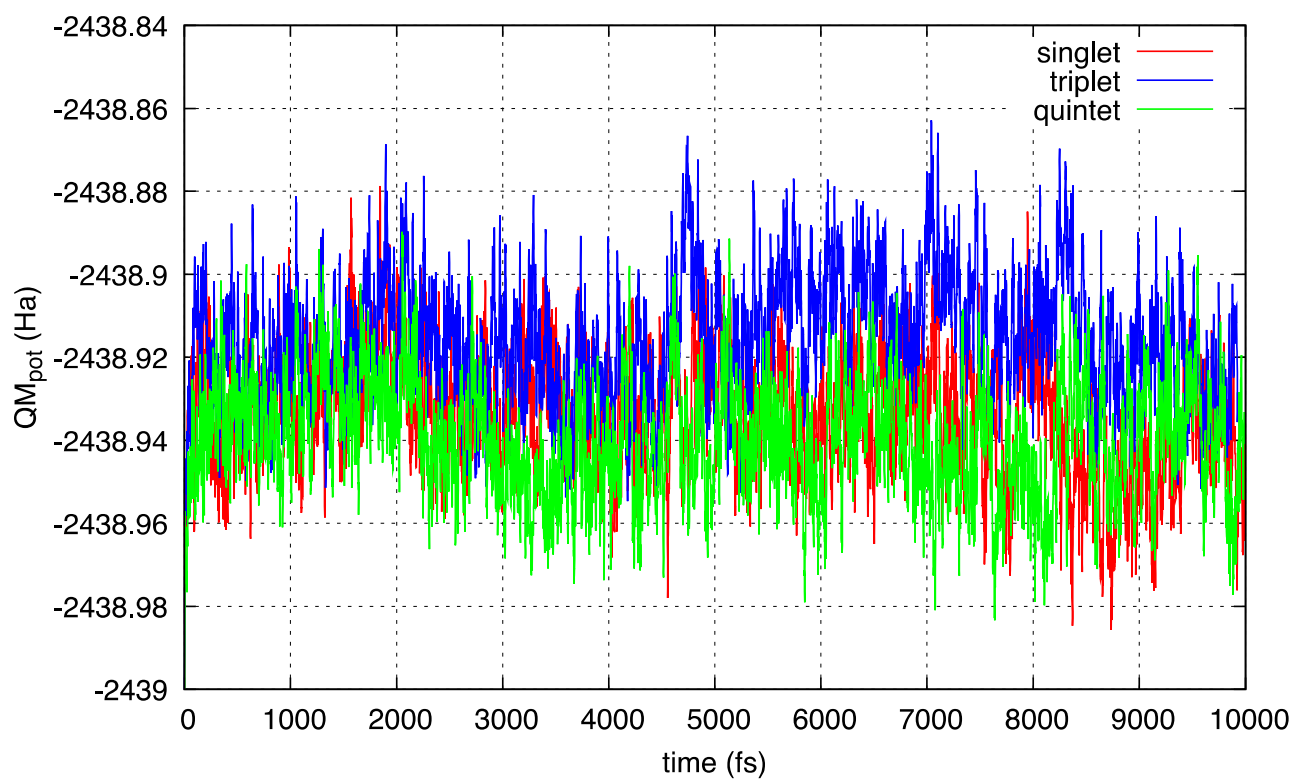
5TS<sub>2A</sub>:

C	-21.7058725590	-6.6962916353	5.0717281496
H	-20.8629248153	-7.3715087103	5.2279922951
H	-21.7344604836	-5.9727607233	5.8962159477
O	-22.9487950278	-7.4330085153	5.0274069594
H	-22.8729842585	-8.4157686378	5.1925893997
C	-24.6302549771	-7.7134019199	13.7131456363
H	-24.5995317070	-6.6223718145	13.6121209445
H	-24.2467368051	-7.9652297584	14.7085605672
N	-22.9834448440	-9.4518800414	12.8588067232
H	-22.6554051825	-9.7698289973	13.7787430650
C	-23.8536132646	-8.3853589572	12.6266892168
C	-22.5325600885	-9.9102210806	11.6506346926
H	-21.8352214814	-10.7225719179	11.5388335704
N	-23.0702628952	-9.1920349084	10.6557172989
C	-23.8995327314	-8.2413481879	11.2495459021
H	-24.4761941249	-7.5432376989	10.6644996922

