Electronic Supplementary Information

Role of Conformational Properties on the Transannular Diels-Alder Reactivities of Macrocyclic Trienes with Varying Linker Lengths

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Table S1: The number of clusters obtained based on conformational differences, the number of unique conformations obtained after molecular mechanics optimization, and the number of unique conformations obtained after optimizations at M06-2X/6-311G(d,p) level**.**

(a) 552 ring system:

	TTT	**TTC**	**TCT**	**TCC**	**CCT**	**CCC**
# of clusters	479	320	885	461	370	567
# of unique structures after MM minimization	11	9	22	21	11	14
# of unique structures after optimization using M06-2X	9	6	18	17	8	9

(b) 662 ring system:

	TTT	**TTC**	**TCT**	**TCC**	**CCT**	**CCC**
# of clusters	1536	1631	1959	1883	1476	1779
# of unique structures after MM minimization	45	30	46	34	30	31
# of unique structures after optimization using M06-2X	25	19	25	23	19	16

(c) 772 ring system:

	TTT	**TTC**	**TCT**	**TCC**	**CCT**	**CCC**
# of clusters	1607	1963	1317	1476	1962	1839
# of unique structures after MM minimization	48	51	39	42	46	45
# of unique structures after optimization using M06-2X	34	29	32	30	31	31

(d) 562 ring system:

	TTT	**TTC**	**TCT**	**TCC**	**CTT**	**CTC**	**CCT**	**CCC**
# of clusters	1494	1070	1987	1724	1620	1771	1141	1514
# of unique structures after MM minimization	39	43	38	44	37	41	26	28
# of unique structures after optimization using M06-2X	28	29	26	28	24	29	21	16

(e) 572 ring system:

	TTT	TTC	TCT	TCC	CTT	CTC	CCT	CCC
# of clusters	1892	1718	1896	2177	2040	2117	1991	1489
# of unique structures after MM minimization	50	47	38	43	42	46	50	37
# of unique structures after optimization using M06-2X	39	30	32	29	30	31	35	26

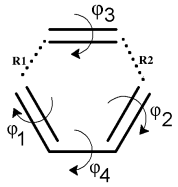
(f) 672 ring system:

	TTT	TTC	TCT	TCC	CTT	CTC	CCT	CCC
# of clusters	1894	2036	1759	1564	1754	1595	1917	2165
# of unique structures after MM minimization	57	50	44	47	46	50	48	56
# of unique structures after optimization using M06-2X	39	35	29	33	33	34	34	38

Table S2: The relative stabilities (ΔE) of the trienes with respect to the most stable triene along with the dihedral angles at the diene and the dienophile for all the trienes at the M06-2X level of theory using 6-311G(d,p) basis set.

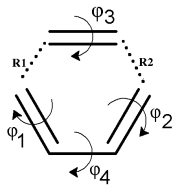
(a) 552 ring system:

	ΔE	φ_1	φ_2	φ_3	φ_4
TTT	7.7	-158.3	158.3	174.9	-19.3
TTC	10.1	149.7	148.1	-0.9	-147.4
TCT	1.2	-167.6	0.1	-179.2	154.2
TCC	0.0	170.1	1.1	-0.4	-155.3
CCT	4.9	-1.6	-1.6	177.8	144.2
CCC	2.7	4.9	4.2	2.7	-141.7



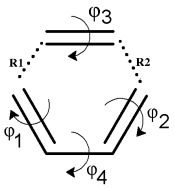
(b) 662 ring system:

	ΔE	φ_1	φ_2	φ_3	φ_4
TTT	5.2	-165.8	-165.6	172.0	168.1
TTC	3.8	-164.1	-164.1	-0.4	161.4
TCT	0.0	179.1	-1.1	-177.6	179.7
TCC	0.2	-176.3	-1.4	-0.6	171.1
CCT	2.9	5.7	5.7	175.8	-148.3
CCC	1.2	-5.6	-5.6	2.9	156.8



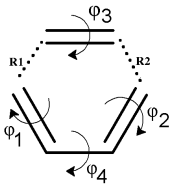
(c) 772 ring system:

	ΔE	φ_1	φ_2	φ_3	φ_4
TTT	0.8	174.4	177.0	179.9	-174.7
TTC	3.2	169.1	168.3	1.0	-169.6
TCT	0.0	177.4	1.2	179.3	-173.8
TCC	1.0	175.3	-0.3	0.6	-173.8
CCT	1.8	2.4	2.9	-179.9	-167.7
CCC	2.4	5.0	4.8	-0.2	-163.9



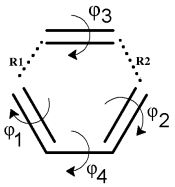
(d) 562 ring system:

	ΔE	φ_1	φ_2	φ_3	φ_4
TTT	3.4	163.5	162.3	175.0	-151.7
TTC	4.4	165.1	159.5	-3.4	-154.3
TCT	0.9	-176.7	-1.5	-178.0	-39.0
TCC	2.1	167.6	-7.0	3.4	-168.2
CTT	1.3	2.2	-176.9	-174.2	-174.4
CTC	0.0	0.1	-179.0	0.3	-178.3
CCT	3.0	1.8	3.7	174.9	-144.5
CCC	1.7	6.1	6.2	-0.3	-142.6



(e) 572 ring system:

	ΔE	φ_1	φ_2	φ_3	φ_4
TTT	2.9	169.2	166.9	175.1	-163.9
TTC	4.1	169.5	162.9	-171.6	2.6
TCT	0.2	-0.2	179.8	177.4	179.2
TCC	1.3	1.9	179.3	-2.3	172.2
CTT	0.0	176.7	1.5	-179.3	173.0
CTC	3.4	178.6	-3.0	-1.4	-173.4
CCT	3.4	0.4	-4.2	-179.6	165.2
CCC	3.3	-4.8	-6.6	0.3	156.6



(f) 672 ring system:

	ΔE	φ_1	φ_2	φ_3	φ_4
TTT	1.4	-163.3	-166.0	-177.6	158.3
TTC	2.2	177.1	174.5	-0.4	-172.2
TCT	0.8	174.9	0.0	176.4	-171.6
TCC	0.6	-175.4	-1.8	2.2	165.3
CTT	0.0	-0.6	-177.7	171.0	-179.7
CTC	1.4	-1.5	173.2	-0.8	-173.4
CCT	1.7	4.3	4.8	175.7	-163.8
CCC	2.2	-4.2	-4.3	-0.6	158.4

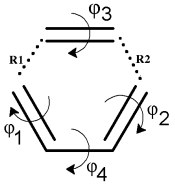


Table S3: The relative energies (kcal/mol) of the reactant, transition states, and the products corresponding to the TADA reactions of the five triene molecules obtained at the hybrid density functional M06-2X level of theory using 6-311G(d,p) basis set. The relative energies were calculated based on the most stable conformation of each of the reactants:

(a) 552 ring system:

	TTT	TTC	TCT	TCC	CCC
Reactant	0.0	0.0	0.0	0.0	0.0
TS-ebe	19.2	20.2	31.6	33.4	38.8
Product	-33.2	-31.1	-28.7	-19.7	-27.7

(b) 662 ring system:

	TTT	TTC	TCT	TCC	CCC
Reactant	0.0	0.0	0.0	0.0	0.0
TS-cbc	21.1	22.1	34.9	35.7	48.8
TS-cbb	24.3	26.7	34.1	37.5	47.1
TS-bbc	24.6	26.7	37.1	39.0	50.1
TS-bbb	28.9	30.5	40.7	41.7	49.8
Product	-40.7	-33.7	-28.8	-26.5	-27.7

(c) 772 ring system:

	TTT	TTC	TCT	TCC	CCC
Reactant	0.0	0.0	0.0	0.0	0.0
TS-cbc	37.1	39.9	52.6	51.0	63.0
TS-cbb	38.0	41.4	45.3	48.2	58.3
TS-bbc	38.0	37.5	50.2	53.7	62.1
TS-bbb	39.0	38.7	46.5	48.3	58.6
Product	-17.2	-19.6	-18	-19.8	-16.2

(d) 562 ring system:

	TTT	TTC	TCT	TCC	CTT	CTC	CCC
Reactant	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS-bbe	25.8	24.5	26.5	34.0	31.1	38.0	45.1
TS-cbe	24.2	20.1	30.1	29.8	33.3	35.9	43.0
Product	-28.8	-34.8	-33.6	-35.2	-33.7	-21.3	-30.8

(e) 572 ring system:

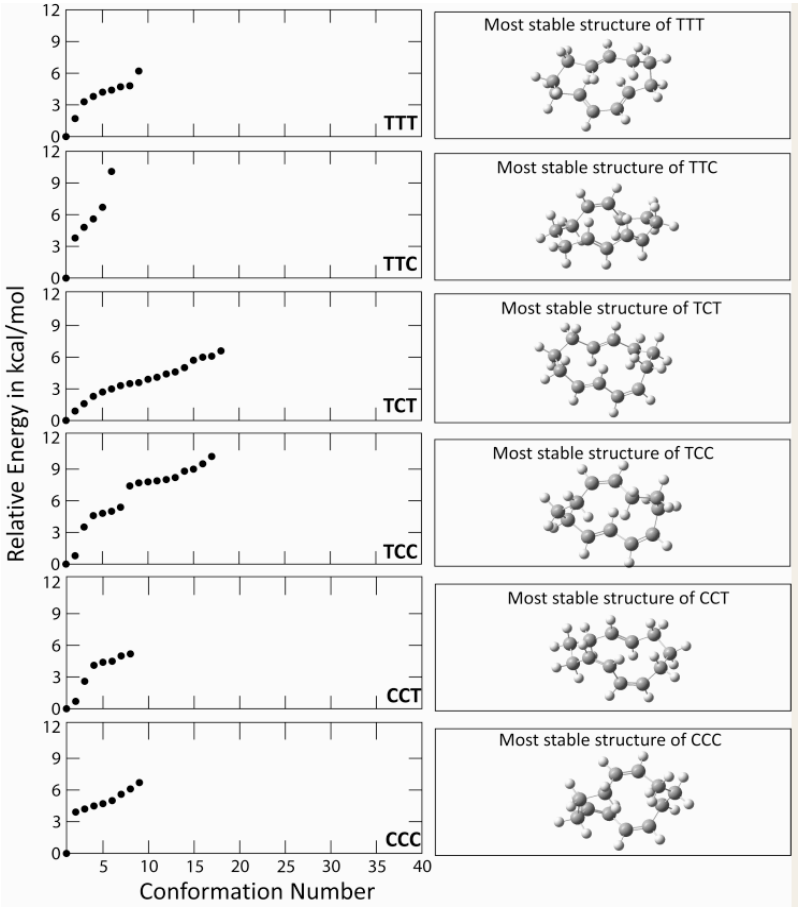
	TTT	TTC	TCT	TCC	CTT	CTC	CCC
Reactant	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS-bbe	33.3	30.4	41.2	40.0	35.3	40.2	49.8
TS-cbe	34.1	27.7	42.0	43.0	34.3	39.5	53.3
Product	-22.3	-23.7	-22.7	-21.6	-22.3	-17.5	-22.7

(f) 672 ring system:

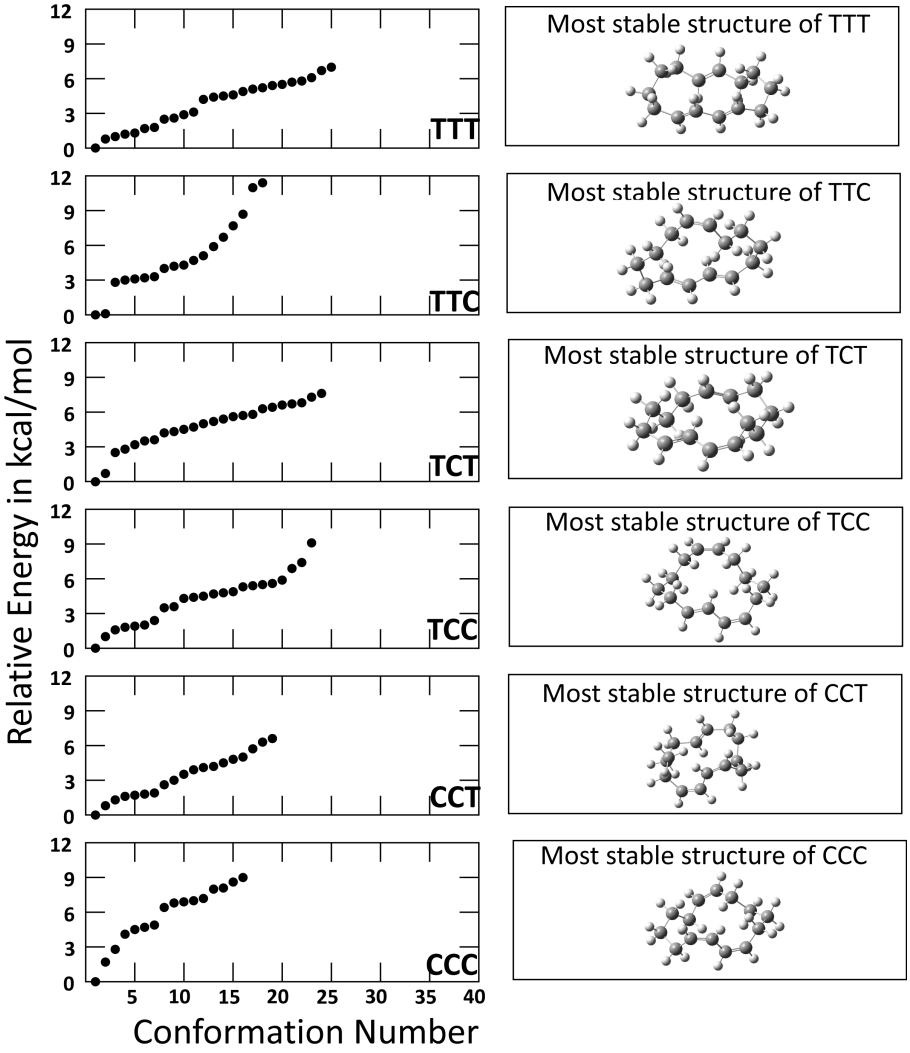
	TTT	TTC	TCT	TCC	CTT	CTC	CCC
Reactant	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS-cbc	29.7	31.2	39.3	40.6	41.9	38.9	53.0
TS-cbb	32.6	30.5	38.2	44.1	44.3	42.5	55.7
TS-bbc	30.1	31.9	41.3	44.0	39.5	38.4	51.4
TS-bbb	33.1	31.7	41.3	43.5	43.0	42.3	51.1
Product	-25.9	-23.8	-24.5	-19.8	-19.5	-20.3	-23.3

Figure S1: The energies of all the unique conformations of the reactants obtained using the M06-2X/6-311G(d,p) level of theory. The most stable conformation of each ofthe six isomers are depicted.

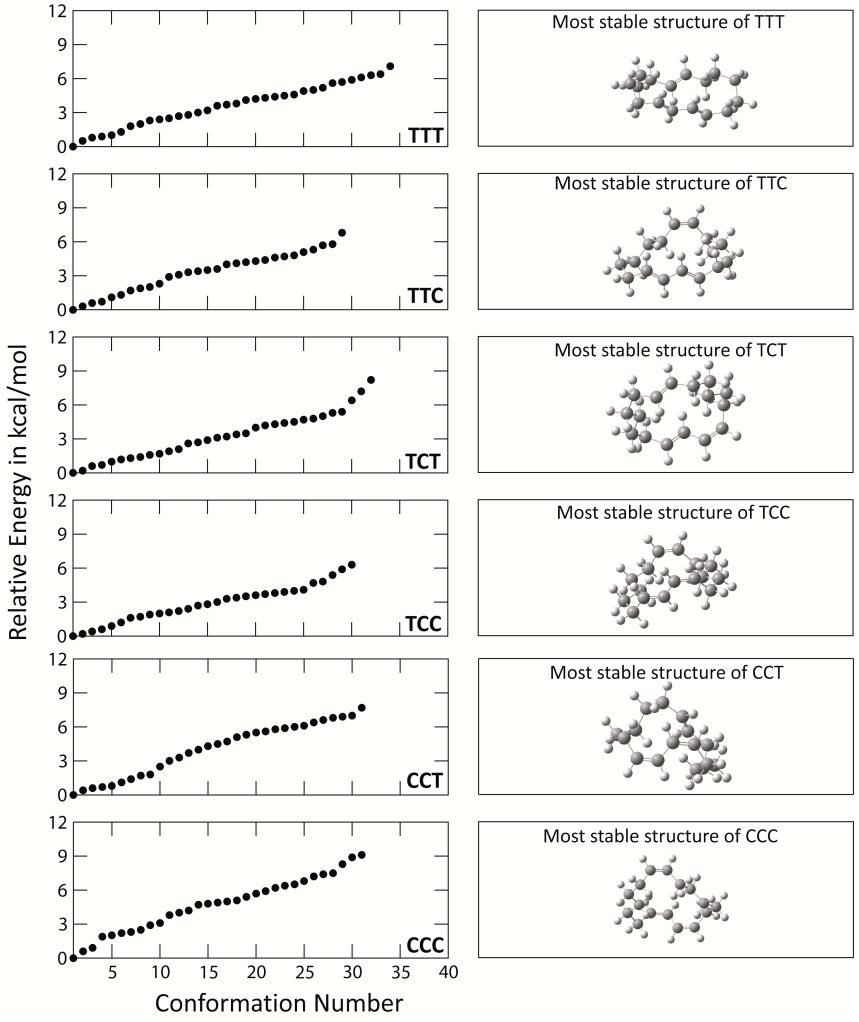
(a) 552 ring system:



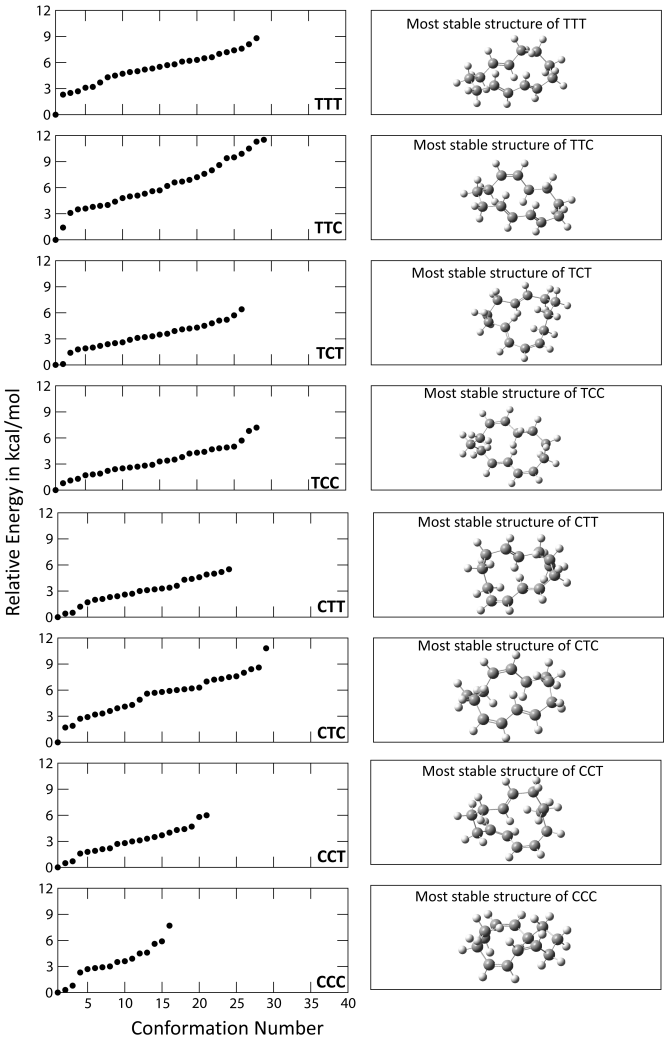
(b) 662 ring system:



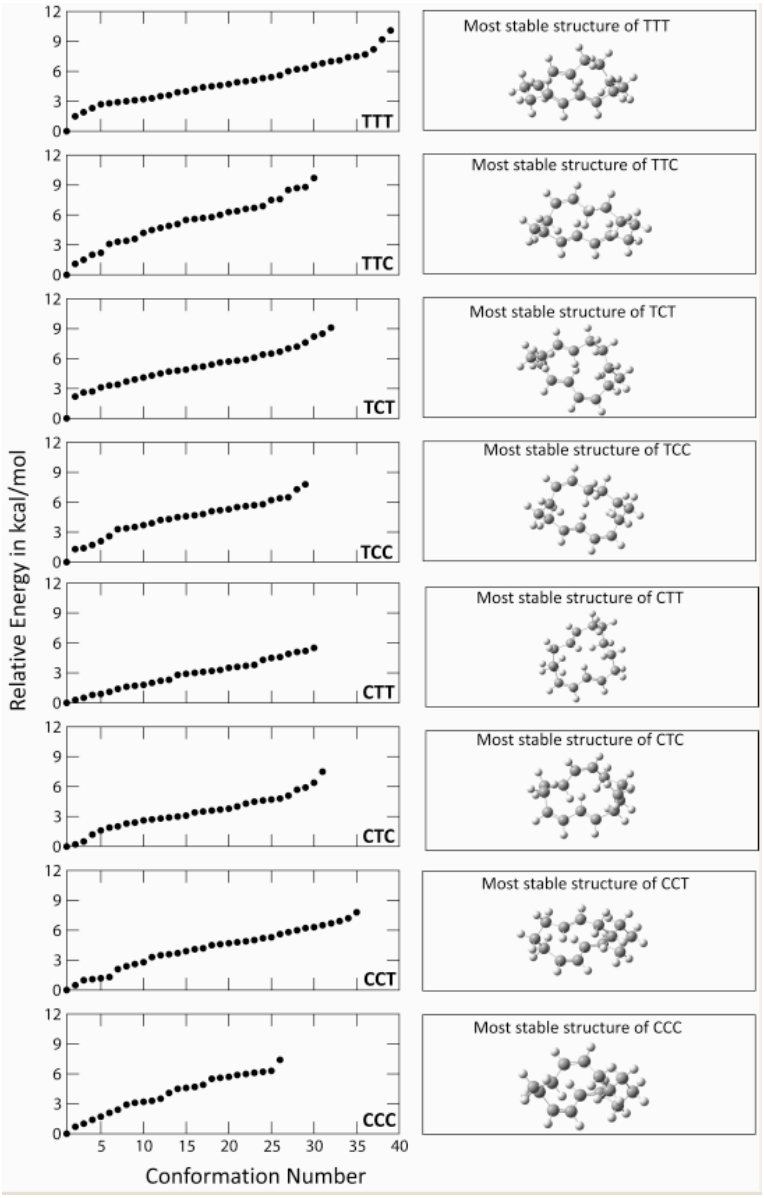
(c) 772 ring system:



(d) 562 ring system



(e) 572 ring system:



(f) 672 ring system:

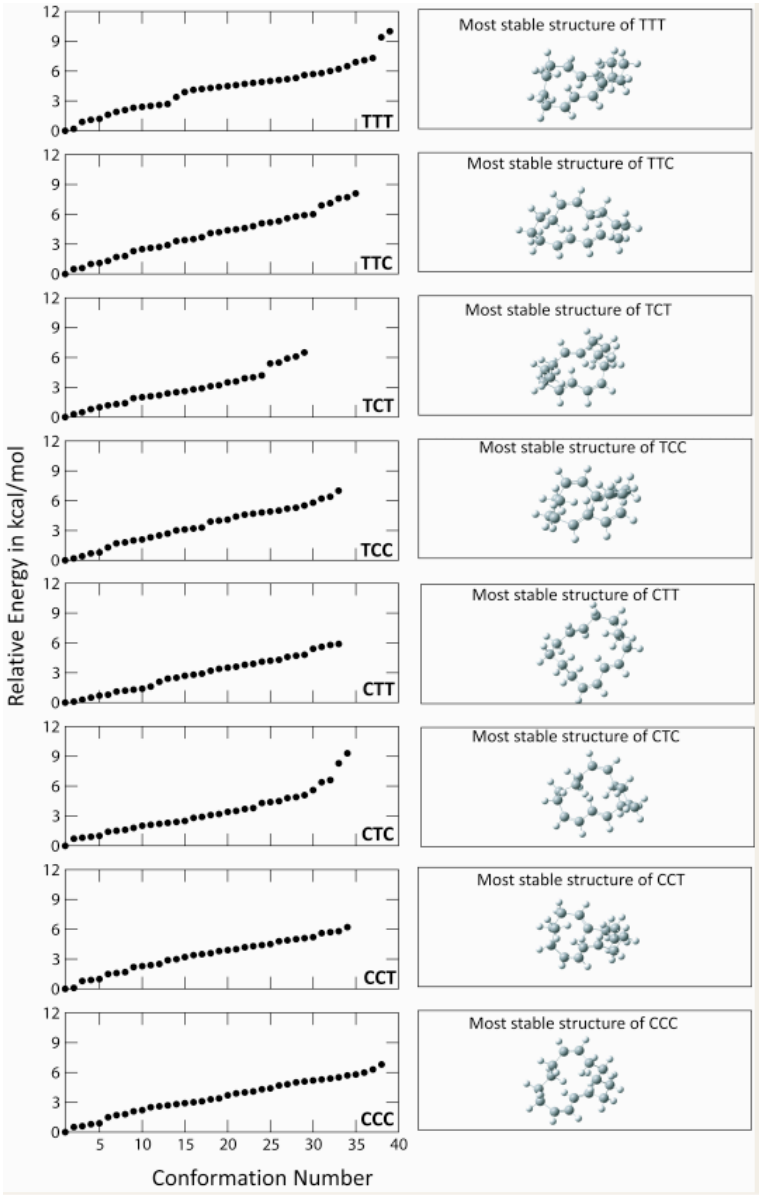


Figure S2: Energy profile diagrams of the macrocyclic trienes undergoing TADA reactions yielding respective tricycles at M06-2X/6-311G(d,p) level of theory. The most stable transition state among the four possibilities in each reaction is depicted here.

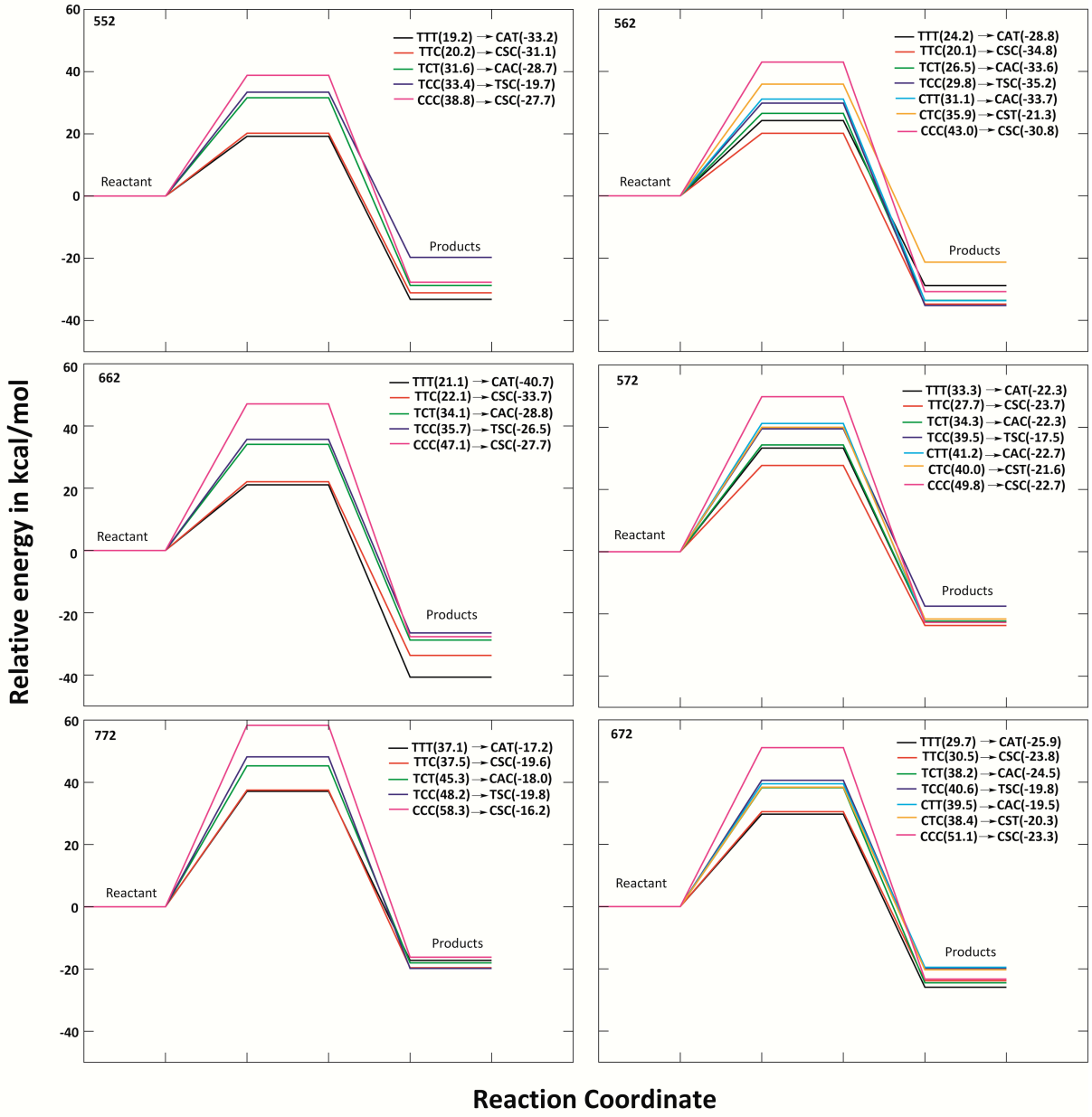
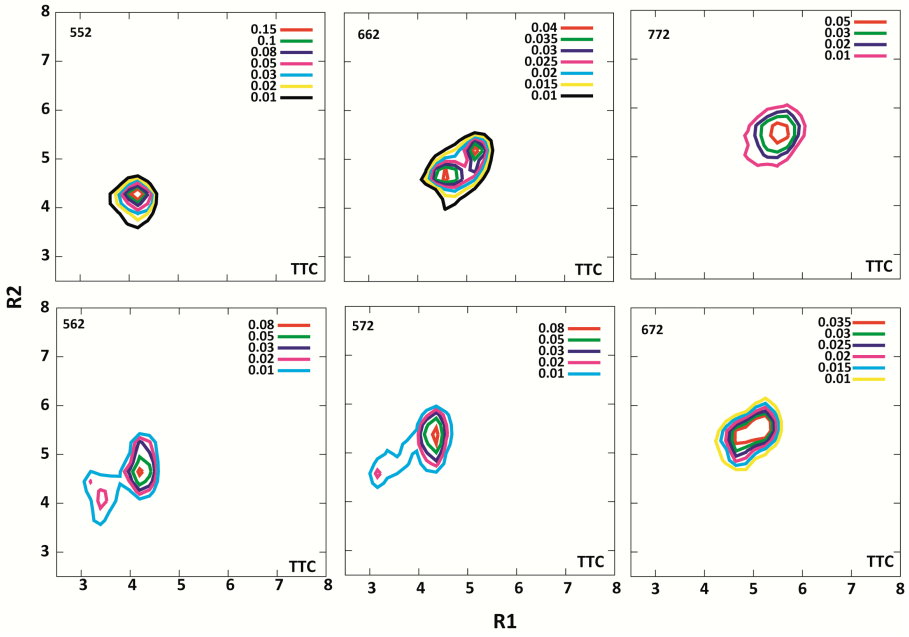
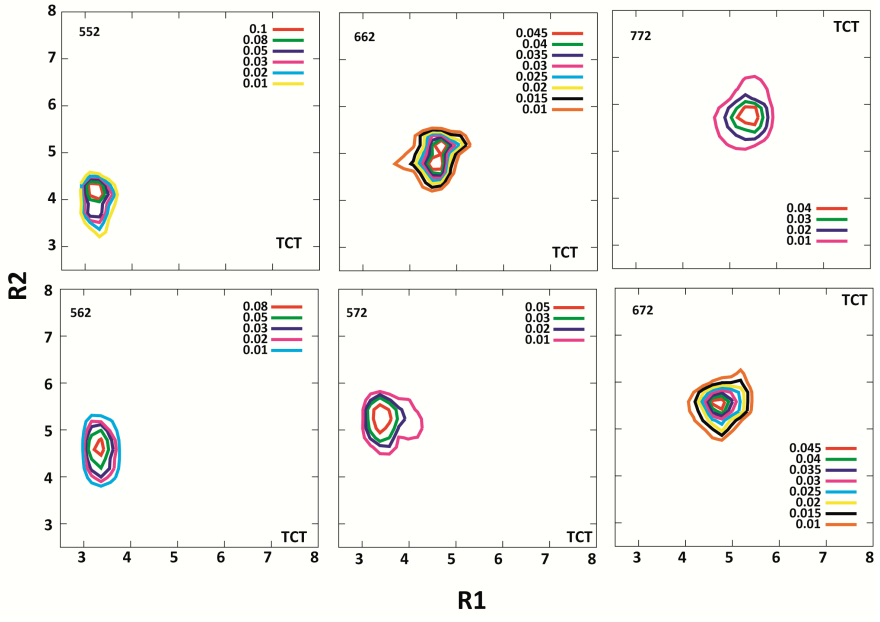


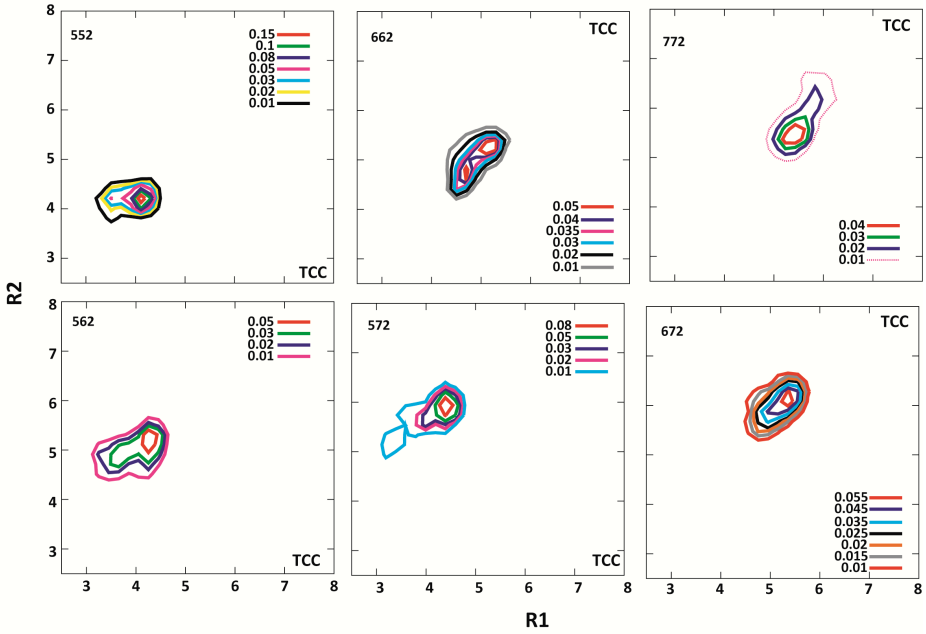
Figure S3: (a) Probability contours with respect to the distances, R1 & R2 of the TTC triene molecules obtained using ReMD simulations.



