Zheng, Z., and Gunner, M. R. (2009) Analysis of the electrochemistry of hemes with Ems spanning 800 mV, Proteins 75, 719-734.

Label	Type	Source	PDB	Resolution[Å]	Heme ID	Heme Type	Exp. Em	Cal. Em	$\Delta\Delta G_{rxn}$	ΔG_{pol}	$\Delta G_{res.prop}$	$\Delta G_{res.prot}$
1	b5	*Rattus N.(wt)*	1AW3*	n/a	96	bis-His *b*	-102	-268	87	24	-79	-77
			1B5A*	n/a	95	bis-His *b*	-102	-166	85	55	-47	-42
2		*B.Taurus(wt)*	1CYO	1.50	201	bis-His *b*	-10	-124	100	123	-73	-49
			1EHB	1.90	A201	bis-His *b*	-10	-131	89	127	-96	-29
3		*B.Taurus(V61H)*	1ES1	2.10	A201	bis-His *b*	12	-106	88	115	-81	-1
4		*Rattus N(V54I/V61I)*	1EUE	1.80	A201	bis-His *b*	-63	-163	89	139	-94	-74
					B201	bis-His *b*	-63	-158	89	97	-74	-42
5	b562	*E.Coli*	1QPU*	n/a	A107	His-Met *b*	168	201	189	-1	-44	66
			256B	1.40	A1	His-Met *b*	168	127	84	24	-52	70
					B1	His-Met *b*	168	109	77	31	-37	73
6	c	*E.Caballus*	1CRC	2.08	A105	His-Met *c*	260	77	169	136	-332	127
					B105	His-Met *c*	260	47	170	131	-287	56
			1HRC	1.90	105	His-Met *c*	260	88	166	125	-284	102
			1WEJ	1.80	F105	His-Met *c*	260	148	154	163	-288	137
			2PCB	2.80	B105	His-Met *c*	260	206	157	84	-104	76
7		*S.Cervisiae*	1YCC	1.23	1	His-Met *c*	290	137	175	140	-294	139
			2YCC	1.90	104	His-Met *c*	290	89	174	122	-321	144
8	c2	*R.Capsulatus*	1C2R	2.50	A120	His-Met *c*	350	98	162	158	-269	70
					B120	His-Met *c*	350	136	163	162	-269	93
9		*R.Centenum*	1JDL	1.70	125	His-Met *c*	293	95	169	146	-303	107
10		*R.Palustris*	1FJ0	1.70	A115	His-Met *c*	350	154	169	163	-305	139
					B115	His-Met *c*	350	144	169	168	-303	139
					C115	His-Met *c*	350	134	169	154	-307	140
					D115	His-Met *c*	350	150	170	166	-307	143
			1I8P	1.95	A115	His-Met *c*	350	130	170	163	-306	127
					B115	His-Met *c*	350	149	166	160	-302	136
					C115	His-Met *c*	350	137	171	152	-309	155
					D115	His-Met *c*	350	165	169	170	-307	156
11		*R.Sphaeroides*	1CXC	1.60	125	His-Met *c*	355	89	165	187	-308	72
12		*R.Viridis*	1CO6	1.60	A108	His-Met *c*	296	100	173	131	-298	121
			1CRY	3.00	108	His-Met *c*	296	86	174	175	-221	5
			1IO3	1.90	A108	His-Met *c*	296	138	167	144	-247	108
13	c3	*D. d. Norway*	1CZJ	2.16	119	bis-His *c*	-318	-326	41	-7	-110	-27
					120	bis-His *c*	-350	-351	22	-30	-88	-35
					121	bis-His *c*	-280	-319	70	-17	-124	-27
					122	bis-His *c*	-150	-221	52	-1	-116	64
14		*D. Gigas*	1GYO	1.20	A111	bis-His *c*	-260	-226	26	1	-65	30
					A112	bis-His *c*	-295	-356	37	-67	-52	-46
					A113	bis-His *c*	-180	-99	64	31	-74	101
					A114	bis-His *c*	-280	-242	44	-86	-72	89
					B111	bis-His *c*	-260	-265	19	11	-81	8
					B112	bis-His *c*	-295	-347	36	-45	-72	-46
					B113	bis-His *c*	-180	-127	48	26	-65	85
					B114	bis-His *c*	-280	-221	71	-90	-65	84
15		*D. vulgaris. M*	1J0O	1.15	A1001	bis-His *c*	-263	-156	53	6	-30	32
					A1002	bis-His *c*	-340	-414	52	-127	-87	-33