C	-18.1415612944	-8.2422839784	5.0813018776
H	-17.5015946032	-7.3541904765	5.0824585238
H	-19.0004644059	-8.0544905408	5.7312420332
N	-17.9488959113	-10.6251480553	6.0228846380
C	-17.3651561683	-9.4481962881	5.5125629463
C	-16.9434207300	-11.5298858440	6.1647183948
H	-17.0340946919	-12.5348323318	6.5477201624
N	-15.7568490867	-10.9736030595	5.7662687405
H	-14.8035357015	-11.3854029523	5.6888666170
C	-16.0082340444	-9.6706852096	5.3611405764
H	-15.2374613384	-9.0446446885	4.9479310765
Fe	-22.3798950122	-9.2648254667	8.5709106595
N	-22.3580910813	-11.3312029097	8.8397092808
N	-24.3695272200	-9.3895218378	7.9873299273
N	-22.5158930887	-7.1985397132	8.4756782317
N	-20.4904188409	-9.1276475861	9.4001702230
C	-21.2361493577	-12.0870148477	9.1350245900
C	-21.5921844761	-13.4971941426	9.0599665254
C	-22.9180600210	-13.5560922594	8.6839647270
C	-23.4070556151	-12.1920521970	8.5888501986
C	-25.1621830908	-10.5178663482	7.9921415604
C	-26.4701616942	-10.1829612937	7.4350873704
C	-26.4053584237	-8.8897741074	6.9704754330
C	-25.1024885547	-8.3867367151	7.3847900295
C	-23.5382687028	-6.5146289922	7.8581788882
C	-23.2779584216	-5.1016318511	7.9471297813
C	-22.1278856195	-4.9207342590	8.6907331300
C	-21.6046632658	-6.2727799641	8.9754627902
C	-19.8246678601	-7.9518185455	9.6804959672
C	-18.4509116819	-8.3058273852	10.0588842269
C	-18.3198855125	-9.6729114813	9.9250286536
C	-19.6248156014	-10.1937033468	9.5506681293
C	-19.9660519365	-11.5558636864	9.4259972882
H	-19.1652438278	-12.2758184552	9.5732815843
C	-24.7249787452	-11.8148574752	8.2837780007
H	-25.4468737897	-12.6199216599	8.1723091861
C	-24.6944839419	-7.0615014074	7.2877866210
H	-25.3477465837	-6.3782938499	6.7582066172
C	-20.3546923307	-6.6477428795	9.5293544659
H	-19.6609084889	-5.8458369254	9.7637605413
O	-23.3486814545	-9.9926649481	5.3952059810
O	-20.2479162403	-15.4081294685	4.6882516273
O	-22.3762245770	-16.1474192399	4.9054312580
N	-21.2869933894	-9.5481361749	6.7822031849
N	-21.5080121673	-15.1947537352	4.7785497258
C	-21.5234470698	-11.5527482293	5.4857507907
C	-22.9241877490	-11.2015517207	5.2353123940
C	-21.0544066267	-12.8427527631	5.2187356398
C	-21.9734979225	-13.8354878266	4.8417859875
C	-23.8153466028	-12.2720156317	4.8647548238
C	-23.3584901030	-13.5600650062	4.6726144887
C	-20.7483796577	-10.5306953025	6.1984779534
H	-20.0154840803	-13.1129909151	5.3727969948
H	-24.8624032034	-12.0131023912	4.7559538395
H	-24.0276253068	-14.3659335636	4.3876833467
H	-19.4350313053	-10.6504449424	6.2053197436
O	-25.3320516962	-7.3611270052	3.9641689724
H	-25.3029773381	-7.8489566590	3.1112201569
H	-24.4090229745	-7.2949201949	4.3419967684



**Figure S1.** Time dependent evolution of the QM potential energy of the reactant states at the three electronic states  $^1\text{RC}$ ,  $^3\text{RC}$  and  $^5\text{RC}$  along the 10 ps of QM/MM MD simulation (Lan12DZ basis set).



**Table S2.** Gibbs free energies (in kcal/mol) for the different states localized and optimized at B3LYP(LanL2DZ)/MM level along the two reaction mechanism in the three different electronic states.

