Towards a Computational Tool Predicting the Stereochemical Outcome of Asymmetric Reactions. 1. Application to Sharpless Asymmetric Dihydroxylation

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Supporting information

Supporting Information

Table S1. Calculated energies, predicted ee's and de's.

computed energies (kcal/mol)			Computed excesses				
E(MM)	polar solvation	non polar	ΔG=E(MM)+ΔGsolv	ΔΔG	K	excess	Pred.-Obs. ee's
2a, 2-(1,2-isopropylidene-xylofuranoside) styrene, obs.: 98%							
208,71	-19,26	8,91	198,36	-0,58	3	**48,8**	-49
218,41	-23,71	8,78	203,48				
215,75	-25,88	9,57	199,44				
210,15	-21,12	8,75	**197,78**	0			**correct isomer**
2b, meta-dioxolane styrene, obs.: 98%							
221,86	-18,36	8,47	211,97	-1,04	7	**74,3**	-24
219,99	-17,58	8,52	**210,93**	0			**correct isomer**
222,69	-19,51	9,09	212,27				
222,16	-19,58	8,56	211,14				
4b, allyl tri-O-benzyl xylopyranoside, obs.: 78%							
203,19	-17,53	9,31	**194,97**	0			**correct isomer**
204,72	-17,29	9,63	197,06				
210,34	-17,86	9,36	201,84				
208,65	-22,26	9,44	195,83	-0,86	5	**65,9**	-12
6, styrene, obs.: 97%							
224,98	-17,62	8,19	215,55	-1,61	19	**90,2**	-7
222,91	-16,9	7,93	**213,94**	0			**correct isomer**
230,49	-20,86	8,59	218,22				
226,06	-19,08	7,96	214,94				
7, alpha-cyclohexyl styrene, obs.: 57%							
218,4	-17,28	8,55	209,67	-0,64	3	**52,9**	-4
220,22	-17,16	8,26	211,32	-2,29			
219,49	-16,44	8,16	211,21	-2,18			
217,08	-16,72	8,67	**209,03**	0			**correct isomer**
8, alpha-adamantyl styrene, obs.: 53%							
215,85	-15,55	8,86	209,16	-0,73	4	**58,6**	6
216,18	-16,16	8,41	208,43	0			**correct isomer**
218,51	-16,58	9,36	211,29				
216,31	-15,88	8,74	209,17				
5, allyl para-methoxy benzoate, obs.: 98%							

	226,49	-16,65	8,2	218,04	-4,73	6068	**100,0**	2
	225,63	-17,72	8,29	216,2				
	229,72	-19,48	8,14	218,38				
	224,99	-19,66	7,98	**213,31**	0			**correct isomer**
9, benzyl tiglate, obs.: 98%								
	232,47	-16,44	8,67	224,7				
	230,51	-16,96	8,36	221,91				
	231,71	-17,35	8,17	222,53	-2,47	95	**97,9**	0
	226,36	-14,38	8,08	**220,06**	0			**correct isomer**
10, isobutyl angelate, obs.: 60%								
	224,79	-15,3	8,49	217,98	-0,57	3	**48,1**	-12
	226,88	-16,67	7,98	218,19				
	229,55	-16,26	7,87	221,16				
	225,36	-16,41	8,46	**217,41**	0			**correct isomer**
11, alpha,beta unsaturated ester, obs.: 97%								
	213,85	-17,15	8,72	205,42				
	203,96	-15,6	8,55	**196,91**	0			**correct isomer**
	209,97	-16,33	9,01	202,65	-5,74	38984	**100,0**	3
	206	-15,36	8,13	198,77				
12, 1-pentene, obs.: 79%								
	214,24	-16,05	8,07	206,26	-3,05	275	**99,3**	20
	211,6	-16,27	7,88	**203,21**	0			**correct isomer**
	219,7	-19,19	8,28	208,79				
	216,96	-17,33	7,87	207,5				
13, Butene, obs.: 72%								
1	226,07	-18,46	7,73	215,34	-3,16	337	**99,4**	27
2	**221,04**	-16,57	7,71	**212,18**	0			**correct isomer**
14, O-benzyl O-TBS 2-butene,1,4-diol, obs.: 90%								
	206,9	-16,11	8,53	199,32				
	198,5	-15,49	8,35	**191,36**	0			**correct isomer**
	200,73	-16,45	9,04	193,32	-1,96	37	**94,7**	5
	199,79	-14,49	8,67	193,97				
15, 2-cyclohexyl propene, obs.: 69%								
	205,39	-15,2	8,21	198,4				
	206,66	-17	8,23	**197,89**	0			**correct isomer**
	206,96	-16,81	7,84	197,99	-0,1	1	**9,2**	-60
	206,72	-16,46	8,09	198,35				
16, 2-methyl-2-heptene, obs.: 98%								
	215,72	-16,53	8,34	207,53	-5,09	11776	**100,0**	2

