Supporting Information

Synthesis and Hydrolysis of a cis-Chlorohydrin Derived from a Benzo[*a*]pyrene 7,8-Diol 9,10-Epoxide

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Figure S1. ^{1}H NMR Spectrum of cis chlorohydrin **9** in THF-d_8 at 200 MHz.

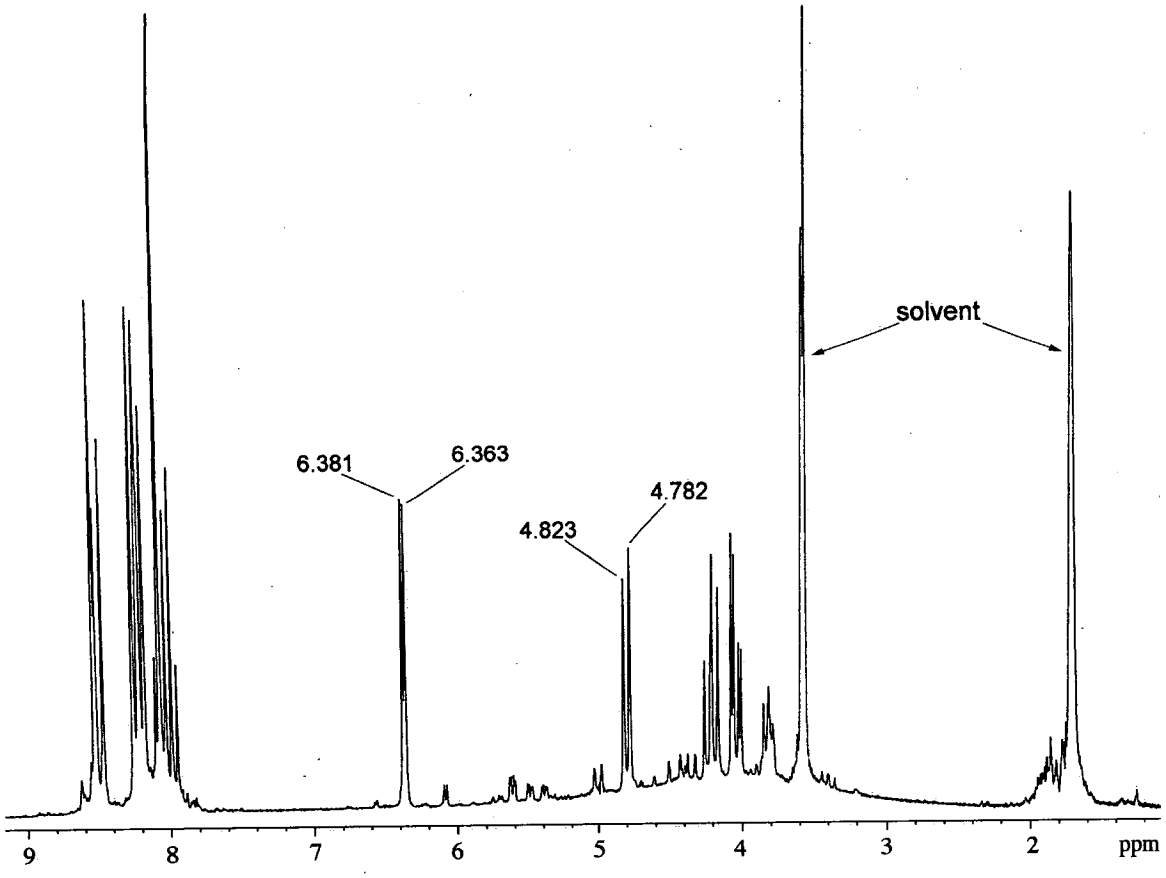
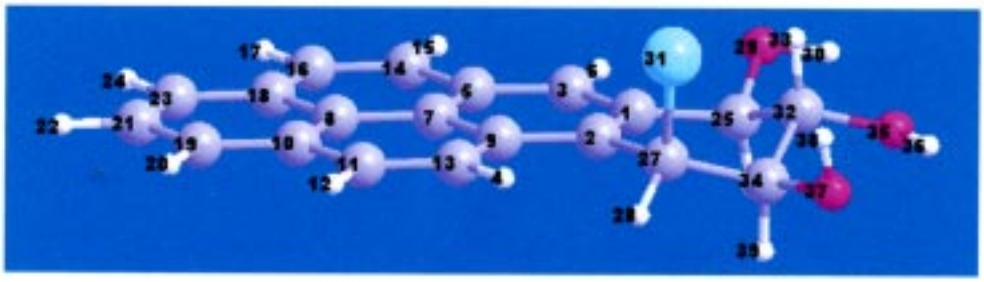


Figure S2. Optimized Structure (B3LYP/6-31G*) of cis Chlorohydrin Conformation **9a**.

