Supporting Information

Can Local Electric Field be a Descriptor of Catalytic Activity? A Case Study on Chorismate Mutase

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Table S1. Comparative Residual Interactions of Chorismate and TSA Inhibitor calculated by MMPBSA. Data are shown as value ± standard error.

Interacting Residues	Binding Energy for Chorismate Reactant (kcal/mol)	Binding Energy for TSA Inhibitor (kcal/mol)
Arg 90	-15.439 ± 2.591	-15.910 ± 1.727
Arg 63	-11.274 ± 3.594	-14.498 ± 6.580
Arg 7	-9.015 ± 5.182	-23.370 ± 2.486
Lys 60	-8.297 ± 4.747	-5.688 ± 4.592
Ala 59	-2.972 ± 0.505	-4.487 ± 0.865
Phe 57	-1.875 ± 0.934	-2.442 ± 0.553
Tyr 108	-0.054 ± 0.745	-3.164 ± 2.139
Cys 75	-0.397 ± 0.430	-0.935 ± 0.558

Table S2. Residue wise energy decompositions for the interaction of Chorismate substrate calculated by MMPBSA. All the energy values are in kcal/mol. Data are shown as value ± standard error.

Interacting Residues	Van der Waals	Electrostatic	Polar Solvation	Non-Polar Solvation	Total
Arg 90	0.019 ± 0.931	-65.424 ± 3.110	50.946 ± 1.827	-0.980 ± 0.294	-15.439 ± 2.591
Arg 63	-0.405 ± 0.928	-62.525 ± 6.371	52.870 ± 3.081	-1.214 ± 0.351	-11.274 ± 3.594
Arg 7	-0.799 ± 0.661	-58.347 ± 7.605	51.177 ± 4.058	-1.047 ± 0.289	-9.015 ± 5.182
Lys 60	-1.959 ± 0.725	-58.084 ± 13.813	53.608 ± 9.928	-1.863 ± 0.570	-8.297 ± 4.747
Ala 59	-0.999 ± 0.295	-0.299 ± 0.974	-0.831 ± 0.741	-0.843 ± 0.126	-2.972 ± 0.505
Phe 57	-1.257 ± 0.737	0.799 ± 0.813	-0.425 ± 0.950	-0.992 ± 0.466	-1.875 ± 0.934
Tyr 108	-0.141 ± 0.081	-1.096 ± 1.884	1.232 ± 1.375	-0.048 ± 0.081	-0.054 ± 0.745
Cys 75	-0.283 ± 0.258	-0.193 ± 0.377	0.102 ± 0.349	-0.168 ± 0.210	-0.397 ± 0.430

Table S3. Residue wise energy decomposition for the interaction of TSA inhibitor calculated by MMPBSA. All the energy values are in kcal/mol. Data are shown as value ± standard error.

Interacting Residues	Van der Waals	Electrostatic	Polar Solvation	Non-Polar Solvation	Total
Arg 90	-0.382 ± 0.805	-62.859 ± 1.925	48.469 ± 1.045	-1.138 ± 0.117	-15.910 ± 1.727
Arg 63	0.542 ± 1.017	-65.243 ± 12.312	50.941 ± 6.045	-0.737 ± 0.277	-14.498 ± 6.580
Arg 7	0.059 ± 0.922	-75.084 ± 2.398	52.868 ± 1.550	-1.213 ± 0.140	-23.370 ± 2.486
Lys 60	-1.189 ± 0.469	-48.870 ± 10.397	45.378 ± 6.134	-1.007 ± 0.315	-5.688 ± 4.592
Ala 59	-1.181 ± 0.213	-1.552 ± 1.283	-0.911 ± 0.855	-0.843 ± 0.114	-4.487 ± 0.865
Phe 57	-1.470 ± 0.351	1.201 ± 0.480	-1.216 ± 0.434	-0.957 ± 0.216	-2.442 ± 0.553
Tyr 108	-0.323 ± 0.519	-6.856 ± 2.812	4.545 ± 1.153	-0.530 ± 0.233	-3.164 ± 2.139
Cys 75	-0.575 ± 0.153	-0.724 ± 0.788	0.795 ± 0.556	-0.432 ± 0.118	-0.935 ± 0.558

Table S4. Total Binding Free Energy of Chorismate and TSA Inhibitor calculated by MMPBSA.

Substrate	Total Binding Free Energy, $\Delta G_{binding}$ (kcal/mol)	Standard Deviation
Chorismate	-31.0394	5.3363
TSA Inhibitor	-46.4348	7.8097

Table S5. The TS dipole moment (**μ**) and B3LYP/Def2-SVP Energy barriers (**ΔE**) for the interconversion reaction of chorismate to prephenate on varying EEF.

EEF (V/Å)	ΔE (kcal/mol)	Overall μ_{TS} (Debye)	TS μ_y (Debye)
+0.200	65.78	13.032	10.486
0.0	32.90	16.243	14.928
-0.200	24.26	20.576	20.099
-0.514	19.80	29.716	29.559
-0.540	19.40	29.689	29.536
-0.617	18.60	29.608	29.456

Table S6. The TS dipole moment (**μ**) and B3LYP-D3/Def2-TZVPP calculated TS energy barriers (**ΔE**) for the interconversion reaction of chorismate to prephenate on varying EEF.

