

Supplementary Information to:

An Investigation of Possible Competing Mechanisms for Ni-containing Methyl-Coenzyme M Reductase

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1. Supplementary figures and table

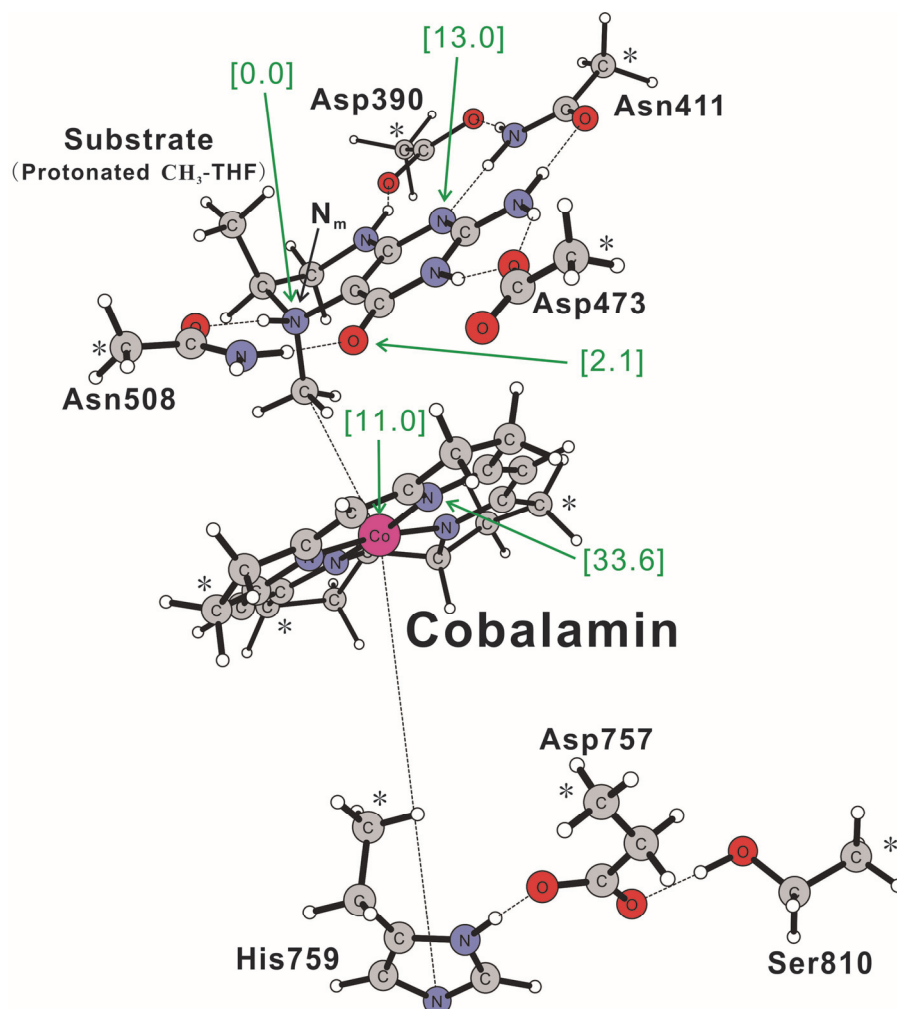
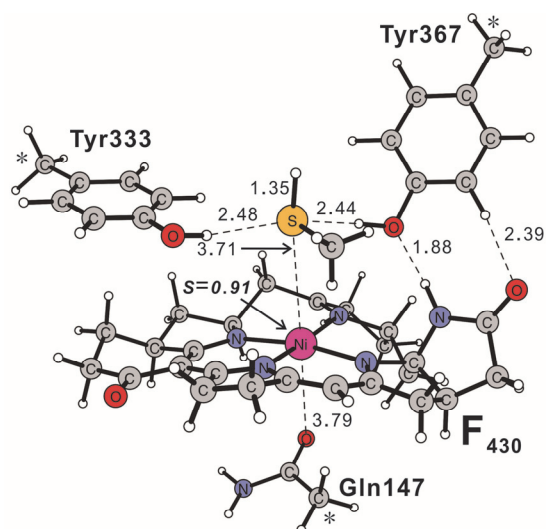
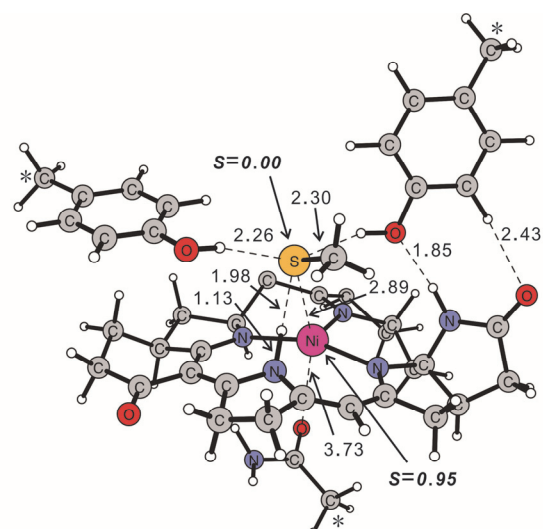


Fig. S1 Optimized structure of the Michaelis complex in cobalamin-dependent methionine synthase (MetH) with a protonated methyl-tetrahydrofolate substrate ($\text{CH}_3\text{-THF}$) bound. This model is the same as the one used in the previous study [S1]. The green arrows indicate the possible positions where a proton is bound and the relative energies (in kcal/mol) for the corresponding protonation states are given in brackets. N_m : the methyl-bound nitrogen of the substrate. Energies are calculated using the same method as employed in the previous study [S1], i.e. using the B3LYP-15% functional including ZPE and solvation effects.

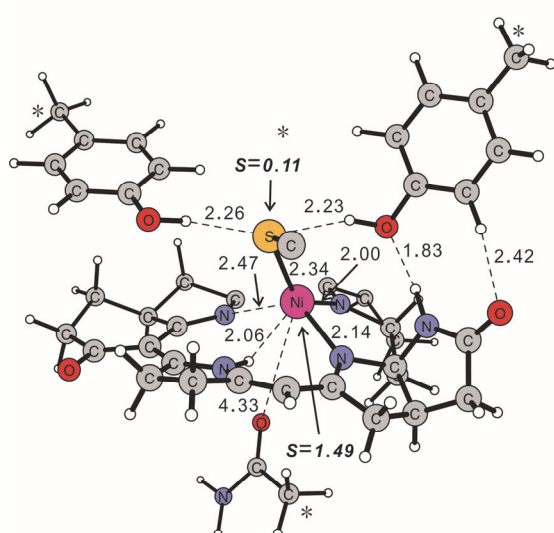
[S1] S. -L. Chen, M. R. A. Blomberg and P. E. M. Siegbahn, *J. Phys. Chem. B*, 2011, **115**, 4066-4077.



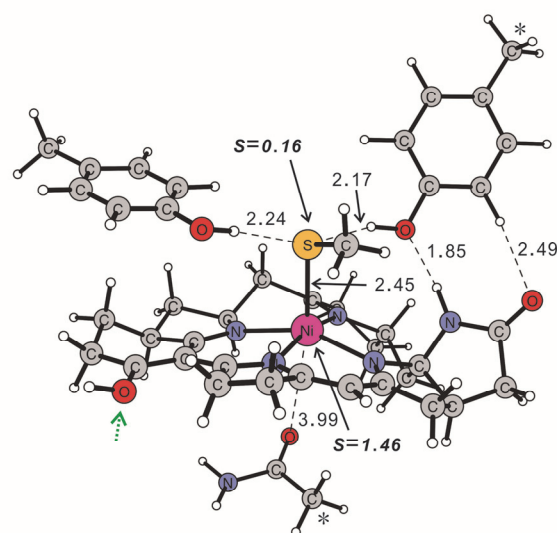
MCR-CoM-SH
(complex 1)
[4.4]



CoMS⁻-Protonated MCR
(complex 2)
[22.3]



CoMS⁻-Protonated MCR
(complex 3)
[18.9]



CoMS⁻-Protonated MCR
(complex 4)
[11.4]

Fig. S2 Optimized structures of several possible complexes of the MCR_{redI} with HSCoM added. For clarity, the methyl hydrogens of CoMS⁻ in **complex 3** are omitted. The relative energies with the B3LYP functional (kcal/mol) are given in the brackets, with **complex H** of Fig. 2 (in the text) as the energy reference. The B3LYP-15% energies of complexes 1-4 are 5.0, 22.0, 19.7, and 13.0 kcal/mol, respectively.

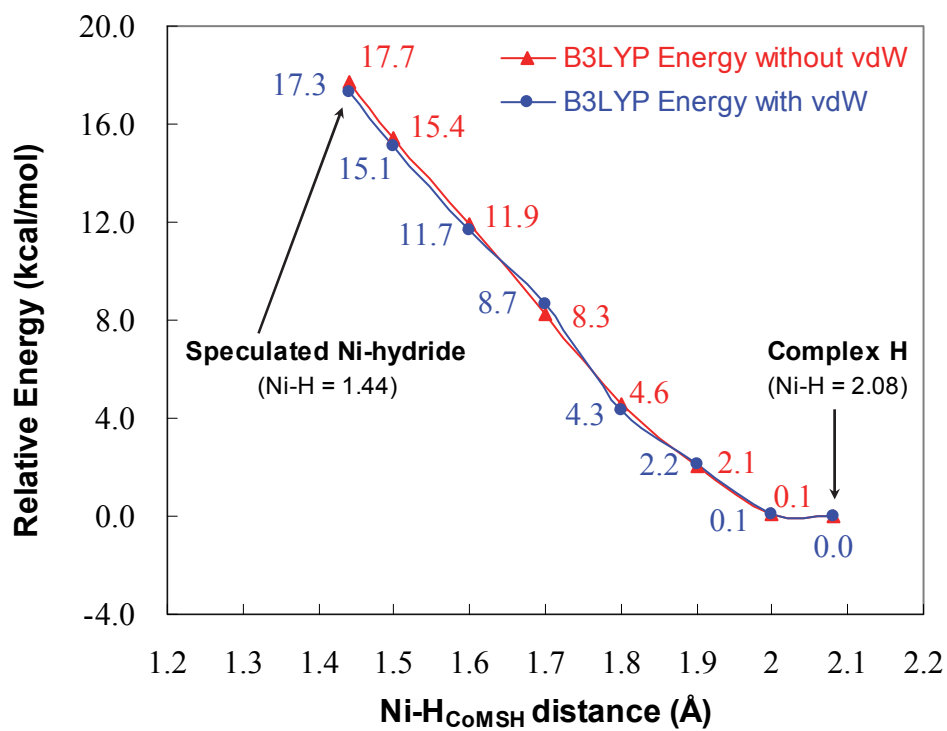


Fig. S3 Potential energy profile for the H transfer from CoM-SH to Ni. The Ni-S distance is fixed to 3.45 Å (the distance in **complex H**). vdW: dispersion correction.

Table S1 Energies for the methyl-Ni(F₄₃₀) formation assuming a protonated CH₃-S-CH₃ as substrate.

Entry	Complex	Energy (kcal/mol)
1	MCR _{red1} with a protonated CH ₃ -S-CH ₃	0.0
2	Transition state for methyl transfer	3.1
3	Methyl-Ni(F ₄₃₀) with a HS-CH ₃	-10.3

2. Cartesian coordinates of all optimized structures

The abbreviations used here are consistent with those in the text.

The MCR active site with a proton bound at position 1 (Fig. 1)

C	5.86195400	4.79089800	2.49137800
C	5.12279400	4.15291600	1.33281600
C	5.80488400	3.77156600	0.16092000
C	3.73519600	3.94248100	1.37714800
C	5.13277200	3.20787700	-0.92466300
C	3.04537300	3.37506700	0.29776700
C	3.74728400	3.00868900	-0.85810600
O	3.14194600	2.43536600	-1.96913600
C	-6.96625300	5.24580400	1.49108800
C	-5.92989200	4.17435600	1.25032300
C	-6.28068300	2.98701000	0.58115600
C	-4.59892000	4.33472400	1.66209300
C	-5.34263700	1.98978500	0.32037700
C	-3.63841100	3.34647100	1.41037100
C	-4.02289900	2.18481300	0.74090100
O	-3.11463700	1.15270700	0.44811900
C	0.57364000	-5.71753100	0.53622000
C	1.34547500	-4.93152800	1.57909800
O	0.78176300	-4.35933900	2.54285100
N	2.69676400	-4.86216400	1.39170400
Ni	0.07985100	-1.38998800	0.08016000
N	-1.14616000	-1.02941500	1.83221500
C	0.63364700	0.13910800	3.02485300
C	-0.62541000	-0.65778300	2.96548900
C	-1.30293600	-1.24704700	4.19117200
C	-2.14416700	-2.36570000	3.53043100
C	-2.38530300	-1.83890900	2.14300400
N	-1.55191800	-2.17214100	-0.81741000
C	-2.65178900	-2.98997100	1.22037500
C	-2.86538300	-2.54507200	-0.19407500
C	-3.51576700	-3.64975200	-1.06568700
C	-2.79222000	-3.41566500	-2.37754800
C	-1.56252000	-2.62004600	-2.06262300
N	-3.83802000	-1.45220800	-0.32359600
C	-5.05838800	-1.81377600	-0.81794300
O	-6.03484200	-1.05264300	-0.99522800

C	5.88238889	5.17280994	1.67559593
C	4.51276153	4.82449961	1.12891588
C	4.35246705	4.40758193	-0.20216152
C	3.36608341	4.87381434	1.93013501
C	3.11156524	4.02427962	-0.70680294
C	2.11229093	4.49402539	1.44106994
C	1.98835198	4.05297498	0.12289351
O	0.78741938	3.62620324	-0.40527629
C	-6.92859594	5.69123696	0.50074800
C	-5.59280503	4.98247498	0.45885940
C	-5.44932171	3.79386007	-0.26943325
C	-4.46957617	5.47279700	1.13882619
C	-4.23526008	3.11216641	-0.32150303
C	-3.24405201	4.79948714	1.10570964
C	-3.14305449	3.61934652	0.37799350
O	-1.88193496	2.96935723	0.28371604
C	0.43459500	-5.41813798	1.06786902
C	0.87691250	-4.57416191	2.25301788
O	0.28225292	-3.55062203	2.58851371
N	1.97902327	-5.01726532	2.91845720
Ni	0.02910562	-1.16498447	0.02534685
N	-1.33916749	-0.40553417	1.72867100
C	0.57845932	0.70781066	2.77328493
C	-0.70557693	-0.05752382	2.79909465
C	-1.29538322	-0.57775408	4.09202075
C	-2.24938901	-1.65967704	3.56921601
C	-2.55942388	-1.16634995	2.14775172
N	-1.56763669	-2.03477398	-0.80177399
C	-2.97118398	-2.29016519	1.20571412
C	-2.94360285	-1.92681044	-0.27971947
C	-3.86694657	-2.82690070	-1.17980947
C	-2.87050788	-3.46771583	-2.15545200
C	-1.54463034	-2.84352658	-1.83777089
N	-3.43873919	-0.57312559	-0.55342303
C	-4.29810724	-0.48035138	-1.60695735
O	-4.54951186	0.54567165	-2.23811267
C	-4.88330147	-1.86615807	-1.83471440
N	1.23550584	-1.80952813	-1.54902163
C	-0.44470593	-3.16167145	-2.66388183
C	0.81905011	-2.65395582	-2.54115326
C	1.93320929	-2.97892972	-3.50365915
C	2.95329595	-1.89466701	-3.16348991
C	2.51544584	-1.43003734	-1.79317752
N	1.70223898	-0.54616850	0.95273265

C	3.34008728	-0.77378186	-0.87418933
C	2.92733396	-0.52728997	0.48271057
C	3.97589133	-0.23543666	1.54988376
C	3.11908899	0.36668497	2.66043595
C	1.73424937	-0.24029007	2.39942180
C	5.13125441	0.61728985	1.03000933
C	5.73835910	-0.05076215	-0.20418283
C	4.70867373	-0.37439022	-1.28690646
O	5.04973736	-0.30788163	-2.46669440
H	6.47157903	5.74258673	0.94841858
H	5.80853225	5.77012484	2.59005867
H	5.21819639	4.37800022	-0.86033856
H	3.44648912	5.21302376	2.96059688
H	3.00734648	3.70302378	-1.73937590
H	1.23669140	4.54509940	2.08657213
H	0.07013461	3.70708361	0.24822880
H	-7.36047789	5.78456149	-0.50200239
H	-6.83833927	6.69605825	0.92444190
H	-6.29822438	3.39170363	-0.81774049
H	-4.54751516	6.39705846	1.70613704
H	-4.15984881	2.20691455	-0.91776966
H	-2.37969029	5.18986787	1.63575060
H	-1.89462322	2.11490442	0.75687535
H	0.38486900	-4.77656559	0.18253921
H	-0.57423093	-5.79766550	1.26178064
H	2.43615246	-5.88758357	2.69249210
H	2.27292087	-4.52395957	3.75051690
H	0.55203668	1.52060970	2.03850227
H	0.77110782	1.14231769	3.76128335
H	-3.14873512	-1.78419728	4.18038338
H	-3.37733634	-0.42952019	2.16993886
H	-2.31163853	-3.15284606	1.34900610
H	-3.98678848	-2.59502451	1.48939407
H	-3.14019733	-3.30494003	-3.20679540
H	-5.04317814	-2.04228524	-2.90181527
H	-5.86603652	-1.90909301	-1.34950664
H	-0.63630313	-3.84348759	-3.48697168
H	2.33330322	-3.97985943	-3.28915850
H	2.90900719	-1.05490865	-3.86888399
H	4.38287478	-1.20853976	1.87448118
H	3.07578105	1.45845596	2.54263173
H	1.60868613	-1.18644877	2.94560577
H	5.89031676	0.75042111	1.81089162
H	4.75848936	1.61702396	0.76991053

