Electronic Supplementary Information

Quantum Chemical Study of HOCl-Induced Transformations of Carbamazepine.

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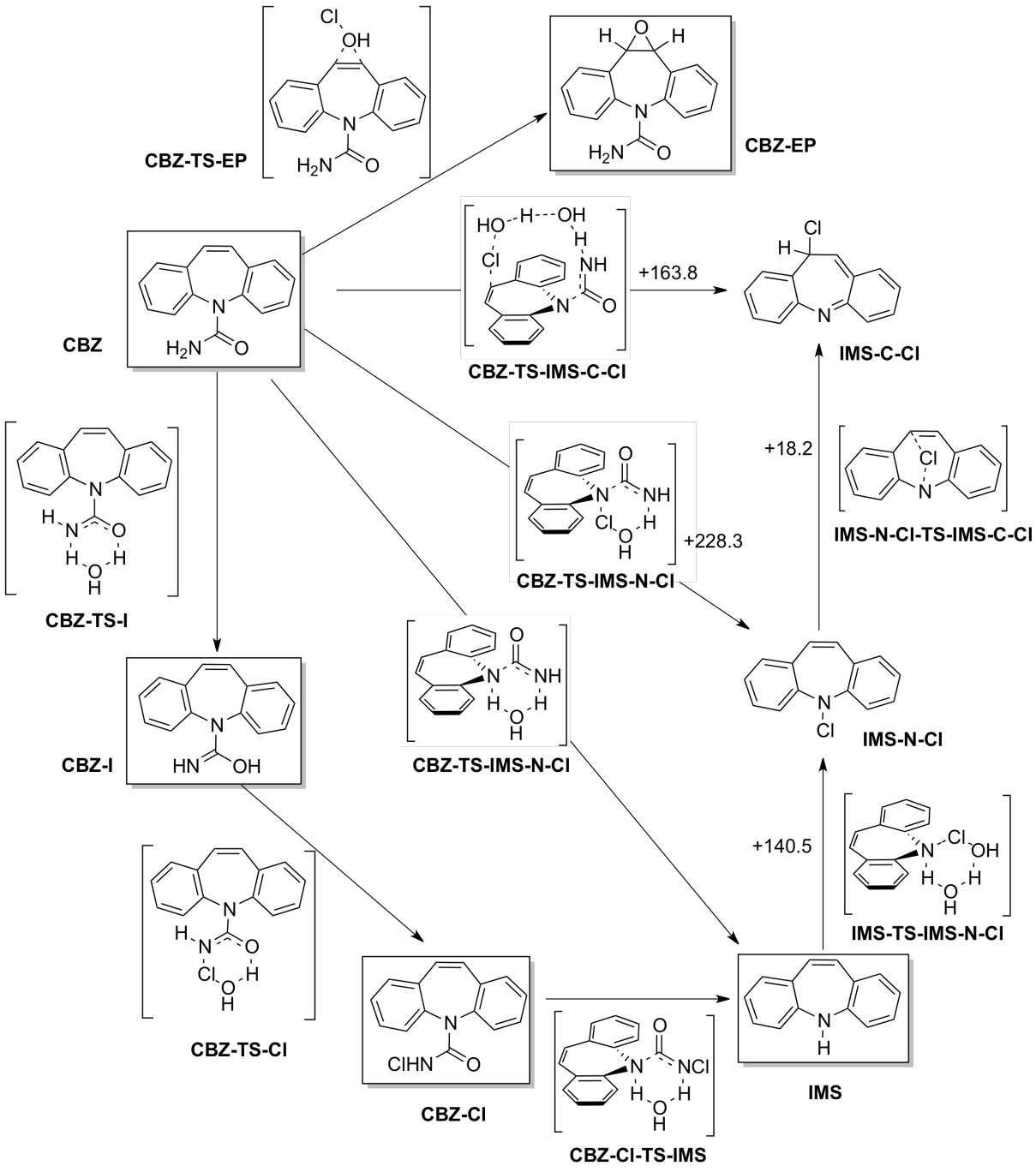


Scheme S1. N-Chlorination and Epoxidation of Carbamazepine

Structures in boxes are discussed in the MS. All optimised structures and corresponding Gibbs free energies (calculated at B3LYP/6-31g(d)) are deposited bellow.

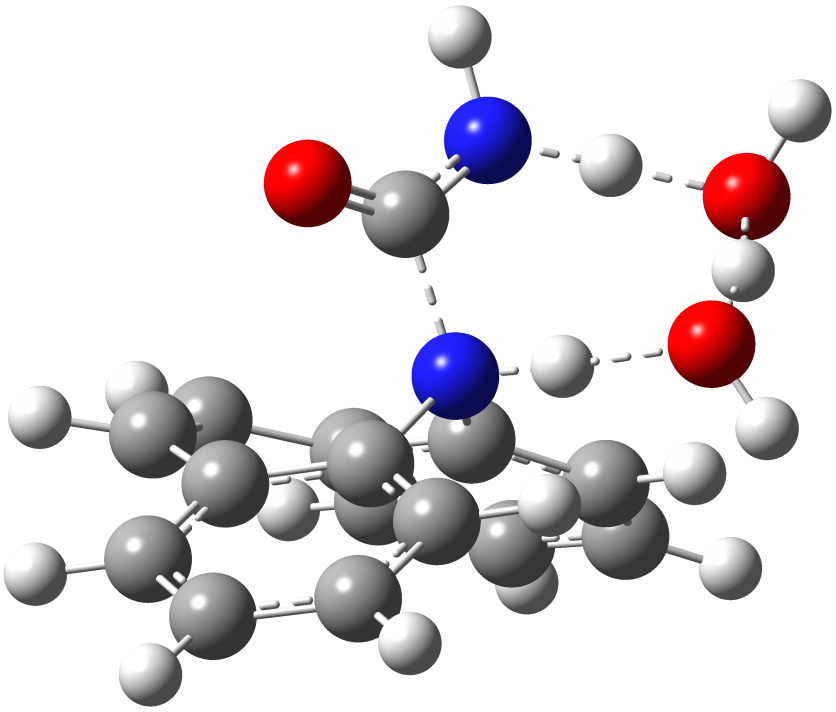


Figure S1. Formation of **IMS** from **CBZ**

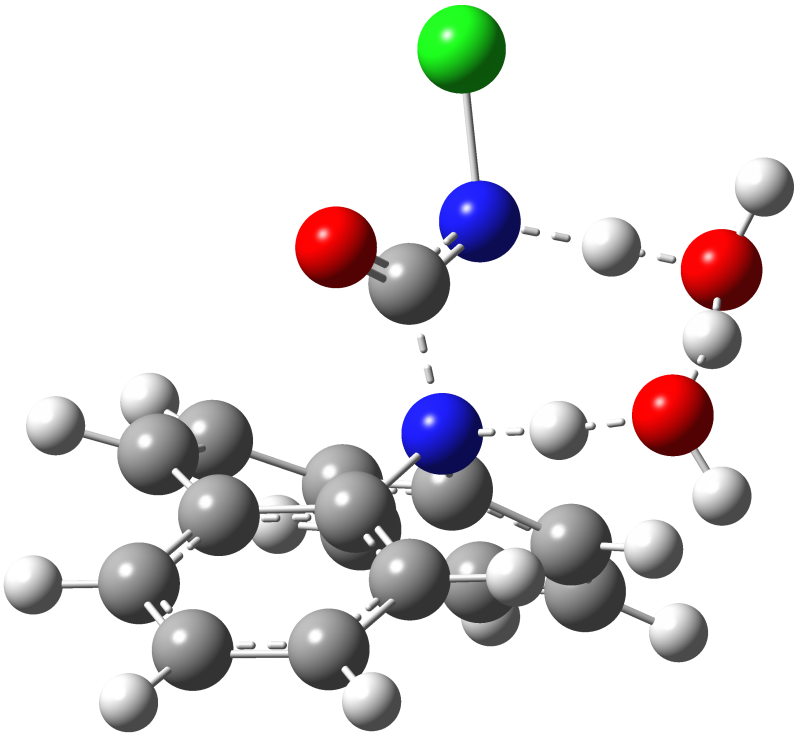
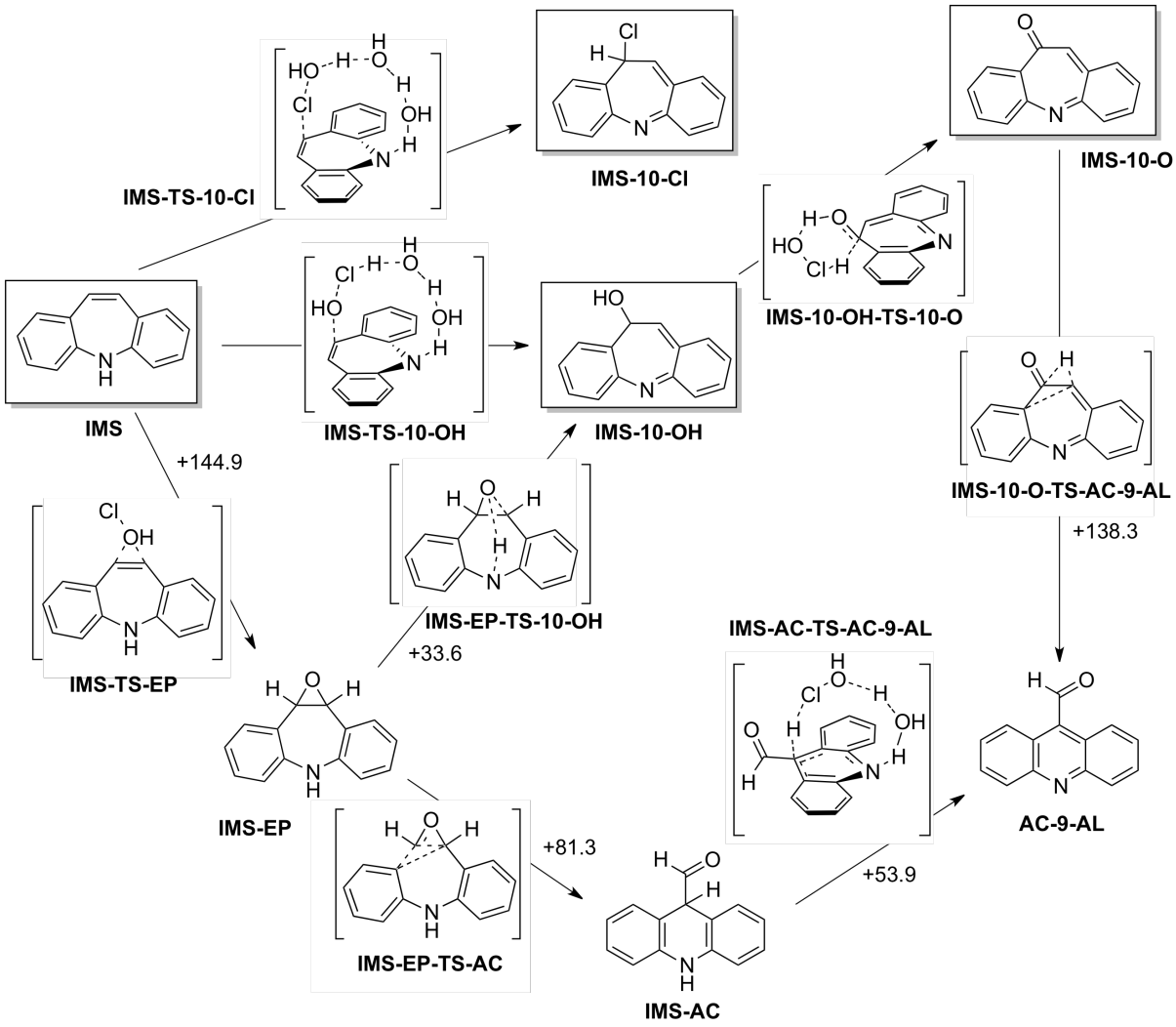
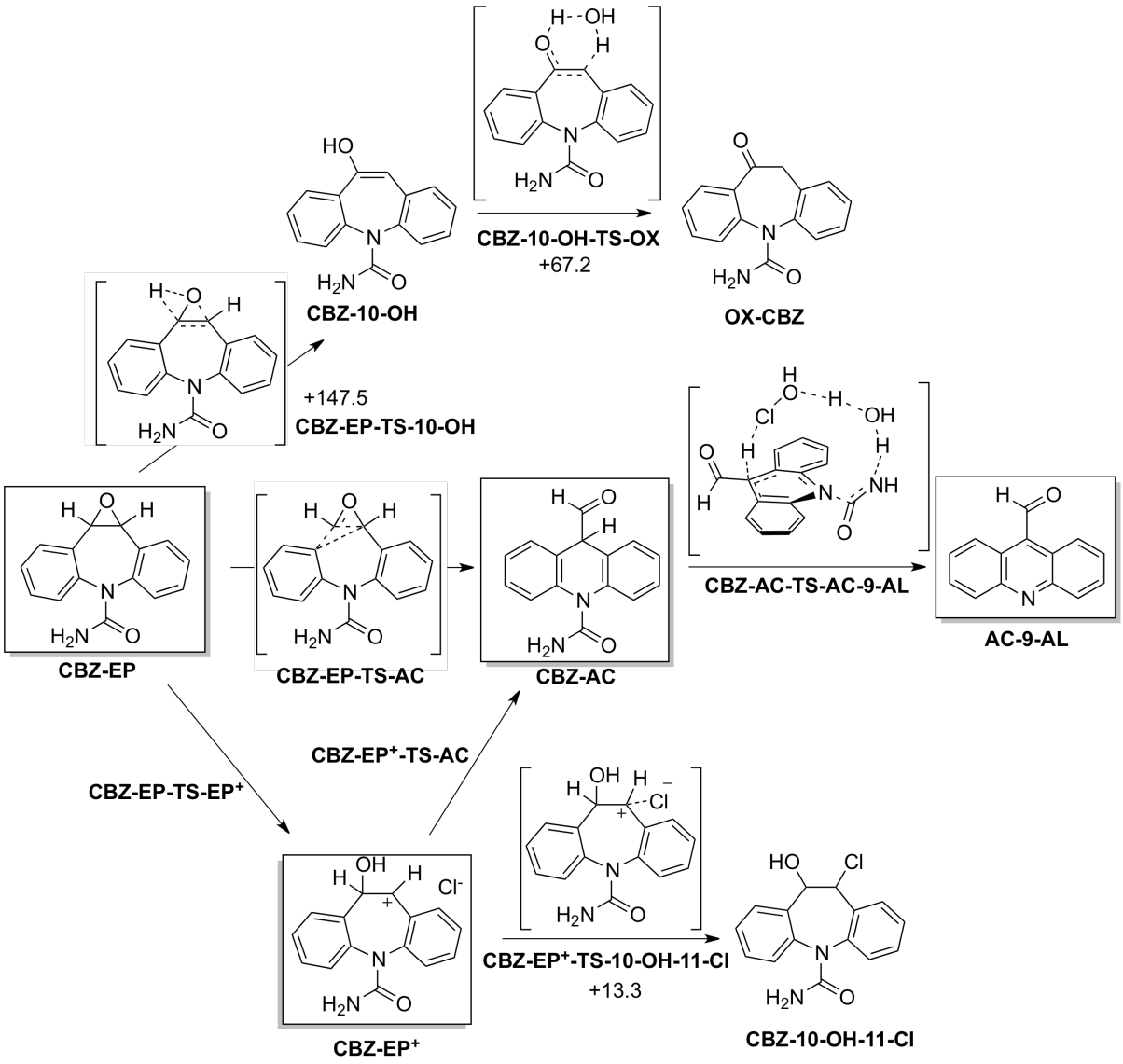


Figure S2. Formation of **IMS** from **CBZ-Cl**



Scheme S2. The formation of 10-Oxoiminostilbene.

Structures in boxes are discussed in the MS. All optimised structures and corresponding Gibbs free energies (calculated at B3LYP/6-31g(d)) are deposited bellow.



Scheme S3. Oxidation of Carbamazepine-10,11-Epoxide

Structures in boxes are discussed in the MS. All optimised structures and corresponding Gibbs free energies (calculated at B3LYP/6-31g(d)) are deposited bellow.

Table S1. Epoxidation power of HOCl compared to typical epoxidizing agents

Relative Gibbs Free Energies (ΔG_{293}, kJ/mol) calculated for epoxidation of ethylene with different epoxidizing agents.

	Gas phase		Water solution[a]		
B2K-PLYP[b]	ΔG_r[c]	$\Delta G^{\#}$	ΔG_r	$\Delta G^{\#}$	*exp*.
ethylene + peroxide	-206.34	175.93	-203.79	149.53	
ethylene + oxaziridine	-110.95	175.86	-103.29	157.37	157.3 [e]
ethylene + dioxirane	-211.33	106.38 [d]	-208.82	71.22	59.0 [f]
ethylene + performic acid	-210.94	123.42 [d]	-207.76	95.3	62.7-75.3 [g]
ethylene + peroxynitrous acid	-179.56	116.57	-182.37	86.14	55.2 [h]
ethylene + HOCl	-121.33	153.58	-122.59	105.26	82.8-94.6 [i]

[a] CPCM/UFF/α=1.1//B3LYP/6-31G(d), no explicit waters

[b] B2K-PLYP/6-311+G(3df,2p)//B3LYP/6-31G(d)

[c] The relative energy of separated reactants set to zero.

[d] *J. Am. Chem. Soc*. **1997**,*119*,10147

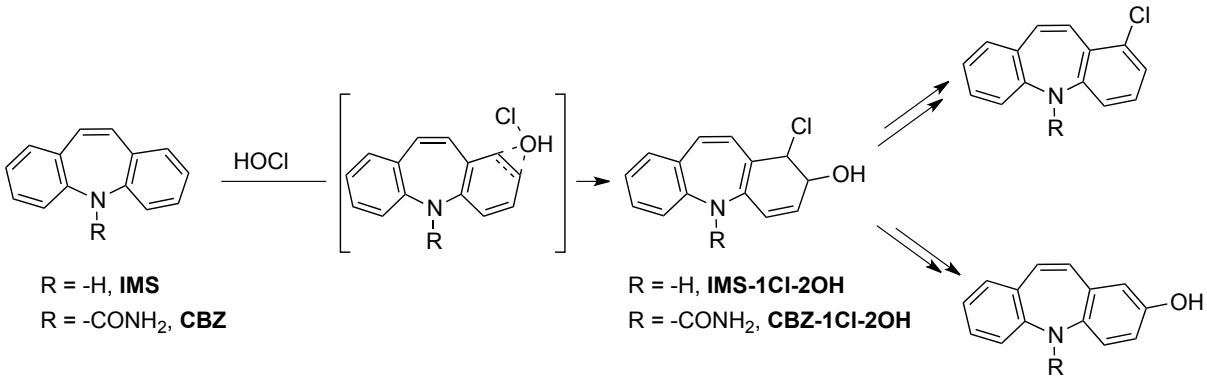
[e] *J. Org. Chem*. **1992**, *57*, 613.

