Supplementary Information:

Quantum Mechanical Methods Predict Accurate Thermodynamics of Biochemical Reactions

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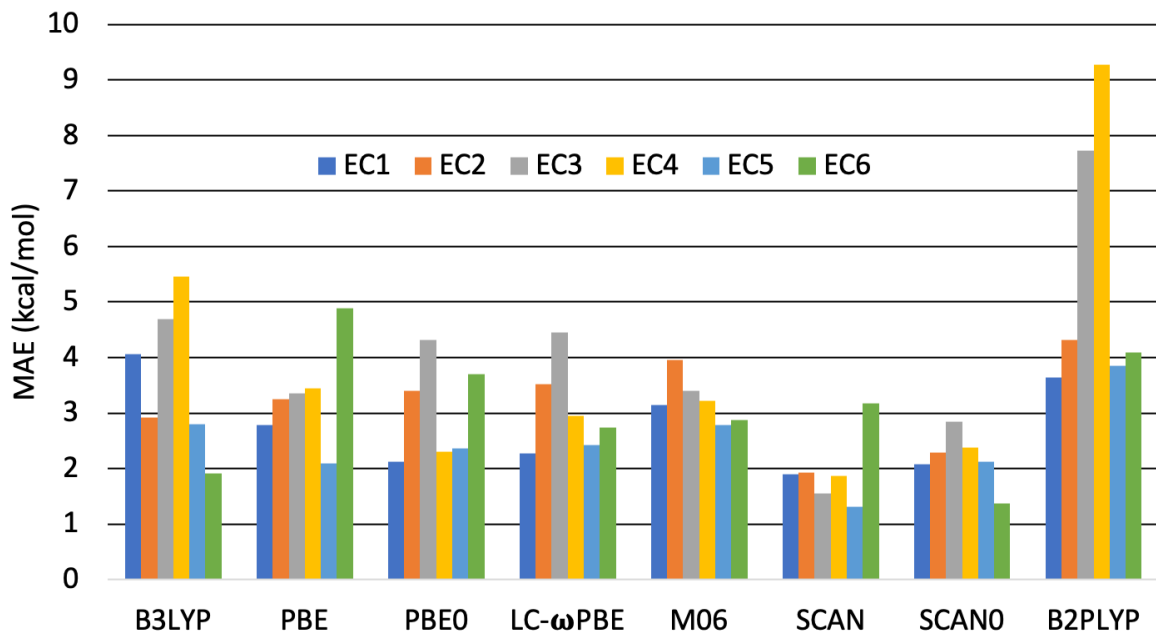
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Figure S1: Bar plot showing performance of different exchange correlation functionals in DFT for each EC category. Error in reaction free energy are calculated with respect to experimental reference.

Regression parameters

Regression parameters used for each type of calibration;

Entire data: y=0.38x+0.84, $R^2 = 0.39$

EC1: y=0.50x+2.3, $R^2 = 0.48$

EC2: y=0.22x+0.29, , $R^2 = 0.19$

EC3: y=0.19x-1.31, $R^2 = 0.12$

EC4: y=0.34x+1.54, $R^2 = 0.31$

EC5: y=0.10x-0.09, $R^2 = 0.19$

EC6: y=0.58x+0.40, $R^2 = 0.28$

Table S1: Different reactions in tricarboxylic acid cycle (TCA)/glycolysis.

| EC-Numbers	Reaction
	TCA cycle
2.3.3.1	oxaloacetate+H2O+acetyl-CoA = citrate+CoA+PROTON
4.2.1.3	citrate = H2O+cis-aconitate
4.2.1.3	cis-aconitate + H2O = D-threo-isocitrate
1.1.1.41	D-threo-isocitrate + NAD^+ = 2-oxoglutarate+NADH +CO2
1.2.1.M9	2-oxoglutarate + CoA + NAD^+ = Succinyl-CoA + NADH + CO2
6.2.1.5	succinyl-CoA + ADP + phosphate=ATP + CoA+succinate
1.3.5.1	succinate + FAD = FADH2 + fumarate
4.2.1.2	fumarate + H2O = malate
1.1.1.37	malate + NAD^+ = NADH + oxaloacetate + PROTON
	glycolysis
5.3.1.9	D-glucopyranose 6-phosphate = β-D-fructofuranose 6-phosphate
3.1.3.11	β-D-fructofuranose 1, 6-phosphate + H2O = β-D-fructofuranose 6-phosphate + phosphate
2.7.1.11	ATP + β-D-fructofuranose 6-phosphate = ADP + β-D-fructofuranose 1, 6-phosphate
4.1.2.13	β-D-fructofuranose 1, 6-phosphate = glycerone phosphate + D-glyceraldehyde 3-phosphate
1.2.1.12	D-glyceraldehyde 3-phosphate + NAD^+ + Phosphate = 3-phospho-D-glyceroyl phosphate + NADH + PROTON
2.7.2.3	3-phospho-D-glycerate + ATP = ADP + 3-phospho-D-glyceroyl phosphate
5.4.2.11	2-phospho-D-glycerate = p3-phospho-D-glycerate
5.4.2.12	2-phospho-D-glycerate = 3-phospho-D-glycerate
4.2.1.11	2-phospho-D-glycerate = phosphoenolpyruvate + water
2.7.9.2	pyruvate + ATP + H2O = AMP + phosphoenolpyruvate + phosphate + water
2.7.1.40	pyruvate+ATP = phosphoenolpyruvate + ADP +PROTON
1.2.1.-	pyruvate + NAD^+ + CoA = acetyl-CoA + NADH + CO2
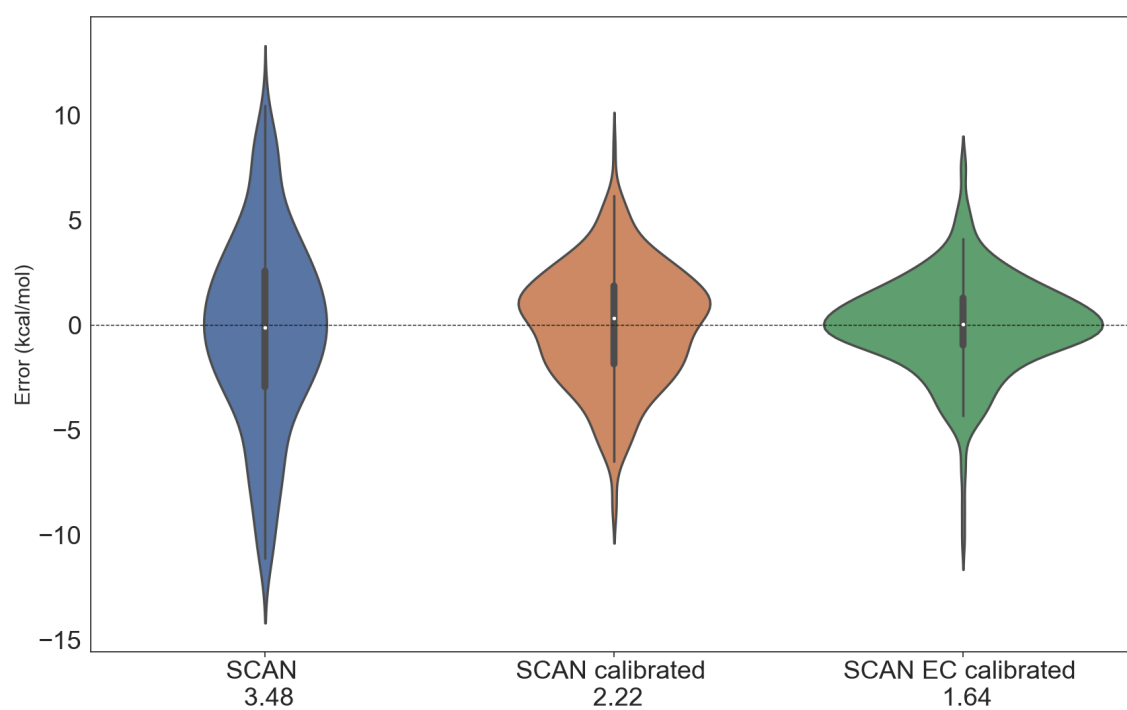
Figure S2: Voilin plot showing improvement in calculated SCAN reaction free energies before and after calibration. Label shows the MAE (kcal/mol) obtained for each case.