H	6.21160597	-1.00227700	0.08632624
H	6.51830120	0.55990130	-0.66818487
H	1.09469874	-6.26558211	0.86063839
H	1.60332982	-2.98074898	-4.54696726
H	3.99074774	-2.22719893	-3.18457128
H	3.49029379	0.15489448	3.66847843
H	-0.52198157	-0.94967522	4.77341725
H	-1.81560372	0.23986259	4.61550911
H	-1.71947807	-2.61437297	3.51318728
H	-2.81500097	-4.55668299	-2.02801476
H	-4.37205950	-3.58422290	-0.57699983
H	-7.64974590	5.13606242	1.11377412
H	6.45515867	4.26813989	1.91869482
C	0.07785415	1.31664810	-2.70879634
H	0.48028029	1.14090443	-3.70858852
H	-0.54725820	0.48541709	-2.37815036
H	0.88688835	1.48511556	-1.99632096
S	-0.87689475	2.87486399	-2.77289757
H	-2.83065003	0.20270716	-0.32444646
C	-2.36993129	2.42610325	-3.73018561
H	-2.96776656	3.33654941	-3.81815614
H	-2.95273420	1.64161456	-3.23873732
H	-2.03338982	2.11825991	-4.72305514
H	-1.38325176	2.85413794	-1.49251178

The MCR active site with a proton bound at position 2 (Fig. 1)

C	5.88238995	5.17280997	1.67559598
C	5.03126459	4.43746614	0.66490877
C	5.56856142	4.00061017	-0.55609956
C	3.67820356	4.17563904	0.90378267
C	4.79772993	3.32303039	-1.49745730
C	2.88904634	3.49790910	-0.02820351
C	3.44847722	3.05917772	-1.23437722
O	2.73832168	2.37396509	-2.17767081
C	-6.92859695	5.69123791	0.50074800
C	-5.96229262	4.53549813	0.39862326
C	-6.37025947	3.31981646	-0.16670168
C	-4.63920074	4.63712895	0.84421282
C	-5.49315974	2.24750062	-0.29500704
C	-3.74710030	3.56688968	0.73661233
C	-4.18072741	2.37426591	0.16039838
O	-3.35007373	1.26949577	0.04772962

C	0.43459499	-5.41813799	1.06786901
C	0.96269446	-4.58952560	2.22852270
O	0.22838505	-3.87238526	2.90533376
N	2.29821188	-4.68955747	2.46727792
Ni	0.03031251	-1.18237816	0.05365936
N	-1.18268918	-0.62133860	1.73559123
C	0.57797858	0.69132926	2.77498871
C	-0.69038063	-0.09598907	2.80537425
C	-1.42088792	-0.46586974	4.07862278
C	-2.24938900	-1.65967701	3.56921593
C	-2.42108025	-1.34125745	2.11895176
N	-1.62632194	-2.06693498	-0.74895184
C	-2.67414475	-2.62907857	1.39019158
C	-2.85496205	-2.43366653	-0.07844244
C	-3.48324152	-3.64798720	-0.78668716
C	-2.87050801	-3.46771688	-2.15545193
C	-1.63142648	-2.64834410	-1.94146177
N	-3.94410762	-1.39272027	-0.33466654
C	-5.06834923	-1.92627191	-0.67410772
O	-6.12906981	-1.18494795	-0.93232807
C	-5.00604565	-3.42706164	-0.73725293
N	1.16383288	-1.62126068	-1.62213713
C	-0.65335156	-2.57258236	-2.93781974
C	0.63239641	-2.08645219	-2.78218019
C	1.63668968	-2.11008676	-3.90540654
C	2.95329601	-1.89466701	-3.16348998
C	2.51940412	-1.50216334	-1.76208969
N	1.72197955	-0.66442136	1.01592746
C	3.39680119	-1.12882595	-0.73787840
C	2.95781860	-0.75379550	0.58584388
C	3.98085510	-0.41961447	1.67077576
C	3.11908900	0.36668500	2.66043599
C	1.74020770	-0.25503499	2.44087058
C	5.22238681	0.26592464	1.11259417
C	5.84016436	-0.64994858	0.06055660
C	4.86213256	-1.13435365	-1.01422690
O	5.33956505	-1.54017430	-2.07087147
H	5.96721172	6.24113301	1.43360504
H	5.45948664	5.10130660	2.68358705
H	6.61813012	4.18882276	-0.77337459
H	3.22691105	4.50429625	1.83856608
H	5.22633381	2.98029079	-2.43467626
H	1.84136990	3.29897093	0.18602556
H	1.83554306	2.20460344	-1.84687967

H	-7.14451234	6.11943519	-0.48657729
H	-6.52906261	6.49505658	1.12701494
H	-7.39315674	3.21348691	-0.52186293
H	-4.29572258	5.56612470	1.29327044
H	-5.81995368	1.31757251	-0.74919980
H	-2.72922996	3.65622967	1.10797647
H	-2.40461546	1.53094434	-0.03044643
H	0.19316093	-4.74004262	0.24092043
H	-0.48534351	-5.91871791	1.38311742
H	2.91414105	-5.24471932	1.89295860
H	2.70215998	-4.13053041	3.20621832
H	0.53543027	1.47898677	2.01400345
H	0.75800627	1.16077566	3.74859735
H	-3.19897769	-1.78407233	4.10203772
H	-3.25686263	-0.64365468	1.96466260
H	-1.83555655	-3.31420081	1.55184874
H	-3.57308302	-3.09155762	1.82274460
H	-3.55432932	-2.93333469	-2.83535936
H	-5.54758663	-3.82423815	-1.60361552
H	-5.46719505	-3.84876676	0.16607745
H	-0.89327252	-3.03070428	-3.89267167
H	1.59587095	-3.04273679	-4.47729720
H	3.59919469	-1.13545041	-3.60787483
H	4.29091590	-1.37353188	2.13398612
H	3.10489028	1.42719603	2.37605873
H	1.63192172	-1.16599805	3.05145718
H	5.94068952	0.47811629	1.91405739
H	4.94445559	1.22800249	0.66526138
H	6.25273747	-1.55020995	0.54267791
H	6.67477920	-0.17875734	-0.46747452
H	1.14222973	-6.17041050	0.70648123
H	1.42565348	-1.29434861	-4.61006092
H	3.56857713	-2.79915795	-3.12370345
H	3.46098808	0.29389959	3.69809698
H	-0.73099639	-0.70640187	4.89499933
H	-2.04315342	0.37588000	4.42015702
H	-1.66474364	-2.57683992	3.68127600
H	-2.65151739	-4.41639677	-2.65849413
H	-3.17947827	-4.58266957	-0.31063605
H	-7.88630656	5.37662474	0.93160904
H	6.90137553	4.77072945	1.71062474
C	-1.25537449	1.39698022	-2.85925920
H	-0.74260464	1.74602359	-3.75990049
H	-2.32676946	1.60390534	-2.93776707

H	-1.09425426	0.32269155	-2.74469266
S	-0.55174720	2.20930416	-1.37969965
H	-3.77365555	-0.36694910	-0.24136077
C	-0.82709453	3.96510957	-1.82707393
H	-0.38284799	4.57587124	-1.03685856
H	-1.89473897	4.18829640	-1.89816290
H	-0.32750663	4.19598811	-2.77196487
H	-6.89307799	-1.73444454	-1.18099287

The MCR active site with a proton bound at position 3 (Fig. 1)

C	5.88238991	5.17280995	1.67559597
C	5.08795735	4.36865339	0.67043166
C	5.67969279	3.86946102	-0.50032592
C	3.72604619	4.10931428	0.86256779
C	4.95293575	3.13293988	-1.43511502
C	2.98314904	3.36941805	-0.05960105
C	3.59574995	2.86772646	-1.21581636
O	2.93623515	2.10730439	-2.13859231
C	-6.92859690	5.69123788	0.50074800
C	-5.89826581	4.58898547	0.48081686
C	-6.26158486	3.29001836	0.09642403
C	-4.56381634	4.81928450	0.82817006
C	-5.33602082	2.25256387	0.05090646
C	-3.61763309	3.78986093	0.79959335
C	-4.01014857	2.51099808	0.40697096
O	-3.12635186	1.44565296	0.38441151
C	0.43459503	-5.41813803	1.06786898
C	0.84598963	-4.76768874	2.38059523
O	0.44486664	-3.65486322	2.71588636
N	1.69078025	-5.49760528	3.16321349
Ni	0.01784503	-1.19235314	0.06883521
N	-1.16674849	-0.64836072	1.73924897
C	0.58002260	0.68316433	2.76987585
C	-0.68987389	-0.10537890	2.80353778
C	-1.44411606	-0.44623624	4.07092148
C	-2.24938904	-1.65967695	3.56921599
C	-2.42782758	-1.34452553	2.11770578
N	-1.62186771	-2.07182608	-0.76386223
C	-2.72798382	-2.59987313	1.35516425
C	-2.93836939	-2.33642956	-0.10806689
C	-3.60353551	-3.52492546	-0.83322376
C	-2.87050800	-3.46771684	-2.15545195
C	-1.62640807	-2.68125699	-1.90942478

N	-3.86917760	-1.25474499	-0.38777680
C	-5.11330343	-1.64546289	-0.80867910
O	-6.05713225	-0.90794193	-1.04285667
C	-5.09579121	-3.17665563	-0.90461797
N	1.20996045	-1.65982871	-1.59608646
C	-0.61290437	-2.60435975	-2.92393750
C	0.63831876	-2.10843993	-2.79750561
C	1.63563742	-2.03232696	-3.92351310
C	2.95329599	-1.89466700	-3.16348994
C	2.51458923	-1.54352672	-1.76299532
N	1.75104826	-0.65647600	1.00369536
C	3.44054353	-1.14827576	-0.71623712
C	2.98372137	-0.74857809	0.61202045
C	3.99579121	-0.43698395	1.70675654
C	3.11908900	0.36668499	2.66043596
C	1.74459613	-0.25356127	2.43420998
C	5.24999414	0.23726103	1.16867950
C	5.83898282	-0.64628957	0.07149898
C	4.81296455	-1.13509560	-0.91953723
O	5.33515023	-1.61451988	-2.05796516
H	5.91921048	6.23538768	1.40135317
H	5.44130097	5.11165658	2.67622937
H	6.73383255	4.06436140	-0.68815076
H	3.23075055	4.48955100	1.75416830
H	5.42010061	2.76214424	-2.34343887
H	1.93090213	3.16991387	0.12584038
H	1.98537462	2.06100040	-1.90975288
H	-7.24774936	5.96118747	-0.51445239
H	-6.53940681	6.59854926	0.97456636
H	-7.29335867	3.08460768	-0.18098714
H	-4.25339708	5.81508609	1.13731623
H	-5.63417864	1.25619060	-0.26734290
H	-2.58849261	3.97821622	1.09988665
H	-2.20510461	1.75085235	0.27363782
H	0.45870877	-4.66061898	0.28013130
H	-0.59734742	-5.77773712	1.15595217
H	1.91473953	-6.45951369	2.95506041
H	1.88296724	-5.16109640	4.09759521
H	0.52836432	1.47902083	2.01759578
H	0.76564845	1.14849295	3.74431003
H	-3.19635734	-1.80102972	4.10098398
H	-3.23762045	-0.61934495	1.97003400
H	-1.91629273	-3.32309036	1.49019875
H	-3.64418209	-3.03584126	1.77587848

H	-3.46907084	-2.95764009	-2.92747589
H	-5.59526196	-3.51447677	-1.81690707
H	-5.65767465	-3.58701526	-0.05680426
H	-0.88653787	-3.00612149	-3.89598706
H	1.59367643	-2.90104372	-4.58608510
H	3.61716146	-1.13594073	-3.58246663
H	4.27949704	-1.39482346	2.17735543
H	3.11185668	1.42166734	2.35635465
H	1.63601778	-1.17898751	3.01866480
H	5.98813206	0.39040425	1.96310753
H	5.00067954	1.22064818	0.75612133
H	6.33245380	-1.53078797	0.50594537
H	6.61429758	-0.10102305	-0.48644567
H	1.07023272	-6.26200617	0.78237350
H	1.44065827	-1.14296477	-4.53750014
H	3.52501262	-2.83048960	-3.15578062
H	3.44306561	0.31347131	3.70478365
H	-0.77209835	-0.65230286	4.91171027
H	-2.08803998	0.39563880	4.36921823
H	-1.64515788	-2.56619835	3.68253055
H	-2.64409111	-4.45626242	-2.57652834
H	-3.40329539	-4.46431311	-0.30885073
H	-7.82874660	5.38900355	1.04920926
H	6.91872390	4.82293155	1.74275823
C	-1.44856365	1.41579584	-2.61949566
H	-1.12758630	1.70385895	-3.62447955
H	-2.49174078	1.70087140	-2.46062444
H	-1.34926862	0.33561070	-2.49507861
S	-0.37840887	2.20319407	-1.36133776
H	-3.65032479	-0.27940962	-0.18317675
C	-0.65597761	3.96629436	-1.78198775
H	-0.00109168	4.56372474	-1.14226069
H	-1.69630829	4.24480473	-1.59499057
H	-0.39728381	4.15514333	-2.82754520
H	6.29908168	-1.48578694	-2.06406485

The MCR active site with a proton bound at position 4a (Fig. 1)

C	5.88238997	5.17280996	1.67559597
C	5.07030226	4.37688030	0.68000941
C	5.65309190	3.86657446	-0.49158479
C	3.70842197	4.12896629	0.87963761
C	4.91923856	3.12931164	-1.41823779
C	2.95707120	3.38680177	-0.03577578

C	3.56189495	2.87290571	-1.18962432
O	2.89441713	2.10481932	-2.10310347
C	-6.92859697	5.69123791	0.50074800
C	-5.88978509	4.60043563	0.48059780
C	-6.22135636	3.32628021	0.00017233
C	-4.58221762	4.81667166	0.92562860
C	-5.28943128	2.29606037	-0.04106652
C	-3.63100981	3.79265218	0.90389540
C	-3.99359197	2.53743841	0.41853970
O	-3.10823847	1.46973482	0.41255068
C	0.43459517	-5.41813816	1.06786889
C	0.90142401	-4.64817868	2.29426977
O	0.47870999	-3.52441071	2.56525194
N	1.79918816	-5.29476343	3.08382634
Ni	-0.07766324	-1.19527350	0.21646439
N	-1.22736276	-0.60167388	1.76275763
C	0.57255612	0.68218668	2.76623454
C	-0.71005533	-0.08758348	2.82328782
C	-1.44248884	-0.45636198	4.09265028
C	-2.24938914	-1.65967679	3.56921600
C	-2.48393039	-1.30090399	2.13839375
N	-1.59840728	-2.12742873	-0.73231537
C	-2.81492682	-2.54288568	1.35632971
C	-2.96173856	-2.29985949	-0.12010830
C	-3.64957345	-3.47318020	-0.85372318
C	-2.87050788	-3.46771685	-2.15545193
C	-1.60336284	-2.76191911	-1.86942419
N	-3.82509323	-1.18379778	-0.46067441
C	-5.06825468	-1.53198643	-0.93056244
O	-5.96470963	-0.76139494	-1.22741563
C	-5.11988310	-3.06290084	-0.98628612
N	1.29417216	-2.03958247	-1.54953989
C	-0.60115536	-2.77024942	-2.88622369
C	0.67002651	-2.35820925	-2.75726118
C	1.63156962	-2.13224087	-3.88038918
C	2.95329585	-1.89466696	-3.16348979
C	2.62716949	-1.69192706	-1.70771541
N	1.73421913	-0.73152690	1.02936158
C	3.45007060	-1.26299503	-0.68814668
C	2.97471054	-0.85042728	0.63097722
C	3.98696758	-0.46609018	1.71024632
C	3.11908900	0.36668490	2.66043587
C	1.73874451	-0.26433011	2.45012266
C	5.24295073	0.19982735	1.15421976