	RC	TS <sub>1</sub>	IC	TS <sub>2</sub>	TS	PC
Singlet	0.0	23.5	19.6	21.5	13.4	-17.3
Triplet	14.3	36.2	28.7	38.8	30.1	-10.1
Quintet-F (ferromagnetic coupling)	3.8	18.7	11.8	9.1	14.6	-34.3
Quintet-A (antiferromagnetic coupling)	3.8	15.4	10.7	8.9	14.6	-34.3

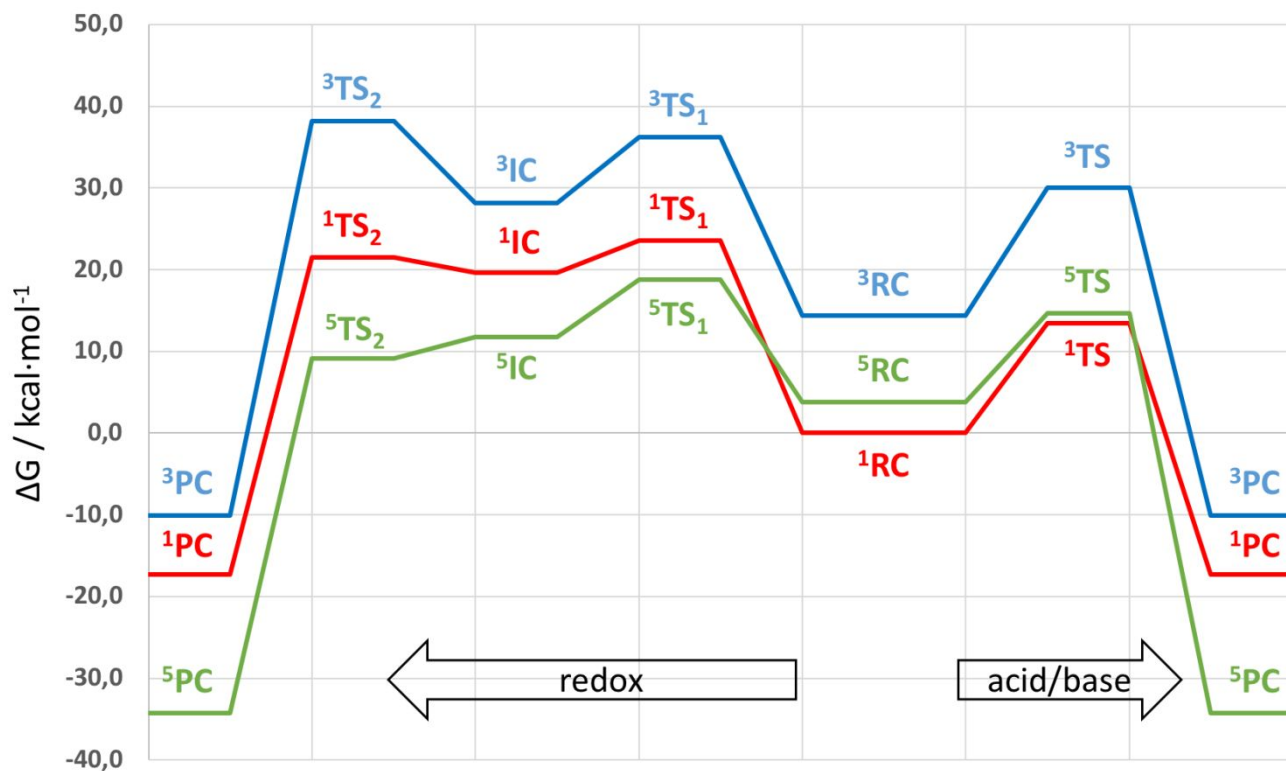
Gibbs free energies (in kcal/mol) considering each reactant species as the base line (LanL2DZ basis set).

	RC	TS <sub>1</sub>	IC	TS <sub>2</sub>	TS	PC
Singlet	0.0	23.5	19.6	21.5	13.4	-17.3
Triplet	0.0	21.8	14.4	24.4	15.7	-24.4
Quintet-F (ferromagnetic coupling)	0.0	15.0	8.0	5.3	10.9	-38.1
Quintet-A (antiferromagnetic coupling)	0.0	11.7	7.0	5.1	10.9	-38.1

Gibbs free energies (in kcal/mol) considering each reactant species as the base line (single point energy calculations using the Def2-TZVP basis set).