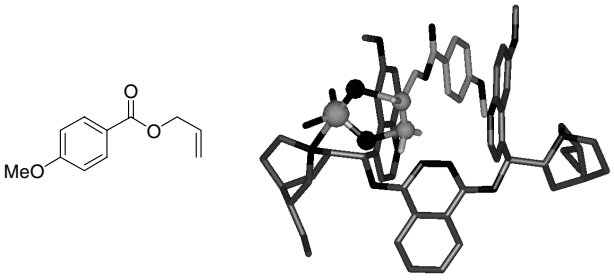
209,61	-15,29	8,12	**202,44**	0			**correct isomer**
216,76	-17,86	8,85	207,75				
213,58	-16,56	8,11	205,13				

17, *E*-methyl enol ether of deoxybenzoin, obs.: 90%							
234,74	-16,13	8,39	227	-1,29	11	**83,0**	-7
234,3	-17	8,41	**225,71**	0			**correct isomer**
240,15	-17,65	8,97	231,47				
239,94	-16,06	8,54	232,42				

18, *Z*-methyl enol ether of deoxybenzoin, obs.: 99%							
236,27	-18,05	8,68	226,9				
228,97	-17,97	8,75	**219,75**	0			**correct isomer**
234,86	-18,51	8,6	224,95	-5,2	14421	**100,0**	10
229,69	-17,28	8,19	220,6				

The data below includes computed energies, predicted ee's with or without the solvation contribution.

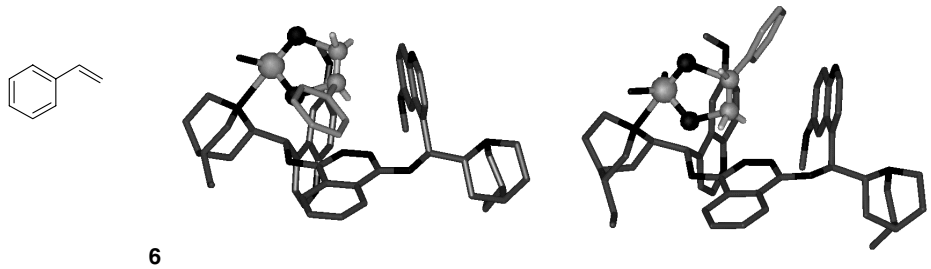
Optimized geometries and Cartesian coordinates for representative transition states.



5

1	4.267	2.187	-5.60	N	18	3.879	-1.06	-6.31	H
2	5.216	0.399	-7.29	C	19	3.072	-0.02	-7.46	H
3	5.612	-0.37	-7.97	H	20	5.029	0.990	-10.4	C
4	4.241	2.697	-6.98	C	21	4.313	1.779	-9.37	C
5	5.016	1.776	-7.99	C	22	4.496	1.093	-11.4	H
6	4.661	3.718	-6.98	H	23	6.058	1.355	-10.6	H
7	3.193	2.813	-7.30	H	24	5.081	-0.08	-10.2	H
8	6.022	2.208	-8.16	H	25	3.283	1.393	-9.27	H
9	5.658	1.877	-5.26	C	26	4.215	2.830	-9.70	H
10	6.187	0.655	-6.10	C	27	-2.21	-1.13	-6.11	C
11	5.731	1.673	-4.18	H	28	-2.73	0.069	-6.48	C
12	6.278	2.773	-5.44	H	29	-4.05	0.239	-6.87	O
13	6.259	-0.25	-5.47	H	30	-1.89	1.141	-6.47	N
14	7.215	0.847	-6.45	H	31	-0.68	1.066	-6.13	N
15	3.477	0.951	-5.49	C	32	-0.08	-0.09	-5.76	C
16	3.850	-0.02	-6.68	C	33	1.251	-0.10	-5.42	O
17	3.789	0.432	-4.56	H	34	-0.85	-1.22	-5.75	C