C	5.87737894	-0.71437211	0.10854123
C	4.91881823	-1.15570135	-0.99109556
O	5.36729725	-1.46162643	-2.08788621
H	6.05556601	6.19925666	1.32595320
H	5.37500704	5.23967724	2.64369360
H	6.70879135	4.04801796	-0.68320443
H	3.21913486	4.51831012	1.77070912
H	5.38279018	2.73879706	-2.31962364
H	1.90393257	3.19569234	0.15640861
H	1.94754792	2.05888014	-1.86358365
H	-7.20733751	5.99936896	-0.51536337
H	-6.56970199	6.58187407	1.02711206
H	-7.23189270	3.13569530	-0.35500261
H	-4.30002667	5.79471817	1.30917680
H	-5.56235578	1.31845510	-0.43053112
H	-2.62524158	3.96529373	1.28249626
H	-2.18691291	1.77042724	0.28758328
H	0.06000593	-4.71328679	0.32329390
H	-0.38973827	-6.08615451	1.34683812
H	2.11967149	-6.23185539	2.88871966
H	2.07770543	-4.86622904	3.95628706
H	0.52268449	1.46378284	1.99925214
H	0.76521406	1.16518827	3.73056723
H	-3.17252914	-1.83672954	4.13207283
H	-3.29260263	-0.56726463	2.03081831
H	-2.04610461	-3.30572966	1.52244386
H	-3.76324431	-2.93302369	1.74942283
H	-3.41253824	-2.92600763	-2.94710540
H	-5.60310443	-3.40475239	-1.90557739
H	-5.72811921	-3.42167631	-0.14710287
H	-0.92081271	-3.09506005	-3.87166744
H	1.65596062	-2.98270850	-4.56825419
H	3.52184370	-1.04949737	-3.55670728
H	4.28378763	-1.40468649	2.21116319
H	3.11447167	1.41555774	2.33762380
H	1.63490735	-1.16863548	3.06725900
H	5.95103907	0.40196873	1.96617116
H	4.98466084	1.16554760	0.70538826
H	6.25306222	-1.63219296	0.58839589
H	6.73598195	-0.25212340	-0.38687123
H	1.22718707	-6.03236829	0.62716546
H	1.32341114	-1.25563042	-4.46298454
H	3.63878465	-2.74660705	-3.24880248
H	3.44823565	0.32386473	3.70280608

H	-0.75742035	-0.68243849	4.91710915
H	-2.08494247	0.37508958	4.42108815
H	-1.62605957	-2.55823636	3.62758640
H	-2.68888654	-4.46995301	-2.56430412
H	-3.50744960	-4.41228210	-0.31022133
H	-7.84814285	5.35926881	0.99753600
H	6.86739808	4.72190707	1.84344799
C	-1.49727615	1.45430084	-2.61592049
H	-1.16114893	1.75388294	-3.61235007
H	-2.53158573	1.76990693	-2.45688890
H	-1.43713019	0.36810652	-2.51751132
S	-0.40886800	2.17821405	-1.33541146
H	-3.59448665	-0.21592080	-0.22342103
C	-0.64011119	3.95900248	-1.70623913
H	0.03441637	4.51962562	-1.05416087
H	-1.67190240	4.25934366	-1.50701322
H	-0.37901424	4.16718425	-2.74731628
H	1.01630621	-2.53449851	-0.69042111

The MCR active site with a proton bound at position 4b (Fig. 1)

C	5.88238995	5.17280995	1.67559596
C	4.97329824	4.46933475	0.69457886
C	5.45559637	4.02174195	-0.54666390
C	3.62187899	4.24649324	0.97735747
C	4.63441764	3.36921955	-1.46273104
C	2.78364340	3.58775675	0.07275819
C	3.28847711	3.14005376	-1.15348984
O	2.53105541	2.46383187	-2.07077177
C	-6.92859693	5.69123786	0.50074800
C	-5.92124474	4.58081813	0.57659703
C	-6.26464636	3.29628133	0.13705338
C	-4.62985246	4.79437493	1.06648641
C	-5.35130405	2.24983108	0.16643797
C	-3.69969484	3.75468646	1.11760991
C	-4.06765788	2.49123370	0.65815624
O	-3.18721905	1.42355604	0.70233619
C	0.43459517	-5.41813816	1.06786889
C	0.91999196	-4.58748870	2.24546039
O	0.50532894	-3.44704884	2.45567374
N	1.83057372	-5.18703406	3.05714628
Ni	-0.14990240	-0.93700586	0.11163990
N	-1.22139414	-0.53191738	1.78712313
C	0.57288057	0.72017683	2.85339361

C	-0.70690312	-0.05793169	2.86759779
C	-1.43799777	-0.47410123	4.12353808
C	-2.24938912	-1.65967677	3.56921592
C	-2.46443671	-1.26881413	2.13814704
N	-1.70146185	-1.90092533	-0.83835408
C	-2.74564609	-2.49257102	1.31177176
C	-2.99794042	-2.20754886	-0.14701272
C	-3.65054893	-3.42178531	-0.85760592
C	-2.87050755	-3.46771670	-2.15545189
C	-1.67566441	-2.56500112	-1.95498528
N	-3.94641013	-1.14294136	-0.39658685
C	-5.17704832	-1.54036685	-0.85400838
O	-6.12600472	-0.80910837	-1.08010209
C	-5.13893389	-3.06633523	-0.99276063
N	1.13041532	-1.23358147	-1.82613624
C	-0.64816481	-2.51503008	-2.96896032
C	0.58022102	-1.95687800	-2.91630942
C	1.65482481	-2.11785279	-3.95588790
C	2.95329555	-1.89466694	-3.16348952
C	2.53210113	-1.25201228	-1.87276794
N	1.67833940	-0.41841687	0.90690124
C	3.36584864	-0.84013860	-0.86137897
C	2.90801651	-0.49840259	0.47678576
C	3.95050847	-0.30097221	1.57164354
C	3.11908893	0.36668477	2.66043564
C	1.71739540	-0.18678410	2.38179025
C	5.18180152	0.44811605	1.07264291
C	5.82042348	-0.35936061	-0.05260147
C	4.85045668	-0.86871621	-1.11671005
O	5.31943162	-1.31232181	-2.15669326
H	6.11572883	6.19401966	1.34696593
H	5.42222234	5.24562632	2.66644948
H	6.50008797	4.18791284	-0.80272036
H	3.20985968	4.59000202	1.92449540
H	5.01880530	3.02986816	-2.42032025
H	1.74083770	3.41226730	0.32854503
H	1.59727662	2.45271251	-1.78359811
H	-7.13657008	5.97540656	-0.53929543
H	-6.58254629	6.59004912	1.02190539
H	-7.26620564	3.11176434	-0.24518158
H	-4.34707099	5.78178573	1.42453587
H	-5.63272516	1.26455290	-0.19706158
H	-2.70541694	3.91855147	1.52789518
H	-2.27316465	1.73790554	0.56277593

H	0.35882376	-4.77277343	0.18903611
H	-0.56762124	-5.80256530	1.29145306
H	2.12529800	-6.14345438	2.92760343
H	2.11548434	-4.71055951	3.90235293
H	0.49921352	1.58712122	2.18608863
H	0.79883232	1.08904586	3.85973713
H	-3.18306177	-1.83606110	4.11368807
H	-3.28863784	-0.55352746	2.04170284
H	-1.91744157	-3.20399633	1.40692865
H	-3.64325990	-2.96709339	1.73070502
H	-3.45812455	-3.09571919	-3.00893428
H	-5.59317654	-3.38228248	-1.93605151
H	-5.74158113	-3.49945326	-0.18567357
H	-0.86998623	-3.06970386	-3.87673080
H	1.61059353	-3.08857575	-4.45558015
H	3.67616316	-1.26558984	-3.68526686
H	4.26113071	-1.30693513	1.90460425
H	3.13056368	1.45605119	2.52176732
H	1.59853760	-1.17416597	2.84969572
H	5.89541651	0.59538487	1.89171258
H	4.88989007	1.44247885	0.71690738
H	6.31758972	-1.25260010	0.35498973
H	6.59775526	0.20192442	-0.58087698
H	1.08435543	-6.26776456	0.83716422
H	1.53509246	-1.34550689	-4.72804750
H	3.49084260	-2.82849549	-2.96425251
H	3.46453544	0.14636483	3.67500346
H	-0.75116202	-0.72621957	4.93889928
H	-2.07769069	0.34783570	4.48009352
H	-1.63769891	-2.56703920	3.62017860
H	-2.54959967	-4.47747924	-2.44131426
H	-3.48957116	-4.33401656	-0.27651681
H	-7.88616968	5.39742658	0.94721214
H	6.83783158	4.64681630	1.78739998
C	-1.94771151	1.93099705	-2.39868827
H	-1.62932360	2.22024935	-3.40371510
H	-2.92897158	2.35823975	-2.17599377
H	-2.01251084	0.84249684	-2.32967413
S	-0.72487742	2.49239549	-1.15591599
H	-3.75437162	-0.18076475	-0.11447649
C	-0.85841194	4.30531790	-1.39594531
H	-0.11501292	4.78003239	-0.75076926
H	-1.85799061	4.64495563	-1.11389094
H	-0.64530867	4.56670896	-2.43584251

H	0.68395425	-0.33915782	-1.55592997
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The MCR active site with a proton bound at position 5 (Fig. 1)

C	5.88238986	5.17280992	1.67559595
C	4.96180280	4.46664379	0.70339999
C	5.44221282	3.98377170	-0.52514493
C	3.60305837	4.28062500	0.97943654
C	4.61191180	3.33641333	-1.43610037
C	2.75398805	3.63103324	0.07760054
C	3.25657969	3.14943858	-1.13692020
O	2.49273851	2.48672586	-2.05481216
C	-6.92859685	5.69123781	0.50074800
C	-5.94323115	4.55698832	0.59610454
C	-6.28763528	3.27714173	0.14148640
C	-4.65891528	4.75079809	1.11519659
C	-5.38098421	2.22117568	0.17370863
C	-3.73860927	3.70300579	1.17023248
C	-4.10311126	2.44736637	0.68490057
O	-3.20805502	1.38352055	0.72065543
C	0.43459499	-5.41813786	1.06786908
C	0.94425526	-4.23176733	1.84351229
O	0.54298846	-3.07999076	1.62561338
N	1.83578016	-4.48815808	2.82570889
Ni	0.09014857	-1.38992714	0.12831110
N	-1.14572261	-0.72712044	1.73114470
C	0.56792689	0.68616899	2.73323961
C	-0.69328820	-0.11581721	2.76795969
C	-1.47807750	-0.40666803	4.02943945
C	-2.24938901	-1.65967707	3.56921589
C	-2.42675832	-1.39221917	2.11482660
N	-1.57344119	-2.21019118	-0.69915817
C	-2.78510261	-2.64497307	1.37795573
C	-2.92704481	-2.38371443	-0.09249267
C	-3.61552803	-3.54120393	-0.84137689
C	-2.87050794	-3.46771671	-2.15545189
C	-1.58762911	-2.77235826	-1.87955250
N	-3.80776372	-1.26503274	-0.40769218
C	-5.06796058	-1.62327084	-0.82413331
O	-5.98990641	-0.85923970	-1.05184379
C	-5.09545659	-3.15266506	-0.92494090
N	1.21985433	-1.79991045	-1.55754708
C	-0.59054056	-2.74954740	-2.87653606
C	0.66734927	-2.24899851	-2.73390559

C	1.64048368	-2.17754922	-3.87558555
C	2.95329596	-1.89466701	-3.16348990
C	2.54724981	-1.56102695	-1.74143884
N	1.75275255	-0.66636163	1.00234452
C	3.42978135	-1.12404991	-0.74442644
C	2.98688065	-0.74216124	0.56714953
C	3.99582149	-0.38795194	1.65541171
C	3.11908897	0.36668491	2.66043588
C	1.74280311	-0.24846235	2.42232072
C	5.21884479	0.33364387	1.09850341
C	5.85736923	-0.54813168	0.02779353
C	4.88918679	-1.05309991	-1.04508221
O	5.35878533	-1.41974828	-2.11722019
H	6.11526264	6.19220188	1.34081029
H	5.43063176	5.25094382	2.67009369
H	6.49281161	4.11771487	-0.77523346
H	3.19227820	4.65205087	1.91672336
H	4.99513392	2.96745604	-2.38304609
H	1.70143506	3.49710209	0.32052562
H	1.56067650	2.46704733	-1.76519051
H	-7.04535731	6.03358662	-0.53606813
H	-6.61081481	6.55360324	1.09583960
H	-7.28356562	3.10298744	-0.26003227
H	-4.37344642	5.73103407	1.49066111
H	-5.65598948	1.23976760	-0.20537618
H	-2.75002979	3.85579612	1.59790423
H	-2.31784036	1.71889202	0.48945482
H	0.45474444	-5.18199724	0.00027806
H	-0.60888094	-5.60351600	1.34647612
H	2.15233548	-5.42347254	3.03584733
H	2.18002142	-3.72735420	3.39597847
H	0.51720369	1.46582255	1.96438260
H	0.73331935	1.17146354	3.70092510
H	-3.19461830	-1.80497598	4.10234685
H	-3.20920998	-0.64166668	1.95852184
H	-2.03443206	-3.42514876	1.54009561
H	-3.74157432	-3.00490177	1.77890373
H	-3.43559304	-2.88652179	-2.90076891
H	-5.59427815	-3.47458875	-1.84325062
H	-5.67893682	-3.54721178	-0.08417145
H	-0.86071832	-3.16280742	-3.84280429
H	1.64451921	-3.09583811	-4.47049944
H	3.53838392	-1.08405184	-3.60194021
H	4.32821570	-1.34323298	2.09910464

H	3.10543026	1.43447018	2.40476011
H	1.62530035	-1.15975922	3.02756165
H	5.93452252	0.54852355	1.90098103
H	4.91596237	1.29618167	0.66946322
H	6.30557688	-1.44038409	0.49229966
H	6.67000281	-0.03927808	-0.49902777
H	1.00740869	-6.33268627	1.24295115
H	1.35717852	-1.35886063	-4.54959774
H	3.63187682	-2.75421029	-3.15751235
H	3.45601570	0.26823030	3.69694403
H	-0.82552906	-0.54608283	4.89841522
H	-2.15095845	0.43330997	4.25953177
H	-1.62914781	-2.55201076	3.71986945
H	-2.69954418	-4.44566585	-2.62278666
H	-3.44179522	-4.49547477	-0.33435809
H	-7.92300379	5.39153403	0.85148395
H	6.83735113	4.64475664	1.78106061
C	-1.96439731	1.89998454	-2.46703499
H	-1.66324686	2.26829117	-3.45106535
H	-2.99472499	2.19485751	-2.25103297
H	-1.89167159	0.80960864	-2.44940321
S	-0.83630984	2.54485685	-1.17774529
H	-3.60520770	-0.30302621	-0.12976511
C	-1.11127233	4.34517701	-1.37444010
H	-0.42291204	4.85680636	-0.69679234
H	-2.14002869	4.60265693	-1.11202443
H	-0.88869921	4.64827562	-2.40095382
H	-0.13710879	-0.14051836	-0.55709004

Transition state for methyl transfer with protonated CH₃-S-CH₃ as substrate (see Table S1)

C	4.96119200	6.12891100	0.31369600
C	3.60681300	5.46720700	0.19086000
C	3.27872400	4.69965800	-0.93897200
C	2.63441800	5.59990500	1.18831200
C	2.03697700	4.08057900	-1.06823200
C	1.38413000	4.98463400	1.07684300
C	1.08873000	4.22154200	-0.05256700
O	-0.11948300	3.56003500	-0.20093200
C	-7.73632800	3.99947200	0.40768900
C	-6.37968100	3.34375200	0.41955500

C	-6.00502100	2.50328200	-0.63725600
C	-5.46687500	3.53161500	1.46321900
C	-4.76950600	1.86915600	-0.65973500
C	-4.21472900	2.90614300	1.45803400
C	-3.87823900	2.07362500	0.39367900
O	-2.65129000	1.42199600	0.29895200
C	1.76442200	-5.28154200	1.65466000
C	2.11659200	-4.14727900	2.60113400
O	1.37273700	-3.18032600	2.76835800
N	3.30720200	-4.26152200	3.24913400
Ni	0.42245800	-1.33785600	0.05784700
N	-0.86976800	-0.69378200	1.85312100
C	0.81006900	0.92717600	2.57036400
C	-0.28738400	-0.05678200	2.80898300
C	-0.72574600	-0.45483000	4.20131100
C	-1.43615700	-1.77968000	3.90849800
C	-1.92239600	-1.56497200	2.46265400
N	-1.04351400	-2.63693100	-0.45094000
C	-2.22569800	-2.84795500	1.70036100
C	-2.38674200	-2.69710700	0.18127300
C	-3.14785800	-3.90261400	-0.49067700
C	-2.10187100	-4.50104500	-1.43730600
C	-0.91434700	-3.58976900	-1.33913700
N	-3.17427100	-1.53853000	-0.22977900
C	-4.07128000	-1.79193900	-1.23294000
O	-4.55619700	-0.96696300	-1.99930100
C	-4.36213100	-3.28497100	-1.20888800
N	1.64367300	-2.04192900	-1.45303300
C	0.18147600	-3.82906700	-2.20645300
C	1.32329000	-3.08366000	-2.28242000
C	2.39687100	-3.31361500	-3.31554200
C	3.18484800	-2.00669800	-3.23623900
C	2.78382400	-1.44784100	-1.89178200
N	2.00656800	-0.30890700	0.76653800
C	3.51121100	-0.49742100	-1.17100000
C	3.16159700	-0.13079700	0.17604900
C	4.20199000	0.51239500	1.08370400
C	3.32090900	1.08178700	2.19534100
C	2.08863400	0.18216800	2.15925400
C	5.10874000	1.49101300	0.33978100
C	5.74076600	0.78716300	-0.86200500
C	4.72740100	0.10076900	-1.77715900
O	4.95701900	0.04118700	-2.98205800
H	5.10493300	6.89376800	-0.45956800