EEF (V/Å)	**ΔE (kcal/mol)**	**Overall μ_{TS} (Debye)**	**TS μ_y (Debye)**
+0.200	57.76	12.845	10.174
0.0	27.00	16.323	14.987
-0.200	18.21	21.052	20.593
-0.514	17.51	30.973	30.778
-0.540	17.13	30.952	30.762
-0.617	16.43	30.903	30.717

Table S7. TS energy barriers (**ΔE**) for the interconversion reaction of chorismate to prephenate in aqueous solution.

Level of Theory	**ΔE (kcal/mol)**
B3LYP/Def2-SVP	25.01
B3LYP-D3/Def2-TZVPP	19.98

Table S8. QM/MM/B3LYP-D3/Def2-TZVPP energies and LEF Quantification along reaction axis of QM/MM optimized geometries.

Species	**Energy (kcal/mol)**	**LEF (V/Å)**
RC	0.00	-0.53
TS	14.88	-0.47
PC	-21.82	-0.09

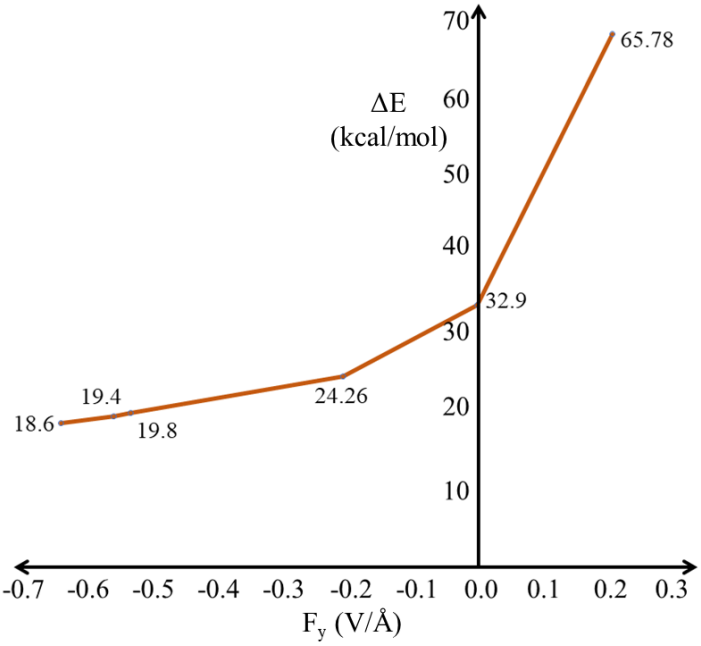

Figure S1. TS energy barriers for the interconversion of chorismate to prephenate vs the electric field strength along y-direction, F_y.

Hydrogen Bond Analysis:

Hydrogen bonding interactions play very commodious role in the protein-ligand binding. The figure shows the number of hydrogen bonds of the active site residues and the chorismate reactant and TSA inhibitor. Initially, the chorismate reactant forms total number of 5 hydrogen bonds and as the simulation proceeds the gradual decrease in the hydrogen bonds with active site residues is seen which can be also observed from the average values present in red that depicts the flexible nature of the reactant. On the other hand, in the case of TSA inhibitor, the active site hydrogen bonds are almost constant throughout the simulation. In this way, the hydrogen bonding interaction present at the active site provide stability and rigidity to transition state analog (TSA).

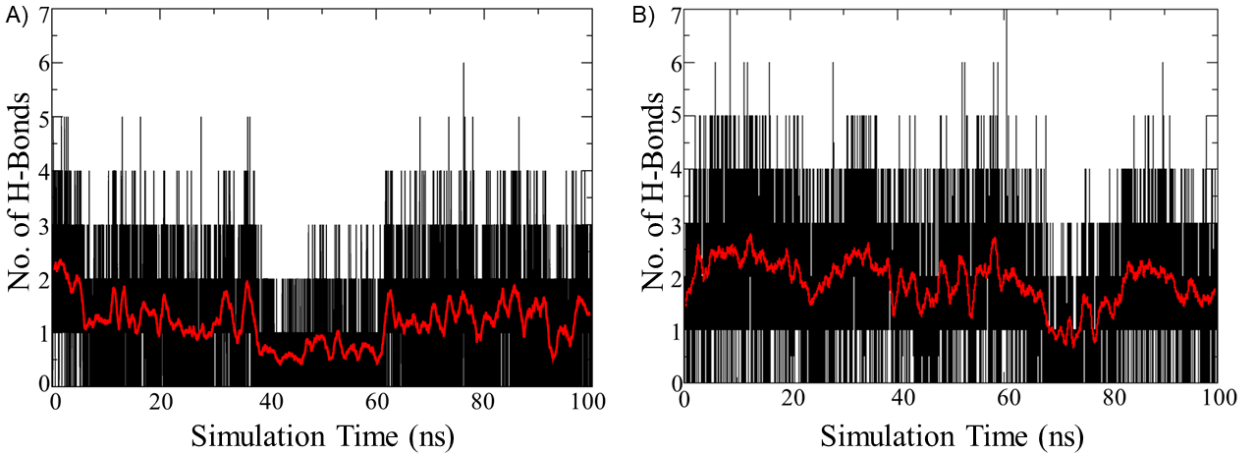

Figure S2. No. of hydrogen bonds vs simulation time in ns between the active site residues of WT chorismate mutase and A) Chorismate Reactant & B) TSA inhibitor.