Inverse Legendre transformation

Each reaction in NIST experimental data has associated error with it. Such error comes mainly from measurements performed and reported at different experimental condition (pH, ionic strength etc.) for a given reaction. We standardized the NIST experimental data to eliminate the effect of varying experimental condition (or to minimize experimental error) by using inverse Legendre transform.[1] For mathematics to carryout such transformation, we refers readers to pioneering work of Alberty.[1,2] We used pKa values for each metabolite which is calculated using Chemaxon.[3]
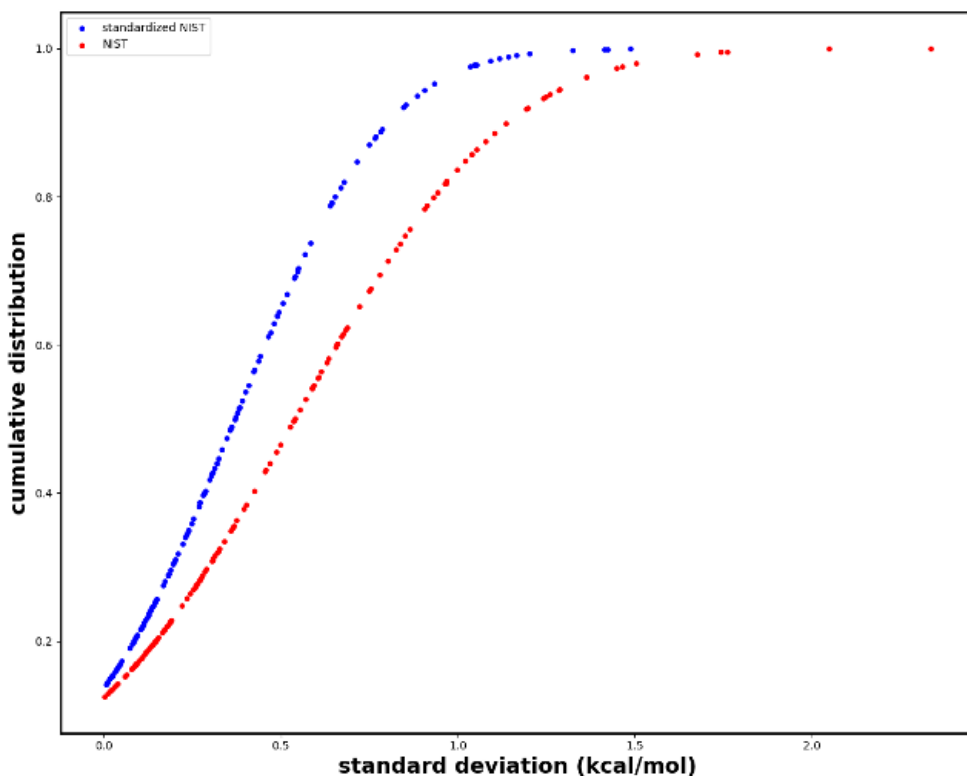
Figure S3: Plot of cumulative distribution functions of the standard deviations in reaction free energy for inverse Legendres transformed (standardized) and for the one directly taken from NIST data. It shows, standardized NIST data have reduced measurement error for each reaction. Only reaction with multiple measurement are considered in this plot.