					A1003	bis-His *c*	-291	-323	61	-39	-130	9
					A1004	bis-His *c*	-318	-336	56	-68	-174	70
			2CDV	1.80	1	bis-His *c*	-318	-339	29	-42	-140	35
					2	bis-His *c*	-340	-408	47	-134	-94	-8
					3	bis-His *c*	-263	-237	44	2	-105	49
					4	bis-His *c*	-291	-301	58	-52	-92	12
16		*D. vulgaris*	2CTH	1.67	A109	bis-His *c*	-305	-305	36	-45	-114	40
					A110	bis-His *c*	-345	-420	33	-119	-90	-24
					A111	bis-His *c*	-250	-230	49	-12	-65	24
					A112	bis-His *c*	-305	-308	59	-50	-118	19
					B109	bis-His *c*	-305	-310	33	-51	-127	58
					B110	bis-His *c*	-345	-415	16	-122	-77	-17
					B111	bis-His *c*	-250	-236	49	-17	-87	42
					B112	bis-His *c*	-305	-327	63	-47	-131	7
17		*D. Africanus*	3CAO	1.60	A104	bis-His *c*	-210	-197	12	114	-103	-12
					A105	bis-His *c*	-270	-352	26	1	-81	-77
					A106	bis-His *c*	-260	-347	82	-18	-116	-86
					A107	bis-His *c*	-240	-228	16	52	-107	35
			3CAR	1.60	A104	bis-His *c*	-210	-194	12	112	-86	-7
					A105	bis-His *c*	-270	-333	33	4	-95	-55
					A106	bis-His *c*	-260	-275	65	-10	-77	-39
					A107	bis-His *c*	-240	-211	35	14	-119	74
18		*S. Oneidensis*	1M1R	1.02	A801	bis-His *c*	-248	-339	3	91	-65	-146
					A802	bis-His *c*	-219	-299	17	15	-66	-47
					A803	bis-His *c*	-138	-187	53	90	-87	-22
					A804	bis-His *c*	-192	-218	3	52	-107	65
19	c4	*P. Stutzeri*	1ETP	2.20	A199	His-Met *c*	237	71	164	29	-209	98
					A200	His-Met *c*	330	177	168	91	-110	42
					B199	His-Met *c*	330	164	164	63	-88	35
					B200	His-Met *c*	237	82	167	76	-223	79

20		*A. Ferrooxidans*	1H1O	2.13	A1184	His-Met *c*	350	118	180	98	-248	106
					A1185	His-Met *c*	450	113	162	-5	-10	-21
					B1185	His-Met *c*	350	177	184	104	-262	176
					B1186	His-Met *c*	450	216	163	63	3	1
21	c549	*Synechocystis sp*	1E29	1.21	A136	bis-His *c*	-250	-209	69	-86	-20	53
22		*C.A.Maxima*	1F1C	2.30	A200	bis-His *c*	-260	-268	75	-96	-12	-11
					B400	bis-His *c*	-260	-269	71	-89	-16	-11
23	c550	*T elongatus*	1MZ4	1.80	A135	bis-His *c*	-240	-255	94	-158	30	6
24		*P versutus*	2BGV	1.90	X1121	His-Met *c*	255	0	158	59	-269	76
25	c551	*P.Aeruginosa*	351C	1.60	0	His-Met c	270	214	160	55	-73	66
			451C	1.60	0	His-Met *c*	270	194	160	61	-81	52
26	c552	*P.Nautica*	1CNO	2.20	A200	His-Met *c*	250	109	163	46	-147	53
					B200	His-Met *c*	250	51	168	42	-246	95
					C200	His-Met *c*	250	79	166	31	-105	36
					D200	His-Met *c*	250	39	166	43	-208	82
					E200	His-Met *c*	250	67	167	47	-52	-69
					F200	His-Met *c*	250	76	168	35	-166	69
					G200	His-Met *c*	250	92	168	35	-107	40
					H200	His-Met *c*	250	119	167	42	-259	105
27		*H.Thermophilus*	1YNR	2.00	A81	His-Met *c*	215	123	128	31	-174	153
					B81	His-Met *c*	215	84	86	30	-139	120
					C81	His-Met *c*	215	139	114	31	-135	143
					D81	His-Met *c*	215	137	125	42	-87	68
28	c553	*B. Pasteurii*	1C75	0.95	A93	His-Met *c*	60	83	152	2	-31	-23