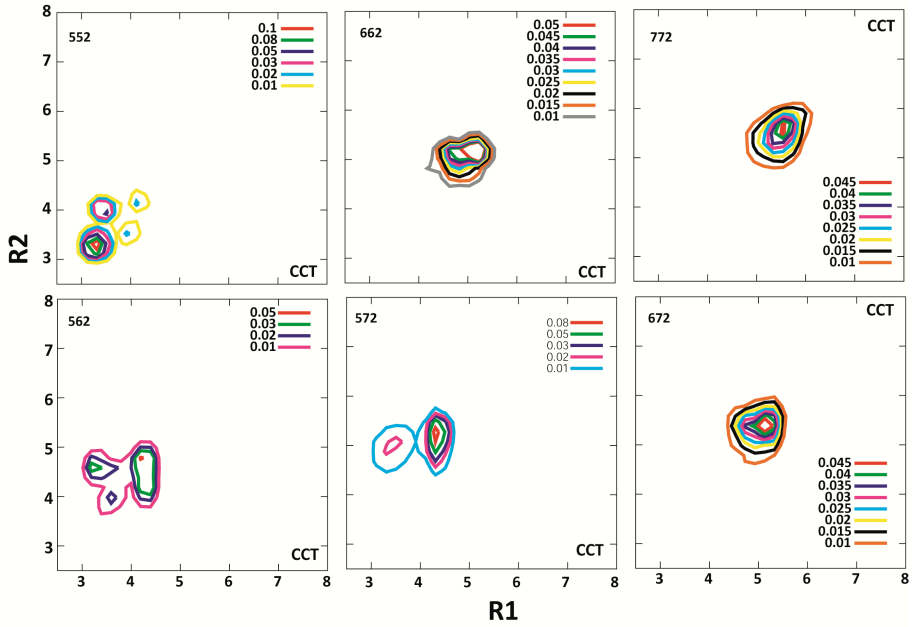
(b) Probability contours with respect to the distances, R1 & R2 of the TCT triene molecules obtained using ReMD simulations.



(c) Probability contours with respect to the distances, R1 & R2 of the TCC triene molecules obtained using ReMD simulations.



(d) Probability contours with respect to the distances, R1 & R2 of the CCT triene molecules obtained using ReMD simulations.



(e) Probability contours with respect to the distances, R1 & R2 of the CCC triene molecules obtained using ReMD simulations.

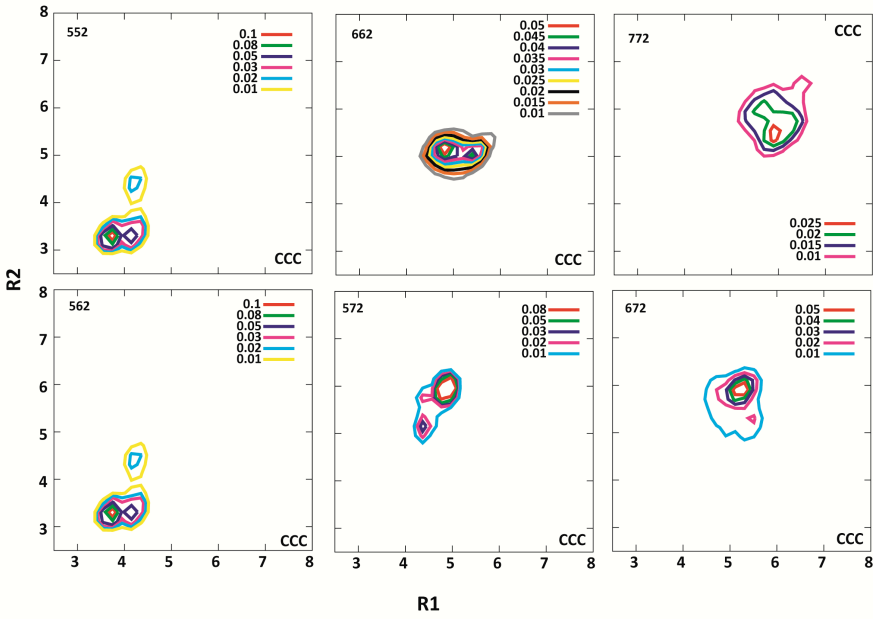
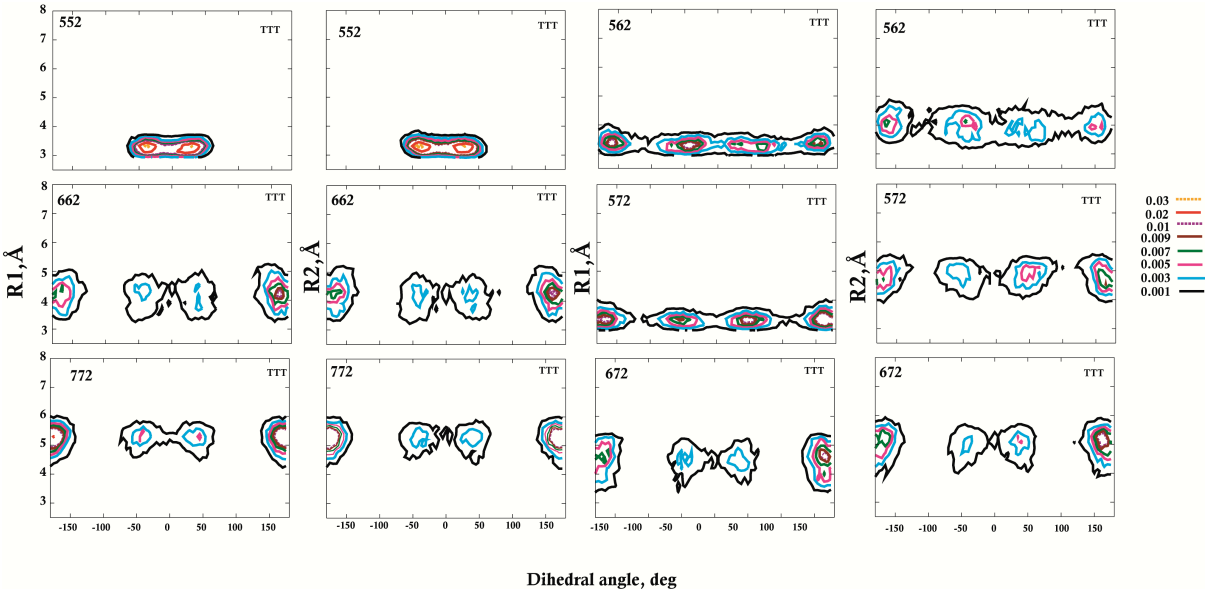
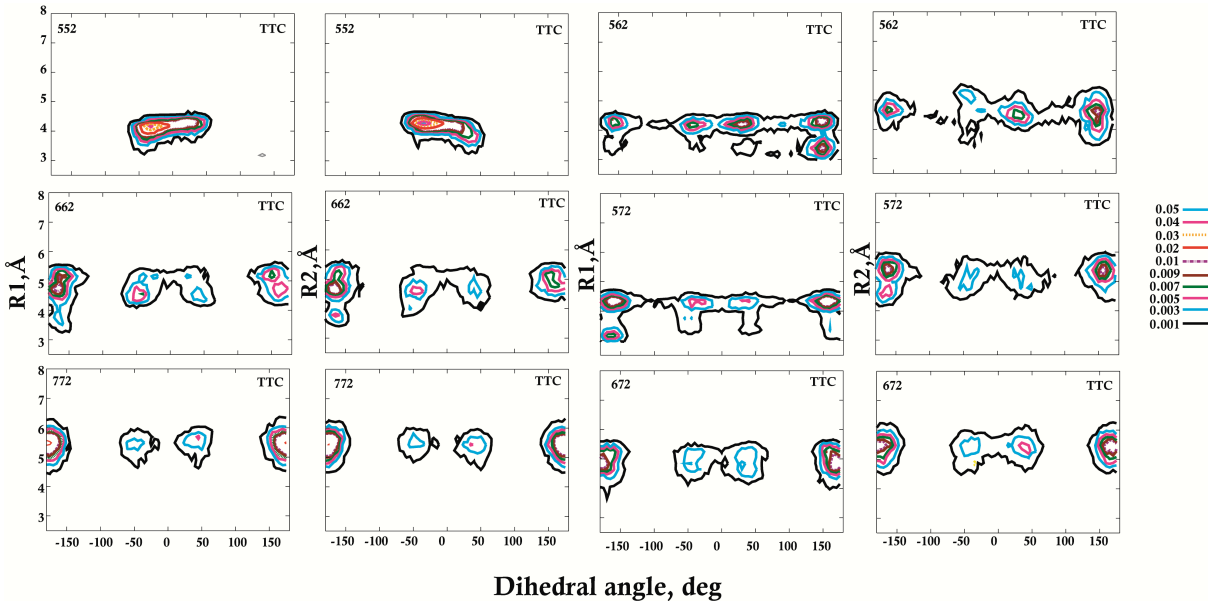


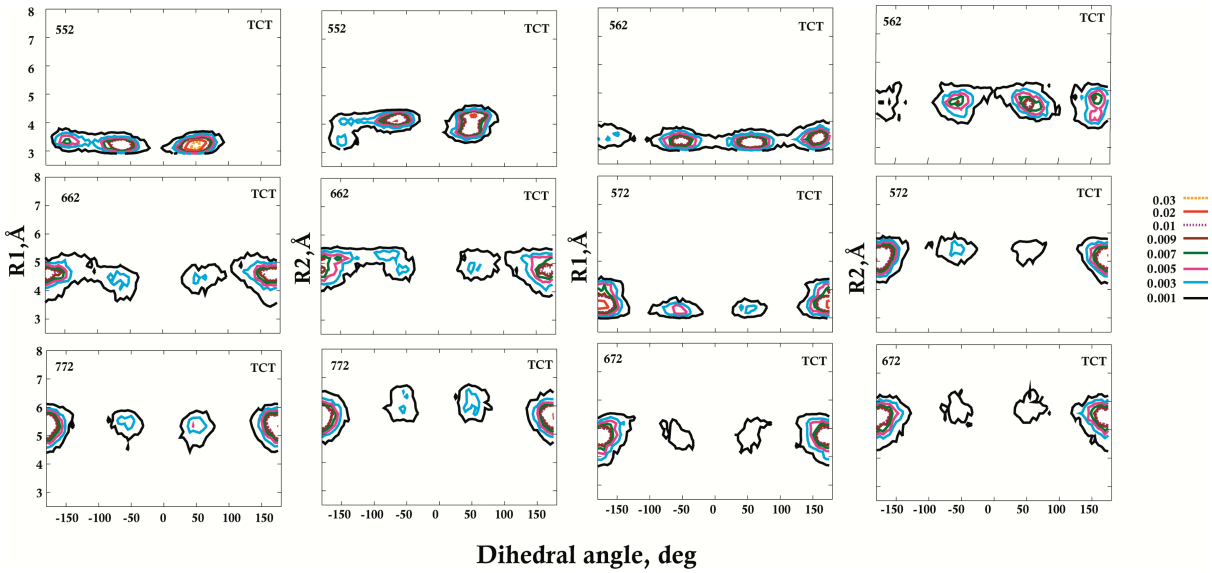
Figure S4: (a) Probability contours corresponding to the diene dihedral angle, φ_4 and distances R1 & R2 between reactive sites for the TTT triene of all the ring systems:



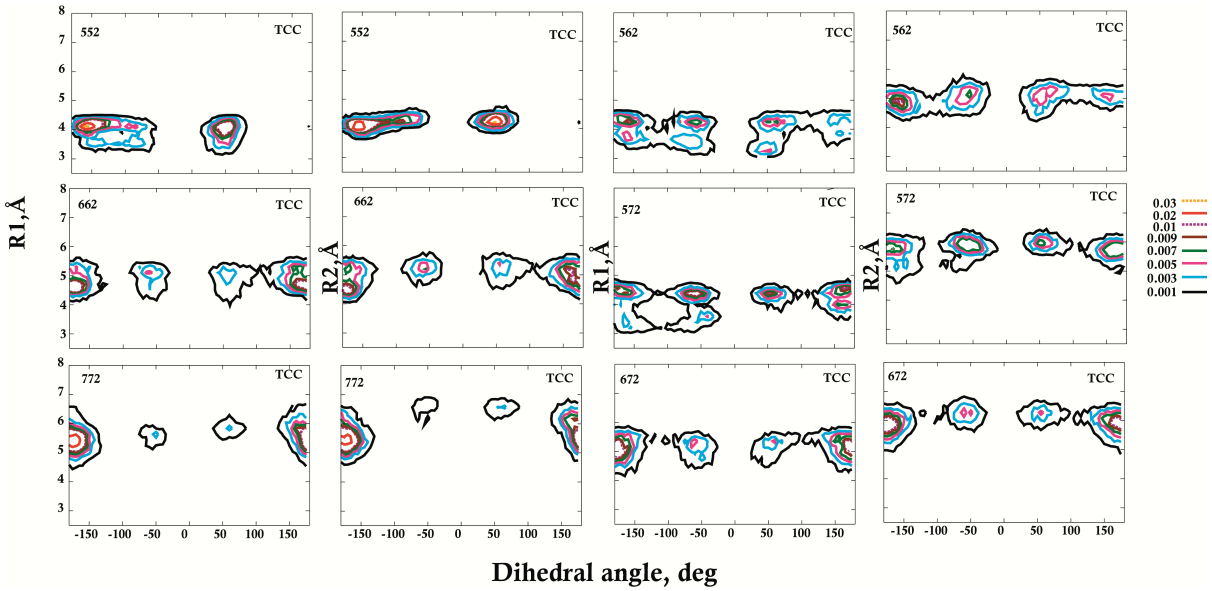
(b) Probability contours corresponding to the diene dihedral angle, φ_4 and distances R1 & R2 between reactive sites for the TTC triene of all the ring systems:



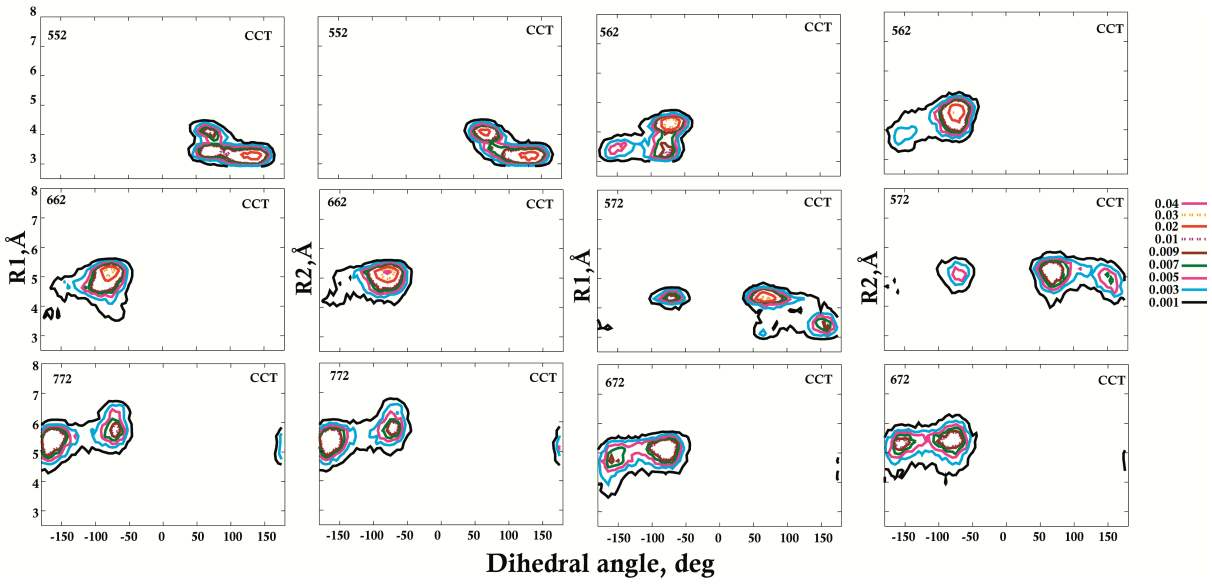
(c) Probability contours corresponding to the diene dihedral angle, φ_4 and distances R1 & R2 between reactive sites for the TCT triene of all the ring systems:



(d) Probability contours corresponding to the diene dihedral angle, φ_4 and distances R1 & R2 between reactive sites for the TCC triene of all the ring systems:



(g) Probability contours corresponding to the diene dihedral angle, φ_4 and distances R1 & R2 between reactive sites for the CCT triene of all the ring systems:



(h) Probability contours corresponding to the diene dihedral angle, φ_4 and distances R1 & R2 between reactive sites for the CCC triene of all the ring systems:

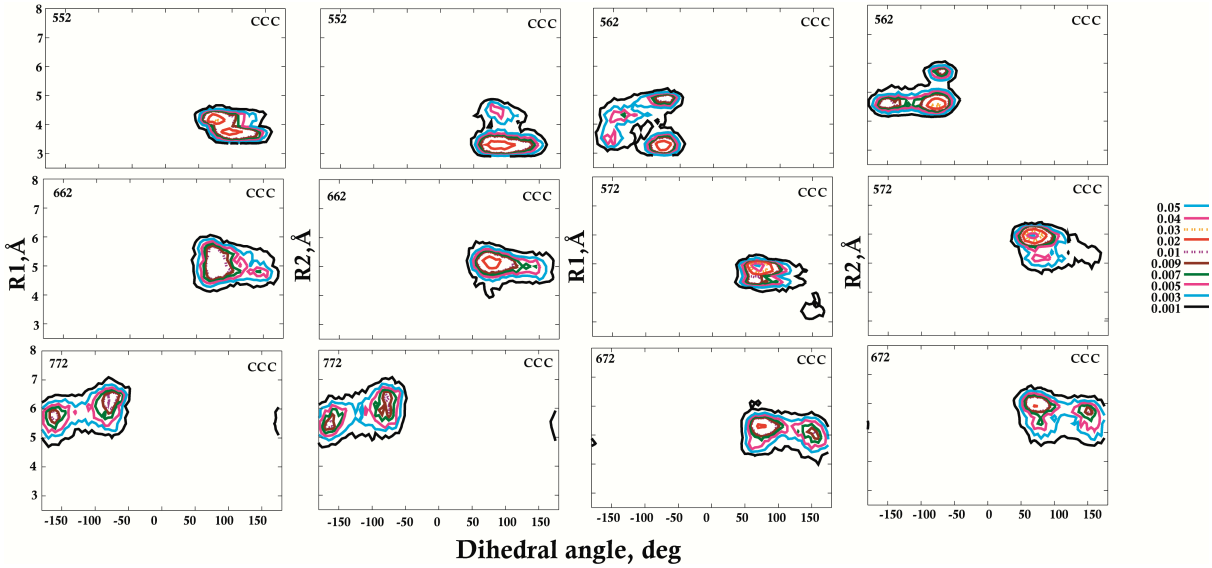
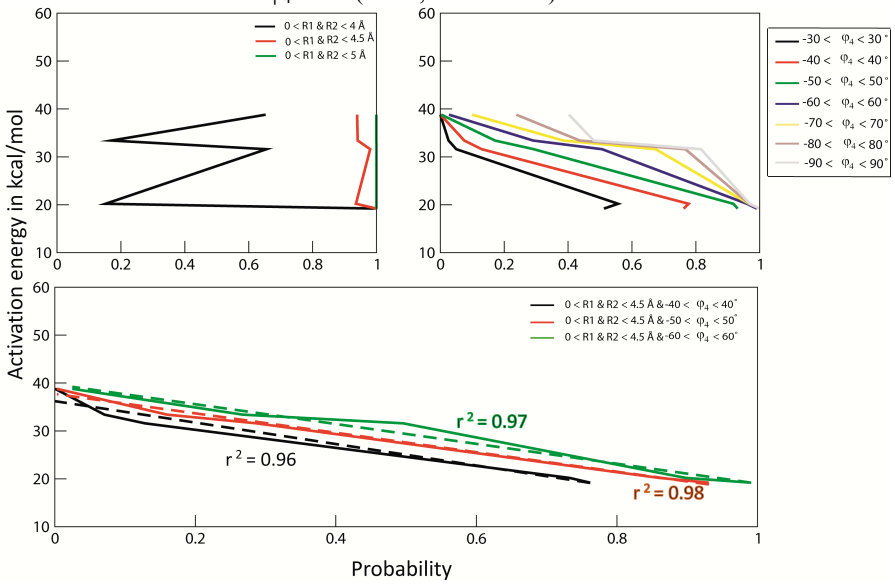
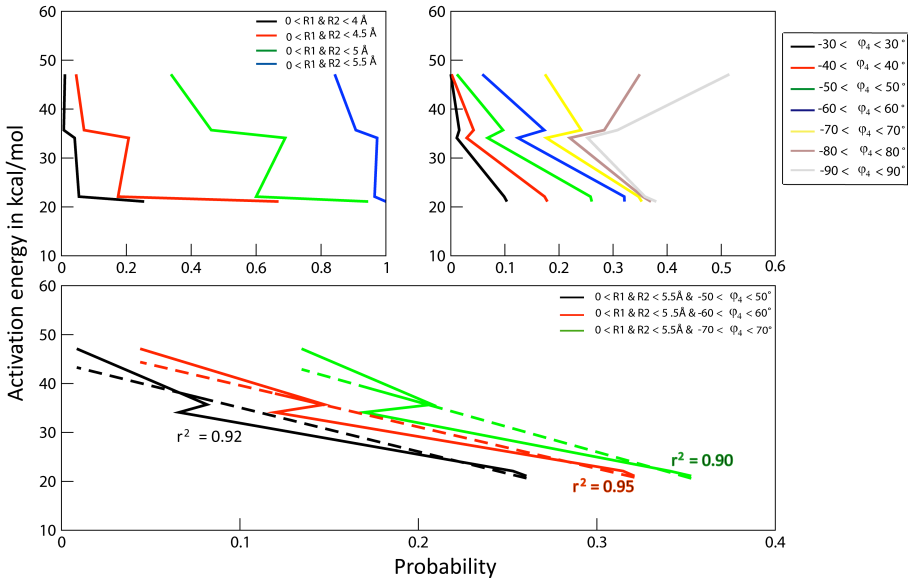


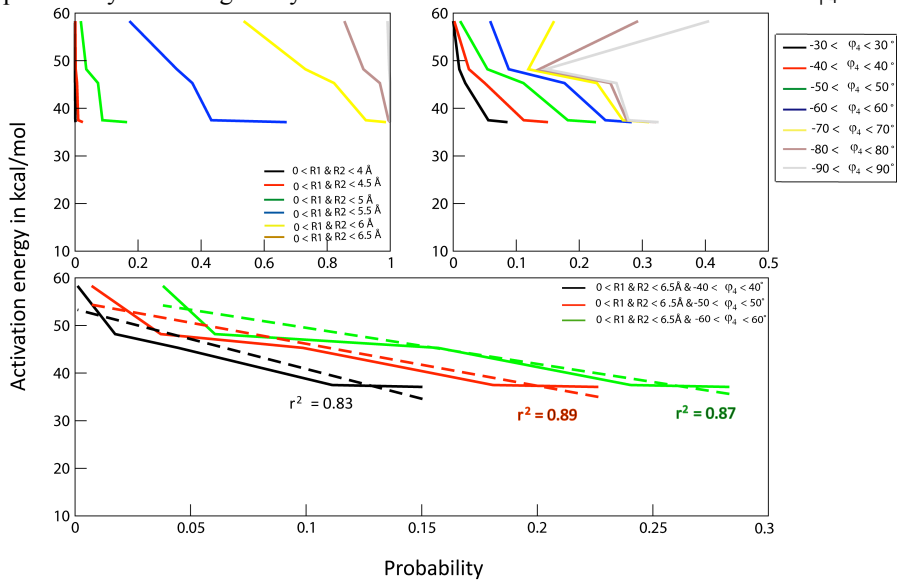
Figure S5: (a) Transition state energy barrier for 552 ring system versus (a) probability of finding the system where the distances R1 and R2 are <4 Å, < 4.5 Å, < 5 Å; (b) Probability of finding the system where the diene dihedral angles satisfies $-x < \varphi_4 < +x$ (x=30, 40, 50, 60, 70, 80, 90°); (c) probability of finding the system where R1 & R2 < 5.5Å and where $-x < \varphi_4 < +x$ (x=40, 50 and 60°).



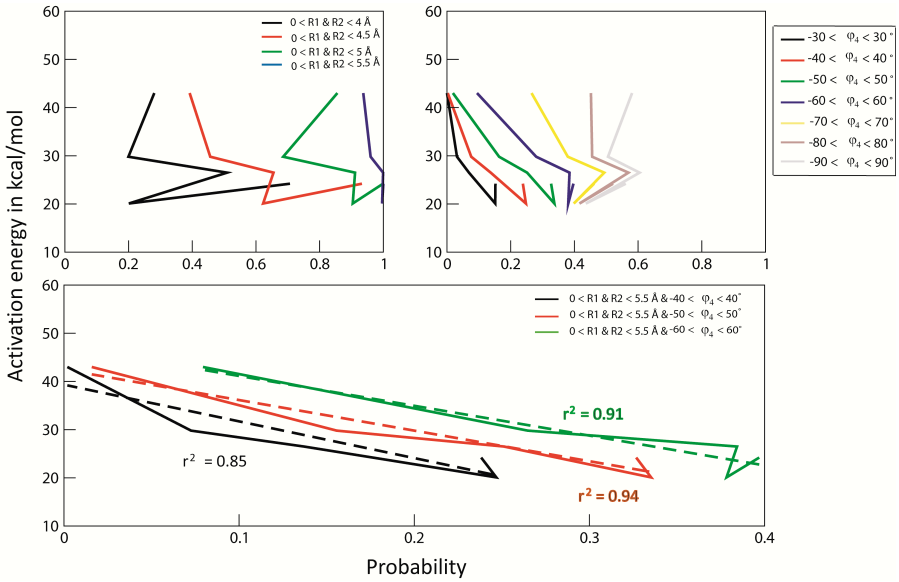
(b) Transition state energy barrier for 662 ring system versus (a) probability of finding the system where the distances R1 and R2 are <4 Å, < 4.5 Å, < 5 Å, < 5.5 Å, ; (b) Probability of finding the system where the diene dihedral angles satisfies $-x < \varphi_4 < +x$ (x=30, 40, 50, 60, 70, 80, 90°); (c) probability of finding the system where R1 & R2 < 5.5Å and where $-x < \varphi_4 < +x$ (x=50, 60 and 70°).



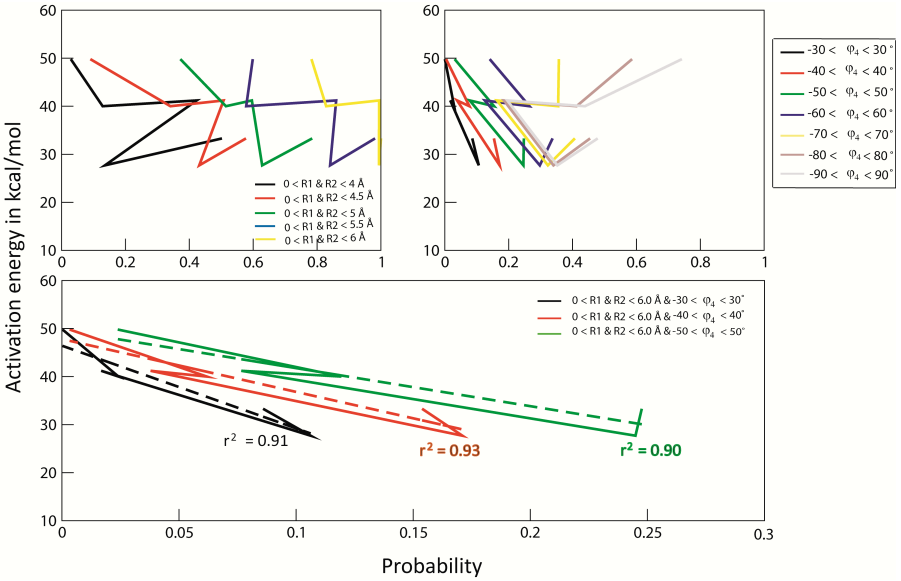
(c) Transition state energy barrier for 772 ring system versus (a) probability of finding the system where the distances R1 and R2 are <4 Å, < 4.5 Å, < 5 Å, < 5.5 Å, < 6 Å, < 6.5 Å; (b) Probability of finding the system where the diene dihedral angles satisfies $-x < \varphi_4 < +x$ (x=30, 40, 50, 60, 70, 80, 90°); (c) probability of finding the system where R1 & R2 < 5.5Å AND where $-x < \varphi_4 < +x$ (x=40, 50 and 60°).



(d) Transition state energy barrier for 562 ring system versus (a) probability of finding the system where the distances R1 and R2 are <4 Å, < 4.5 Å, < 5 Å, < 5.5 Å; (b) Probability of finding the system where the diene dihedral angles satisfies $-x < \varphi_4 < +x$ (x=30, 40, 50, 60, 70, 80, 90°); (c) probability of finding the system where R1 & R2 < 5.5Å AND where $-x < \varphi_4 < +x$ (x=40, 50 and 60°).



(e) Transition state energy barrier for 572 ring system versus (a) probability of finding the system where the distances R1 and R2 are <4 Å, < 4.5 Å, < 5 Å, < 5.5 Å, < 6 Å; (b) Probability of finding the system where the diene dihedral angles satisfies $-x < \varphi_4 < +x$ (x=30, 40, 50, 60, 70, 80, 90°); (c) probability of finding the system where R1 & R2 < 5.5Å AND where $-x < \varphi_4 < +x$ (x=30, 40 and 50°).



(f) Transition state energy barrier for 672 ring system versus (a) probability of finding the system where the distances R1 and R2 are <4 Å, < 4.5 Å, < 5 Å, < 5.5 Å, < 6 Å, < 6.5 Å; (b) Probability of finding the system where the diene dihedral angles satisfies $-x < \varphi_4 < +x$ (x=30, 40, 50, 60, 70, 80, 90°); (c) probability of finding the system where R1 & R2 < 5.5Å AND where $-x < \varphi_4 < +x$ (x=50, 60 and 70°).

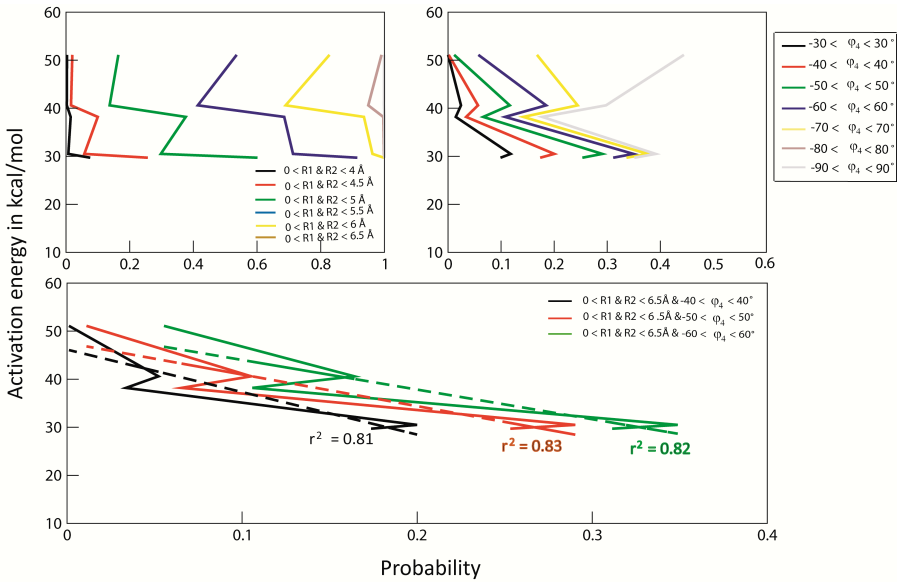


Figure S6: Transition state energy barrier for trienes of all the ring system versus probability of finding the system where R1 & R2 < 6.0 Å and where $-x < \varphi_4 < +x$ (x=30, 40 and 50°).