QM region for the QM/MM optimized geometry

RC

C	39.3967928	39.3828278	25.8409806
H	38.4534224	39.9583056	25.8329735
H	39.1577055	38.3729971	26.2017133
C	40.3215588	40.0915777	26.8545844
O	39.9852000	39.9384832	28.0659629
O	41.2798913	40.7989673	26.4653455
C	39.6239175	42.1378931	30.6760587
H	39.4896607	43.1201574	31.1519854
H	38.6378387	41.7761748	30.3440902
N	40.4801589	42.1777724	29.5118095
H	40.4093382	41.3212739	28.9069587
C	41.4885636	43.0220061	29.2777939
N	41.7248528	44.0783059	30.0824812
H	41.0092212	44.4453962	30.7210869
H	42.3935037	44.7672896	29.7563415
N	42.2814612	42.7791843	28.2318018
H	42.0275627	42.0126510	27.5773323
H	43.0463450	43.4234052	28.0092507
C	37.9066237	48.6199165	28.6731485
C	39.0148931	47.9610136	28.2714705
C	36.9473399	47.9636584	29.5725903
C	37.0834449	46.6698779	29.9160919
C	38.1447438	45.8105880	29.2729725
C	39.3831260	46.6187108	28.8369741
O	40.3778188	46.8073839	29.8924309
C	39.9943799	47.4381109	31.0629056
C	40.0657938	48.7710271	31.1823553
C	39.5553923	46.5313279	32.2124348
O	39.0663610	47.0888088	33.2385715
O	39.6978064	45.2880341	32.0750994
O	37.5936522	45.1515735	28.1196032
H	37.4188653	45.8554317	27.4771232
C	37.6913197	50.0983201	28.3400993
O	38.6315097	50.7087341	27.7659977
O	36.6056178	50.5950217	28.7160897
H	39.7351129	48.4765788	27.6360587
H	36.1477636	48.5933549	29.9682633
H	36.3931297	46.2007099	30.6201244
H	38.4715376	45.0106807	29.9482655
H	39.9163262	46.0032651	28.0972981
H	40.3976311	49.4051458	30.3588511
H	39.7708251	49.2655891	32.1053294
H	39.7806559	39.2997870	24.8242110
H	40.0054959	41.4381836	31.4196122

TS

C	39.3945877	39.3889171	25.8447745
H	38.4513172	39.9643503	25.8339767
H	39.1556895	38.3796515	26.2073874
C	40.3180165	40.1006845	26.8584555
O	39.9736198	39.9603798	28.0687406
O	41.2840487	40.7972758	26.4679838
C	39.6600245	42.1673707	30.6979884
H	39.5516508	43.1502369	31.1797246
H	38.6628933	41.8304698	30.3730549
N	40.5048781	42.1963087	29.5254858
H	40.4131803	41.3454141	28.9168709
C	41.5296549	43.0212297	29.2871504
N	41.7978628	44.0675124	30.0936572
H	41.0876369	44.4640195	30.7210259
H	42.4606040	44.7540508	29.7490205
N	42.3055435	42.7666674	28.2313140
H	42.0370626	42.0030725	27.5791040
H	43.0798534	43.3988392	28.0068777
C	38.0187379	48.3639932	29.0626916
C	38.9399040	47.7510431	28.2132097
C	37.1530211	47.5276631	29.8985268

C	37.3055823	46.1901743	29.9319278
C	38.3341573	45.4768267	29.0974243
C	39.2960991	46.4223197	28.4204393
O	40.6830118	46.8497153	29.9703588
C	40.0908648	47.4465243	30.9450697
C	39.7803973	48.7981662	30.8920395
C	39.5968040	46.5886699	32.1373840
O	39.0556546	47.1898331	33.1127046
O	39.7614482	45.3444634	32.0695609
O	37.6914488	44.6711912	28.0838235
H	37.4884533	45.2784870	27.3579496
C	37.6932076	49.8499104	28.8924231
O	38.5413454	50.5561822	28.2755222
O	36.6087026	50.2364026	29.3700387
H	39.5113331	48.3736992	27.5276266
H	36.3976715	48.0480903	30.4914915
H	36.6800243	45.5653038	30.5743170
H	38.8919057	44.7658592	29.7179786
H	40.0483311	45.9475815	27.7865186
H	40.1967485	49.4339347	30.1123082
H	39.2537605	49.2878642	31.7112803
H	39.7786704	39.3034064	24.8282925
H	40.0333297	41.4568121	31.4354278