We note that, inverse Legendre transform does not completely eliminate the condition dependance in NIST experimental data as shown in Figure S3. It however reduces the

mean/median of standard deviation for Set2 from 0.54/0.37 to 0.37/0.28 kcal/mol. We note that, standard deviation is calculated for each reaction in experimentally measured multiple reaction free energies and then mean/median is calculated on entire Set2. Ideally, multiple experimental measurements in NIST data should give a single value for reaction free energy after such transformation. Such ideal situation is not observed after inverse Legendre transformation, thus showing remaining noise in the standardized data, which may arise from measurement errors and inaccuracies in the inverse Legendre transform as discussed by Noor et al.[4] in their work.

Data

SCAN predicted reaction free energies for each reaction in Set-2 along with corresponding experimental values, error on experimental value, absolute deviation between DFT and experimental values and corresponding reactions are provided.

EC	DFT	Expt	Error	DFT-Expt	Reactions
1.1.1.-	8.56	7.23	0.09	1.33	cpd00795+cpd00003=cpd00024+cpd00004
1.1.1.1	8.35	5.73	1.16	2.62	cpd00363+cpd00003=cpd00071+cpd00004
1.1.1.1	8.95	3.29	0.02	5.66	cpd00365+cpd00003=cpd00304+cpd00004
1.1.1.1	5.85	5.55	0.01	0.29	cpd00435+cpd00003=C00261+cpd00004
1.1.1.1	9.49	6.58	0.00	2.91	cpd00562+cpd00003=cpd01088+cpd00004
1.1.1.1	4.96	2.62	0.31	2.34	cpd00636+cpd00003=cpd00329+cpd00004
1.1.1.1	3.05	2.30	0.09	0.75	cpd01269+cpd00003=cpd00178+cpd00004
1.1.1.1	8.10	6.29	0.00	1.81	cpd03662+cpd00003=cpd01011+cpd00004
1.1.1.1	8.36	6.83	0.00	1.53	cpd05400+cpd00003=cpd00613310+cpd00004
1.1.1.108	1.83	6.32	0.03	4.49	cpd00266+cpd00003=cpd01715+cpd00004
1.1.1.108	1.80	6.95	0.01	5.15	cpd10719+cpd00003=cpd01715+cpd00004
1.1.1.125	3.80	7.43	0.00	3.63	cpd01795+cpd00003=cpd02441+cpd00004
1.1.1.129	5.37	4.93	1.14	0.44	cpd01138+cpd00003=cpd01961+cpd00004
1.1.1.14	3.91	5.28	0.20	1.37	cpd00306+cpd00003=cpd00259+cpd00004
1.1.1.14	2.02	2.60	0.08	0.57	cpd00314+cpd00003=cpd00082+cpd00004
1.1.1.14	4.41	5.23	0.00	0.82	cpd00366+cpd00003=cpd00258+cpd00004
1.1.1.14	3.15	3.24	0.38	0.09	cpd00588+cpd00003=cpd00082+cpd00004
1.1.1.14	5.16	2.54	0.00	2.62	cpd01066+cpd00003=cpd00212+cpd00004
1.1.1.14	2.43	3.27	0.00	0.84	cpd01171+cpd00003=cpd00589+cpd00004

EC	DFT	Expt	Error	DFT-Expt	Reactions
1.1.1.14	4.67	4.92	0.00	0.26	cpd01307+cpd00003=cpd00258+cpd00004
1.1.1.140	2.99	3.79	0.00	0.80	cpd00804+cpd00003=cpd00072+cpd00004
1.1.1.24	-2.35	4.53	0.00	6.88	cpd00248+cpd00003=cpd00699+cpd00004
1.1.1.26	15.37	11.28	0.18	4.10	cpd00139+cpd00003=cpd00040+cpd00004
1.1.1.26	9.92	7.99	0.25	1.94	cpd00223+cpd00003=cpd00145+cpd00004
1.1.1.27	11.62	7.10	0.55	4.52	cpd00159+cpd00003=cpd00020+cpd00004
1.1.1.28	11.60	6.38	1.33	5.22	cpd00221+cpd00003=cpd00020+cpd00004
1.1.1.29	9.92	8.17	0.32	1.76	cpd00223+cpd00003=cpd00145+cpd00004
1.1.1.3	8.57	4.82	0.00	3.75	cpd00227+cpd00003=cpd00346+cpd00004
1.1.1.30	8.42	3.29	0.38	5.13	cpd00797+cpd00003=cpd00142+cpd00004
1.1.1.31	8.17	5.71	0.36	2.46	cpd00876+cpd00003=cpd00287+cpd00004
1.1.1.37	11.16	7.27	0.00	3.89	cpd00023+cpd00130+cpd00003=cpd00041+cpd00024+cpd00004
1.1.1.37	9.21	7.63	0.36	1.57	cpd00130+cpd00003=cpd00032+cpd00004
1.1.1.37	11.34	7.19	0.19	4.15	cpd00432+cpd00003=cpd00718+cpd00004
1.1.1.37	13.87	10.18	0.00	3.69	cpd00432+cpd00003=cpd02186+cpd00004
1.1.1.39	5.99	3.53	0.00	2.46	cpd00130+cpd00003+cpd00001=cpd00020+cpd00004+cpd00242
1.1.1.4	5.73	4.34	0.05	1.39	cpd01947+cpd00003=cpd19008+cpd00004
1.1.1.47	-2.65	-0.66	0.77	1.99	cpd00027+cpd00003=cpd00170+cpd00004
1.1.1.48	-6.95	-3.12	0.20	3.83	cpd00108+cpd00003=cpd02143+cpd00004
1.1.1.51	1.69	1.23	0.43	0.46	cpd00420+cpd00003=cpd00237+cpd00004
1.1.1.56	4.41	5.01	0.55	0.60	cpd00366+cpd00003=cpd00258+cpd00004
1.1.1.59	10.51	6.29	0.00	4.22	cpd00745+cpd00003=cpd00191+cpd00004
1.1.1.60	10.61	8.52	1.09	2.09	cpd00223+cpd00003=cpd00843+cpd00004
1.1.1.62	-0.82	1.77	0.04	2.59	cpd00702+cpd00003=cpd00362+cpd00004
1.1.1.67	2.02	3.47	1.41	1.44	cpd00314+cpd00003=cpd00082+cpd00004
1.1.1.8	7.34	6.48	0.49	0.86	cpd00080+cpd00003=cpd00095+cpd00004
1.1.1.9	3.91	5.37	0.30	1.45	cpd00306+cpd00003=cpd00259+cpd00004
1.1.1.9	4.41	5.86	0.05	1.44	cpd00366+cpd00003=cpd00258+cpd00004
1.1.1.9	3.15	3.98	0.05	0.83	cpd00588+cpd00003=cpd00082+cpd00004
1.1.1.9	5.16	3.97	0.05	1.19	cpd01066+cpd00003=cpd00212+cpd00004
1.1.1.90	5.85	5.67	0.00	0.18	cpd00435+cpd00003=C00261+cpd00004
1.1.1.95	15.33	8.66	1.12	6.67	cpd00169+cpd00003=cpd02069+cpd00004
1.1.99.7	2.42	-0.61	0.36	3.03	cpd00159+cpd00032=cpd00130+cpd00020
1.2.1.12	-0.56	-0.55	0.67	0.01	cpd00102+cpd00008+cpd00003+cpd00009=cpd00169+cpd00002+cpd00004
1.2.1.12	-2.24	3.21	0.85	5.46	cpd00102+cpd00009+cpd00003=cpd00203+cpd00004
1.2.1.2	2.00	-4.27	0.00	6.27	cpd00047+cpd00003+cpd00001=cpd00242+cpd00004
1.3.99.11	6.74	3.52	0.18	3.21	cpd00282+cpd00003=cpd00247+cpd00004
1.4.1.1	6.74	9.71	0.35	2.96	cpd00035+cpd00003+cpd00001=cpd00020+cpd00004+cpd00013
1.4.1.11	1.51	4.95	1.42	3.44	cpd00874+cpd00003+cpd00001=cpd02294+cpd00004+cpd00013
1.4.1.12	4.35	7.73	0.00	3.38	cpd02448+cpd00003+cpd00001=cpd02121+cpd00004+cpd00013