[f] *Tetrahedron* **1976**, *32*, 2855.

[g] *Chem. Rev*. **1989**, *89*, 1187

[h] *J. Am. Chem. Soc*. **1996**, *118*, 13002.

[i] *J. Phys. Chem. A* **2008**, *112*, 3631.

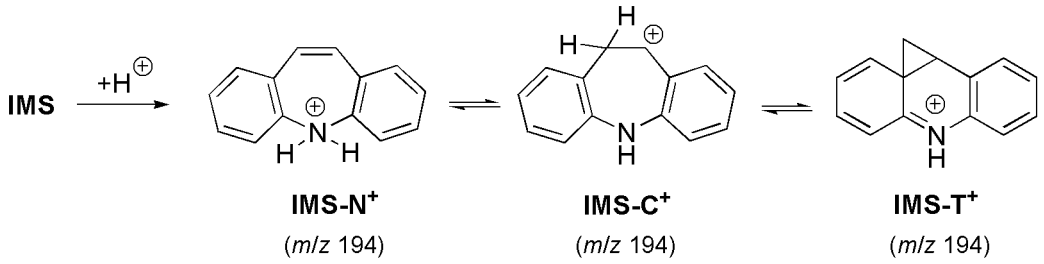


Scheme S4. Ring Oxidation of Carbamazepine and Iminostilbene.

Table S2. Ring Oxidation of Carbamazepine and Iminostilbene
Relative Gibbs Energy (ΔG_{293}, kJ/mol) of Reactants,[a] Intermediates, Products, and Transition State Structures Involved in Various Oxidations[b] (Scheme S4) of Carbamazepine and Iminostilbene, Calculated at Different Levels of Theory in Water as the Model Solvent[c]

Entry	B3LYP[c]	B2K-PLYP[d]	B2-PLYPD[e]	MP2[f]	MP2[g]
CBZ-HOCl	0.0	0.0	0.0	0.0	0.0
CBZ-1Cl-2OH	-58.0	-77.3	-62.4	-75.3	-69.1
CBZ-TS-CBZ-1Cl-2OH	90.3	130.8	132.3	169.5	167.1
IMS-HOCl	0.0	0.0	0.0	0.0	0.0
IMS-1Cl-2OH	-73.2	-70.7	-90.2	-88.3	-79.6
IMS-TS-IMS-1Cl-2OH	58.2	83.6	79.4	82.0	81.9

[a] Gibbs free energy of reactants (HOCl Complexes of **CBZ** and **IMS** without explicit water molecules) set to zero. [b] Products of these reactions were not found in MS spectra obtained by Soufan et al.[30] and Kotcharaksa.[32] [c] CPCM(UFF,α=1.1)//B3LYP/6-31G(d) model (ε = 78.4) [d] B3LYP/6-31G(d) [e] B2K-PLYP/6-311+G(3df,2p)//B3LYP/6-31G(d) [f] B2PLYP-D/6-311+G(3df,2p) [g] MP2/6-311+G(3df,2p)//B3LYP/6-31G(d) [h] MP2/G3MP2Large//B3LYP/6-31G(d)



Scheme S5. Fast rearrangement of N-protonated iminostilbene occurs during LC-ITMS analysis.

In addition to N-protonated iminostilbene **IMS-N**$^+$ (Scheme S5), another protonated isomer of iminostilbene (*m*/*z* 194.2) showed up at 13.8 min retention time in the chromatogram.[MS-32] It is known that iminostilbene undergoes fast acid-catalyzed rearrangement to homotropylium cation **IMS-T**$^+$ (Scheme 4).[SI-1] It has been reported that this prototropic tautomerism proceeded via the quinone imonium ion **IMS-C**$^+$.[SI-2,3] Therefore, both **IMS-T**$^+$ and **IMS-C**$^+$ are good candidates to which the retention peak (13.8 min) could be assigned, but no definitive answer is possible. In any case, the formation of these intermediates is not HOCl-induced process, but most probably occurs during LC-ITMS analysis, and is not discussed in details in MS. Structures and transition states are deposited with the rest of structures.

[1] C. Dardonville, M.-L. Jimeno, I. Alkorta and J. Elguero, *Org. Biomol. Chem*., 2004, **2**, 1587.

[2] E.-C. Elliott, J.-L. Maggs, B. K. Park, P. M. O'Neill and A. V. Stachulski, *Org. Biomol. Chem*., 2013, **11**, 8426.

[3] L. J. Kricka and A. Ledwith, *Chem. Rev*., 1974, **74**, 101.

Cartesian coordinates and Gibbs free energies (B3LYP/6-31G(d)) for all structures

Optimized structures at B3LYP/6-31G(d) level of theory with corresponding Gibbs free energies.

Structures from Table 1/Scheme S1.

CBZ
G = -763.365568

C 3.668105 -1.083134 0.797652
C 3.295806 0.084863 1.469771
C 2.067443 0.680209 1.191255
C 1.206822 0.125027 0.236265
C 1.552676 -1.075127 -0.423520
C 2.805327 -1.650677 -0.133447
C -1.249557 0.161911 0.208993
C -1.590504 -1.045340 -0.434682
C -0.694550 -1.741295 -1.356753
C 0.656988 -1.750963 -1.360438
C -2.132046 0.757821 1.112678
C -3.370506 0.177846 1.374655
C -3.733188 -1.009742 0.732612
C -2.853213 -1.607076 -0.161733
N -0.007184 0.802936 -0.102243
C -0.039285 2.044972 -0.749884
N 1.198704 2.567495 -1.086200
O -1.080641 2.645459 -0.967859
H 4.626947 -1.550739 1.003435
H 3.960910 0.533601 2.202111
H 1.770484 1.598956 1.686982
H 3.088553 -2.566786 -0.646079
H -1.192038 -2.401088 -2.066015
H 1.146849 -2.417798 -2.068216
H -1.849206 1.695744 1.577443
H -4.056136 0.658599 2.066703
H -4.700751 -1.464085 0.927079
H -3.131553 -2.532209 -0.660689
H 1.124154 3.335386 -1.739334
H 1.974359 1.937966 -1.241981

CBZ 1H2O
G = -839.774827

C -3.809959 -1.361300 -0.460529
C -3.371162 -0.515336 -1.483466
C -2.093313 0.036690 -1.421989
C -1.249632 -0.241548 -0.339857
C -1.664859 -1.122843 0.682615
C -2.965590 -1.657810 0.603767
C 1.201613 -0.402956 -0.337649
C 1.469358 -1.351104 0.670766
C 0.552779 -1.622566 1.776981
C -0.794969 -1.519400 1.788360
C 2.093501 -0.220492 -1.396493
C 3.273080 -0.957669 -1.458245
C 3.565522 -1.888297 -0.456751
C 2.674636 -2.076142 0.593072
N 0.022974 0.407146 -0.249869
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N -0.990281 2.489666 0.153005
O 1.278444 2.306609 0.016345
H -4.807187 -1.790875 -0.496487
H -4.022265 -0.281535 -2.320890
H -1.741508 0.711142 -2.196489
H -3.302525 -2.326447 1.392180
H 1.020291 -2.046638 2.664318
H -1.312368 -1.868877 2.680278
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H 1.045140 4.094568 0.481533
O 0.518931 4.843243 0.847482
H 0.748879 4.839194 1.789117

CBZ 2H2O
G = -916.186679

C 2.557236 -3.379165 -0.358807
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C 0.900720 -1.125170 -0.358983
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C 2.561053 -2.507689 0.724698
C 0.524761 1.299406 -0.358557
C 1.295611 1.753020 0.731415
C 1.653799 0.902653 1.865348
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C 0.254304 2.144159 -1.437231
C 0.722843 3.455219 -1.440188
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N -0.016324 -0.026957 -0.337924
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H 1.731914 -3.790524 -2.313614
H 0.259203 -1.781276 -2.296331
H 3.208978 -2.704425 1.575378
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H 2.210658 -0.877172 2.802135
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H 0.493319 4.109363 -2.276575
H 1.834261 4.953090 -0.350807
H 2.333515 3.452223 1.552193
H -2.839044 -1.614414 0.172363
H -1.202644 -2.213280 0.121847
H -3.860477 0.875423 0.102195
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CBZ EP TS EP+ 1H2O
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C -0.947777 -0.325903 -1.214233
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C -0.300225 -1.224015 -0.361533
C 1.915894 -0.251090 0.116694
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N 0.706681 -0.791348 0.566901
H -1.602871 -0.458328 1.726021
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Cl -3.468948 0.778237 1.122751
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CBZ EP TS EP+ 2H2O
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C -2.139239 -0.699859 -1.049427
C -0.225729 1.468454 0.076118
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N -0.983234 0.491537 0.808404
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O -1.317037 -0.413501 2.932362
N 0.766795 0.332151 2.364364
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O 0.593955 -1.313980 -0.857808
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CBZ-I
G = -763.336575

C 3.713179 -1.033442 0.752160
C 3.332980 0.110649 1.459793
C 2.094242 0.696851 1.208174
C 1.232784 0.153720 0.248876
C 1.589141 -1.017454 -0.452963
C 2.851131 -1.584821 -0.189138
C -1.222219 0.138948 0.246634
C -1.552675 -1.041385 -0.451484
C -0.651779 -1.679375 -1.409953
C 0.699820 -1.669352 -1.412610
C -2.093639 0.663032 1.204799
C -3.317653 0.049138 1.457555
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N 0.003503 0.820595 -0.050274
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N 1.039952 2.685512 -1.181250
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H -1.140913 -2.314541 -2.146795
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H -1.811180 1.573320 1.723463
H -3.994665 0.474654 2.192927
H -4.631046 -1.585037 0.938612
H -3.074699 -2.538349 -0.731713
H 1.923600 2.220779 -0.982738
H -1.067826 3.319464 -1.474828

CBZ-I 1H2O
G = -839.750975

C -3.879348 -1.185576 -0.459423
C -3.409490 -0.357353 -1.483034
C -2.110828 0.143921 -1.422694
C -1.277867 -0.169804 -0.343067
C -1.726124 -1.030073 0.681899
C -3.046806 -1.513803 0.604776
C 1.159951 -0.445733 -0.348930
C 1.392764 -1.393764 0.668922
C 0.469682 -1.612444 1.781355
C -0.872778 -1.454220 1.790262
C 2.043459 -0.327245 -1.424261
C 3.185542 -1.121007 -1.489091
C 3.447474 -2.046311 -0.474264
C 2.561822 -2.175346 0.589038
N 0.021751 0.422282 -0.261286
C 0.149936 1.770679 0.055453
N -0.806924 2.609233 0.273196
O 1.428513 2.155835 0.113616
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H -1.731689 0.802008 -2.198831
H -3.409741 -2.167041 1.394528
H 0.920132 -2.046686 2.672530

H -1.404109 -1.772379 2.685649
H 1.838838 0.415650 -2.188052
H 3.874820 -1.009576 -2.321296
H 4.340567 -2.663699 -0.514096
H 2.760376 -2.899507 1.375468
H -1.726807 2.182186 0.209657
H 1.431398 3.131720 0.335550
O 0.840977 4.711358 0.718972
H 0.891961 4.813035 1.682362
H -0.024473 4.237857 0.573871

CBZ-I 2H2O
G = -916.163720

C -1.896467 3.760114 -0.357818
C -1.139697 3.360046 -1.463319
C -0.531054 2.106765 -1.464537
C -0.666240 1.249665 -0.366574
C -1.453961 1.625681 0.742701
C -2.047962 2.902877 0.726300
C -0.744693 -1.198974 -0.369970
C -1.565764 -1.510919 0.733488
C -1.745344 -0.611831 1.872117
C -1.695179 0.739132 1.879412
C -0.664952 -2.065714 -1.462359
C -1.369139 -3.266736 -1.462646
C -2.165063 -3.605995 -0.364291
C -2.256787 -2.738335 0.717472
N 0.036068 0.003818 -0.355103
C 1.413624 -0.021698 -0.136949
N 2.163216 1.017563 0.034685
O 1.889009 -1.259244 -0.142265
H -2.368924 4.738337 -0.344375
H -1.018096 4.022907 -2.315227
H 0.075162 1.782796 -2.305254
H -2.645970 3.210751 1.580528
H -2.051067 -1.098016 2.797227
H -1.963667 1.240969 2.807472
H -0.019034 -1.799556 -2.292483
H -1.287199 -3.941614 -2.309963
H -2.711233 -4.545149 -0.353880
H -2.881428 -2.997151 1.569047
H 3.874356 1.183268 0.349902
H 1.619373 1.876827 0.042869
H 2.878661 -1.281222 0.061156
O 4.459779 -1.493889 0.436028
H 4.501166 -1.787203 1.359105
H 4.790281 -0.549659 0.459091
O 4.870247 1.132169 0.478040
H 5.232425 1.417294 -0.374877

CBZ-Cl
G = -1222.923391

C -2.288182 3.181426 0.602815
C -2.335817 2.215778 1.612354
C -1.542691 1.073693 1.509516
C -0.712143 0.882508 0.398050
C -0.620052 1.869245 -0.607075
C -1.439836 3.007870 -0.485646
C 1.444856 -0.289191 0.326740
C 2.155569 0.395146 -0.680254
C 1.502978 1.139386 -1.756285
C 0.306047 1.767686 -1.732516
C 2.118648 -0.950018 1.354591
C 3.510751 -0.957705 1.389995
C 4.234571 -0.300534 0.390788
C 3.562891 0.361431 -0.630240
N 0.012213 -0.346685 0.266700
C -0.574335 -1.553970 -0.129200
N -1.933608 -1.418235 -0.472398
O 0.040354 -2.594777 -0.228600
H -2.907512 4.071394 0.669329
H -2.986928 2.348753 2.471435
H -1.565246 0.308844 2.281174
H -1.393506 3.768272 -1.261221
H 2.107120 1.269187 -2.652605
H 0.036114 2.355949 -2.607622
H 1.539466 -1.481139 2.102374
H 4.028722 -1.487375 2.184322
H 5.320806 -0.309356 0.407357
H 4.125679 0.874298 -1.406309
H -2.458996 -0.684344 -0.010388
Cl -2.862254 -2.881078 -0.487703

CBZ-Cl 1H2O
G = -1299.325793

C -2.567840 -3.344347 0.485290

C -1.697651 -3.065003 1.543103
C -0.894942 -1.926230 1.491216
C -0.947932 -1.072043 0.383029
C -1.852810 -1.315728 -0.672224
C -2.643005 -2.479252 -0.601297
C -0.594189 1.359681 0.356792
C -1.431109 1.799276 -0.688643
C -1.845005 0.941311 -1.797661
C -2.019164 -0.399617 -1.798270
C -0.261994 2.206153 1.414757
C -0.742323 3.513014 1.442887
C -1.558765 3.975503 0.406596
C -1.892373 3.129420 -0.644484
N -0.040260 0.035346 0.305111
C 1.302299 -0.098588 -0.037194
N 1.673080 -1.409709 -0.357907
O 2.063334 0.852209 -0.110131
H -3.191787 -4.233083 0.512821
H -1.641762 -3.729442 2.400342
H -0.209380 -1.690698 2.300796
H -3.332733 -2.691197 -1.414362
H -2.129844 1.473062 -2.703887
H -2.430839 -0.846815 -2.701077
H 0.399142 1.839194 2.192691
H -0.467281 4.172555 2.260727
H -1.929743 4.996452 0.417990
H -2.529211 3.488661 -1.449009
O 4.993154 1.276328 -0.168432
H 4.040670 1.109354 -0.049114
H 1.144903 -2.168766 0.056688
Cl 3.365471 -1.758673 -0.341651
H 5.064022 1.429103 -1.121842

CBZ-Cl 2H2O
G = -1375.732910

C 2.365782 -3.722221 -0.427555
C 1.584277 -3.308714 -1.510370
C 0.983928 -2.050673 -1.484632
C 1.149634 -1.207943 -0.378936
C 1.970772 -1.592958 0.702343
C 2.555401 -2.873417 0.657817
C 1.207791 1.247810 -0.366447
C 2.076327 1.548812 0.702243
C 2.309376 0.640716 1.824177
C 2.257302 -0.710419 1.831110
C 1.055101 2.131137 -1.435703
C 1.747809 3.339099 -1.451980
C 2.599084 3.665871 -0.392249
C 2.755024 2.782693 0.669637
N 0.439263 0.035950 -0.330313
C -0.917234 0.124844 -0.023127
N -1.523774 -1.089350 0.260344
O -1.499904 1.202446 0.037523
H 2.831283 -4.703652 -0.434115
H 1.439591 -3.961562 -2.366153
H 0.368286 -1.710418 -2.312851
H 3.176516 -3.191888 1.491222
H 2.653584 1.122769 2.737624
H 2.562967 -1.214657 2.745933
H 0.366746 1.873314 -2.233667
H 1.612424 4.028974 -2.279899
H 3.136695 4.609872 -0.394598
H 3.419596 3.035307 1.492121
O -4.256963 2.057887 0.206928
H -5.358109 0.590816 0.219944
O -5.825808 -0.278210 0.193063
H -6.059618 -0.375823 -0.742287
H -3.349356 1.704729 0.084234
H -1.118159 -1.942761 -0.102548
Cl -3.257903 -1.107617 0.262992
H -4.247352 2.393456 1.115877

CBZ-EP
G = -838.551999

C -0.752839 -1.703378 1.250117
C 0.734159 -1.729362 1.225942
C 1.560817 -1.018351 0.215014
C -1.596590 -0.982209 0.259827
C 1.207135 0.235348 -0.324176
C -1.246546 0.261807 -0.295737
H -1.238097 -2.582705 1.678123
N -0.007630 0.892870 0.052338
H 1.895868 1.838026 1.453409
C -0.046272 2.077995 0.796786
O -1.082090 2.691919 0.998392
N 1.188219 2.529020 1.238541
H 1.089751 3.256884 1.934197
C -2.798679 -1.581670 -0.140318