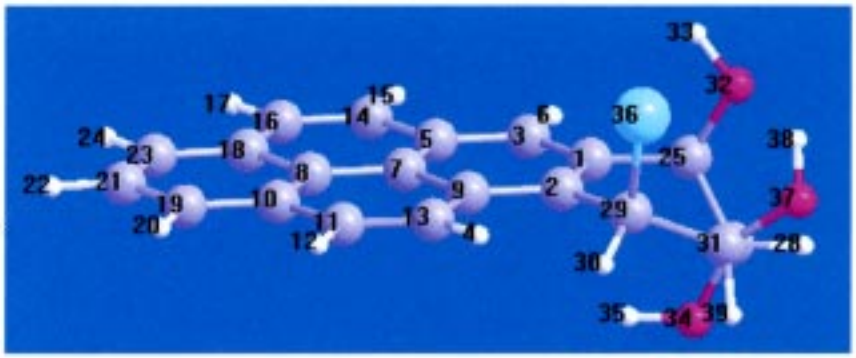


Atom	X	Y	Z
C(1)	1.835	-0.815	0.129
C(2)	1.451	0.541	0.123
C(3)	0.866	-1.818	0.095
C(5)	-0.500	-1.519	0.071
C(7)	-0.910	-0.153	0.088
C(8)	-2.302	0.164	0.080
C(9)	0.072	0.884	0.106
C(10)	-2.727	1.524	0.091
C(11)	-1.724	2.546	0.098
C(13)	-0.396	2.245	0.098
C(14)	-1.501	-2.550	0.042
C(16)	-2.826	-2.245	0.038
C(18)	-3.276	-0.881	0.058
C(19)	-4.102	1.815	0.088
C(21)	-5.045	0.791	0.071
C(23)	-4.638	-0.543	0.055
C(25)	3.288	-1.236	0.266
C(27)	2.488	1.628	0.114
O(29)	3.507	-2.440	-0.455
Cl(31)	2.621	2.390	-1.611
C(32)	4.250	-0.143	-0.175
C(34)	3.883	1.160	0.530
O(35)	5.560	-0.558	0.183
O(37)	4.896	2.141	0.367

Atom	X	Y	Z
H(6)	1.192	-2.853	0.085
H(12)	-2.045	3.585	0.094
H(4)	0.322	3.057	0.075
H(15)	-1.170	-3.585	0.025
H(17)	-3.574	-3.035	0.018
H(20)	-4.424	2.854	0.096
H(22)	-6.104	1.032	0.068
H(24)	-5.380	-1.338	0.038
H(26)	3.490	-1.411	1.339
H(28)	2.199	2.489	0.716
H(30)	4.450	-2.645	-0.343
H(33)	4.169	-0.013	-1.265
H(39)	3.844	0.969	1.611
H(36)	6.104	0.249	0.177
H(38)	4.781	2.521	-0.524

E = -1457.05826 Hartree
Frequency Analysis: No Imaginary Frequencies

Figure S3. Optimized Structure (B3LYP/6-31G*) of cis Chlorohydrin Conformation **9b**.