PC

C	39.3685279	39.4047821	25.8336684
H	38.4050405	39.9451599	25.8093096
H	39.1616199	38.3943227	26.2118455
C	40.2557077	40.1679391	26.8402195
O	39.8883400	40.0609113	28.0474109
O	41.2132110	40.8761896	26.4494710
C	39.5556986	42.2509694	30.6737171
H	39.4654312	43.2181329	31.1887340
H	38.5451482	41.9316911	30.3766429
N	40.3505548	42.3285978	29.4632838
H	40.2732543	41.4647137	28.8671233
C	41.4520020	43.0813645	29.2859745
N	41.7674811	44.0752514	30.1339641
H	41.0989187	44.4580184	30.8130530
H	42.4931614	44.7252758	29.8501822
N	42.2342166	42.8088031	28.2422496
H	41.9490277	42.0653413	27.5716025
H	43.0442021	43.4068635	28.0491871
C	38.2255619	48.2405567	29.4666669
C	38.7923747	47.5714760	28.2343845
C	37.2411906	47.3263265	30.1571430
C	37.2687656	45.9962377	30.0004641
C	38.2101342	45.2933814	29.0588626
C	38.7618169	46.2484450	28.0303288
O	41.1153047	47.0066491	30.3149953
C	40.1439201	47.3864671	30.9460512
C	39.3641817	48.6019438	30.5130964
C	39.6667350	46.5728345	32.1944919
O	39.0848854	47.2192079	33.1080517
O	39.8930923	45.3404915	32.1920774
O	37.5265847	44.1752622	28.4815510
H	38.1874271	43.5611627	28.1308532
C	37.6227339	49.6482590	29.0918409
O	38.3855553	50.3987036	28.4134864
O	36.4929567	49.9303878	29.5219386
H	39.2409255	48.2310542	27.4904200
H	36.5435488	47.8060220	30.8490276
H	36.6325633	45.3410326	30.6019593
H	39.0577588	44.9060134	29.6564113
H	39.1986879	45.8128390	27.1248404
H	40.0522622	49.3078545	30.0268950
H	38.8958519	49.0926539	31.3776793
H	39.7622835	39.3152871	24.8212385
H	39.9544703	41.5183370	31.3753566

QM-only DFT geometry

1. **No EEF**

Reactant

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.35193800
C	1.28571100	0.00000000	-0.71586600
C	2.45469400	0.23397000	-0.08870700
C	2.46055700	0.61455900	1.37232300
C	1.27272100	0.01880200	2.16311400
O	1.56070100	-1.33686300	2.56223000
C	2.38868400	-1.58741700	3.62546300
C	3.21336700	-2.64959000	3.53174200
C	2.27886000	-0.78291200	4.97239600
O	3.16012400	-1.04707200	5.81643300
O	1.30837300	0.00401200	5.06557400
O	2.46509900	2.05212200	1.48734000
H	1.65329800	2.33625700	1.04261700
C	-1.30993000	-0.02337100	-0.84686900
O	-1.13282000	-0.13020800	-2.08749100
O	-2.38235200	0.06713600	-0.21336400
H	-0.96221000	-0.04431200	1.87018300
H	1.20874300	-0.18680000	-1.79092000
H	3.40553000	0.25513900	-0.63621300
H	3.38829200	0.28643300	1.86756200
H	1.14827700	0.61938400	3.07787100
H	3.81542800	-2.91151400	4.40157000
H	3.25808200	-3.24642000	2.61442700

TS

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39868000
C	1.29350700	0.00000000	-0.68429000
C	2.45878200	-0.12342700	-0.01652500
C	2.51578600	-0.27994400	1.47659400
C	1.13854600	-0.38857900	2.09213900
O	0.90398200	-2.46525500	1.93539600
C	0.80132900	-2.82086100	0.70768000
C	-0.35357100	-2.55634200	-0.03566200
C	2.03343000	-3.48900900	-0.00895200
O	1.73710800	-4.22881900	-0.97693800
O	3.16240000	-3.24237000	0.47517400
O	3.23532300	0.83649700	2.07867100
H	2.75538500	1.61990900	1.77225600
C	-1.28374900	0.41215700	-0.77721400
O	-1.09254800	0.81818400	-1.94782200
O	-2.35869100	0.32297500	-0.13960000
H	-0.97251200	0.08612400	1.89075700
H	1.24660700	0.11236100	-1.77006200
H	3.41942300	-0.13293000	-0.54128200
H	3.09431000	-1.18513400	1.71747400
H	1.13180500	-0.43020300	3.18508800
H	-0.38070800	-2.87328900	-1.07923500
H	-1.27064400	-2.18643800	0.42270100

Product

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.50048700
C	1.39997000	0.00000000	-0.53927600
C	2.49501200	-0.21629700	0.20244600
C	2.45484700	-0.49064100	1.68018300
C	1.08800400	-0.22320200	2.25283800
O	-1.12855000	-3.15468400	0.86556400
C	-0.39038600	-2.60417500	0.05720400
C	-0.79339800	-1.24704200	-0.53368600
C	0.88264000	-3.30564500	-0.48881700
O	0.78150500	-3.55846800	-1.71412500
O	1.79928900	-3.57269000	0.31536500
O	3.46076700	0.29090900	2.37932400
H	3.21393200	1.20847000	2.19275000
C	-0.82754900	1.28652900	-0.56040100

O	-0.43444700	1.74014200	-1.65326300
O	-1.78782200	1.64587100	0.15133900
H	-0.97381000	0.19802000	1.95577400
H	1.47446100	0.19091800	-1.61233600
H	3.49175300	-0.23477100	-0.25533700
H	2.74191800	-1.54358000	1.85784600
H	1.02521500	-0.22704400	3.34910300
H	-0.67074900	-1.28709700	-1.62725100
H	-1.85669900	-1.09073700	-0.28845000