EC	DFT	Expt	Error	DFT-Expt	Reactions
1.4.1.2	9.96	10.08	1.20	0.12	cpd00023+cpd00003+cpd00001=cpd00024+cpd00004+cpd00013
1.4.1.3	9.96	9.58	0.10	0.38	cpd00023+cpd00003+cpd00001=cpd00024+cpd00004+cpd00013
1.4.1.9	7.98	10.02	0.00	2.04	cpd00107+cpd00003+cpd00001=cpd00200+cpd00004+cpd00013
1.5.1.11	4.37	8.62	0.00	4.25	cpd02553+cpd00003+cpd00001=cpd00051+cpd00020+cpd00004
1.5.1.7	7.45	10.21	0.00	2.76	cpd00351+cpd00003+cpd00001=cpd00039+cpd00024+cpd00004
1.8.1.4	9.35	1.78	0.46	7.56	cpd00449+cpd00003=cpd00213+cpd00004
2.1.2.1	-9.10	-4.86	0.00	4.24	cpd00033+cpd00055=cpd00054
2.1.2.1	0.07	-2.44	0.00	2.52	cpd00033+cpd00071=cpd00161
2.1.2.7	9.76	5.05	0.00	4.71	cpd01432=cpd00117+cpd00055
2.1.2.7	9.34	5.01	0.00	4.34	cpd01958=cpd00550+cpd00055
2.1.3.2	-11.73	-5.00	0.00	6.73	cpd00146+cpd00041=cpd00009+cpd00343
2.1.3.3	-15.03	-7.61	0.00	7.42	cpd00146+cpd00064=cpd00274+cpd00009
2.1.4.1	2.62	-0.13	0.00	2.75	cpd00051+cpd00033=cpd00064+cpd00451
2.2.1.1	3.37	1.72	0.36	1.65	cpd00072+cpd00102=cpd00236+cpd00198
2.2.1.1	2.56	2.48	0.00	0.08	cpd00072+cpd00229=cpd01395+cpd00236
2.2.1.1	6.70	0.26	0.28	6.44	cpd00238+cpd00102=cpd00101+cpd00198
2.2.1.2	4.65	0.80	0.00	3.86	cpd00082+cpd00102=cpd00072+cpd00448
2.2.1.2	10.71	0.26	0.37	10.45	cpd00238+cpd00102=cpd00236+cpd00072
2.3.1.2	9.37	1.96	0.91	7.41	cpd00196+cpd01116=cpd01677+cpd00009
2.3.1.35	-0.33	1.23	0.00	1.57	cpd00342+cpd00023=cpd00064+cpd00477
2.3.1.8	-4.01	-1.97	0.00	2.04	cpd00020+cpd00009=cpd00196+cpd00047
2.4.1.13	-7.28	0.96	0.55	8.25	cpd00026+cpd00082=cpd00014+cpd00076
2.4.1.15	-10.62	-1.89	0.00	8.73	cpd00026+cpd00079=cpd00014+cpd00523
2.4.1.20	10.11	0.75	0.14	9.37	cpd00158+cpd00009=cpd00027+cpd00089
2.4.1.20	4.26	0.55	0.00	3.71	cpd03721+cpd00009=cpd00158+cpd00089
2.4.1.216	9.17	2.02	0.04	7.15	cpd00523+cpd00009=cpd00089+cpd00079
2.4.1.31	8.24	0.58	0.00	7.66	cpd01397+cpd00009=cpd00027+cpd00089
2.4.1.64	3.45	1.17	0.49	2.28	cpd00794+cpd00009=cpd00027+cpd00089
2.4.1.67	2.13	-0.83	0.01	2.97	cpd00910+cpd00382=cpd00121+cpd01133
2.4.1.7	5.83	-1.94	0.13	7.78	cpd00076+cpd00009=cpd00089+cpd00082
2.4.1.8	0.35	0.85	0.00	0.50	cpd00179+cpd00009=cpd00027+cpd00089
2.4.2.1	0.47	3.55	0.00	3.08	cpd00133+cpd00475=cpd02016+cpd00009
2.4.2.1	-0.06	2.09	0.78	2.14	cpd00182+cpd00009=cpd00128+cpd00475
2.4.2.1	-4.53	2.29	0.31	6.82	cpd00246+cpd00009=cpd00226+cpd00475
2.4.2.1	-6.52	2.64	0.00	9.16	cpd00311+cpd00009=cpd00207+cpd00475
2.4.2.1	-6.35	2.47	0.00	8.82	cpd01217+cpd00009=cpd00309+cpd00475
2.4.2.1	5.86	2.22	0.13	3.63	cpd03279+cpd00009=cpd00226+cpd00509
2.4.2.10	-5.89	-3.90	0.64	1.98	cpd00810+cpd00012=cpd00247+cpd00103
2.4.2.11	-2.27	1.89	0.00	4.16	cpd00873+cpd00012=cpd00218+cpd00103
2.4.2.15	-6.52	2.39	0.00	8.91	cpd00311+cpd00009=cpd00207+cpd00475