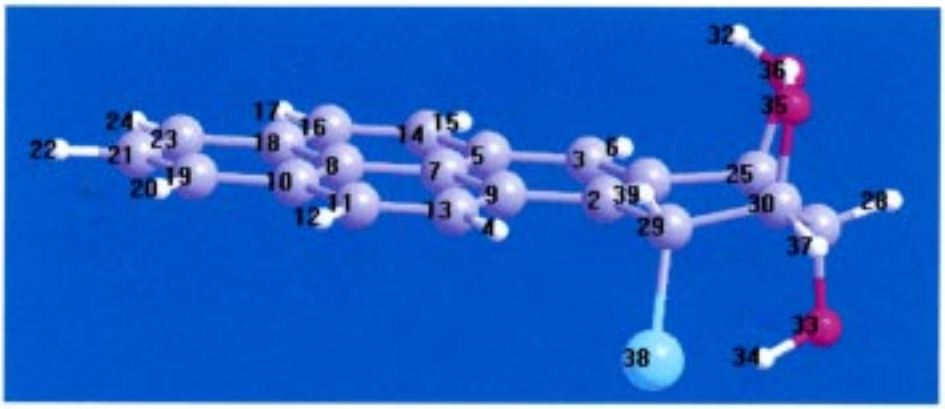


Atom	X	Y	Z
C(1)	2.342	-0.813	-0.179
C(2)	1.968	0.544	-0.133
C(3)	1.378	-1.820	-0.164
C(5)	0.010	-1.522	-0.118
C(7)	-0.392	-0.154	-0.081
C(8)	-1.784	0.165	-0.032
C(9)	0.591	0.887	-0.096
C(10)	-2.206	1.526	-0.003
C(11)	-1.203	2.549	-0.036
C(13)	0.124	2.248	-0.084
C(14)	-0.992	-2.551	-0.098
C(16)	-2.316	-2.243	-0.047
C(18)	-2.760	-0.878	-0.013
C(19)	-3.579	1.818	0.047
C(21)	-4.524	0.796	0.067
C(23)	-4.121	-0.538	0.037
C(25)	3.812	-1.169	-0.180
C(27)	4.523	-0.282	0.848
C(29)	3.036	1.611	-0.163
C(31)	4.461	1.198	0.399
O(32)	4.449	-0.908	-1.444
O(34)	4.005	-0.499	2.153
Cl(36)	3.153	2.257	-1.896
O(37)	5.529	1.503	-0.463

Atom	X	Y	Z
H(6)	1.697	-2.860	-0.175
H(12)	-1.525	3.588	-0.033
H(4)	0.842	3.058	-0.142
H(15)	-0.665	-3.588	-0.124
H(17)	-3.065	-3.031	-0.033
H(20)	-3.898	2.857	0.067
H(22)	-5.582	1.039	0.106
H(24)	-4.864	-1.332	0.051
H(26)	3.935	-2.227	0.089
H(28)	5.582	-0.546	0.904
H(30)	2.705	2.487	0.391
H(39)	4.624	1.802	1.297
H(33)	3.820	-1.109	-2.153
H(35)	3.040	-0.388	2.115
H(38)	5.441	0.894	-1.219

E = -1457.04389 Hartree
Frequency Analysis: No Imaginary Frequencies

Figure S4. Optimized Structure (B3LYP/6-31G*) of trans Chlorohydrin Conformation **10a**.

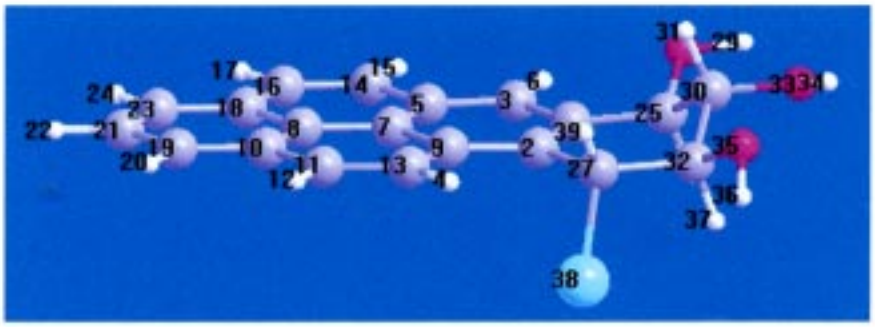


Atom	X	Y	Z
C(1)	2.262	-0.757	-0.001
C(2)	1.860	0.591	-0.060
C(3)	1.306	-1.774	0.049
C(5)	-0.066	-1.502	0.022
C(7)	-0.491	-0.143	-0.066
C(8)	-1.887	0.153	-0.107
C(9)	0.476	0.909	-0.099
C(10)	-2.329	1.506	-0.189
C(11)	-1.340	2.542	-0.220
C(13)	-0.008	2.261	-0.171
C(14)	-1.053	-2.545	0.073
C(16)	-2.382	-2.258	0.032
C(18)	-2.848	-0.902	-0.061
C(19)	-3.707	1.777	-0.231
C(21)	-4.637	0.741	-0.190
C(23)	-4.214	-0.584	-0.104
C(25)	3.718	-1.171	-0.116
C(27)	4.724	-0.079	0.276
C(29)	2.893	1.686	-0.035
C(30)	4.335	1.260	-0.377
O(31)	4.018	-1.505	-1.498
O(33)	4.883	-0.011	1.681
O(35)	4.444	1.200	-1.790
Cl(38)	2.878	2.504	1.664