C -2.102546 0.887705 -1.204793
C -3.301107 0.284569 -1.579809
H -3.960944 0.785938 -2.282251
C -3.647132 -0.960677 -1.053198
H -4.577461 -1.441149 -1.342670
H -1.820147 1.856648 -1.600961
H -3.074286 -2.543618 0.286058
H 1.210700 -2.624162 1.631806
C 2.743813 -1.628989 -0.223792
H 3.019180 -2.596384 0.190084
C 2.044034 0.846883 -1.265731
C 3.224714 0.232318 -1.677626
H 3.863711 0.723237 -2.406178
C 3.572805 -1.016557 -1.160572
H 4.487310 -1.508474 -1.479446
H 1.752570 1.812898 -1.665249
O 0.021231 -0.962289 2.206022

CBZ-EP 1H2O
G = -914.960794

C -0.540886 -1.483660 1.777012
C 0.935779 -1.301753 1.776551
C 1.729673 -0.963445 0.565684
C -1.401898 -1.363917 0.570005
C 1.255826 -0.109510 -0.450792
C -1.178338 -0.420270 -0.448932
H -0.936627 -2.168276 2.529729
N -0.053511 0.467507 -0.386337
H 1.681441 2.173023 0.376167
C -0.277223 1.825966 -0.164049
O -1.420601 2.294098 -0.198088
N 0.831350 2.600209 0.038221
H 0.611476 3.544838 0.360365
C -2.486790 -2.242309 0.444370
C -2.042443 -0.353968 -1.543964
C -3.125228 -1.224777 -1.645223
H -3.793964 -1.157745 -2.498673
C -3.343489 -2.180181 -0.651556
H -4.182313 -2.866685 -0.723637
H -1.858980 0.395726 -2.305773
H -2.665003 -2.974018 1.229140
H 1.494718 -1.869338 2.523386
C 3.004825 -1.528276 0.426777
H 3.374265 -2.188246 1.208324
C 2.064337 0.169056 -1.559229
C 3.336505 -0.388907 -1.671990
H 3.952792 -0.159460 -2.536549
C 3.805891 -1.248835 -0.677994
H 4.793102 -1.694821 -0.758225
H 1.678490 0.831612 -2.327492
O 0.065797 -0.310721 2.340222
H -1.090469 4.790753 1.657407
O -0.846311 4.850795 0.721138
H -1.314135 4.083970 0.316453

CBZ-EP 2H2O
G = -991.370506

C -1.011492 -0.145848 1.936785
C 0.304106 -0.841491 2.002934
C 0.893583 -1.613013 0.875645
C -1.893302 -0.129707 0.739606
C 0.745415 -1.238375 -0.476578
C -1.403220 -0.074725 -0.578225
H -1.550293 -0.054507 2.881195
N 0.008342 -0.065224 -0.842259
H 2.495049 0.363696 -0.857449
C 0.624360 1.178598 -1.046957
O -0.062973 2.200702 -1.146807
N 1.979550 1.176982 -1.163566
H 2.432491 2.086918 -0.991746
C -3.279107 -0.179822 0.940568
C -2.292342 -0.049868 -1.653200
C -3.668633 -0.088646 -1.437040
H -4.350130 -0.062182 -2.282542
C -4.164281 -0.162722 -0.134674
H -5.235068 -0.196492 0.044741
H -1.886606 0.007144 -2.658043
H -3.664144 -0.220549 1.956960
H 0.613159 -1.197587 2.987055
C 1.609274 -2.779714 1.174121
H 1.727386 -3.073962 2.214449
C 1.320420 -2.020920 -1.483032
C 2.040142 -3.173137 -1.166651
H 2.483800 -3.769072 -1.959016
C 2.179015 -3.557201 0.167367
H 2.734325 -4.454248 0.425643
H 1.191520 -1.708859 -2.514858
O 0.223835 0.592145 1.920449

O 0.686890 3.518366 1.197314
H 0.234769 3.233222 0.372352
H 0.690238 2.699978 1.723019
O 3.032218 3.658882 -0.225314
H 2.827296 4.372321 -0.848672
H 2.277570 3.690651 0.418523

IMS
G = -594.680783

C 4.020564 0.177306 0.000004
C 3.676459 -1.170706 0.000002
C 2.333278 -1.542939 0.000000
C 1.297707 -0.594499 -0.000002
C 1.635207 0.782615 -0.000001
C 2.997122 1.123917 0.000002
C -1.297707 -0.594499 -0.000002
C -1.635207 0.782615 -0.000001
C -0.672422 1.887012 -0.000003
C 0.672422 1.887012 -0.000003
C -2.333278 -1.542939 0.000000
C -3.676459 -1.170706 0.000002
C -4.020564 0.177306 0.000004
C -2.997122 1.123917 0.000002
N 0.000000 -1.117535 -0.000005
H 5.059902 0.490830 0.000006
H 4.443062 -1.940730 0.000003
H 2.073686 -2.600404 -0.000001
H 3.250493 2.181604 0.000003
H -1.144527 2.867816 -0.000004
H 1.144527 2.867816 -0.000004
H -2.073686 -2.600404 -0.000001
H -4.443062 -1.940730 0.000003
H -5.059902 0.490830 0.000006
H -3.250493 2.181604 0.000003
H 0.000000 -2.127965 -0.000007

IMS 1H2O
G = -671.083619

C 4.019940 -0.566322 -0.000002
C 3.675042 0.781784 -0.000002
C 2.333191 1.158872 -0.000001
C 1.294003 0.211013 0.000002
C 1.633688 -1.166969 0.000002
C 2.994689 -1.511065 0.000000
C -1.294017 0.211042 0.000001
C -1.633733 -1.166932 -0.000002
C -0.672212 -2.272737 0.000002
C 0.672142 -2.272753 0.000005
C -2.333183 1.158924 -0.000002
C -3.675043 0.781866 -0.000008
C -4.019971 -0.566231 -0.000012
C -2.994741 -1.510998 -0.000008
N -0.000001 0.739645 0.000007
H 5.059162 -0.880979 -0.000003
H 4.443812 1.550398 -0.000004
H 2.069934 2.213585 -0.000001
H 3.246367 -2.569337 0.000001
H -1.145374 -3.253268 0.000003
H 1.145283 -3.253293 0.000008
H -2.069902 2.213632 0.000001
H -4.443796 1.550497 -0.000010
H -5.059200 -0.880865 -0.000016
H -3.246443 -2.569264 -0.000011
H 0.000011 1.754986 0.000008
O 0.000133 3.815405 0.000012
H 0.000163 4.403094 0.770092
H 0.000152 4.403098 -0.770064

IMS 2H2O
G = -747.491468

C -4.058965 -0.151216 0.493417
C -3.541873 1.096474 0.153180
C -2.215185 1.215893 -0.261095
C -1.379070 0.093808 -0.358656
C -1.891115 -1.179673 -0.013417
C -3.229172 -1.266734 0.404143
C 1.127098 -0.249488 -0.442463
C 1.290384 -1.609596 -0.071192
C 0.213347 -2.602952 -0.094721
C -1.119792 -2.422461 -0.079650
C 2.261281 0.585535 -0.461612
C 3.528311 0.110128 -0.112145
C 3.690679 -1.214487 0.281869
C 2.573788 -2.050052 0.287548
N -0.084465 0.300017 -0.891242
H -5.090530 -0.259142 0.815628

H -4.164865 1.985469 0.207415
H -1.812896 2.190525 -0.523532
H -3.620330 -2.248801 0.660586
H 0.564086 -3.633766 -0.086050
H -1.729409 -3.324570 -0.058417
H 2.137968 1.609372 -0.803223
H 4.383162 0.780389 -0.162573
H 4.667167 -1.600779 0.558169
H 2.691235 -3.094864 0.566288
H 0.036883 1.270642 -1.176565
O 0.315448 3.313955 -0.896547
H 0.683585 4.092376 -1.338787
H 0.653136 3.345435 0.027105
O 1.412011 2.871982 1.636756
H 2.287976 3.236574 1.835485
H 1.586115 1.932451 1.444257

CBZ-TS-I
G = -763.295512

C 3.712639 -1.045364 0.765839
C 3.342580 0.142393 1.402746
C 2.102098 0.714938 1.129027
C 1.231131 0.112897 0.215621
C 1.573594 -1.101681 -0.413168
C 2.837602 -1.653497 -0.127394
C -1.246720 0.126937 0.203155
C -1.577543 -1.095410 -0.415278
C -0.675964 -1.810971 -1.316979
C 0.674983 -1.812470 -1.321066
C -2.132299 0.742483 1.089678
C -3.371790 0.166435 1.356814
C -3.727960 -1.035290 0.738925
C -2.841200 -1.651237 -0.136444
N -0.001466 0.766282 -0.115814
C 0.013712 1.999169 -0.701298
N 1.035467 2.733672 -1.103251
O -1.065894 2.676926 -0.953904
H 4.680399 -1.495740 0.967687
H 4.017746 0.624437 2.103883
H 1.805362 1.647148 1.599394
H 3.121751 -2.582093 -0.616177
H -1.169884 -2.491576 -2.008501
H 1.167152 -2.493558 -2.013166
H -1.854248 1.691691 1.533926
H -4.061450 0.661114 2.034632
H -4.696019 -1.486816 0.936848
H -3.115724 -2.586940 -0.617164
H -0.084902 3.404932 -1.408269
H 1.989781 2.396324 -1.169473

CBZ-TS-I 1H2O
G = -839.743523

C 3.783642 -1.391478 0.508360
C 3.361672 -0.496181 1.495607
C 2.095597 0.079440 1.408370
C 1.249529 -0.226474 0.336734
C 1.646134 -1.154880 -0.649178
C 2.935218 -1.713117 -0.545379
C -1.206360 -0.340603 0.336085
C -1.492484 -1.317197 -0.639478
C -0.579388 -1.647906 -1.732418
C 0.770393 -1.574824 -1.741524
C -2.089995 -0.107800 1.391722
C -3.283845 -0.818925 1.479445
C -3.597338 -1.773787 0.507563
C -2.712544 -2.013784 -0.536894
N -0.010397 0.443006 0.220233
C -0.074601 1.783932 -0.112737
N 0.984625 2.535089 -0.336597
O -1.262769 2.302602 -0.195661
H 4.771615 -1.839888 0.563840
H 4.016394 -0.242556 2.324330
H 1.754491 0.789025 2.156256
H 3.260045 -2.419254 -1.305596
H -1.053385 -2.093761 -2.605402
H 1.282812 -1.967144 -2.618244
H -1.844509 0.658411 2.119206
H -3.973041 -0.619320 2.294972
H -4.530569 -2.327020 0.565270
H -2.952406 -2.760125 -1.290302
H 0.538520 3.724131 -0.599183
H 1.895344 2.100299 -0.275638
H -1.073090 3.418600 -0.464990
O -0.394449 4.491397 -0.730088
H -0.487863 4.661449 -1.681655

CBZ-TS-I 2H2O

G = -916.157595

C 2.235649 -3.554689 -0.376874
C 1.428414 -3.232673 -1.472186
C 0.694408 -2.048529 -1.462948
C 0.754394 -1.183841 -0.363886
C 1.592528 -1.477249 0.733586
C 2.313304 -2.687240 0.706983
C 0.577981 1.260068 -0.368045
C 1.385236 1.654331 0.718633
C 1.675727 0.781051 1.854452
C 1.760799 -0.568185 1.865466
C 0.384593 2.113967 -1.455947
C 0.963189 3.380149 -1.469292
C 1.745474 3.798580 -0.388432
C 1.948129 2.945531 0.689622
N -0.073311 -0.017145 -0.337657
C -1.446298 -0.105356 -0.116104
N -2.041013 -1.266384 0.059622
O -2.064735 1.025809 -0.116333
H 2.805525 -4.479620 -0.371775
H 1.365242 -3.903142 -2.324463
H 0.047987 -1.787646 -2.295577
H 2.951327 -2.932890 1.552351
H 1.947461 1.298565 2.773144
H 2.094273 -1.037434 2.789454
H -0.250614 1.784095 -2.271102
H 0.793333 4.043521 -2.312591
H 2.193816 4.788221 -0.388407
H 2.561421 3.266748 1.528065
H -3.297500 -1.419338 0.271941
H -1.421440 -2.067311 0.090374
H -3.203445 1.007758 0.155477
O -4.424392 0.981030 0.448375
H -4.514725 1.318997 1.353439
H -4.600661 -0.153300 0.498374
O -4.489484 -1.436921 0.497484
H -4.923997 -1.757351 -0.308840

CBZ-TS-Cl
G = -1299.225623

C 1.209687 -0.504152 -0.497125
N 2.242847 0.336761 -0.592200
O 1.401189 -1.771002 -0.552639
H 2.608590 -1.921491 -0.497913
O 3.795141 -1.906556 -0.373454
Cl 3.919952 -0.332396 1.115595
H 2.054190 1.256482 -0.193232
N -0.097754 -0.062074 -0.387083
C -1.187997 -0.993765 -0.313012
C -1.430288 -1.874924 -1.368859
C -1.981890 -1.026567 0.851115
C -2.443052 -2.825267 -1.270183
H -0.796902 -1.830276 -2.247967
C -2.989191 -2.007883 0.932331
C -3.221776 -2.895343 -0.111364
H -2.614778 -3.517277 -2.089579
H -3.600058 -2.054011 1.830496
H -4.007304 -3.640677 -0.024338
C -0.407360 1.335705 -0.424634
C -0.093804 2.086482 -1.563958
C -0.992626 1.947768 0.704432
C -0.319675 3.460718 -1.584979
H 0.349728 1.583772 -2.417640
C -1.195622 3.340712 0.661515
C -0.868076 4.089644 -0.463508
H -0.060713 4.037448 -2.467995
H -1.627943 3.830201 1.530581
H -1.040088 5.162196 -0.468215
C -1.825275 -0.080235 1.954212
C -1.400852 1.201257 1.892812
H -2.190353 -0.433437 2.917093
H -1.455103 1.787186 2.808522
H 4.042025 -2.636641 0.226041

CBZ-TS-Cl 1H2O
G = -1375.682496

C -0.959812 -0.057333 -0.250444
N -1.564819 -1.230406 -0.154451
O -1.562461 1.076799 -0.245617
O -3.886778 1.713205 0.167674
H -4.178677 2.158068 -0.643662
H -2.702153 1.253892 -0.036782
O -5.343232 -0.326178 0.453934
H -4.591817 0.905587 0.330466
Cl -3.464084 -1.111562 0.171526
H -1.017038 -2.075953 -0.057674
N 0.418086 0.001496 -0.405417

C 1.097393 1.265659 -0.368142
C 1.012457 2.131575 -1.459556
C 1.819674 1.628838 0.786334
C 1.617370 3.384758 -1.410379
H 0.443615 1.821518 -2.329987
C 2.408654 2.907980 0.819212
C 2.313830 3.775303 -0.262573
H 1.534515 4.059379 -2.257680
H 2.956588 3.208073 1.708956
H 2.780621 4.755054 -0.213641
C 1.219267 -1.186159 -0.384396
C 1.222140 -2.036126 -1.495902
C 1.962821 -1.508016 0.771537
C 1.929771 -3.235960 -1.463207
H 0.646408 -1.752313 -2.371710
C 2.656930 -2.733811 0.784762
C 2.643773 -3.586813 -0.313233
H 1.917328 -3.896240 -2.325419
H 3.222745 -3.003289 1.673053
H 3.191576 -4.524174 -0.276191
C 2.000375 0.734666 1.928625
C 2.059687 -0.616152 1.925571
H 2.205914 1.233955 2.873969
H 2.308969 -1.104129 2.866105
H -5.488263 -0.461557 1.406142

CBZ-TS-Cl 2H2O
G = -1452.100095

C -0.621591 0.056048 -0.342354
N -1.300945 -1.078841 -0.424313
O -1.154968 1.207148 -0.233428
O -3.385435 2.028709 -0.563778
O -5.509931 1.059817 0.229412
H -3.320069 2.865298 -0.075871
H -6.102743 0.999509 -0.535960
H -4.304550 1.537967 -0.215489
H -2.363625 1.473242 -0.395353
O -5.081087 -1.312987 0.821454
H -5.373996 0.036176 0.544988
Cl -3.147866 -1.224060 0.193714
H -0.779380 -1.945711 -0.388319
N 0.770334 0.033479 -0.410940
C 1.512101 1.255047 -0.296033
C 1.499585 2.177305 -1.344577
C 2.223043 1.525688 0.890960
C 2.166307 3.393219 -1.220499
H 0.937821 1.940259 -2.242212
C 2.877470 2.768704 0.999001
C 2.854707 3.691010 -0.040246
H 2.139893 4.110572 -2.035871
H 3.418713 2.996075 1.914185
H 3.371621 4.640624 0.066530
C 1.508454 -1.193498 -0.424925
C 1.508519 -1.988112 -1.577060
C 2.197009 -1.609953 0.734941
C 2.150397 -3.225036 -1.581478
H 0.979943 -1.632088 -2.456258
C 2.824678 -2.870535 0.709877
C 2.804091 -3.669227 -0.428259
H 2.132862 -3.841340 -2.475618
H 3.344889 -3.211712 1.601457
H 3.299398 -4.636045 -0.419682
C 2.324911 0.572573 1.994678
C 2.308770 -0.777862 1.931525
H 2.533067 1.017198 2.966502
H 2.504921 -1.320487 2.854631
H -4.970093 -1.396714 1.783376

CBZ-TS-EP
G = -1299.282068

C -0.647235 -0.049571 -1.878695
C 0.701445 -0.410461 -2.016679
C 1.797624 -0.169080 -1.125195
C -1.111923 1.006173 -0.956808
C 1.656031 0.174364 0.250737
C -0.605989 1.126153 0.348391
H -1.235387 -0.122143 -2.789289
N 0.370064 0.204581 0.849420
H -1.852552 -0.895265 1.463544
C 0.116940 -0.639628 1.961530
O 1.019153 -1.144359 2.610896
N -1.219335 -0.799666 2.252828
H -1.353733 -1.528676 2.943120
C -2.077337 1.922543 -1.398207
C -1.058326 2.157103 1.178983
C -2.020436 3.057598 0.727484
H -2.370189 3.846997 1.386549
C -2.531187 2.942541 -0.567059