H	5.07997200	6.61627600	1.28617100
H	4.00545100	4.59170300	-1.74106900
H	2.85125000	6.19443300	2.07217900
H	1.79237500	3.50179400	-1.95368000
H	0.64628400	5.10314700	1.86848600
H	-0.76232700	3.93625500	0.42089100
H	-7.81504600	4.74204000	-0.39649800
H	-7.94573600	4.51344600	1.35114300
H	-6.70378300	2.32266600	-1.45067200
H	-5.73304200	4.17287800	2.29967400
H	-4.53062200	1.15456000	-1.43850600
H	-3.52131500	3.06329500	2.28286000
H	-2.20211500	1.38701200	1.15869500
H	1.57921800	-4.86495000	0.65964600
H	0.83563800	-5.74942700	1.99666200
H	3.89014500	-5.08107600	3.17051700
H	3.55414700	-3.56418000	3.93815000
H	0.55027400	1.64317600	1.78183000
H	1.00665000	1.49148000	3.48877000
H	-2.24946200	-2.00951800	4.60273200
H	-2.84156300	-0.95848800	2.46475500
H	-1.43097500	-3.58085500	1.87693700
H	-3.15324500	-3.25748800	2.11898600
H	-2.45396400	-4.57128400	-2.47346100
H	-4.52265900	-3.66357900	-2.22132500
H	-5.29445400	-3.43935600	-0.65320000
H	0.07073800	-4.64899500	-2.90912800
H	3.02182900	-4.16899600	-3.02436200
H	2.88891300	-1.30305300	-4.02424400
H	4.82581500	-0.30663900	1.48033200
H	3.03752300	2.11366900	1.94882500
H	2.21556900	-0.69325800	2.81137800
H	5.88393100	1.87888200	1.01143300
H	4.51556300	2.35113000	0.00381700
H	6.43140500	0.00503000	-0.50907300
H	6.32937800	1.46845200	-1.48248700
H	2.53894200	-6.05039300	1.58232400
H	1.98621800	-3.53373100	-4.30467900
H	4.26348000	-2.11897200	-3.34310800
H	3.80724300	1.09515300	3.17580700
H	0.12346600	-0.53361400	4.88852700
H	-1.40201700	0.30927700	4.61550000
H	-0.70702200	-2.59464500	3.92149500
H	-1.81338600	-5.52001000	-1.14840800

H	-3.45591000	-4.62714200	0.26546200
H	-8.53242300	3.26377300	0.24457100
H	5.77481700	5.40225400	0.20158000
C	-0.30986400	0.41809800	-1.58418500
H	0.52673900	0.13670900	-2.20746900
H	-1.17176500	-0.23116600	-1.56727100
H	-0.11516300	1.06111600	-0.73841300
S	-1.19612200	2.02662000	-2.85907200
H	-2.84822500	-0.58710400	-0.06992400
C	-2.38545100	1.06637900	-3.87259000
H	-3.06577400	1.76055300	-4.36995000
H	-2.94736300	0.36526400	-3.25106100
H	-1.80244400	0.53230300	-4.62578000
H	-2.03640300	2.38316200	-1.86780500

**Intermediate resulted from methyl transfer with protonated CH₃-S-CH₃
as substrate (see Table S1)**

C	5.88238898	5.17281000	1.67559601
C	4.44396924	4.86895123	1.31322358
C	4.10955501	4.34363521	0.05487772
C	3.40109325	5.07751392	2.22355662
C	2.79719994	4.01154247	-0.27766192
C	2.07971189	4.74846503	1.90964269
C	1.77820719	4.20408674	0.65896233
O	0.50582717	3.81404070	0.30295011
C	-6.92859598	5.69123699	0.50074800
C	-5.70885366	4.81049457	0.61083817
C	-5.19454560	4.17349525	-0.52681535
C	-5.08158429	4.56887275	1.83722944
C	-4.10782758	3.31035034	-0.45216335
C	-3.98721954	3.70465720	1.93443575
C	-3.51511354	3.07283869	0.78673885
O	-2.44869844	2.18122669	0.81749359
C	0.43459505	-5.41813799	1.06786902
C	0.77809477	-4.27296137	1.99599664
O	0.35904274	-3.12504127	1.81074511
N	1.55205783	-4.58607419	3.06463457
Ni	0.07289587	-1.18302954	0.01255420
N	-1.22406533	-0.55141645	1.73826998
C	0.59972322	0.67504649	2.79385273
C	-0.67786817	-0.09758924	2.81095290
C	-1.37868541	-0.50805796	4.08987621

C	-2.24938906	-1.65967701	3.56921597
C	-2.50656005	-1.21460848	2.12530836
N	-1.55839218	-2.04705722	-0.81017598
C	-2.99797846	-2.28772005	1.16800358
C	-2.94946141	-1.86922003	-0.31021652
C	-3.86988590	-2.74365438	-1.24356716
C	-2.87050799	-3.46771595	-2.15545194
C	-1.53287539	-2.86895170	-1.82776605
N	-3.41004422	-0.51169023	-0.55294732
C	-4.25245496	-0.36645800	-1.62917079
O	-4.52802523	0.68113801	-2.19045248
C	-4.79993437	-1.74966797	-1.96677701
N	1.29084932	-1.91469413	-1.49053876
C	-0.41859236	-3.21647276	-2.63272462
C	0.84748102	-2.72074719	-2.50839072
C	1.94452786	-2.99152621	-3.50565213
C	2.95329600	-1.89466700	-3.16349000
C	2.55088183	-1.48280691	-1.76779360
N	1.73992027	-0.57909243	0.96392891
C	3.37138637	-0.80396009	-0.86316495
C	2.96039173	-0.54481598	0.48813994
C	3.99668331	-0.21314699	1.55220543
C	3.11908900	0.36668496	2.66043595
C	1.75407485	-0.25944568	2.40692347
C	5.11985724	0.67557189	1.02121316
C	5.75037431	0.01156306	-0.20385149
C	4.73982321	-0.38574149	-1.28028061
O	5.08837086	-0.37004235	-2.45549253
H	6.44922835	5.52252526	0.80585210
H	5.94623360	5.94455819	2.44987265
H	4.89202573	4.20049065	-0.68775375
H	3.61883911	5.50533065	3.19988345
H	2.54687916	3.62204528	-1.26018070
H	1.28667717	4.92434516	2.63556050
H	-0.13623452	4.19201134	0.92405035
H	-6.87475367	6.34453268	-0.37751181
H	-7.04917798	6.32688110	1.38406922
H	-5.66646369	4.34115668	-1.49223935
H	-5.45266027	5.05493153	2.73660049
H	-3.76072705	2.77616664	-1.32798654
H	-3.51490313	3.52513884	2.90014801
H	-2.20181799	2.01167371	1.73896058
H	0.53475579	-5.07981292	0.03298222
H	-0.61257601	-5.70109176	1.22587266

H	1.86478608	-5.52812765	3.24731128
H	1.76357221	-3.87251982	3.74876386
H	0.55980270	1.50318179	2.07595847
H	0.79755600	1.09285858	3.78736480
H	-3.16837684	-1.81313100	4.14316503
H	-3.26118680	-0.41276509	2.12110178
H	-2.40837092	-3.20416167	1.28113151
H	-4.03452063	-2.51909421	1.44250939
H	-3.10070635	-3.35335625	-3.22132127
H	-4.83490910	-1.88400473	-3.05152035
H	-5.83268315	-1.80708341	-1.60438254
H	-0.61805382	-3.87219908	-3.47422427
H	2.37197480	-3.98897961	-3.33235691
H	2.85897852	-1.02823132	-3.83053583
H	4.43499333	-1.17278533	1.87550913
H	3.05549449	1.45721222	2.54429583
H	1.63865311	-1.20650182	2.95111883
H	5.87296564	0.84400021	1.80030238
H	4.70699604	1.65683273	0.75445929
H	6.27106798	-0.91029623	0.10070939
H	6.49830920	0.64839137	-0.68444230
H	1.05819682	-6.30343462	1.22046971
H	1.58404090	-2.96639326	-4.53749690
H	3.99733491	-2.19834377	-3.22961737
H	3.49713164	0.16416096	3.66777733
H	-0.66683203	-0.78230022	4.87652058
H	-1.98017225	0.32623595	4.48432967
H	-1.67415954	-2.59156661	3.56406862
H	-2.84218021	-4.54936197	-1.96730976
H	-4.44203325	-3.45774327	-0.64746088
H	-7.84292254	5.09162868	0.40064932
H	6.39675159	4.28148176	2.06046342
C	-0.10616109	0.55514275	-1.11301477
H	0.92540686	0.84331379	-1.28809136
H	-0.64329708	0.19887664	-1.98409617
H	-0.66291848	1.20036158	-0.44033461
S	-0.82034500	3.05375645	-3.20121527
H	-2.91050695	0.29896487	-0.19420051
C	-2.37513564	2.82932839	-4.15422285
H	-2.85823997	3.79241034	-4.33521463
H	-3.06225703	2.14741572	-3.64774651
H	-2.08331099	2.39971161	-5.11590292
H	-1.36427826	3.59766064	-2.09343623

Complex H (Fig. 4)

C	5.88238964	5.17280980	1.67559580
C	5.03027928	4.50182120	0.62185467
C	5.59886825	4.00904057	-0.56372066
C	3.64746343	4.35996334	0.77796978
C	4.82882883	3.39255438	-1.54627630
C	2.85706011	3.74747925	-0.19772530
C	3.44624469	3.25045447	-1.36689844
O	2.73952933	2.63310958	-2.35445450
C	-6.92859657	5.69123757	0.50074797
C	-5.91505593	4.57783879	0.47605627
C	-6.31744790	3.25807391	0.22915332
C	-4.55441704	4.82636339	0.67405352
C	-5.40136100	2.21396746	0.17693606
C	-3.61720537	3.79352119	0.63498565
C	-4.04790376	2.49070276	0.38721385
O	-3.17052374	1.42872085	0.37013071
C	0.43459500	-5.41813761	1.06786909
C	1.13446216	-4.35079483	1.89446908
O	0.56500557	-3.71726444	2.77762143
N	2.45489870	-4.15496713	1.58916748
Ni	0.02901768	-1.21734401	0.07238606
N	-1.16514799	-0.64987798	1.74530977
C	0.58745069	0.67014242	2.78797108
C	-0.68545623	-0.11119697	2.81081529
C	-1.44174579	-0.45290074	4.07705150
C	-2.24938899	-1.65967718	3.56921584
C	-2.42590019	-1.34323195	2.11943431
N	-1.61848819	-2.08248794	-0.75298113
C	-2.72888950	-2.60188503	1.36215337
C	-2.92407020	-2.34971758	-0.10552702
C	-3.58161297	-3.54772967	-0.82205791
C	-2.87050790	-3.46771641	-2.15545182
C	-1.62237568	-2.67922743	-1.91662898
N	-3.88440879	-1.28184117	-0.38237941
C	-5.13308212	-1.69996037	-0.74459096
O	-6.11160090	-0.98877836	-0.92701882
C	-5.08175115	-3.23041827	-0.85896106
N	1.18412181	-1.66029719	-1.60413323
C	-0.62531486	-2.62089233	-2.92283828
C	0.63753781	-2.12363367	-2.77896831
C	1.63608181	-2.08587593	-3.90883553
C	2.95329592	-1.89466701	-3.16348981

C	2.52000728	-1.51910678	-1.75717883
N	1.73402175	-0.67516315	1.01887237
C	3.41085097	-1.12125256	-0.73925817
C	2.96991818	-0.74458150	0.57879168
C	3.99337149	-0.38576315	1.65718821
C	3.11908888	0.36668483	2.66043593
C	1.74928747	-0.26960782	2.44399355
C	5.20003361	0.34477583	1.08044283
C	5.83959240	-0.54996411	0.02340984
C	4.86458481	-1.10639807	-1.02349483
O	5.35766403	-1.54634247	-2.06319979
H	6.20628040	6.17367146	1.35910179
H	5.33415142	5.28992967	2.61665476
H	6.67207964	4.10468767	-0.71993473
H	3.16903706	4.74015053	1.67911098
H	5.28020093	3.00691250	-2.45588008
H	1.78248282	3.66188161	-0.05584417
H	1.80751392	2.52693133	-2.07906081
H	-7.30007452	5.92325782	-0.50679673
H	-6.50346438	6.61365803	0.91124048
H	-7.37137682	3.04258657	0.06401555
H	-4.21630987	5.84251431	0.86733497
H	-5.72238548	1.19969455	-0.04910258
H	-2.56181276	3.99722863	0.79946855
H	-2.26161868	1.73342340	0.16395689
H	-0.06507834	-4.93248108	0.22051547
H	-0.32671574	-5.90481477	1.68185366
H	2.81886166	-4.48390591	0.70531871
H	2.87057921	-3.30269257	1.94158410
H	0.54533929	1.47345022	2.04245402
H	0.76948863	1.12684336	3.76770669
H	-3.19742279	-1.80266927	4.10028281
H	-3.23611529	-0.61841261	1.97093912
H	-1.92523968	-3.33209513	1.50816444
H	-3.65023099	-3.02874588	1.78247636
H	-3.48845512	-2.94839343	-2.90527952
H	-5.59287701	-3.56678076	-1.76598095
H	-5.61924040	-3.66232905	-0.00560021
H	-0.88468263	-3.05299111	-3.88515528
H	1.60098362	-2.98750500	-4.52847882
H	3.60949449	-1.13706476	-3.59522268
H	4.34938274	-1.32738733	2.11545991
H	3.08514843	1.43132955	2.39053120
H	1.64587789	-1.18214921	3.05218224

H	5.91972002	0.59251350	1.87124842
H	4.87477796	1.29162484	0.63192591
H	6.31799789	-1.41763827	0.50440385
H	6.63118323	-0.03766070	-0.53275251
H	1.12409896	-6.17352215	0.67728046
H	1.42011746	-1.23379906	-4.56757333
H	3.55823773	-2.80717942	-3.13377747
H	3.47000213	0.28876455	3.69509750
H	-0.76984525	-0.66720981	4.91593732
H	-2.08243619	0.39067425	4.37854032
H	-1.64689684	-2.56832295	3.68036357
H	-2.64734266	-4.44908442	-2.59401509
H	-3.35144556	-4.48414939	-0.30384836
H	-7.80270435	5.42881817	1.10938828
H	6.79058092	4.59556683	1.88854353
C	-1.49890719	1.38911987	-2.68747915
H	-0.93313625	0.74522597	-3.36278984
H	-1.81404341	2.29112990	-3.21654615
H	-2.37789461	0.86099218	-2.31396080
S	-0.44435434	1.92737539	-1.28157586
H	-3.68461880	-0.30350758	-0.17195896
H	-0.12968756	0.65873650	-0.80498267

Complex 1 (Fig. S2)

C	5.88238986	5.17280991	1.67559594
C	5.05737575	4.44778227	0.63609424
C	5.63867835	3.98116628	-0.55341509
C	3.69004314	4.21666826	0.81655606
C	4.89614123	3.30494833	-1.51692544
C	2.92846828	3.53949128	-0.13830809
C	3.52978296	3.07022208	-1.31265005
O	2.85285842	2.39216995	-2.27917750
C	-6.92859683	5.69123776	0.50074800
C	-5.90477538	4.58597028	0.45041065
C	-6.28897240	3.27826598	0.12141471
C	-4.55328005	4.82751001	0.71068874
C	-5.36652165	2.24123738	0.04880840
C	-3.60942878	3.80039530	0.65291027
C	-4.02197120	2.51005196	0.32145648
O	-3.14518065	1.44979710	0.28307853
C	0.43459499	-5.41813769	1.06786913
C	1.04644714	-4.53269544	2.14186952
O	0.36376232	-3.85812548	2.90655724

N	2.40975048	-4.53509169	2.19740635
Ni	0.02529669	-1.19270758	0.05353886
N	-1.17423871	-0.63584371	1.74001101
C	0.58111300	0.68165605	2.77937061
C	-0.68946671	-0.10330106	2.80639495
C	-1.43447160	-0.45678800	4.07702176
C	-2.24938902	-1.65967713	3.56921586
C	-2.42935940	-1.33716152	2.11923147
N	-1.61926638	-2.06997119	-0.75997139
C	-2.72621435	-2.59380396	1.35779885
C	-2.92208105	-2.33908572	-0.10908580
C	-3.58382630	-3.53735799	-0.82294142
C	-2.87050792	-3.46771665	-2.15545187
C	-1.62286307	-2.67609745	-1.92066355
N	-3.88141063	-1.26962853	-0.38441467
C	-5.12198018	-1.68046431	-0.77168178
O	-6.09037281	-0.96217805	-0.98680110
C	-5.08208223	-3.21196224	-0.86667563
N	1.17813007	-1.63427180	-1.61612347
C	-0.62591830	-2.61828352	-2.92607184
C	0.63733272	-2.11594374	-2.78456415
C	1.63931339	-2.09514186	-3.91146189
C	2.95329594	-1.89466702	-3.16348988
C	2.51729571	-1.50898204	-1.76110912
N	1.72687745	-0.66238403	1.01160489
C	3.40799513	-1.12502529	-0.73757812
C	2.96523452	-0.74959090	0.58114396
C	3.98537413	-0.41202383	1.66965222
C	3.11908894	0.36668482	2.66043584
C	1.74300985	-0.25814229	2.43666833
C	5.22343500	0.27827187	1.11204245
C	5.84171784	-0.63259927	0.05671851
C	4.86174815	-1.13180041	-1.01387739
O	5.35520010	-1.54721578	-2.06435918
H	6.17268808	6.17552592	1.33673030
H	5.32804402	5.29163650	2.61152584
H	6.70071978	4.14329289	-0.72671641
H	3.20327168	4.56948708	1.72374129
H	5.35786785	2.93720191	-2.42812032
H	1.86981473	3.36615706	0.03375065
H	1.93597646	2.23227818	-1.99353825
H	-7.27516946	5.96593600	-0.50372034
H	-6.52204563	6.59525028	0.96457544
H	-7.33501308	3.06624978	-0.08917774