35	-2.47	-3.52	-5.71	C
36	-3.09	-4.42	-5.69	H
37	-3.03	-2.31	-6.08	C
38	-4.08	-2.27	-6.35	H
39	-0.30	-2.49	-5.37	C
40	0.741	-2.59	-5.10	H
41	-1.11	-3.61	-5.36	C
42	-0.69	-4.58	-5.07	H
43	1.908	1.172	-5.32	C
44	1.546	1.802	-6.14	H
45	-4.42	1.539	-7.36	C
46	-3.91	2.295	-6.75	H
47	1.406	3.735	-2.45	C
48	1.136	2.920	-1.39	N
49	1.133	1.614	-1.62	C
50	0.929	1.005	-0.74	H
51	1.389	1.044	-2.86	C
52	1.393	-0.04	-2.93	H
53	1.628	1.840	-3.96	C
54	1.623	3.231	-3.74	C
55	1.752	5.983	-3.14	C
56	1.799	7.034	-2.87	H
57	1.465	5.062	-2.15	C
58	1.297	5.384	-1.12	H
59	1.877	4.198	-4.74	C
60	2.029	3.883	-5.77	H
61	1.970	5.555	-4.47	C
62	-3.15	3.149	-10.6	C
63	-2.93	2.058	-11.4	N
64	-3.20	0.869	-10.9	C
65	-3.01	0.031	-11.5	H
66	-3.68	0.684	-9.63	C
67	-3.86	-0.33	-9.30	H
68	-3.91	1.766	-8.80	C
69	-3.63	3.038	-9.35	C
70	-3.03	5.511	-10.5	C
71	-2.78	6.461	-11.0	H
72	-2.85	4.342	-11.2	C
73	-2.48	4.359	-12.2	H
74	-3.81	4.258	-8.64	C
75	-4.17	4.221	-7.62	H
76	-3.51	5.489	-9.21	C
77	-8.02	0.263	-7.61	C
78	-8.59	-0.36	-8.32	H
79	-6.86	0.349	-5.36	C
80	-7.72	-0.55	-6.31	C
81	-7.33	0.423	-4.37	H
82	-5.84	-0.01	-5.21	H
83	-8.69	-0.71	-5.81	H
84	-8.07	2.344	-6.19	C
85	-8.87	1.507	-7.22	C
86	-8.63	2.394	-5.24	H
87	-7.94	3.377	-6.54	H
88	-9.08	2.112	-8.12	H
89	-9.84	1.205	-6.80	H
90	-5.95	1.744	-7.32	C
91	-6.71	0.759	-8.27	C
92	-6.13	2.765	-7.71	H
93	-6.93	1.264	-9.23	H
94	-6.09	-0.11	-8.53	H
95	-6.94	-2.80	-5.31	C
96	-7.13	-1.95	-6.57	C
97	-6.55	-3.80	-5.55	H
98	-6.22	-2.33	-4.61	H
99	-7.89	-2.93	-4.77	H
100	-7.80	-2.50	-7.26	H
101	-6.16	-1.87	-7.10	H
102	-3.66	6.707	-8.57	O
103	2.273	6.412	-5.51	O
104	2.333	7.810	-5.25	C
105	-4.29	6.740	-7.29	C
106	3.130	8.031	-4.52	H
107	1.369	8.172	-4.86	H
108	2.553	8.345	-6.18	H
109	-4.33	7.779	-6.93	H
110	-3.73	6.140	-6.56	H
111	-5.32	6.359	-7.37	H
112	-2.75	3.641	-2.67	C
113	-2.60	2.422	-3.30	C
114	-3.10	3.647	-1.64	H
115	-2.80	1.498	-2.77	H
116	-2.01	2.342	-4.20	H
117	-5.62	3.239	-4.30	Os
118	-4.75	4.248	-3.15	O
119	-4.31	2.064	-4.47	O
120	-5.78	4.310	-5.66	O
121	-6.97	2.692	-3.36	O
122	-6.74	1.784	-5.91	N
123	-2.11	4.906	-3.16	C
124	-2.80	5.759	-3.06	H
125	-1.26	5.153	-2.51	H
126	-1.67	4.782	-4.52	O
127	-1.29	5.903	-5.19	C
128	-1.35	7.014	-4.71	O
129	-0.19	4.009	-8.37	C
130	-0.17	2.967	-8.68	H
131	0.242	5.050	-9.20	C
132	0.149	6.368	-8.72	C
133	0.476	7.199	-9.35	H
134	-0.35	6.634	-7.46	C
135	-0.39	7.671	-7.13	H
136	-0.78	5.604	-6.60	C
137	-0.70	4.291	-7.11	C
138	-1.02	3.447	-6.51	H
139	0.756	4.854	-10.4	O
140	0.882	3.516	-10.9	C
141	-0.10	3.035	-11.0	H
142	1.530	2.929	-10.2	H
143	1.335	3.530	-11.9	H