H -3.283006 3.639806 -0.924823
H -0.659299 2.231236 2.185254
H -2.477274 1.823734 -2.404118
H 0.966272 -0.912771 -2.946322
C 3.107079 -0.289508 -1.655768
H 3.218494 -0.558871 -2.702964
C 2.796328 0.399878 1.025892
C 4.068977 0.290900 0.469038
H 4.940780 0.470516 1.091644
C 4.227978 -0.054937 -0.878319
H 5.220400 -0.145104 -1.309621
H 2.672615 0.633359 2.074966
Cl -2.701837 -2.887643 -0.211094
O -1.219885 -1.570184 -1.052235
H -0.824963 -2.295371 -1.576312

CBZ-TS-EP 1H2O
G = -1375.691774

C -0.708377 -0.247060 -1.680020
C 0.489116 -0.957350 -1.650287
C 1.703762 -0.652913 -0.938199
C -0.881055 1.126652 -1.185917
C 1.769840 0.196297 0.198425
C -0.242720 1.590746 -0.021117
H -1.406076 -0.531676 -2.461769
N 0.576787 0.721392 0.767039
H -1.767389 0.461350 1.734460
C 0.242552 0.347543 2.089390
O 1.061601 -0.142571 2.850661
N -1.061560 0.625150 2.445644
H -1.294246 0.179216 3.324871
C -1.699465 2.010733 -1.906635
C -0.417748 2.916994 0.388445
C -1.233949 3.780909 -0.338299
H -1.368573 4.805154 -0.002565
C -1.876932 3.327043 -1.492130
H -2.517006 3.993803 -2.062486
H 0.079054 3.252900 1.292693
H -2.202318 1.651306 -2.800914
H 0.536185 -1.835279 -2.292208
C 2.902602 -1.239767 -1.407278
H 2.855744 -1.897175 -2.271792
C 3.001275 0.445781 0.807573
C 4.168827 -0.132428 0.312778
H 5.116426 0.070884 0.803429
C 4.121186 -0.979016 -0.799895
H 5.029422 -1.435202 -1.182551
H 3.026285 1.072926 1.689669
Cl -3.009657 -2.014548 0.979936
O -1.459901 -1.316507 -0.285176
H -1.329822 -2.228756 -0.661768
O -1.471431 -3.995976 -1.016553
H -2.352491 -3.933299 -0.602030
H -0.923248 -4.369203 -0.307195

CBZ-TS-EP 2H2O
G = -1452.097726

C -0.511234 0.696335 -1.898567
C 0.611753 -0.098782 -2.121726
C 1.780931 -0.261407 -1.295649
C -0.606559 1.742986 -0.868789
C 1.823057 0.025792 0.093826
C -0.044551 1.591246 0.412039
H -1.146315 0.865481 -2.762987
N 0.627818 0.382240 0.782876
H -1.797803 0.039913 1.513948
C 0.159798 -0.459428 1.808072
O 0.900621 -1.307065 2.316854
N -1.123967 -0.239768 2.217840
H -1.449835 -0.967402 2.858696
C -1.272817 2.939645 -1.176111
C -0.142069 2.629543 1.344615
C -0.808357 3.809846 1.023093
H -0.884820 4.603585 1.760659
C -1.375185 3.967197 -0.243599
H -1.898263 4.883445 -0.501204
H 0.295548 2.490949 2.327807
H -1.717581 3.055496 -2.161187
H 0.641145 -0.620888 -3.076325
C 2.964688 -0.719624 -1.920036
H 2.935542 -0.952109 -2.981513
C 3.020574 -0.115035 0.797017
C 4.177203 -0.548737 0.151236
H 5.097993 -0.657739 0.717077
C 4.149803 -0.855171 -1.213102
H 5.047539 -1.201532 -1.716622
H 3.025881 0.088419 1.860360
Cl -3.251373 -1.624905 -0.398741

O -1.483512 -0.738162 -1.153161
H -1.436963 -1.405064 -1.891999
O -1.802674 -2.767524 -3.012105
H -2.702624 -2.736577 -2.635592
H -1.398020 -3.518265 -2.547722
H -0.141594 -2.378641 3.461667
O -0.938139 -2.544558 4.013426
H -0.696036 -2.170944 4.874503

CBZ-TS-IMS
G = -763.289268

C -3.760958 -0.924205 -0.789700
C -3.394234 0.239135 -1.468238
C -2.135593 0.795616 -1.247666
C -1.235153 0.199374 -0.361597
C -1.576644 -0.993775 0.311048
C -2.861965 -1.523374 0.086087
C 1.235157 0.199377 -0.361596
C 1.576649 -0.993772 0.311049
C 0.674099 -1.718926 1.202462
C -0.674092 -1.718928 1.202462
C 2.135596 0.795622 -1.247663
C 3.394238 0.239144 -1.468234
C 3.760964 -0.924196 -0.789696
C 2.861972 -1.523367 0.086089
N 0.000001 0.901567 -0.098367
C -0.000008 1.808319 1.312877
N -0.000015 2.951252 0.648886
O -0.000006 1.353312 2.422698
H -4.743087 -1.362570 -0.942548
H -4.085914 0.720074 -2.153815
H -1.845933 1.713601 -1.750707
H -3.143843 -2.434220 0.608412
H 1.168115 -2.396577 1.895972
H -1.168108 -2.396579 1.895972
H 1.845934 1.713607 -1.750703
H 4.085919 0.720085 -2.153810
H 4.743094 -1.362558 -0.942543
H 3.143851 -2.434212 0.608414
H -0.000029 3.821953 1.174455
H -0.000009 2.164898 -0.390426

CBZ-TS-IMS 1H2O
G = -839.716514

C -3.683260 -1.182057 -0.916215
C -3.400123 0.116645 -1.339795
C -2.178030 0.702633 -1.014380
C -1.232764 -0.012219 -0.274668
C -1.478771 -1.336908 0.140532
C -2.734436 -1.887821 -0.186477
C 1.266583 0.114027 -0.281534
C 1.661376 -1.172554 0.135851
C 0.813292 -2.126937 0.842062
C -0.530843 -2.196017 0.844270
C 2.122263 0.919432 -1.036222
C 3.398758 0.476506 -1.374351
C 3.826882 -0.779217 -0.941662
C 2.967942 -1.580974 -0.199540
N -0.008707 0.719800 0.110371
C -0.037161 1.176081 1.668725
N -0.540036 2.396749 1.689523
O 0.373581 0.404758 2.501975
H -4.638238 -1.642927 -1.152450
H -4.131724 0.684844 -1.906716
H -1.955950 1.725983 -1.302230
H -2.947087 -2.904066 0.135190
H 1.353432 -2.913778 1.363846
H -0.983109 -3.037123 1.365229
H 1.780044 1.900789 -1.348508
H 4.055278 1.114960 -1.957936
H 4.824665 -1.133524 -1.184181
H 3.296174 -2.564721 0.125676
H -0.607808 2.792604 2.620852
H -0.580394 2.982662 0.627944
O -0.441827 3.137810 -0.651386
H -0.075703 1.716404 -0.400216
H 0.307340 3.737783 -0.790041

CBZ-TS-IMS 2H2O
G = -916.124588

C 2.889119 2.348310 -1.045856
C 2.880372 1.090581 -1.651213
C 1.920094 0.148222 -1.287521
C 0.964643 0.472651 -0.325844
C 0.915738 1.751472 0.262300
C 1.920408 2.667503 -0.101071

C -1.363994 -0.268308 -0.288026
C -2.047377 0.815766 0.293102
C -1.423240 1.786502 1.187145
C -0.134473 2.188549 1.178673
C -1.979894 -1.110928 -1.212310
C -3.314273 -0.903971 -1.556350
C -4.030718 0.136216 -0.960152
C -3.403204 0.977194 -0.047824
N 0.014886 -0.570396 0.105125
C 0.132358 -0.996471 1.649025
N 1.393252 -1.281964 1.932951
O -0.893295 -1.030220 2.289608
H 3.647248 3.079451 -1.311866
H 3.632454 0.828319 -2.388975
H 1.932720 -0.842611 -1.724619
H 1.911704 3.653385 0.356695
H -2.103517 2.291447 1.869489
H 0.142811 2.998548 1.850191
H -1.408261 -1.921809 -1.652934
H -3.793800 -1.562115 -2.274873
H -5.076043 0.293886 -1.210179
H -3.957228 1.795503 0.404598
H 1.481952 -1.584330 2.899026
H 2.170156 -1.759373 1.151243
O 0.817786 -2.799138 -1.012558
H 0.302701 -1.520043 -0.397326
H 0.343416 -3.561918 -0.646128
O 2.859820 -2.407396 0.232549
H 1.835887 -2.753538 -0.473344
H 3.252979 -3.193974 0.641212

CBZ-Cl-TS-IMS
G = -1222.861301

C -3.749603 -1.634890 -0.583899
C -3.386173 -0.668753 -1.524016
C -2.133349 -0.064948 -1.438934
C -1.239430 -0.423649 -0.428578
C -1.574036 -1.418741 0.513558
C -2.854748 -1.997050 0.416862
C 1.241409 -0.419310 -0.428400
C 1.579386 -1.413269 0.513733
C 0.677737 -1.896202 1.556543
C -0.670814 -1.898548 1.556468
C 2.134136 -0.057550 -1.438717
C 3.388995 -0.657113 -1.523791
C 3.755693 -1.622024 -0.583683
C 2.862054 -1.987224 0.417063
N -0.000310 0.322369 -0.335300
C -0.002650 1.491255 0.783363
N -0.004183 2.441733 -0.158874
O -0.002748 1.360398 1.973706
H -4.728130 -2.104061 -0.630902
H -4.076487 -0.374319 -2.308848
H -1.847735 0.707143 -2.147452
H -3.135245 -2.755365 1.143376
H 1.172496 -2.381028 2.395481
H -1.163974 -2.385089 2.395354
H 1.845913 0.713539 -2.147269
H 4.078310 -0.360339 -2.308620
H 4.735808 -2.087869 -0.630679
H 3.145091 -2.744588 1.143586
H -0.002425 1.474050 -0.989235
Cl -0.008343 4.122007 0.288785

CBZ-Cl-TS-IMS 1H2O
G = -1299.282563

C -2.151087 3.445586 0.411337
C -2.274205 2.545597 1.470626
C -1.546993 1.356900 1.460103
C -0.686179 1.070775 0.397974
C -0.513293 1.979676 -0.666363
C -1.285806 3.158195 -0.636909
C 1.441876 -0.217254 0.385913
C 2.167219 0.354427 -0.678665
C 1.582015 1.119687 -1.774211
C 0.429042 1.815704 -1.769356
C 2.097326 -0.845529 1.446969
C 3.486442 -0.944923 1.462090
C 4.224269 -0.424114 0.397819
C 3.568760 0.210839 -0.650096
N -0.022546 -0.250541 0.408263
C -0.627007 -1.247541 -0.673064
N -1.696198 -1.790049 -0.076848
O -0.106578 -1.382062 -1.750179
H -2.726493 4.366878 0.402064
H -2.949019 2.752719 2.295827
H -1.667101 0.630142 2.256664
H -1.176853 3.863136 -1.456966

H 2.201929 1.186516 -2.665325
H 0.198579 2.402577 -2.655821
H 1.512272 -1.260475 2.261357
H 3.983821 -1.438639 2.291501
H 5.307082 -0.508906 0.387454
H 4.144505 0.629993 -1.471026
H -1.653979 -1.819424 1.132208
O -1.134487 -1.509072 2.284149
H -0.366190 -0.786892 1.410341
H -0.686057 -2.306026 2.609829
Cl -2.566884 -2.974503 -0.993810

CBZ-Cl-TS-IMS 2H2O
G = -1375.693947

C -1.490809 3.678903 -0.000295
C -1.548057 3.029540 1.234256
C -0.993430 1.758779 1.377451
C -0.374352 1.140120 0.290544
C -0.251688 1.801934 -0.948152
C -0.852310 3.067660 -1.073834
C 1.588011 -0.275302 0.396459
C 2.268669 0.003598 -0.805346
C 1.600257 0.478520 -2.013922
C 0.498508 1.257873 -2.077217
C 2.282479 -0.633556 1.551289
C 3.670835 -0.753224 1.523927
C 4.361930 -0.529565 0.331197
C 3.665546 -0.161237 -0.814845
N 0.128635 -0.229999 0.441097
C -0.508585 -1.303067 -0.496715
N -1.830321 -1.077606 -0.545008
O 0.213651 -2.163112 -0.948640
H -1.937644 4.661330 -0.123594
H -2.039229 3.499059 2.081362
H -1.058920 1.241193 2.328119
H -0.787602 3.580180 -2.030251
H 2.107079 0.246413 -2.948132
H 0.187266 1.610002 -3.058495
H 1.733566 -0.820857 2.468913
H 4.206064 -1.036043 2.425667
H 5.442227 -0.638271 0.296532
H 4.204782 0.026590 -1.739731
H -2.556150 -0.844247 0.596335
O -0.817303 -1.150300 2.589212
H -0.280155 -0.701063 1.579279
H -0.575466 -2.088839 2.659001
O -3.013079 -0.820586 1.647909
H -1.984493 -1.062543 2.250595
H -3.629073 -1.569900 1.695438
Cl -2.687567 -2.308450 -1.465311

Structures from Table 2/Scheme S2/Scheme S5.

IMS-10+
G = -593.844117

C -3.953143 -0.137391 0.000001
C -3.592639 1.233302 0.000000
C -2.267287 1.588407 0.000000
C -1.223166 0.604231 0.000000
C -1.603712 -0.806103 0.000000
C -2.985410 -1.121298 0.000000
C 1.223166 0.604231 -0.000001
C 1.603712 -0.806103 0.000000
C 0.689870 -1.887076 0.000000
C -0.689870 -1.887076 -0.000001
C 2.267287 1.588407 0.000000
C 3.592639 1.233302 0.000000
C 3.953143 -0.137391 0.000001
C 2.985410 -1.121298 0.000000
N 0.000000 1.139996 -0.000001
H -5.002424 -0.416761 0.000001
H -4.365325 1.995263 0.000001
H -1.952421 2.625749 0.000000
H -3.278569 -2.166760 0.000000
H -1.151264 -2.871902 -0.000001
H 1.952421 2.625749 0.000000
H 4.365325 1.995263 0.000001
H 5.002424 -0.416761 0.000001
H 3.278569 -2.166760 0.000001
H 1.151264 -2.871902 -0.000001

IMS-10-Cl
G = -1054.261528

C 3.915904 -0.326069 -0.719197
C 3.693553 -1.227755 0.383307
C 2.445830 -1.413080 0.885541
C 1.286390 -0.734764 0.331100
C 1.552747 0.329631 -0.661765
C 2.890114 0.403467 -1.225016
C -1.120001 -0.896785 0.225663
C -1.554006 0.339544 -0.329643
C -0.672802 1.538160 -0.391878
C 0.649286 1.293994 -1.007483
C -2.072786 -1.941826 0.343177
C -3.365773 -1.806597 -0.128333
C -3.774802 -0.594591 -0.704472
C -2.877257 0.460651 -0.785768
N 0.127935 -1.224179 0.701873
H 4.916776 -0.222271 -1.128476
H 4.534919 -1.781121 0.791422
H 2.243229 -2.128241 1.675894
H 3.059533 1.117362 -2.027249
H 0.958524 2.020559 -1.757098
H -1.730293 -2.866101 0.796593
H -4.064133 -2.634590 -0.043962
H -4.793101 -0.471365 -1.061822
H -3.201399 1.413462 -1.197524
H -1.183451 2.341134 -0.921229
Cl -0.447913 2.308032 1.333467

IMS-10-Cl 1H2O
G = -1130.665384

C -3.900785 -0.334101 -0.879284
C -3.703366 0.886594 -0.140464
C -2.465073 1.259235 0.275668
C -1.290852 0.457144 -0.018790
C -1.523331 -0.875383 -0.615079
C -2.855124 -1.164226 -1.118599
C 1.127806 0.629546 -0.159114
C 1.585376 -0.708773 -0.304478
C 0.730077 -1.883434 0.021406
C -0.595210 -1.877543 -0.634836
C 2.059608 1.681778 -0.357114
C 3.358285 1.429061 -0.761034
C 3.790319 0.107636 -0.946353
C 2.912094 -0.939233 -0.703751
N -0.137649 1.054954 0.184367
H -4.896567 -0.590614 -1.229020
H -4.556962 1.529296 0.056203
H -2.291221 2.209324 0.771156
H -3.001440 -2.106849 -1.639773
H -0.885038 -2.812497 -1.111406
H 1.707139 2.696491 -0.199326
H 4.042523 2.256213 -0.927475
H 4.812382 -0.099578 -1.249933
H 3.255702 -1.965971 -0.803617
H 1.259808 -2.801854 -0.226604
Cl 0.510644 -2.065187 1.898967

O -0.287804 3.836932 1.039617
H -0.000609 3.807074 1.964922
H -0.239637 2.897198 0.755872

IMS-10-Cl 2H2O
G = -1207.070795

C -3.007868 -2.187727 -1.175818
C -3.404448 -0.952204 -0.551190
C -2.482360 -0.065021 -0.091868
C -1.059363 -0.318588 -0.227288
C -0.667708 -1.679849 -0.655050
C -1.696384 -2.527900 -1.233546
C 1.099643 0.796042 -0.254205
C 2.051481 -0.254451 -0.134754
C 1.678841 -1.621415 0.325324
C 0.568608 -2.219549 -0.448229
C 1.581233 2.092135 -0.575055
C 2.918135 2.324076 -0.844387
C 3.842649 1.272900 -0.768195
C 3.405247 0.008270 -0.402684
N -0.267090 0.721008 -0.058736
H -3.767416 -2.854964 -1.572879
H -4.461183 -0.714541 -0.466663
H -2.803762 0.876318 0.346999
H -1.384750 -3.482842 -1.648901
H 0.741561 -3.228649 -0.818608
H 0.861473 2.902798 -0.614578
H 3.248775 3.325256 -1.105959
H 4.896205 1.449791 -0.963873
H 4.122685 -0.802151 -0.299492
H 2.550766 -2.272094 0.282043
Cl 1.271681 -1.640583 2.171777
O -3.902486 2.687311 1.262914
H -3.073526 3.079273 0.908304
H -3.708107 2.558566 2.203382
O -1.477779 3.336841 0.021176
H -1.806859 3.385662 -0.890275
H -1.088922 2.426899 0.080398