H	-4.22803948	5.83215178	0.97201181
H	-5.67734393	1.23607322	-0.22809988
H	-2.56385551	3.99859773	0.87610576
H	-2.22746061	1.74454101	0.14065634
H	0.10223991	-4.77646267	0.24477906
H	-0.44190190	-5.92064899	1.48251067
H	2.97211776	-4.99509953	1.49985867
H	2.85937528	-3.88581616	2.82551673
H	0.53608305	1.47637313	2.02619046
H	0.76272685	1.14340461	3.75626372
H	-3.19617961	-1.79868658	4.10215173
H	-3.24466667	-0.61684916	1.97293799
H	-1.91877117	-3.31856006	1.50324204
H	-3.64562024	-3.02555260	1.77604127
H	-3.48670227	-2.95504183	-2.91044997
H	-5.59391704	-3.55503624	-1.76991714
H	-5.62362379	-3.62821239	-0.00894398
H	-0.88004840	-3.06192335	-3.88425328
H	1.60526708	-3.00580932	-4.51675227
H	3.60989875	-1.13863509	-3.59668265
H	4.30023829	-1.36456279	2.13308566
H	3.10026274	1.42728040	2.37742986
H	1.63676384	-1.17040493	3.04635750
H	5.94220585	0.49538967	1.91203707
H	4.93836435	1.23844433	0.66562044
H	6.26781722	-1.52711427	0.53649064
H	6.66610053	-0.15397510	-0.47988213
H	1.12798819	-6.16603525	0.67361553
H	1.42517853	-1.25376008	-4.58345406
H	3.56243298	-2.80332370	-3.12381032
H	3.46003329	0.29506897	3.69844583
H	-0.75505561	-0.67741546	4.90753673
H	-2.06984691	0.38549316	4.39161989
H	-1.65083162	-2.57047815	3.67485850
H	-2.64719017	-4.45179303	-2.58506625
H	-3.36033119	-4.47199712	-0.29995647
H	-7.81431946	5.39303557	1.07300851
H	6.80818988	4.63203581	1.90313510
C	-1.38389456	1.21967607	-2.71580650
H	-1.04245641	1.49575758	-3.71400261
H	-2.45504524	1.39356544	-2.60848257
H	-1.16516936	0.16873210	-2.52559889
S	-0.45825377	2.16653464	-1.44073675
H	-3.66778489	-0.28883584	-0.20822311

H	-0.80008898	3.40238985	-1.86638896
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Complex 2 (Fig. S2)

C	5.88238984	5.17280991	1.67559593
C	5.00518334	4.58120589	0.59263054
C	5.54274980	4.19376076	-0.64541389
C	3.63041079	4.39668394	0.77978630
C	4.75295640	3.62687254	-1.64237913
C	2.81988242	3.83198291	-0.20816701
C	3.37964660	3.42677778	-1.42948342
O	2.66033193	2.84910600	-2.42144026
C	-6.92859679	5.69123774	0.50074799
C	-5.88317857	4.60896166	0.35001808
C	-6.27077580	3.26806202	0.21562726
C	-4.51410561	4.89379350	0.32109722
C	-5.33877233	2.24814898	0.06727997
C	-3.55700159	3.88363918	0.18024159
C	-3.97214598	2.55621025	0.06029657
O	-3.09667248	1.50356511	-0.03639204
C	0.43459502	-5.41813751	1.06786910
C	1.11244665	-4.15019858	1.55274351
O	0.69574715	-3.50564600	2.51031095
N	2.21792320	-3.77936762	0.83852917
Ni	-0.15078152	-0.84148203	0.04509799
N	-1.18581101	-0.56525850	1.79044873
C	0.58521996	0.70263941	2.86542317
C	-0.69297541	-0.07346842	2.87186220
C	-1.44393185	-0.47147158	4.12463474
C	-2.24938894	-1.65967714	3.56921572
C	-2.43448802	-1.28356510	2.12920667
N	-1.68712115	-1.91445504	-0.83550920
C	-2.70074637	-2.51947830	1.32120509
C	-2.95806205	-2.24998303	-0.13760528
C	-3.58867340	-3.48561678	-0.82406381
C	-2.87050774	-3.46771666	-2.15545185
C	-1.66629254	-2.56351901	-1.96203606
N	-3.95087649	-1.21541210	-0.37611859
C	-5.18028246	-1.66248534	-0.77008871
O	-6.17072352	-0.97806342	-0.97642856
C	-5.09445360	-3.19344406	-0.87597196
N	1.11677619	-1.13439152	-1.87592297
C	-0.63727215	-2.50167775	-2.97230129
C	0.58280162	-1.91082066	-2.92966186

C	1.65881019	-2.09825416	-3.96977351
C	2.95329569	-1.89466693	-3.16348941
C	2.50312897	-1.18283766	-1.91002430
N	1.67948497	-0.39099125	0.89579944
C	3.34699771	-0.72646609	-0.91009290
C	2.90261420	-0.40574759	0.43727144
C	3.96105276	-0.19179427	1.51637203
C	3.11908890	0.36668458	2.66043551
C	1.72631576	-0.19688442	2.37069558
C	5.10555962	0.67287210	0.99646617
C	5.77157489	-0.05042218	-0.17124941
C	4.82085220	-0.72278002	-1.16753997
O	5.32589469	-1.24764010	-2.15634708
H	6.22769281	6.18278187	1.41557278
H	5.34414908	5.24741902	2.62682645
H	6.60715831	4.33114917	-0.83097672
H	3.17481577	4.70154926	1.72106516
H	5.18157946	3.32261176	-2.59343525
H	1.75367346	3.70237047	-0.04274527
H	1.74885278	2.62656702	-2.10272019
H	-7.49638154	5.83756500	-0.42804602
H	-6.47478538	6.65358560	0.76205843
H	-7.32954988	3.01469878	0.21906411
H	-4.17909003	5.92528915	0.41461133
H	-5.66562245	1.22110775	-0.07312695
H	-2.49634324	4.12380940	0.16522266
H	-2.17248663	1.76100733	-0.28472052
H	-0.34955689	-5.14870597	0.34923137
H	-0.03856073	-5.92149421	1.91380184
H	2.41164812	-4.21785343	-0.05066023
H	2.51312337	-2.81607643	0.92932468
H	0.50737417	1.57940806	2.21130264
H	0.81729035	1.05322740	3.87749862
H	-3.19339326	-1.83152392	4.09853459
H	-3.26087507	-0.57182670	1.99985266
H	-1.86299358	-3.21859218	1.42414751
H	-3.59053671	-3.00447953	1.74626893
H	-3.50057516	-3.05128921	-2.95681804
H	-5.58967399	-3.54072763	-1.78752161
H	-5.63131621	-3.63588284	-0.02802344
H	-0.84151862	-3.08203049	-3.86873690
H	1.59935651	-3.06785791	-4.47131972
H	3.71311755	-1.31613085	-3.68922830
H	4.36646052	-1.18071296	1.79599988

H	3.09930605	1.46357157	2.59984660
H	1.60855961	-1.19165957	2.82306747
H	5.83407921	0.87058377	1.79245852
H	4.71023288	1.64179399	0.67354363
H	6.43296281	-0.84904250	0.19484869
H	6.40685322	0.62286295	-0.75734250
H	1.12654454	-6.10958425	0.57546403
H	1.56227271	-1.32024490	-4.74024799
H	3.44368025	-2.84180139	-2.90855311
H	3.48785477	0.08885963	3.65292751
H	-0.76791551	-0.72082081	4.95022009
H	-2.08709016	0.35426197	4.46643101
H	-1.64098648	-2.56887329	3.63712336
H	-2.56755656	-4.46243679	-2.50729899
H	-3.35330062	-4.39690697	-0.26530366
H	-7.65532004	5.44246833	1.28413581
H	6.77909700	4.56397710	1.84763516
C	-1.21810042	1.68388245	-2.95228173
H	-0.62594712	1.42166430	-3.83472397
H	-1.62688518	2.68763360	-3.10089252
H	-2.05287817	0.98203613	-2.86241793
S	-0.17728210	1.65102593	-1.42346788
H	-3.72359468	-0.22171560	-0.27706212
H	0.65196200	-0.12661416	-1.68791859

Complex 3 (Fig. S2)

C	5.88238978	5.17280985	1.67559587
C	5.05037360	4.41200848	0.66225600
C	5.63404027	3.87276539	-0.49567682
C	3.67154742	4.22731330	0.82449829
C	4.88603571	3.17109806	-1.43785845
C	2.90182359	3.52762915	-0.11005075
C	3.50686990	2.97999896	-1.25187264
O	2.83702761	2.26881983	-2.18986140
C	-6.92859679	5.69123774	0.50074799
C	-5.90467717	4.60631752	0.29174678
C	-6.31681858	3.28355030	0.08256157
C	-4.53337057	4.87662388	0.28125385
C	-5.40089404	2.26103920	-0.12506759
C	-3.59253574	3.86376826	0.08221130
C	-4.03173834	2.55399405	-0.11575933
O	-3.17086160	1.50226018	-0.27987145
C	0.43459504	-5.41813762	1.06786906

C	1.43707652	-4.66771711	1.93236710
O	1.28094969	-3.49099107	2.23539814
N	2.51312611	-5.39213181	2.35623794
Ni	-0.52219624	-0.30188020	-0.07862125
N	-1.25869674	-0.51844265	1.76873789
C	0.56181281	0.73030879	2.78404931
C	-0.70839100	-0.05780109	2.83750992
C	-1.39636765	-0.49761564	4.11269258
C	-2.24938891	-1.65967708	3.56921562
C	-2.48077361	-1.26686128	2.13307652
N	-1.77165646	-1.85900355	-0.84815280
C	-2.74563942	-2.49689306	1.30827043
C	-3.03282260	-2.22390048	-0.14930686
C	-3.63590200	-3.47361286	-0.84403666
C	-2.87050766	-3.46771656	-2.15545172
C	-1.70008141	-2.55965668	-1.93839025
N	-4.04915581	-1.20973014	-0.36604605
C	-5.24987619	-1.66843509	-0.82968062
O	-6.23532328	-0.99297677	-1.08484422
C	-5.14259670	-3.19723905	-0.94051488
N	1.27058967	-1.86767543	-1.60040285
C	-0.67574469	-2.51065542	-2.94301562
C	0.61750244	-2.16056294	-2.78557616
C	1.62038346	-2.04577050	-3.89922530
C	2.95329568	-1.89466693	-3.16348948
C	2.59708865	-1.59914772	-1.73812534
N	1.71618660	-0.53280304	0.93262875
C	3.43949331	-1.15796035	-0.73221412
C	2.95365367	-0.72545683	0.57476255
C	3.97003811	-0.44370756	1.68191044
C	3.11908884	0.36668459	2.66043566
C	1.71933914	-0.19949901	2.38173563
C	5.23707163	0.22020355	1.14817214
C	5.86406140	-0.67481600	0.08255982
C	4.89806153	-1.14500952	-1.00719961
O	5.37867152	-1.54708485	-2.06599504
H	6.17979044	6.16107832	1.29890887
H	5.32737532	5.33230050	2.60663187
H	6.70268105	4.00065844	-0.66307467
H	3.17782660	4.64364838	1.70169326
H	5.35253288	2.75363505	-2.32601830
H	1.83066667	3.40917028	0.03412069
H	1.88639869	2.14118380	-1.94008891
H	-7.49208440	5.90071021	-0.41891145

H	-6.46144322	6.63081645	0.81645060
H	-7.38001934	3.04954367	0.07353142
H	-4.18687701	5.89710178	0.43436929
H	-5.73864152	1.24608878	-0.31908373
H	-2.52785450	4.08498912	0.07742509
H	-2.23768866	1.76770890	-0.49995103
H	0.24522552	-4.83107521	0.16464630
H	-0.51120702	-5.49966105	1.61403537
H	2.68090837	-6.34183869	2.06246410
H	3.22290865	-4.92408844	2.90267385
H	0.48128973	1.54740436	2.05647422
H	0.77587969	1.16649862	3.76675481
H	-3.17666840	-1.82078184	4.12976452
H	-3.32735356	-0.57350832	2.03481596
H	-1.89147099	-3.18171329	1.37987565
H	-3.61693564	-3.00417202	1.74595936
H	-3.47957333	-3.06976088	-2.98314555
H	-5.60564718	-3.54270145	-1.86947420
H	-5.70067162	-3.65201218	-0.11283236
H	-0.97343145	-2.82511532	-3.93979376
H	1.58574700	-2.90577481	-4.57451101
H	3.59264269	-1.11171046	-3.57402625
H	4.23841044	-1.41355697	2.13668969
H	3.15727667	1.43207304	2.39669504
H	1.60208866	-1.15302365	2.91656764
H	5.94707958	0.40089187	1.96536039
H	4.98577851	1.19756271	0.71957792
H	6.27420880	-1.58544815	0.54769171
H	6.70186035	-0.18959663	-0.42813926
H	0.75954926	-6.42298322	0.78078653
H	1.39587501	-1.15231695	-4.49457112
H	3.56392492	-2.80415955	-3.20364519
H	3.42235172	0.25494246	3.70689895
H	-0.68333610	-0.78286300	4.89459146
H	-2.00874811	0.32346804	4.51633016
H	-1.66115951	-2.58502446	3.60816911
H	-2.55263226	-4.46652507	-2.48059142
H	-3.41031537	-4.37826753	-0.27065402
H	-7.66294706	5.41282837	1.26725548
H	6.80542558	4.63486643	1.92578081
C	-1.18341152	1.31124753	-3.05871771
H	-1.19376878	2.25125860	-3.61843340
H	-2.21554075	1.01830913	-2.84586223
H	-0.71983255	0.53798606	-3.67847436

S	-0.24645271	1.54740531	-1.48391717
H	-3.81866440	-0.21266583	-0.32295044
H	0.79731596	-1.75899367	-0.69863043

Complex 4 (Fig. S2)

C	5.88238986	5.17280992	1.67559595
C	4.97203102	4.43704154	0.71275399
C	5.45712699	3.93864511	-0.50716481
C	3.61525951	4.23174359	0.99098276
C	4.63736058	3.24763646	-1.39621296
C	2.77499806	3.54367970	0.11114831
C	3.28388139	3.02708999	-1.09091345
O	2.54046570	2.32409109	-1.97514804
C	-6.92859681	5.69123777	0.50074800
C	-5.91941408	4.56940130	0.45551750
C	-6.34355326	3.24017992	0.31471528
C	-4.54449407	4.81142445	0.53140536
C	-5.43851613	2.18705695	0.25747917
C	-3.61636614	3.76848857	0.48380224
C	-4.06711956	2.45337388	0.35261535
O	-3.21458883	1.37997471	0.34896758
C	0.43459496	-5.41813765	1.06786912
C	1.15860139	-4.46718666	2.00830356
O	0.56703419	-3.63976480	2.69469893
N	2.51758193	-4.60218718	2.04805983
Ni	-0.06134102	-0.87064768	-0.10162758
N	-1.15953865	-0.63971404	1.75283611
C	0.58045005	0.69558518	2.78971727
C	-0.68443919	-0.10010126	2.81620392
C	-1.44467100	-0.44901606	4.07933286
C	-2.24938895	-1.65967715	3.56921582
C	-2.41723563	-1.34110737	2.11675374
N	-1.63888227	-2.03357301	-0.77662082
C	-2.70041295	-2.59726798	1.35307968
C	-2.92412757	-2.33625336	-0.11015340
C	-3.55263300	-3.56087458	-0.80925801
C	-2.87050787	-3.46771668	-2.15545183
C	-1.63475750	-2.64659240	-1.94089464
N	-3.92731832	-1.30428192	-0.36173284
C	-5.16830781	-1.76737573	-0.68927696
O	-6.18053144	-1.09690774	-0.83762582
C	-5.06318337	-3.29610363	-0.81430137
N	1.17864795	-1.61500386	-1.61994182

C	-0.63956970	-2.58648557	-2.93353547
C	0.63132354	-2.08586814	-2.78102233
C	1.63139522	-2.06045813	-3.91136736
C	2.95329591	-1.89466701	-3.16348985
C	2.52389915	-1.47925408	-1.77261698
N	1.73970294	-0.58151098	0.97008821
C	3.43670682	-1.08073867	-0.75535126
C	2.97136333	-0.68813932	0.56453622
C	3.98833584	-0.39311511	1.66480792
C	3.11908889	0.36668480	2.66043581
C	1.73908655	-0.23330454	2.41134254
C	5.22066370	0.32704454	1.13106967
C	5.85048734	-0.53092876	0.03613545
C	4.83624754	-1.07849692	-0.92678674
O	5.38292217	-1.67451885	-2.03589631
H	6.16785047	6.16204244	1.29259310
H	5.39474704	5.32652802	2.64441033
H	6.50438375	4.09054113	-0.76570810
H	3.19682255	4.62129166	1.91804933
H	5.02648237	2.86204197	-2.33482125
H	1.72194418	3.40870428	0.34333907
H	1.64198437	2.11886699	-1.60388105
H	-7.40614961	5.84722123	-0.47626436
H	-6.46209345	6.63930109	0.79079317
H	-7.40792160	3.02401208	0.23924685
H	-4.18503361	5.83378531	0.63480404
H	-5.78141581	1.16563115	0.11113778
H	-2.54998455	3.97075605	0.54892227
H	-2.28052149	1.61222801	0.08455426
H	0.05478241	-4.84203360	0.21653717
H	-0.42350190	-5.84841133	1.59166034
H	3.01524462	-5.17250390	1.38107894
H	3.04511493	-3.91838029	2.57340262
H	0.51271548	1.51188906	2.06121659
H	0.77552953	1.13154740	3.77615259
H	-3.20141670	-1.79958728	4.09320335
H	-3.22813565	-0.61938775	1.95975486
H	-1.87757393	-3.30885655	1.48232316
H	-3.60670470	-3.04804037	1.78145989
H	-3.51604587	-2.95980162	-2.88940122
H	-5.57872224	-3.64304089	-1.71503961
H	-5.56933590	-3.75412840	0.04460604
H	-0.88074007	-3.03629362	-3.89239876
H	1.58298011	-2.95411332	-4.54184845