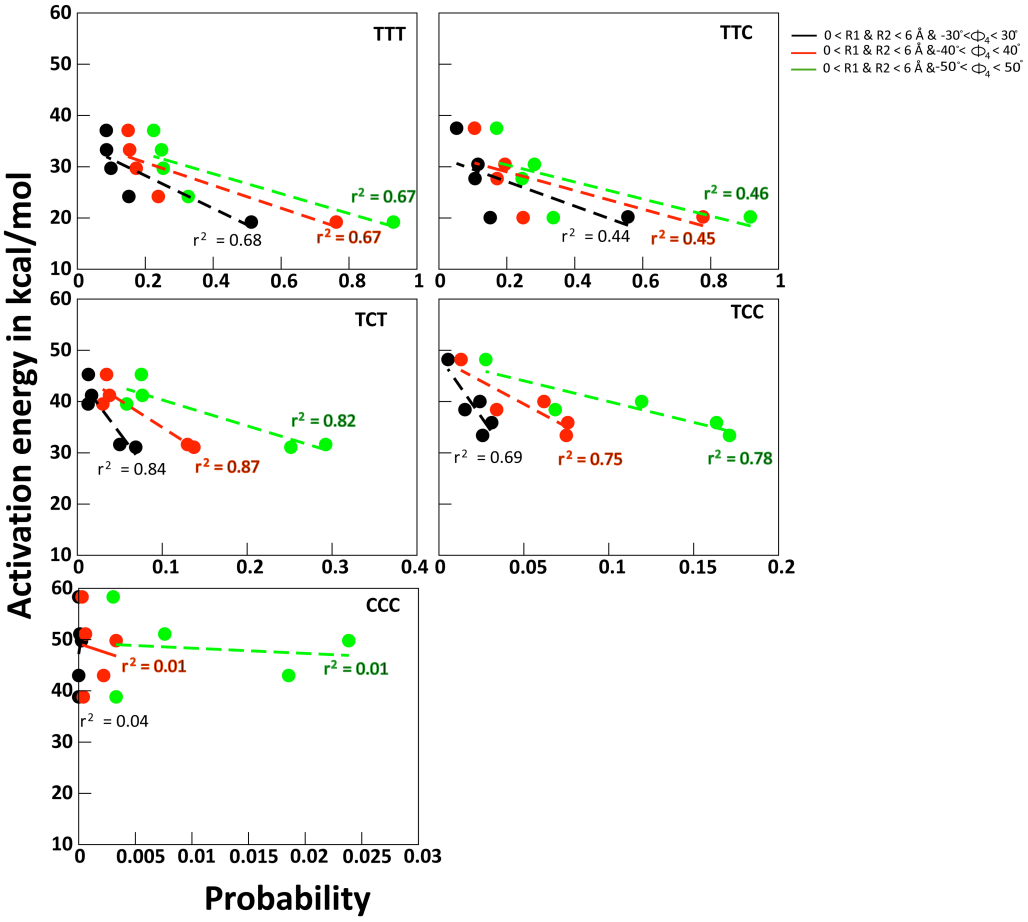


Table S4: The Cartesian coordinates for the TTC, TCT, TCC and CCC trienes along with their four possible TS and respective adducts at M06-2X/6-311G(d,p) level of theory**.**

552 ring systems:

TTT :

6	0.738506	1.913348	0.410790
6	-0.719712	1.822188	0.544809
1	1.285503	2.445070	1.186115
1	-1.118339	2.017087	1.539075
6	1.409122	1.185661	-0.486508
6	-1.546547	1.338127	-0.384647
1	0.832777	0.624770	-1.214087
1	-1.172933	1.172961	-1.394220
6	0.610285	-1.433889	0.440311
6	-0.549206	-1.583440	-0.196624
1	-0.535663	-1.824700	-1.261540
1	0.587712	-1.177683	1.500444
6	2.859198	0.831663	-0.444400
1	3.262563	0.749810	-1.458496
1	3.443234	1.588331	0.086231
6	1.989270	-1.608198	-0.150292
1	2.378050	-2.576370	0.186441
1	1.923211	-1.667093	-1.242760
6	3.008798	-0.531909	0.273814
1	2.898401	-0.363973	1.350617
1	4.022224	-0.910773	0.114103
6	-2.920671	0.818743	-0.113117
1	-3.201517	1.038547	0.921844
6	-1.914723	-1.510669	0.441369
1	-1.819961	-1.108594	1.456131
1	-2.291463	-2.535104	0.545039
6	-2.967517	-0.706597	-0.345062
1	-2.842991	-0.909252	-1.415054
1	-3.966493	-1.063217	-0.078822
1	-3.665140	1.290005	-0.763724

TTT-TS:

6	-0.623209	1.834534	-0.439717
6	0.772616	1.790591	-0.367409
1	-1.090684	2.342527	-1.279077
1	1.336456	2.225202	-1.189210
6	-1.386884	0.981035	0.335502
6	1.453931	0.985970	0.530004
1	-0.989412	0.702833	1.306035
1	1.050735	0.844629	1.527147
6	-0.682092	-0.933030	-0.336176
6	0.600419	-1.077742	0.171189
1	0.661533	-1.420470	1.206704
1	-0.758016	-0.760927	-1.410217
6	-2.872660	0.776488	0.201500
1	-3.362760	1.035401	1.144381
1	-3.285451	1.432488	-0.568265
6	-1.926964	-1.540513	0.272599
1	-2.044600	-2.574868	-0.067983
1	-1.824153	-1.574236	1.363046
6	-3.143427	-0.710749	-0.139923

1	-3.272359	-0.810575	-1.222190
1	-4.061931	-1.074580	0.325045
6	2.908697	0.662620	0.319695
1	3.259865	1.190757	-0.571616
6	1.838706	-1.371959	-0.639967
1	1.751557	-0.895724	-1.622952
1	1.929857	-2.451540	-0.809409
6	3.069659	-0.856905	0.103018
1	3.124461	-1.361328	1.073891
1	3.997219	-1.083967	-0.427885
1	3.524936	0.992352	1.160668

CAT adduct:

6	0.684101	2.032562	-0.079408
6	-0.648154	2.042191	-0.094361
1	1.236466	2.945390	0.126898
1	-1.181642	2.966914	0.113221
6	1.439478	0.765002	-0.349699
6	-1.504135	0.842616	-0.409084
1	1.642104	0.687759	-1.429463
1	-2.082618	1.076570	-1.312483
6	0.607876	-0.448893	0.058768
6	-0.730348	-0.487969	-0.659916
1	-0.537081	-0.607540	-1.731748
1	0.410845	-0.341663	1.136764
6	2.754675	0.519074	0.394981
1	3.592274	1.088455	-0.011913
1	2.632609	0.813503	1.442015
6	1.585894	-1.607789	-0.140651
1	1.318661	-2.498470	0.430843
1	1.599242	-1.890822	-1.198618
6	2.961443	-1.016441	0.281300
1	3.300796	-1.434868	1.230081
1	3.727006	-1.252849	-0.459765
6	-2.522841	0.482308	0.685954
1	-2.017612	0.442501	1.657498
6	-1.667055	-1.610714	-0.138869
1	-1.213400	-2.081136	0.739399
1	-1.824104	-2.399341	-0.876486
6	-2.978331	-0.916813	0.270231
1	-3.650098	-0.838460	-0.590394
1	-3.511233	-1.452180	1.057788
1	-3.337831	1.205439	0.760883

TTC:

6	-0.731804	1.860552	-0.370618
6	0.731834	1.860564	-0.370587
1	-1.188899	2.210719	-1.294512
1	1.188968	2.210780	-1.294442
6	-1.528572	1.263025	0.519648
6	1.528562	1.262995	0.519688
1	-1.117602	0.889631	1.454715
1	1.117549	0.889553	1.454715
6	-0.667294	-1.643283	0.473737
6	0.667298	-1.643266	0.473724
1	1.136370	-1.960032	1.405425
1	-1.136341	-1.960097	1.405434
6	2.914367	0.828700	0.163368

1	3.647143	1.090038	0.932247
6	1.660757	-1.337949	-0.620235
1	1.927745	-2.285940	-1.102327
1	1.216422	-0.705224	-1.394017
6	2.957282	-0.710615	-0.064747
1	3.791669	-0.932501	-0.734737
6	-1.660782	-1.337962	-0.620195
1	-1.216463	-0.705249	-1.393995
1	-1.927792	-2.285957	-1.102267
6	-2.914364	0.828720	0.163290
1	-3.647186	1.090148	0.932097
6	-2.957284	-0.710607	-0.064672
1	-3.791720	-0.932567	-0.734577
1	-3.187997	-1.206164	0.883669
1	3.213186	1.336972	-0.757603
1	3.188075	-1.206264	0.883526
1	-3.213117	1.336903	-0.757753

TTC-TS:

6	0.698728	-1.615128	-0.538755
6	-0.698911	-1.615109	-0.538688
1	1.185649	-1.805018	-1.492792
1	-1.185929	-1.804970	-1.492681
6	1.476354	-1.083886	0.473556
6	-1.476398	-1.083836	0.473707
1	1.165778	-1.196251	1.505529
1	-1.165693	-1.196234	1.505635
6	0.692462	0.975049	0.628904
6	-0.692441	0.975070	0.628845
1	-1.148138	1.093252	1.610432
1	1.148058	1.093170	1.610546
6	-2.906909	-0.709457	0.165421
1	-3.580460	-0.960406	0.987062
6	-1.615598	1.358154	-0.499900
1	-1.660987	2.448019	-0.611144
1	-1.242637	0.951669	-1.445450
6	-3.004914	0.810905	-0.162750
1	-3.721919	0.992160	-0.966014
6	1.615761	1.358228	-0.499701
1	1.242897	0.951866	-1.445344
1	1.661214	2.448104	-0.610804
6	2.906853	-0.709623	0.165075
1	3.580608	-0.961062	0.986403
6	3.004997	0.810851	-0.162445
1	3.722218	0.992405	-0.965451
1	3.373195	1.347675	0.717168
1	-3.234057	-1.284975	-0.704277
1	-3.373342	1.348085	0.716549
1	3.233637	-1.284794	-0.704987

CSC Adduct:

6	0.664699	-1.670732	-0.525065
6	-0.664974	-1.670692	-0.524967
1	1.218493	-2.263751	-1.247801
1	-1.218911	-2.263672	-1.247626
6	1.434269	-0.865906	0.489337

6	-1.434338	-0.865784	0.489528
1	1.420227	-1.412019	1.439467
1	-1.420177	-1.411835	1.439692
6	0.772399	0.529080	0.679336
6	-0.772348	0.529166	0.679271
1	-1.116826	0.916258	1.644751
1	1.116828	0.915908	1.644938
6	-2.890462	-0.558469	0.054388
1	-3.608413	-0.837917	0.826920
6	-1.475650	1.363388	-0.401088
1	-1.309398	2.437041	-0.290272
1	-1.115921	1.064265	-1.390467
6	-2.941961	0.959483	-0.238436
1	-3.550988	1.198093	-1.111624
6	1.475866	1.363523	-0.400745
1	1.116169	1.064729	-1.390237
1	1.309735	2.437164	-0.289630
6	2.890360	-0.558682	0.053991
1	3.608465	-0.838696	0.826175
6	2.942109	0.959385	-0.238117
1	3.551267	1.198309	-1.111128
1	3.372509	1.491244	0.615128
1	-3.145460	-1.134831	-0.838311
1	-3.372396	1.491789	0.614512
1	3.144981	-1.134634	-0.839082

TCT:

6	-0.204576	1.955051	0.614589
6	-1.632507	2.146968	0.295338
1	0.076445	2.157781	1.648338
1	-2.073907	3.066926	0.672824
6	0.755638	1.602148	-0.239619
6	-2.433174	1.283912	-0.337208
1	0.500504	1.453708	-1.288284
6	1.114741	-1.620565	-0.262109
6	0.102250	-1.904965	0.550351
1	-3.477259	1.561299	-0.460250
1	0.982818	-1.760267	-1.336517
1	0.236413	-1.747470	1.620974
6	2.462847	-1.126389	0.178858
1	3.212559	-1.882345	-0.082173
1	2.478515	-1.031085	1.269785
6	2.892680	0.204272	-0.459191
1	3.971879	0.318916	-0.323271
1	2.723020	0.159516	-1.541692
6	2.209015	1.456594	0.109777
1	2.742487	2.330136	-0.285215
1	2.330317	1.482005	1.197911
6	-2.037513	-0.091297	-0.800172
1	-0.982426	-0.102726	-1.065690
6	-1.271910	-2.332214	0.123783
1	-1.601375	-3.179036	0.733330
1	-1.258415	-2.666732	-0.918805
6	-2.265406	-1.165428	0.282528
1	-2.122026	-0.715384	1.269792
1	-3.294842	-1.532505	0.247703
1	-2.597213	-0.361264	-1.700317

TCT-TS:

6	-0.823355	1.724167	-0.197495
6	0.411684	1.851113	-0.832565
1	-1.664328	2.180699	-0.716519
1	0.393968	2.390085	-1.776085
6	-1.140308	0.801445	0.788844
6	1.555368	1.110094	-0.582689
1	-0.456693	0.599715	1.599695
6	-0.507078	-1.066081	-0.135017
6	0.770919	-1.019789	-0.676528
1	2.288029	1.152417	-1.390926
1	-0.576346	-1.560599	0.833679
1	0.877332	-0.971649	-1.755254
6	-1.804035	-1.085479	-0.905058
1	-1.954084	-2.057835	-1.387167
1	-1.770919	-0.331474	-1.697967
6	-2.938554	-0.817910	0.086744
1	-3.898284	-0.691299	-0.417807
1	-3.036046	-1.696081	0.731949
6	-2.595186	0.427184	0.962928
1	-2.836046	0.227358	2.008583
1	-3.212805	1.272605	0.649745
6	2.228094	0.752604	0.716726
1	1.520119	0.661790	1.541677
6	1.917545	-1.610950	0.124119
1	2.374647	-2.440216	-0.423502
1	1.506195	-2.033215	1.045765
6	2.972997	-0.560444	0.501580
1	3.689960	-0.428147	-0.315650
1	3.541690	-0.866956	1.382685
1	2.925071	1.557075	0.977566

CAC adduct:

6	-0.657639	1.485807	0.613527
6	0.366505	1.652154	-0.219532
1	-1.148005	2.361974	1.032942
1	0.688287	2.661721	-0.466895
6	-1.212765	0.146066	1.018745
6	1.165838	0.537119	-0.842300
1	-0.955593	-0.051274	2.065803
6	-0.705446	-0.967813	0.086233
6	0.772925	-0.843260	-0.267919
1	1.012196	0.568375	-1.925708
1	-0.857974	-1.926187	0.595535
1	1.015552	-1.606787	-1.018560
6	-1.650338	-0.903437	-1.142628
1	-1.926502	-1.909237	-1.464971
1	-1.148219	-0.425635	-1.987114
6	-2.886329	-0.078792	-0.706922
1	-2.865952	0.902127	-1.186539
1	-3.828867	-0.555729	-0.978866
6	-2.733878	0.088590	0.812604
1	-3.131699	-0.788717	1.332148
1	-3.250075	0.969525	1.201445
6	2.685406	0.692538	-0.520568
1	2.851073	1.613277	0.043921
6	1.740966	-1.024606	0.906670
1	1.776157	-2.054120	1.270012

1	1.435328	-0.380975	1.739174
6	3.071344	-0.537348	0.328388
1	3.491930	-1.318001	-0.312216
1	3.816112	-0.303505	1.090610
1	3.286716	0.761065	-1.428506

TCC:

6	-0.263399	2.034427	-0.412092
6	1.106906	1.859091	-0.895606
1	-0.872587	2.776111	-0.923706
1	1.312668	2.343685	-1.846734
6	-0.830203	1.218705	0.480257
6	2.096504	1.104628	-0.390738
1	-0.198926	0.476837	0.938701
6	-0.809763	-1.221673	-1.090279
6	0.509753	-1.406565	-1.138041
1	2.997165	1.048377	-0.996961
1	0.983408	-1.192674	-2.091373
1	-1.278338	-0.873325	-2.010078
6	-2.276880	1.041450	0.802350
1	-2.398997	0.955089	1.887298
1	-2.871821	1.897061	0.473022
6	2.205742	0.431947	0.959652
1	1.761458	1.093018	1.711696
1	3.273109	0.387529	1.189547
6	1.447866	-1.894378	-0.054889
1	1.109785	-2.873727	0.301889
1	2.429932	-2.060679	-0.507073
6	-1.793225	-1.416685	0.037701
1	-2.361906	-2.331204	-0.168021
6	-2.808441	-0.255358	0.134533
1	-3.699782	-0.590024	0.671482
6	1.625440	-0.996980	1.180071
1	2.296386	-1.517498	1.869518
1	-1.289627	-1.580662	0.994847
1	0.674549	-0.936313	1.712551
1	-3.128279	-0.013259	-0.884119

TCC_TS:

6	0.385845	2.040261	0.140909
6	-0.945786	2.029996	0.575475
1	1.053856	2.795152	0.548194
1	-1.204808	2.733786	1.361684
6	0.938266	0.939830	-0.484582
6	-1.845573	1.004941	0.323672
1	0.294027	0.331703	-1.100025
6	0.619211	-0.618412	1.012868
6	-0.745865	-0.798626	1.173230
1	-2.731171	1.019164	0.956385
1	-1.163815	-0.527837	2.134320
1	1.117617	-0.092792	1.825100
6	2.401054	0.710180	-0.745786
1	2.580608	0.694321	-1.824881
1	3.000251	1.524713	-0.332222
6	-2.098130	0.328985	-1.019852
1	-1.598392	0.895895	-1.808991
1	-3.170740	0.423697	-1.210312
6	-1.561887	-1.734320	0.313495

1	-1.110068	-2.731843	0.271454
1	-2.553896	-1.852234	0.758307
6	1.567635	-1.476077	0.204782
1	1.851246	-2.362810	0.783142
6	2.818008	-0.651017	-0.122329
1	3.500768	-1.200625	-0.773234
6	-1.712271	-1.165238	-1.101462
1	-2.459237	-1.728669	-1.665805
1	1.090302	-1.838532	-0.710195
1	-0.772998	-1.282030	-1.648479
1	3.353414	-0.464071	0.813038

TSC adduct:

6	-0.311794	2.060184	0.048018
6	0.936425	2.030745	-0.415940
1	-0.859485	2.991676	0.156217
1	1.450533	2.945206	-0.694330
6	-0.964322	0.753806	0.388019
6	1.685710	0.723714	-0.507025
1	-0.542135	0.371988	1.329035
6	-0.669083	-0.276668	-0.719260
6	0.826735	-0.475323	-1.032152
1	2.535256	0.845604	-1.182677
1	0.934680	-0.543300	-2.117107
1	-1.127215	0.151829	-1.620327
6	-2.490377	0.696120	0.486095
1	-2.866580	1.050681	1.447153
1	-2.922514	1.334928	-0.290135
6	2.233954	0.250449	0.883811
1	1.845383	0.878328	1.687354
1	3.321860	0.342139	0.903688
6	1.495028	-1.687421	-0.370503
1	0.887921	-2.593697	-0.412471
1	2.432678	-1.898260	-0.895955
6	-1.536786	-1.461497	-0.289637
1	-1.715118	-2.179428	-1.092853
6	-2.842522	-0.794847	0.217725
1	-3.208767	-1.287797	1.119515
6	1.808446	-1.222321	1.053362
1	2.578854	-1.827958	1.533800
1	-1.049573	-2.000498	0.528814
1	0.910153	-1.289413	1.674258
1	-3.634409	-0.873665	-0.529055

CCC:

6	1.560914	1.286187	-1.059187
6	2.582774	0.447092	-0.398375
1	1.759210	1.435024	-2.119414
1	3.605641	0.661462	-0.700444
6	0.456969	1.874376	-0.585221
6	2.379504	-0.608391	0.399299
6	-1.836150	-0.017608	-1.050897
6	-1.384527	-1.272297	-1.053892
1	3.244580	-1.179251	0.728662
1	-0.149830	2.406470	-1.315717
1	-1.127376	-1.686231	-2.028055
1	-1.913282	0.451333	-2.028819
6	-0.032407	1.990823	0.835835

1	0.769351	1.701886	1.521188
1	-0.216549	3.056654	1.005888
6	-2.314571	0.855271	0.096295
1	-2.701085	1.782675	-0.336669
1	-3.174904	0.370140	0.570678
6	-1.073732	-2.199093	0.089508
1	-1.522282	-3.176704	-0.111995
1	-1.501903	-1.835080	1.029172
6	1.022177	-1.053927	0.844119
1	0.983028	-1.113891	1.938394
1	0.339888	-0.275802	0.542404
6	0.458877	-2.351513	0.240930
1	0.700474	-3.221434	0.856929
1	0.895250	-2.523614	-0.747886
6	-1.327823	1.217071	1.223228
1	-1.065264	0.308098	1.762979
1	-1.876973	1.830321	1.942859

CCC-TS:

6	-1.092085	2.046518	-0.254204
6	0.286490	2.270973	-0.219776
1	-1.637961	2.778322	-0.844966
1	0.591938	3.162449	-0.762333
6	-1.777350	0.867054	0.003327
6	1.317629	1.376723	0.030126
6	-0.688065	-0.557300	-1.292102
6	0.697915	-0.403219	-1.271132
1	2.261837	1.704218	-0.411583
1	-2.755484	0.835224	-0.476966
1	1.134319	0.123527	-2.112049
1	-1.199850	-0.146030	-2.154257
6	-1.750667	-0.011365	1.241519
1	-1.104816	0.427969	2.001241
1	-2.761816	0.022459	1.657818
6	-1.404761	-1.687786	-0.576706
1	-2.444808	-1.704127	-0.913366
1	-0.974986	-2.660669	-0.837784
6	1.611683	-1.387917	-0.567131
1	2.291813	-1.822374	-1.305400
1	1.026945	-2.218619	-0.170107
6	1.599228	0.407340	1.144897
1	2.169872	0.934461	1.918684
1	0.693348	0.037649	1.614695
6	2.423609	-0.742234	0.572759
1	2.692102	-1.475421	1.337345
1	3.359767	-0.335649	0.176150
6	-1.375729	-1.478227	0.941057
1	-0.375877	-1.692805	1.325769
1	-2.053729	-2.173942	1.441297

CSC adduct:

6	-0.214162	2.012968	0.334185
6	1.069625	1.785423	0.069843
1	-0.492079	2.896899	0.903214
1	1.816140	2.495373	0.419069
6	-1.330588	1.117257	-0.117986
6	1.591615	0.584695	-0.681168
6	-0.869709	-0.010214	-1.061555

6	0.532991	-0.534690	-0.741835
1	1.879929	0.904623	-1.688482
1	-2.047042	1.732730	-0.675105
1	0.817268	-1.227881	-1.544908
1	-0.831185	0.375238	-2.086025
6	-2.113747	0.427886	1.035356
1	-1.514551	0.405078	1.947991
1	-3.021668	0.986803	1.269423
6	-1.980290	-1.061970	-0.927520
1	-2.814897	-0.784520	-1.578131
1	-1.651171	-2.059581	-1.230348
6	0.753186	-1.278807	0.583963
1	0.268020	-2.256455	0.610331
1	0.371042	-0.683192	1.418239
6	2.803698	-0.059167	0.048355
1	3.625816	-0.248673	-0.643790
1	3.185817	0.614481	0.818626
6	2.281077	-1.378886	0.666721
1	2.640813	-1.535009	1.684577
1	2.618812	-2.230485	0.069854
6	-2.434801	-1.005334	0.544760
1	-1.889498	-1.736844	1.142565
1	-3.494930	-1.243540	0.644183

562 ring systems:

TTT:

6	-0.402917	2.140477	-0.398322
6	1.056360	1.960966	-0.426194
1	-0.825003	2.929351	-1.016881
1	1.586333	2.364519	-1.287338
6	-1.217539	1.341671	0.294854
6	1.740655	1.272407	0.489272
1	-0.770396	0.536582	0.869583
1	1.209030	0.903882	1.363227
6	-0.224546	-1.798248	0.244557
6	0.915334	-1.509938	-0.378162
1	-0.198543	-2.085228	1.297449
1	0.865420	-1.220215	-1.428734
6	2.307573	-1.611031	0.194133
1	2.710373	-2.589741	-0.092167
1	2.269631	-1.603752	1.289315
6	3.280704	-0.539075	-0.326304
6	-1.572022	-1.843567	-0.431770
1	-1.480173	-1.383755	-1.420600
1	-1.804038	-2.899585	-0.611205
6	-2.771521	-1.218210	0.329949
6	3.168944	0.837284	0.361812
1	3.742222	1.568352	-0.215617
1	4.308096	-0.899099	-0.222104
1	3.100632	-0.406415	-1.398575
1	3.626600	0.776915	1.354050
1	-3.584239	-1.947516	0.334038
1	-2.507619	-1.065087	1.383210
6	-2.709821	1.381439	0.321225
1	-3.046770	1.483869	1.360422
1	-3.082726	2.251903	-0.225835
6	-3.326410	0.095890	-0.258308
1	-4.406218	0.135324	-0.089425

1	-3.181384	0.089289	-1.343270

TTT-TS1:

6	0.369961	1.896697	0.485602
6	-1.026208	1.820078	0.572308
1	0.906739	2.364576	1.307445
1	-1.526055	2.244156	1.438915
6	1.102302	1.189296	-0.447098
6	-1.724776	0.965875	-0.257979
1	0.673954	0.997186	-1.425511
1	-1.302117	0.780187	-1.239977
6	0.407417	-0.982365	-0.053874
6	-0.930394	-0.929543	0.307511
1	0.620215	-1.326858	-1.065880
1	-1.129596	-0.838445	1.375822
6	-2.065070	-1.569907	-0.463287
1	-2.120563	-2.639264	-0.233941
1	-1.873237	-1.485971	-1.538583
6	-3.379061	-0.884039	-0.079017
6	1.505373	-1.210311	0.964425
1	1.462783	-0.412517	1.713653
1	1.323817	-2.144776	1.508334
6	2.904661	-1.285637	0.333295
6	-3.193813	0.654828	-0.165910
1	-3.637538	1.149364	0.701170
1	-4.209758	-1.228911	-0.697595
1	-3.617640	-1.158063	0.952748
1	-3.702044	1.043304	-1.053120
6	2.609615	1.148611	-0.391227
1	3.014255	1.892496	-1.087514
1	3.047437	-2.279334	-0.103813
6	3.169803	-0.230263	-0.748815
1	2.724010	-0.546561	-1.697985
1	4.246282	-0.162029	-0.926436
1	3.652000	-1.187302	1.126752
1	2.948206	1.438840	0.609920

TTT-TS2:

6	-0.590207	1.730946	-0.373299
6	0.778070	1.752073	-0.705083
1	-1.300027	2.106993	-1.105710
1	1.081027	2.121959	-1.680871
6	-1.067794	1.035412	0.715752
6	1.679544	1.058049	0.068561
1	-0.420543	0.910125	1.574510
1	1.431251	0.940794	1.117692
6	-0.327636	-1.097067	0.229506
6	0.996136	-0.999367	-0.154837
1	-0.547788	-1.400479	1.252633
1	1.174251	-1.012745	-1.230288
6	2.206282	-1.401006	0.655077
1	2.352674	-2.485412	0.611525
1	2.050273	-1.149019	1.709444
6	3.447165	-0.695275	0.086206
6	-1.380484	-1.414808	-0.811502
1	-1.201311	-0.779143	-1.688167
1	-1.228469	-2.447620	-1.149797
6	-2.835174	-1.271574	-0.355202

6	3.128425	0.798104	-0.222799
1	3.355879	1.038055	-1.264165
1	4.296209	-0.791250	0.765378
1	3.731410	-1.199454	-0.841101
1	3.750390	1.449297	0.398601
1	-3.481572	-1.739145	-1.103618
1	-2.976261	-1.839973	0.572977
6	-2.544040	0.873669	0.993510
1	-2.675682	0.297368	1.915214
1	-2.992147	1.856898	1.178416
6	-3.298759	0.167909	-0.135817
1	-4.367986	0.170387	0.095776
1	-3.180754	0.729975	-1.068891

CAT-adduct:

6	-0.544185	1.782732	-0.285525
6	0.756849	1.856318	-0.571127
1	-1.269433	2.463554	-0.723031
1	1.164004	2.590050	-1.260117
6	-1.000921	0.743146	0.714081
6	1.637448	0.837877	0.090111
1	-0.530027	1.007315	1.671053
1	1.647389	1.033589	1.174573
6	-0.443488	-0.663596	0.334832
6	1.027534	-0.562811	-0.107760
1	-0.517160	-1.289337	1.234322
1	1.066102	-0.741414	-1.191102
6	2.080515	-1.461819	0.541025
1	2.012455	-2.502717	0.218531
1	1.951865	-1.445727	1.628034
6	3.429178	-0.800014	0.142413
6	-1.285280	-1.313087	-0.772197
1	-1.132678	-0.742102	-1.696600
1	-0.908463	-2.323921	-0.960819
6	-2.778714	-1.336527	-0.455459
6	3.079138	0.627894	-0.367758
1	3.120025	0.663855	-1.460737
1	4.108668	-0.757895	0.995120
1	3.934748	-1.374124	-0.635649
1	3.764157	1.387603	0.012101
1	-3.329452	-1.807199	-1.274271
1	-2.959714	-1.941731	0.441528
6	-2.515725	0.723684	0.945075
1	-2.725507	0.151658	1.856527
1	-2.866322	1.744402	1.126914
6	-3.282267	0.085989	-0.213058
1	-4.354217	0.087769	0.000997
1	-3.136929	0.677654	-1.125290

TTC:

6	0.516459	-2.277804	-0.422164
6	-0.933088	-2.082911	-0.591181
1	1.025015	-3.020996	-1.031646
1	-1.319386	-2.155293	-1.607388
6	1.218544	-1.444234	0.349095
6	-1.743292	-1.663680	0.381876
1	0.657124	-0.678308	0.881505

1	-1.356946	-1.641448	1.400541
6	0.194926	2.466191	0.047538
6	-1.131753	2.324587	0.074629
1	-1.703300	3.080069	0.611914
1	0.615245	3.330697	0.560214
6	-3.062767	-0.985823	0.176475
1	-3.827202	-1.387319	0.847979
6	-1.952500	1.226787	-0.546112
1	-2.570095	1.648468	-1.346957
1	-1.296992	0.493074	-1.016799
6	-2.871671	0.519730	0.473711
1	-2.438344	0.613769	1.475060
1	-3.845316	1.016072	0.509859
6	2.704450	-1.326732	0.463703
1	2.987648	-1.351280	1.522630
1	3.201091	-2.167767	-0.027198
6	1.207388	1.566942	-0.606948
1	0.737854	0.647149	-0.956946
1	1.609197	2.060961	-1.500260
6	2.393009	1.233825	0.323353
1	3.044946	2.110115	0.380197
1	2.025899	1.067475	1.342641
6	3.202307	0.007685	-0.138740
1	4.255686	0.130382	0.125903
1	3.157840	-0.057611	-1.231265
1	-3.412038	-1.125590	-0.851389

TTC-TS1:

6	0.575559	1.602762	0.611912
6	-0.809891	1.555234	0.796209
1	1.199679	1.767219	1.487256
1	-1.187015	1.626519	1.813674
6	1.189372	1.169298	-0.549906
6	-1.690477	1.164864	-0.195692
1	0.667183	1.293784	-1.491006
1	-1.474806	1.436046	-1.223745
6	0.430936	-0.899119	-0.618941
6	-0.944618	-0.841585	-0.793834
1	-1.270508	-0.740711	-1.828528
1	1.016904	-0.986015	-1.526710
6	-3.105686	0.779655	0.148309
1	-3.836435	1.388490	-0.390400
6	-2.005353	-1.450110	0.093839
1	-2.115090	-2.518318	-0.128467
1	-1.722585	-1.366241	1.147389
6	-3.323163	-0.718604	-0.158068
1	-4.143815	-1.127654	0.435776
6	1.064642	-1.454006	0.630897
1	0.447468	-1.176793	1.490350
1	1.019656	-2.548882	0.570815
6	2.698365	1.034089	-0.617441
1	3.068495	1.368631	-1.590130
6	2.527703	-1.011013	0.888400
1	2.546229	-0.278748	1.702054
1	3.105369	-1.869492	1.237910
6	3.224632	-0.385989	-0.322114
1	3.114641	-1.033361	-1.197107
1	4.298421	-0.318156	-0.128984

1	-3.261660	0.949850	1.217562
1	-3.595228	-0.844155	-1.211447
1	3.130970	1.705138	0.132330

TTC-TS2:

6	0.567510	-1.614161	-0.535713
6	-0.817343	-1.579037	-0.744901
1	1.195365	-1.759138	-1.410032
1	-1.168449	-1.661291	-1.771185
6	1.150775	-1.161582	0.630680
6	-1.727848	-1.177626	0.211304
1	0.618143	-1.302669	1.564250
1	-1.543052	-1.413183	1.253423
6	0.408115	0.910624	0.690386
6	-0.971282	0.865904	0.797955
1	-1.358883	0.782983	1.812279
1	0.963659	0.993475	1.621238
6	-3.121449	-0.773699	-0.192661
1	-3.885307	-1.334247	0.352338
6	-1.968013	1.442061	-0.178024
1	-2.074828	2.521496	-0.013741
1	-1.616889	1.303026	-1.205603
6	-3.312077	0.745042	0.030162
1	-3.638966	0.927050	1.059393
1	-4.088877	1.142604	-0.627042
6	2.644987	-0.950376	0.737349
1	2.874617	-0.478672	1.698661
1	3.160201	-1.917652	0.738509
6	1.114852	1.446450	-0.529525
1	0.765066	0.906209	-1.418482
1	0.832045	2.496268	-0.679449
6	2.640652	1.352259	-0.412693
1	3.100313	1.895585	-1.243153
1	2.949269	1.870354	0.504042
6	3.202544	-0.073532	-0.392324
1	4.290776	-0.021615	-0.292957
1	3.008063	-0.550193	-1.358315
1	-3.250794	-0.994354	-1.256140

CSC-adduct:

6	0.795795	-1.809627	-0.140528
6	-0.463819	-1.911715	-0.556775
1	1.547187	-2.496794	-0.523937
1	-0.735397	-2.679074	-1.277644
6	1.253706	-0.764238	0.853006
6	-1.572937	-1.043076	-0.036726
1	1.142118	-1.185582	1.861315
1	-2.280896	-1.701745	0.485384
6	0.345084	0.478129	0.753175
6	-1.114073	0.036506	0.976480
1	-1.144247	-0.396572	1.981154
1	0.612149	1.159529	1.573160
6	-2.400922	-0.275989	-1.082653
1	-3.051285	-0.932330	-1.665225
6	-2.167007	1.169461	0.863766
1	-2.663308	1.349650	1.818665
1	-1.690708	2.110148	0.580372
6	-3.174756	0.726047	-0.219508

1	-4.022488	0.216163	0.247884
1	-3.574391	1.565168	-0.791306
6	2.733671	-0.403619	0.663812
1	3.054387	0.217833	1.507850
1	3.338414	-1.315733	0.692776
6	0.613469	1.223314	-0.564164
1	0.347726	0.583198	-1.410113
1	-0.008479	2.119365	-0.632282
6	2.089930	1.606101	-0.695715
1	2.254368	2.147174	-1.631329
1	2.366508	2.285715	0.119978
6	2.975487	0.361367	-0.637506
1	4.030799	0.633551	-0.723544
1	2.739832	-0.284369	-1.491913
1	-1.744056	0.248750	-1.781234

TCT:

6	0.316769	-1.943732	-0.326043
6	-0.996951	-1.947356	-0.976657
1	1.044777	-2.602357	-0.800090
1	-0.992748	-2.460151	-1.935559
6	0.760413	-1.186465	0.681870
6	-2.175620	-1.418801	-0.621716
1	0.095920	-0.496959	1.180044
6	0.429995	1.702708	-0.041552
6	-0.827436	1.573337	-0.454627
1	-2.982266	-1.546754	-1.342816
1	0.603141	1.994740	0.996518
1	-1.025756	1.279278	-1.484887
6	1.666038	1.526763	-0.882672
1	1.902895	2.499328	-1.330499
1	1.452333	0.846029	-1.713630
6	2.920560	1.058018	-0.119660
1	3.794489	1.421766	-0.667822
1	2.953881	1.555684	0.857648
6	2.209063	-1.157335	1.093289
1	2.315379	-0.667546	2.065838
1	2.574143	-2.182235	1.214728
6	3.116207	-0.451864	0.068984
1	4.153696	-0.615309	0.378631
1	2.999166	-0.948916	-0.900406
6	-2.616263	-0.708733	0.625853
1	-1.847563	-0.709666	1.398692
6	-2.019964	1.808048	0.429531
1	-2.483875	2.766917	0.167825
1	-1.675935	1.903626	1.465525
6	-3.108185	0.728481	0.353404
1	-3.581359	0.758541	-0.634388
1	-3.888675	0.986428	1.074710
1	-3.459394	-1.280862	1.029917

TCT-TS1:

6	-0.496692	1.684362	-0.297399
6	0.663796	1.682450	-1.079058
1	-1.368343	2.147318	-0.751795
1	0.550173	2.081213	-2.084216
6	-0.710331	0.861770	0.795604
6	1.825818	0.973930	-0.830894

1	0.100269	0.653617	1.478248
6	-0.332763	-1.093379	-0.068316
6	0.991423	-1.165380	-0.466839
1	2.474115	0.859367	-1.701187
1	-0.554204	-1.475298	0.927157
1	1.210200	-1.323709	-1.518569
6	-1.474793	-1.159597	-1.052541
1	-1.423379	-2.108946	-1.598168
1	-1.347642	-0.366804	-1.800533
6	-2.846634	-1.054632	-0.375578
1	-3.628503	-1.249603	-1.115124
1	-2.922487	-1.854148	0.372392
6	-2.104159	0.686348	1.363989
1	-2.079608	-0.084943	2.141403
1	-2.422748	1.611050	1.858502
6	-3.137921	0.288202	0.302186
1	-4.124643	0.238911	0.772118
1	-3.204371	1.069193	-0.461565
6	2.616352	0.844728	0.446790
1	2.015685	1.062024	1.330793
6	2.053947	-1.548744	0.534481
1	2.414184	-2.564084	0.338924
1	1.600947	-1.560423	1.532189
6	3.217960	-0.554986	0.528999
1	3.844702	-0.722606	-0.354225
1	3.856241	-0.679271	1.407435
1	3.413399	1.596712	0.417669

TCT-TS2:

6	0.491723	1.706809	0.245743
6	-0.668038	1.711987	1.024839
1	1.353593	2.224958	0.661134
1	-0.569086	2.152398	2.013840
6	0.733385	0.846376	-0.815872
6	-1.812452	0.967103	0.789174
1	-0.071782	0.570333	-1.479481
6	0.362523	-1.068143	0.160253
6	-0.975966	-1.139050	0.513786
1	-2.470254	0.870841	1.654611
1	0.619066	-1.495634	-0.804597
1	-1.226568	-1.273915	1.561727
6	2.138100	0.728658	-1.380184
1	2.105211	0.606194	-2.465902
6	-2.591434	0.810801	-0.494399
1	-3.395582	1.555411	-0.484050
1	-1.983354	1.022152	-1.374860
6	1.452688	-1.082216	1.202174
1	1.608230	-2.125656	1.501890
1	1.084597	-0.561436	2.092268
6	-2.000003	-1.574285	-0.507390
1	-2.349798	-2.589178	-0.292570
6	2.806662	-0.476854	0.760423
1	2.907765	0.534283	1.166055
1	3.618401	-1.062643	1.197460
6	2.984422	-0.402726	-0.757586
1	2.736653	-1.368138	-1.209509
1	4.034444	-0.215798	-0.996823
6	-3.176348	-0.596529	-0.560775
1	-3.826608	-0.750563	0.307816

1	2.658916	1.671978	-1.184907
1	-1.518323	-1.607854	-1.491197
1	-3.787092	-0.749319	-1.454023

CAC- adduct:

6	-0.328151	1.657844	0.040072
6	0.700464	1.511885	-0.791349
1	-0.809906	2.630024	0.125910
1	1.036499	2.364811	-1.377375
6	-0.868290	0.550159	0.909985
6	1.476511	0.233983	-0.976574
1	-0.409203	0.655215	1.902042
6	-0.472170	-0.823804	0.337955
6	1.023097	-0.868880	0.011025
1	1.346907	-0.098243	-2.011933
1	-0.681513	-1.580248	1.106950
1	1.238329	-1.842572	-0.448519
6	-1.305645	-1.175529	-0.903711
1	-1.044155	-2.186965	-1.231195
1	-1.039211	-0.496752	-1.721784
6	-2.809092	-1.066598	-0.649186
1	-3.363598	-1.311428	-1.558995
1	-3.106346	-1.798162	0.112668
6	-2.386780	0.666143	1.110740
1	-2.691198	-0.028657	1.902312
1	-2.629143	1.673776	1.463252
6	-3.166197	0.337820	-0.161668
1	-4.240582	0.421256	0.022026
1	-2.915286	1.065116	-0.943182
6	2.994333	0.447878	-0.678136
1	3.171924	1.489504	-0.399286
6	1.982995	-0.703965	1.193884
1	1.973869	-1.562986	1.868639
1	1.719800	0.187253	1.773694
6	3.330647	-0.485018	0.502579
1	3.705043	-1.443114	0.130153
1	4.093244	-0.068490	1.162429
1	3.614186	0.239143	-1.551502

TCC:

6	-0.262886	1.855894	-0.718105
6	1.164775	2.187637	-0.640662
1	-0.676788	1.857666	-1.726651
1	1.489869	2.959588	-1.334689
6	-1.093298	1.584091	0.288007
6	2.110673	1.618489	0.112788
1	-0.727413	1.629729	1.312672
6	-0.232224	-1.293025	-1.048944
6	1.096956	-1.354508	-1.091127
1	3.125226	1.994879	-0.009899
1	1.605610	-0.993361	-1.982253
6	-2.547502	1.258580	0.109554
1	-3.137292	2.061136	0.568667
1	-2.794462	1.259169	-0.957683
6	1.991267	0.480630	1.084920
6	1.977554	-1.849716	0.021467
1	2.639642	-2.635675	-0.357914
1	1.366650	-2.308066	0.803739

6	2.837021	-0.738857	0.650263
1	3.373437	-1.158153	1.505510
6	-1.101510	-1.749176	0.102553
1	-0.695969	-1.385375	1.053756
1	-1.040387	-2.842266	0.156601
6	-2.585706	-1.351603	0.009412
1	-3.182284	-2.163792	0.434086
1	-2.882708	-1.281038	-1.043594
6	-2.997244	-0.067623	0.741072
1	-2.637606	-0.114569	1.776261
1	-4.089879	-0.053297	0.800288
1	-0.758941	-0.905977	-1.918523
1	0.948755	0.178954	1.194889
1	2.329367	0.831356	2.065498
1	3.597909	-0.415777	-0.067941

TCC-TS1:

6	0.120630	2.108052	0.218371
6	-1.216625	2.041109	0.603044
1	0.715807	2.913392	0.643043
1	-1.524135	2.729916	1.385465
6	0.811202	1.083104	-0.406630
6	-2.092716	1.003989	0.313113
1	0.289241	0.419409	-1.080669
6	0.401880	-0.570801	1.060600
6	-0.972663	-0.807852	0.983107
1	-2.975763	0.987363	0.954876
1	-1.569942	-0.656308	1.874586
1	0.727845	0.012411	1.916688
6	2.290426	1.220594	-0.676304
1	2.429332	1.300960	-1.761918
1	2.659421	2.152786	-0.240109
6	-2.402377	0.337660	-1.006403
1	-1.580887	0.419866	-1.719392
1	-3.258778	0.857784	-1.449991
6	-1.529584	-1.750658	-0.058661
1	-0.768174	-1.929811	-0.824694
1	-1.779838	-2.723998	0.377779
6	-2.749818	-1.125044	-0.740026
1	-3.020652	-1.660919	-1.652772
1	-3.614889	-1.167146	-0.068713
6	1.406846	-1.634349	0.610814
1	1.967394	-1.899841	1.515126
6	2.442675	-1.290146	-0.466576
1	1.972141	-1.252414	-1.456871
1	3.171101	-2.104567	-0.501447
6	3.134335	0.040148	-0.179851
1	4.117048	0.081134	-0.655956
1	3.300062	0.128735	0.899951
1	0.878405	-2.543592	0.317434

TCC-TS2:

6	-0.156095	2.118415	-0.275562
6	1.210176	2.078415	-0.549449
1	-0.733574	2.871743	-0.808213
1	1.556879	2.772896	-1.310321
6	-0.873067	1.108550	0.341510

6	2.093344	1.066844	-0.211041
1	-0.424080	0.536042	1.142320
6	-0.367114	-0.618921	-0.938412
6	1.017022	-0.777046	-1.007763
1	3.019293	1.090909	-0.789225
1	1.500460	-0.521671	-1.942635
6	-2.381883	1.196333	0.382144
1	-2.669412	1.966427	1.108496
1	-2.743385	1.541701	-0.593330
6	2.315048	0.319905	1.079368
6	1.747619	-1.762156	-0.118116
1	2.188501	-2.555896	-0.729298
1	1.041623	-2.249318	0.555860
6	2.831720	-1.072456	0.726668
1	3.081146	-1.659843	1.613621
6	-1.256498	-1.617166	-0.209786
1	-0.934862	-1.740191	0.829804
1	-1.126130	-2.597652	-0.683719
6	-2.742581	-1.254964	-0.210327
1	-3.322736	-2.138599	0.070448
1	-3.053037	-0.986668	-1.227408
6	-3.076127	-0.113278	0.746719
1	-2.784462	-0.406536	1.762708
1	-4.157473	0.048367	0.767459
1	-0.840533	-0.162166	-1.803654
1	1.416770	0.253728	1.694033
1	3.063585	0.866549	1.664726
1	3.752032	-0.964668	0.142605

TSC-adduct:

6	0.068092	1.948925	0.252359
6	1.263329	1.823861	-0.318582
1	-0.255413	2.923283	0.612186
1	1.897292	2.701871	-0.423519
6	-0.887146	0.800923	0.429566
6	1.853741	0.525508	-0.806769
1	-0.785532	0.417153	1.456956
6	-0.548639	-0.334453	-0.543710
6	0.938300	-0.687019	-0.510076
1	2.029390	0.612696	-1.884025
1	1.120840	-1.446384	-1.281491
6	-2.350100	1.225462	0.257261
1	-2.587411	2.033491	0.956526
1	-2.484677	1.628543	-0.754292
6	3.196581	0.216983	-0.072503
6	1.486385	-1.246066	0.810091
1	1.143695	-2.261349	1.019418
1	1.185885	-0.606094	1.647195
6	3.000286	-1.151804	0.605221
1	3.570290	-1.247051	1.530713
6	-1.467171	-1.532824	-0.299329
1	-1.296205	-1.918939	0.713522
1	-1.219888	-2.342175	-0.994305
6	-2.937923	-1.132425	-0.447301
1	-3.587714	-1.986205	-0.236831
1	-3.124398	-0.840214	-1.487677
6	-3.291865	0.039054	0.473889
1	-3.212756	-0.290601	1.517027
1	-4.329786	0.343874	0.316067

1	-0.761684	0.049825	-1.553235
1	3.383257	0.983786	0.683785
1	4.049048	0.221961	-0.753451
1	3.322541	-1.954220	-0.065274

CTT:

6	0.281214	2.135275	0.972627
6	-1.079039	1.623977	0.785040
1	0.427879	2.748599	1.858323
1	-1.627304	1.427469	1.706722
6	1.369578	1.868260	0.239235
6	-1.682572	1.325392	-0.365945
6	0.410422	-1.331739	1.043446
6	-0.465505	-1.639729	0.092589
1	2.303103	2.317705	0.576891
1	-1.190750	1.554619	-1.308074
6	1.918324	-1.337703	0.957087
1	2.299651	-0.500895	1.553129
1	2.269992	-2.242430	1.467583
6	1.504761	1.042091	-1.009240
1	1.581921	1.737463	-1.854382
1	0.608159	0.445361	-1.178579
6	2.537900	-1.278096	-0.445352
1	3.513824	-1.771210	-0.416073
1	-0.116783	-1.906500	-0.904224
6	-2.981790	0.583104	-0.444890
1	-3.503965	0.657649	0.514668
6	-1.960354	-1.684994	0.275624
1	-2.271443	-2.735161	0.231575
1	-2.217186	-1.327275	1.278862
6	-2.773271	-0.907085	-0.778164
1	-3.758940	-1.369518	-0.881981
1	1.934628	-1.863377	-1.145132
6	2.749974	0.134542	-1.005550
1	3.127018	0.036649	-2.027411
1	-3.633421	1.026316	-1.204292
1	-2.285170	-0.999653	-1.755308
1	0.015316	-1.063109	2.023070
1	3.545612	0.627525	-0.434409

CTT-TS1:

6	0.032063	1.960498	0.970474
6	-1.236375	1.758480	0.418784
1	0.051279	2.430738	1.949616
1	-2.075350	2.086521	1.029577
6	1.192430	1.309816	0.578631
6	-1.536645	0.906531	-0.626255
6	0.543502	-0.757500	0.973908
6	-0.516123	-1.050785	0.129149
1	2.017704	1.400027	1.286735
1	-0.878138	0.801936	-1.473904
6	1.925423	-1.380390	0.807196
1	2.609220	-0.938054	1.539579
1	1.845688	-2.441814	1.068524
6	1.694259	1.121406	-0.836960
1	1.964381	2.113206	-1.218602
1	0.920746	0.739009	-1.501043
6	2.552400	-1.250141	-0.581317

1	3.452731	-1.869533	-0.620592
1	-0.264634	-1.452858	-0.853063
6	-2.933102	0.373453	-0.784078
1	-3.587664	0.873461	-0.064308
6	-1.901756	-1.431219	0.596847
1	-1.921887	-2.498922	0.848956
1	-2.144065	-0.880969	1.513110
6	-2.931087	-1.142974	-0.492895
1	-3.929836	-1.489219	-0.215924
1	1.870693	-1.648913	-1.340266
6	2.906786	0.194775	-0.922431
1	3.329688	0.243193	-1.929608
1	-3.332579	0.565890	-1.783510
1	-2.641992	-1.689648	-1.397054
1	0.278686	-0.566482	2.011534
1	3.684680	0.550741	-0.236076

CTT-TS2:

6	0.045422	1.804376	1.042279
6	-1.211235	1.689724	0.453605
1	0.061775	2.208709	2.050702
1	-2.054568	2.018544	1.057746
6	1.205561	1.178660	0.615234
6	-1.507864	0.896549	-0.646001
6	0.517541	-0.982413	0.650409
6	-0.719102	-1.053951	0.018249
1	2.007472	1.207205	1.353006
1	-0.834747	0.853559	-1.489483
6	1.711485	-1.654804	-0.011742
1	1.802794	-2.657433	0.421584
1	1.489368	-1.808017	-1.074382
6	1.746515	1.053077	-0.791270
1	1.864375	2.050951	-1.227980
1	1.059608	0.510968	-1.442348
6	3.050791	-0.928201	0.117567
1	3.210520	-0.665902	1.167632
1	3.867238	-1.601040	-0.156906
6	3.099238	0.327838	-0.764298
1	3.379784	0.052271	-1.785148
1	-0.688638	-1.444147	-1.000043
6	-2.943755	0.473404	-0.851459
1	-3.589611	1.163971	-0.302907
6	-2.047725	-1.289326	0.697223
1	-2.130886	-2.333862	1.018655
1	-2.118563	-0.667933	1.596033
6	-3.156456	-0.964366	-0.302179
1	-4.150842	-1.075342	0.135144
1	-3.235824	0.524769	-1.902327
1	-3.090013	-1.682509	-1.125415
1	3.873937	1.007660	-0.395871
1	0.534323	-0.965823	1.736606

CAC-adduct:

6	0.185823	2.205411	0.388716
6	-1.049288	2.056641	-0.081550
1	0.546461	3.196223	0.652322
1	-1.694284	2.926356	-0.182955
6	1.137803	1.053961	0.560332

6	-1.625199	0.744071	-0.524136
6	0.371039	-0.269224	0.723657
6	-0.669263	-0.472582	-0.388877
1	1.708803	1.215564	1.485007
1	-1.894558	0.844382	-1.584230
6	1.348982	-1.448098	0.837689
1	1.905792	-1.348607	1.777187
1	0.797533	-2.390764	0.901058
6	2.157572	0.996354	-0.592225
1	2.708125	1.941015	-0.636959
1	1.618460	0.906368	-1.542185
6	2.354018	-1.499858	-0.316991
1	3.048830	-2.330002	-0.164462
1	-0.148694	-0.620989	-1.338308
6	-2.906376	0.311285	0.208443
1	-2.754225	0.384041	1.291229
6	-1.600456	-1.681634	-0.094893
1	-1.409530	-2.531222	-0.753133
1	-1.431975	-2.028217	0.929856
6	-3.039112	-1.152717	-0.212712
1	-3.746107	-1.720407	0.394472
1	1.833323	-1.699009	-1.260465
6	3.119919	-0.180737	-0.430478
1	3.818996	-0.214794	-1.270400
1	-3.771307	0.925099	-0.052087
1	-3.380281	-1.200243	-1.251711
1	-0.186896	-0.197429	1.666849
1	3.718763	-0.034605	0.477066

CTC:

6	2.738952	1.126290	0.697163
6	1.642762	1.929510	0.131392
1	3.389964	1.639422	1.400765
1	1.872313	2.968000	-0.105485
6	3.024426	-0.147759	0.398081
6	0.408601	1.471351	-0.090572
6	-1.696000	-1.519071	0.997493
6	-2.189168	-0.281706	1.015745
1	3.863904	-0.607884	0.913463
1	0.172455	0.461851	0.222839
6	-1.374802	-2.350795	-0.224341
1	-1.287957	-3.398523	0.076474
1	-2.197817	-2.302049	-0.943605
6	-2.607209	0.566568	-0.156115
1	-2.318313	0.099198	-1.102795
1	-3.702893	0.604062	-0.153624
6	2.292574	-1.001695	-0.601428
1	3.001643	-1.672265	-1.094090
1	1.881676	-0.346036	-1.374810
6	-0.706360	2.227710	-0.750451
1	-0.776193	1.899394	-1.796923
6	-0.076654	-1.910979	-0.924278
1	0.140522	-2.588835	-1.756132
1	-0.241839	-0.924475	-1.371233
6	-2.084692	2.019145	-0.107072
1	-2.796698	2.663225	-0.629862
1	-2.060867	2.360583	0.933307
1	-2.341549	0.185165	1.987795
1	-0.463747	3.294496	-0.777999

6	1.133090	-1.824803	0.012209
1	0.827622	-1.353649	0.950009
1	-1.468668	-1.973473	1.958230
1	1.473324	-2.830796	0.276738

CTC-TS1:

6	-0.234340	2.188555	-0.821894
6	1.037121	1.975953	-0.281439
1	-0.291959	2.811496	-1.710590
1	1.874678	2.529620	-0.699001
6	-1.338581	1.411834	-0.495488
6	1.308973	0.835750	0.460162
6	-0.565677	-0.642646	-1.235804
6	0.798720	-0.680876	-0.945843
1	-2.181848	1.497107	-1.177398
1	0.519401	0.424198	1.069894
6	-1.544556	-1.667514	-0.683356
1	-2.015738	-2.171842	-1.533313
1	-0.986609	-2.439560	-0.144362
6	1.515922	-1.681951	-0.065866
1	0.934500	-1.892790	0.837218
1	1.647530	-2.635819	-0.589305
6	-1.763888	1.141219	0.942905
1	-2.715842	1.674058	1.056781
1	-1.064638	1.630510	1.624935
6	2.681811	0.352226	0.848376
1	2.775703	0.355438	1.938106
1	3.452004	1.021452	0.458009
6	-2.631446	-1.146785	0.263149
1	-3.368852	-0.548473	-0.283668
1	-3.168236	-2.003796	0.678966
6	2.879713	-1.090501	0.305841
1	3.410651	-1.721081	1.021417
1	3.492907	-1.052072	-0.599184
6	-2.011229	-0.309074	1.378996
1	-1.074847	-0.788065	1.690917
1	1.447849	-0.257687	-1.707583
1	-0.826222	-0.254070	-2.211806
1	-2.655698	-0.295758	2.261535

CTC-TS2:

6	0.353591	2.213133	0.722552
6	-0.888149	2.036436	0.099368
1	0.371487	2.892166	1.571376
1	-1.708424	2.679613	0.409715
6	1.447002	1.376309	0.551078
6	-1.204303	0.862924	-0.565481
6	0.455341	-0.628205	1.296558
6	-0.900567	-0.553201	0.998028
1	2.229089	1.472982	1.304633
1	-0.416398	0.332049	-1.078031
6	1.336567	-1.724960	0.730868
1	2.229961	-1.813083	1.357124
1	0.806115	-2.681533	0.818672
6	-1.695970	-1.559062	0.195621
1	-1.107626	-1.936554	-0.646205
1	-1.950208	-2.424876	0.818295
6	2.012941	0.996778	-0.802791

1	2.752122	1.777817	-1.024715
1	1.260117	1.086058	-1.586813
6	-2.587374	0.458882	-1.005229
1	-2.599649	0.319805	-2.090115
6	1.805467	-1.554648	-0.717759
1	2.339027	-2.463644	-1.010830
1	0.949758	-1.469079	-1.397820
6	-2.970518	-0.870747	-0.300843
1	-3.557015	-1.520541	-0.953351
1	-3.594919	-0.645156	0.568923
1	-1.509102	-0.006303	1.713373
1	-3.313014	1.241815	-0.772879
6	2.723945	-0.352233	-0.904612
1	3.528596	-0.398805	-0.160056
1	0.757541	-0.240990	2.260052
1	3.204699	-0.410173	-1.885505

CST-adduct:

6	-0.307939	2.244348	-0.493206
6	0.901341	2.073235	0.040792
1	-0.649222	3.228284	-0.799944
1	1.587776	2.904343	0.173714
6	-1.269905	1.079573	-0.590471
6	1.319635	0.683116	0.420252
6	-0.568824	-0.213861	-1.123789
6	0.918204	-0.291831	-0.697380
1	-2.063807	1.323426	-1.305581
1	0.802840	0.375051	1.340375
6	-1.407629	-1.473906	-0.848862
1	-2.271902	-1.462672	-1.524255
1	-0.825352	-2.361356	-1.111442
6	1.548246	-1.607499	-0.227255
1	0.915386	-2.088758	0.523076
1	1.689982	-2.324418	-1.038337
6	-1.957715	0.910944	0.785983
1	-2.565908	1.800949	0.973554
1	-1.199682	0.889432	1.574515
6	2.807163	0.376377	0.591402
1	3.205952	0.710880	1.550675
6	-1.943781	-1.574676	0.578464
1	-2.518825	-2.497381	0.694220
1	-1.116673	-1.620349	1.297499
6	2.895579	-1.164319	0.410402
1	3.050080	-1.662255	1.369092
1	3.741278	-1.432975	-0.224387
1	1.506787	0.039599	-1.562395
1	3.370398	0.886833	-0.196077
6	-2.804959	-0.353678	0.889151
1	-3.637346	-0.307045	0.176241
1	-0.555258	-0.100624	-2.211597
1	-3.243005	-0.427912	1.888161

CCC:

6	-1.514652	1.442554	1.142373
6	-2.541175	1.177935	0.108503
1	-1.867261	1.316235	2.164862
1	-3.460898	1.751299	0.206350
6	-0.250677	1.839108	0.982104

6	-2.480723	0.241482	-0.841783
6	1.569871	-0.966719	1.069202
6	0.518669	-1.780538	1.149587
1	-3.341455	0.111219	-1.493045
1	0.342167	1.979533	1.885026
1	-0.034210	-1.794340	2.087682
1	1.808608	-0.378988	1.952903
6	0.445721	2.233093	-0.291148
1	-0.142008	1.936448	-1.164224
1	0.459956	3.330363	-0.297027
6	2.490855	-0.775939	-0.108385
1	3.497381	-0.591872	0.281818
1	2.554120	-1.700477	-0.688806
6	2.138525	0.373979	-1.072646
1	2.967750	0.448970	-1.782265
1	1.266199	0.099046	-1.669785
6	1.910158	1.763446	-0.438383
1	2.406571	1.816302	0.537924
1	2.416587	2.500731	-1.065959
6	-0.091211	-2.616133	0.059137
1	-0.205960	-3.647589	0.406770
1	0.548200	-2.639939	-0.828569
6	-1.317488	-0.688057	-1.025130
1	-1.120737	-0.851765	-2.090100
1	-0.437567	-0.213877	-0.600742
6	-1.473998	-2.045705	-0.316789
1	-2.023438	-2.754544	-0.941996
1	-2.057250	-1.907799	0.599343

CCC-TS1:

6	0.078811	2.324386	-0.459896
6	1.428051	1.988897	-0.343195
1	-0.120210	3.127312	-1.165913
1	2.086804	2.633154	-0.920602
6	-1.007697	1.536962	-0.104208
6	2.010051	0.779688	0.022428
6	-0.568397	-0.224528	-1.374760
6	0.745904	-0.681614	-1.215505
1	3.019423	0.686490	-0.386182
1	-1.931086	1.816722	-0.609516
1	1.447212	-0.418684	-1.998687
1	-0.712191	0.421100	-2.232630
6	-1.274989	0.998849	1.289214
1	-0.411709	1.165937	1.932755
1	-2.061927	1.653239	1.685913
6	-1.791400	-1.099920	-1.071494
1	-2.431617	-1.069043	-1.957599
1	-1.462973	-2.138493	-0.984744
6	-2.650858	-0.785087	0.165395
1	-3.275406	-1.657457	0.374825
6	1.107468	-1.904105	-0.404429
1	1.462057	-2.698205	-1.069826
1	0.224452	-2.293395	0.103849
6	1.872972	-0.178324	1.176930
1	2.598680	0.107547	1.947657
1	0.888793	-0.160048	1.633851
6	2.173484	-1.581059	0.655484
1	2.178973	-2.325328	1.455762
1	3.169994	-1.587248	0.201053

6	-1.791924	-0.440905	1.378926
1	-0.958424	-1.147847	1.436006
1	-2.361822	-0.558068	2.303808
1	-3.337881	0.042879	-0.039122

CCC-TS2:

6	-0.244557	2.340067	-0.482537
6	1.097811	2.189067	-0.128524
1	-0.418887	3.117281	-1.223888
1	1.748526	2.945373	-0.560098
6	-1.277621	1.432671	-0.299836
6	1.776384	1.051119	0.296853
6	-0.326800	-0.292755	-1.439576
6	1.042998	-0.448028	-1.210948
1	2.848740	1.134081	0.102054
1	-2.129349	1.585668	-0.965666
1	1.702546	0.030639	-1.924709
1	-0.582333	0.290106	-2.315756
6	-1.726176	0.880020	1.032433
1	-0.907111	0.852793	1.747065
1	-2.420541	1.632665	1.428973
6	-1.348401	-1.372154	-1.109153
1	-2.280371	-1.125310	-1.628094
1	-1.005936	-2.319189	-1.543487
6	-1.689446	-1.602019	0.367681
1	-2.288094	-2.515368	0.439590
1	-0.782303	-1.785982	0.951446
6	-2.479098	-0.450460	0.979465
1	-3.399357	-0.311600	0.398251
1	-2.791572	-0.714918	1.993783
6	1.615849	-1.653800	-0.490434
1	2.363122	-2.127270	-1.132662
1	0.834525	-2.399022	-0.332347
6	1.562006	-0.004557	1.351046
1	2.002289	0.341618	2.293897
1	0.513834	-0.212701	1.532235
6	2.249609	-1.277398	0.867950
1	2.158438	-2.090367	1.592411
1	3.318485	-1.079139	0.740483

CSC adduct:

6	0.186482	2.127978	0.097008
6	1.456177	1.786929	-0.104745
1	-0.039297	3.102532	0.524243
1	2.240281	2.497252	0.149245
6	-0.990033	1.246424	-0.217934
6	1.922054	0.459761	-0.645377
6	-0.568802	0.037308	-1.077145
6	0.779294	-0.582090	-0.681349
1	2.319418	0.619672	-1.653556
1	-1.685473	1.835236	-0.834362
1	1.024798	-1.312439	-1.464142
1	-0.388973	0.445136	-2.080585
6	-1.774000	0.891424	1.059878
1	-1.109692	0.426395	1.793578
1	-2.136535	1.819192	1.514349
6	-1.705219	-0.989649	-1.219385
1	-2.448750	-0.584938	-1.916652

1	-1.311654	-1.901630	-1.680713
6	-2.432210	-1.323192	0.086895
1	-3.264632	-2.000035	-0.124892
1	-1.766830	-1.849478	0.778126
6	-2.939626	-0.049166	0.761412
1	-3.652659	0.453617	0.095962
1	-3.477510	-0.289070	1.682311
6	0.932318	-1.324978	0.653800
1	0.385014	-2.268734	0.684715
1	0.591395	-0.701300	1.484587
6	3.019411	-0.165422	0.268533
1	3.970895	-0.283173	-0.252255
1	3.200204	0.488731	1.125351
6	2.448491	-1.514614	0.745658
1	2.790563	-1.785553	1.745697
1	2.753411	-2.315699	0.065503

572 ring systems:

TTT:

6	0.333167	2.011146	0.614327
6	-1.029918	1.619848	0.986770
1	0.942156	2.520877	1.358510
1	-1.152548	1.294663	2.020211
6	0.904121	1.563426	-0.504968
6	-2.058069	1.463908	0.154423
1	0.284217	0.992042	-1.193559
1	-1.971592	1.822543	-0.870594
6	0.055364	-1.639089	-0.320588
6	-1.248057	-1.628651	-0.050022
1	0.371796	-1.286403	-1.300465
1	-1.594367	-1.992401	0.918288
6	-2.298625	-1.182256	-1.035926
1	-2.650415	-2.056783	-1.596393
1	-1.823489	-0.525516	-1.771975
6	-3.543754	-0.491565	-0.452743
6	1.136100	-2.115626	0.609816
1	0.655584	-2.621368	1.452831
1	1.747899	-2.871555	0.101068
6	2.069251	-1.023470	1.175405
6	-3.286201	0.685008	0.518463
1	-3.159314	0.302078	1.534869
1	-4.140182	-0.134919	-1.297876
1	-4.162332	-1.233169	0.062058
1	-4.177488	1.321237	0.527862
6	2.359246	1.623221	-0.847977
1	2.495382	2.166811	-1.789662
1	2.529992	-1.436197	2.079016
1	1.465676	-0.174334	1.497545
1	2.909860	2.171722	-0.076357
6	3.232392	-0.563778	0.280094
1	3.895588	0.056239	0.895311
1	3.816983	-1.453145	0.016048
6	2.956290	0.211084	-1.017635
1	3.914086	0.310957	-1.537850
1	2.314669	-0.372605	-1.685520

TTT-TS1:

6	0.200810	1.834849	0.597689
6	-1.170115	1.713652	0.863675
1	0.842148	2.275703	1.357474
1	-1.550667	1.999094	1.840325
6	0.800971	1.227187	-0.488529
6	-1.962932	0.978816	0.001632
1	0.198292	1.019029	-1.365381
1	-1.673614	1.000958	-1.044662
6	0.158186	-1.006528	-0.095018
6	-1.214003	-0.970151	0.127801
1	0.491420	-1.244428	-1.100986
1	-1.518618	-1.101883	1.166043
6	-2.279778	-1.401863	-0.855798
1	-2.347095	-2.493457	-0.895123
1	-2.007153	-1.069653	-1.863086
6	-3.631413	-0.807227	-0.417098
6	1.065500	-1.435081	1.040200
1	0.519749	-1.291512	1.978582
1	1.209277	-2.521188	0.944477
6	2.439804	-0.784382	1.196862
6	-3.405329	0.606006	0.194142
1	-3.654708	0.616663	1.258213
1	-4.328819	-0.772746	-1.255843
1	-4.080642	-1.460934	0.334068
1	-4.052476	1.341047	-0.292669
6	2.270787	1.370079	-0.806123
1	2.357976	2.082098	-1.635303
1	2.950714	-1.296272	2.019105
1	2.307430	0.249392	1.525000
1	2.800838	1.819261	0.040471
6	3.365592	-0.819932	-0.021692
1	4.352173	-0.483882	0.314595
1	3.495885	-1.855281	-0.355678
6	2.953250	0.059124	-1.217128
1	3.850344	0.286336	-1.799708
1	2.289561	-0.485638	-1.893612

TTT-TS2:

6	-0.174698	1.988562	0.154634
6	-1.530283	1.725571	-0.041402
1	0.093882	2.710245	0.922784
1	-2.239033	2.211466	0.625227
6	0.841655	1.239092	-0.404609
6	-1.995465	0.683290	-0.829401
1	0.656789	0.743783	-1.350687
1	-1.469015	0.442830	-1.746485
6	0.233113	-0.884904	0.338195
6	-1.127505	-1.026118	0.087911
1	-1.371243	-1.670514	-0.758648
1	0.522488	-0.592270	1.341033
6	2.281572	1.569505	-0.053316
1	2.287779	2.554807	0.421077
6	1.198103	-1.782597	-0.419685
1	1.387129	-2.655804	0.220615
1	0.673044	-2.172015	-1.298495
6	2.554705	-1.248473	-0.886837

1	3.072616	-2.076010	-1.382313
1	2.410987	-0.487345	-1.658779
6	-3.439936	0.258316	-0.683397
1	-3.847753	-0.095230	-1.631868
6	-2.219620	-0.993442	1.132051
1	-2.042251	-0.160037	1.818614
1	-2.211690	-1.911972	1.728979
6	-3.557477	-0.855294	0.402394
1	-3.781820	-1.809757	-0.082364
1	-4.378347	-0.652874	1.092797
1	2.874870	1.664181	-0.970489
6	2.983399	0.582743	0.893100
1	3.846213	1.082302	1.343098
1	2.308088	0.349005	1.718817
6	3.475157	-0.697057	0.201207
1	4.443307	-0.483675	-0.264219
1	3.660575	-1.472766	0.952367
1	-4.032945	1.126491	-0.386129

CAT-adduct:

6	-0.163292	2.146574	-0.390005
6	-1.482991	1.976981	-0.446039
1	0.241465	3.156197	-0.374464
1	-2.142309	2.839620	-0.494143
6	0.869329	1.039406	-0.354020
6	-2.075456	0.601856	-0.468497
1	1.529618	1.223309	-1.208396
1	-2.239288	0.300762	-1.515474
6	0.247189	-0.375758	-0.528152
6	-1.114965	-0.405230	0.156508
1	0.078902	-0.536409	-1.602961
1	-0.974902	-0.099013	1.204738
6	-1.938932	-1.695814	0.143585
1	-1.595913	-2.429507	0.874906
1	-1.868057	-2.163059	-0.844969
6	-3.394661	-1.217298	0.420139
6	1.145270	-1.501402	-0.010855
1	1.208682	-1.424341	1.081485
1	0.647952	-2.455295	-0.212436
6	2.558308	-1.565787	-0.598145
6	-3.372672	0.330356	0.295925
1	-3.311989	0.796360	1.284309
1	-4.087069	-1.653948	-0.301825
1	-3.733732	-1.526737	1.409761
1	-4.259376	0.725761	-0.202783
6	1.723270	1.183404	0.924423
1	1.916391	2.250210	1.067784
1	2.496811	-1.760833	-1.673713
1	3.053650	-2.437292	-0.158671
1	1.112280	0.881620	1.781175
6	3.434539	-0.321636	-0.346121
1	4.481234	-0.633638	-0.293899
1	3.378070	0.365496	-1.193669
6	3.080942	0.425629	0.942439
1	3.093054	-0.288107	1.772026
1	3.879255	1.141166	1.154110

TTC:

6	0.573045	-1.720007	-0.352429
6	-0.838472	-1.678612	-0.746073
1	1.280686	-1.980616	-1.134705
1	-1.024888	-1.669281	-1.818978
6	1.032572	-1.286040	0.824204
6	-1.881954	-1.501442	0.068497
1	0.311378	-1.016305	1.588831
1	-1.736142	-1.539226	1.146566
6	-0.097504	1.539711	0.787238
6	-1.414264	1.371151	0.916183
1	-1.812873	1.270510	1.925076
1	0.499227	1.568167	1.697557
6	-3.239375	-1.091683	-0.406143
1	-4.014636	-1.772118	-0.038663
6	-2.451514	1.360422	-0.178283
1	-2.897399	2.361162	-0.231338
1	-1.981045	1.177960	-1.150157
6	-3.579435	0.341030	0.060172
1	-3.818899	0.325842	1.129214
1	-4.488115	0.663529	-0.455209
6	2.468451	-1.005543	1.162700
1	2.477587	-0.163934	1.864278
1	2.908063	-1.843964	1.716437
6	0.655077	1.741926	-0.504572
1	0.301348	1.011040	-1.241038
1	0.376057	2.723016	-0.905607
6	2.199619	1.668869	-0.396701
1	2.611865	2.540515	-0.909117
1	2.499570	1.782376	0.650731
6	3.373808	-0.664827	-0.027846
1	4.335415	-0.338283	0.381228
1	3.587899	-1.572722	-0.601479
1	-3.263528	-1.129099	-1.499660
6	2.860944	0.410888	-1.006034
1	2.159576	-0.033420	-1.715173
1	3.722868	0.719803	-1.604272

TTC-TS1:

6	-0.003568	2.176255	-0.315472
6	1.347468	2.020237	0.024410
1	-0.274064	2.974745	-1.001949
1	2.077703	2.712327	-0.386925
6	-0.949263	1.217228	-0.010748
6	1.793017	0.855088	0.618111
1	-0.811026	0.648402	0.901088
1	1.099183	0.325075	1.264962
6	-0.111525	-0.714317	-0.887752
6	1.271842	-0.602194	-0.873789
1	1.711056	-0.063091	-1.709562
1	-0.628348	-0.401924	-1.787596
6	3.236761	0.484982	0.838730
1	3.896236	1.296252	0.522085
1	3.412902	0.322108	1.905923
6	2.238141	-1.557619	-0.209046
1	2.414947	-2.424501	-0.856438
1	1.821326	-1.941429	0.727313
6	3.549131	-0.814229	0.052678

1	4.275871	-1.438855	0.575982
1	3.990164	-0.549781	-0.913333
6	-2.354530	1.267909	-0.556273
1	-2.635263	2.307242	-0.754512
1	-2.381179	0.767756	-1.531607
6	-0.813645	-1.757869	-0.048821
1	-0.484570	-2.743512	-0.403734
1	-0.462570	-1.697224	0.990970
6	-2.352435	-1.741908	-0.047599
1	-2.720741	-1.574540	-1.066735
1	-2.681462	-2.747736	0.225504
6	-3.403511	0.621360	0.353422
1	-3.627437	1.293435	1.187698
1	-4.332591	0.516419	-0.215686
6	-3.012810	-0.748919	0.929316
1	-2.348566	-0.615441	1.789303
1	-3.922021	-1.201747	1.334246

TTC-TS2:

6	0.460757	-1.526592	-0.537278
6	-0.896920	-1.504661	-0.879885
1	1.183838	-1.611608	-1.341374
1	-1.151872	-1.499758	-1.937297
6	0.897518	-1.155527	0.720530
6	-1.899903	-1.227200	0.030439
1	0.243461	-1.353999	1.563096
1	-1.794822	-1.586944	1.048133
6	0.063071	0.893854	0.839346
6	-1.314808	0.738631	0.901100
1	-1.716234	0.506767	1.886879
1	0.599821	0.934406	1.781980
6	-3.283882	-0.858504	-0.436084
1	-4.036640	-1.558779	-0.064057
6	-2.323442	1.392861	-0.013510
1	-2.513759	2.422847	0.312860
1	-1.934294	1.443395	-1.035090
6	-3.615305	0.579015	0.018340
1	-3.992046	0.562149	1.046669
1	-4.398056	1.019218	-0.603700
6	2.350768	-1.017505	1.092450
1	2.438324	-0.249189	1.868756
1	2.684016	-1.946313	1.571798
6	0.702533	1.619262	-0.314826
1	0.364648	1.158936	-1.253619
1	0.300712	2.641194	-0.329391
6	2.237975	1.695561	-0.310015
1	2.522278	2.590584	-0.869617
1	2.600811	1.855269	0.712614
6	3.320604	-0.689197	-0.046711
1	4.295489	-0.495076	0.411144
1	3.459259	-1.575859	-0.673736
1	-3.307286	-0.902056	-1.528991
6	2.955508	0.499017	-0.958141
1	2.338209	0.157493	-1.793098
1	3.887303	0.853233	-1.408490

CSC-adduct:

6	0.630226	-1.706155	-0.293730
6	-0.597799	-1.765913	-0.802845
1	1.435551	-2.276757	-0.749275
1	-0.799030	-2.382953	-1.675308
6	0.948015	-0.846297	0.909060
6	-1.768396	-1.050631	-0.189794
1	0.625334	-1.404873	1.798812
1	-2.421689	-1.820855	0.243386
6	0.063040	0.421044	0.888593
6	-1.404060	-0.063359	0.959408
1	-1.491603	-0.601391	1.907696
1	0.274710	0.975928	1.812968
6	-2.656683	-0.240894	-1.149310
1	-3.258627	-0.879468	-1.799925
6	-2.495722	1.037553	0.903196
1	-2.980588	1.170145	1.871849
1	-2.063454	2.003122	0.637583
6	-3.497131	0.599871	-0.183949
1	-4.274674	-0.032643	0.255647
1	-3.993608	1.444462	-0.664508
6	2.449008	-0.586044	1.121880
1	2.541257	0.228825	1.847589
1	2.887606	-1.464399	1.605901
6	0.334010	1.370998	-0.288406
1	-0.020332	0.915858	-1.218578
1	-0.259924	2.276289	-0.142336
6	1.791518	1.797390	-0.506363
1	1.783551	2.657941	-1.181180
1	2.232181	2.153213	0.433063
6	3.297604	-0.265933	-0.116081
1	4.244372	0.154936	0.237451
1	3.560341	-1.193338	-0.633882
1	-2.046142	0.405822	-1.786410
6	2.660693	0.696933	-1.126744
1	2.039183	0.130904	-1.828216
1	3.459649	1.147853	-1.721821

TCT:

6	-0.055699	-1.938658	-0.293109
6	-1.261618	-1.844787	-1.122395
1	0.715446	-2.581496	-0.712670
1	-1.131538	-2.269019	-2.115260
6	0.256382	-1.228868	0.794500
6	-2.454436	-1.285570	-0.886920
1	-0.471526	-0.547453	1.213070
6	0.428591	1.848952	0.140297
6	-0.827684	1.723714	-0.281392
1	-3.156559	-1.291944	-1.719102
1	0.604148	1.874603	1.218367
1	-1.038339	1.698376	-1.350174
6	1.654983	2.049577	-0.704748
1	1.947898	3.103459	-0.620240
1	1.416496	1.875237	-1.758984
6	2.855133	1.182705	-0.287139
1	3.759671	1.618124	-0.718932
1	2.979850	1.258677	0.799612
6	1.622391	-1.190862	1.431814

1	1.710887	-0.246146	1.978083
1	1.714209	-1.977312	2.189935
6	2.788722	-1.310309	0.439064
1	3.726338	-1.190320	0.992404
6	-3.013082	-0.678312	0.365808
1	-2.420201	-0.938877	1.243801
6	-2.010801	1.720041	0.653262
1	-2.377856	2.752222	0.718177
1	-1.671757	1.462084	1.663720
6	-3.215916	0.848442	0.279190
1	-4.033765	1.123605	0.951380
1	-3.551729	1.107826	-0.731244
1	-3.999531	-1.129645	0.519407
1	2.812731	-2.321764	0.021929
6	2.746823	-0.297377	-0.712704
1	1.820304	-0.436768	-1.275414
1	3.562079	-0.535613	-1.401039

TCT-TS1:

6	0.080133	1.819262	0.358591
6	-1.111529	1.696513	1.073067
1	0.858915	2.429007	0.812415
1	-1.116687	2.127754	2.070706
6	0.463445	1.001474	-0.693862
6	-2.155980	0.837570	0.755332
1	-0.282709	0.606413	-1.368777
6	0.205109	-0.978557	0.316532
6	-1.157551	-1.140526	0.528691
1	-2.852392	0.660742	1.576651
1	0.597998	-1.390104	-0.605385
1	-1.492932	-1.328578	1.544810
6	1.156632	-0.908469	1.479921
1	1.291235	-1.928282	1.864702
1	0.674185	-0.341716	2.285840
6	2.532469	-0.300969	1.188695
1	2.457674	0.788354	1.201556
1	3.199729	-0.562240	2.015403
6	1.843976	1.129303	-1.308210
1	1.729461	1.558863	-2.309939
1	2.434750	1.848927	-0.732283
6	-2.851919	0.665064	-0.576034
1	-2.220825	0.970022	-1.411584
6	-2.035152	-1.649019	-0.590876
1	-2.297275	-2.699227	-0.428367
1	-1.467398	-1.605595	-1.527321
6	-3.293293	-0.788058	-0.725754
1	-3.811203	-0.968877	-1.670626
1	-3.994085	-1.029649	0.081435
1	-3.722820	1.329870	-0.581546
6	2.630067	-0.182649	-1.442952
1	3.462807	-0.011536	-2.130608
1	1.996795	-0.922636	-1.938987
6	3.206884	-0.743899	-0.118160
1	3.220638	-1.838579	-0.164336
1	4.254393	-0.435173	-0.053638

TCT-TS2:

6	0.353814	-1.499300	-0.557804
6	-0.751662	-1.369108	-1.404915
1	1.271862	-1.855064	-1.014232
1	-0.558451	-1.528631	-2.462921
6	0.441622	-0.905556	0.690952
6	-1.962576	-0.780359	-1.075790
1	-0.447173	-0.828338	1.300713
6	0.012747	1.183669	0.175576
6	-1.323814	1.230507	-0.189588
1	-2.568784	-0.492347	-1.936054
1	0.244121	1.361815	1.222752
1	-1.574759	1.632492	-1.167208
6	1.079875	1.565380	-0.816936
1	0.894953	2.603873	-1.116998
1	0.939614	0.962881	-1.725573
6	2.536549	1.451162	-0.339646
1	3.130091	2.148336	-0.937075
1	2.616428	1.804046	0.695988
6	1.722041	-0.868774	1.487756
1	1.716588	0.035778	2.106133
1	1.720537	-1.702201	2.201091
6	3.030255	-0.920220	0.692040
1	3.841763	-0.736942	1.403064
6	-2.831149	-1.033326	0.134126
1	-2.269114	-1.472012	0.959983
6	-2.398381	1.272130	0.868828
1	-2.808640	2.283335	0.957875
1	-1.946069	1.028928	1.837293
6	-3.507617	0.265251	0.562386
1	-4.172269	0.121507	1.417828
1	-4.121422	0.634442	-0.267242
1	-3.585885	-1.773285	-0.155649
1	3.189782	-1.936296	0.316968
6	3.175351	0.060167	-0.488285
1	2.777347	-0.388410	-1.402053
1	4.247149	0.186351	-0.666882

CAC adduct:

6	0.220715	-1.543948	-0.305289
6	-0.780094	-1.267069	-1.138084
1	0.791590	-2.459527	-0.441780
1	-1.006318	-1.954444	-1.950401
6	0.585686	-0.654471	0.855062
6	-1.677984	-0.063270	-1.021991
1	-0.024372	-0.979244	1.708478
6	0.157104	0.800810	0.581964
6	-1.330543	0.837104	0.197109
1	-1.601120	0.510616	-1.951378
1	0.283633	1.350360	1.524731
1	-1.576933	1.870809	-0.076924
6	0.947448	1.550783	-0.504192
1	0.623529	2.596582	-0.461788
1	0.642284	1.178305	-1.489010
6	2.477061	1.498348	-0.447367
1	2.858118	2.257979	-1.135932
1	2.839537	1.781294	0.548012
6	2.037256	-0.815825	1.340042

1	2.247981	0.010898	2.026965
1	2.098063	-1.725951	1.945675
6	3.138743	-0.892092	0.276411
1	4.097327	-0.767242	0.790362
6	-3.163878	-0.492334	-0.801761
1	-3.208318	-1.571273	-0.631238
6	-2.341928	0.415158	1.268892
1	-2.423199	1.142690	2.079604
1	-2.064386	-0.550411	1.704809
6	-3.630651	0.250598	0.460706
1	-4.417169	-0.283439	0.996412
1	-4.021327	1.238063	0.196064
1	-3.788388	-0.275579	-1.669849
1	3.162138	-1.896344	-0.157762
6	3.037626	0.132401	-0.861166
1	2.397492	-0.267104	-1.654498
1	4.030475	0.255809	-1.302573

CTT:

6	0.200172	1.919536	-0.929673
6	1.633343	2.110084	-0.631256
1	-0.021482	1.632274	-1.958594
1	2.184502	2.757909	-1.309310
6	-0.813922	2.001240	-0.070315
6	2.321466	1.458033	0.314141
1	-0.612561	2.328117	0.950102
6	-0.054719	-1.444728	-1.259486
6	1.235600	-1.128391	-1.180193
1	3.393541	1.636837	0.377502
1	1.607314	-0.441111	-1.934484
6	-2.234007	1.610032	-0.378315
1	-2.856313	2.505017	-0.492805
1	-2.261281	1.081415	-1.337197
6	1.743791	0.478883	1.294646
6	2.278515	-1.607102	-0.196221
6	2.278639	-0.959138	1.211200
1	1.663155	-1.561819	1.886764
6	-0.881429	-2.335155	-0.374763
1	-0.337609	-2.597131	0.539181
1	-1.082568	-3.272405	-0.906939
6	-2.220658	-1.660737	-0.025299
1	-2.932505	-2.412434	0.325338
1	-2.645006	-1.250152	-0.948774
6	-2.846578	0.743481	0.737722
1	-3.885116	0.507182	0.482383
1	-0.616691	-0.998772	-2.080514
1	0.669160	0.448787	1.152936
1	1.917036	0.846469	2.312621
1	3.298171	-1.007028	1.606303
1	-2.883366	1.347015	1.651185
6	-2.078812	-0.550530	1.032264
1	-1.020617	-0.307399	1.142183
1	-2.400500	-0.938829	2.002649
1	3.252949	-1.425584	-0.656290
1	2.201386	-2.691411	-0.070958

CTT-TS1:

6	0.296208	2.224393	-0.119440
6	1.652545	2.058760	-0.388064
1	-0.186930	3.105199	-0.536545
1	2.105022	2.768689	-1.074744
6	-0.525641	1.240445	0.402691
6	2.367972	0.900826	-0.102255
1	-0.107328	0.505494	1.072454
6	-0.057277	-0.497544	-1.093215
6	1.337606	-0.598048	-1.197379
1	3.334333	0.843006	-0.601416
1	1.784714	-0.221038	-2.108887
1	-0.529804	0.084998	-1.874756
6	-2.011678	1.515155	0.530748
1	-2.309429	1.403769	1.581452
1	-2.178903	2.564228	0.271685
6	2.368058	0.140808	1.220211
1	1.730121	0.643909	1.948138
1	3.387446	0.203647	1.611956
6	2.106785	-1.665653	-0.445442
1	1.752453	-2.676141	-0.670625
1	3.159562	-1.628730	-0.738651
6	1.981148	-1.343655	1.045788
1	0.945761	-1.500274	1.363609
1	2.602907	-1.998436	1.660279
6	-0.892770	-1.669458	-0.575295
1	-1.467009	-2.033203	-1.438043
6	-1.884283	-1.502678	0.586187
1	-1.396600	-1.027693	1.442211
1	-2.164246	-2.505335	0.924579
6	-2.946891	0.652760	-0.329302
1	-3.917728	1.152289	-0.400087
1	-0.222258	-2.488539	-0.311550
1	-2.554371	0.602418	-1.348339
6	-3.165760	-0.751897	0.230198
1	-3.735820	-1.343523	-0.494544
1	-3.788013	-0.680009	1.129239

CTT-TS2:

6	0.056462	2.278349	-0.196357
6	1.451203	2.219299	-0.113639
1	-0.355272	3.118772	-0.752454
1	1.985983	3.015155	-0.624894
6	-0.805516	1.238678	0.091223
6	2.204448	1.110137	0.240527
1	-0.586965	0.573297	0.909972
6	0.071918	-0.492609	-1.110903
6	1.457631	-0.393307	-1.184153
1	3.259209	1.180997	-0.033570
1	1.860766	0.154825	-2.026676
6	-2.248725	1.289257	-0.347207
1	-2.582589	2.331114	-0.384740
1	-2.325398	0.921787	-1.377603
6	2.001242	0.128726	1.367940
6	2.373213	-1.435187	-0.568235
6	2.545577	-1.249242	0.962401
1	2.034896	-2.037098	1.521241
6	-0.565839	-1.682716	-0.422119

1	-0.137832	-1.811836	0.580146
1	-0.253046	-2.574486	-0.982874
6	-2.099103	-1.727440	-0.312116
1	-2.374939	-2.778394	-0.193786
1	-2.547260	-1.407522	-1.260469
6	-3.200283	0.478326	0.535274
1	-4.169263	0.416390	0.029928
1	-0.497333	-0.065306	-1.928981
1	0.956266	0.054604	1.657779
1	2.534471	0.500478	2.249777
1	3.604866	-1.326870	1.219744
1	-3.374615	1.011929	1.474716
6	-2.714434	-0.941618	0.861309
1	-1.986539	-0.908747	1.679085
1	-3.567998	-1.499292	1.256173
1	3.349269	-1.350260	-1.049521
1	2.006560	-2.443449	-0.786656

CAC-adduct:

6	0.483278	2.136385	-0.177801
6	1.772430	1.940106	-0.425573
1	0.070918	3.141075	-0.190582
1	2.431106	2.776221	-0.638017
6	-0.460261	0.987800	0.107217
6	2.341894	0.556774	-0.348708
1	-0.315532	0.657743	1.148106
6	-0.120540	-0.186824	-0.857321
6	1.406443	-0.528545	-0.953310
1	3.288379	0.517253	-0.893228
1	1.632105	-0.635293	-2.017451
6	-1.910337	1.481755	-0.063797
1	-1.948619	2.544810	0.191568
1	-2.161478	1.427506	-1.129244
6	2.607502	0.099528	1.126097
6	1.889688	-1.782477	-0.203684
6	2.016657	-1.319101	1.247486
1	1.026179	-1.277223	1.711859
6	-0.945308	-1.466517	-0.654570
1	-0.631448	-1.959768	0.271565
1	-0.678200	-2.150624	-1.467673
6	-2.471408	-1.344035	-0.592489
1	-2.883360	-2.351594	-0.698468
1	-2.855537	-0.767272	-1.441496
6	-2.991813	0.783653	0.763903
1	-3.962707	1.131624	0.396788
1	-0.393414	0.208890	-1.843914
1	2.149214	0.792749	1.833365
1	3.680324	0.095193	1.329274
1	2.633653	-1.983232	1.855175
1	-2.922233	1.121047	1.802926
6	-2.959579	-0.749151	0.732853
1	-2.305112	-1.120309	1.529585
1	-3.959093	-1.124605	0.967627
1	2.885864	-2.033628	-0.584734
1	1.267107	-2.666670	-0.334855

CTC:

6	-1.424328	1.820843	-1.311796
6	-0.164263	2.253927	-0.690183
1	-1.526422	2.034305	-2.373651
1	0.203504	3.246017	-0.948793
6	-2.428658	1.179303	-0.706145
6	0.572735	1.474620	0.103355
6	1.332858	-2.035106	-0.865563
6	2.415792	-1.287743	-0.657520
1	-3.260679	0.869318	-1.334578
1	0.225445	0.461758	0.287961
6	0.173448	-2.260245	0.061247
1	0.102119	-3.323594	0.318735
1	0.329216	-1.731027	1.003893
6	2.826465	-0.536964	0.581116
1	2.105601	-0.675960	1.391613
1	3.764487	-0.978548	0.933733
6	-2.594200	0.916817	0.770849
1	-3.660657	1.036108	0.986954
1	-2.068764	1.698154	1.327209
6	1.870124	1.859926	0.745532
1	1.756698	1.788436	1.834968
1	2.097325	2.905709	0.518728
6	-1.144620	-1.818048	-0.599900
1	-0.978378	-0.876638	-1.127240
1	-1.414429	-2.554081	-1.364187
6	3.055371	0.971699	0.333533
1	3.934181	1.305112	0.891728
1	3.274241	1.135498	-0.726137
6	-2.150638	-0.455712	1.334146
1	-2.730030	-0.635226	2.243988
1	3.128738	-1.206950	-1.476616
1	1.233810	-2.508446	-1.841217
1	-1.110887	-0.384038	1.663015
6	-2.303430	-1.659353	0.393375
1	-2.376612	-2.574563	0.991269
1	-3.248456	-1.575135	-0.153662

CTC-TS1:

6	0.254673	2.193556	-0.969032
6	1.497174	1.878715	-0.415149
1	0.259761	2.755781	-1.899505
1	2.388951	2.306240	-0.866922
6	-0.933701	1.586246	-0.579692
6	1.643411	0.758002	0.394118
6	-0.327825	-0.608865	-1.252592
6	1.010940	-0.772942	-0.889302
1	-1.767340	1.733713	-1.261714
1	0.817355	0.483595	1.032453
6	-1.422713	-1.571359	-0.830591
1	-1.529091	-2.282867	-1.658794
1	-1.110496	-2.170071	0.030513
6	1.563057	-1.797827	0.077311
1	0.925756	-1.874064	0.964424
1	1.594049	-2.794003	-0.377531
6	-1.350521	1.505505	0.886293
1	-2.223856	2.164349	0.978979

1	-0.564755	1.972341	1.486162
6	2.958699	0.164371	0.828756
1	3.080230	0.296428	1.907662
1	3.790514	0.684263	0.347571
6	-2.794905	-0.948266	-0.544900
1	-2.952816	-0.103331	-1.219517
1	-3.581816	-1.672111	-0.775347
6	2.976333	-1.349991	0.471150
1	3.373927	-1.953182	1.289260
1	3.636368	-1.507226	-0.386396
6	-1.725321	0.165427	1.519598
1	-1.915314	0.342364	2.583198
1	1.736937	-0.476774	-1.640978
1	-0.494523	-0.195790	-2.241053
1	-0.871831	-0.518173	1.474213
6	-2.950462	-0.520537	0.919506
1	-3.161015	-1.415478	1.515700
1	-3.824028	0.131784	1.024771

CTC-TS2:

6	-0.209018	2.205523	0.882597
6	-1.489247	1.953079	0.383976
1	-0.145668	2.825368	1.772723
1	-2.333159	2.425399	0.882185
6	0.927794	1.497493	0.518282
6	-1.739082	0.860743	-0.434245
6	0.227818	-0.641313	1.222982
6	-1.108587	-0.718625	0.825571
1	1.793462	1.671916	1.155623
1	-0.984209	0.583971	-1.151484
6	1.238060	-1.725125	0.835818
1	1.821413	-1.923759	1.740755
1	0.676216	-2.646216	0.641106
6	-1.667483	-1.708782	-0.168584
1	-1.009454	-1.771931	-1.042525
1	-1.715539	-2.716376	0.261403
6	1.304106	1.118226	-0.901871
1	1.020863	1.939909	-1.570358
1	0.761408	0.241600	-1.254272
6	-3.097348	0.303230	-0.764355
1	-3.858400	0.760725	-0.127524
6	2.264257	-1.581506	-0.304653
1	2.849065	-2.505531	-0.292802
1	1.768253	-1.564249	-1.280746
6	-3.076630	-1.243986	-0.568395
1	-3.766803	-1.510691	0.235902
1	-1.836709	-0.395726	1.563468
6	2.792981	0.812919	-1.036197
1	3.384655	1.695228	-0.771933
1	3.011619	0.586786	-2.085069
1	0.386459	-0.242534	2.216078
6	3.211414	-0.379473	-0.169782
1	3.252907	-0.078341	0.882692
1	4.229090	-0.671304	-0.441833
1	-3.357179	0.547513	-1.798196
1	-3.422491	-1.766164	-1.462077

CST adduct:

6	0.046541	2.110975	0.051602
6	1.251286	1.886645	0.575999
1	-0.369977	3.115306	0.097676
1	1.794869	2.698009	1.053462
6	-0.845578	1.069124	-0.596521
6	1.872483	0.524438	0.529205
6	-0.313248	-0.375412	-0.394731
6	1.207263	-0.322849	-0.551606
1	-0.855492	1.269757	-1.677746
1	1.731883	0.026169	1.500903
6	-0.765510	-0.966330	0.950029
1	-0.137529	-1.830262	1.181422
1	-0.562767	-0.230369	1.734556
6	2.054064	-1.597439	-0.554845
1	1.744856	-2.269404	0.249798
1	1.972365	-2.151243	-1.491915
6	-2.278167	1.265520	-0.080325
1	-2.597096	2.282113	-0.332738
1	-2.264578	1.220633	1.014057
6	3.354319	0.402464	0.159372
1	4.025534	0.657997	0.981133
1	3.573193	1.080672	-0.670864
6	-2.256966	-1.407850	1.027213
1	-2.298763	-2.469115	1.284851
1	-2.751247	-0.883317	1.850828
6	3.498245	-1.077862	-0.292914
1	3.989418	-1.674226	0.477822
1	4.114573	-1.151061	-1.190191
6	-3.320947	0.280756	-0.615324
1	-3.393529	0.382766	-1.703267
1	1.404952	0.196066	-1.501799
1	-0.706755	-0.998658	-1.202810
1	-4.291887	0.590211	-0.216709
6	-3.081904	-1.200118	-0.248137
1	-4.050458	-1.689722	-0.114846
1	-2.602856	-1.724695	-1.077729

CCC :

6	-1.992839	1.265504	-1.276932
6	-1.589202	2.454976	-0.499773
1	-2.008106	1.401162	-2.356889
1	-2.176124	3.354867	-0.672554
6	-2.365542	0.076420	-0.797636
6	-0.541599	2.536563	0.323317
6	2.292071	-1.314872	-0.839923
6	2.933461	-0.164778	-0.635877
1	-0.349420	3.490861	0.811138
1	-2.623800	-0.690254	-1.525828
6	-2.569619	-0.305608	0.643589
1	-2.552370	0.594440	1.263718
1	-3.582623	-0.719991	0.712061
6	1.307393	-1.984582	0.075608
1	1.684670	-2.966861	0.383653
1	1.184182	-1.397162	0.987455
6	-0.049182	-2.173001	-0.628846