2. At EEF, F_y = -0.200 V/Å

Reactant

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.35254500
C	1.28560800	0.00000000	-0.71659000
C	2.46805600	0.07343000	-0.07526200
C	2.52127700	0.19085000	1.43093800
C	1.25758300	-0.38010600	2.10789100
O	1.31086800	-1.83145900	2.04407200
C	2.08655400	-2.59378600	2.86992200
C	2.76995400	-3.61642900	2.31279300
C	2.04785000	-2.42386300	4.43152100
O	2.75594200	-3.23832500	5.06856700
O	1.29746500	-1.52458900	4.86634500
O	2.73600200	1.55792900	1.81082900
H	1.99204700	2.05015000	1.43381200
C	-1.31160300	-0.01261300	-0.84302500
O	-1.13989400	-0.27061000	-2.06217300
O	-2.37632700	0.18398100	-0.22318800
H	-0.96004300	0.03297500	1.87514500
H	1.20022300	-0.03875100	-1.80630000
H	3.41365500	0.15286300	-0.62636900
H	3.38838100	-0.35808300	1.83422500
H	1.24214500	-0.07663800	3.16401800
H	3.30027700	-4.29926500	2.97718900
H	2.77022400	-3.76419200	1.22731500

TS

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.40397800
C	1.28888200	0.00000000	-0.68174400
C	2.44655300	-0.19982600	-0.01660800
C	2.48797000	-0.48377400	1.45919300
C	1.12487700	-0.38402700	2.10437200
O	0.60837200	-2.59396500	2.11237700
C	0.52989000	-3.01652000	0.91335100
C	-0.52700100	-2.65748900	0.06312400
C	1.67403700	-3.94706400	0.35808000
O	1.28976000	-4.82591900	-0.45633800
O	2.82624700	-3.76226600	0.81447100
O	3.43336100	0.38681200	2.12934200
H	3.12803500	1.28568700	1.93848100
C	-1.29629200	0.31853300	-0.79516400
O	-1.12257300	0.63067500	-1.99523800
O	-2.36343400	0.22358500	-0.14495200
H	-0.96688600	0.13087500	1.89574600
H	1.24309000	0.17480600	-1.75955200
H	3.41347500	-0.19617700	-0.53206600
H	2.87070600	-1.51185700	1.60785800
H	1.12715000	-0.41548400	3.19659700
H	-0.52964800	-3.03908500	-0.95969600
H	-1.39865200	-2.10500200	0.41365300

Product

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.49940400
C	1.40132100	0.00000000	-0.53644400
C	2.48447900	-0.29687700	0.19538500
C	2.41577000	-0.65917900	1.65562400
C	1.07628900	-0.29443900	2.24422600
O	-1.03025100	-3.00157600	1.10382000

C	-0.42650300	-2.63274400	0.10201200
C	-0.77323200	-1.27790800	-0.53314700
C	0.56487400	-3.59944200	-0.60193100
O	0.13093900	-3.99610400	-1.71331600
O	1.60311100	-3.92982500	0.00964600
O	3.49382200	-0.04138800	2.39872000
H	3.34572300	0.90989000	2.29315900
C	-0.86959900	1.23628200	-0.59669500
O	-0.47061200	1.68068400	-1.68915600
O	-1.86625200	1.54274600	0.08568500
H	-0.96006400	0.25582300	1.95494800
H	1.47972000	0.26529300	-1.59393600
H	3.48757900	-0.30786600	-0.24930300
H	2.59589700	-1.74671800	1.76467700
H	1.02440400	-0.29790100	3.34083700
H	-0.63258300	-1.33101400	-1.62342500
H	-1.83891900	-1.09656800	-0.31649100

3. At EEF, F_y = -0.514 V/Å

Reactant

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.35307600
C	1.27939800	0.00000000	-0.72000600
C	2.46332600	-0.13356500	-0.09215600
C	2.57340100	-0.24989200	1.40544000
C	1.21682800	-0.42766800	2.14904400
O	1.08269700	-1.76136600	2.75931700
C	1.13969000	-2.96976100	2.12877700
C	1.11379800	-3.19602000	0.80001600
C	1.24999300	-4.20537400	3.11477900
O	1.32552300	-5.33949600	2.55844900
O	1.25573500	-3.96608800	4.33783900
O	3.29587700	0.87531700	1.92440700
H	2.87057100	1.66688300	1.56330900
C	-1.29925200	-0.21121400	-0.82979200
O	-1.06695000	-0.71642600	-1.96119200
O	-2.38750100	0.02261000	-0.27716300
H	-0.96396800	0.03765300	1.87019700
H	1.20391800	0.08011100	-1.80721300
H	3.41161900	-0.09582700	-0.64218700
H	3.19397100	-1.12189900	1.67396700
H	1.31669600	0.18721100	3.05705000
H	1.17696100	-4.24467900	0.50503300
H	0.99301500	-2.42332600	0.04410300

TS

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.44406900
C	1.28365800	0.00000000	-0.66511200
C	2.44827000	-0.03897300	0.02456300
C	2.49913100	-0.19775300	1.51896000
C	1.14801000	-0.04769500	2.16098400
O	-0.32209900	-3.76292700	1.74166500
C	-0.19725600	-3.68275800	0.51132000
C	-0.61555500	-2.51409700	-0.25606600
C	0.32212100	-4.97594100	-0.28710500
O	0.89771200	-4.77729400	-1.38134600
O	0.08966200	-6.08153900	0.27083000
O	3.49358600	0.64541500	2.12648400
H	3.20692500	1.55592700	1.95965900
C	-1.30827900	0.24125800	-0.80670500
O	-1.15044700	0.32296400	-2.04275600
O	-2.35478400	0.25303900	-0.12109700
H	-0.98354600	0.08412000	1.91207800
H	1.24237600	0.09090000	-1.75315900
H	3.41711600	-0.00301300	-0.48664000
H	2.87578900	-1.22345600	1.74462500
H	1.13831100	-0.02349900	3.25629700
H	-0.45229500	-2.50108800	-1.33392500
H	-1.48739800	-1.97671800	0.11993800