	RC	TS <sub>1</sub>	IC	TS <sub>2</sub>	TS	PC
Singlet	0.0	27.7	23.8	28.4	24.8	-17.5
Triplet	0.0	29.8	26.0	32.9	23.9	-22.0
Quintet-F (ferromagnetic coupling)	0.0	32.6	15.4	14.9	19.9	-32.3
Quintet-A (antiferromagnetic coupling)	0.0	10.8	6.0	6.6	19.9	-32.3

**Figure S2.** B3LYP(LanI2DZ)/MM free energy profiles for the redox Kemp elimination in the singlet (red line), triplet (blue line) and quintet states (green line), catalysed by the promiscuous OxDa enzyme by means of two different mechanisms starting from the same reactant complex (RC): acid/base (from RC to the right) and redox (from RC to the left).



## Computational Details:

### Linear response approximation (LRA) data

Averages and root mean square deviations of the potential energy (in kcal/mol) for each reactant at different spin states. The  $\langle \rangle_x$  denotes that the averages have been carried out using the geometrical data for this spin state.

Molecular dynamics using the Lanl2DZ basis set:

$\langle 1 \rangle_1$  -1739484.85 ±164.26  
 $\langle 1 \rangle_3$  -1739486.86 ±171.98  
 $\langle 1 \rangle_5$  -1739523.66 ±163.39  
 $\langle 3 \rangle_1$  -1739466.21 ±163.39  
 $\langle 3 \rangle_3$  -1739476.81 ±172.35  
 $\langle 5 \rangle_1$  -1739470.65 ±161.70  
 $\langle 5 \rangle_5$  -1739529.85 ±163.76

$$\Delta F_{\text{LRA}}(1 \rightarrow 3) = 14.34 \pm 0.59$$

$$\Delta F_{\text{LRA}}(1 \rightarrow 5) = 3.76 \pm 0.56$$

Single point energy calculations using the Def2-TZVP basis set:

$\langle 1 \rangle_1$  -2246774.84 ±161.8  
 $\langle 5 \rangle_1$  -2246762.49 ±176.8  
 $\langle 1 \rangle_5$  -2246774.61 ±175.1  
 $\langle 5 \rangle_5$  -2246781.44 ±164.0

$$\Delta F_{\text{LRA}}(1 \rightarrow 5) = 2.76 \pm 0.62$$

The error of the free energy differences has been evaluated by means a first order expansion [eqs 20 and 21 of ref 44 of the manuscript]:

$$\varepsilon(\Delta F_{i \rightarrow j}) \approx \pm RT \frac{\delta \varepsilon}{\left\langle e^{-\frac{U_j - U_i}{RT}} \right\rangle_i} \quad \delta \varepsilon^2 = \frac{1 + 2\tau}{N} \left( \left\langle e^{-2\frac{U_j - U_i}{RT}} \right\rangle_i - \left\langle e^{-\frac{U_j - U_i}{RT}} \right\rangle_i^2 \right)$$
$$1 + 2\tau = \frac{1 + r_1}{1 - r_1} \quad r_1 = \frac{\sum (x_i - \bar{x})(x_{i-1} - \bar{x})}{\sum (x_i - \bar{x})^2}$$

**Table S3.** Second order perturbation theory analysis results (in kcal/mol) of the different states located along the two reaction mechanisms at the three different electronic states (Lan12DZ basis set).