Atom	X	Y	Z
H(6)	1.637	-2.809	0.120
H(12)	-1.675	3.575	-0.277
H(4)	0.700	3.081	-0.174
H(15)	-0.711	-3.575	0.145
H(17)	-3.120	-3.056	0.070
H(20)	-4.041	2.809	-0.294
H(22)	-5.699	0.968	-0.223
H(24)	-4.946	-1.388	-0.069
H(26)	3.904	-2.049	0.515
H(28)	5.699	-0.376	-0.125
H(39)	2.633	2.508	-0.700
H(37)	5.015	2.042	-0.027
H(32)	3.264	-2.001	-1.854
H(34)	4.160	0.518	2.058
H(36)	4.268	0.276	-2.058

E = -1457.05332 Hartree
Frequency Analysis: No Imaginary Frequencies

Figure S5. Optimized Structure (B3LYP/6-31G*) of trans Chlorohydrin Conformation **10b**.

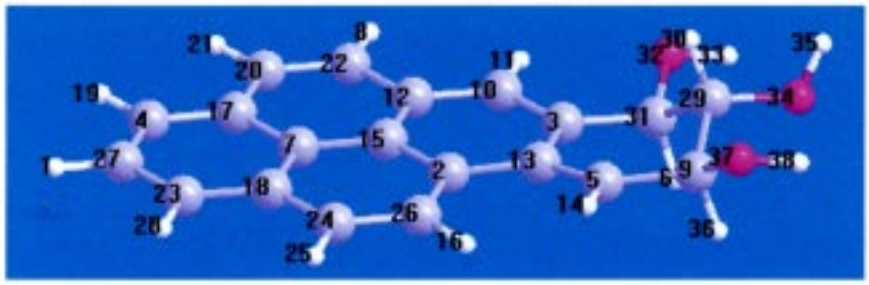


Atom	X	Y	Z
C(1)	1.863	-0.833	0.154
C(2)	1.495	0.528	0.141
C(3)	0.889	-1.830	0.137
C(5)	-0.473	-1.521	0.101
C(7)	-0.869	-0.153	0.028
C(8)	-2.257	0.171	-0.059
C(9)	0.121	0.878	0.032
C(10)	-2.671	1.531	-0.167
C(11)	-1.658	2.544	-0.196
C(13)	-0.334	2.237	-0.099
C(14)	-1.482	-2.545	0.109
C(16)	-2.804	-2.231	0.046
C(18)	-3.240	-0.865	-0.045
C(19)	-4.041	1.830	-0.248
C(21)	-4.992	0.814	-0.224
C(23)	-4.598	-0.520	-0.124
C(25)	3.321	-1.251	0.135
C(27)	2.557	1.603	0.151
O(28)	3.449	-2.515	-0.496
C(30)	4.158	-0.199	-0.583
C(32)	4.010	1.109	0.176
O(33)	5.506	-0.646	-0.566
O(35)	4.898	2.051	-0.415
Cl(38)	2.403	2.763	1.619

Atom	X	Y	Z
H(6)	1.208	-2.867	0.136
H(12)	-1.967	3.581	-0.297
H(4)	0.388	3.042	-0.116
H(15)	-1.160	-3.581	0.168
H(17)	-3.558	-3.015	0.057
H(20)	-4.352	2.868	-0.330
H(22)	-6.049	1.061	-0.286
H(24)	-5.346	-1.309	-0.109
H(26)	3.701	-1.318	1.171
H(39)	2.439	2.278	-0.699
H(29)	4.406	-2.662	-0.589
H(31)	3.798	-0.090	-1.619
H(37)	4.307	0.913	1.215
H(34)	6.049	0.110	-0.848
H(36)	4.963	2.811	0.186

E = -1457.05432 Hartree
Frequency Analysis: No Imaginary Frequencies

Figure S6. Optimized Structure (B3LYP/6-31G*) of Carbocation Conformation **2a**.