Product

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.49758700
C	1.39481200	0.00000000	-0.54674100
C	2.49291200	-0.21369900	0.19339400
C	2.44618000	-0.52072500	1.66774700
C	1.08937100	-0.21752000	2.24950900
O	0.83683200	-2.96026600	0.52930700
C	-0.15940900	-2.74945600	-0.14660800
C	-0.70772800	-1.35365400	-0.48100900
C	-0.97282300	-4.00651800	-0.64903700
O	-2.14263800	-4.09547400	-0.20401800
O	-0.34981100	-4.82923900	-1.36645900
O	3.49756900	0.15807000	2.38734500
H	3.31966200	1.10288900	2.26712400
C	-0.97619900	1.10171900	-0.67196100
O	-0.70421800	1.35348400	-1.85937000
O	-1.92234500	1.45263700	0.05207500
H	-0.97005300	0.23423800	1.94630800
H	1.45775500	0.23005400	-1.61476600
H	3.49542600	-0.18678900	-0.25390500
H	2.67574100	-1.59582300	1.82122700
H	1.03893600	-0.19139100	3.34621200
H	-0.79577500	-1.29749700	-1.58297000
H	-1.75307400	-1.34358800	-0.12499400

4. At EEF, F_y = -0.540 V/Å

Reactant

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.35335400
C	1.27963300	0.00000000	-0.71991900
C	2.46262400	-0.14230500	-0.09251100
C	2.57150000	-0.27168100	1.40397000
C	1.21344400	-0.44534700	2.14553600
O	1.07138100	-1.78757800	2.74032100
C	1.11592500	-2.99006500	2.09728400
C	1.05891500	-3.20518800	0.76746300
C	1.24661200	-4.23614300	3.06824800
O	1.30694100	-5.36603700	2.50007500
O	1.28073500	-4.01090700	4.29370000
O	3.30397100	0.84152200	1.93327900
H	2.88720500	1.64102900	1.57963700
C	-1.29637400	-0.22898600	-0.82813800
O	-1.05565500	-0.76737000	-1.94314000
O	-2.38811300	0.01727500	-0.28931900
H	-0.96376700	0.03799800	1.87091800
H	1.20675600	0.08761300	-1.80663900
H	3.41145100	-0.10205700	-0.64140400
H	3.18392700	-1.15181700	1.66518400
H	1.31822200	0.15633100	3.06156500
H	1.11571200	-4.25165300	0.46313800
H	0.91643100	-2.42807400	0.01976400

TS

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.44519800
C	1.28567700	0.00000000	-0.66417900
C	2.44885300	-0.04494200	0.02623500
C	2.49749100	-0.21238600	1.52004500
C	1.14709000	-0.05436600	2.16192300
O	-0.30036700	-3.71739500	1.74447000
C	-0.18611300	-3.64353300	0.51316400
C	-0.61048500	-2.47592100	-0.25638300
C	0.32148400	-4.94536000	-0.28181600
O	0.86589300	-4.76190400	-1.39458400
O	0.10919000	-6.04520800	0.29674100
O	3.49890200	0.61749000	2.13292900
H	3.22161500	1.53199900	1.97201900
C	-1.30696700	0.25310800	-0.80769900
O	-1.14705800	0.33372700	-2.04326700

O	-2.35351800	0.26894900	-0.12273800
H	-0.98320300	0.08929200	1.91293900
H	1.24534500	0.09636000	-1.75179500
H	3.41847200	-0.00801500	-0.48348400
H	2.86388500	-1.24312500	1.73964800
H	1.13747500	-0.03042100	3.25723400
H	-0.45580600	-2.47112200	-1.33568400
H	-1.49302600	-1.95395700	0.11664800

Product

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.49744100
C	1.39431200	0.00000000	-0.54753500
C	2.49249100	-0.21470400	0.19225000
C	2.44601700	-0.52249000	1.66659100
C	1.08956200	-0.21821900	2.24895600
O	0.84537400	-2.96476100	0.53675400
C	-0.15066700	-2.75570900	-0.14017000
C	-0.70227700	-1.36135600	-0.47703300
C	-0.95796400	-4.01898300	-0.63969300
O	-0.33243900	-4.83737600	-1.36067500
O	-2.12410400	-4.12000700	-0.18740800
O	3.49882000	0.15299200	2.38647200
H	3.32370600	1.09861400	2.26809800
C	-0.98616900	1.08920300	-0.67786300
O	-0.71543800	1.33678900	-1.86623500
O	-1.93748000	1.43100400	0.04345000
H	-0.96998500	0.23486300	1.94609100
H	1.45664600	0.23091000	-1.61544400
H	3.49495100	-0.18725500	-0.25512500
H	2.67358500	-1.59830300	1.81879300
H	1.03968400	-0.19147300	3.34566200
H	-0.79085400	-1.30778100	-1.57910200
H	-1.74766800	-1.35292700	-0.12080400