H	3.61831491	-1.16010676	-3.62246156
H	4.30102231	-1.36084576	2.09750430
H	3.11395953	1.43434001	2.40360181
H	1.62404699	-1.17658677	2.96725783
H	5.94206736	0.51516189	1.93512054
H	4.92637218	1.29858902	0.71966720
H	6.42059278	-1.36462086	0.48566721
H	6.58915593	0.06596054	-0.52642677
H	1.06803213	-6.22793241	0.69291824
H	1.42538182	-1.19544186	-4.55737122
H	3.51774605	-2.83459817	-3.12829352
H	3.44692519	0.26610497	3.70095943
H	-0.77412175	-0.65912639	4.92044527
H	-2.08894413	0.39294591	4.37671485
H	-1.64820719	-2.56842154	3.68391954
H	-2.63556800	-4.44411743	-2.59834255
H	-3.27916325	-4.48514778	-0.28957893
H	-7.73192545	5.48325418	1.21871381
H	6.81293987	4.61958599	1.85581829
C	-1.21460960	1.23835913	-2.54184101
H	-1.26574039	2.21677201	-3.02879213
H	-2.23123694	0.86011503	-2.40272023
H	-0.66723726	0.54855782	-3.18962905
S	-0.36806903	1.41716746	-0.91300691
H	-3.74435695	-0.31325237	-0.18290802
H	6.31030978	-1.39850065	-2.10775413

Complex M (Fig. 5)

C	6.34085500	3.71474600	2.78470500
C	5.54495400	3.66988900	1.49819100
C	6.12202500	3.18479300	0.31299600
C	4.22040700	4.11467900	1.43408900
C	5.41102900	3.13914800	-0.88178000
C	3.48982200	4.07759600	0.24321200
C	4.08212000	3.58396800	-0.92505700
O	3.43226300	3.49758400	-2.11628700
C	-6.34788100	5.60754900	1.69672100
C	-5.41053000	4.44456000	1.49614300
C	-5.55567700	3.59513900	0.39192400
C	-4.37135000	4.18609600	2.39674300
C	-4.69309100	2.52314600	0.18229600
C	-3.49327700	3.12168300	2.19589000
C	-3.65091300	2.29161800	1.08615400

O	-2.80495000	1.21181800	0.94346300
C	-0.03213500	-6.06414100	0.34045500
C	0.76925600	-5.16604900	1.27036500
O	0.26224800	-4.57049500	2.21545100
N	2.10424700	-5.08299300	0.98256000
Ni	-0.08187400	-0.84774600	-0.12855400
N	-1.24982400	-1.18764900	1.87419100
C	0.65099800	-0.40423000	3.17580000
C	-0.69432200	-1.02676400	3.01944000
C	-1.44210200	-1.62772200	4.19117000
C	-2.40831500	-2.56236100	3.45137700
C	-2.54677400	-1.89237500	2.10107500
N	-1.78231800	-2.13611100	-0.91675500
C	-2.91053400	-2.94382500	1.08849200
C	-3.10870200	-2.39744700	-0.29900700
C	-3.88385200	-3.38885700	-1.21267500
C	-3.08980000	-3.29037100	-2.50111700
C	-1.78947100	-2.61862400	-2.12284200
N	-3.95823700	-1.21453000	-0.32783700
C	-5.18542800	-1.36999500	-0.91099100
O	-6.01917400	-0.49399200	-1.08173400
C	-5.31994800	-2.85165700	-1.28741200
N	1.09300600	-1.71538800	-1.69247600
C	-0.74613900	-2.52301800	-3.09660100
C	0.52834100	-2.08851500	-2.90186400
C	1.56100700	-2.06111700	-4.00079800
C	2.86936000	-2.11097000	-3.21157000
C	2.43236900	-1.78500800	-1.79460200
N	1.66494700	-1.43755600	1.09416600
C	3.33912200	-1.65585200	-0.71877700
C	2.89539600	-1.52853800	0.64227000
C	3.94008600	-1.50336300	1.76457700
C	3.13676600	-0.91353800	2.91655800
C	1.70541600	-1.34872900	2.57965800
C	5.20395100	-0.75573700	1.35203800
C	5.79750200	-1.45777700	0.13751600
C	4.79294700	-1.75282800	-0.98454400
O	5.26787700	-2.07723800	-2.07405700
H	7.13641800	4.47108800	2.74449000
H	5.70201400	3.95834800	3.64066700
H	7.15363000	2.83630400	0.32622700
H	3.74182800	4.50158300	2.33231600
H	5.86366400	2.76160500	-1.79413100
H	2.45975200	4.42671200	0.21920500

H	2.53814300	3.89005400	-2.05603500
H	-6.05331400	6.47564800	1.08996400
H	-6.36545700	5.93566600	2.74204700
H	-6.37235500	3.76215500	-0.30787500
H	-4.24651300	4.82549900	3.26884000
H	-4.86070900	1.83682200	-0.64262200
H	-2.68637700	2.91696600	2.89468400
H	-2.31325000	1.25908800	0.06958100
H	-0.47333400	-5.44923100	-0.45369600
H	-0.84518800	-6.52652500	0.90471400
H	2.45217600	-5.38298700	0.08282000
H	2.62541500	-4.34675000	1.43943200
H	0.69259300	0.57602100	2.69543100
H	0.87728800	-0.26363200	4.23909800
H	-3.36940700	-2.69237000	3.95994700
H	-3.31789400	-1.11389100	2.12228400
H	-2.14169700	-3.72456500	1.06951900
H	-3.84847200	-3.40617700	1.42706500
H	-3.59918600	-2.66895600	-3.25332100
H	-5.78990000	-2.96030700	-2.26912600
H	-5.98070100	-3.33339700	-0.55608800
H	-0.99885800	-2.86457800	-4.09656000
H	1.43899900	-2.87769200	-4.71844800
H	3.63455600	-1.41771000	-3.56239600
H	4.21736100	-2.54614300	2.00190400
H	3.20901100	0.18314100	2.90135800
H	1.50749200	-2.35907900	2.96849900
H	5.92120200	-0.72741700	2.18238700
H	4.95335100	0.28532800	1.10834200
H	6.23411500	-2.42381600	0.43409000
H	6.61206900	-0.88604600	-0.31900500
H	0.57671200	-6.84566000	-0.12539500
H	1.46927400	-1.11811400	-4.55643300
H	3.34437000	-3.09739800	-3.24015500
H	3.46246800	-1.25748700	3.90402600
H	-0.76921400	-2.12955200	4.89575700
H	-1.95765500	-0.82894800	4.74589400
H	-1.93873900	-3.54456000	3.33190000
H	-2.91387900	-4.25868000	-2.98626900
H	-3.83310400	-4.40131000	-0.80080000
H	-7.37470100	5.35176900	1.40970800
H	6.82600300	2.75302700	2.99472600
C	-2.35292400	0.51413300	-2.91933500
H	-2.70510300	1.43379600	-3.39949100

H	-3.21251900	0.00102400	-2.48391400
H	-1.89223400	-0.11960000	-3.68075000
S	-1.12262900	1.01197100	-1.65003800
H	-3.67016600	-0.32886300	0.09276600
C	0.96263900	1.04136400	0.15258400
H	1.73446700	0.91795300	0.90047700
H	0.14881400	1.69466100	0.46076700
H	1.35200300	1.22910400	-0.84278600
H	-0.33329500	3.31599100	-2.36229900
S	0.24967600	4.42187000	-2.89807600
C	-0.82612500	5.69680700	-2.10868700
H	-0.45207100	6.64807000	-2.50146900
H	-1.84316200	5.56587500	-2.49098600
C	-0.81028900	5.69355600	-0.58251100
H	-1.20046100	4.75190400	-0.18171700
H	0.20512200	5.83856800	-0.19787800
H	-1.44125300	6.50489600	-0.19718500

Complex C (Fig. 5)

C	-4.99737700	6.35998300	-1.87713900
C	-4.14295800	5.57369400	-0.90631700
C	-4.55603000	5.38775700	0.42298400
C	-2.92308500	5.00614000	-1.28789600
C	-3.79841800	4.65445900	1.33038000
C	-2.14640500	4.26812200	-0.38929100
C	-2.58908200	4.07896100	0.92294700
O	-1.89129400	3.36235800	1.85392400
C	7.38484000	2.87668200	-2.44080500
C	6.09965900	2.11777300	-2.26385000
C	6.12511600	0.77461100	-1.86333200
C	4.85842900	2.73149300	-2.45089600
C	4.95486800	0.06284100	-1.63312100
C	3.67030100	2.03727900	-2.22109400
C	3.72941400	0.71113900	-1.80434200
O	2.60262400	-0.03201300	-1.55093300
C	-2.94529400	-5.27392900	-0.24710100
C	-3.40335600	-4.11941300	-1.12541700
O	-2.84404200	-3.82193400	-2.17623400
N	-4.50284400	-3.44696900	-0.66426300
Ni	-0.90359300	-0.99246500	0.06960700
N	-0.04676600	-1.28098900	-1.93465900
C	-1.55254900	0.33598300	-2.95671200
C	-0.58813600	-0.80831500	-3.00280600

C	-0.28241300	-1.58965400	-4.26458200
C	0.26789100	-2.88841200	-3.64876100
C	0.81060400	-2.43363400	-2.32450900
N	0.42422600	-2.46334700	0.76714900
C	0.81104800	-3.59208800	-1.36705700
C	1.39001000	-3.25857900	-0.01711200
C	1.74453000	-4.53756900	0.78136000
C	1.29399900	-4.12824900	2.16815600
C	0.38669000	-2.94494200	1.97949100
N	2.68570300	-2.58768000	-0.09783800
C	3.77483000	-3.36788300	0.15358600
O	4.94605900	-3.02887300	0.03476300
C	3.25582200	-4.74310500	0.59245500
N	-2.00479000	-1.09331000	1.87729800
C	-0.38009600	-2.46365300	3.07898200
C	-1.45256500	-1.61950400	3.02474300
C	-2.23477200	-1.20511400	4.24909400
C	-3.52923400	-0.66658500	3.63806400
C	-3.21087000	-0.56417200	2.15795900
N	-2.66281700	-0.25947600	-0.78666500
C	-4.10940300	-0.02750700	1.20608900
C	-3.79777900	0.04290100	-0.19932200
C	-4.86791700	0.49581000	-1.19560400
C	-4.00947800	0.84210100	-2.40780600
C	-2.83696600	-0.12249100	-2.24904300
C	-5.75967100	1.59129900	-0.62531300
C	-6.41323300	1.06036200	0.64533900
C	-5.44146700	0.42962900	1.65422800
O	-5.85430500	0.31375000	2.81090900
H	-5.03100500	7.42599300	-1.61581900
H	-4.61161900	6.28483500	-2.89943600
H	-5.49894500	5.81992000	0.75309100
H	-2.56528100	5.14033900	-2.30711900
H	-4.13162600	4.50367000	2.35287200
H	-1.19543400	3.84403300	-0.70716700
H	-1.16490100	2.88190900	1.42638600
H	7.79838900	3.21071600	-1.47972300
H	7.24330200	3.77365900	-3.05416600
H	7.08213500	0.27557700	-1.72501600
H	4.81425900	3.77038200	-2.77041200
H	4.98780400	-0.97167300	-1.29976900
H	2.70812900	2.52697700	-2.36216400
H	1.78762400	0.47522900	-1.68499500
H	-2.19019100	-4.90386000	0.45767200

H	-2.48347400	-6.03920900	-0.87483800
H	-4.77049800	-3.52773000	0.30722100
H	-4.69553800	-2.55311400	-1.09665200
H	-1.13558900	1.19694400	-2.41920600
H	-1.79724900	0.66363000	-3.97385500
H	1.02020800	-3.38100700	-4.27461400
H	1.82928500	-2.04671900	-2.43383000
H	-0.20856500	-3.97221000	-1.24161600
H	1.41117400	-4.39129700	-1.82550700
H	2.14655700	-3.83147100	2.79979200
H	3.78019100	-5.08039800	1.49186500
H	3.48175900	-5.46655600	-0.20045400
H	-0.12898900	-2.87704500	4.05212000
H	-2.38578900	-2.03307700	4.94927700
H	-3.85073200	0.29385900	4.04429700
H	-5.50644700	-0.37330400	-1.44103100
H	-3.65505300	1.87941400	-2.32667800
H	-3.10425100	-1.11377700	-2.65086600
H	-6.51623900	1.89811200	-1.35944100
H	-5.15138100	2.47635100	-0.39951400
H	-7.15369000	0.28581000	0.39036700
H	-6.96258800	1.83593900	1.18861300
H	-3.76437100	-5.71900500	0.32715000
H	-1.68713900	-0.42174300	4.79085500
H	-4.38114600	-1.33593000	3.79495300
H	-4.53169900	0.73302500	-3.36514700
H	-1.16987300	-1.72552600	-4.89321300
H	0.46330400	-1.05119100	-4.87060100
H	-0.56240300	-3.58597800	-3.49128100
H	0.79265900	-4.93468100	2.71880100
H	1.15976600	-5.38756500	0.41660500
H	8.15463900	2.26272300	-2.92336300
H	-6.03304000	5.99837800	-1.88440300
C	5.15669500	-0.25538000	2.07198300
H	5.67736900	-0.64371100	2.94993100
H	5.82196900	-0.24604900	1.20770800
H	4.29963200	-0.89547900	1.84438100
S	4.47053200	1.41022000	2.41629500
H	2.77541100	-1.65611700	-0.49351500
C	0.12095000	0.82412000	0.69086600
H	-0.69149600	1.06860800	0.00294100
H	0.73533900	1.74413200	0.78318400
H	-0.23614600	0.59676900	1.69414800
H	0.82885900	0.07258500	0.33919400

S	6.15539300	2.49312400	2.99295300
C	6.74858200	3.26146200	1.42250800
H	7.75914600	3.60956600	1.67306800
H	6.84189400	2.47513700	0.66810000
C	5.87583500	4.41110900	0.93098000
H	4.86381400	4.05869600	0.70709300
H	5.80863800	5.20476700	1.68219100
H	6.29427500	4.83618100	0.01019700

The proton-bound MetH active site with an energy of 0.0 kcal/mol (Fig. S1)

C	-8.78344200	0.02518200	-5.27860400
C	-8.32361600	0.65251800	-3.95622100
O	-8.67716600	1.86337800	-3.72684000
O	-7.59580800	-0.09517400	-3.19794200
C	-8.68129000	5.11921300	-1.92476900
C	-7.71088400	4.29978500	-1.09217200
O	-7.14288300	4.83168900	-0.07963000
N	-7.51214800	3.03849500	-1.48617200
C	-2.79862900	4.88996300	5.31746000
C	-2.62916100	3.52877900	4.62226400
O	-3.37986100	3.34689400	3.56287300
O	-1.80352200	2.69311300	5.09290500
C	-3.34093900	-4.98493500	4.51000800
C	-3.33751600	-3.74953400	3.63159500
O	-3.95578700	-3.77973900	2.51699300
N	-2.69314100	-2.66320000	4.07447500
N	-5.61502600	1.45013700	0.13897700
C	-4.98833100	2.06001400	1.16979900
N	-5.23755000	3.34177900	1.46087800
N	-4.06713600	1.40001000	1.96192700
C	-3.75169600	0.06459000	1.76788000
O	-2.88117800	-0.51018700	2.51093200
C	-4.43436900	-0.57393800	0.70419100
N	-4.13395600	-1.99861300	0.45232700
C	-5.27009000	-2.67637200	-0.33273200
C	-5.59687900	-1.81075600	-1.55899500
N	-5.95170800	-0.45737300	-1.15981100
C	-5.32895100	0.14087400	-0.11830500
C	-6.46952100	-2.91060700	0.58935700
C	-2.77700400	-2.19979200	-0.19828400
H	-9.52363100	0.66145100	-5.76965100
H	-9.20293800	-0.97103700	-5.09723300