EC	DFT	Expt	Error	DFT-Expt	Reactions
2.4.2.28	2.47	2.62	0.00	0.15	cpd00147+cpd00009=cpd00128+cpd02574
2.4.2.6	-4.58	-1.71	0.00	2.87	cpd00184+cpd00128=cpd00438+cpd00151
2.4.2.6	-2.20	-0.20	0.00	2.00	cpd03279+cpd00128=cpd00438+cpd00226
2.4.2.8	-2.14	8.53	0.00	10.67	cpd00114+cpd00012=cpd00226+cpd00103
2.4.2.8	-5.52	0.55	0.00	6.07	cpd00126+cpd00226=cpd00114+cpd00207
2.4.2.8	2.14	-6.71	0.00	8.85	cpd00226+cpd00103=cpd00114+cpd00012
2.6.1.-	-5.77	0.43	0.00	6.21	cpd00035+cpd01504=cpd00020+cpd00726
2.6.1.1	-1.95	1.04	0.18	3.00	cpd00041+cpd00024=cpd00032+cpd00023
2.6.1.1	-1.41	-1.61	0.00	0.20	cpd21080+cpd00024=cpd02186+cpd00023
2.6.1.15	-1.13	-3.57	0.00	2.44	cpd00053+cpd00020=cpd00695+cpd00035
2.6.1.15	-7.04	-3.82	0.00	3.21	cpd00053+cpd00040=cpd00695+cpd00033
2.6.1.18	-0.55	0.92	0.00	1.47	cpd00035+cpd00191=cpd00085+cpd00020
2.6.1.19	-0.25	1.03	0.57	1.28	cpd00281+cpd00024=cpd00199+cpd00023
2.6.1.2	-3.22	-0.23	0.25	2.99	cpd00035+cpd00024=cpd00020+cpd00023
2.6.1.21	-3.23	0.01	0.00	3.24	cpd00117+cpd00024=cpd00020+cpd00186
2.6.1.30	-2.68	-0.28	0.00	2.40	cpd00419+cpd00020=cpd00215+cpd00035
2.6.1.35	4.64	2.06	0.00	2.58	cpd00033+cpd00032=cpd00040+cpd00041
2.6.1.37	-0.03	0.69	0.00	0.72	cpd02233+cpd00020=cpd02024+cpd00035
2.6.1.39	1.97	-0.17	0.00	2.15	cpd00705+cpd00024=cpd00269+cpd00023
2.6.1.42	-1.98	-0.79	0.20	1.19	cpd00107+cpd00024=cpd00200+cpd00023
2.6.1.42	-5.17	-0.71	0.00	4.46	cpd00156+cpd00024=cpd03737+cpd00023
2.6.1.5	3.57	-0.41	0.02	3.97	cpd00066+cpd00024=cpd00143+cpd00023
2.6.1.5	-2.27	-0.29	0.01	1.98	cpd00069+cpd00024=cpd00868+cpd00023
2.6.1.51	0.61	-0.96	0.14	1.57	cpd00035+cpd00145=cpd00054+cpd00020
2.6.1.52	1.55	2.54	0.00	0.99	cpd00738+cpd00024=cpd02069+cpd00023
2.6.1.52	-1.55	-3.15	0.38	1.60	cpd02069+cpd00023=cpd00024+cpd00738
2.6.2.1	-1.95	1.14	0.03	3.10	cpd00041+cpd00024=cpd00032+cpd00023
2.7.1.1	-0.11	-5.36	0.40	5.24	cpd00002+cpd00027=cpd00008+cpd00079
2.7.1.11	-4.32	-2.31	0.51	2.01	cpd00002+cpd00072=cpd00008+cpd00290
2.7.1.23	-2.88	-2.71	0.00	0.17	cpd00002+cpd00003=cpd00008+cpd00006
2.7.1.24	6.54	1.75	0.00	4.79	cpd00002+cpd00655=cpd00008+cpd00010
2.7.1.40	7.88	6.46	0.44	1.43	cpd00002+cpd00020=cpd00008+cpd00061
2.7.1.40	7.88	6.03	0.93	1.86	cpd00002+cpd00020=cpd00061+cpd00008
2.7.1.6	-1.60	-3.55	0.15	1.94	cpd00002+cpd00108=cpd00008+cpd19025
2.7.2.2	10.13	3.73	0.47	6.40	cpd00002+cpd01101=cpd00008+cpd00146
2.7.2.3	-1.68	4.80	0.28	6.49	cpd00002+cpd00169=cpd00008+cpd00203
2.7.3.2	-7.95	2.45	0.85	10.40	cpd00002+cpd00250=cpd00008+cpd01550
2.7.3.3	8.45	0.20	1.05	8.26	cpd00002+cpd00051=cpd00008+cpd03535
2.7.3.4	-1.02	-0.71	1.49	0.31	cpd00002+cpd01345=cpd00008+cpd02015
2.7.3.5	-5.27	-1.77	0.00	3.49	cpd00002+cpd09876=cpd00008+cpd09877