5. At EEF, F_y = -0.617 V/Å

Reactant

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.35409700
C	1.28058700	0.00000000	-0.71887700
C	2.46078400	-0.16604300	-0.09261000
C	2.56598500	-0.33792800	1.39963400
C	1.20303900	-0.49321100	2.13601600
O	1.03186600	-1.85552300	2.69434100
C	1.05825400	-3.04347800	2.02440000
C	0.96140400	-3.23216800	0.69233000
C	1.21079800	-4.31481900	2.96118000
O	1.24943800	-5.43451800	2.36699800
O	1.28052300	-4.12462600	4.19149200
O	3.33445000	0.73204700	1.96187200
H	2.94831700	1.55784300	1.63432800
C	-1.29002500	-0.26630800	-0.82476200
O	-1.02974400	-0.86019000	-1.90857600
O	-2.38981500	-0.00963700	-0.31095600
H	-0.96322900	0.04083000	1.87260600
H	1.21420800	0.11172800	-1.80365200
H	3.41138400	-0.11877700	-0.63776400
H	3.14921000	-1.24546300	1.63428100
H	1.32181000	0.07450900	3.07127100
H	1.00809700	-4.27299000	0.36671300
H	0.79210100	-2.44312800	-0.03761200

TS

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.44874500
C	1.29225700	0.00000000	-0.66057400
C	2.45093600	-0.06480500	0.03210300
C	2.49264700	-0.25638300	1.52408900
C	1.14397900	-0.07569200	2.16519900
O	-0.25901000	-3.60188100	1.74445100
C	-0.16801800	-3.53997300	0.51207400

C	-0.59882900	-2.36923100	-0.26102500
C	0.30428200	-4.86592600	-0.27460600
O	0.77196000	-4.72327300	-1.42770000
O	0.13756800	-5.95027200	0.35050300
O	3.51255300	0.53643800	2.15163200
H	3.26150900	1.46128600	2.00668500
C	-1.30197600	0.28906900	-0.81119900
O	-1.13467600	0.36858500	-2.04502300
O	-2.34930900	0.31474500	-0.12922200
H	-0.98194200	0.10547500	1.91574000
H	1.25557600	0.11342900	-1.74670800
H	3.42295100	-0.02593800	-0.47306100
H	2.83079600	-1.30015800	1.72724800
H	1.13426400	-0.05221200	3.26050600
H	-0.46259000	-2.38594800	-1.34308300
H	-1.51196600	-1.89236100	0.10021900

Product

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.49745400
C	1.39269400	0.00000000	-0.54977200
C	2.49055700	-0.22056600	0.18901300
C	2.44493300	-0.52781900	1.66405100
C	1.09027500	-0.21780100	2.24811400
O	0.84437300	-2.98034200	0.59692700
C	-0.15489000	-2.77500900	-0.07714100
C	-0.68318800	-1.38494600	-0.46789500
C	-0.90135300	-4.05534300	-0.63162300
O	-0.86691000	-4.20089100	-1.87795600
O	-1.36713700	-4.85197700	0.22424000
O	3.50349500	0.13789300	2.38230200
H	3.33784800	1.08583200	2.26762500
C	-1.02004200	1.04907600	-0.68751400
O	-0.71146900	1.36664800	-1.84723700
O	-2.03128700	1.28030700	-0.00203900
H	-0.97101500	0.23306200	1.94533800
H	1.45411200	0.23717700	-1.61632500
H	3.49302900	-0.19223400	-0.25839500
H	2.66446900	-1.60571000	1.81557900
H	1.04182200	-0.18877800	3.34472100
H	-0.73797200	-1.37887200	-1.57132400
H	-1.74080000	-1.34119600	-0.14385000

6. At EEF, F_y = +0.200 V/Å

Reactant

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.35202000
C	1.29767400	0.00000000	-0.69547800
C	2.46250600	-0.10345200	-0.02728200
C	2.52219100	-0.24416400	1.48468200
C	1.26579600	0.37873700	2.09740800
O	1.20726600	0.06080900	3.49903700
C	1.06639300	1.04574400	4.43260700
C	0.24688200	0.83035600	5.47886300
C	1.95658100	2.32790300	4.39260200
O	1.63304600	3.25123900	5.16288800
O	2.94714600	2.30064800	3.60810300
O	3.70842000	0.30123700	2.01149400
H	3.45464800	1.01796800	2.65518500
C	-1.30973500	0.07782000	-0.83999700
O	-1.13133300	0.32542400	-2.06044400
O	-2.38383400	-0.05528700	-0.21661000
H	-0.95572400	0.00606900	1.88472000
H	1.24202900	0.06878600	-1.78549900
H	3.42826700	-0.16082300	-0.54447700
H	2.48492400	-1.33663100	1.72287200
H	1.38560600	1.47501600	2.00026700
H	0.20339800	1.58187000	6.26676800
H	-0.34591100	-0.08617100	5.54683900

TS

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39801900
C	1.29480600	0.00000000	-0.68716500
C	2.46395300	-0.02887200	-0.01622500
C	2.51877400	-0.09314200	1.48323500
C	1.15768600	-0.35830600	2.08550600
O	1.11427100	-2.37143700	1.84315000
C	0.99875500	-2.68293500	0.60129100
C	-0.21532400	-2.51301000	-0.07168300
C	2.26962500	-3.11483700	-0.22079900
O	2.02434000	-3.67495400	-1.31163600
O	3.37794000	-2.85122900	0.30225200
O	3.05045300	1.16005600	2.03087100
H	2.44506700	1.82849900	1.67741200
C	-1.26553500	0.50745300	-0.75618400
O	-1.04839700	0.98760000	-1.89585600
O	-2.34696900	0.44901400	-0.12686600
H	-0.97498300	0.05198800	1.89049300
H	1.25174700	0.04264100	-1.77731700
H	3.42169000	-0.05071400	-0.54320500
H	3.22117400	-0.88130900	1.78573400
H	1.14671900	-0.41581700	3.17833400
H	-0.26184800	-2.78776000	-1.12608000
H	-1.14172400	-2.29649500	0.46098000