H	-9.50961800	5.45465100	-1.29011000
H	-9.07647200	4.54996100	-2.77005400
H	-6.86136200	2.45323400	-0.95088400
H	-7.97684200	2.62474900	-2.31618900
H	-3.83929900	5.01833300	5.63987400
H	-2.57549100	5.69866200	4.61107700
H	-2.69573200	-4.88570400	5.38745100
H	-3.01389600	-5.84573200	3.91940300
H	-2.20689200	-2.66598100	4.95710500
H	-2.70015800	-1.79073000	3.50579800
H	-4.72203300	3.75429300	2.24235700
H	-5.91905600	3.88391700	0.90509100
H	-4.85673900	-3.63701100	-0.65597600
H	-6.44830200	-2.22668700	-2.10255100
H	-4.74382900	-1.81270700	-2.25572300
H	-6.62512100	0.01889800	-1.79426900
H	-6.17184100	-3.49416100	1.46490800
H	-6.90696800	-1.96427700	0.91684800
H	-2.57318000	-3.27156300	-0.25569600
H	-2.02682800	-1.71329700	0.42320200
H	-2.77564300	-1.74587500	-1.18778900
C	8.30658900	2.86147700	2.71760900
C	9.05511900	3.31960000	1.46218600
H	7.32246500	2.45574700	2.45718700
C	9.37555700	2.17986100	0.47781800
H	8.50020600	4.08943500	0.91223200
H	10.01532400	3.78263500	1.74284600
O	9.32652300	0.97648600	0.93344200
O	9.70379400	2.50835800	-0.72446100
H	9.49833500	-0.30716400	-0.04275400
O	8.92360600	4.91810400	-1.56156700
N	9.63166700	-1.13930100	-0.67964500
C	10.02929200	5.82691500	-1.63892400
H	9.22711300	3.98957200	-1.28904000
C	9.31730000	-2.46974900	-0.43666100
C	10.18552000	-1.07019300	-1.92951600
C	9.48388600	7.20147300	-2.02834300
H	10.77334700	5.50057800	-2.38837800
H	10.56574800	5.90183600	-0.67545600
C	8.65406300	-2.94285000	0.82218800
C	9.71098800	-3.15294100	-1.57731200
N	10.25655900	-2.27498100	-2.51441400
H	10.50125700	-0.13264400	-2.35615500
H	8.75872600	7.54022500	-1.28016100

C	7.20236000	-2.43699700	0.98942400
H	9.23789700	-2.62657800	1.69979900
H	8.66238200	-4.04183000	0.82200300
H	9.63129200	-4.21098300	-1.77889600
Co	0.60025100	-1.27715600	-0.56739300
H	6.57991000	-2.75514700	0.14518800
N	0.39076300	-0.07119700	-1.97257200
N	0.37632100	0.12072800	0.73298100
N	0.57742100	-2.53523500	-1.93957800
C	0.62033800	-0.60083100	-3.35058900
C	0.06884300	1.21265300	-2.00492000
C	0.01117400	1.44130000	0.43998500
C	0.47307200	-0.03052700	2.08883800
C	0.90269900	-3.82320100	-1.98071500
C	0.14825100	-2.05382900	-3.28962300
C	-0.10326200	0.41833700	-4.26094900
C	-0.02701200	1.73503700	-3.43323500
C	-0.13916700	1.96159000	-0.82300600
C	-0.18914200	2.24441700	1.71598000
C	0.14629100	1.24306900	2.84203100
C	0.85282600	-1.21571300	2.71627400
C	1.33414200	-4.51365300	-0.82503900
C	0.77317800	-4.39703900	-3.38836300
C	0.73320400	-3.10655100	-4.25940600
H	-0.89466800	2.38661200	-3.58176200
H	-0.69526300	1.12367500	3.53272200
C	1.13817700	-2.41152300	2.07889900
H	0.93071800	-1.19388700	3.79914900
C	1.40962400	-3.92594200	0.41808300
H	1.75322600	-2.81979200	-4.54598100
N	1.04185200	-2.61975500	0.72676700
C	1.54990400	-3.68316300	2.80925800
C	1.95301700	-4.62872100	1.65607300
H	1.55244500	-5.64275600	1.76479100
H	-3.60755400	1.97870300	2.73173700
H	0.46586200	3.12359500	1.72747400
H	1.00267400	1.56982800	3.44576900
H	-0.42818500	3.00295300	-0.91556300
H	0.86793100	2.31922300	-3.69465400
H	0.35433100	0.50749300	-5.25106500
H	-1.15230000	0.12225500	-4.39456000
H	1.70375800	-0.59446200	-3.54744300
H	-0.95321000	-2.06476400	-3.33259300
H	0.14136200	-3.22172900	-5.17304300

H	-0.15596500	-4.97845800	-3.49724600
H	1.60352700	-5.06321000	-3.64800500
H	1.65003700	-5.54738000	-0.92533000
H	3.04570500	-4.71923000	1.58401200
H	0.70132600	-4.08451500	3.38292800
H	2.36293800	-3.50272200	3.52065800
H	7.18489700	-1.34249900	1.03053700
H	6.75507500	-2.82125900	1.91576600
H	-7.23840100	-3.46448300	0.03961200
H	8.15862500	3.69167700	3.42200500
H	8.86034700	2.06090200	3.21683500
H	8.96752300	7.13722800	-2.99253200
H	10.28950200	7.94444700	-2.10480100
H	-4.06630900	-2.51330900	1.37352800
H	-1.21734700	2.61300700	1.80424500
H	-2.13247200	4.95958100	6.18046200
H	-8.17166800	6.01640300	-2.29357500
H	-4.36470000	-5.18621500	4.84378600
H	-7.91895400	-0.10031000	-5.94338900

The proton-bound MetH active site with an energy of 13.0 kcal/mol (Fig. S1)

C	-8.91128400	0.46927900	-5.00098600
C	-8.38045700	1.29019400	-3.82564700
O	-8.52587800	2.57098300	-3.87627500
O	-7.78677900	0.63391100	-2.89521800
C	-8.74218200	5.21166300	-1.16836500
C	-7.42121800	4.49472600	-0.95678000
O	-6.75532600	4.66237900	0.11405200
N	-7.01006700	3.70272600	-1.96438000
C	-2.67727800	4.31088700	5.86822900
C	-2.49820000	3.06100300	4.99926400
O	-3.19588500	3.04740100	3.88027500
O	-1.72373500	2.14340000	5.37984100
C	-3.20509700	-5.44088700	4.11210300
C	-4.00623400	-4.79001400	2.99395600
O	-4.94906100	-5.41569100	2.43306400
N	-3.64818800	-3.53439800	2.65886200
N	-5.58239000	1.57084200	0.50017200
C	-4.84749100	2.08057200	1.53721600
N	-5.00224600	3.34751000	1.92644700
N	-3.96440400	1.27491500	2.15781000
C	-3.73933400	-0.08779300	1.81856600

O	-2.89896200	-0.74553400	2.48189300
C	-4.50055500	-0.57541000	0.70029400
N	-4.34547700	-1.93840200	0.27661800
C	-5.52477200	-2.47068100	-0.46576600
C	-5.91519900	-1.47625900	-1.58537000
N	-6.13556900	-0.14341300	-1.01797500
C	-5.39490500	0.25767800	0.03639200
C	-6.67750300	-2.79882400	0.49229000
C	-3.03596400	-2.25065900	-0.34807500
H	-9.62138700	1.05237100	-5.59209800
H	-9.38161700	-0.44916800	-4.63644800
H	-9.28502700	5.25796600	-0.22124800
H	-9.34828900	4.71471300	-1.93047800
H	-6.08669000	3.29280700	-1.90463800
H	-7.63284500	3.35524400	-2.74422700
H	-3.73130000	4.42461900	6.15046100
H	-2.39329600	5.20552000	5.30073300
H	-2.38840800	-4.81164800	4.47762300
H	-2.79113200	-6.38741800	3.74905700
H	-2.92319900	-3.00739900	3.12235800
H	-4.09253500	-3.03851500	1.87928000
H	-4.42777500	3.64176500	2.73421100
H	-5.60143500	3.97596200	1.38614100
H	-5.19123200	-3.40030900	-0.93986100
H	-6.83248700	-1.76519400	-2.10197500
H	-5.10846000	-1.44250900	-2.33389700
H	-6.78957700	0.44927600	-1.56164800
H	-6.37730600	-3.60443500	1.17045200
H	-6.96220900	-1.92358900	1.08536700
H	-2.92068500	-3.33710800	-0.40919200
H	-2.23263900	-1.85446000	0.27348000
H	-2.93637200	-1.81851000	-1.35721100
C	8.36562800	2.61263900	2.80718000
C	9.06059400	3.22768300	1.58927200
H	7.42982300	2.12354300	2.51495600
C	9.48390700	2.19699000	0.52613700
H	8.43031200	3.97658300	1.09324500
H	9.97209500	3.76281700	1.90146900
O	9.48349700	0.95919600	0.87747300
O	9.83472700	2.64703400	-0.62818600
H	9.75609100	-0.31075100	-0.08329800
O	8.95281700	5.05777400	-1.32227100
N	9.96153700	-1.17512700	-0.65530400
C	9.99323400	6.03252100	-1.17856100

H	9.29274900	4.12802600	-1.09880500
C	9.59080300	-2.48444200	-0.37907400
C	10.69889400	-1.19413100	-1.80846300
C	9.40710700	7.40265300	-1.51910500
H	10.84668300	5.82054700	-1.84848600
H	10.39844300	6.05027300	-0.15030500
C	8.72691300	-2.86672500	0.78517100
C	10.13753400	-3.24452300	-1.40178300
N	10.83300000	-2.43444000	-2.29911700
H	11.10173900	-0.29474200	-2.24385300
H	8.57114300	7.62739400	-0.84746200
C	7.23665500	-2.49807700	0.59680000
H	9.09624900	-2.38299400	1.70060200
H	8.81792800	-3.95055500	0.94261400
H	10.07020100	-4.31270100	-1.54537000
Co	0.60935500	-1.22838700	-0.67759800
H	6.82916100	-2.97422000	-0.30248600
N	0.35659000	0.10638500	-1.95044200
N	0.41955300	0.03497900	0.76003700
N	0.55552400	-2.34791000	-2.16405800
C	0.53158400	-0.28735900	-3.38101200
C	0.03543200	1.38771400	-1.84773300
C	0.06731000	1.37963400	0.60828800
C	0.53350800	-0.25663300	2.09216700
C	0.88532000	-3.62182500	-2.34031000
C	0.06898700	-1.74331900	-3.44187600
C	-0.23166800	0.80949500	-4.15910000
C	-0.11701200	2.04292100	-3.21535200
C	-0.12236700	2.02108700	-0.59337100
C	-0.06684800	2.06259200	1.96218400
C	0.21658300	0.93292300	2.97604400
C	0.91140900	-1.49914800	2.59221200
C	1.35423000	-4.41810500	-1.27019600
C	0.70563600	-4.05929000	-3.79063200
C	0.61983600	-2.69214600	-4.53186800
H	-0.98715500	2.70671700	-3.26783800
H	-0.64658800	0.74773200	3.62447700
C	1.18884200	-2.62322500	1.83207300
H	0.99265300	-1.59070200	3.67091600
C	1.45017900	-3.95631700	0.02272700
H	1.62471200	-2.36799200	-4.83252100
N	1.08012600	-2.68962200	0.46742200
C	1.60965200	-3.96129300	2.42389500
C	2.01361900	-4.77581000	1.17603800

H	1.62622800	-5.80040800	1.18158400
H	-3.43815000	1.74547000	2.96435200
H	0.65188000	2.88726900	2.04778600
H	1.05872500	1.16863000	3.63823000
H	-0.39619100	3.07099200	-0.57521600
H	0.76842000	2.64907900	-3.45971800
H	0.18062000	0.99268200	-5.15637300
H	-1.28552700	0.52175400	-4.27196200
H	1.60606000	-0.25249500	-3.62046000
H	-1.03281000	-1.76062500	-3.43822300
H	-0.00975200	-2.72677700	-5.42683400
H	-0.22223500	-4.63861200	-3.91708300
H	1.53029700	-4.68794200	-4.14505200
H	1.66979900	-5.43555700	-1.47832700
H	3.10705200	-4.84348200	1.08683400
H	0.76610800	-4.42760900	2.95330900
H	2.42350200	-3.85190100	3.14862500
H	7.12521600	-1.41401900	0.48777200
H	6.63794900	-2.81719400	1.45997600
H	-7.55926300	-3.12575800	-0.07261500
H	8.13285800	3.37495100	3.56362400
H	8.99982300	1.84325000	3.25745900
H	9.02236300	7.39854700	-2.54506800
H	10.16185000	8.19549500	-1.42531700
H	-6.28013700	2.16450700	0.06833100
H	-1.06354700	2.49400300	2.10632500
H	-2.06135500	4.23473100	6.76661800
H	-8.54401800	6.23992900	-1.49445000
H	-3.87337800	-5.67634100	4.94775400
H	-8.07151200	0.17802200	-5.64507700

The proton-bound MetH active site with an energy of 2.1 kcal/mol (Fig. S1)

C	8.51480400	-0.65543200	5.53436300
C	8.22092600	0.07130400	4.20490100
O	8.59987700	1.29881600	4.12416900
O	7.60522900	-0.59640800	3.29121600
C	8.64607600	4.62653300	2.48618200
C	8.59507200	3.68470000	1.31046200
O	8.62480500	4.17271900	0.12916100
N	8.46222500	2.38660500	1.59193800
C	2.89601100	5.02435000	-4.85456800
C	3.45363300	3.74781000	-4.22220700

O	4.71217600	3.72727600	-3.94548300
O	2.64662300	2.76083900	-3.98535400
C	3.09244300	-4.89369000	-4.62310800
C	3.46439700	-4.26969200	-3.28327500
O	3.86164700	-5.00096500	-2.33750200
N	3.38937800	-2.91849000	-3.19769900
N	6.68398100	1.20003100	-0.45287000
C	6.37699000	1.98494000	-1.49199200
N	7.12944500	3.05147200	-1.81933200
N	5.26367800	1.75081700	-2.26422400
C	4.44277400	0.66970000	-2.03931700
O	3.37563700	0.54405100	-2.85448700
C	4.73175800	-0.19464700	-0.98736800
N	3.97434900	-1.38881900	-0.72188400
C	4.69093000	-2.34379000	0.18959900
C	5.17935100	-1.57784100	1.43529500
N	6.06752600	-0.49841900	1.00641900
C	5.83586900	0.17365200	-0.13470800
C	5.83675000	-3.06916800	-0.53116600
C	2.55241200	-1.16508800	-0.35097700
H	9.28527500	-0.12033100	6.09445600
H	8.82798800	-1.68615000	5.33847300
H	9.41864800	5.38433100	2.32323400
H	8.82888100	4.10014500	3.42681000
H	8.17988400	1.76057700	0.83831300
H	8.47578400	2.00918000	2.56567000
H	3.49780600	5.29059700	-5.72950200
H	2.97595600	5.84760500	-4.13558800
H	2.46417900	-4.24251700	-5.23963500
H	2.56876700	-5.83503000	-4.43978300
H	3.04488200	-2.35204500	-3.95719300
H	3.65366100	-2.41792300	-2.33392800
H	6.80928800	3.65269000	-2.56691400
H	7.83136900	3.41252300	-1.14143000
H	3.94282900	-3.08319200	0.49278700
H	5.74425000	-2.21168800	2.12176800
H	4.31723000	-1.17437600	1.98853800
H	6.81472700	-0.25068400	1.68088100
H	5.43012200	-3.77715500	-1.25680200
H	6.50327800	-2.36441700	-1.03783700
H	2.03350900	-2.12605300	-0.32151300
H	2.07878200	-0.54533200	-1.11091700
H	2.43989500	-0.67221700	0.62636900
C	-8.31768800	3.23157300	-2.56573400

C	-9.07507900	3.66082000	-1.30625200
H	-7.37267200	2.74253400	-2.30328700
C	-9.49809100	2.48426000	-0.40741800
H	-8.49180900	4.35887200	-0.69347800
H	-9.99501700	4.20081200	-1.58388100
O	-9.49004600	1.31123800	-0.93743200
O	-9.86156400	2.75798100	0.79723100
H	-9.84807800	-0.06894900	-0.17640000
O	-8.97270600	5.05284100	1.80554700
N	-10.11164400	-0.99526700	0.25818800
C	-10.04393900	5.98973700	1.97483600
H	-9.31651200	4.15945200	1.46832000
C	-9.79169200	-2.26800200	-0.19557300
C	-10.88427300	-1.14335400	1.37839600
C	-9.43802300	7.32456900	2.40798500
H	-10.76629300	5.64865300	2.73893500
H	-10.61785600	6.12912000	1.04072100
C	-8.91464400	-2.52027800	-1.38491600
C	-10.40176500	-3.13918000	0.69394700
N	-11.08807300	-2.43312300	1.68162900
H	-11.25901900	-0.29679600	1.92944600
H	-8.73924000	7.68280400	1.64383200
C	-7.42394700	-2.19384600	-1.13541000
H	-9.26474700	-1.92804000	-2.24270600
H	-9.01503200	-3.57680600	-1.67010300
H	-10.38595300	-4.21887500	0.68389000
Co	-0.92105800	-1.32614900	0.60644800
H	-7.03327100	-2.77814700	-0.29423600
N	-0.66306400	-0.22616600	2.08245100
N	-0.69004300	0.15980100	-0.60068000
N	-0.91828100	-2.67811400	1.89553800
C	-0.87318400	-0.84080800	3.43031700
C	-0.30124500	1.04276100	2.19479300
C	-0.29504900	1.44666500	-0.22413700
C	-0.80623700	0.09849900	-1.96294900
C	-1.26698200	-3.95736400	1.85655200
C	-0.44985700	-2.29956900	3.26377500
C	-0.09017200	0.09040700	4.38359000
C	-0.14334900	1.46048200	3.64668000
C	-0.10450000	1.87224600	1.06686900
C	-0.08434200	2.33119100	-1.44596100
C	-0.49962800	1.43052700	-2.62883800
C	-1.17338600	-1.04155600	-2.66751300
C	-1.69484600	-4.56263800	0.65178800