EC	DFT	Expt	Error	DFT-Expt	Reactions
2.7.4.4	-2.54	0.36	0.15	2.91	cpd00002+cpd00014=cpd00008+cpd00062
2.7.4.6	4.62	-0.02	0.00	4.65	cpd00002+cpd00031=cpd00008+cpd00038
2.7.7.1	-2.15	-0.38	0.00	1.77	cpd00002+cpd00355=cpd00003+cpd00012
2.7.7.12	-1.55	-0.68	0.00	0.87	cpd19025=cpd00089
2.7.7.12	0.86	-0.25	0.27	1.11	cpd00026+cpd19025=cpd00089+cpd00043
2.7.7.15	-8.55	1.54	0.00	10.09	cpd00052+cpd00457=cpd00012+cpd00256
2.7.7.27	-8.58	-1.05	0.00	7.53	cpd00002+cpd00089=cpd00387+cpd00012
2.7.7.33	2.86	-0.82	0.23	3.68	cpd00052+cpd00089=cpd00390+cpd00012
2.8.3.5	6.61	1.66	0.49	4.96	cpd00078+cpd00142=cpd00036+cpd00279
2.8.3.8	-0.74	1.21	0.00	1.95	cpd00022+cpd00142=cpd00279+cpd00029
3.1.1.21	-3.41	5.13	0.00	8.53	cpd01691+cpd00001=cpd00365+cpd00214
3.1.3.1	-14.18	-3.10	0.00	11.08	cpd00018+cpd00001=cpd00182+cpd00009
3.1.3.1	-5.60	-3.25	0.14	2.34	cpd00072+cpd00001=cpd00082+cpd00009
3.1.3.1	-5.50	-2.53	0.48	2.97	cpd00079+cpd00001=cpd00027+cpd00009
3.1.3.1	-2.02	-2.99	0.00	0.97	cpd00114+cpd00001=cpd00246+cpd00009
3.1.3.1	-12.83	-2.26	0.00	10.57	cpd00235+cpd00001=cpd00138+cpd00009
3.1.3.1	-1.29	-3.11	0.00	1.82	cpd00290+cpd00001=cpd00072+cpd00009
3.1.3.1	-5.64	-3.61	0.00	2.03	cpd00290+cpd00001=cpd00802+cpd00009
3.1.3.1	-1.24	-2.62	0.00	1.38	cpd00802+cpd00001=cpd00082+cpd00009
3.1.3.1	-3.00	-2.77	0.00	0.22	cpd00818+cpd00001=cpd00108+cpd00009
3.1.3.1	5.97	-2.41	0.58	8.38	cpd00738+cpd00001=cpd00054+cpd00009
3.1.3.11	-1.29	-4.57	0.64	3.28	cpd00290+cpd00001=cpd00072+cpd00009
3.1.3.2	-5.60	-2.99	0.00	2.61	cpd00072+cpd00001=cpd00082+cpd00009
3.1.3.2	-1.29	-1.94	0.00	0.65	cpd00290+cpd00001=cpd00072+cpd00009
3.1.3.2	-5.64	-2.21	0.00	3.43	cpd00290+cpd00001=cpd00802+cpd00009
3.1.3.2	-1.24	-2.70	0.00	1.45	cpd00802+cpd00001=cpd00082+cpd00009
3.1.3.3	5.97	-2.37	0.32	8.34	cpd00738+cpd00001=cpd00054+cpd00009
3.1.3.5	-14.18	-3.08	0.00	11.10	cpd00018+cpd00001=cpd00182+cpd00009
3.2.1.23	-1.32	-2.31	0.41	0.99	cpd00208+cpd00001=cpd00108+cpd00027
3.2.1.23	-3.07	-2.57	0.42	0.50	cpd04349+cpd00001=cpd00108+cpd00082
3.2.2.2	-3.56	-2.81	0.00	0.74	cpd00246+cpd00001=cpd00226+cpd00105
3.2.2.4	-2.54	-3.07	0.00	0.53	cpd00018+cpd00001=cpd00128+cpd00101
3.2.2.7	0.92	-2.35	0.00	3.27	cpd00182+cpd00001=cpd00128+cpd00105
3.3.1.1	-3.03	8.30	0.00	11.33	cpd00019+cpd00001=cpd00182+cpd00135
3.5.1.11	5.72	-0.11	0.00	5.83	cpd03325+cpd00001=cpd19069+cpd00033
3.5.1.11	2.08	-1.14	0.52	3.22	cpd04194+cpd00001=cpd01896+cpd02202
3.5.1.14	3.09	-0.77	0.01	3.86	cpd01756+cpd00001=cpd00029+cpd00060
3.5.1.14	3.09	-0.63	0.00	3.72	cpd01756+cpd00001=cpd00060+cpd00029
3.5.1.2	-5.55	-3.60	0.02	1.95	cpd00053+cpd00001=cpd00023+cpd00013
3.5.1.22	1.78	1.65	0.15	0.13	cpd00644+cpd00001=cpd00408+cpd00085