Product

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.50295600
C	1.41126000	0.00000000	-0.52540000
C	2.44300400	0.46586200	0.19582700
C	2.25647400	1.06245500	1.57255900
C	1.02552000	0.47380600	2.22753600
O	-0.05383000	-3.09113100	0.42569400
C	-0.22852200	-2.50390300	-0.63037700
C	-0.85795700	-1.10629500	-0.64573900
C	0.18253100	-3.07543200	-2.02272500
O	0.87938500	-2.27264700	-2.70019800
O	-0.22168100	-4.21421100	-2.30862800
O	2.16871300	2.49575300	1.51875100
H	1.36543100	2.62011300	0.93818700
C	-0.67976100	1.48599000	-0.37823700
O	-0.02577500	2.50023000	-0.02140100
O	-1.77416200	1.45343500	-0.95266000
H	-0.91097200	-0.35786800	1.99716700
H	1.54438600	-0.43749200	-1.52196700
H	3.45639300	0.47669100	-0.22696700
H	3.14905000	0.85139200	2.19750300
H	0.95919200	0.52872800	3.32237900
H	-1.07883700	-0.80199600	-1.67533600
H	-1.81932100	-1.15670200	-0.10563600

7. In Aqueous Solution

Reactant

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.34964900
C	1.28058000	0.00000000	-0.72567900
C	2.46010700	0.17513200	-0.10010500
C	2.50896300	0.46987500	1.37768600
C	1.27204000	-0.04342800	2.14757700
O	1.46702600	-1.41802000	2.54620500
C	2.13024800	-1.67941400	3.71857300
C	3.07574400	-2.63485400	3.72178100
C	1.65870100	-0.99264600	5.03008300
O	2.38995200	-1.16361900	6.02982700
O	0.57812000	-0.35639900	4.96555100
O	2.69233800	1.87629400	1.59164500
H	2.02017300	2.33241000	1.06404600
C	-1.31472700	-0.02507300	-0.81086100
O	-1.18474100	-0.11436100	-2.05771600
O	-2.38396500	0.03808700	-0.15988700

H	-0.95166400	-0.02798600	1.88625100
H	1.21575700	-0.13912900	-1.80712200
H	3.40210200	0.19414600	-0.65785000
H	3.39319000	-0.00378300	1.83447200
H	1.16908800	0.57100600	3.05298000
H	3.53966600	-2.91864300	4.66567600
H	3.36400500	-3.14858600	2.80037000

TS

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39540000
C	1.28968900	0.00000000	-0.69346400
C	2.45582100	-0.12155100	-0.03007900
C	2.51411100	-0.32617900	1.45767600
C	1.13614300	-0.41743500	2.07976300
O	0.84237200	-2.47383600	1.86986000
C	0.67875600	-2.78724700	0.63444000
C	-0.50720200	-2.51286500	-0.03787600
C	1.88307200	-3.37376100	-0.17181800
O	1.61653900	-3.82043300	-1.31516300
O	2.99990800	-3.36644700	0.39931000
O	3.29472100	0.69353700	2.10139600
H	2.89170200	1.54578600	1.87724600
C	-1.27862400	0.35658500	-0.79145100
O	-1.12653200	0.54865100	-2.02220200
O	-2.34275500	0.42252200	-0.13154000
H	-0.95802300	0.11401800	1.90668400
H	1.25007000	0.12875600	-1.77682700
H	3.41594900	-0.07495800	-0.55357800
H	3.03857100	-1.27427600	1.65363100
H	1.13182300	-0.46406700	3.17149600
H	-0.60032300	-2.78217500	-1.08995800
H	-1.39633200	-2.17678700	0.49417200

Product

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.50601600
C	1.40279100	0.00000000	-0.54348500
C	2.50355900	-0.15442300	0.20403800
C	2.47840600	-0.34721400	1.69715600
C	1.09596500	-0.15055600	2.26316800
O	-0.92047900	-3.14245600	0.88763700
C	-0.32590400	-2.57026400	-0.01441900
C	-0.81019800	-1.23011200	-0.54114400
C	0.91532800	-3.21318700	-0.69189600
O	0.88544100	-3.18070400	-1.94549400
O	1.77532300	-3.71433800	0.06348300
O	3.43843200	0.49339600	2.35488300
H	3.17813900	1.40797800	2.16902400
C	-0.80991500	1.28596400	-0.51589200
O	-0.24812900	1.98785800	-1.38347300
O	-1.94111800	1.44463200	-0.00756800
H	-0.97916000	0.14305500	1.97164600
H	1.49059000	0.13201700	-1.62425200
H	3.49800600	-0.15341700	-0.25676500
H	2.82283700	-1.37367100	1.92952200
H	1.02737900	-0.13347900	3.35688100
H	-0.74374600	-1.23514200	-1.63958500
H	-1.85760300	-1.09295900	-0.23525400