IMS-10-OH-TS-O
G = -1205.778330

C 0.603763 -0.552403 1.723097
C -0.658132 0.104150 1.435083
C -1.540371 -0.606852 0.467306
C 1.543770 -0.919543 0.790970
C -1.059035 -0.876585 -0.841821
C 1.347122 -0.711969 -0.658496
N 0.210857 -0.623976 -1.322124
H -2.008140 1.126575 2.352408
C 2.843680 -1.353859 1.248694
C 2.542973 -0.679581 -1.474923
C 3.759891 -1.024536 -0.972771
H 4.630553 -1.038653 -1.622385
C 3.910641 -1.400967 0.406071
H 4.888329 -1.696119 0.774960
H 2.400288 -0.442517 -2.523848
H 2.958806 -1.582862 2.304893
H -0.295721 1.228275 0.797539
C -2.858692 -0.939300 0.807891
H -3.205819 -0.748353 1.818469
C -1.961984 -1.415507 -1.787158
C -3.260098 -1.748439 -1.433843
H -3.927914 -2.182544 -2.172252
C -3.710386 -1.517867 -0.126664
H -4.728202 -1.771770 0.154781
H -1.588293 -1.581533 -2.792046
O -1.259959 0.557525 2.599573
Cl 0.052124 4.204713 -0.660175
O -0.158545 2.221860 0.132878
H -0.011174 1.836675 -0.754684
H 0.854356 -0.634985 2.779785

IMS-10-OH-TS-O 1H2O
G = -1282.155346

C 0.486807 -0.334024 -1.082482
C -0.530362 -1.141537 -0.365650
C -1.878368 -0.470931 -0.268803
C 0.909743 0.936499 -0.738495
C -2.029575 0.855276 0.249427
C 0.207825 1.801289 0.218130
N -1.059435 1.743048 0.604961
H 0.441258 -2.908185 -0.333795
C 2.168051 1.380210 -1.261526
C 0.922875 2.952599 0.707070
C 2.165862 3.286112 0.238531
H 2.673537 4.166254 0.622430

C 2.791055 2.501355 -0.772455
H 3.773558 2.780617 -1.140340
H 0.404134 3.564614 1.437198
H 2.663531 0.753873 -1.995131
H -0.110459 -1.099127 0.724480
C -3.014516 -1.214661 -0.592661
H -2.866710 -2.223939 -0.958506
C -3.353215 1.347821 0.456777
C -4.462184 0.606183 0.108128
H -5.459760 1.009472 0.254718
C -4.290093 -0.683017 -0.427597
H -5.158357 -1.277862 -0.697987
H -3.441813 2.342087 0.881390
O -0.575308 -2.446209 -0.740882
O 1.410558 -3.160955 0.341396
H 1.896728 -3.942867 0.031615
H 1.588642 -0.926976 2.050972
O 0.764639 -1.413933 2.238096
H 0.996280 -2.296276 1.857184
H 1.049144 -0.870582 -1.842087
Cl 3.270811 -1.531925 0.079641

IMS-10-OH-TS-O 2H2O
G = -1358.565927

C 0.413739 -0.010532 -1.099314
C -0.464968 -1.040343 -0.546000
C -1.915787 -0.691553 -0.375908
C 0.542119 1.305789 -0.685221
C -2.349675 0.545105 0.202324
C -0.378534 1.973876 0.244365
N -1.604299 1.620111 0.594347
H 0.765955 -2.538721 -0.862615
C 1.698805 2.023623 -1.133675
C 0.037352 3.250142 0.771755
C 1.186315 3.866252 0.356861
H 1.460451 4.835460 0.763792
C 2.021993 3.254929 -0.622730
H 2.930557 3.754668 -0.944141
H -0.635817 3.714562 1.484162
H 2.363889 1.527226 -1.831160
H -0.071065 -1.022750 0.618695
C -2.868437 -1.659764 -0.708605
H -2.514177 -2.593760 -1.127332
C -3.744134 0.720020 0.437308
C -4.670244 -0.239583 0.079871
H -5.728720 -0.072185 0.255977
C -4.227397 -1.437592 -0.503052
H -4.944166 -2.204073 -0.784712
H -4.042803 1.655501 0.898047
O -0.266421 -2.297656 -1.040031
Cl 3.664838 -0.765315 -0.530638
O 2.558893 -2.263432 2.157517
H 3.262062 -1.606707 2.012150
O 2.058468 -2.670893 -0.393465
H 2.445796 -2.622968 1.229510
H 2.637264 -3.177035 -0.986992
H 1.222553 -1.432352 2.174478
O 0.301746 -0.982279 2.112588
H -0.303896 -1.609809 2.540970
H 1.171609 -0.385607 -1.781162

IMS-10-OH
G = -669.858452

C 3.826281 -0.040843 -0.766356
C 3.632751 -1.159168 0.122535
C 2.406130 -1.438824 0.635897
C 1.239026 -0.643175 0.298059
C 1.489449 0.620783 -0.430113
C 2.795655 0.797126 -1.042895
C -1.169520 -0.738774 0.193771
C -1.578121 0.608808 -0.004791
C -0.652112 1.737095 0.371862
C 0.591728 1.649438 -0.466735
C -2.132307 -1.762339 0.004158
C -3.408206 -1.478947 -0.450415
C -3.786957 -0.149274 -0.691256
C -2.879761 0.875152 -0.454714
N 0.077108 -1.189943 0.583304
H 4.808398 0.133934 -1.196293
H 4.478529 -1.801324 0.353769
H 2.227301 -2.314032 1.252306
H 2.941206 1.669788 -1.675131
H -1.149442 2.687734 0.162716
H 0.835693 2.512472 -1.085060
H -1.812996 -2.782207 0.193259
H -4.116699 -2.286144 -0.615298
H -4.792901 0.081342 -1.030686
H -3.181242 1.910237 -0.598148

O -0.374664 1.791382 1.775359
H -0.024517 0.924399 2.038525

IMS-10-OH 1H2O
G = -746.261115

C -3.454347 -0.932743 1.068406
C -3.252467 -1.676789 -0.150540
C -2.053332 -1.647033 -0.791421
C -0.933676 -0.871141 -0.285212
C -1.226002 0.062802 0.824701
C -2.472002 -0.125032 1.549542
C 1.458933 -0.683175 -0.369510
C 1.736283 0.598341 0.185510
C 0.654960 1.648107 0.224614
C -0.426770 1.130762 1.128055
C 2.543169 -1.582164 -0.540694
C 3.816623 -1.272941 -0.097312
C 4.066964 -0.026682 0.497685
C 3.034827 0.894400 0.621692
N 0.241268 -1.175022 -0.782056
H -4.401860 -1.017287 1.593197
H -4.060853 -2.295448 -0.531094
H -1.856260 -2.255400 -1.668628
H -2.629851 0.467928 2.447837
H 1.072148 2.562795 0.673564
H -0.642604 1.696017 2.034294
H 2.321239 -2.541165 -0.997779
H 4.622347 -1.992342 -0.215842
H 5.069510 0.231392 0.827566
H 3.233283 1.879330 1.037856
O 0.210845 1.905432 -1.098903
H -0.713799 2.233220 -1.065939
O -2.608999 2.208649 -1.304582
H -2.893191 1.644292 -0.566601
H -2.582737 1.598900 -2.059250

IMS-10-OH 2H2O
G = -822.674782

C -4.123178 -0.622262 -0.378183
C -3.815475 0.735633 -0.745449
C -2.533078 1.189826 -0.747997
C -1.425539 0.322067 -0.403894
C -1.770618 -0.980931 0.196547
C -3.136813 -1.449578 0.053611
C 0.933332 -0.022206 -0.743785
C 1.287067 -0.995293 0.228526
C 0.417022 -1.157976 1.456041
C -0.893722 -1.697106 0.961216
C 1.857438 0.253925 -1.780725
C 3.037918 -0.461259 -1.903655
C 3.354878 -1.458369 -0.968696
C 2.487060 -1.707864 0.087692
N -0.229862 0.729823 -0.776782
H -5.151384 -0.968205 -0.428963
H -4.622826 1.392414 -1.058578
H -2.285748 2.188651 -1.095209
H -3.361717 -2.460388 0.385152
H 0.881743 -1.911449 2.112181
H -1.188759 -2.693924 1.285909
H 1.589227 1.020093 -2.501668
H 3.716835 -0.247195 -2.724465
H 4.286536 -2.011026 -1.051160
H 2.746885 -2.447194 0.841887
O 0.193069 0.049567 2.152423
H 1.018999 0.597275 2.123932
O 2.295641 1.793022 1.800578
H 1.789919 2.414753 1.218370
H 2.944724 1.389205 1.204622
O 0.634496 3.274972 0.151255
H -0.071489 3.486788 0.781843
H 0.272686 2.509311 -0.357917

IMS-10-O
G = -668.696998

C 4.042622 0.169068 0.000001
C 3.749324 -1.238998 -0.000001
C 2.461524 -1.669071 -0.000002
C 1.331574 -0.755311 -0.000001
C 1.635222 0.689182 0.000001
C 3.034828 1.078256 0.000002
C -1.107401 -0.850010 0.000000
C -1.575264 0.501202 0.000000
C -0.746004 1.735867 0.000000
C 0.713499 1.706317 0.000001
C -2.083908 -1.889110 0.000000
C -3.438868 -1.631050 0.000001

C -3.886616 -0.299484 0.000001
C -2.964826 0.733500 0.000001
N 0.165828 -1.357269 -0.000001
H 5.077358 0.499756 0.000002
H 4.567319 -1.953874 -0.000001
H 2.207473 -2.723576 -0.000003
H 3.253333 2.142545 0.000004
H 1.109312 2.720065 0.000002
H -1.701485 -2.904119 0.000000
H -4.151153 -2.451499 0.000001
H -4.950415 -0.078590 0.000002
H -3.284191 1.769490 0.000001
O -1.285325 2.849816 -0.000003

IMS-10-O 1H2O
G = -745.101743

C -3.955174 -0.628568 -0.005540
C -3.531827 -2.001729 0.001334
C -2.208637 -2.310101 0.004837
C -1.172491 -1.293582 0.002016
C -1.608650 0.114035 -0.004115
C -3.036685 0.372241 -0.007611
C 1.262448 -1.153581 0.004988
C 1.599691 0.238536 -0.005218
C 0.654686 1.378364 -0.013177
C -0.790998 1.219499 -0.006033
C 2.335555 -2.094464 0.012820
C 3.658489 -1.708747 0.010461
C 3.977406 -0.339450 -0.000590
C 2.963135 0.601124 -0.008408
N 0.047497 -1.781024 0.007255
H -5.016214 -0.396026 -0.010290
H -4.278946 -2.790407 0.003096
H -1.856978 -3.336162 0.009557
H -3.352060 1.411677 -0.016079
H -1.288952 2.188652 -0.006048
H 2.051040 -3.141022 0.020270
H 4.446061 -2.457088 0.016424
H 5.015266 -0.018275 -0.003617
H 3.186636 1.661498 -0.018076
O 1.102654 2.543180 -0.024134
O -0.978990 4.486066 -0.060512
H -0.155227 3.960624 -0.143332
H -0.954111 4.788259 0.859903

IMS-10-O 2H2O
G = -821.504329

C 3.877717 -0.892727 -0.054075
C 3.241173 -2.180038 -0.038632
C 1.886009 -2.282764 -0.019532
C 1.022867 -1.115507 -0.017059
C 1.676016 0.205715 -0.024820
C 3.126958 0.238554 -0.048397
C -1.370744 -0.580542 -0.027543
C -1.472053 0.847668 0.001338
C -0.354442 1.816953 0.046759
C 1.046733 1.427043 -0.002079
C -2.585220 -1.330541 -0.068765
C -3.823514 -0.724932 -0.085695
C -3.912125 0.676982 -0.055508
C -2.755257 1.433394 -0.010786
N -0.265480 -1.393395 -0.015098
H 4.961909 -0.830551 -0.068860
H 3.853254 -3.077485 -0.045157
H 1.393309 -3.249570 -0.015234
H 3.598569 1.216852 -0.054344
H 1.693849 2.303765 -0.007666
H -2.498231 -2.411777 -0.091463
H -4.723097 -1.332832 -0.121864
H -4.881707 1.166711 -0.066649
H -2.797435 2.515792 0.016781
O -0.603936 3.036937 0.113432
O 1.784402 4.597349 0.122061
H 0.881391 4.230319 0.223766
H 1.778359 4.952155 -0.779691
O -0.859732 -4.285908 0.078017
H -0.923270 -4.426118 1.035290
H -0.669119 -3.326063 0.001458

IMS-C+-TS-T+
G = -595.032718

C 0.623221 1.488645 1.356858
C -0.178215 1.578361 0.143181
C -1.302412 0.711550 -0.099526
C 1.407168 0.654785 0.348477
C -1.287373 -0.641191 0.322725

C 1.164646 -0.759788 0.288630
H 1.147084 2.389106 1.666879
N -0.067600 -1.266206 0.594412
C 2.611482 1.175294 -0.229523
C 2.202368 -1.615618 -0.138866
C 3.374939 -1.078981 -0.629363
H 4.150191 -1.746675 -0.992650
C 3.572566 0.324951 -0.708947
H 4.498000 0.716203 -1.117710
H 2.044032 -2.690542 -0.142736
H 2.771926 2.249423 -0.217300
H -0.058871 2.456074 -0.487141
C -2.481553 1.222508 -0.687519
H -2.488285 2.246270 -1.050070
C -2.466277 -1.404864 0.300539
C -3.629896 -0.848434 -0.204457
H -4.537948 -1.442494 -0.228006
C -3.635409 0.460415 -0.721321
H -4.548311 0.877072 -1.133554
H -2.450867 -2.436213 0.643272
H -0.117824 -2.278164 0.665291
H 0.212538 0.917590 2.187501

IMS-C+
G = -595.042155

C -3.784843 0.175534 -0.572692
C -3.444404 -1.183445 -0.604872
C -2.183814 -1.596256 -0.197915
C -1.249198 -0.644573 0.244160
C -1.604385 0.713093 0.339843
C -2.867969 1.113217 -0.108237
C 1.260266 -0.587921 0.333942
C 1.452394 0.773658 -0.146788
C 0.549825 1.783844 0.084891
C -0.630614 1.675312 0.990243
C 2.392965 -1.435849 0.437352
C 3.608524 -1.029899 -0.060009
C 3.778635 0.239609 -0.688978
C 2.726988 1.103771 -0.748631
N 0.037441 -1.107306 0.598912
H -4.773471 0.495735 -0.885510
H -4.160085 -1.917526 -0.960648
H -1.904985 -2.645269 -0.256671
H -3.144693 2.161486 -0.044255
H -0.323725 1.291351 1.973081
H 2.275924 -2.432803 0.853809
H 4.453731 -1.709456 -0.002501
H 4.745322 0.511527 -1.098375
H 2.840665 2.094559 -1.178141
H 0.056857 -2.093570 0.844910
H -1.094457 2.651474 1.141674
H 0.740620 2.743076 -0.393611

IMS-N+-TS-C+
G = -594.997020

C 0.669168 1.810159 0.761948
C -0.640222 1.939881 0.261032
C -1.480756 0.840446 -0.084652
C 1.626419 0.789256 0.219341
C -1.202166 -0.442395 0.476530
C 1.239674 -0.525911 0.463725
H 1.112992 2.719878 1.161267
N -0.001904 -0.558244 1.237530
C 2.822245 1.036885 -0.455563
C 1.977719 -1.623831 0.045712
C 3.170942 -1.366208 -0.635940
H 3.783768 -2.197565 -0.969191
C 3.585794 -0.052753 -0.882210
H 4.518046 0.124507 -1.409124
H 1.655219 -2.640953 0.246629
H 3.151991 2.053196 -0.646909
H -1.104842 2.925296 0.279086
C -2.707801 1.019525 -0.772328
H -2.935013 1.992776 -1.197108
C -2.133533 -1.478192 0.391019
C -3.311101 -1.275665 -0.320267
H -4.021984 -2.090655 -0.415069
C -3.593869 -0.031025 -0.912794
H -4.520074 0.107491 -1.460553
H -1.926040 -2.439911 0.851423
H -0.038154 -1.300353 1.938890
H 0.202341 0.812981 1.624646

IMS-N+
G = -595.037896

C -0.015733 -0.826160 3.639781

C -1.327306 -0.516427 3.266388
C -1.567613 0.140678 2.060021
C -0.482765 0.450745 1.250921
C 0.844846 0.132364 1.568928
C 1.052643 -0.498842 2.810093
C -0.482765 0.450745 -1.250921
C 0.844846 0.132364 -1.568928
C 1.971662 0.414282 -0.678074
C 1.971662 0.414282 0.678074
C -1.567613 0.140678 -2.060021
C -1.327306 -0.516427 -3.266388
C -0.015733 -0.826160 -3.639781
C 1.052643 -0.498842 -2.810093
N -0.698613 1.224419 0.000000
H 0.172811 -1.324107 4.585472
H -2.158565 -0.765976 3.917322
H -2.579916 0.413995 1.772175
H 2.067076 -0.750177 3.105005
H 2.931676 0.539124 1.173109
H -2.579916 0.413995 -1.772175
H -2.158565 -0.765976 -3.917322
H 0.172811 -1.324107 -4.585472
H 2.067076 -0.750177 -3.105005
H 2.931676 0.539124 -1.173109
H -1.644035 1.623643 0.000000
H -0.040643 2.020033 0.000000

IMS-T+
G = -595.033878

C 3.576304 -0.392413 -0.648737
C 3.446244 1.020372 -0.479525
C 2.274302 1.601295 -0.053316
C 1.149243 0.788427 0.220564
C 1.301904 -0.659061 0.214164
C 2.538747 -1.207408 -0.315186
C -1.294071 0.683541 0.221276
C -1.300946 -0.688871 -0.090392
C -0.086464 -1.500845 0.106011
C 0.635385 -1.449847 1.379095
C -2.472970 1.439290 0.185342
C -3.659176 0.829963 -0.202375
C -3.670902 -0.520689 -0.575051
C -2.499065 -1.268776 -0.528621
N -0.062559 1.332061 0.442268
H 4.509459 -0.803925 -1.017498
H 4.290143 1.659065 -0.723481
H 2.183297 2.682053 0.009775
H 2.628899 -2.288075 -0.381460
H 0.236196 -0.838803 2.183429
H -2.451389 2.496663 0.436933
H -4.574983 1.411329 -0.231741
H -4.598069 -0.990273 -0.886845
H -2.513859 -2.322423 -0.792139
H -0.103891 2.345276 0.498147
H 1.201426 -2.318688 1.698254
H -0.000525 -2.406483 -0.488740