1	0.052876	-2.970164	-1.372568
6	2.884009	0.721221	0.582570
1	3.888269	1.118207	0.755652
1	2.618467	0.148391	1.475972
6	0.447206	1.444591	0.604652
1	0.326507	1.099709	1.640200
1	0.244011	0.590328	-0.045064
6	1.900288	1.894807	0.423685
1	2.132462	2.673667	1.157490
1	2.023389	2.344275	-0.567303
6	-1.599121	-1.345223	1.249146
1	-0.698546	-0.836626	1.594549
1	-0.284879	-1.263957	-1.187392
1	3.564868	0.204267	-1.441561
1	-2.076359	-1.743777	2.148560
1	2.447926	-1.815562	-1.794279
6	-1.198347	-2.508319	0.331056
1	-0.897142	-3.362750	0.946867
1	-2.072111	-2.839270	-0.241693

CCC-TS1:

6	0.456627	2.297010	-0.621347
6	1.779578	1.885539	-0.475518
1	0.307152	3.054569	-1.387839
1	2.480853	2.439845	-1.094283
6	-0.679903	1.626247	-0.188248
6	2.276319	0.662751	-0.025019
6	-0.289228	-0.286815	-1.388283
6	1.001486	-0.786529	-1.153989
1	3.278814	0.481107	-0.421208
1	-1.584560	1.945077	-0.699805
6	-0.938137	1.252565	1.259075
1	-0.024900	1.402124	1.835907
1	-1.638752	2.013554	1.629401
6	-1.543352	-1.142978	-1.206683
1	-1.759648	-1.536589	-2.206898
1	-1.335888	-2.022063	-0.593175
6	-2.816944	-0.474693	-0.677848
1	-3.678985	-1.057460	-1.015991
6	1.282687	-1.979156	-0.264674
1	1.596967	-2.833558	-0.872481
1	0.379100	-2.287558	0.261597
6	2.097341	-0.192197	1.204218
1	2.824965	0.130245	1.958069
1	1.108593	-0.109820	1.646119
6	2.351086	-1.638432	0.787260
1	2.311923	-2.326830	1.634681
1	3.352408	-1.717035	0.350593
6	-1.545706	-0.114438	1.557285
1	-0.828518	-0.894425	1.289944
1	-2.933340	0.510197	-1.132897
1	1.734569	-0.614191	-1.933604
1	-1.698179	-0.194882	2.638555
1	-0.366299	0.351481	-2.262671
6	-2.875995	-0.396872	0.857787
1	-3.245795	-1.357945	1.231043
1	-3.615628	0.352140	1.160842

CCC-TS2:

6	-0.481696	2.399526	0.434343
6	-1.750107	2.020117	-0.007525
1	-0.511452	3.201482	1.170256
1	-2.548425	2.658416	0.362471
6	0.721483	1.704889	0.382344
6	-2.182038	0.777736	-0.453541
6	-0.018137	-0.163337	1.511351
6	-1.321771	-0.534820	1.171348
1	-3.262601	0.651180	-0.348835
1	1.425832	2.048157	1.143429
6	1.511907	1.301307	-0.854510
1	0.936089	0.771877	-1.610078
1	1.765495	2.261450	-1.320030
6	1.166855	-1.110407	1.356667
1	2.048419	-0.638302	1.799509
1	0.959220	-1.983474	1.987024
6	1.509230	-1.591561	-0.066876
1	1.637193	-2.678038	-0.069452
1	0.668313	-1.395955	-0.731719
6	2.827597	0.568018	-0.549183
1	3.605491	0.926653	-1.228446
6	-1.647509	-1.830655	0.453551
1	-2.462944	-2.325238	0.986738
1	-0.797052	-2.512920	0.504816
6	-1.647277	-0.204139	-1.455490
1	-2.073777	0.027372	-2.439195
1	-0.571142	-0.131989	-1.546132
6	-2.062151	-1.609951	-1.026438
1	-1.630834	-2.370819	-1.681943
1	-3.149399	-1.694041	-1.118122
1	-2.106479	-0.136851	1.802372
1	3.158072	0.855028	0.454106
1	0.061878	0.480271	2.379212
6	2.767763	-0.958385	-0.662377
1	2.827545	-1.243803	-1.718155
1	3.655657	-1.380488	-0.179804

CSC-adduct:

6	0.447675	1.996721	-0.243903
6	1.704061	1.681146	-0.541395
1	0.208863	3.027934	0.008155
1	2.462442	2.460906	-0.532169
6	-0.721232	1.045316	-0.263461
6	2.172220	0.290069	-0.880779
6	-0.322007	-0.362437	-0.777829
6	1.125966	-0.750087	-0.443093
1	2.352798	0.234819	-1.959809
1	-1.415039	1.470508	-0.997144
6	-1.462373	1.062975	1.090153
1	-0.860134	0.540211	1.836750
1	-1.501541	2.105050	1.420831
6	-1.278124	-1.464066	-0.311371
1	-0.904835	-2.424274	-0.684322
1	-1.236015	-1.531189	0.780992
6	-2.739471	-1.310107	-0.741714
1	-3.291725	-2.165068	-0.338262
6	1.486641	-0.987238	1.031180

1	1.007585	-1.870759	1.457328
1	1.199196	-0.118357	1.629413
6	3.458381	-0.088206	-0.093955
1	4.214449	-0.518055	-0.753146
1	3.900324	0.801476	0.360273
6	3.014218	-1.105196	0.985666
1	3.484187	-0.921696	1.952837
1	3.288298	-2.118480	0.679285
6	-2.909235	0.489412	1.086171
1	-2.979556	-0.330411	1.808285
1	-2.811920	-1.385292	-1.831660
1	1.338877	-1.686378	-0.976835
1	-3.593830	1.261260	1.446237
1	-0.374557	-0.318646	-1.874481
6	-3.422877	-0.013870	-0.266825
1	-4.498865	-0.192011	-0.187886
1	-3.312057	0.771865	-1.017736

672 ring systems:

TTT:

6	-0.142414	-2.530443	-0.012897
6	-1.530382	-2.146824	-0.308555
1	0.164068	-3.540617	-0.281086
1	-1.927401	-2.499553	-1.260371
6	0.767643	-1.681154	0.465930
6	-2.310757	-1.379535	0.453786
1	0.456896	-0.654504	0.657131
1	-1.949318	-1.070311	1.433854
6	0.928388	2.071781	0.555669
6	-0.178458	2.266669	-0.155250
1	0.824430	1.662681	1.562882
1	-0.100829	2.674986	-1.163181
6	-1.556819	1.949111	0.354131
1	-2.034037	2.858770	0.740165
1	-1.463383	1.268768	1.206810
6	-2.490663	1.331146	-0.697263
6	2.342826	2.310854	0.114416
1	2.359125	2.701671	-0.908309
1	2.800217	3.069244	0.758951
6	3.161156	1.011548	0.201026
6	-3.649904	-0.866292	0.009552
1	-3.858352	-1.269379	-0.986356
1	-2.795065	2.111607	-1.400144
1	-1.938686	0.584013	-1.276786
1	-4.440355	-1.229533	0.674934
6	2.225627	-1.993552	0.641387
1	2.369743	-3.075112	0.712361
1	4.230623	1.234448	0.142899
1	2.583759	-1.566366	1.583160
1	2.994810	0.573682	1.191806
6	2.784081	0.007456	-0.893327
1	3.324651	0.263768	-1.809783
1	1.720074	0.110844	-1.129324
6	3.068641	-1.454197	-0.535389
1	4.131627	-1.584570	-0.304097
1	2.854215	-2.074031	-1.411533
6	-3.723848	0.675742	-0.046717
1	-4.636595	0.947853	-0.582373

1	-3.840917	1.067789	0.969398

TTT-TS-cbc:

6	0.814486	-1.617230	-0.228068
6	-0.471789	-1.741879	-0.787685
1	1.660317	-1.967649	-0.810155
1	-0.567028	-2.132790	-1.797740
6	1.043714	-0.865977	0.902288
6	-1.565092	-1.173289	-0.177957
1	0.233577	-0.747301	1.613653
1	-1.534517	-1.083486	0.903185
6	0.279946	1.158252	0.170102
6	-1.061936	1.006039	-0.119150
1	0.556643	1.530361	1.154956
1	-1.338683	1.063896	-1.170625
6	-2.165034	1.388343	0.847228
1	-2.091166	2.460860	1.060291
1	-2.019427	0.881116	1.810199
6	-3.570679	1.103749	0.304642
6	1.240256	1.438552	-0.962805
1	1.054277	0.700814	-1.755500
1	0.955841	2.407706	-1.391247
6	2.745997	1.486381	-0.649592
6	-2.958262	-1.158635	-0.752334
1	-2.944733	-0.727954	-1.760276
1	-4.307966	1.568815	0.965493
1	-3.669886	1.601518	-0.667779
1	-3.321866	-2.187158	-0.858740
6	2.401556	-0.604717	1.494673
1	2.565901	-1.306023	2.322356
1	3.200424	2.166999	-1.374457
1	2.387732	0.387383	1.960068
1	2.909572	1.949230	0.331049
6	3.492255	0.144770	-0.749178
1	4.513287	0.335418	-1.091807
1	3.020235	-0.438115	-1.544571
6	3.591682	-0.692995	0.539729
1	4.477882	-0.377706	1.099188
1	3.767882	-1.738719	0.267714
6	-3.922735	-0.377432	0.143912
1	-4.938423	-0.459454	-0.253117
1	-3.936065	-0.851352	1.133025

TTT-TS-cbb:

6	0.795707	-1.624760	-0.125530
6	-0.489989	-1.779364	-0.673224
1	1.638789	-2.005118	-0.692325
1	-0.586529	-2.235543	-1.655274
6	1.030604	-0.804826	0.956566
6	-1.588152	-1.169188	-0.109161
1	0.228903	-0.658562	1.672340
1	-1.566086	-1.020526	0.965332
6	0.266408	1.153485	0.114525
6	-1.086377	0.993594	-0.127770
1	0.568564	1.585875	1.066397
1	-1.387367	1.020238	-1.171620

6	-2.134583	1.458170	0.864186
1	-2.330521	2.515020	0.646519
1	-1.706865	1.435002	1.872435
6	-3.487767	0.707362	0.849835
6	1.197524	1.366494	-1.054898
1	1.000272	0.580158	-1.796737
1	0.899215	2.305689	-1.537217
6	2.707466	1.440959	-0.770866
6	-2.974940	-1.237768	-0.695718
1	-2.922176	-1.502037	-1.755661
6	-3.793903	0.053322	-0.499145
1	-3.587036	0.764979	-1.304247
1	-4.857464	-0.186814	-0.566899
1	-3.505084	-0.067217	1.624046
1	-4.280602	1.411200	1.112307
1	-3.508087	-2.054001	-0.191420
6	2.395954	-0.507040	1.515385
1	2.573141	-1.157998	2.380721
1	3.148638	2.072048	-1.546883
1	2.387231	0.510688	1.921798
1	2.883898	1.969026	0.173971
6	3.458514	0.099233	-0.788491
1	4.475690	0.271763	-1.151685
1	2.984418	-0.538094	-1.539628
6	3.575066	-0.651145	0.552191
1	4.465845	-0.295412	1.079111
1	3.754023	-1.711526	0.347306

TTT-bbc:

6	0.606405	1.911420	0.261745
6	-0.735686	1.913389	0.670657
1	1.332298	2.446296	0.869939
1	-0.998736	2.397214	1.607802
6	1.078540	1.091919	-0.742167
6	-1.669029	1.126741	0.027966
1	0.388550	0.753158	-1.507983
1	-1.510096	0.946148	-1.031209
6	0.442502	-0.936629	0.179233
6	-0.935945	-0.908423	0.309839
1	0.848528	-1.413717	-0.706767
1	-1.321133	-0.879790	1.327349
6	-1.859860	-1.572040	-0.693568
1	-1.623095	-2.640777	-0.741986
1	-1.673618	-1.175126	-1.700372
6	-3.341593	-1.420733	-0.332746
6	1.297931	-0.964691	1.422862
1	0.787359	-0.380154	2.197717
1	1.307813	-2.001146	1.788215
6	2.742863	-0.475834	1.307404
6	-3.111318	1.011673	0.454987
1	-3.168168	0.721472	1.510570
1	-3.939198	-2.059115	-0.989805
1	-3.486784	-1.802208	0.685306
1	-3.590607	1.994303	0.376243
6	2.527207	1.083399	-1.176740
1	2.582192	1.554041	-2.165140
1	3.280463	-0.808436	2.200762

1	2.759305	0.615464	1.342091
1	3.123101	1.710629	-0.505850
6	3.529887	-0.951130	0.079620
1	4.584077	-0.730356	0.272929
1	3.461795	-2.042092	0.001790
6	3.155532	-0.313396	-1.278941
1	4.063009	-0.245505	-1.885287
1	2.476843	-0.958461	-1.842473
6	-3.879203	0.010197	-0.411224
1	-4.934593	0.011969	-0.124382
1	-3.838719	0.351023	-1.453016

TTT-bbb:

6	0.577894	1.924860	0.096665
6	-0.765934	1.951823	0.493730
1	1.295018	2.509069	0.668820
1	-1.037211	2.516402	1.381903
6	1.064164	1.025216	-0.830190
6	-1.697350	1.105936	-0.075899
1	0.385871	0.635816	-1.582435
1	-1.536508	0.839320	-1.116082
6	0.430581	-0.903089	0.247919
6	-0.953287	-0.889733	0.335365
1	0.868000	-1.452267	-0.578957
1	-1.361174	-0.803706	1.338765
6	-1.808579	-1.672421	-0.643874
1	-1.893878	-2.690846	-0.246158
1	-1.272045	-1.765188	-1.594304
6	-3.235974	-1.134784	-0.895135
6	1.250037	-0.809945	1.511623
1	0.728813	-0.139168	2.205681
1	1.234651	-1.801423	1.985224
6	2.704676	-0.353984	1.376977
6	-3.142761	1.065880	0.357106
1	-3.242823	1.485419	1.362188
6	-3.777018	-0.336217	0.291948
1	-3.585587	-0.887177	1.217993
1	-4.861846	-0.232545	0.214958
1	-3.255063	-0.495549	-1.784241
1	-3.895474	-1.977074	-1.115371
1	-3.707080	1.722552	-0.317222
6	2.521001	0.984983	-1.236122
1	2.594176	1.372399	-2.258803
1	3.226848	-0.617941	2.301592
1	2.738851	0.735913	1.320169
1	3.101687	1.668000	-0.607886
6	3.498585	-0.942544	0.202795
1	4.554333	-0.728452	0.394147
1	3.408168	-2.034523	0.213447
6	3.156742	-0.411357	-1.210554
1	4.079122	-0.384163	-1.797162
1	2.496489	-1.102615	-1.740387

CAT adduct:

6	0.768365	-1.689691	-0.231860
6	-0.481082	-1.831105	-0.673358
1	1.589696	-2.285131	-0.618769
1	-0.749992	-2.548492	-1.443578
6	1.004833	-0.650542	0.834747
6	-1.541641	-0.959088	-0.056650
1	0.380818	-0.938393	1.693574
1	-1.642822	-1.260625	0.999267
6	0.400297	0.704586	0.372222
6	-1.080977	0.519577	-0.059016
1	0.432837	1.366474	1.247980
1	-1.161309	0.847923	-1.104216
6	-2.070757	1.362175	0.748024
1	-1.752845	2.410216	0.750598
1	-2.060976	1.024686	1.792959
6	-3.485004	1.241946	0.171431
6	1.151920	1.402029	-0.771765
1	0.960857	0.843528	-1.696069
1	0.680581	2.382484	-0.909087
6	2.667276	1.577812	-0.640370
6	-2.927132	-1.076047	-0.690201
1	-2.873982	-0.748058	-1.735938
1	-4.192748	1.816214	0.775371
1	-3.491983	1.685117	-0.831736
1	-3.247341	-2.122672	-0.698807
6	2.432394	-0.557749	1.390334
1	2.577842	-1.371047	2.108140
1	2.984729	2.298528	-1.399328
1	2.497634	0.366393	1.974689
1	2.929126	2.019986	0.328131
6	3.429496	0.264241	-0.861621
1	4.423180	0.473346	-1.267253
1	2.899883	-0.301028	-1.636478
6	3.592319	-0.608425	0.390275
1	4.496860	-0.304687	0.926845
1	3.766747	-1.643170	0.079036
6	-3.939141	-0.218113	0.074230
1	-4.922532	-0.275504	-0.399954
1	-4.051267	-0.625717	1.086106

TTC:

6	0.934798	-1.737983	-0.000387
6	-0.286717	-1.880686	-0.507436
1	1.737489	-2.390775	-0.334206
1	-0.475053	-2.647393	-1.255778
6	1.246012	-0.685146	1.035656
6	-1.477845	-1.069339	-0.070359
1	0.917623	-1.080653	2.006773
1	-2.125600	-1.762396	0.486511
6	0.355842	0.554842	0.793306
6	-1.113672	0.091017	0.907995
1	-1.213435	-0.318952	1.920829
1	0.543388	1.248265	1.625324
6	-2.329939	-0.572945	-1.248742
1	-2.492313	-1.387530	-1.960031
6	-2.142301	1.229494	0.801958
1	-2.077942	1.861190	1.692650

1	-1.926631	1.871938	-0.056665
6	-3.547769	0.652276	0.630704
1	-3.727970	-0.076724	1.428406
1	-4.306914	1.429240	0.743276
6	2.744422	-0.385756	1.207199
1	2.828787	0.538362	1.788626
1	3.184689	-1.169413	1.832017
6	0.636807	1.318304	-0.509265
1	0.280408	0.732388	-1.362783
1	0.043553	2.236129	-0.492846
6	2.094460	1.702744	-0.790076
1	2.088280	2.440309	-1.597577
1	2.535284	2.206966	0.078348
6	3.596365	-0.270315	-0.063767
1	4.540935	0.205846	0.218276
1	3.863872	-1.269079	-0.421740
6	-3.680728	-0.028326	-0.748161
1	-4.074860	0.686003	-1.476114
1	-1.786501	0.206241	-1.789935
1	-4.406893	-0.843562	-0.685024
6	2.961774	0.512617	-1.219847
1	2.338782	-0.158442	-1.820375
1	3.761970	0.857259	-1.880640

TTC-TS-cbc:

6	0.335531	-1.673518	-0.600787
6	-1.066684	-1.598450	-0.609929
1	0.833366	-1.825539	-1.553733
1	-1.574582	-1.670450	-1.567785
6	1.089807	-1.367516	0.511327
6	-1.780336	-1.204272	0.501018
1	0.641972	-1.522248	1.485748
1	-1.361986	-1.429893	1.475055
6	0.392541	0.798549	0.890191
6	-0.991804	0.834834	0.800161
1	-1.550427	0.830267	1.732896
1	0.816204	0.703347	1.886035
6	-3.277047	-0.991303	0.473895
1	-3.777796	-1.953890	0.320139
1	-3.606152	-0.627261	1.453132
6	-1.667615	1.525648	-0.361739
1	-1.391500	2.588562	-0.345060
1	-1.267846	1.126419	-1.302178
6	-3.194159	1.419061	-0.358159
1	-3.572366	1.787880	0.603852
1	-3.597962	2.086317	-1.124917
6	2.605062	-1.416833	0.499018
1	2.992834	-0.982277	1.426036
1	2.892788	-2.474401	0.529335
6	1.270979	1.512510	-0.118708
1	1.173336	1.040957	-1.103504
1	0.882666	2.530395	-0.246121
6	2.749296	1.590015	0.308393
1	3.101776	2.621409	0.226486
1	2.817891	1.344258	1.372762
6	3.275542	-0.744564	-0.711435

1	4.151788	-1.324301	-1.012981
6	-3.728776	0.006265	-0.596586
1	-3.407638	-0.339916	-1.584796
1	-4.821952	0.034070	-0.618814
1	2.595714	-0.775532	-1.565447
6	3.725149	0.704306	-0.475991
1	3.924954	1.161814	-1.450607
1	4.680001	0.701615	0.060464

TTC-TS-cbb:

6	0.775985	-1.523978	-0.582371
6	-0.579443	-1.564286	-0.934717
1	1.513574	-1.579946	-1.375937
1	-0.832992	-1.597130	-1.991841
6	1.177021	-1.158644	0.688815
6	-1.592532	-1.328934	-0.026787
1	0.506435	-1.388141	1.510058
1	-1.447221	-1.632498	1.004910
6	0.312934	0.857522	0.805018
6	-1.072297	0.726165	0.765836
1	-1.556279	0.534266	1.720438
1	0.781301	0.886616	1.784265
6	-3.033882	-1.233821	-0.465084
1	-3.504187	-2.217281	-0.349854
6	-1.932069	1.436895	-0.257777
1	-1.711300	2.512049	-0.254236
1	-1.676311	1.084758	-1.262384
6	-3.433410	1.245301	0.002522
1	-3.744258	1.899374	0.823537
1	-3.986318	1.574464	-0.882558
6	2.616197	-1.016981	1.110589
1	2.675226	-0.255166	1.895993
1	2.931505	-1.949661	1.594467
6	1.014678	1.625105	-0.286555
1	0.712644	1.213551	-1.259338
1	0.617389	2.649022	-0.269787
6	2.547903	1.702802	-0.223792
1	2.846738	2.615521	-0.746046
1	2.875048	1.833630	0.814639
6	3.623888	-0.680635	0.009450
1	4.586091	-0.502303	0.499316
1	3.773645	-1.556914	-0.629426
6	-3.824920	-0.200562	0.341029
1	-4.896467	-0.333610	0.171859
1	-3.078715	-0.987951	-1.532289
1	-3.658460	-0.396566	1.405535
6	3.289821	0.528694	-0.884276
1	2.699537	0.209039	-1.747415
1	4.234129	0.897035	-1.295303

TTC-TS-bbc:

6	0.115407	-1.742088	-0.822350
6	-1.245709	-1.653322	-0.513626
1	0.375559	-1.936960	-1.861486
1	-1.953517	-1.793496	-1.325174

6	1.142578	-1.377635	0.023370
6	-1.694440	-1.123014	0.680224
1	1.032093	-1.485694	1.097022
1	-1.084127	-1.274651	1.563920
6	0.484717	0.826840	0.520374
6	-0.901920	0.879975	0.570862
1	-1.338113	1.010869	1.558669
1	0.962144	0.773319	1.490444
6	-3.164535	-0.863227	0.927940
1	-3.693555	-1.817134	1.032008
6	-1.722960	1.431395	-0.568881
1	-1.431417	2.474872	-0.746239
1	-1.476220	0.887343	-1.489535
6	-3.231284	1.382555	-0.301387
1	-3.435973	1.933644	0.625311
6	1.310067	1.428099	-0.594585
1	1.225990	0.818141	-1.499076
1	0.887172	2.402190	-0.870695
6	2.543047	-1.368034	-0.546174
1	2.824538	-2.404220	-0.771516
6	2.795590	1.657040	-0.217454
1	3.394216	1.681662	-1.134525
1	2.878798	2.655533	0.222433
1	-3.755476	1.915222	-1.099913
1	2.513487	-0.860043	-1.517129
6	-3.816678	-0.026703	-0.179065
1	-3.718795	-0.542542	-1.139427
1	-4.889601	0.050087	0.018951
1	-3.282343	-0.340250	1.883188
6	3.661652	-0.755859	0.296097
1	3.854748	-1.391530	1.166767
1	4.573444	-0.787609	-0.309573
6	3.436902	0.682031	0.780396
1	2.853378	0.668523	1.703006
1	4.408964	1.094394	1.068112

TTC-TS-bbb:

6	0.557108	1.680968	0.862736
6	-0.832569	1.619675	0.999220
1	1.159264	1.822171	1.757360
1	-1.254267	1.665572	2.000277
6	1.200078	1.334407	-0.311287
6	-1.664601	1.272698	-0.050921
1	0.662161	1.459863	-1.245306
1	-1.377663	1.570819	-1.054515
6	0.463622	-0.772480	-0.466107
6	-0.920116	-0.729315	-0.625131
1	-1.268430	-0.635471	-1.650993
1	1.051679	-0.822912	-1.373327
6	-3.152054	1.106036	0.158139
1	-3.649402	2.049963	-0.092196
6	-1.870653	-1.465211	0.298743
1	-1.565835	-2.514737	0.395628
1	-1.810065	-1.041953	1.306394
6	-3.320524	-1.412470	-0.204977
1	-3.984220	-1.737535	0.601916
6	-3.747645	-0.019398	-0.691302

1	-3.433937	0.130038	-1.729648
1	-4.838429	0.047564	-0.690728
6	1.060653	-1.426018	0.752445
1	0.457130	-1.162284	1.628104
1	0.948981	-2.513665	0.631333
6	2.705198	1.410460	-0.456508
1	2.932593	2.274867	-1.090862
6	2.526570	-1.103104	1.052386
1	2.581182	-0.153142	1.589103
1	2.903423	-1.857034	1.749835
1	-3.355454	0.917427	1.218299
1	-3.447956	-2.131429	-1.020497
1	3.161622	1.618918	0.516065
6	3.365632	0.176195	-1.086614
1	2.826614	-0.075394	-2.003836
1	4.372827	0.452862	-1.409100
6	3.475526	-1.056471	-0.153094
1	3.356138	-1.972517	-0.742256
1	4.494685	-1.087816	0.242596

CSC-adduct:

6	0.934798	-1.737983	-0.000387
6	-0.286717	-1.880686	-0.507436
1	1.737489	-2.390775	-0.334206
1	-0.475053	-2.647393	-1.255778
6	1.246012	-0.685146	1.035656
6	-1.477845	-1.069339	-0.070359
1	0.917623	-1.080653	2.006773
1	-2.125600	-1.762396	0.486511
6	0.355842	0.554842	0.793306
6	-1.113672	0.091017	0.907995
1	-1.213435	-0.318952	1.920829
1	0.543388	1.248265	1.625324
6	-2.329939	-0.572945	-1.248742
1	-2.492313	-1.387530	-1.960031
6	-2.142301	1.229494	0.801958
1	-2.077942	1.861190	1.692650
1	-1.926631	1.871938	-0.056665
6	-3.547769	0.652276	0.630704
1	-3.727970	-0.076724	1.428406
1	-4.306914	1.429240	0.743276
6	2.744422	-0.385756	1.207199
1	2.828787	0.538362	1.788626
1	3.184689	-1.169413	1.832017
6	0.636807	1.318304	-0.509265
1	0.280408	0.732388	-1.362783
1	0.043553	2.236129	-0.492846
6	2.094460	1.702744	-0.790076
1	2.088280	2.440309	-1.597577
1	2.535284	2.206966	0.078348
6	3.596365	-0.270315	-0.063767
1	4.540935	0.205846	0.218276
1	3.863872	-1.269079	-0.421740
6	-3.680728	-0.028326	-0.748161
1	-4.074860	0.686003	-1.476114
1	-1.786501	0.206241	-1.789935
1	-4.406893	-0.843562	-0.685024

6	2.961774	0.512617	-1.219847
1	2.338782	-0.158442	-1.820375
1	3.761970	0.857259	-1.880640

TCT:

6	-1.208009	-2.117296	0.605058
6	0.063539	-2.850012	0.663676
1	-1.695054	-1.921470	1.559350
1	0.104496	-3.694928	1.346748
6	-1.780129	-1.689206	-0.521459
6	1.169432	-2.538882	-0.019774
1	-1.307060	-1.950710	-1.465126
6	0.786096	2.397186	-0.381653
6	1.461159	1.844754	0.623375
1	2.039852	-3.179075	0.118750
1	1.279660	2.472593	-1.350836
1	0.974834	1.755766	1.595591
6	-0.612100	2.955804	-0.298271
1	-0.706328	3.760027	-1.032486
1	-0.763988	3.412321	0.685382
6	-1.725051	1.919104	-0.536886
1	-2.638492	2.433968	-0.856823
1	-1.428664	1.259379	-1.360337
6	-3.043716	-0.870364	-0.596438
1	-3.060356	-0.338117	-1.551596
1	-3.912390	-1.538505	-0.619768
6	-3.212500	0.135980	0.549607
1	-4.125477	0.712961	0.366868
6	1.375035	-1.367333	-0.941218
1	0.633401	-0.590285	-0.734530
6	2.890683	1.382478	0.549885
1	3.418979	1.795427	1.415960
1	3.362648	1.817172	-0.337583
6	3.112748	-0.140209	0.528656
1	4.162930	-0.321382	0.773556
1	2.524879	-0.615890	1.322190
6	2.794197	-0.799286	-0.823858
1	3.502489	-1.614666	-1.005187
1	2.957665	-0.070606	-1.624745
1	1.213241	-1.686186	-1.978377
1	-3.374783	-0.398563	1.490483
6	-2.032398	1.098822	0.715317
1	-1.137390	0.542813	1.010533
1	-2.259002	1.788713	1.535887

TCT-TS-cbc:

6	-0.619158	-1.471205	0.691628
6	0.445973	-1.325432	1.594710
1	-1.571670	-1.788459	1.103739
1	0.193365	-1.370119	2.651553
6	-0.609024	-0.919754	-0.576167
6	1.702265	-0.856396	1.252089
1	0.328854	-0.812369	-1.096817
6	-0.185928	1.211480	-0.036274

6	1.054833	1.267245	0.577808
1	2.340702	-0.559586	2.084480
1	-0.234643	1.437812	-1.100774
1	1.047589	1.499485	1.638292
6	-1.407415	1.558061	0.785286
1	-1.288048	2.599803	1.107716
1	-1.378815	0.961609	1.707647
6	-2.792259	1.423680	0.129692
1	-3.446679	2.154530	0.612265
1	-2.740134	1.725699	-0.923102
6	-1.800886	-0.906709	-1.497034
1	-1.745782	-0.003568	-2.115369
1	-1.705670	-1.740793	-2.203771
6	-3.180232	-0.982549	-0.842048
1	-3.921304	-0.857535	-1.637345
1	-3.340989	-1.988022	-0.440108
6	2.493635	-1.410411	0.081593
1	3.084217	-2.230223	0.511074
1	1.831510	-1.885488	-0.641558
6	2.297729	1.719710	-0.166366
1	3.104570	1.884503	0.555370
1	2.091896	2.695693	-0.620086
6	2.814965	0.763025	-1.240954
1	2.000839	0.470426	-1.915716
1	3.550269	1.289588	-1.855822
6	3.467080	-0.471849	-0.630336
1	3.982626	-1.044086	-1.407129
1	4.239099	-0.142218	0.075982
6	-3.463790	0.047005	0.268677
1	-3.181106	-0.360146	1.243063
1	-4.547429	0.188060	0.312582

TCT-TS-cbb:

6	-0.727563	-1.490970	0.611275
6	0.410921	-1.391446	1.419374
1	-1.653447	-1.761233	1.108744
1	0.244534	-1.480973	2.490080
6	-0.808121	-0.955678	-0.662026
6	1.651325	-0.921133	1.020118
1	0.070876	-0.953117	-1.287375
6	-0.247355	1.142315	-0.212031
6	1.068194	1.168372	0.226518
1	2.325134	-0.683088	1.844622
1	-0.424297	1.327763	-1.269557
1	1.240051	1.504773	1.246269
6	-1.334210	1.579813	0.742354
1	-1.117093	2.618053	1.021308
1	-1.230148	0.997834	1.668644
6	-2.791082	1.514699	0.253629
1	-3.348500	2.276662	0.804911
1	-2.845669	1.813444	-0.800314
6	-2.090138	-0.879653	-1.450652
1	-2.052709	0.015020	-2.082066
1	-2.118382	-1.722752	-2.152171
6	-3.394692	-0.873390	-0.651795
1	-4.205892	-0.709689	-1.367777
6	2.418566	-1.317056	-0.223717

1	1.846685	-1.170843	-1.136752
6	2.211163	1.441930	-0.726286
1	2.257344	2.524864	-0.890251
1	1.998443	0.999434	-1.707617
6	3.566185	0.959046	-0.202515
1	4.379615	1.474763	-0.718608
1	3.639823	1.247411	0.851489
6	3.744455	-0.560052	-0.346331
1	4.447525	-0.922755	0.410027
1	4.187769	-0.789921	-1.319795
1	2.619160	-2.393073	-0.169024
1	-3.568929	-1.867196	-0.227005
6	-3.507170	0.172268	0.474309
1	-3.142582	-0.244794	1.416861
1	-4.572173	0.365014	0.632019

TCT-TS-bbc:

6	-0.399322	2.127460	-0.596852
6	0.960427	2.122632	-0.911454
1	-1.040831	2.669526	-1.291021
1	1.241602	2.644427	-1.821679
6	-1.050255	1.316379	0.308634
6	1.904437	1.253198	-0.379257
1	-0.586561	0.981264	1.223076
6	-0.107339	-0.840069	-0.509283
6	1.124342	-0.583695	-1.100275
1	2.861735	1.267185	-0.902238
1	-0.073546	-1.350626	0.448943
1	1.086605	-0.296268	-2.149862
6	-2.559260	1.286844	0.258296
1	-2.930661	2.275560	0.555557
6	2.080043	0.900360	1.084234
1	2.365802	1.817594	1.611749
1	1.149353	0.558894	1.535087
6	-1.370036	-1.064702	-1.314635
1	-1.151963	-1.770689	-2.125724
1	-1.675000	-0.141879	-1.815841
6	2.361132	-1.417522	-0.763597
1	3.226495	-1.010170	-1.297443
1	2.199990	-2.422612	-1.168861
6	-2.524820	-1.677654	-0.489466
1	-3.464282	-1.548117	-1.038553
1	-2.351871	-2.757570	-0.439420
6	-3.248953	0.232996	1.122627
1	-4.317332	0.246282	0.882664
6	3.142751	-0.176517	1.302038
1	3.343164	-0.282004	2.371650
1	-2.875743	1.160405	-0.783367
6	2.710830	-1.520733	0.720422
1	3.511791	-2.254424	0.845564
1	1.852599	-1.902395	1.284039
1	4.082343	0.139921	0.833206
1	-3.167999	0.514728	2.177918
6	-2.710253	-1.189224	0.954113
1	-1.766631	-1.282804	1.496979
1	-3.401396	-1.874746	1.454302