6

Conformer 1:

1	2.969	-1.48	10.51	N
2	3.194	-0.18	11.15	C
3	4.708	0.078	11.50	C
4	5.550	-1.01	10.78	C
5	6.634	-0.83	10.88	H
6	2.579	-0.14	12.07	H
7	2.793	0.605	10.50	H
8	4.855	-0.06	12.58	H
9	3.573	-2.52	11.35	C
10	5.139	-2.38	11.40	C
11	3.282	-3.51	10.96	H
12	3.138	-2.45	12.36	H
13	5.627	-3.20	10.86	H
14	5.497	-2.46	12.45	H
15	3.605	-1.52	9.188	C
16	5.117	-1.07	9.291	C
17	3.611	-2.57	8.855	H
18	5.756	-1.76	8.716	H
19	5.274	-0.08	8.817	H
20	4.395	2.584	12.05	C
21	5.129	1.538	11.19	C
22	3.309	2.565	11.87	H
23	4.562	2.406	13.12	H
24	4.754	3.600	11.82	H
25	6.215	1.648	11.37	H
26	4.966	1.770	10.13	H
27	2.984	0.817	3.563	C
28	1.964	1.649	3.930	C
29	1.333	2.510	3.049	O
30	1.560	1.617	5.227	N
31	2.060	0.843	6.081	N
32	3.055	-0.03	5.797	C
33	3.494	-0.89	6.787	O
34	3.551	-0.04	4.524	C
35	4.463	-0.10	1.866	C
36	4.823	-0.13	0.840	H
37	3.458	0.776	2.213	C
38	3.031	1.423	1.454	H
39	4.598	-0.94	4.141	C
40	5.046	-1.61	4.865	H
41	5.036	-0.96	2.833	C
42	5.828	-1.64	2.536	H
43	2.824	-0.73	8.051	C
44	2.893	0.332	8.302	H
45	0.250	3.281	3.609	C
46	-0.33	2.615	4.259	H
47	-1.04	-0.95	8.202	C
48	-1.25	-2.23	7.779	N
49	-0.18	-2.96	7.474	C
50	-0.40	-3.97	7.146	H
51	1.120	-2.49	7.559	C
52	1.933	-3.16	7.283	H
53	1.371	-1.20	7.984	C
54	0.248	-0.41	8.309	C
55	-2.05	1.057	8.940	C
56	-2.95	1.613	9.185	H
57	-2.16	-0.24	8.506	C
58	-3.14	-0.71	8.412	H
59	0.332	0.932	8.748	C
60	1.306	1.400	8.834	H
61	-0.79	1.673	9.069	C
62	0.574	5.985	6.379	C
63	1.801	6.512	6.118	N
64	2.480	6.003	5.099	C
65	3.454	6.454	4.934	H
66	2.006	4.975	4.288	C
67	2.646	4.631	3.478	H
68	0.761	4.421	4.515	C
69	0.034	4.946	5.607	C
70	-1.32	6.064	7.790	C
71	-1.83	6.509	8.642	H
72	-0.07	6.539	7.440	C
73	0.381	7.345	8.007	H
74	-1.24	4.477	5.994	C
75	-1.70	3.668	5.431	H
76	-1.93	5.019	7.072	C
77	-0.29	4.776	0.129	C
78	0.210	5.560	-0.46	H
79	-0.59	2.280	0.480	C
80	0.077	3.365	-0.42	C
81	-1.21	1.606	-0.12	H
82	0.138	1.656	1.011	H
83	-0.39	3.287	-1.42	H
84	-2.49	3.821	0.849	C
85	-1.82	4.951	0.040	C
86	-3.11	3.185	0.196	H
87	-3.15	4.216	1.635	H