IMS-TS-10-Cl
G = -1130.593706

C -4.262781 0.368805 0.003482
C -3.535860 1.441199 -0.528092
C -2.159888 1.352030 -0.651699
C -1.439197 0.202202 -0.225045
C -2.191506 -0.920249 0.263467
C -3.588305 -0.786708 0.375697
C 0.940740 -0.595630 -0.274853
C 0.847395 -1.987567 0.079350
C -0.347440 -2.640775 0.562127
C -1.620438 -2.185317 0.664294
C 2.215704 -0.076231 -0.631046
C 3.340405 -0.881927 -0.671761
C 3.247829 -2.240790 -0.345573
C 2.017989 -2.765840 0.030253
N -0.074817 0.323282 -0.295577
H -5.343233 0.423565 0.094429
H -4.048209 2.335605 -0.870423
H -1.595922 2.150850 -1.120987
H -4.149784 -1.632761 0.763361
H -2.342943 -2.886415 1.076873
H 2.292621 0.974011 -0.881120
H 4.294464 -0.448402 -0.955716
H 4.126487 -2.877953 -0.374984
H 1.944120 -3.814851 0.305003
H 0.293006 1.493499 -0.406738
H -0.184269 -3.662267 0.899716
O 0.636572 2.676205 -0.610547
H 0.099683 3.258877 -0.045323
Cl 2.309250 3.018495 0.974454

IMS-TS-10-Cl 1H2O
G = -1206.995817

C -3.767948 -1.566416 -0.199001
C -3.601484 -0.520246 -1.156119
C -2.385461 0.074478 -1.366158
C -1.224056 -0.370807 -0.659817
C -1.425354 -1.284928 0.456843
C -2.712669 -1.919910 0.589878
C 1.250748 -0.355115 -0.750875
C 1.638990 -0.735680 0.547124
C 0.683992 -0.597628 1.692545
C -0.554234 -1.331660 1.538336
C 2.188318 -0.372227 -1.792297
C 3.492370 -0.803395 -1.563183
C 3.871781 -1.219258 -0.285786
C 2.947038 -1.182925 0.756929
N -0.043270 0.112139 -1.068903
H -4.737163 -2.039119 -0.076425
H -4.457435 -0.197340 -1.742691
H -2.255675 0.862546 -2.100428
H -2.832969 -2.656081 1.380441
H -0.905174 -1.889220 2.406571
H 1.872640 -0.061548 -2.783942
H 4.207168 -0.817729 -2.380751
H 4.888593 -1.550509 -0.095989
H 3.248460 -1.472369 1.760434
H -0.093257 1.127277 -1.459619
H 1.163784 -0.795519 2.649463
Cl 0.201284 1.353020 1.704226
O -0.378939 2.652693 -1.474158
H 0.289964 3.170567 -1.946779
O -0.184193 3.478056 0.884407
H -0.315422 3.019652 -0.429524
H -1.099590 3.581386 1.197208

IMS-TS-10-Cl 2H2O
G = -1283.413146

C -3.770068 -1.793596 -0.262898
C -3.605921 -0.707421 -1.175405
C -2.389235 -0.111209 -1.365373
C -1.225954 -0.578256 -0.674108
C -1.414165 -1.563646 0.380563
C -2.707572 -2.194033 0.491029
C 1.262982 -0.482758 -0.791400
C 1.671988 -1.015453 0.446280
C 0.744741 -1.048194 1.623239
C -0.504045 -1.761662 1.405237
C 2.202509 -0.293014 -1.818588
C 3.522260 -0.693203 -1.647471
C 3.921526 -1.281565 -0.444788
C 2.999810 -1.431978 0.589124
N -0.051556 -0.079608 -1.075286
H -4.741557 -2.263427 -0.149258
H -4.464265 -0.354014 -1.740277
H -2.259821 0.706463 -2.066240
H -2.822838 -2.971249 1.241708
H -0.820252 -2.440671 2.196428
H 1.876646 0.170719 -2.743955
H 4.237183 -0.546476 -2.451548
H 4.952144 -1.592304 -0.300867
H 3.319008 -1.841454 1.544054
H -0.116303 0.776956 -1.706575
H 1.258335 -1.416922 2.509991
Cl 0.258161 0.799947 2.041450
O -0.094123 2.267557 -2.230487
H -0.570806 2.661619 -2.973894
O -0.154468 3.094329 2.110903
H -0.291901 2.882593 -1.374436
H 0.748653 3.409420 2.281738
O -0.589381 3.674798 -0.216983
H -1.538510 3.865390 -0.190747
H -0.342907 3.353962 0.906118

IMS-TS-10-OH
G = -1130.600557

C -0.616689 0.580554 1.408125
C 0.767975 0.695664 1.519770
C 1.812607 0.119911 0.725921
C -1.352601 -0.517130 0.750393
C 1.610704 -0.655435 -0.454535
C -0.869108 -1.231062 -0.364004
H -1.176607 1.025660 2.225816
N 0.372261 -0.988108 -0.980152
C -2.621457 -0.837517 1.248940
C -1.676870 -2.218970 -0.945474

C -2.942001 -2.509805 -0.441038
H -3.545274 -3.276123 -0.919252
C -3.420086 -1.822719 0.672125
H -4.404029 -2.036202 1.077590
H -1.302020 -2.767464 -1.806970
H -2.995563 -0.276953 2.101716
H 1.119222 1.368786 2.300348
C 3.145898 0.405435 1.113582
H 3.292702 0.998841 2.012574
C 2.740085 -1.075563 -1.184254
C 4.029960 -0.770016 -0.775608
H 4.872180 -1.116726 -1.367730
C 4.244087 -0.029274 0.394059
H 5.249997 0.210069 0.723407
H 2.588299 -1.659515 -2.089416
Cl -1.738043 3.334216 -1.150890
O -0.737091 1.960572 0.168621
H -0.422759 2.725032 0.688853
H 0.446466 -1.449322 -1.877731

IMS-TS-10-OH 1H2O
G = -1207.009822

C 0.528563 -0.638190 -1.849613
C -0.850992 -0.744543 -1.855433
C -1.768238 -0.807945 -0.754283
C 1.431692 -0.985461 -0.745485
C -1.414234 -0.480045 0.590732
C 1.094106 -0.770217 0.605983
H 1.006152 -0.633828 -2.826176
N -0.131625 -0.228998 1.025619
C 2.698936 -1.497502 -1.052249
C 2.044951 -1.043631 1.599476
C 3.306940 -1.537317 1.272140
H 4.025570 -1.737757 2.061996
C 3.636550 -1.779986 -0.060410
H 4.615046 -2.166911 -0.328137
H 1.777470 -0.870531 2.638375
H 2.957191 -1.652231 -2.097171
H -1.324413 -0.734668 -2.836710
C -3.132995 -1.043424 -1.054068
H -3.391714 -1.292950 -2.080457
C -2.450296 -0.332919 1.538091
C -3.775476 -0.559790 1.203447
H -4.542789 -0.447466 1.964642
C -4.128174 -0.943201 -0.100235
H -5.164666 -1.132739 -0.360531
H -2.183668 -0.049534 2.552325
Cl 0.742350 3.297400 -0.764294
O 0.335801 1.354466 -1.483165
H 0.017697 1.676799 -2.350743
H -0.052042 0.405466 1.826089
O 0.367355 2.183169 2.416744
H 1.306114 2.293006 2.632385
H 0.302222 2.574457 1.520584

IMS-TS-10-OH 2H2O
G = -1283.477887

C 0.528563 -0.63819000 -1.84961300
C -0.850992 -0.74454300 -1.85543300
C -1.768238 -0.80794500 -0.75428300
C 1.431692 -0.98546100 -0.74548500
C -1.414234 -0.48004500 0.59073200
C 1.094106 -0.77021700 0.60598300
H 1.006152 -0.63382800 -2.82617600
N -0.131625 -0.22899800 1.02561900
C 2.698936 -1.49750200 -1.05224900
C 2.044951 -1.04363100 1.59947600
C 3.306940 -1.53731700 1.27214000
H 4.025570 -1.73775700 2.06199600
C 3.636550 -1.77998600 -0.06041000
H 4.615046 -2.16691100 -0.32813700
H 1.777470 -0.87053100 2.63837500
H 2.957191 -1.65223100 -2.09717100
H -1.324413 -0.73466800 -2.83671000
C -3.132995 -1.04342400 -1.05406800
H -3.391714 -1.29295000 -2.08045700
C -2.450296 -0.33291900 1.53809100
C -3.775476 -0.55979000 1.20344700
H -4.542789 -0.44746600 1.96464200
C -4.128174 -0.94320100 -0.10023500
H -5.164666 -1.13273900 -0.36053100
H -2.183668 -0.04953400 2.55232500
Cl 0.742350 3.29740000 -0.76429400
O 0.335801 1.35446600 -1.48316500
H 0.017697 1.67679900 -2.35074300
H -0.052042 0.40546600 1.82608900
O 0.367355 2.18316900 2.41674400
H 1.306114 2.29300600 2.63238500

H 0.302222 2.57445700 1.52058400
H -0.286329 -1.44666487 1.88779876
O -0.385340 -2.22597167 2.43959380
H -0.420763 -1.96297704 3.36218742

IMS-1-Cl-2-OH
G = -1130.842349

C 0.019228 -1.724005 -0.010663
C 1.352767 -1.890475 0.040104
C 2.390373 -0.854389 -0.030190
C -0.740840 -0.482130 -0.070029
C 2.185005 0.479128 0.375201
C -0.307338 0.710429 0.440823
H -0.589024 -2.626036 -0.023133
N 0.966883 0.910195 0.977962
C -2.149103 -0.577536 -0.535387
C -1.219572 1.849618 0.552044
C -2.389296 1.869546 -0.096594
H -3.074385 2.707973 -0.034023
H -0.917323 2.686710 1.176631
H -2.296631 -1.353112 -1.282024
H 1.724936 -2.911535 0.057504
C 3.656793 -1.202825 -0.516914
H 3.825004 -2.231237 -0.822390
C 3.221605 1.405929 0.267218
C 4.477957 1.031899 -0.211075
H 5.273215 1.767821 -0.265160
C 4.698083 -0.280879 -0.608355
H 5.668762 -0.590570 -0.980141
H 3.051920 2.432606 0.581317
C -2.745416 0.739372 -1.022707
O -4.121214 0.664290 -1.334374
H -4.581699 0.265727 -0.581131
Cl -3.258998 -1.237599 0.891525
H -2.249790 0.936510 -1.985824
H 1.068051 1.826550 1.390862

IMS-TS-IMS-1-Cl-2-OH
G = -1130.594212

C 0.475349 1.637582 0.991286
C 1.761886 1.791276 0.631111
C 2.716756 0.841277 0.063691
C -0.406933 0.470133 0.941292
C 2.454977 -0.523218 -0.202645
C -0.008428 -0.838183 0.501066
H -0.016124 2.524259 1.385315
N 1.234915 -1.184043 0.042496
C -1.712099 0.636134 1.368599
C -0.958708 -1.893870 0.530760
C -2.247217 -1.701863 0.964326
H -2.946114 -2.531651 0.983072
H -0.643775 -2.882838 0.204017
H -2.021635 1.619276 1.711009
H 2.176671 2.786718 0.773141
C 3.999907 1.325080 -0.241781
H 4.206363 2.372724 -0.039435
C 3.463747 -1.327981 -0.751142
C 4.726078 -0.817004 -1.042848
H 5.483272 -1.469187 -1.467444
C 5.000594 0.523807 -0.786760
H 5.977275 0.943268 -1.006518
H 3.252873 -2.376378 -0.953551
C -2.716871 -0.392041 1.315335
O -3.736378 0.007822 -0.054834
H -3.097158 0.027622 -0.791545
Cl -5.186486 0.665180 -1.656395
H -3.536875 -0.320740 2.022320
H 1.287879 -2.162182 -0.214223

CBZ-1-Cl-2-OH
G = -1299.330856

C 0.212642 -1.294677 -1.490418
C -1.125982 -1.504415 -1.564326
C -2.145030 -1.105881 -0.599797
C 0.929805 -0.617859 -0.428727
C -2.011894 0.026775 0.231306
C 0.406929 0.387742 0.335192
H 0.835015 -1.761299 -2.252547
N -0.892158 0.901475 0.049761
H 0.887095 2.354758 -1.050402
C -1.100554 2.181084 -0.483053
O -2.214362 2.658423 -0.630455
N 0.062599 2.873864 -0.772932
H -0.112378 3.714731 -1.306683
C 2.369750 -1.006527 -0.194716
C 1.168020 1.004620 1.421733

C 2.319186 0.461922 1.847435
H 2.911908 0.892911 2.647976
H 0.768565 1.913038 1.860029
H 2.564078 -2.029113 -0.525359
H -1.481842 -2.129408 -2.381657
C -3.306612 -1.892542 -0.463950
H -3.428271 -2.760825 -1.106967
C -2.984612 0.328605 1.186164
C -4.117847 -0.471378 1.309445
H -4.882144 -0.216177 2.037938
C -4.280102 -1.584369 0.478163
H -5.166732 -2.206213 0.564761
H -2.860679 1.216942 1.795568
C 2.785587 -0.844663 1.272669
O 4.169893 -0.980492 1.513566
H 4.471991 -1.815585 1.123264
Cl 3.454054 0.012557 -1.314379
H 2.221417 -1.648667 1.793104

CBZ-TS-CBZ-1-Cl-2-OH
G = -1299.260491

C -0.366377 -1.995694 -1.174444
C -1.647927 -1.676072 -1.451155
C -2.546712 -0.792821 -0.714788
C 0.462166 -1.529956 -0.066707
C -2.108643 0.268910 0.101650
C 0.210990 -0.327207 0.657852
H 0.108006 -2.739146 -1.811338
N -0.713313 0.611135 0.187127
H 1.730093 1.384577 -0.395511
C -0.298747 1.944185 -0.151991
O -1.116753 2.826628 -0.343742
N 1.052014 2.122762 -0.225554
H 1.333011 3.036445 -0.554265
C 1.637484 -2.198891 0.240875
C 0.961332 -0.006676 1.828733
C 2.083992 -0.705400 2.152564
H 2.674404 -0.455200 3.027547
H 0.622381 0.829504 2.430846
H 1.935908 -3.050329 -0.366249
H -2.108800 -2.198390 -2.287400
C -3.932231 -1.032302 -0.799795
H -4.280462 -1.842143 -1.435745
C -3.026212 1.024385 0.836037
C -4.390970 0.761341 0.739284
H -5.094922 1.370540 1.298632
C -4.847326 -0.269206 -0.085171
H -5.910387 -0.474744 -0.170611
H -2.665016 1.843197 1.445562
C 2.608358 -1.656383 1.177884
O 3.405102 -0.628466 0.171207
H 3.815606 -1.174246 -0.529765
Cl 4.412302 1.073647 -1.193776
H 3.358280 -2.353918 1.546796

Structures from Table 3/Scheme S3.

CBZ-EP+ 1H2O
G = -1375.739610

C 1.215058 -2.155506 0.104316
C -0.161395 -2.000027 -0.450453
C -0.820922 -1.247852 0.695500
C 2.130825 -1.129954 0.134732
C -0.454648 0.092266 0.958934
C 1.778323 0.265646 -0.099904
H 1.532957 -3.139892 0.443324
N 0.570778 0.769618 0.256173
H -1.391099 1.904841 -0.986840
C 0.373967 2.266100 0.135674
O 1.118890 3.012119 0.741453
N -0.629590 2.564160 -0.684561
H -0.871335 3.547051 -0.730088
C 3.529253 -1.477280 0.228063
C 2.806603 1.118382 -0.603493
C 4.110154 0.691962 -0.625201
H 4.875194 1.376083 -0.980892
C 4.495893 -0.598053 -0.156450
H 5.543529 -0.880181 -0.144190
H 2.571784 2.130451 -0.900363
H 3.776468 -2.496896 0.509854
H -0.641079 -2.984253 -0.540898
C -1.812108 -1.853686 1.482685
H -2.092850 -2.880170 1.264422
C -1.131853 0.806745 1.968434
C -2.121208 0.193136 2.715970
H -2.624474 0.755452 3.496227
C -2.467467 -1.144411 2.475341
H -3.260166 -1.614726 3.049051
H -0.843786 1.828602 2.188148
Cl -3.242667 1.128346 -1.360685
O -0.119508 -1.317903 -1.664795
H -1.049777 -1.360626 -2.042659
H -2.982426 -0.766123 -2.040659
O -2.633564 -1.620919 -2.433220
H -2.755307 -1.489134 -3.386459

CBZ-EP+ 2H2O
G = -1452.146760

C -1.635312 -2.082347 -0.320116
C -0.315070 -2.049837 0.370908
C 0.482764 -1.257136 -0.651963
C -2.499289 -1.010729 -0.354476
C 0.201220 0.115554 -0.840161
C -2.111065 0.341086 0.026833
H -1.959745 -3.017756 -0.772699
N -0.845148 0.795152 -0.166724
H 1.147840 1.623863 1.252375
C -0.551972 2.238909 0.150380
O -1.225631 3.117645 -0.350671
N 0.455436 2.362639 1.016199
H 0.765274 3.311224 1.188489
C -3.893769 -1.279116 -0.609469
C -3.144889 1.203074 0.499718
C -4.462179 0.842533 0.361072
H -5.227918 1.536294 0.696115
C -4.855480 -0.384221 -0.247176
H -5.907885 -0.610308 -0.383663
H -2.898125 2.177792 0.894091
H -4.155399 -2.259393 -0.997772
H 0.101159 -3.064486 0.429423
C 1.529958 -1.847650 -1.377068
H 1.747771 -2.899006 -1.211426
C 1.006486 0.871468 -1.716228
C 2.057944 0.276142 -2.388766
H 2.693177 0.873887 -3.031471
C 2.327945 -1.090476 -2.216945
H 3.187629 -1.533720 -2.706643
H 0.784944 1.920859 -1.877812
Cl 3.050041 0.736520 1.650239
O -0.427231 -1.451867 1.626939
H 0.460660 -1.578818 2.074573
H 2.478906 -1.158635 2.245409
O 2.002017 -1.972386 2.571820
H 2.076761 -1.904915 3.536316
H 4.204143 0.504255 -0.334328
O 4.767767 0.472806 -1.136863
H 5.618951 0.800382 -0.810417