TCT-TS-bbb:

6	-0.436464	1.792119	-0.691677
6	0.718258	1.625167	-1.457235
1	-1.287873	2.280972	-1.160469
1	0.651451	1.846033	-2.519096
6	-0.664392	1.105362	0.491815
6	1.827575	0.928778	-0.989484
1	0.174538	0.802748	1.101041
6	-0.367890	-0.984203	-0.350781
6	0.960493	-1.098881	-0.756831
1	2.559529	0.660801	-1.748393
1	-0.611646	-1.401706	0.620560
1	1.117912	-1.186815	-1.827481
6	-1.465547	-1.010373	-1.384573
1	-1.568741	-2.052073	-1.718223
1	-1.122602	-0.450165	-2.263084
6	-2.841780	-0.488469	-0.960717
1	-2.871492	0.596527	-1.078456
1	-3.581463	-0.880199	-1.665384
6	-1.966557	1.233066	1.253098
1	-1.762651	1.783444	2.178587
1	-2.673642	1.843865	0.683160
6	2.471647	1.266002	0.352559
1	1.875184	2.029247	0.856235
6	1.951044	-1.884526	0.093163
1	2.238766	-2.780039	-0.467989
1	1.428856	-2.238767	0.988800
6	3.204766	-1.149189	0.569153
1	3.774053	-1.816793	1.221524
1	3.858845	-0.897900	-0.273620
6	2.803696	0.120597	1.315414
1	3.598905	0.451909	1.987648
1	1.939164	-0.112786	1.949260
1	3.419156	1.750024	0.086229
6	-2.617039	-0.105439	1.630171
1	-3.366801	0.078038	2.404574
1	-1.858683	-0.735123	2.102303
6	-3.302783	-0.850393	0.457485
1	-3.206317	-1.931657	0.606465
1	-4.374611	-0.637289	0.506439

CAC-adduct:

6	-0.596317	-1.611961	-0.164380
6	0.408763	-1.626023	0.708353
1	-1.207747	-2.502443	-0.291628
1	0.601586	-2.525606	1.289637
6	-0.916088	-0.410292	-1.016274
6	1.361468	-0.479836	0.934572
1	-0.333933	-0.511959	-1.942175
6	-0.392856	0.875760	-0.348311
6	1.105775	0.710368	-0.030113
1	1.228680	-0.124209	1.964744
1	-0.492178	1.679710	-1.090583
1	1.427337	1.627968	0.479998

6	-1.126241	1.334082	0.923003
1	-0.732976	2.326505	1.170543
1	-0.852494	0.681814	1.759120
6	-2.656224	1.397452	0.880283
1	-2.986897	1.961640	1.757046
1	-2.997631	1.965122	0.006591
6	-2.378717	-0.345777	-1.489831
1	-2.541467	0.650449	-1.915088
1	-2.501493	-1.046468	-2.322114
6	-3.475599	-0.651697	-0.462830
1	-4.428056	-0.334641	-0.899837
6	2.820284	-0.987061	0.821668
1	2.887161	-1.731735	0.020766
6	1.991981	0.554553	-1.269178
1	1.703073	1.276094	-2.039343
1	1.842550	-0.441480	-1.699188
6	3.473774	0.735953	-0.892620
1	4.101857	0.236821	-1.635537
1	3.735802	1.797378	-0.921961
6	3.771445	0.167401	0.510573
1	3.640994	0.946375	1.269153
1	4.812091	-0.157607	0.575609
1	3.102109	-1.497398	1.746272
1	-3.556279	-1.734164	-0.323310
6	-3.304351	0.008383	0.911996
1	-2.689054	-0.635840	1.548755
1	-4.285623	0.065841	1.391063

TCC:

6	-0.684754	2.035473	-0.996763
6	0.687994	2.556570	-1.107823
1	-1.170129	1.761431	-1.933277
1	0.867086	3.240018	-1.934476
6	-1.379653	1.910866	0.135803
6	1.723797	2.244375	-0.320254
1	-0.920568	2.236874	1.069109
6	-0.008321	-1.508668	-1.398235
6	1.257263	-1.262974	-1.065343
1	2.679948	2.721340	-0.528266
1	1.749934	-0.448548	-1.594091
6	-2.766801	1.346018	0.241675
1	-3.459229	2.136592	0.552432
1	-3.098949	1.010520	-0.744894
6	1.711477	1.244392	0.798114
1	1.649082	1.760585	1.763718
6	2.116386	-1.982139	-0.059502
1	3.034858	-2.282448	-0.578033
1	1.636695	-2.903726	0.276501
6	2.526794	-1.140551	1.167303
1	3.348647	-1.657077	1.670422
6	-0.969330	-2.498186	-0.801212
1	-0.501542	-3.075730	0.001038
1	-1.281418	-3.210746	-1.572284
6	-2.207113	-1.763906	-0.258840
1	-3.007861	-2.478226	-0.044615
1	-2.583653	-1.104801	-1.048694

6	2.934039	0.299683	0.816815
1	3.670354	0.665152	1.536536
1	3.432554	0.308335	-0.158817
6	-2.856624	0.201705	1.269472
1	-2.650490	0.614896	2.262687
1	-3.885641	-0.172681	1.296775
1	1.697238	-1.107000	1.882177
1	0.801716	0.650452	0.713599
1	-0.443919	-0.881881	-2.175681
6	-1.887880	-0.951501	0.999053
1	-0.876643	-0.545502	0.904323
1	-1.871710	-1.624790	1.862234

TCC-TS-cbc:

6	-0.462990	2.355174	-0.256493
6	0.931743	2.450333	-0.277284
1	-1.005701	3.110680	-0.822264
1	1.340456	3.254137	-0.883647
6	-1.177749	1.244267	0.140375
6	1.824380	1.458071	0.097553
1	-0.820927	0.631029	0.952766
6	-0.147801	-0.407820	-1.137424
6	1.198783	-0.114000	-1.327147
1	2.848737	1.639724	-0.232951
1	1.404922	0.558292	-2.151382
6	-2.638133	1.109954	-0.218761
1	-3.108298	2.098607	-0.194588
1	-2.719255	0.775983	-1.260506
6	1.802491	0.607237	1.349360
1	1.949342	1.278415	2.203771
6	2.338181	-1.097645	-1.079455
1	3.257616	-0.639932	-1.458712
1	2.156839	-1.979836	-1.708306
6	2.614208	-1.581873	0.349414
1	3.472627	-2.259329	0.311686
6	-0.613079	-1.678738	-0.460255
1	-0.180540	-1.760527	0.541298
1	-0.194208	-2.524490	-1.025498
6	-2.130522	-1.886449	-0.325391
1	-2.302280	-2.962906	-0.247874
1	-2.637532	-1.568422	-1.243891
6	2.904184	-0.454638	1.336485
1	3.021428	-0.875200	2.339033
1	3.858026	0.024096	1.083935
6	-3.434065	0.150345	0.667192
1	-3.621048	0.619115	1.638506
1	-4.414416	-0.005746	0.205958
1	1.778004	-2.178426	0.719642
1	0.842334	0.115468	1.507960
1	-0.835263	-0.001286	-1.869880
6	-2.769369	-1.212953	0.905947
1	-2.004479	-1.118152	1.684212
1	-3.527960	-1.878891	1.326039

TCC-TS-cbb:

6	-0.192791	2.347268	-0.420281
6	1.199676	2.350064	-0.516054
1	-0.729158	3.101646	-0.992831
1	1.638532	3.037186	-1.234666
6	-0.939002	1.293687	0.077631
6	2.003040	1.337598	-0.011143
1	-0.545988	0.667027	0.863327
6	-0.115695	-0.421540	-1.245637
6	1.277070	-0.303569	-1.294316
1	3.030503	1.336285	-0.372177
1	1.663282	0.285685	-2.114122
6	-2.434577	1.275581	-0.125133
1	-2.827486	2.292285	-0.022654
1	-2.646775	0.984316	-1.161236
6	1.870239	0.798408	1.405205
6	2.202724	-1.434840	-0.856316
1	3.101104	-1.386266	-1.475768
1	1.722904	-2.386508	-1.106568
6	2.634743	-1.479453	0.631133
1	2.709045	-2.523316	0.945542
6	-0.771934	-1.714959	-0.799408
1	-0.233006	-2.159858	0.041216
1	-0.628097	-2.421153	-1.630959
6	-2.266778	-1.710906	-0.454390
1	-2.590815	-2.754922	-0.445199
1	-2.836499	-1.230599	-1.257746
6	-3.190340	0.345199	0.823086
1	-4.232897	0.287752	0.493983
1	-0.669950	0.106753	-2.014489
6	1.704665	-0.713874	1.568782
1	0.667041	-1.003393	1.390081
1	1.925292	-0.977377	2.606862
1	1.072447	1.332774	1.925580
1	2.802376	1.079858	1.910380
1	3.639883	-1.055815	0.736896
1	-3.204956	0.779780	1.827618
6	-2.611177	-1.072328	0.904089
1	-1.713055	-1.069517	1.530846
1	-3.332897	-1.700633	1.432583

TCC-TS-bbc:

6	0.359797	-1.995018	-0.347362
6	-0.826354	-2.036977	-1.086668
1	1.192369	-2.612691	-0.677416
1	-0.793394	-2.554384	-2.042074
6	0.611798	-0.984212	0.566710
6	-1.930895	-1.231683	-0.824165
1	-0.229910	-0.505332	1.039876
6	0.379564	0.721005	-0.857439
6	-0.980117	0.814655	-1.154782
1	-2.670468	-1.186680	-1.624079
1	-1.251963	0.591449	-2.177546
6	1.879724	-0.870946	1.382189
1	1.898214	-1.700503	2.099313
6	-2.584018	-1.131007	0.543570
1	-3.350041	-1.917444	0.544405
6	-1.877311	1.808610	-0.449527

1	-2.763760	1.989018	-1.065928
1	-1.353179	2.770416	-0.375703
6	-2.356596	1.395868	0.945118
1	-2.890317	2.239082	1.392918
6	1.143337	1.710476	-0.005285
1	0.842745	1.627635	1.043423
1	0.859903	2.729807	-0.296643
6	2.684585	1.595649	-0.146710
1	3.152114	1.980583	0.766309
1	2.993768	2.272494	-0.948616
6	-3.281552	0.183866	0.897174
1	-3.771513	0.054798	1.866625
1	-4.079207	0.378819	0.169310
1	-1.501955	1.189724	1.601221
1	-1.885790	-1.410218	1.332524
1	0.963694	0.241724	-1.630980
6	3.203424	-0.849812	0.616808
1	3.398402	-1.829794	0.170036
1	1.823073	0.033914	1.993480
6	3.283148	0.219083	-0.480330
1	2.826185	-0.167923	-1.393187
1	4.337493	0.372055	-0.730112
1	4.002329	-0.683893	1.347046

TCC-TS-bbb:

6	-0.268230	2.352462	-0.162105
6	1.091142	2.381791	-0.471071
1	-0.896122	3.129582	-0.592933
1	1.413471	3.108553	-1.211656
6	-0.906930	1.270662	0.419768
6	1.972800	1.352120	-0.147675
1	-0.351040	0.627551	1.080507
6	-0.192701	-0.420377	-1.081454
6	1.169442	-0.210328	-1.326988
1	2.935615	1.409059	-0.653341
1	1.381984	0.385299	-2.205832
1	-0.861932	0.083559	-1.764312
6	-2.414156	1.273923	0.578312
1	-2.669539	1.063431	1.624634
1	-2.771448	2.286391	0.369303
6	2.088045	0.762820	1.257104
1	1.436111	1.326094	1.929886
1	3.113879	0.969929	1.583066
6	2.252426	-1.253278	-1.065283
1	1.983146	-2.171997	-1.597157
1	3.161956	-0.888984	-1.547455
6	2.576885	-1.596523	0.413347
1	2.347283	-2.647452	0.608223
1	3.653703	-1.487176	0.577684
6	-0.717483	-1.729696	-0.519369
1	-1.130502	-2.291813	-1.369635
6	-1.792753	-1.700612	0.574680
1	-1.433073	-1.143162	1.444744
1	-1.936758	-2.728747	0.922357
6	-3.195958	0.299198	-0.317741
1	-4.242628	0.617787	-0.341333
6	1.839872	-0.736268	1.434934

1	2.159397	-1.022011	2.441222
1	0.119324	-2.330676	-0.154681
1	0.771541	-0.950528	1.384338
1	-2.833838	0.386597	-1.344454
6	-3.159742	-1.158535	0.153167
1	-3.573251	-1.799854	-0.632964
1	-3.833239	-1.255594	1.012030

TSC-adduct:

6	-0.348045	2.311419	-0.042226
6	0.976399	2.405786	-0.065252
1	-0.959552	3.208300	0.010581
1	1.460585	3.377258	-0.035861
6	-1.057174	0.981228	0.015239
6	1.831219	1.173631	-0.138564
1	-1.033003	0.684340	1.074154
6	-0.333406	-0.145792	-0.789623
6	1.182182	0.137414	-1.078002
1	2.796399	1.446202	-0.585472
1	1.192183	0.613458	-2.063499
6	-2.540780	1.095998	-0.391644
1	-2.859396	2.139581	-0.316217
1	-2.634357	0.835154	-1.450424
6	2.139577	0.567585	1.239449
1	2.558655	1.334636	1.896974
6	2.107701	-1.089440	-1.185390
1	3.008631	-0.758777	-1.716790
1	1.657614	-1.862792	-1.814055
6	2.551565	-1.679198	0.160180
1	3.309629	-2.447546	-0.017949
6	-0.666200	-1.517209	-0.184384
1	-0.303600	-1.568468	0.848995
1	-0.136383	-2.293876	-0.741068
6	-2.159572	-1.880677	-0.179514
1	-2.233554	-2.953041	0.022126
1	-2.585220	-1.728359	-1.179097
6	3.112099	-0.604158	1.094753
1	3.339488	-1.037861	2.072300
1	4.057906	-0.225611	0.687704
6	-3.513685	0.245422	0.440865
1	-3.793468	0.799616	1.342349
1	-4.436019	0.118520	-0.134444
1	1.716435	-2.179538	0.654525
1	1.206314	0.227796	1.705030
1	-0.801210	-0.147837	-1.781358
6	-2.994861	-1.134679	0.869458
1	-2.392937	-1.039121	1.779813
1	-3.857250	-1.746015	1.149615

CTT:

6	-0.314380	-2.108087	1.382225
6	1.068856	-2.072185	0.885135
1	-0.422709	-2.275591	2.451589
1	1.771630	-2.760411	1.352910

6	-1.436125	-1.984327	0.661023
6	1.513199	-1.231571	-0.051182
6	-0.634140	1.684306	0.744029
6	0.453131	2.237339	0.212563
1	-2.375694	-2.031881	1.206857
1	0.809726	-0.508911	-0.457588
6	-2.058540	2.085450	0.470847
1	-2.376259	2.746512	1.286039
1	-2.111949	2.681078	-0.447637
6	-1.554008	-1.888574	-0.835537
1	-2.371626	-2.551159	-1.143395
1	-0.637432	-2.276444	-1.288717
6	-3.052310	0.912994	0.409160
1	-2.816312	0.213843	1.216379
1	-4.053340	1.299713	0.623116
6	-1.841181	-0.497443	-1.433060
1	-1.921785	-0.634081	-2.516242
1	0.342258	3.029643	-0.528594
6	2.912460	-1.160535	-0.587665
1	3.515246	-1.971940	-0.170716
6	1.851665	1.817695	0.563740
1	2.363786	2.632403	1.087829
1	1.788992	0.987739	1.272678
6	2.710158	1.399917	-0.654410
1	2.060858	1.156699	-1.503366
1	3.320167	2.247510	-0.975721
1	-0.501528	0.882821	1.472920
1	-0.989552	0.166670	-1.270841
6	-3.122773	0.185958	-0.940334
1	-3.428685	0.923461	-1.691158
1	-3.929702	-0.556154	-0.901620
1	2.865130	-1.322727	-1.671831
6	3.611060	0.193221	-0.348021
1	4.511588	0.223160	-0.967165
1	3.944785	0.253100	0.693188

CTT-TS-cbc:

6	0.069214	1.888048	-1.129936
6	1.136019	1.754791	-0.229834
1	0.326085	2.263564	-2.117869
1	2.091484	2.157779	-0.554824
6	-1.181922	1.317412	-0.984686
6	1.142820	0.855828	0.818185
6	-0.443573	-0.906132	-1.059504
6	0.735278	-1.028045	-0.343460
1	-1.790400	1.311197	-1.889903
1	0.225654	0.626361	1.335542
6	-1.698194	-1.664927	-0.662635
1	-2.525924	-1.371014	-1.313517
1	-1.515747	-2.722143	-0.885981
6	-2.051548	1.427409	0.259575
1	-2.284837	2.496887	0.324991
1	-1.520807	1.200913	1.182231
6	-2.114942	-1.514924	0.810961
1	-2.287113	-2.495890	1.260550
1	0.699098	-1.583984	0.593021

6	2.408073	0.522607	1.576450
1	2.699284	1.375673	2.200496
6	2.063307	-1.060292	-1.069658
1	2.073176	-1.936862	-1.729130
1	2.127231	-0.185074	-1.728428
6	3.289138	-1.137229	-0.152925
1	4.169781	-1.369358	-0.758839
1	-1.290694	-1.071317	1.377051
6	-3.375244	0.648518	0.207669
1	-3.632093	0.455613	-0.838284
1	2.201923	-0.304496	2.264318
1	3.156531	-1.983345	0.533593
6	3.572242	0.124330	0.664636
1	4.463288	-0.040409	1.277558
1	3.815438	0.948675	-0.013028
1	-0.337415	-0.745296	-2.128632
1	-4.181221	1.276310	0.596215
6	-3.374061	-0.663438	1.000640
1	-3.487409	-0.440367	2.066818
1	-4.254954	-1.247164	0.713180

CTT-TS-cbb:

6	0.056061	2.097474	1.064207
6	-1.155802	1.984045	0.380521
1	0.019529	2.574749	2.039495
1	-2.025590	2.428837	0.859903
6	1.201930	1.375911	0.756911
6	-1.401883	1.101921	-0.652237
6	0.485270	-0.618368	1.180593
6	-0.661895	-0.879951	0.440285
1	1.981662	1.430741	1.516108
1	-0.635722	0.852888	-1.369277
6	1.783222	-1.402938	0.985396
1	2.598827	-0.900248	1.515405
1	1.635282	-2.351366	1.513062
6	1.774095	1.204737	-0.644634
1	1.724991	2.185429	-1.129047
1	1.163355	0.540621	-1.255718
6	2.217477	-1.701890	-0.459917
1	2.544061	-2.742340	-0.530976
1	-0.544332	-1.446364	-0.479850
6	-2.815067	0.815094	-1.094444
1	-2.998762	1.300474	-2.060120
1	-3.520450	1.253164	-0.379457
6	-2.016598	-1.012544	1.104691
1	-1.967089	-1.774366	1.892547
1	-2.261780	-0.074940	1.614732
6	-3.130141	-1.413571	0.122313
1	-3.070159	-2.491201	-0.062796
1	-4.099652	-1.237655	0.599109
6	-3.089118	-0.685740	-1.227320
1	-2.316002	-1.123413	-1.867301
1	-4.038856	-0.844473	-1.745429
1	1.358182	-1.625078	-1.129527
6	3.221877	0.682410	-0.647879
1	3.819558	1.249756	-1.365275
1	0.311786	-0.374702	2.226526
1	3.672158	0.878683	0.329705

6	3.353241	-0.812826	-0.985964
1	3.404204	-0.935987	-2.072448
1	4.308795	-1.175793	-0.594503

CTT-TS-bbc:

6	0.054155	-1.443875	1.626457
6	1.180287	-1.530145	0.799826
1	0.229275	-1.462961	2.699479
1	2.130153	-1.749786	1.278949
6	-1.198054	-1.060342	1.177849
6	1.198716	-1.007016	-0.484048
6	-0.546060	1.142304	0.619770
6	0.673759	1.080073	-0.044591
1	-1.912023	-0.812590	1.959031
1	0.296146	-1.022477	-1.073566
6	-1.749285	1.825394	-0.011305
1	-1.766055	2.838316	0.408415
1	-1.576553	1.956102	-1.085326
6	-1.828561	-1.672917	-0.068293
1	-2.702443	-2.232503	0.289927
1	-1.135945	-2.423074	-0.458247
6	-3.127983	1.189081	0.201232
1	-3.179097	0.749576	1.200072
1	-3.895692	1.967726	0.173950
6	-2.301337	-0.786967	-1.221665
1	-2.617840	-1.442953	-2.038914
1	0.658298	1.335729	-1.105506
6	2.482124	-0.893447	-1.276084
1	2.822840	-1.892073	-1.572333
6	1.958833	1.434089	0.678678
1	1.890124	2.480836	0.999536
1	2.026477	0.839837	1.597936
6	3.228341	1.275451	-0.164165
1	3.101273	1.845890	-1.093250
1	4.066246	1.736051	0.366992
1	-0.495056	1.272773	1.697622
1	-1.462367	-0.199993	-1.608824
6	-3.456582	0.149894	-0.877657
1	-3.744630	0.683552	-1.790257
1	-4.329022	-0.439381	-0.575601
1	2.278943	-0.349456	-2.204674
6	3.594345	-0.167458	-0.513895
1	4.503840	-0.170629	-1.121539
1	3.836907	-0.713226	0.403475

CTT-TS-bbb:

6	-0.127247	1.747097	-1.491039
6	1.082252	1.777578	-0.796531
1	-0.085769	1.944113	-2.559138
1	1.958331	2.112167	-1.347687
6	-1.291035	1.199501	-0.970862
6	1.314494	1.107188	0.394941
6	-0.548704	-0.930642	-0.888764
6	0.679251	-0.977551	-0.230656

1	-2.083443	1.047418	-1.698195
1	0.530496	0.985145	1.129086
6	-1.707178	-1.781440	-0.366190
1	-1.757878	-2.647735	-1.035123
1	-1.437298	-2.185890	0.615672
6	-1.791975	1.577226	0.419495
1	-2.712897	2.151124	0.252288
1	-1.079874	2.282351	0.853978
6	-3.104965	-1.162562	-0.259742
1	-3.300705	-0.517877	-1.118853
1	-3.851518	-1.960699	-0.308552
6	-2.113162	0.487411	1.441667
1	-2.337147	0.973523	2.396397
1	0.638800	-1.376636	0.782092
6	2.728611	0.988585	0.917355
1	2.839080	1.608433	1.814254
1	3.423200	1.388117	0.169971
6	1.987994	-1.218860	-0.952881
1	1.914884	-2.137765	-1.546519
1	2.155746	-0.412517	-1.673391
6	3.181230	-1.362213	0.013541
1	3.240355	-2.400487	0.355144
1	4.107702	-1.167175	-0.535236
6	3.123713	-0.452630	1.248938
1	2.412064	-0.853161	1.977564
1	4.099391	-0.461511	1.742649
1	-0.504501	-0.887445	-1.973615
1	-1.226401	-0.131415	1.612644
6	-3.294603	-0.402091	1.058048
1	-3.447952	-1.133975	1.858848
1	-4.206720	0.202320	1.011803

CAC-adduct:

6	0.013725	-1.722803	1.387360
6	1.161460	-1.692254	0.713864
1	-0.119178	-2.367767	2.250204
1	2.008228	-2.310200	1.001533
6	-1.133380	-0.848513	0.924597
6	1.265820	-0.801494	-0.499603
6	-0.563347	0.582940	0.688437
6	0.741340	0.616208	-0.154572
1	-1.838992	-0.756638	1.753059
1	0.582933	-1.208580	-1.256112
6	-1.582429	1.666467	0.234460
1	-1.384787	2.576894	0.807194
1	-1.406397	1.934204	-0.812744
6	-1.891524	-1.534386	-0.248271
1	-2.687045	-2.154210	0.180215
1	-1.217090	-2.229107	-0.754633
6	-3.055874	1.280489	0.388112
1	-3.213215	0.794166	1.354280
1	-3.669328	2.185167	0.408408
6	-2.493922	-0.597716	-1.293550
1	-2.948153	-1.202496	-2.084411
1	0.539998	1.118637	-1.109754
6	2.661010	-0.771026	-1.135319
1	3.013971	-1.797411	-1.276500

6	1.807730	1.435922	0.588463
1	1.427823	2.450242	0.751026
1	1.950908	0.988724	1.580167
6	3.154320	1.467187	-0.129557
1	3.043181	1.949602	-1.108553
1	3.871677	2.062790	0.441302
1	-0.262967	0.871265	1.701554
1	-1.682846	-0.037359	-1.772520
6	-3.545954	0.378031	-0.759251
1	-3.868049	1.013143	-1.591112
1	-4.430857	-0.180981	-0.437871
1	2.580343	-0.326118	-2.134180
6	3.669399	0.041829	-0.324950
1	4.639480	0.043899	-0.828920
1	3.820128	-0.423151	0.657053

CTC:

6	-0.581979	2.024293	-1.339471
6	0.842945	1.938522	-1.008590
1	-0.781078	2.181407	-2.396829
1	1.516214	2.290672	-1.788811
6	-1.653819	1.919623	-0.541652
6	1.396841	1.384938	0.074637
6	-0.562484	-1.412383	-1.312223
6	0.744829	-1.337747	-1.073633
1	-2.626152	1.987695	-1.023803
1	0.765922	0.981083	0.857824
6	-1.622247	-2.077221	-0.476475
1	-1.938603	-2.980545	-1.010410
1	-1.210031	-2.421186	0.478163
6	1.488210	-1.890994	0.119307
1	0.952302	-1.665348	1.050173
1	1.489261	-2.984402	0.042627
6	-1.667802	1.773012	0.953773
1	-2.565246	2.264788	1.343293
1	-0.809650	2.310497	1.370091
6	2.868813	1.200073	0.296674
1	3.243669	2.019851	0.922292
6	-2.864501	-1.189577	-0.232239
1	-2.925184	-0.437562	-1.023929
1	-3.768868	-1.798920	-0.314797
6	2.950747	-1.422857	0.243430
1	3.508193	-2.208336	0.761388
1	3.391206	-1.351263	-0.758205
6	-1.654029	0.328701	1.492278
1	-1.565315	0.392503	2.581576
1	1.361988	-0.844200	-1.819918
1	3.403472	1.266767	-0.657002
6	3.209747	-0.116652	1.009736
1	4.271788	-0.087822	1.271402
1	2.663755	-0.151174	1.960804
1	-0.929371	-0.968755	-2.235901
1	-0.762249	-0.192106	1.133769
6	-2.883029	-0.518707	1.147127
1	-2.971092	-1.313677	1.895912
1	-3.788386	0.091891	1.244209

CTC-TS-cbc:

6	0.257016	2.348473	0.824058
6	-1.096911	2.184110	0.514173
1	0.493633	3.006263	1.655775
1	-1.818286	2.749746	1.100745
6	1.267895	1.521320	0.363367
6	-1.570717	1.125619	-0.239286
6	0.509909	-0.400380	1.392650
6	-0.801189	-0.590879	0.965007
1	2.233162	1.658266	0.848718
1	-0.971163	0.744318	-1.050915
6	1.603543	-1.446256	1.185753
1	2.364477	-1.269181	1.952113
1	1.154506	-2.417042	1.435735
6	-1.208517	-1.714912	0.037970
1	-0.682165	-1.639269	-0.921563
1	-0.892155	-2.672687	0.474557
6	1.370966	0.972596	-1.045961
1	1.003274	1.731297	-1.747129
1	0.735142	0.098538	-1.188326
6	-3.036638	0.795581	-0.360759
1	-3.530352	1.565470	-0.965800
6	2.364207	-1.636337	-0.140831
1	2.923274	-2.569453	-0.026991
1	1.677322	-1.808257	-0.975918
6	-2.719300	-1.757546	-0.212050
1	-2.969465	-2.681733	-0.740867
1	-3.231508	-1.805145	0.756684
1	-1.578404	-0.279024	1.653943
1	-3.511108	0.826877	0.627307
6	-3.267054	-0.571998	-1.011922
1	-4.338877	-0.718563	-1.172337
1	-2.802482	-0.566961	-2.005803
6	2.794511	0.564183	-1.413453
1	3.452528	1.438951	-1.408854
1	2.788340	0.180462	-2.438785
1	0.611658	0.128025	2.331760
6	3.356448	-0.511661	-0.477868
1	3.691834	-0.054530	0.459148
1	4.251814	-0.937850	-0.938280

CTC-TS-cbb:

6	0.156134	2.349016	0.754873
6	-1.190233	2.154740	0.438024
1	0.376957	3.039696	1.563838
1	-1.927216	2.741090	0.982374
6	1.178883	1.509645	0.336220
6	-1.640271	1.066030	-0.286886
6	0.488916	-0.349326	1.389672
6	-0.806104	-0.622965	0.951075
1	2.135395	1.679577	0.827930
1	-1.010524	0.664587	-1.062882
6	1.643041	-1.347920	1.246950
1	2.370843	-1.096302	2.024874

1	1.241993	-2.330272	1.528153
6	-1.139152	-1.821464	0.088530
1	-0.259409	-2.149036	-0.470169
1	-1.382719	-2.644891	0.775381
6	1.316337	0.938851	-1.063613
1	0.914718	1.662193	-1.782493
1	0.729653	0.026606	-1.190263
6	-3.102748	0.741544	-0.452249
1	-3.702498	1.331663	0.246418
6	2.461005	-1.555665	-0.044896
1	3.075271	-2.441226	0.142689
1	1.822918	-1.817329	-0.894674
6	-2.327870	-1.649475	-0.878516
1	-2.727561	-2.638163	-1.115956
1	-1.602233	-0.323026	1.620548
6	2.766293	0.606576	-1.408017
1	3.366635	1.521427	-1.434308
1	2.793502	0.183101	-2.417253
1	0.543800	0.201311	2.319986
6	3.389838	-0.393154	-0.426826
1	3.702628	0.120054	0.488405
1	4.306061	-0.789904	-0.872488
1	-3.399751	1.048358	-1.463268
1	-1.985911	-1.223962	-1.828936
6	-3.431144	-0.758904	-0.301159
1	-4.381034	-0.960603	-0.801346
1	-3.579070	-1.010127	0.754346

CTC-TS-bbc:

6	-0.313061	2.337000	-0.907670
6	1.012398	2.146170	-0.521450
1	-0.483997	2.930874	-1.802238
1	1.779821	2.699135	-1.059026
6	-1.371499	1.588169	-0.414926
6	1.429648	1.057996	0.234007
6	-0.617773	-0.437469	-1.316633
6	0.745366	-0.579572	-1.033131
1	-2.294401	1.677981	-0.981706
1	0.772792	0.637632	0.985110
6	-1.628355	-1.515556	-0.955805
1	-1.781634	-2.097541	-1.873187
1	-1.207115	-2.216777	-0.230010
6	1.289791	-1.756204	-0.243019
1	0.786838	-1.842343	0.727299
1	1.053748	-2.680408	-0.785523
6	-1.590929	1.363744	1.074361
1	-2.499532	1.926179	1.326722
1	-0.779541	1.852939	1.618871
6	2.900595	0.815331	0.468459
1	3.267326	1.545793	1.199684
6	-2.996774	-1.051567	-0.442210
1	-3.314572	-0.165106	-0.995274
1	-3.741893	-1.823334	-0.656663
6	2.799737	-1.693145	-0.005096
1	3.138581	-2.659016	0.380365
1	3.309653	-1.543227	-0.964546
6	-1.770860	-0.057594	1.604849
1	-1.848562	-0.004143	2.695686

1	1.433296	-0.210529	-1.786985
1	3.449527	1.007794	-0.461087
6	3.217518	-0.592898	0.969315
1	4.290413	-0.669019	1.167050
1	2.710999	-0.755499	1.928832
1	-0.854510	0.065303	-2.246250
1	-0.872185	-0.643329	1.390145
6	-2.998386	-0.795043	1.070820
1	-3.056007	-1.763720	1.579723
1	-3.903532	-0.245799	1.351787

CTC-TS-bbb:

6	-0.175563	2.191685	-1.085327
6	1.069566	2.043907	-0.476214
1	-0.203295	2.698259	-2.046647
1	1.922702	2.561229	-0.910875
6	-1.307091	1.489372	-0.677569
6	1.323727	1.016817	0.425601
6	-0.546028	-0.610604	-1.198779
6	0.801824	-0.688246	-0.831473
1	-2.137691	1.521985	-1.377992
1	0.516544	0.660614	1.044877
6	-1.559343	-1.646429	-0.740475
1	-1.589302	-2.404894	-1.532883
1	-1.205730	-2.168064	0.153827
6	1.360296	-1.718356	0.129610
1	0.949814	-1.557109	1.133750
1	1.043709	-2.726606	-0.160648
6	-1.750009	1.482860	0.784404
1	-2.675832	2.072232	0.811552
1	-1.017768	2.055123	1.359487
6	2.717440	0.756052	0.967024
1	2.653937	0.407615	2.002590
1	3.277155	1.695797	0.985120
6	-2.985247	-1.140120	-0.492074
1	-3.218494	-0.347718	-1.207632
1	-3.699981	-1.944380	-0.687236
6	2.898659	-1.681084	0.183984
1	3.229705	-2.189656	1.094442
1	3.299249	-2.257637	-0.655716
6	3.499548	-0.269379	0.136532
1	3.537971	0.088024	-0.897178
1	4.535310	-0.308927	0.484299
6	-2.027372	0.166973	1.510431
1	-2.247319	0.403670	2.556538
1	1.505800	-0.357401	-1.585749
1	-0.731247	-0.270573	-2.211036
1	-1.121323	-0.447441	1.524237
6	-3.185846	-0.655497	0.949351
1	-3.317437	-1.533589	1.591355
1	-4.113833	-0.078245	1.021360