	singlet						triplet					
	<sup>1</sup> RC	<sup>1</sup> TS <sub>1</sub>	<sup>1</sup> IC	<sup>1</sup> TS <sub>2</sub>	<sup>1</sup> TS	<sup>1</sup> PC	<sup>3</sup> RC	<sup>3</sup> TS <sub>1</sub>	<sup>3</sup> IC	<sup>3</sup> TS <sub>2</sub>	<sup>3</sup> TS	<sup>3</sup> PC
LP(Fe28):BD*(O57-N60)	0.8	2.1	2.0	0.0	0.0	0.0	0.1	1.5	0.0	0.0	0.0	0.0
BD(O57-N60):BD*(C68-H72)	3.3	2.7	2.5	0.0	3.9	0.0	3.4	2.9	0.0	0.0	2.9	0.0
LP(N60):RY*(Fe28)	0.2	0.6	0.6	0.4	0.3	1.0	0.0	0.1	0.4	0.2	0.0	0.0
BD(C68-H72):BD*(O57-N60)	7.5	6.8	6.9	0.0	25.9	0.0	7.8	5.2	0.0	0.0	30.6	0.0
LP(Fe28):RY*(N60)	1.0	3.1	3.1	3.0	0.2	0.1	0.5	1.3	2.0	1.2	0.0	0.0
BD(O57-N60):RY*(Fe28)	0.5	0.0	0.0	0.0	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0
LP(N60):BD*(C68-H72)	0.0	0.5	0.6	0.3	0.0	0.0	0.5	0.5	7.2	1.0	0.0	0.0
BD(O57-N60):LP*(Fe28)	5.4	3.1	3.0	0.0	3.5	0.0	2.2	2.0	0.0	0.0	1.1	0.0
BD(C68-H72):RY*(N60)	0.8	1.8	1.8	1.0	1.3	0.0	0.8	1.2	1.5	2.0	1.4	0.0
CR(N60):LP*(Fe28)	8.3	18.2	17.8	18.2	3.5	1.3	2.7	10.2	10.2	8.5	0.6	0.0
LP(N60):LP*(Fe28)	56.8	139.6	127.2	158.0	29.0	11.9	19.3	69.0	82.5	73.8	7.6	0.0
CR(Fe28):LP*(N60)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.4	0.0	0.0
CR(Fe28):RY*(N60)	0.4	2.1	2.1	2.4	0.0	0.0	0.0	0.4	1.1	0.7	0.0	0.0
CR(Fe28):BD*(O57-N60)	0.2	0.2	0.2	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0
CR(N60):RY*(Fe28)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LP(Fe28):LP*(N60)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.3	0.3	0.0	0.0
BD(C68-H72):LP*(N60)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	9.6	31.2	0.0	0.0

	quintet-F (ferromagnetic)						quintet-A (antiferromagnetic)					
	<sup>5</sup> RC	<sup>5</sup> TS <sub>1</sub>	<sup>5</sup> IC	<sup>5</sup> TS <sub>2</sub>	<sup>5</sup> TS	<sup>5</sup> PC	<sup>5</sup> RC	<sup>5</sup> TS <sub>1</sub>	<sup>5</sup> IC	<sup>5</sup> TS <sub>2</sub>	<sup>5</sup> TS	<sup>5</sup> PC
LP(Fe28):BD*(O57-N60)	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.7	1.2			
BD(O57-N60):BD*(C68-H72)	3.5	1.5	0.0	0.0	3.0	0.0	2.5	2.6	0.9			
LP(N60):RY*(Fe28)	0.0	0.7	0.8	0.7	0.0	0.1	0.4	0.3	0.2			
BD(C68-H72):BD*(O57-N60)	7.9	7.6	0.0	0.0	30.1	0.0	7.1	6.9	17.9			
LP(Fe28):RY*(N60)	0.4	1.4	1.4	2.0	0.0	0.1	2.6	2.6	2.1			
BD(O57-N60):RY*(Fe28)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2			
LP(N60):BD*(C68-H72)	0.0	7.1	7.4	8.6	0.0	0.0	0.3	0.3	0.0			
BD(O57-N60):LP*(Fe28)	1.8	5.3	0.0	0.0	1.0	0.0	3.2	3.1	2.5			
BD(C68-H72):RY*(N60)	0.8	1.6	1.6	1.9	1.4	0.0	1.5	1.5	2.1			
CR(N60):LP*(Fe28)	2.0	7.2	8.5	10.7	0.6	0.3	12.3	12.1	10.7			
LP(N60):LP*(Fe28)	16.2	69.2	82.8	111.5	7.7	3.7	99.5	97.3	93.4			
CR(Fe28):LP*(N60)	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0			
CR(Fe28):RY*(N60)	0.0	0.3	0.4	0.5	0.0	0.0	0.8	0.8	0.3			
CR(Fe28):BD*(O57-N60)	0.0	0.1	0.0	0.0	0.0	0.0	0.1	0.1	0.8			
CR(N60):RY*(Fe28)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			
LP(Fe28):LP*(N60)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			
BD(C68-H72):LP*(N60)	0.0	0.0	9.8	23.0	0.0	0.0	0.0	0.0	0.0			