C	-1.14723100	-4.62721100	3.22609600
C	-1.04949800	-3.39587600	4.17586600
H	0.75192300	2.07007300	3.81124100
H	0.30223600	1.34693000	-3.36995900
C	-1.44671800	-2.28058100	-2.10776300
H	-1.24996100	-0.95436600	-3.74727500
C	-1.73780300	-3.89624400	-0.55053000
H	-2.05389300	-3.09728200	4.50326100
N	-1.36861700	-2.57027000	-0.77128400
C	-1.83102600	-3.50385500	-2.92543500
C	-2.23926800	-4.52260400	-1.84229000
H	-1.81555600	-5.51956400	-2.00459500
H	5.02641400	2.46572000	-3.01274300
H	-0.68468300	3.24540800	-1.37923400
H	-1.38506200	1.81441500	-3.15251500
H	0.21191300	2.89722800	1.22922200
H	-1.00649600	2.05733800	3.97836800
H	-0.51707100	0.12884500	5.39042300
H	0.95047200	-0.24968600	4.46615900
H	-1.95038400	-0.81073700	3.65643000
H	0.65049300	-2.34801500	3.27766100
H	-0.44312300	-3.58812600	5.06645900
H	-0.24053100	-5.24833000	3.28220200
H	-2.00115400	-5.27587700	3.45027400
H	-2.01263400	-5.60004200	0.67497100
H	-3.33124200	-4.63947600	-1.80152200
H	-0.97057800	-3.85960100	-3.51012900
H	-2.63603600	-3.28748600	-3.63580100
H	-7.30401000	-1.13163100	-0.89675800
H	-6.81729600	-2.41474300	-2.02364600
H	6.43675200	-3.62706500	0.19806600
H	-8.09095500	4.09161500	-3.21124100
H	-8.90646700	2.50346300	-3.13134100
H	-8.87805500	7.19310000	3.34052500
H	-10.21504000	8.08532200	2.56421600
H	3.11066900	1.43238400	-3.36106000
H	0.96329900	2.63955700	-1.53980700
H	1.85164600	4.88915600	-5.14087800
H	7.68434300	5.14921400	2.55855700
H	4.00775000	-5.12374200	-5.18193100
H	7.59953100	-0.69515300	6.13981700

The proton-bound MetH active site with an energy of 33.6 kcal/mol (Fig. S1)

C	-8.86431800	0.07789200	-5.10447800
C	-8.36635300	0.79019600	-3.84140400
O	-8.64452300	2.03790100	-3.71368000
O	-7.68123400	0.06561300	-3.03112000
C	-8.68725200	5.20397700	-1.80301000
C	-7.66174800	4.39863500	-1.01279300
O	-7.08302900	4.92681700	-0.00505700
N	-7.43568800	3.15191300	-1.44032200
C	-2.76065900	4.98556600	5.40364800
C	-2.23430900	3.87254100	4.47225300
O	-3.02640400	3.51548300	3.49724400
O	-1.08435900	3.38308600	4.70971800
C	-3.41139000	-4.89068800	4.69949300
C	-3.89819700	-4.48752200	3.31178200
O	-4.57794600	-5.30100100	2.62483100
N	-3.58120400	-3.24471600	2.89864500
N	-5.49399700	1.49709500	0.16151700
C	-4.83906000	2.09087000	1.16811600
N	-5.07722000	3.37607600	1.49475600
N	-3.88164600	1.42043900	1.90561800
C	-3.56633200	0.06557900	1.70153600
O	-2.66538300	-0.47653200	2.44417900
C	-4.26746700	-0.56597600	0.63826600
N	-4.04973500	-1.97065000	0.35234900
C	-5.17771000	-2.60925800	-0.39341300
C	-5.54137000	-1.72793100	-1.60920700
N	-5.84710200	-0.37702700	-1.16598000
C	-5.19017700	0.18575900	-0.12491400
C	-6.37005800	-2.87843900	0.53371100
C	-2.71841500	-2.27636400	-0.20669900
H	-9.60415300	0.68733100	-5.63067200
H	-9.29420900	-0.89464900	-4.84068400
H	-9.51945200	5.47284900	-1.14197500
H	-9.07004500	4.64503500	-2.66087400
H	-6.77496000	2.56045500	-0.92235300
H	-7.90914500	2.74989800	-2.27138100
H	-3.69110800	4.65793500	5.88350100
H	-2.99640800	5.88235400	4.81776400
H	-2.66776500	-4.20056900	5.11060800
H	-2.98499100	-5.89708800	4.64881300
H	-3.06212700	-2.57237200	3.44597300
H	-3.87877800	-2.87768000	1.97805000

H	-4.53698400	3.78229100	2.25925400
H	-5.77928600	3.92005900	0.97697900
H	-4.79609200	-3.57090000	-0.75826100
H	-6.41396700	-2.10323400	-2.14919800
H	-4.69365800	-1.73106800	-2.31827700
H	-6.56885700	0.11920200	-1.71330300
H	-6.09821100	-3.62822500	1.28316300
H	-6.68803600	-1.96200300	1.03942800
H	-2.56982000	-3.36285300	-0.21793500
H	-1.96315000	-1.82697800	0.43999900
H	-2.58472200	-1.88640500	-1.23223900
C	8.30572100	2.81437000	2.75393300
C	8.95880400	3.22709500	1.43166600
H	7.28298500	2.45675100	2.58829500
C	9.12998200	2.07064300	0.43115800
H	8.39820500	4.02436800	0.92815800
H	9.96309000	3.64009900	1.61942900
O	9.02500800	0.87042200	0.88841100
O	9.39955500	2.37809700	-0.79102400
H	9.18715400	-0.37476600	-0.14501900
O	8.76867800	4.85703000	-1.57221800
N	9.29905700	-1.17993700	-0.81896300
C	9.94076700	5.67894700	-1.67004000
H	9.01049000	3.90569200	-1.32336600
C	9.04808000	-2.52671000	-0.59449600
C	9.73891200	-1.05312500	-2.10889200
C	9.49765400	7.09387900	-2.04301900
H	10.64067100	5.29814100	-2.43554800
H	10.50014800	5.70596700	-0.71739700
C	8.52221300	-3.05534800	0.70591900
C	9.35870500	-3.16103500	-1.78761000
N	9.79308200	-2.23640100	-2.73799900
H	9.98855100	-0.09232500	-2.52736500
H	8.81602500	7.48500000	-1.27960600
C	7.13501600	-2.48927600	1.08643000
H	9.22547100	-2.82965100	1.52229200
H	8.46916300	-4.15060600	0.63583200
H	9.29478400	-4.21438700	-2.01730100
Co	0.75795800	-1.25125700	-0.49100200
H	6.39766300	-2.71634000	0.30690000
N	0.45670900	-0.05018600	-1.88663900
N	0.67764600	0.28977600	0.84567900
N	0.62137000	-2.52723200	-1.82950100
C	0.59726500	-0.61339200	-3.27153300

C	0.11080700	1.21937600	-1.91347900
C	0.10087600	1.56923200	0.53650300
C	0.64030400	0.06156600	2.22857400
C	0.88931400	-3.81877300	-1.84716600
C	0.10612900	-2.05804900	-3.15159500
C	-0.17828700	0.39374500	-4.14804700
C	-0.07875400	1.71397200	-3.33214800
C	-0.10100700	2.00597800	-0.73494300
C	-0.20272000	2.28360400	1.83346300
C	-0.07180100	1.18661400	2.91363500
C	1.13059600	-1.08919600	2.80215600
C	1.32373900	-4.49965700	-0.67993900
C	0.65755200	-4.42542300	-3.23039300
C	0.59414800	-3.15157400	-4.13118800
H	-0.96639600	2.34698300	-3.43141000
H	-1.07121700	0.81182600	3.18812900
C	1.43519400	-2.28493500	2.13692500
H	1.18391200	-1.10644900	3.88488400
C	1.45624700	-3.89403500	0.54284300
H	1.59847000	-2.90486600	-4.49856100
N	1.20820400	-2.54682800	0.82105300
C	1.96850700	-3.50225200	2.86754700
C	1.86745800	-4.61885300	1.80852900
H	1.11181400	-5.36606800	2.08115200
H	-3.39244600	1.96304400	2.64302800
H	0.52361200	3.09110600	2.00083300
H	0.39915400	1.54366300	3.83018900
H	-0.50797600	3.00209800	-0.86327300
H	0.78549300	2.31847100	-3.64490100
H	0.23471000	0.48587000	-5.15599500
H	-1.22808200	0.08769900	-4.23390200
H	1.66820400	-0.61950300	-3.52450000
H	-0.99302800	-2.04848100	-3.10004000
H	-0.06642900	-3.27321500	-4.99391600
H	-0.29030900	-4.98174600	-3.25339200
H	1.45382200	-5.11847300	-3.51999500
H	1.54484800	-5.55879400	-0.75288200
H	2.81256400	-5.15521300	1.67093700
H	1.37996800	-3.70919700	3.76775100
H	3.00260000	-3.32909600	3.19220800
H	7.18860500	-1.40067500	1.19869300
H	6.78208200	-2.91599300	2.03511700
H	-7.22075200	-3.25503900	-0.04759100
H	8.26400400	3.65506900	3.45975900

H	8.86172600	1.99016200	3.21041200
H	8.96007900	7.07668600	-2.99756500
H	10.35790500	7.77098400	-2.13169700
H	1.61919800	0.06864100	0.35867600
H	-1.19341900	2.74615400	1.85600900
H	-2.01518900	5.22476600	6.16551500
H	-8.22771600	6.13808200	-2.14507000
H	-4.26648800	-4.93080600	5.38449800
H	-8.01554200	-0.11001800	-5.77561000

The proton-bound MetH active site with an energy of 11.0 kcal/mol (Fig. S1)

C	-8.70355200	0.34689400	-5.21254100
C	-8.31985000	1.01748500	-3.88745200
O	-8.51068500	2.28312300	-3.78080900
O	-7.80021600	0.24126500	-3.00467600
C	-8.51487800	5.35821300	-1.73995100
C	-7.49243600	4.52452100	-0.97954800
O	-6.90006800	5.01880700	0.03711400
N	-7.28721900	3.28718000	-1.44178300
C	-2.65589500	4.84945500	5.50722800
C	-2.23280600	3.64750900	4.62966200
O	-2.93610100	3.44013300	3.54802300
O	-1.24279000	2.94489300	5.00942500
C	-3.38029900	-4.99195800	4.46726700
C	-4.10301300	-4.49868400	3.22346300
O	-4.84700400	-5.28397100	2.56977000
N	-3.89498100	-3.21269500	2.88871300
N	-5.45603600	1.57494200	0.15816100
C	-4.75218100	2.11808300	1.16059500
N	-4.90928800	3.41283000	1.49630400
N	-3.83006000	1.38126300	1.87947700
C	-3.61275200	0.00525100	1.67095200
O	-2.73025300	-0.59394700	2.38752300
C	-4.39802900	-0.57738900	0.63224000
N	-4.35066100	-2.00415400	0.38365300
C	-5.54451300	-2.54009500	-0.33673100
C	-5.82372900	-1.65126400	-1.56643900
N	-5.99500600	-0.27234900	-1.14061900
C	-5.26928500	0.24223700	-0.12017800
C	-6.74772000	-2.66550600	0.60691600
C	-3.06707300	-2.51121200	-0.12998000
H	-9.35612700	0.99499000	-5.80425900

H	-9.19563800	-0.61234300	-5.01910100
H	-9.35030100	5.59929700	-1.07192000
H	-8.89481100	4.83293500	-2.62000800
H	-6.64309600	2.66954600	-0.93163000
H	-7.77220100	2.92076600	-2.28088900
H	-3.67279300	4.68970900	5.88679500
H	-2.67358400	5.76544200	4.90458600
H	-2.70392000	-4.24591100	4.89607200
H	-2.81099500	-5.89395200	4.21747400
H	-3.27676200	-2.57997400	3.37833500
H	-4.26404300	-2.81701300	2.00633700
H	-4.35331400	3.78001300	2.27047200
H	-5.59952600	3.98867700	0.99732100
H	-5.26730500	-3.54399400	-0.68012100
H	-6.72963000	-1.94424700	-2.10180100
H	-4.97949000	-1.74868500	-2.27311000
H	-6.68786400	0.27122000	-1.67807400
H	-6.53608600	-3.41200900	1.37873000
H	-6.97441500	-1.70808300	1.08477200
H	-3.07524400	-3.60753200	-0.10612600
H	-2.27984000	-2.15177200	0.53419500
H	-2.85402900	-2.17644200	-1.16254400
C	8.41609900	2.67494800	2.88381000
C	9.07932000	3.12764400	1.57967000
H	7.39677400	2.31740200	2.69878800
C	9.26252400	2.00268000	0.54592500
H	8.52087100	3.93805300	1.09497300
H	10.08068400	3.53799700	1.78773600
O	9.14768100	0.78865000	0.96273400
O	9.55216900	2.34825700	-0.66144100
H	9.30638300	-0.42057400	-0.11026700
O	8.94384200	4.85191000	-1.37814300
N	9.41358000	-1.20389900	-0.81093500
C	10.11773500	5.67607300	-1.41295300
H	9.17835700	3.89287800	-1.15289700
C	9.14621500	-2.55447200	-0.63312200
C	9.86301900	-1.03925100	-2.09327300
C	9.68618900	7.10206700	-1.75657200
H	10.84238900	5.31888200	-2.16678300
H	10.64595000	5.67390400	-0.44228600
C	8.60659100	-3.11922100	0.64623100
C	9.45642200	-3.15218300	-1.84505300
N	9.90789600	-2.20155100	-2.76127300
H	10.12701300	-0.06804900	-2.47752600

H	8.97902600	7.46939500	-1.00466500
C	7.21759200	-2.56002800	1.02952300
H	9.30264000	-2.91853700	1.47510000
H	8.55147800	-4.21193200	0.54450000
H	9.38236400	-4.19658000	-2.11005900
Co	0.67321200	-1.22948100	-0.51908500
H	6.48631500	-2.76488000	0.23810600
N	0.54910600	0.02006200	-1.91586300
N	0.48033500	0.14355400	0.81243800
N	0.69818400	-2.45616200	-1.94652100
C	0.72623700	-0.49280000	-3.31262200
C	0.20049900	1.29307800	-1.89717500
C	0.10710200	1.47230200	0.55409700
C	0.49129100	-0.06934900	2.15698200
C	0.97150600	-3.74409800	-1.99831800
C	0.21334100	-1.93427000	-3.25957300
C	-0.00887900	0.55846900	-4.17497900
C	0.07855000	1.84893600	-3.30922200
C	-0.02437400	2.01499300	-0.70116600
C	-0.11477600	2.22233400	1.85040700
C	0.10942200	1.15591500	2.93747300
C	0.83482800	-1.28411400	2.76225500
C	1.38816300	-4.47277700	-0.85724500
C	0.76407700	-4.29640900	-3.40650000
C	0.71619500	-2.99539400	-4.26557900
H	-0.79379600	2.50002300	-3.41752000
H	-0.80363300	0.98778600	3.51906600
C	1.13578800	-2.45235900	2.10065100
H	0.83516400	-1.30268100	3.84573000
C	1.45448800	-3.91764400	0.39914700
H	1.72581300	-2.73792200	-4.60994600
N	1.11227100	-2.61436400	0.73550100
C	1.49276000	-3.75347900	2.79810700
C	1.92659800	-4.66815200	1.63357800
H	1.49493500	-5.67188800	1.68647600
H	-3.32010600	1.87813200	2.63336600
H	0.58985300	3.05822900	1.93481900
H	0.87822000	1.43609000	3.66466200
H	-0.33448900	3.04995700	-0.77798300
H	0.96744200	2.44592400	-3.55766000
H	0.43717700	0.68042600	-5.16557600
H	-1.05912700	0.26916200	-4.30447900
H	1.80285300	-0.50717700	-3.54225400
H	-0.88692800	-1.91389600	-3.23101400

H	0.06868200	-3.08833100	-5.14129900
H	-0.18611900	-4.84669500	-3.45445200
H	1.55954800	-4.98527200	-3.70710600
H	1.66527600	-5.51324600	-0.97800900
H	3.01801900	-4.78362400	1.60050200
H	0.60928200	-4.14830600	3.31604400
H	2.27354400	-3.60719500	3.55015900
H	7.27256900	-1.47491400	1.17048000
H	6.85537600	-3.00969700	1.96388800
H	-7.63559000	-2.98118400	0.04545600
H	8.36405200	3.49561900	3.61218100
H	8.97197800	1.84110000	3.32268700
H	9.18103200	7.11469500	-2.72874000
H	10.54840400	7.78138900	-1.79511700
H	-0.73187100	-1.39474600	-0.45869500
H	-1.12079900	2.65242200	1.92423400
H	-1.96400900	4.96538900	6.34450700
H	-8.05728400	6.30659600	-2.04316900
H	-4.11682100	-5.27571900	5.22768000
H	-7.79307900	0.13951700	-5.79086100