29	c6	*M. braunii*	1CTJ	1.10	91	His-Met *c*	358	106	160	-44	-44	52
30		*chloroplast*	1CYI	1.90	200	His-Met *c*	370	63	159	-65	-29	18
31		*C.A.Maxima*	1F1F	2.70	A200	His-Met *c*	314	112	163	-54	-44	61
32		*C. glomerata*	1LS9	1.30	A92	His-Met *c*	352	149	160	-84	-53	128
33	c7	*D. acetoxidans*	1HH5	1.90	A69	bis-His *c*	-200	-277	-10	10	-59	-3
					A70	bis-His *c*	-140	-165	60	27	-86	58
					A71	bis-His *c*	-200	-181	16	28	-77	72
34	Q.A.Dehydrogenase	*P denitrificans*	1JJU	2.05	A991	His-Met *c*	235	103	110	8	-145	155
					A992	bis-His *c*	149	2	127	20	-142	216
35	Hemoglobin	*monoeric clam*	1EBT	1.90	144	mono-his b	103	95	202	39	-116	107
			1BOB	2.30	144	mono-His b	103	59	218	59	-135	67
			1FLP	1.50	143	mono-His b	103	48	190	23	-97	58
			1MOH	1.90	143	mono-His b	103	67	205	38	-122	89
36	Myoglobin	*sperm whale*	1A6G	1.15	154	mono-His b	50	57	272	55	-151	51
			1A6K	1.10	154	mono-His b	50	5	210	39	-120	29
			1A6M	1.00	154	mono-His b	50	22	245	60	-149	40
			1HJT	2.50	160	mono-His b	50	53	305	63	-149	-7
			1JP6	2.30	A200	mono-His b	50	-29	209	42	-137	22
			1JP9	1.70	A200	mono-His b	50	9	235	44	-128	8
37	Cyt. *c* Peroxidase	*P.aeruginosa*	1EB7	2.40	A401	bis-His c	-330	-265	99	49	-138	-57
					A402	his-met c	320	133	179	54	-177	83
					B401	bis-His c	-330	-260	101	48	-131	-66
					B402	his-met c	320	123	180	51	-166	73
38		*N europaea*	1IQC	1.80	A401	mono-His c	-260	-175	223	69	-180	-168
					A402	His-Met *c*	450	264	197	102	-67	54
					B401	mono-His c	-260	-244	214	63	-206	-203
					B402	His-Met *c*	450	246	191	122	-105	61
					C401	mono-His c	-260	-178	222	64	-190	-159
					C402	His-Met *c*	450	261	195	96	-72	67
					D401	mono-His c	-260	-148	135	-34	-11	-261
					D402	His-Met *c*	450	306	195	97	-38	54
39	c"	*M. methylotrophus*	1GU2	1.19	A125	bis-His *c*	-60	-230	9	39	-106	48
					B125	bis-His *c*	-60	-184	14	49	-91	65
40	bc1	*B.Taurus*	1BE3	3.00	C1	bis-His *b*	-10	4	280	-23	-164	136
					C2	bis-His *b*	100	100	247	49	-243	345
					D3	His-Met *c*	250	213	283	61	-113	-3
41	Cyto c Oxi	*Rb. Sphaeroides*	2GSM	2.00	A2001	bis-His *a*	300	261	205	131	-522	507
42	RC	*R.Viridis*	1DXR	2.00	C401	His-Met *c*	-60	14	156	5	-161	25
					C402	His-Met *c*	310	283	205	2	-153	243
					C403	His-Met *c*	380	336	169	-3	-207	348
					C404	bis-His *c*	20	-197	107	-21	-124	71

Table SIII: Experimental, calculated E_ms and decomposed energy terms for each protein. *: NMR structures. The experimental E_ms are from: 1[93], 2,3[88], 4[111], 5[94], 6[90], 7[112], 8, 25[113], 9[114], 10[115], 11[87], 12[116], 13[92], 14[117], 15[118], 16[119], 17[120], 18[83], 19[121], 20[91], 21[122], 22[123], 23[86], 24[124], 26[125], 27[126], 28[107], 29[127], 30[128], 31[129], 32[130], 33[131], 34[102], 35, 36[84], 37[132], 38[16], 39[133], 40[134], 41[101], 42[100].