88	-2.12	5.936	0.437	H
89	-2.16	4.916	-1.00	H
90	-0.65	3.872	2.506	C
91	0.113	4.907	1.619	C
92	-1.45	4.421	3.033	H
93	-0.09	5.929	1.981	H
94	1.203	4.775	1.698	H
95	1.941	1.823	-1.34	C
96	1.591	3.151	-0.65	C
97	1.628	0.957	-0.74	H
98	1.448	1.746	-2.32	H
99	3.028	1.740	-1.50	H
100	1.979	3.977	-1.27	H
101	2.135	3.212	0.301	H
102	-3.18	4.593	7.498	O
103	-0.76	2.985	9.516	O
104	0.507	3.618	9.660	C
105	-3.88	3.634	6.711	C
106	1.132	3.071	10.38	H
107	0.360	4.642	10.03	H
108	1.027	3.668	8.691	H
109	-4.07	4.036	5.706	H
110	-4.84	3.409	7.188	H
111	-3.30	2.699	6.634	H
112	-0.83	-1.14	4.377	C
113	-2.13	-1.43	4.733	C
114	-0.24	-0.52	5.050	H
115	-2.66	-2.24	4.258	H
116	-2.55	-1.06	5.664	H
117	-2.66	1.152	2.798	Os
118	-3.44	-0.12	3.721	O
119	-1.02	0.628	3.197	O
120	-3.15	0.773	1.180	O
121	-3.18	2.574	3.640	O
122	-1.49	2.888	1.542	N
123	-0.07	-1.92	3.347	C
124	1.951	-3.11	2.673	C
125	2.952	-3.47	2.907	H
126	1.394	-3.37	1.414	C
127	1.960	-3.93	0.670	H
128	0.099	-2.92	1.122	C
129	-0.33	-3.12	0.147	H
130	-0.62	-2.21	2.077	C
131	-1.62	-1.87	1.804	H
132	1.225	-2.40	3.623	C
133	1.689	-2.22	4.590	H

Conformer 2:

1	4.718	5.341	9.146	N
2	6.156	5.214	8.897	C
3	6.865	4.196	9.867	C
4	5.747	3.423	10.63	C
5	6.161	2.614	11.25	H
6	6.615	6.214	8.986	H
7	6.309	4.925	7.844	H
8	7.440	4.767	10.62	H
9	4.527	5.658	10.56	C
10	4.983	4.470	11.48	C
11	3.466	5.906	10.73	H
12	5.088	6.578	10.80	H
13	5.609	4.845	12.31	H
14	4.113	3.997	11.97	H
15	4.025	4.079	8.849	C
16	4.732	2.875	9.593	C
17	3.003	4.156	9.267	H
18	3.974	2.237	10.07	H
19	5.245	2.206	8.879	H
20	9.078	4.091	8.536	C
21	7.899	3.308	9.132	C
22	8.743	4.814	7.777	H
23	9.797	3.410	8.052	H
24	9.618	4.648	9.319	H
25	7.406	2.738	8.324	H
26	8.301	2.556	9.835	H
27	3.218	0.084	4.410	C
28	3.681	0.900	3.416	C
29	3.889	0.469	2.117	O
30	3.925	2.200	3.728	N
31	3.745	2.674	4.878	N
32	3.263	1.942	5.917	C
33	3.069	2.560	7.139	O
34	2.982	0.625	5.689	C
35	2.419	-2.07	5.175	C
36	2.196	-3.12	4.990	H
37	2.929	-1.29	4.162	C
38	3.101	-1.73	3.184	H
39	2.455	-0.21	6.726	C
40	2.267	0.185	7.721	H
41	2.181	-1.53	6.461	C
42	1.780	-2.17	7.244	H
43	3.819	3.778	7.301	C
44	4.818	3.594	6.885	H
45	3.934	1.527	1.139	C
46	3.202	2.286	1.440	H
47	3.051	6.909	5.156	C
48	1.772	7.183	5.533	N
49	1.199	6.364	6.405	C
50	0.176	6.621	6.663	H
51	1.840	5.261	6.965	C
52	1.293	4.647	7.677	H
53	3.144	4.969	6.624	C
54	3.754	5.811	5.671	C
55	4.878	7.572	3.799	C
56	5.298	8.266	3.073	H
57	3.590	7.776	4.252	C
58	3.009	8.620	3.888	H
59	5.074	5.624	5.181	C
60	5.656	4.781	5.539	H
61	5.645	6.484	4.256	C