EC	DFT	Expt	Error	DFT-Expt	Reactions
3.5.1.5	-13.67	-3.55	0.24	10.12	cpd01101+cpd00001=cpd00013+cpd00242
3.5.1.a	0.74	3.18	1.05	2.44	cpd08505+cpd00001=cpd00162+cpd00188
3.5.1.a	2.34	5.54	0.00	3.21	cpd16300+cpd00001=cpd00162+cpd00214
3.5.3.4	8.05	-0.27	0.00	8.32	cpd00388+cpd00001=cpd00465+cpd00073
3.5.4.16	-5.80	-7.21	0.00	1.41	cpd00038+cpd00001=cpd03518
3.5.4.4	-7.31	-5.45	0.68	1.86	cpd00182+cpd00001=cpd00246+cpd00013
3.6.1.38	-5.61	-6.45	0.00	0.84	cpd00002+cpd00001=cpd00008+cpd00009
4.-	-1.66	-1.64	0.00	0.02	cpd00216+cpd00013=cpd08210+cpd00001
4.1.2.-	11.27	6.10	0.00	5.17	cpd03583=cpd00171+cpd00055
4.1.2.13	-1.82	3.52	0.64	5.34	cpd00290=cpd00095+cpd00102
4.1.2.13	2.88	7.40	0.33	4.52	cpd00802=cpd00448+cpd00095
4.1.2.14	8.31	3.13	0.11	5.18	cpd02711=cpd00020+cpd00102
4.1.2.17	-3.28	4.73	0.00	8.02	cpd00806=cpd00095+cpd00334
4.1.2.18	2.58	4.73	0.00	2.14	cpd00520=cpd00020+cpd00229
4.1.2.18	-0.59	5.40	0.00	5.99	cpd03674=cpd00020+cpd00334
4.1.2.19	-4.88	1.53	0.00	6.42	cpd00831=cpd00095+cpd00334
4.1.2.2	3.94	4.64	0.00	0.70	cpd02148=cpd00055+cpd00095
4.1.2.21	-1.81	2.55	0.00	4.36	cpd00945=cpd00020+cpd00102
4.1.2.4	3.12	4.97	0.14	1.85	cpd00510=cpd00102+cpd00071
4.1.2.43	-11.27	-6.10	0.00	5.17	cpd00171+cpd00055=cpd03583
4.1.2.a	5.96	4.38	0.00	1.59	cpd00176=cpd00020+cpd00448
4.1.3.1	0.66	2.50	1.03	1.83	cpd00260=cpd00036+cpd00040
4.1.3.16	7.12	2.59	0.39	4.53	cpd00830=cpd00020+cpd00040
4.1.3.22	-0.61	0.25	0.77	0.86	cpd01701=cpd00029+cpd00020
4.1.3.27	-5.59	-1.90	0.02	3.69	cpd00216+cpd00013=cpd17073+cpd00001
4.1.3.3	6.64	1.89	0.44	4.75	cpd00232=cpd00492+cpd00020
4.1.3.3	5.81	1.48	0.00	4.33	cpd02155=cpd02219+cpd00020
4.1.3.32	0.55	0.02	0.00	0.53	cpd01705=cpd00141+cpd00020
4.1.3.6	-6.83	-0.01	0.54	6.81	cpd00137=cpd00029+cpd00032
4.1.3.7	-7.70	-6.67	0.28	1.03	cpd00032+cpd00022+cpd00001=cpd00137+cpd00010
4.1.99.1	-3.52	5.32	0.24	8.84	cpd00065+cpd00001=cpd00359+cpd00020+cpd00013
4.2.1.10	-2.38	-1.63	0.00	0.76	cpd00699=cpd01716+cpd00001
4.2.1.11	1.22	-0.74	0.13	1.96	cpd00482=cpd00061+cpd00001
4.2.1.2	-1.45	-0.85	0.11	0.60	cpd00106+cpd00001=cpd00130
4.2.1.3	2.13	1.89	0.13	0.24	cpd00137=cpd00331+cpd00001
4.2.1.3	-1.69	-1.30	0.32	0.38	cpd00260=cpd00137
4.2.1.3	0.44	0.34	0.11	0.10	cpd00260=cpd00331+cpd00001
4.2.1.31	1.45	4.52	0.00	3.07	cpd00386=cpd00996+cpd00001
4.2.1.34	3.48	1.05	0.00	2.43	cpd01701=cpd01194+cpd00001
4.2.1.35	4.59	2.75	0.00	1.84	cpd01700=cpd01502+cpd00001

EC	DFT	Expt	Error	DFT-Expt	Reactions
4.2.1.48	-8.06	-2.03	0.13	6.02	cpd00186=cpd01512+cpd00001
4.2.1.85	4.19	0.99	0.65	3.20	cpd01705=cpd00684+cpd00001
4.2.1.89	3.61	-0.25	0.00	3.86	cpd00266=cpd02543+cpd00001
4.3.1.1	0.25	3.79	0.31	3.55	cpd00041=cpd00106+cpd00013
4.3.1.2	0.32	1.71	0.08	1.39	cpd02273=cpd01194+cpd00013
4.3.2.1	-3.28	3.51	0.00	6.79	cpd02152=cpd00106+cpd00051
4.3.2.2	4.78	1.38	0.21	3.40	cpd02375=cpd00106+cpd00018
4.3.2.2	6.62	1.01	0.00	5.61	cpd19032=cpd00106+cpd02851
4.3.2.3	-7.82	1.17	0.02	8.99	cpd00465=cpd00040+cpd00073
4.4.1.5	5.79	5.62	0.00	0.17	cpd02182=cpd00042+cpd00428
4.6.1.1	-1.15	1.33	0.20	2.47	cpd00002=cpd00446+cpd00012
5.1.1.1	0.02	0.02	0.08	0.00	cpd00035=cpd00117
5.1.1.10	1.77	0.00	0.00	1.77	cpd00107=cpd01106
5.1.1.3	0.01	0.00	0.00	0.01	cpd00023=cpd00186
5.1.1.5	-0.23	0.00	0.00	0.23	cpd00039=cpd00549
5.1.1.7	1.45	-0.40	0.00	1.85	cpd00504=cpd00516
5.1.1.8	0.07	0.01	0.00	0.06	cpd00851=cpd02175
5.1.3.1	-7.71	-0.28	0.29	7.43	cpd00171=cpd00198
5.1.3.10	9.32	-0.16	0.00	9.48	cpd02264=cpd02265
5.1.3.15	-7.55	-0.31	0.00	7.24	cpd19006=cpd00863
5.1.3.18	9.31	0.40	0.00	8.90	cpd00083=cpd01536
5.1.3.2	-1.55	-0.66	0.02	0.88	cpd19025=cpd00089
5.1.3.2	2.41	0.71	0.04	1.70	cpd00026=cpd00043
5.1.3.4	-7.01	-0.12	0.17	6.89	cpd00808=cpd00198
5.1.3.5	6.13	-0.03	0.09	6.16	cpd00691=cpd00163
5.1.3.6	5.03	-0.26	0.27	5.29	cpd00144=cpd00472
5.1.3.8	9.38	0.89	0.09	8.49	cpd00122=cpd00492
5.1.3.9	9.17	0.52	0.00	8.65	cpd00293=cpd02612
5.2.1.5	0.37	-2.52	0.00	2.88	cpd01122=cpd02510
5.3.1.-	-4.92	-3.17	0.00	1.75	cpd03583=cpd00072
5.3.1.1	-4.70	-1.88	0.13	2.82	cpd00102=cpd00095
5.3.1.10	2.53	0.89	0.03	1.65	cpd00288+cpd00001=cpd00072+cpd00013
5.3.1.12	-0.44	0.15	0.00	0.59	cpd00164=cpd00672
5.3.1.12	-4.93	0.32	0.75	5.25	cpd00280=cpd00437
5.3.1.13	2.59	0.59	0.23	2.00	cpd00817=cpd00171
5.3.1.14	-0.71	-0.04	0.30	0.67	cpd00396=cpd00642
5.3.1.15	-2.18	0.87	0.00	3.05	cpd00368=cpd00259
5.3.1.2	-0.37	-0.51	0.00	0.14	cpd01239=cpd01383
5.3.1.20	1.59	0.47	0.08	1.12	cpd00105=cpd00258
5.3.1.27	-4.92	-3.17	0.00	1.75	cpd03583=cpd00072