CBZ-AC
G = -838.586586

C -3.523185 -1.222566 -0.869952
C -3.475746 0.127526 -1.220195
C -2.321761 0.879665 -1.004680
C -1.207749 0.277897 -0.409330
C -1.248314 -1.077427 -0.047991
C -2.404709 -1.820049 -0.292040
C 1.224111 0.241580 -0.391525
C 1.231709 -1.123187 -0.050101
C 0.088424 -1.396686 2.098565
C -0.024840 -1.686689 0.590644
C 2.355672 0.811387 -0.991951
C 3.496057 0.038431 -1.204645
C 3.511314 -1.314002 -0.857290
C 2.374803 -1.889417 -0.290710
N 0.022284 0.984926 -0.193099
H -4.421650 -1.806386 -1.048665
H -4.339040 0.602299 -1.678284
H -2.282134 1.924523 -1.277423
H -2.427289 -2.872110 -0.016643
H 0.888616 -1.988160 2.599549
H -0.027951 -2.779562 0.481424
H 2.335789 1.854178 -1.287222
H 4.367981 0.493032 -1.666582
H 4.396066 -1.917700 -1.036893
H 2.368709 -2.945887 -0.032622
O -0.564854 -0.585233 2.708221
C -0.010605 2.277853 0.373457
O -1.011778 2.974265 0.373796
N 1.187328 2.725030 0.902754
H 1.059030 3.558381 1.461724
H 1.836566 2.049545 1.284377

CBZ-AC 1H2O
G = -914.991044

C -3.888591 -1.069657 -0.146128
C -3.786331 0.145498 -0.823391
C -2.551664 0.771135 -0.992755
C -1.397060 0.187445 -0.452951
C -1.494882 -1.033894 0.237804
C -2.736621 -1.656134 0.373783
C 0.996744 -0.143545 -0.761455
C 0.932860 -1.399684 -0.132710
C 0.224815 -1.024773 2.120684
C -0.239651 -1.645835 0.805028
C 2.079073 0.145402 -1.606080
C 3.089379 -0.793474 -1.791667
C 3.027695 -2.043153 -1.168227
C 1.945794 -2.340090 -0.344148
N -0.092368 0.759856 -0.601646
H -4.851732 -1.557942 -0.028357
H -4.673664 0.610833 -1.244127
H -2.470195 1.704827 -1.529005
H -2.796920 -2.605252 0.901990
H 1.040530 -1.589216 2.620497
H -0.359456 -2.724300 0.969700
H 2.125174 1.103930 -2.108455
H 3.922283 -0.552899 -2.446467
H 3.811811 -2.777387 -1.327418
H 1.878298 -3.310092 0.143254
O -0.159299 0.039145 2.565542
C 0.084862 2.172004 -0.574714
O -0.763377 2.952884 -0.980016
N 1.297964 2.582082 -0.076405
H 1.346220 3.591564 -0.018038
H 1.707625 2.095888 0.726832
O 2.140310 1.670340 2.619332
H 1.327997 1.189102 2.872355
H 2.093250 2.500954 3.116306

CBZ-AC 2H2O
G = -991.401018

C 4.027856 -0.537238 -0.768886
C 3.946785 -0.368245 0.613838
C 2.710961 -0.265819 1.251843
C 1.534845 -0.309261 0.492439
C 1.609691 -0.469922 -0.902486
C 2.854796 -0.593807 -1.519327
C -0.776005 -1.062363 0.485014
C -0.737725 -1.267241 -0.903621
C -0.246414 0.890389 -1.976677
C 0.317409 -0.501719 -1.681305
C -1.731994 -1.736940 1.256256
C -2.655825 -2.577248 0.639900
C -2.622075 -2.781991 -0.741941
C -1.656218 -2.130076 -1.505779
N 0.228889 -0.241316 1.077281
H 4.993646 -0.627746 -1.257917

H 4.853541 -0.330882 1.211618
H 2.645945 -0.141120 2.322725
H 2.901346 -0.724890 -2.598245
H -1.232252 0.882221 -2.480224
H 0.461113 -0.979532 -2.661888
H -1.749617 -1.595102 2.330216
H -3.393276 -3.093093 1.248816
H -3.334427 -3.450425 -1.216813
H -1.609769 -2.289888 -2.580844
O 0.295958 1.936132 -1.676837
C -0.037147 0.665711 2.136981
O 0.841124 1.081523 2.879835
N -1.357403 1.021512 2.269301
H -1.474639 1.737646 2.974366
H -1.937590 1.137835 1.431502
O -1.485223 4.001061 -1.108080
H -0.779449 3.431029 -1.486605
H -1.042116 4.467365 -0.382475
O -2.722899 1.734077 -0.185017
H -2.394184 2.627288 -0.453705
H -3.673997 1.740188 -0.363298

CBZ-EP-TS-AC
G = -838.491023

C -3.724299 -1.112077 -0.856423
C -3.642702 0.301797 -0.764107
C -2.466872 0.944116 -0.440296
C -1.295634 0.185065 -0.189859
C -1.406414 -1.252495 -0.109523
C -2.623545 -1.868302 -0.549729
C 1.179641 0.198010 -0.354000
C 1.574823 -0.992945 0.282356
C 0.639094 -1.463308 1.435722
C -0.434499 -2.022384 0.528479
C 2.047052 0.853900 -1.238695
C 3.280867 0.284072 -1.538690
C 3.655920 -0.934183 -0.957737
C 2.804783 -1.569423 -0.058086
N -0.082539 0.798224 -0.095777
H -4.656904 -1.583183 -1.150385
H -4.519336 0.900285 -0.996992
H -2.402110 2.025461 -0.459053
H -2.673001 -2.953988 -0.558462
H 1.150953 -2.326158 1.917998
H -0.518815 -3.106330 0.420101
H 1.729699 1.782487 -1.702852
H 3.944823 0.781846 -2.239468
H 4.622414 -1.372185 -1.191950
H 3.107041 -2.495014 0.425320
O 0.252382 -0.503411 2.273771
C -0.011864 2.199394 0.432462
O -0.254092 3.168749 -0.260636
N 0.349550 2.115741 1.715026
H 0.463345 2.973355 2.238118
H 0.438394 1.145538 2.126552

CBZ-EP-TS-AC 1H2O
G = -914.903012

C -3.987575 -0.954871 -0.567389
C -3.798620 0.443380 -0.422518
C -2.554025 0.995755 -0.221305
C -1.397448 0.170103 -0.156239
C -1.601863 -1.266416 -0.116991
C -2.907704 -1.780961 -0.425471
C 1.055280 0.045508 -0.550954
C 1.427334 -1.190310 0.015264
C 0.562497 -1.760354 1.156684
C -0.646869 -2.159836 0.349502
C 1.890267 0.659648 -1.503171
C 3.063419 0.037084 -1.907109
C 3.424105 -1.206193 -1.372173
C 2.604246 -1.810706 -0.428572
N -0.150644 0.720214 -0.200329
H -4.977105 -1.356259 -0.760616
H -4.654282 1.107929 -0.505762
H -2.448341 2.071137 -0.195067
H -3.025323 -2.860542 -0.461788
H 1.067723 -2.695487 1.490541
H -0.867792 -3.220509 0.212387
H 1.588603 1.599135 -1.953576
H 3.690609 0.514996 -2.654033
H 4.348027 -1.686787 -1.681644
H 2.886629 -2.762291 0.014693
O 0.242717 -0.903963 2.136823
C -0.027322 2.212041 -0.183927
O -0.462488 2.881462 -1.104604
N 0.596792 2.632144 0.917132
H 0.787754 3.625114 0.956453

H 1.004319 2.003694 1.660303
O 1.745685 1.042661 2.798450
H 1.393309 1.250636 3.677629
H 1.241181 0.178218 2.543723

CBZ-EP-TS-AC 2H2O
G = -991.313778

C 3.894618 -1.264648 -0.805175
C 3.818215 -0.457833 0.361927
C 2.619393 0.002049 0.851049
C 1.394093 -0.325075 0.199685
C 1.478139 -0.990180 -1.087698
C 2.748298 -1.529917 -1.497496
C -1.048709 -0.688091 0.529357
C -1.531223 -0.819410 -0.792902
C -0.779945 -0.128506 -1.946113
C 0.439117 -1.012573 -2.002255
C -1.829704 -1.167944 1.601120
C -3.042844 -1.795765 1.357106
C -3.506415 -1.965181 0.046799
C -2.745896 -1.486903 -1.010059
N 0.211244 -0.095418 0.831033
H 4.853621 -1.640473 -1.146350
H 4.728115 -0.221220 0.906286
H 2.605100 0.560947 1.777400
H 2.776572 -2.093074 -2.426167
H -1.372071 -0.338111 -2.863745
H 0.570878 -1.663336 -2.868638
H -1.453782 -1.090180 2.612887
H -3.621083 -2.173282 2.195442
H -4.460860 -2.449495 -0.139480
H -3.106715 -1.579553 -2.031244
O -0.508120 1.173083 -1.756612
C 0.286457 0.622656 2.153404
O 0.433679 -0.008005 3.183834
N 0.169126 1.938048 1.989035
H 0.229218 2.491823 2.834516
H 0.204900 2.430842 1.053190
O 0.459224 3.220644 -0.370936
H 0.444788 2.415066 -0.946493
H -0.441162 3.566521 -0.581524
O -2.129082 3.230239 -1.326670
H -1.707395 2.339051 -1.511658
H -2.119898 3.662304 -2.194322

CBZ-EP+-TS-AC
G = -1299.331684

C -4.193669 -0.812684 -0.030070
C -3.967339 0.580814 0.003207
C -2.692542 1.110465 -0.010955
C -1.568443 0.250562 -0.038585
C -1.791140 -1.159500 0.112361
C -3.117338 -1.666464 0.005093
C 0.761596 -0.090768 -0.726156
C 1.031112 -1.334547 -0.092901
C 0.401584 -1.625612 1.280069
C -0.765894 -2.050008 0.493632
C 1.575607 0.305388 -1.810820
C 2.550598 -0.542156 -2.297072
C 2.762464 -1.812890 -1.721637
C 2.006298 -2.204357 -0.640513
N -0.305619 0.723756 -0.348942
H -5.206144 -1.202355 -0.057455
H -4.814321 1.260709 0.000656
H -2.557457 2.180769 -0.072570
H -3.262375 -2.742428 0.050502
H 0.929849 -2.473582 1.734756
H -0.892733 -3.111793 0.292825
H 1.383217 1.252295 -2.302436
H 3.144115 -0.231811 -3.151670
H 3.538240 -2.464076 -2.111929
H 2.192793 -3.154237 -0.147855
Cl 2.705513 0.975891 2.017971
O 0.180424 -0.568646 2.120209
H 1.053042 -0.067052 2.241973
C -0.118381 2.193860 -0.587986
O -0.787320 2.774684 -1.421621
N 0.824628 2.687826 0.213659
H 1.058681 3.663708 0.085287
H 1.414396 2.117705 0.864677

CBZ-EP+-TS-AC 1H2O
G = -1375.741184

C 4.221355 -1.514546 -0.093186
C 4.253014 -0.149695 -0.453704
C 3.114525 0.632418 -0.450580

C 1.867610 0.064111 -0.097126
C 1.801496 -1.358632 0.091859
C 3.012463 -2.101506 0.193747
C -0.349176 0.383646 0.909410
C -0.951963 -0.871441 0.642311
C -0.600067 -1.599680 -0.670173
C 0.586276 -2.073337 0.049811
C -0.870492 1.180169 1.949059
C -1.898247 0.701993 2.741274
C -2.452259 -0.574075 2.517868
C -1.979280 -1.356353 1.485620
N 0.763918 0.847564 0.195007
H 5.137750 -2.095184 -0.065521
H 5.202639 0.315577 -0.701955
H 3.188916 1.692897 -0.642533
H 2.947442 -3.164411 0.410277
H -1.361389 -2.366984 -0.841375
H 0.549402 -3.064231 0.498083
H -0.416850 2.142105 2.162109
H -2.266889 1.315303 3.558105
H -3.272525 -0.925904 3.135600
H -2.450122 -2.301713 1.239479
O -3.692945 -1.974067 -1.055108
H -3.558309 -1.008063 -1.179488
H -3.972957 -2.265211 -1.935978
Cl -2.713236 1.018124 -1.833451
O -0.325013 -0.816577 -1.768356
H -1.136959 -0.259914 -1.957586
C 0.815979 2.320280 -0.030508
O 1.721003 2.997255 0.419786
N -0.225993 2.733647 -0.759880
H -0.296747 3.729175 -0.922619
H -0.985626 2.126976 -1.118493

CBZ-EP+-TS-AC 2H2O

C -4.208649 -0.467449 -1.578070
C -4.112526 -1.426046 -0.567685
C -3.013957 -1.455894 0.290452
C -1.981702 -0.525541 0.122533
C -2.064025 0.428456 -0.906587
C -3.183090 0.462313 -1.739626
C -0.331898 0.808535 1.295514
C -0.395355 1.818882 0.315393
C 0.355773 0.807569 -1.591344
C -0.919054 1.397632 -1.061902
C 0.178295 1.119992 2.565635
C 0.628844 2.408133 2.835681
C 0.563329 3.412050 1.861492
C 0.054900 3.113156 0.602512
N -0.848011 -0.475486 0.994258
H -5.074235 -0.443030 -2.233569
H -4.908536 -2.152797 -0.431476
H -2.939927 -2.193190 1.076877
H -3.242075 1.213555 -2.524050
H 1.195939 1.477752 -1.842759
H -1.185464 2.282837 -1.649058
H 0.216653 0.348981 3.326485
H 1.021102 2.636489 3.822532
H 0.909083 4.416531 2.084860
H 0.006168 3.879110 -0.167237
O 3.100937 2.191815 -2.245037
H 3.475970 1.367811 -1.875535
H 3.363477 2.154972 -3.177659
Cl 3.253881 -0.947615 -1.450941
O 0.533128 -0.429132 -1.611685
H 1.674546 -0.735047 -1.631701
C -0.137817 -1.690670 1.289874
O -0.701132 -2.771750 1.263364
N 1.182146 -1.531183 1.608366
H 1.738346 -2.391061 1.560564
H 1.680616 -0.729717 1.240505
H 3.460589 -2.767190 0.129405
O 3.243731 -3.401802 0.839977
H 2.941116 -4.189638 0.363238

AC-9-AL
G = -668.729527

C -3.605071 -0.073441 -0.012829
C -3.438295 -1.486708 -0.009146
C -2.180514 -2.023985 0.000054
C -1.027107 -1.178538 0.003955
C -1.191545 0.259332 -0.000928
C -2.525800 0.774968 -0.008533
C 1.278380 -1.031765 0.012458
C 1.254041 0.415495 0.007329
C -0.070165 2.540604 0.090115
C -0.015456 1.057037 0.017478
C 2.530921 -1.723255 0.010897

C 3.711478 -1.034063 -0.008641
C 3.697651 0.388683 -0.034167
C 2.518115 1.088886 -0.029322
N 0.169516 -1.783862 0.016588
H -4.608817 0.342960 -0.020702
H -4.312506 -2.131912 -0.012908
H -2.005499 -3.094950 0.004829
H -2.668147 1.845745 -0.020115
H 0.891755 3.030711 0.324920
H 2.491674 -2.807690 0.019580
H 4.660271 -1.562950 -0.012106
H 4.638988 0.930484 -0.064309
H 2.563404 2.169980 -0.071486
O -1.057192 3.240646 -0.062017

AC-9-AL 1H2O
G = -745.131200

C 3.556897 0.978064 -0.020909
C 3.975054 -0.380947 0.024374
C 3.040283 -1.379272 0.048074
C 1.644240 -1.070490 0.026101
C 1.213893 0.310042 -0.020331
C 2.226548 1.318787 -0.041992
C -0.524586 -1.869932 0.025755
C -1.089133 -0.537531 -0.023467
C -0.744633 1.931300 -0.026880
C -0.185905 0.563635 -0.032820
C -1.387492 -3.010937 0.045110
C -2.745636 -2.861167 0.007359
C -3.309396 -1.556104 -0.055957
C -2.517021 -0.436219 -0.072331
N 0.793647 -2.106882 0.053363
H 4.306844 1.764266 -0.040726
H 5.035162 -0.618110 0.039899
H 3.311340 -2.429435 0.083236
H 1.927212 2.355787 -0.081935
H -1.835278 2.011398 0.085536
H -0.910795 -3.984897 0.085758
H -3.398364 -3.729271 0.019920
H -4.389250 -1.443603 -0.096516
H -3.000165 0.530606 -0.137153
O -0.109601 2.978178 -0.122682
O -2.558014 4.433365 0.060988
H -1.614617 4.240125 -0.102182
H -2.565373 4.763592 0.971654

AC-9-AL 2H2O
G = -821.534878

C 0.152934 3.696349 -0.014683
C 1.564981 3.527195 0.034070
C 2.100506 2.268701 0.055016
C 1.247637 1.122453 0.027495
C -0.187875 1.284402 -0.020259
C -0.699045 2.619438 -0.040540
C 1.100250 -1.195842 0.025747
C -0.345411 -1.167615 -0.021431
C -2.462888 0.148183 -0.024988
C -0.983540 0.105276 -0.032766
C 1.801458 -2.442508 0.046290
C 1.110033 -3.621335 0.011563
C -0.311954 -3.608781 -0.051166
C -1.016862 -2.431871 -0.068833
N 1.841761 -0.079580 0.050785
H -0.260550 4.700995 -0.032268
H 2.211474 4.399856 0.055769
H 3.170771 2.089716 0.095806
H -1.768053 2.767160 -0.083280
H -2.977748 -0.811926 0.121319
H 2.885944 -2.398064 0.089549
H 1.638863 -4.569835 0.027391
H -0.851268 -4.551042 -0.089736
H -2.096471 -2.481968 -0.133462
O -3.159530 1.150132 -0.153289
O -5.467354 -0.524803 0.065456
H -4.932331 0.272074 -0.112658
H -5.800840 -0.377420 0.962972
O 4.726246 -0.553525 0.078797
H 4.895049 -0.564610 -0.875222
H 3.776596 -0.316579 0.137532