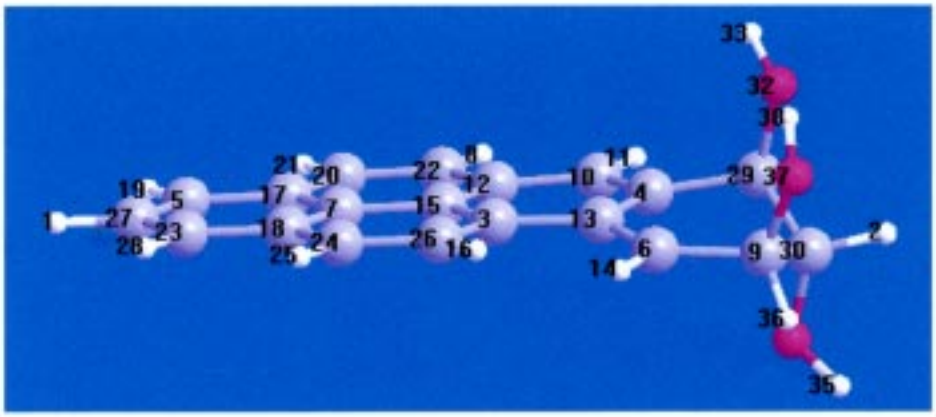


Atom	X	Y	Z
C(2)	-0.098	0.963	-0.148
C(3)	-1.959	-0.732	-0.260
C(4)	4.519	-0.671	0.189
C(5)	-2.481	1.645	-0.089
C(7)	2.219	0.136	0.013
C(9)	-3.949	1.395	-0.120
C(10)	-1.045	-1.741	-0.173
C(12)	0.351	-1.472	-0.066
C(13)	-1.534	0.661	-0.196
C(15)	0.822	-0.118	-0.066
C(17)	3.142	-0.947	0.106
C(18)	2.704	1.472	0.000
C(20)	2.636	-2.280	0.112
C(22)	1.288	-2.533	0.026
C(23)	4.097	1.703	0.083
C(24)	1.764	2.530	-0.102
C(26)	0.411	2.283	-0.179
C(27)	4.991	0.644	0.178
C(29)	-4.262	-0.015	0.406
C(31)	-3.431	-1.026	-0.403
O(37)	-4.594	2.412	0.612

Atom	X	Y	Z
H(19)	5.221	-1.497	0.261
H(14)	-2.203	2.685	0.057
H(36)	-4.267	1.418	-1.182
H(11)	-1.389	-2.769	-0.184
H(21)	3.339	-3.106	0.182
H(8)	0.921	-3.555	0.027
H(28)	4.463	2.726	0.071
H(25)	2.124	3.555	-0.126
H(16)	-0.263	3.126	-0.275
H(1)	6.057	0.836	0.243
H(30)	-3.981	-0.074	1.465
H(6)	-3.706	-0.884	-1.465
H(38)	-5.548	2.325	0.450
O(32)	-3.695	-2.350	-0.004
H(33)	-4.643	-2.499	-0.157
O(34)	-5.640	-0.300	0.219
H(35)	-6.057	-0.440	1.082

E = -996.610839 Hartree
Frequency Analysis: No Imaginary Frequencies

Figure S7. Optimized Structure (B3LYP/6-31G*) of Carbocation Conformation **2b**.



Atom	X	Y	Z
C(3)	0.463	-0.950	0.172
C(4)	2.310	0.756	0.212
C(5)	-4.183	0.643	0.011
C(6)	2.849	-1.601	-0.042
C(7)	-1.869	-0.142	0.103
C(9)	4.330	-1.340	-0.126
C(10)	1.385	1.757	0.180
C(12)	-0.016	1.481	0.107
C(13)	1.893	-0.635	0.141
C(15)	-0.471	0.125	0.127
C(17)	-2.804	0.932	0.038
C(18)	-2.341	-1.481	0.145
C(20)	-2.312	2.268	0.003
C(22)	-0.963	2.533	0.041
C(23)	-3.732	-1.726	0.120
C(24)	-1.387	-2.532	0.215
C(26)	-0.034	-2.275	0.227
C(27)	-4.641	-0.674	0.052
C(29)	3.784	1.054	0.413
C(30)	4.650	0.132	-0.445
O(32)	4.155	0.776	1.772
O(34)	4.315	0.437	-1.790
O(37)	4.877	-1.804	1.102

Atom	X	Y	Z
H(19)	-4.895	1.462	-0.041
H(14)	2.572	-2.650	-0.080
H(36)	4.760	-1.971	-0.911
H(11)	1.706	2.795	0.206
H(21)	-3.024	3.087	-0.049
H(8)	-0.607	3.559	0.021
H(28)	-4.089	-2.751	0.154
H(25)	-1.738	-3.559	0.264
H(16)	0.650	-3.112	0.292
H(1)	-5.707	-0.878	0.031
H(31)	3.993	2.099	0.153
H(2)	5.707	0.321	-0.218
H(33)	3.673	1.370	2.369
H(35)	5.028	0.125	-2.369
H(38)	4.676	-1.121	1.771

E = -996.605013 Hartree
Frequency Analysis: No Imaginary Frequencies