EC	DFT	Expt	Error	DFT-Expt	Reactions
5.3.1.3	3.18	1.08	0.10	2.10	cpd00185=cpd00258
5.3.1.3	-6.84	1.30	0.00	8.14	cpd00751=cpd01186
5.3.1.4	2.06	1.17	0.12	0.89	cpd00224=cpd00397
5.3.1.5	-0.92	-0.05	0.07	0.86	cpd00027=cpd00082
5.3.1.5	-3.67	0.49	0.00	4.15	cpd00027=cpd00138
5.3.1.5	3.57	0.87	0.17	2.70	cpd00154=cpd00259
5.3.1.5	1.59	0.73	0.11	0.86	cpd00185=cpd00105
5.3.1.5	3.18	1.59	0.24	1.60	cpd00185=cpd00258
5.3.1.5	-0.37	-0.60	0.13	0.23	cpd01239=cpd01383
5.3.1.5	-0.20	0.05	0.10	0.25	cpd01239=cpd03879
5.3.1.5	-0.30	-0.62	0.11	0.32	cpd03884=cpd01055
5.3.1.5	3.81	0.80	0.00	3.02	cpd03884=cpd03880
5.3.1.6	1.80	0.68	0.28	1.12	cpd00101=cpd00171
5.3.1.7	2.75	-0.60	0.09	3.35	cpd00138=cpd00082
5.3.1.7	-2.18	0.57	0.00	2.75	cpd00368=cpd00259
5.3.1.8	-4.49	-0.14	0.27	4.35	cpd00235=cpd00072
5.3.1.9	-0.82	0.80	0.22	1.62	cpd00079=cpd00072
5.3.2.1	-5.96	1.36	0.00	7.33	cpd00143=cpd01784
5.3.2.2	10.16	1.36	0.00	8.80	cpd00032=cpd02469
5.3.3.2	-7.24	-1.17	0.00	6.07	cpd00113=cpd00202
5.3.3.5	-8.51	-1.63	0.00	6.88	cpd03222=cpd03221
5.3.3.6	-3.59	-0.75	0.00	2.85	cpd01545=cpd00684
5.4.2.1	-6.77	-1.43	0.37	5.34	cpd00482=cpd00169
5.4.2.2	1.09	-1.71	0.03	2.80	cpd00089=cpd00079
5.4.2.2	1.42	0.57	0.12	0.85	cpd00288=cpd03671
5.4.2.3	-11.48	-1.10	0.00	10.38	cpd02611=cpd00293
5.4.2.6	1.09	-1.60	0.72	2.69	cpd00089=cpd00079
5.4.2.8	1.09	-0.20	0.00	1.29	cpd00089=cpd00079
5.4.2.8	-1.42	-0.97	0.89	0.45	cpd00485=cpd00235
5.4.3.2	-3.01	-1.11	0.13	1.90	cpd00039=cpd00840
5.4.3.5	2.49	1.70	0.00	0.79	cpd00404=cpd02448
5.4.99.1	-1.88	-1.39	0.00	0.48	cpd02273=cpd00023
5.4.99.4	3.16	0.90	0.00	2.26	cpd01876=cpd01545
5.4.99.6	-5.59	-1.32	0.00	4.27	cpd00216+cpd00013=cpd17073+cpd00001
5.4.99.6	-5.04	0.23	0.13	5.27	cpd00216=cpd00658
5.5.1.1	11.16	3.42	0.79	7.74	cpd02536=cpd01630
5.5.1.3	5.59	-2.40	0.00	7.99	cpd02033=cpd02112
6.2.1.4	-3.06	0.98	0.54	4.04	cpd00038+cpd00036+cpd00010=cpd00031+cpd00009+cpd00078
6.3.1.2	-0.06	-4.38	0.38	4.33	cpd00002+cpd00023+cpd00013=cpd00008+cpd00009+cpd00053
6.3.4.4	4.70	4.89	0.00	0.19	cpd00038+cpd00114+cpd00041=cpd00031+cpd00009+cpd02375

EC	DFT Expt	Error	DFT-Expt	Reactions
6.4.1.1	-2.39 -0.36	1.05	2.03	cpd00002+cpd00020+cpd00242=cpd00008+cpd00009+cpd00032

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