62	6.746	4.186	0.834	C
63	7.853	3.467	1.169	N
64	7.681	2.188	1.474	C
65	8.593	1.660	1.738	H
66	6.443	1.550	1.472	C
67	6.411	0.499	1.750	H
68	5.300	2.243	1.125	C
69	5.470	3.606	0.799	C
70	5.910	6.318	0.225	C
71	6.099	7.368	0.010	H
72	6.972	5.502	0.557	C
73	7.980	5.907	0.608	H
74	4.399	4.468	0.439	C
75	3.392	4.067	0.404	H
76	4.601	5.809	0.148	C
77	4.026	-1.12	-1.62	C
78	4.815	-1.76	-2.06	H
79	2.034	-1.02	-0.06	C
80	3.090	-1.97	-0.71	C
81	1.015	-1.37	-0.27	H
82	2.130	-0.96	1.031	H
83	2.540	-2.66	-1.38	H
84	2.062	0.362	-2.11	C
85	3.176	-0.49	-2.75	C
86	2.095	1.406	-2.46	H
87	1.067	-0.03	-2.37	H
88	3.810	0.127	-3.41	H
89	2.732	-1.27	-3.39	H
90	3.594	1.016	-0.27	C
91	4.678	0.027	-0.81	C
92	3.611	1.909	-0.93	H
93	5.399	0.577	-1.44	H
94	5.267	-0.41	0.002	H
95	2.912	-3.87	1.029	C
96	3.828	-2.87	0.304	C
97	2.420	-4.54	0.312	H
98	2.124	-3.35	1.602	H
99	3.487	-4.49	1.736	H
100	4.613	-3.44	-0.22	H
101	4.352	-2.25	1.053	H
102	3.587	6.686	-0.20	O
103	6.931	6.345	3.756	O
104	7.696	5.215	4.165	C
105	2.371	6.125	-0.69	C
106	8.655	5.214	3.625	H
107	7.165	4.280	3.934	H
108	7.901	5.262	5.245	H
109	1.758	6.923	-1.13	H
110	1.804	5.668	0.133	H
111	2.571	5.368	-1.46	H
112	-0.87	2.983	3.177	C
113	0.122	2.118	3.583	C
114	-1.89	2.609	3.138	H
115	-0.11	1.101	3.876	H
116	1.085	2.500	3.902	H
117	0.347	1.792	0.326	Os
118	-0.91	2.783	1.041	O
119	1.068	1.348	1.875	O
120	1.253	2.970	-0.56	O
121	-0.56	0.533	-0.43	O
122	2.133	0.403	-0.58	N
123	-0.70	4.475	3.162	C
124	0.638	6.464	2.707	C
125	1.581	6.906	2.395	H
126	-0.44	7.288	3.029	C
127	-0.34	8.369	2.977	H
128	-1.66	6.711	3.417	C
129	-2.51	7.346	3.665	H
130	-1.79	5.323	3.475	C
131	-2.75	4.914	3.765	H
132	0.514	5.078	2.785	C
133	1.383	4.480	2.517	H