CBZ-AC-TS-AC-9-AL
G = -1374.500523

C -4.010770 -0.211472 0.110330
C -3.652137 -1.516365 -0.246192
C -2.329074 -1.840335 -0.520243
C -1.340998 -0.847390 -0.432406

C -1.688283 0.478749 -0.060182
C -3.037482 0.774221 0.207576
C 0.850417 -0.105941 -1.183779
C 0.532116 1.234975 -0.873006
C -0.783655 2.855809 0.572521
C -0.563081 1.433619 0.114997
C 1.940919 -0.399684 -2.017883
C 2.700156 0.632973 -2.549091
C 2.375477 1.968468 -2.275128
C 1.303303 2.262827 -1.444002
N 0.021377 -1.125432 -0.684841
H -5.049156 0.035936 0.310312
H -4.412580 -2.288018 -0.328096
H -2.048883 -2.840311 -0.820939
H -3.302084 1.784075 0.488720
H 0.163138 3.408842 0.732501
H 0.054583 1.028118 1.148606
H 2.169921 -1.431265 -2.261169
H 3.535773 0.398893 -3.202145
H 2.956612 2.773496 -2.714180
H 1.055848 3.300521 -1.248370
O -1.846679 3.382125 0.824293
C 0.564058 -2.443560 -0.415142
O 0.069497 -3.465274 -0.852676
N 1.675741 -2.388948 0.363985
H 1.851671 -1.596269 0.973503
H 2.058785 -3.280891 0.646246
O 0.809800 0.502357 2.105686
H 0.135495 0.338548 2.795198
Cl 2.324960 -0.355650 3.245715

CBZ-AC-TS-AC-9-AL 1H2O
G = -1450.910266

C -2.082711 3.385810 -0.029325
C -3.006686 2.542429 0.604098
C -2.791058 1.175677 0.652558
C -1.634594 0.625555 0.065288
C -0.692415 1.464330 -0.582963
C -0.943164 2.849694 -0.609791
C -0.489147 -1.377231 -0.715916
C 0.491954 -0.600846 -1.381215
C 1.445182 1.642908 -2.041097
C 0.581602 0.856583 -1.056926
C -0.545270 -2.770975 -0.914542
C 0.358844 -3.386980 -1.763012
C 1.328754 -2.631715 -2.437288
C 1.389240 -1.260245 -2.242638
N -1.400616 -0.747582 0.125285
H -2.257609 4.456536 -0.070612
H -3.905817 2.955392 1.052330
H -3.524199 0.522942 1.111264
H -0.239549 3.502169 -1.108847
H 2.497537 1.299053 -2.077917
H 1.346902 0.860541 -0.105287
H -1.322156 -3.351117 -0.430123
H 0.300092 -4.460706 -1.915507
H 2.029867 -3.114517 -3.110737
H 2.147827 -0.693979 -2.770271
O 1.077038 2.574815 -2.718098
C -2.247941 -1.580937 1.003739
O -3.332991 -1.989444 0.640194
N -1.645436 -1.795257 2.183220
H -0.736626 -1.371993 2.429151
H -2.152972 -2.339536 2.867739
O 2.386378 0.813867 0.884367
H 2.359019 1.749513 1.170397
Cl 3.975156 0.384091 2.168967
O 0.799682 -0.553521 2.843894
H 1.508303 -1.058701 3.270073
H 1.277706 -0.055352 2.147695

CBZ-AC-TS-AC-9-AL 2H2O
G = -1527.316626

C -2.892314 2.544689 0.554253
C -2.138571 3.241151 -0.399316
C -0.852446 2.833212 -0.721166
C -0.294455 1.699215 -0.099046
C -1.051797 0.974976 0.859449
C -2.349197 1.426409 1.175550
C 1.705521 0.431584 0.469321
C 0.994813 -0.331601 1.425415
C -1.193341 -1.097153 2.445468
C -0.493429 -0.310904 1.354897
C 3.112654 0.411182 0.460901
C 3.805903 -0.366287 1.376351
C 3.115010 -1.121025 2.332831
C 1.727667 -1.096079 2.354462
N 0.994865 1.240912 -0.428590

H -3.889240 2.881880 0.823023
H -2.549300 4.122806 -0.883490
H -0.259406 3.394269 -1.429350
H -2.916576 0.888397 1.922585
H -0.806829 -2.129750 2.548960
H -0.704824 -1.130920 0.412029
H 3.654746 1.020737 -0.252500
H 4.891815 -0.367199 1.359575
H 3.657837 -1.714305 3.062020
H 1.207155 -1.668162 3.114011
O -2.114942 -0.718576 3.134723
C 1.648634 1.689831 -1.660034
O 1.785256 2.870681 -1.927891

N 2.044998 0.657729 -2.427301
H 1.867631 -0.333994 -2.206130
H 2.546310 0.893393 -3.272499
O -1.136102 -1.995989 -0.455626
H -2.068841 -1.642302 -0.532723
Cl -1.387011 -3.266026 -2.066000
O 1.689004 -2.090714 -1.878512
H 1.779666 -2.287781 -0.933972
H 0.800560 -2.433441 -2.098172
O -3.579632 -0.821369 -0.827255
H -3.674552 -0.919576 -1.787969
H -3.452593 0.130442 -0.671699

Structures from Table S1.

vinil dioxirane
G = -268.126872

C 1.673813 -0.685096 0.025513
C 1.674340 0.684940 0.024375
H 1.531530 -1.250976 0.940358
H 1.532308 1.252455 0.938245
O -0.163438 -0.000348 -0.423164
O -2.036452 -0.000420 -0.398983
C -1.185725 0.000752 0.611955
H -1.117991 0.913725 1.235570
H -1.117882 -0.910815 1.237619
H 1.898703 1.248479 -0.873892
H 1.897890 -1.250297 -0.871783

---
vinil dioxirane 1H2O
G = -344.531125

C -1.447038 1.089254 0.041818
C -2.382869 0.095919 0.019007
H -0.962907 1.410282 0.957875
H -2.641310 -0.462391 0.913754
O -0.307390 -0.467316 -0.455495
O 1.304843 -1.310240 -0.389359
C 0.397282 -1.137661 0.590055
H -0.123508 -2.042915 0.940133
H 0.670415 -0.461053 1.414192
H -2.901049 -0.171458 -0.895540
H -1.236838 1.688282 -0.836798
H 1.825352 0.592771 -0.355422
O 1.897117 1.483072 0.043478
H 2.809032 1.517276 0.367531

---
vinil HOCl
G = -614.466251

C -1.597286 0.716703 0.036236
C -2.389721 -0.432660 -0.037488
H -1.523092 1.260613 0.974972
H -2.706142 -0.957810 0.858694
O -0.173139 -0.178323 -0.077440
H -0.137993 -0.687297 0.757376
H -1.481933 1.338379 -0.846430
H -2.621349 -0.885729 -0.994284
Cl 1.986921 -0.020343 -0.007253

---
vinil HOCl 1H2O
G = -690.878074

C 1.932777 -0.527626 0.673960
C 2.408688 -0.060151 -0.532140
H 1.811830 0.141681 1.520135
H 2.513520 1.003754 -0.720606
O 0.285790 -0.485235 -0.142102
H 0.137134 0.503179 -0.116651
H 1.959299 -1.585758 0.908359
H 2.643738 -0.739841 -1.343028
Cl -1.822334 -0.758436 -0.056963
O -0.537139 2.112508 0.159237
H -0.786557 2.447454 -0.717180
H -1.337295 1.631427 0.449344

---
vinil oxaziridine
G = -248.245654

C 1.312311 -0.610921 0.365210
C 2.026188 0.432410 -0.230046
H 1.086908 -0.560307 1.429761
H 2.057406 1.418259 0.221968
O -0.120752 -0.191404 -0.377626
C -1.139818 0.524090 0.388414
H -1.115146 1.594303 0.133217
H -0.986946 0.375753 1.465714
H 2.447217 0.323376 -1.223088
H 1.458066 -1.622288 -0.004241
N -2.116654 -0.306434 -0.152470
H -2.357000 0.073704 -1.076507

---
vinil oxaziridine 1H2O
G = -324.648600

C 1.874426 -0.137967 -0.477603
C 2.062589 0.988287 0.335325
H 2.217875 -1.107469 -0.118365
H 2.178408 0.887605 1.409107

O 0.243477 -0.179656 -0.248859
C -0.367540 -1.243461 0.599687
H -0.606579 -0.811396 1.581242
H 0.337089 -2.079542 0.688306
H 1.957915 1.990684 -0.064907
H 1.958048 -0.020523 -1.555014
N -1.365642 -1.440393 -0.337689
H -2.073320 -0.714797 -0.157737
O -2.031239 1.592638 0.088841
H -2.396097 1.727924 -0.798791
H -1.128605 1.265248 -0.084332

---
vinil performic acid
G = -343.387015

C -2.189757 0.154758 -0.684388
C -2.189709 0.154540 0.684424
H -1.962014 1.051861 -1.251664
H -1.961950 1.051479 1.251933
O -0.398434 -0.507105 -0.000035
H 0.019098 0.412194 0.000064
O 1.370744 -1.064984 -0.000071
C 2.019728 0.047358 -0.000005
H 3.117000 -0.089498 -0.000031
O 1.520408 1.180846 0.000069
H -2.497802 -0.717811 -1.248340
H -2.497638 -0.718227 1.248140

---
vinil performic acid 1H2O
G = -419.793931

C 2.092798 -0.166636 0.916890
C 2.590217 -0.268015 -0.353997
H 1.781158 0.790982 1.319496
H 2.638609 0.598470 -1.005382
O 0.539920 -0.714845 -0.175975
H 0.341354 0.234992 -0.438753
O -1.184061 -1.249167 -0.532385
C -2.094512 -0.563454 0.068609
H -3.070584 -1.090541 0.017234
O -2.029040 0.530603 0.637347
H 2.119294 -1.007267 1.600638
H 2.970648 -1.206859 -0.739782
O 0.023691 1.908277 -0.365778
H -0.339306 2.265804 -1.190795
H -0.776276 1.604102 0.142650

---
vinil peroxide
G = -230.013891

C -1.028844 0.706006 0.000635
C -1.851507 -0.436790 0.046342
H -0.895750 1.299032 0.904161
H -2.050891 -0.944960 0.984110
O 0.311411 -0.174623 -0.175693
H 0.604765 -0.462191 0.710866
O 2.239502 -0.000481 0.123735
H 2.424847 -0.494994 -0.693822
H -1.030061 1.307858 -0.904358
H -2.178106 -0.919203 -0.867161

---
vinil peroxide 1H2O
G = -306.430530

C 1.640652 -0.265854 0.624000
C 2.085453 0.546893 -0.422832
H 1.376019 0.184506 1.578089
H 1.887516 1.613619 -0.426871
O 0.202517 -0.503657 -0.186552
H -0.279835 0.369652 -0.072408
O -1.565744 -1.231292 -0.018360
H -1.510171 -1.633474 -0.902110
H 2.012622 -1.282627 0.706360
H 2.530051 0.113426 -1.310781
O -1.693741 1.356274 0.003778
H -2.001084 0.403477 -0.092435
H -1.916008 1.574585 0.922217

---
vinil peroxynitrous acid
G = -359.353605

C 2.115183 -0.161171 0.674372
C 2.402880 0.421542 -0.532918
H 1.877660 0.439896 1.546774
H 2.273215 1.487614 -0.693667
O 0.404913 -0.453881 -0.127922
H 0.020438 0.456409 -0.014933

O -1.422555 -0.993221 -0.169742
O -1.637107 1.115385 0.150664
H 2.352587 -1.201853 0.862383
H 2.733073 -0.172093 -1.377806
N -2.161051 0.011648 0.000646

---
vinil peroxynitrous acid 1H2O
G = -435.757635

C -2.684265 -0.225204 -0.306913
C -2.025592 -0.350117 0.886485
H -2.776618 0.739527 -0.795479
H -1.697402 0.526127 1.435484
O -0.493550 -0.698355 -0.243687
H -0.353896 0.258324 -0.482855
O 1.295273 -1.147782 -0.636788
O 1.959495 0.381352 0.746540
H -3.092693 -1.089702 -0.818475
H -2.013126 -1.291629 1.423583
N 2.208076 -0.574161 0.016343
O -0.052181 1.995226 -0.305388
H 0.363374 2.405412 -1.079782
H 0.700671 1.679462 0.240286

Structures form Table S2/Scheme S4.

CBZ-1Cl-2OH
G = -1299.330856

C 0.212642 -1.294677 -1.490418
C -1.125982 -1.504415 -1.564326
C -2.145030 -1.105881 -0.599797
C 0.929805 -0.617859 -0.428727
C -2.011894 0.026775 0.231306
C 0.406929 0.387742 0.335192
H 0.835015 -1.761299 -2.252547
N -0.892158 0.901475 0.049761
H 0.887095 2.354758 -1.050402
C -1.100554 2.181084 -0.483053
O -2.214362 2.658423 -0.630455
N 0.062599 2.873864 -0.772932
H -0.112378 3.714731 -1.306683
C 2.369750 -1.006527 -0.194716
C 1.168020 1.004620 1.421733
C 2.319186 0.461922 1.847435
H 2.911908 0.892911 2.647976
H 0.768565 1.913038 1.860029
H 2.564078 -2.029113 -0.525359
H -1.481842 -2.129408 -2.381657
C -3.306612 -1.892542 -0.463950
H -3.428271 -2.760825 -1.106967
C -2.984612 0.328605 1.186164
C -4.117847 -0.471378 1.309445
H -4.882144 -0.216177 2.037938
C -4.280102 -1.584369 0.478163
H -5.166732 -2.206213 0.564761
H -2.860679 1.216942 1.795568
C 2.785587 -0.844663 1.272669
O 4.169893 -0.980492 1.513566
H 4.471991 -1.815585 1.123264
Cl 3.454054 0.012557 -1.314379
H 2.221417 -1.648667 1.793104

CBZ-TS-CBZ-1Cl-2OH
G = -1299.260491

C -0.366377 -1.995694 -1.174444
C -1.647927 -1.676072 -1.451155
C -2.546712 -0.792821 -0.714788
C 0.462166 -1.529956 -0.066707
C -2.108643 0.268910 0.101650
C 0.210990 -0.327207 0.657852
H 0.108006 -2.739146 -1.811338
N -0.713313 0.611135 0.187127
H 1.730093 1.384577 -0.395511
C -0.298747 1.944185 -0.151991
O -1.116753 2.826628 -0.343742
N 1.052014 2.122762 -0.225554
H 1.333011 3.036445 -0.554265
C 1.637484 -2.198891 0.240875
C 0.961332 -0.006676 1.828733
C 2.083992 -0.705400 2.152564
H 2.674404 -0.455200 3.027547
H 0.622381 0.829504 2.430846
H 1.935908 -3.050329 -0.366249
H -2.108800 -2.198390 -2.287400
C -3.932231 -1.032302 -0.799795
H -4.280462 -1.842143 -1.435745
C -3.026212 1.024385 0.836037
C -4.390970 0.761341 0.739284
H -5.094922 1.370540 1.298632
C -4.847326 -0.269206 -0.085171
H -5.910387 -0.474744 -0.170611
H -2.665016 1.843197 1.445562
C 2.608358 -1.656383 1.177884
O 3.405102 -0.628466 0.171207
H 3.815606 -1.174246 -0.529765
Cl 4.412302 1.073647 -1.193776
H 3.358280 -2.353918 1.546796

IMS-1Cl-2OH
G = -1130.842349
C 0.019228 -1.724005 -0.010663
C 1.352767 -1.890475 0.040104
C 2.390373 -0.854389 -0.030190
C -0.740840 -0.482130 -0.070029
C 2.185005 0.479128 0.375201
C -0.307338 0.710429 0.440823
H -0.589024 -2.626036 -0.023133
N 0.966883 0.910195 0.977962
C -2.149103 -0.577536 -0.535387
C -1.219572 1.849618 0.552044
C -2.389296 1.869546 -0.096594

H -3.074385 2.707973 -0.034023
H -0.917323 2.686710 1.176631
H -2.296631 -1.353112 -1.282024
H 1.724936 -2.911535 0.057504
C 3.656793 -1.202825 -0.516914
H 3.825004 -2.231237 -0.822390
C 3.221605 1.405929 0.267218
C 4.477957 1.031899 -0.211075
H 5.273215 1.767821 -0.265160
C 4.698083 -0.280879 -0.608355
H 5.668762 -0.590570 -0.980141
H 3.051920 2.432606 0.581317
C -2.745416 0.739372 -1.022707
O -4.121214 0.664290 -1.334374
H -4.581699 0.265727 -0.581131
Cl -3.258998 -1.237599 0.891525
H -2.249790 0.936510 -1.985824
H 1.068051 1.826550 1.390862

IMS-TS-IMS-1Cl-2OH
G = -1130.594212

C 0.475349 1.637582 0.991286
C 1.761886 1.791276 0.631111
C 2.716756 0.841277 0.063691
C -0.406933 0.470133 0.941292
C 2.454977 -0.523218 -0.202645
C -0.008428 -0.838183 0.501066
H -0.016124 2.524259 1.385315
N 1.234915 -1.184043 0.042496
C -1.712099 0.636134 1.368599
C -0.958708 -1.893870 0.530760
C -2.247217 -1.701863 0.964326
H -2.946114 -2.531651 0.983072
H -0.643775 -2.882838 0.204017
H -2.021635 1.619276 1.711009
H 2.176671 2.786718 0.773141
C 3.999907 1.325080 -0.241781
H 4.206363 2.372724 -0.039435
C 3.463747 -1.327981 -0.751142
C 4.726078 -0.817004 -1.042848
H 5.483272 -1.469187 -1.467444
C 5.000594 0.523807 -0.786760
H 5.977275 0.943268 -1.006518
H 3.252873 -2.376378 -0.953551
C -2.716871 -0.392041 1.315335
O -3.736378 0.007822 -0.054834
H -3.097158 0.027622 -0.791545
Cl -5.186486 0.665180 -1.656395
H -3.536875 -0.320740 2.022320
H 1.287879 -2.162182 -0.214223