**Table S4.** Second order perturbation theory analysis results (in kcal/mol) of the different states located along the two reaction mechanisms at the different electronic states (single point energy calculations using the Def2-TZVP basis set).

	singlet						quintet-F (ferromagnetic)						quintet-A (antiferromagnetic)					
	<sup>1</sup> RC	<sup>1</sup> TS <sub>1</sub>	<sup>1</sup> IC	<sup>1</sup> TS <sub>2</sub>	<sup>1</sup> TS	<sup>1</sup> PC	<sup>5</sup> RC	<sup>5</sup> TS <sub>1</sub>	<sup>5</sup> IC	<sup>5</sup> TS <sub>2</sub>	<sup>5</sup> TS	<sup>5</sup> PC	<sup>5</sup> RC	<sup>5</sup> TS <sub>1</sub>	<sup>5</sup> IC	<sup>5</sup> TS <sub>2</sub>	<sup>5</sup> TS	<sup>5</sup> PC
LP(Fe28):BD*(O57-N60)	0.8	2.8	2.6	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.7	0.7	0.0			
BD(O57-N60):BD*(C68-H72)	3.8	2.8	2.6	0.0	4.1	0.0	3.9	2.0	0.0	0.0	3.3	0.0	2.5	2.7	0.0			
LP(N60):RY*(Fe28)	0.9	1.1	1.1	1.2	1.0	0.0	0.7	0.9	1.1	1.8	0.9	0.0	1.5	1.5	1.2			
BD(C68-H72):BD*(O57-N60)	6.3	6.5	6.6	0.0	23.2	0.0	6.5	7.1	0.0	0.0	27.2	0.0	6.8	6.6	0.0			
LP(Fe28):RY*(N60)	4.0	10.5	10.5	9.6	1.2	0.6	5.3	13.5	13.4	18.4	2.4	1.3	23.7	23.4	22.1			
BD(O57-N60):RY*(Fe28)	1.6	0.1	0.1	0.0	1.2	0.0	1.0	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.0			
LP(N60):BD*(C68-H72)	0.0	0.7	0.8	0.5	0.0	0.0	0.0	8.6	8.4	9.1	0.0	0.0	0.6	0.6	0.3			
BD(O57-N60):LP*(Fe28)	2.0	1.9	1.9	0.0	1.0	0.0	0.9	2.9	0.0	0.0	0.5	0.0	2.2	2.1	0.0			
BD(C68-H72):RY*(N60)	0.8	1.5	1.5	0.9	1.3	0.0	0.7	1.1	1.4	1.5	1.6	0.0	1.5	1.5	0.9			
CR(N60):LP*(Fe28)	6.2	12.3	12.0	21.2	1.2	0.1	0.8	5.3	6.6	10.5	0.1	0.0	7.5	7.2	8.6			
LP(N60):LP*(Fe28)	62.6	88.1	86.5	174.6	21.8	4.7	11.8	70.8	91.0	153.9	3.5	0.9	83.6	80.5	97.1			
CR(Fe28):LP*(N60)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.3	0.0	0.0	0.0	0.0	0.0			
CR(Fe28):RY*(N60)	0.1	0.6	0.4	0.6	0.0	0.0	0.0	0.1	0.1	0.1	0.0	0.0	0.1	0.2	0.1			
CR(Fe28):BD*(O57-N60)	0.3	0.4	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.0			
CR(N60):RY*(Fe28)	0.1	0.1	0.1	0.1	0.0	0.0	0.0	0.3	0.3	0.4	0.0	0.0	0.5	0.5	0.4			
LP(Fe28):LP*(N60)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			
BD(C68-H72):LP*(N60)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	9.2	22.0	0.0	0.0	0.0	0.0	0.0			

### Intramolecular proton transfer:

The intramolecular proton transfer between C<sub>68</sub> and O<sub>57</sub> was studied for the quintet-A (antiferromagnetic coupling) state at the B3LYP(LanI2DZ)/MM level. Starting from the intermediate compound, a nudged elastic band calculation was performed until reaching the species where the H<sub>72</sub> was finally bonded to O<sub>57</sub>, as shown in the Figure S2 and Table S5.

**Figure S3.** Single point energy calculations using the Def2-TZVP basis set on the B3LYP(LanI2DZ)/MM potential energy surface (in kcal/mol) for the internal proton transfer in the quintet-A (antiferromagnetic coupling) state.