CST-adduct:

6	-0.299317	2.262316	-0.670593
6	1.006100	2.154602	-0.444040
1	-0.729525	3.190727	-1.034275
1	1.682557	2.986950	-0.619984
6	-1.214313	1.092968	-0.397225
6	1.563595	0.867178	0.096573
6	-0.571457	-0.210851	-0.938774
6	0.956392	-0.356680	-0.629748
1	-2.129502	1.244638	-0.979251
1	1.269580	0.794392	1.153873
6	-1.404617	-1.462952	-0.617508
1	-1.098704	-2.261803	-1.300267
1	-1.180400	-1.832551	0.384846
6	1.394144	-1.621151	0.123564
1	1.010930	-1.590341	1.151957
1	0.980459	-2.518131	-0.342777
6	-1.642058	1.091437	1.086397
1	-2.077924	2.077476	1.280204
1	-0.762479	1.022956	1.731591
6	3.091290	0.792721	0.064794
1	3.516737	1.674703	0.553918
6	-2.917759	-1.261561	-0.764255
1	-3.117357	-0.811795	-1.742647
1	-3.383959	-2.249649	-0.791016
6	2.923224	-1.727698	0.150232
1	3.227276	-2.618854	0.706237
1	3.282287	-1.858885	-0.877694
6	-2.668886	0.013748	1.489375
1	-3.277713	0.406017	2.308689
1	1.460454	-0.395057	-1.604456
1	3.429403	0.810402	-0.978976
6	3.579351	-0.483055	0.752642
1	4.667999	-0.561609	0.689125
1	3.327084	-0.425987	1.818524
1	-0.638331	-0.087747	-2.025630
1	-2.160919	-0.863504	1.896550
6	-3.598690	-0.419135	0.352121
1	-4.420344	-0.997523	0.781550
1	-4.059612	0.473854	-0.081426

CCC:

6	-0.007801	1.851158	-1.522484
6	1.331102	2.240248	-1.046527
1	-0.060344	1.722282	-2.602537
1	1.832344	2.962911	-1.687489
6	-1.153070	1.687424	-0.852731
6	2.025139	1.778010	-0.000987
6	-0.576959	-1.572514	-1.234447
6	0.749481	-1.647589	-1.151227
1	3.023304	2.185590	0.154763
1	-2.021512	1.422155	-1.450554
6	-1.425173	1.901400	0.608154
1	-0.565690	2.392539	1.071615
1	-2.266378	2.601385	0.687980
6	-1.627058	-2.006217	-0.243346
1	-1.949628	-3.014382	-0.526774
1	-1.206184	-2.104061	0.762127

6	-2.868866	-1.081817	-0.233041
1	-3.772268	-1.696525	-0.272305
6	1.597464	-2.196686	-0.036577
1	1.915258	-3.204056	-0.329148
1	1.009500	-2.319715	0.879948
6	1.576137	0.748836	0.990512
1	1.267094	1.256347	1.913264
1	0.696232	0.249504	0.589532
6	2.856443	-1.353501	0.257838
1	3.664444	-2.015004	0.581655
6	2.644640	-0.292355	1.339589
1	2.351837	-0.800420	2.264812
1	3.196714	-0.876569	-0.668328
6	-1.790075	0.648908	1.431601
1	-0.933435	-0.023557	1.493966
1	-2.874730	-0.493582	-1.153211
1	1.316132	-1.285177	-2.007993
1	3.593458	0.213158	1.551215
1	-1.971578	0.991163	2.455622
1	-0.982945	-1.158910	-2.155960
6	-3.014759	-0.160332	0.991282
1	-3.300742	-0.791148	1.840170
1	-3.860746	0.516245	0.821970

CCC-TS-cbc:

6	0.168399	2.486512	-0.472342
6	1.522407	2.158505	-0.575278
1	-0.133149	3.334760	-1.082084
1	2.060103	2.759980	-1.305531
6	-0.866806	1.671713	-0.032461
6	2.168944	0.980928	-0.209901
6	-0.487759	0.041201	-1.565829
6	0.800199	-0.474017	-1.390588
1	3.089342	0.819203	-0.775741
1	-1.856630	2.027284	-0.318816
6	-0.877468	0.830566	1.222589
1	-0.290340	-0.071504	1.077514
1	-0.389279	1.392912	2.025913
6	-1.739562	-0.827283	-1.501620
1	-2.543359	-0.280193	-2.003508
1	-1.538720	-1.701219	-2.135472
6	-2.317302	-1.347198	-0.173719
1	-2.997781	-2.162244	-0.435897
1	-1.538969	-1.800185	0.448833
6	-2.279560	0.441272	1.686339
1	-2.176814	-0.199593	2.568430
6	1.072050	-1.867863	-0.849650
1	1.915152	-2.275540	-1.417702
1	0.215720	-2.516369	-1.074184
6	2.306075	0.323922	1.142894
1	3.173130	0.815210	1.603992
1	1.469052	0.533296	1.801961
6	2.598321	-1.179060	1.095082
1	2.907123	-1.501109	2.093540
6	1.420889	-2.034187	0.636790
1	0.552738	-1.826722	1.270493
1	1.662670	-3.088796	0.800459

1	1.520413	-0.144172	-2.125539
1	3.454125	-1.358735	0.431628
1	-0.562909	0.803242	-2.331505
1	-2.823606	1.333664	2.012409
6	-3.102330	-0.295676	0.625708
1	-3.534476	0.422895	-0.078941
1	-3.952510	-0.772078	1.121665

CCC-TS-cbb:

6	0.299297	2.511113	0.512524
6	-1.045877	2.416923	0.165953
1	0.503523	3.280753	1.254599
1	-1.669335	3.189202	0.610009
6	1.305908	1.560002	0.361392
6	-1.755247	1.320802	-0.306442
6	0.313469	-0.083439	1.532588
6	-1.066510	-0.189233	1.316288
1	-2.830121	1.442890	-0.161657
1	2.130217	1.727041	1.057798
6	1.878319	1.014744	-0.941095
1	1.138815	0.586195	-1.614419
1	2.245865	1.909048	-1.457990
6	1.262598	-1.264378	1.334022
1	2.243214	-0.983259	1.730351
1	0.906640	-2.072334	1.984509
6	1.446894	-1.821601	-0.092234
1	1.387366	-2.913786	-0.067686
1	0.623761	-1.500439	-0.728663
6	3.074884	0.070762	-0.736323
1	3.828730	0.273459	-1.501731
6	-1.716006	-1.473139	0.831343
1	-2.015371	-2.032644	1.727289
1	-0.999215	-2.112496	0.313503
6	-1.475984	0.327298	-1.403770
1	-1.427004	0.846888	-2.368940
1	-0.515511	-0.149930	-1.256588
6	-2.945081	-1.272864	-0.058289
1	-3.486793	-2.216895	-0.161315
6	-2.578717	-0.741293	-1.450494
1	-2.246212	-1.568924	-2.084810
1	-3.627499	-0.579797	0.443292
1	-1.698704	0.392747	1.977596
1	-3.473040	-0.322852	-1.923520
1	3.550075	0.324241	0.216776
1	0.591169	0.534145	2.377503
6	2.758297	-1.428567	-0.772141
1	2.711964	-1.763303	-1.813785
1	3.589994	-1.972732	-0.312062

CCC-TS-bbc:

6	-0.127994	2.452985	-0.708111
6	1.252316	2.282528	-0.575824
1	-0.404796	3.119669	-1.523171
1	1.839990	2.906163	-1.244934

6	-1.151321	1.639343	-0.237409
6	1.933076	1.178181	-0.067894
6	-0.355346	-0.271298	-1.416633
6	1.039272	-0.358298	-1.392333
1	2.974872	1.131987	-0.392441
1	-2.075131	1.753720	-0.802280
6	-1.435979	1.285885	1.210832
1	-0.618560	1.635987	1.842726
1	-2.298096	1.908785	1.485638
6	-1.266227	-1.432024	-1.065202
1	-1.293326	-2.067759	-1.961325
1	-0.846424	-2.061780	-0.278386
6	-2.705885	-1.033575	-0.714285
1	-3.389209	-1.825119	-1.034295
6	1.782735	-1.614159	-0.953520
1	2.814831	-1.530561	-1.309430
1	1.347838	-2.474137	-1.479131
6	1.753474	0.488975	1.259557
1	2.116461	1.179428	2.031274
1	0.705368	0.310378	1.470431
6	2.505386	-0.837478	1.365741
1	2.544691	-1.145429	2.414376
6	1.837454	-1.933928	0.543536
1	0.831342	-2.102660	0.939216
1	2.379380	-2.875574	0.671907
6	-1.787035	-0.158521	1.564251
1	-0.903087	-0.789474	1.443890
1	-2.976232	-0.153424	-1.303454
1	1.542114	0.170036	-2.191891
1	3.543500	-0.704938	1.036674
1	-2.036242	-0.188977	2.630132
1	-0.766111	0.330892	-2.218515
6	-2.945149	-0.787131	0.786977
1	-3.849271	-0.182588	0.918013
1	-3.156572	-1.753541	1.256876

CCC-TS-bbb:

6	-0.255565	2.373842	-0.799112
6	1.127349	2.225551	-0.722038
1	-0.591847	3.019590	-1.607543
1	1.678618	2.833487	-1.435200
6	-1.216121	1.532598	-0.248080
6	1.863887	1.173364	-0.182669
6	-0.531558	-0.336870	-1.368496
6	0.846532	-0.558323	-1.239398
1	2.880782	1.154458	-0.579602
1	-2.189755	1.627666	-0.723389
6	-1.342841	1.216976	1.228771
1	-0.437593	1.521814	1.753499
1	-2.129412	1.892397	1.592808
6	-1.548248	-1.428322	-1.044769
1	-1.681553	-1.980686	-1.983445
1	-1.143099	-2.155766	-0.338477
6	-2.929557	-0.976684	-0.558212
1	-3.662422	-1.746344	-0.816973
6	1.403859	-1.747826	-0.482191
1	1.360326	-2.622359	-1.143778

1	0.778481	-1.994639	0.381742
6	1.822893	0.486711	1.162198
1	2.006905	1.224450	1.952238
1	0.848320	0.052648	1.363470
6	2.840298	-1.537095	0.000441
1	3.303766	-2.496449	0.243077
6	2.889098	-0.615177	1.228494
1	2.730316	-1.203069	2.137576
1	3.425987	-1.110907	-0.820351
6	-1.735265	-0.202975	1.624417
1	-0.905881	-0.883005	1.409483
1	-3.232161	-0.085289	-1.111576
1	1.470068	-0.240973	-2.067580
1	3.882735	-0.164005	1.314401
1	-1.874243	-0.228346	2.709991
1	-0.819607	0.230891	-2.246582
6	-3.004793	-0.747179	0.964114
1	-3.229246	-1.707839	1.439243
1	-3.849280	-0.089273	1.196163

CSC-adduct:

6	-0.030377	2.207227	0.070428
6	1.244587	2.054924	-0.278228
1	-0.363767	3.165326	0.463242
1	1.925824	2.897187	-0.174097
6	-1.075939	1.129285	-0.051771
6	1.860181	0.769073	-0.771171
6	-0.537302	-0.018586	-0.924982
6	0.901356	-0.427293	-0.573702
1	2.063663	0.869715	-1.845635
1	-1.911549	1.571772	-0.611488
6	-1.646623	0.779692	1.338250
1	-0.841967	0.495079	2.018939
1	-2.062153	1.711901	1.738651
6	-1.476071	-1.225495	-1.044481
1	-1.178390	-1.792089	-1.933124
1	-1.337202	-1.908724	-0.203431
6	-2.960038	-0.861847	-1.174095
1	-3.498868	-1.757059	-1.494256
6	1.134707	-1.004510	0.828011
1	0.347972	-1.703995	1.121862
1	1.115762	-0.186843	1.554547
6	3.212432	0.534287	-0.052740
1	4.001705	1.097695	-0.557055
1	3.152881	0.926886	0.968635
6	2.508441	-1.700237	0.874618
1	2.856226	-1.748872	1.910187
6	3.546534	-0.955829	0.008573
1	4.552135	-1.110585	0.405818
1	2.412196	-2.732300	0.525521
6	-2.748892	-0.294619	1.361029
1	-2.309124	-1.284700	1.505600
1	-3.070452	-0.139420	-1.989598
1	1.181266	-1.209753	-1.292206
1	3.549853	-1.360367	-1.008900
1	-3.378953	-0.121934	2.238033
1	-0.472337	0.417514	-1.932796

6	-3.635244	-0.304707	0.111953
1	-4.526732	-0.898433	0.328416
1	-3.994503	0.713827	-0.067015

772 ring systems:

TTT:

6	0.732242	-2.963477	0.072862
6	-0.731001	-2.963629	-0.072105
1	1.278204	-3.862467	-0.208267
1	-1.276877	-3.862647	0.209121
6	1.400870	-1.900944	0.524785
6	-1.399778	-1.901418	-0.524553
1	0.819303	-1.041250	0.856840
1	-0.818447	-1.041557	-0.856573
6	0.463182	2.626006	0.477830
6	-0.464291	2.625922	-0.477542
1	0.135502	2.622196	1.518240
1	-0.136528	2.622373	-1.517927
6	-1.951109	2.700206	-0.251561
1	-2.358204	3.447367	-0.939889
1	-2.146212	3.068280	0.761161
6	-2.698894	1.370749	-0.451837
6	1.949935	2.700782	0.251837
1	2.144992	3.069144	-0.760776
1	2.356868	3.447822	0.940405
6	2.698131	1.371434	0.451870
6	-2.888869	-1.744260	-0.535564
1	-3.371128	-2.722697	-0.460183
1	-3.756600	1.574917	-0.651872
6	2.889891	-1.743189	0.535151
1	3.372460	-2.721461	0.459519
1	3.755749	1.575950	0.651990
1	-3.211082	-1.297722	-1.481760
1	-2.305362	0.866732	-1.341805
6	-3.354210	-0.860187	0.638378
1	-4.425050	-0.655595	0.530341
1	-3.228416	-1.429690	1.564200
6	-2.593532	0.462501	0.771387
1	-2.987187	1.003956	1.638542
1	-1.537461	0.265932	0.987952
1	3.212437	-1.296554	1.481194
1	2.304652	0.867071	1.341648
6	3.354339	-0.858969	-0.639019
1	4.425159	-0.653998	-0.531524
1	3.228262	-1.428504	-1.564793
6	2.593226	0.463515	-0.771706
1	2.986903	1.005446	-1.638546
1	1.537267	0.266702	-0.988521

TTT-TS-cbc:

6	1.022817	-1.618514	0.030968
6	-0.209381	-1.801593	-0.618577
1	1.897407	-2.097817	-0.395400
1	-0.225310	-2.378357	-1.540347
6	1.192758	-0.668297	1.016153
6	-1.339366	-1.106542	-0.250542
1	0.337086	-0.411884	1.633754
1	-1.431919	-0.828908	0.792695
6	0.622768	1.170367	-0.103229
6	-0.730356	1.079680	-0.371139
1	0.919515	1.706130	0.796583
1	-1.032979	1.022330	-1.413376
6	-1.731312	1.695452	0.586137
1	-1.559350	2.778316	0.574843
1	-1.494119	1.375674	1.610766
6	-3.232041	1.470140	0.325690
6	1.613950	1.174807	-1.241775
1	1.427718	0.290563	-1.867073
1	1.379936	2.039749	-1.874037
6	3.105232	1.246011	-0.871096
6	-2.622399	-1.158188	-1.040810
1	-2.670997	-2.095383	-1.603830
1	-3.760950	2.285231	0.826543
6	2.519622	-0.347871	1.652021
1	2.595715	-0.887504	2.604183
1	3.622329	1.724942	-1.706931
1	-2.617358	-0.362519	-1.794716
1	-3.442227	1.593962	-0.743427
6	-3.881131	-1.006698	-0.181598
1	-4.735261	-0.852314	-0.848468
1	-4.072747	-1.940012	0.356663
6	-3.825894	0.143068	0.835725
1	-4.846774	0.322479	1.183912
1	-3.267238	-0.168701	1.724176
1	2.525311	0.713224	1.925803
1	3.242183	1.918273	-0.015174
6	3.767448	-0.655827	0.821545
1	4.624043	-0.254172	1.371574
1	3.921757	-1.738853	0.781594
6	3.800249	-0.102033	-0.617176
1	4.852669	-0.009372	-0.900636
1	3.373776	-0.828854	-1.313444

TTT-TS-cbb:

6	-1.094960	1.621395	0.131761
6	0.193586	1.911601	-0.336538
1	-1.936938	2.061839	-0.390684
1	0.290950	2.544485	-1.215522
6	-1.322944	0.622183	1.060299
6	1.320742	1.285245	0.153928
1	-0.542109	0.423047	1.788065
1	1.285709	0.952542	1.183729

6	-0.532365	-1.112346	-0.002108
6	0.839088	-0.944642	-0.122145
1	-0.883711	-1.700198	0.844040
1	1.227647	-0.860955	-1.129337
6	1.768093	-1.550962	0.909406
1	1.919689	-2.602294	0.629189
1	1.248972	-1.575842	1.875612
6	3.150956	-0.918059	1.107683
6	-1.379410	-1.170639	-1.252055
1	-1.166941	-0.277266	-1.855081
1	-1.022608	-2.020776	-1.846148
6	-2.898682	-1.325565	-1.072081
6	2.694676	1.601010	-0.404933
1	2.584737	2.414665	-1.128024
1	3.068778	0.014099	1.672855
1	3.732839	-1.592723	1.743174
1	3.327725	1.987767	0.403455
6	-2.697561	0.219170	1.530225
1	-2.908273	0.731219	2.477065
1	-3.282232	-1.803866	-1.977294
6	3.440098	0.452729	-1.103434
1	2.794811	0.040908	-1.881306
1	4.297505	0.880783	-1.630976
6	3.961715	-0.655866	-0.166416
1	4.063591	-1.589619	-0.730545
1	4.973299	-0.382899	0.150240
1	-2.681344	-0.847465	1.779852
1	-3.106836	-2.027406	-0.255118
6	-3.854945	0.490053	0.567015
1	-4.747887	0.029566	1.000745
1	-4.060192	1.564873	0.535827
6	-3.684910	-0.019006	-0.876698
1	-4.687825	-0.149200	-1.293444
1	-3.208414	0.746917	-1.493820

TTT-TS-bbc:

6	0.840132	1.910023	-0.178440
6	-0.446043	2.022083	0.363134
1	1.611122	2.583185	0.188894
1	-0.611889	2.741299	1.161352
6	1.228384	0.851251	-0.976169
6	-1.442184	1.114054	0.063419
1	0.476261	0.345611	-1.574458
1	-1.421279	0.673366	-0.927058
6	0.764905	-0.833823	0.467341
6	-0.610593	-0.857764	0.636870
1	1.171790	-1.511422	-0.275880
1	-0.990677	-0.650189	1.633514
6	-1.442340	-1.799248	-0.214202
1	-1.141140	-2.820024	0.049406
1	-1.155906	-1.674583	-1.268045
6	-2.975833	-1.735836	-0.105226

6	1.664233	-0.485652	1.625666
1	1.178042	0.306485	2.208408
1	1.708625	-1.362750	2.285463
6	3.092814	-0.053722	1.280866
6	-2.788697	1.149977	0.744878
1	-2.988597	2.164258	1.104025
1	-3.353165	-2.694945	-0.469873
6	2.637459	0.740168	-1.520226
1	2.595302	0.909865	-2.601986
1	3.697292	-0.129325	2.189758
1	3.097694	1.004260	1.010302
1	3.253756	1.545513	-1.107936
6	3.797124	-0.854871	0.176770
1	4.860564	-0.604231	0.232410
1	3.730116	-1.924516	0.405041
6	3.328883	-0.609650	-1.279532
1	4.203421	-0.667001	-1.933438
1	2.662826	-1.407689	-1.616826
1	-2.764015	0.520762	1.641787
1	-3.269645	-1.685229	0.950131
6	-3.943236	0.685511	-0.147136
1	-4.832486	0.559806	0.478581
1	-4.182841	1.468588	-0.873115
6	-3.674297	-0.622128	-0.906969
1	-4.635404	-0.995876	-1.270550
1	-3.084056	-0.417457	-1.806161

TTT-TS-bbb:

6	0.904928	1.921715	-0.180793
6	-0.440305	2.077975	0.165059
1	1.641311	2.542206	0.324118
1	-0.695368	2.793438	0.942867
6	1.361118	0.870526	-0.956589
6	-1.426764	1.231160	-0.307356
1	0.684277	0.438413	-1.687459
1	-1.263609	0.798117	-1.286983
6	0.677084	-0.806949	0.321719
6	-0.711994	-0.800583	0.330467
1	1.147523	-1.481514	-0.385820
1	-1.177737	-0.618567	1.290612
6	-1.467112	-1.708070	-0.622066
1	-1.528711	-2.696449	-0.146735
1	-0.856089	-1.850493	-1.521932
6	-2.883183	-1.310106	-1.053835
6	1.428537	-0.552326	1.605278
1	0.904662	0.237862	2.156756
1	1.344365	-1.457928	2.221151
6	2.908611	-0.181904	1.477031
6	-2.876206	1.433626	0.100016
1	-2.926683	2.340267	0.710220
1	-2.848353	-0.475250	-1.758679
1	-3.301226	-2.149413	-1.618429

1	-3.469098	1.634957	-0.801201
6	2.827853	0.734497	-1.314024
1	2.931983	0.955919	-2.382125
1	3.379699	-0.331608	2.453179
1	3.002119	0.885528	1.267171
1	3.404105	1.501338	-0.786799
6	3.715991	-0.971491	0.437086
1	4.773087	-0.777279	0.640448
1	3.571210	-2.044383	0.605857
6	3.450266	-0.644497	-1.054448
1	4.401197	-0.696967	-1.591359
1	2.815944	-1.406152	-1.514889
6	-3.554323	0.302432	0.887927
1	-2.947330	0.068705	1.764503
1	-4.498524	0.688971	1.282869
6	-3.862995	-0.967824	0.073582
1	-3.948376	-1.822219	0.753976
1	-4.849420	-0.846580	-0.385647

CAT-adduct:

6	1.031184	-1.663572	0.093855
6	-0.166258	-1.855800	-0.452719
1	1.856379	-2.347591	-0.078280
1	-0.372804	-2.709365	-1.091627
6	1.214406	-0.435262	0.943712
6	-1.284188	-0.892395	-0.128908
1	0.521585	-0.527378	1.794345
1	-1.536930	-1.066080	0.929388
6	0.688370	0.792689	0.155369
6	-0.801921	0.586952	-0.245997
1	0.745025	1.643296	0.847020
1	-0.890515	0.841154	-1.309737
6	-1.695213	1.562915	0.528066
1	-1.312534	2.573189	0.345001
1	-1.566932	1.378484	1.603908
6	-3.193497	1.537746	0.204184
6	1.499839	1.163701	-1.092972
1	1.316515	0.408559	-1.866498
1	1.078782	2.100092	-1.477528
6	3.014896	1.320908	-0.932483
6	-2.546082	-1.143641	-0.971565
1	-2.536347	-2.173262	-1.340935
1	-3.646998	2.417128	0.670112
6	2.608425	-0.244686	1.558634
1	2.685434	-0.874434	2.450324
1	3.393997	1.817971	-1.829798
1	-2.501578	-0.509352	-1.863065
1	-3.345780	1.652245	-0.876262
6	-3.879110	-0.919051	-0.242347
1	-4.664821	-0.805535	-0.995945
1	-4.132625	-1.817939	0.328453
6	-3.919209	0.284252	0.709852

1	-4.967402	0.521811	0.911217
1	-3.487149	0.005500	1.677131
1	2.671592	0.787905	1.918081
1	3.249308	1.986379	-0.092810
6	3.820419	-0.547037	0.666980
1	4.700298	-0.116141	1.155141
1	3.996802	-1.626801	0.638333
6	3.736759	-0.023613	-0.772841
1	4.753182	0.051978	-1.168815
1	3.220599	-0.756455	-1.402067

TTC:

6	0.825557	-1.785527	-0.916289
6	-0.546975	-1.859574	-0.391384
1	0.924347	-1.545349	-1.975309
1	-1.309891	-2.322923	-1.011844
6	1.928838	-1.846592	-0.171156
6	-0.876685	-1.255030	0.753140
1	1.834922	-2.140817	0.874275
1	-0.080470	-0.748702	1.293790
6	0.244962	2.063681	0.558579
6	-1.086887	2.016055	0.526492
1	-1.645646	2.314250	1.411890
1	0.733008	2.390274	1.475025
6	-2.238136	-1.117421	1.367460
1	-2.315164	-1.805827	2.218205
6	-1.891507	1.646308	-0.693157
1	-1.950238	2.542195	-1.323803
1	-1.331640	0.911713	-1.280262
6	-3.327183	1.121345	-0.448200
6	1.141376	1.718056	-0.607870
1	0.858934	0.733810	-0.994322
1	0.962956	2.429629	-1.423303
6	3.289462	-1.403858	-0.622800
1	3.963443	-2.258596	-0.747323
6	2.634205	1.720149	-0.256657
1	3.211975	1.511812	-1.163305
1	2.913067	2.732768	0.050272
6	3.920746	-0.443012	0.403235
1	4.854780	-0.046223	-0.008145
1	-4.008537	1.691202	-1.083436
1	3.203697	-0.919748	-1.601052
1	-2.296380	-0.113890	1.805435
1	-3.636703	1.337160	0.581235
6	-3.437061	-1.330044	0.443237
1	-4.341309	-1.217088	1.050644
1	-3.446696	-2.362401	0.077762
6	-3.538123	-0.375004	-0.755899
1	-2.831439	-0.670676	-1.535887
1	-4.533196	-0.511951	-1.189159
1	4.195865	-1.024183	1.290218
6	3.025105	0.719471	0.852336

1	2.115569	0.312822	1.307567
1	3.548583	1.246709	1.654440

TTC-TS-cbc:

6	0.700927	-1.726888	-0.526769
6	-0.700832	-1.726919	-0.526816
1	1.198043	-1.890251	-1.477639
1	-1.197883	-1.890287	-1.477721
6	1.444063	-1.334191	0.566796
6	-1.444066	-1.334285	0.566702
1	1.013076	-1.494755	1.548525
1	-1.013147	-1.494844	1.548460
6	0.695449	0.769535	0.853150
6	-0.695433	0.769534	0.853215
1	-1.172466	0.717085	1.827703
1	1.172563	0.717184	1.827602
6	-2.959778	-1.309275	0.545717
1	-3.299491	-2.346250	0.650336
6	-1.491217	1.506992	-0.206096
1	-1.046889	2.501082	-0.332730
1	-1.375240	1.013094	-1.178650
6	-2.978758	1.680379	0.158222
6	1.491131	1.506881	-0.206316
1	1.375185	1.012768	-1.178767
1	1.046716	2.500907	-0.333137
6	2.959778	-1.309148	0.545945
1	3.299502	-2.346102	0.650736
6	2.978663	1.680468	0.157962
1	3.276855	2.717878	-0.014948
1	3.090390	1.522654	1.235199
1	-3.277037	2.717800	-0.014468
1	3.329304	-0.790789	1.436969
6	3.588437	-0.693807	-0.715651
1	4.485230	-1.255624	-0.989103
1	-3.329394	-0.791045	1.436780
1	-3.090478	1.522329	1.235424
6	-3.588336	-0.693764	-0.715847
1	-4.485054	-1.255596	-0.989512
1	-2.901746	-0.811147	-1.556418
6	-3.975856	0.785687	-0.588051
1	-4.134526	1.184460	-1.595336
1	-4.940902	0.862486	-0.075889
1	2.901965	-0.811407	-1.556287
6	3.975838	0.785700	-0.588115
1	4.134498	1.184290	-1.595473
1	4.940870	0.862676	-0.075953

TTC-TS-cbb:

6	0.873995	-1.782928	-0.504992
6	-0.489849	-1.803730	-0.811239
1	1.560332	-1.998691	-1.316297
1	-0.760142	-1.997734	-1.847918
6	1.361137	-1.260617	0.678557
6	-1.496091	-1.378238	0.031165
1	0.735269	-1.356900	1.559808
1	-1.390084	-1.494617	1.104503
6	0.635176	0.790106	0.567684
6	-0.753458	0.772088	0.484245
1	-1.246335	0.721424	1.445929
1	1.033208	0.870029	1.575350
6	-2.897395	-1.314047	-0.533534
1	-3.223622	-2.340061	-0.744396
6	-1.544727	1.415659	-0.631331
1	-1.078656	2.370818	-0.900725
1	-1.480703	0.806105	-1.537991
6	-3.022469	1.713974	-0.267645
1	-3.615432	1.735924	-1.188414
6	1.513053	1.410396	-0.500256
1	1.555092	0.763829	-1.385481
1	1.035777	2.336637	-0.839146
6	2.845893	-1.162647	0.972979
1	3.173495	-2.145788	1.329516
6	2.923491	1.750954	0.017637
1	3.228006	2.725532	-0.373099
1	2.860090	1.882899	1.102730
1	-2.850787	-0.819492	-1.510696
1	-3.067882	2.727268	0.142433
6	-3.985600	-0.645774	0.305932
1	-4.191507	-1.255044	1.192373
1	-4.903674	-0.660547	-0.290726
6	-3.708430	0.795466	0.753241
1	-3.133078	0.787658	1.681032
1	-4.665410	1.254459	1.019921
1	3.003484	-0.478167	1.814164
6	3.723957	-0.736589	-0.216132
1	4.670535	-1.281944	-0.178735
1	3.248600	-1.046751	-1.147719
6	4.053448	0.761033	-0.305458
1	4.888998	0.984992	0.366050
1	4.421625	0.957531	-1.317591

TTC-TS-bbc:

6	0.238617	-1.651958	-0.892801
6	-1.085175	-1.576096	-0.452519
1	0.405668	-1.799087	-1.958442
1	-1.873030	-1.712663	-1.184993

6	1.339742	-1.343499	-0.116495
6	-1.405000	-1.078462	0.797790
1	1.319272	-1.541569	0.950046
1	-0.686062	-1.235461	1.595629
6	0.791568	0.805201	0.616530
6	-0.596020	0.919261	0.654927
1	-1.044142	1.038989	1.636840
1	1.249686	0.648270	1.586690
6	-2.821517	-0.902850	1.282756
1	-3.098531	-1.781146	1.878390
6	-1.331349	1.577839	-0.482487
1	-0.942952	2.600953	-0.575520
1	-1.057045	1.075271	-1.420248
6	-2.861658	1.653591	-0.366962
6	1.659398	1.500787	-0.408079
1	1.553634	1.025938	-1.387177
1	1.293758	2.525549	-0.552075
6	2.692783	-1.327313	-0.792593
1	2.891580	-2.336173	-1.174258
6	3.146114	1.599236	0.007030
1	3.752945	1.776158	-0.887881
1	3.258258	2.492886	0.629134
6	3.895348	-0.897564	0.048181
1	4.760275	-0.833369	-0.620372
1	-3.192554	2.493259	-0.983993
1	2.632541	-0.691733	-1.682860
1	-2.849696	-0.061794	1.984338
1	-3.143441	1.910270	0.661696
6	-3.891807	-0.694290	0.208285
1	-4.825379	-0.461112	0.729421
1	-4.071721	-1.638583	-0.315236
6	-3.622677	0.403850	-0.839634
1	-3.078902	-0.011989	-1.692144
1	-4.593683	0.715197	-1.235208
1	4.129072	-1.682613	0.775224
6	3.740121	0.427543	0.799852
1	3.150554	0.260466	1.704229
1	4.728965	0.732428	1.156076

TTC-TS-bbb:

6	0.471142	1.749976	0.979430
6	-0.899755	1.775854	0.722188
1	0.796440	1.907409	2.005963
1	-1.573917	1.997945	1.546074
6	1.422002	1.332087	0.064387
6	-1.444271	1.295464	-0.455722
1	1.261068	1.517795	-0.992853
1	-0.835855	1.342115	-1.353585
6	0.664604	-0.761984	-0.447150
6	-0.723739	-0.781630	-0.330217
1	-1.273228	-0.919163	-1.252158
1	1.021186	-0.709489	-1.469128

6	-2.937400	1.343566	-0.711646
1	-3.118180	2.119169	-1.464408
6	-1.373277	-1.317921	0.916891
1	-1.257798	-2.411732	0.908666
1	-0.808960	-0.965945	1.788556
6	-2.852403	-0.971699	1.106580
1	-2.935556	0.033214	1.527245
6	1.580929	-1.477058	0.524864
1	1.631006	-0.933770	1.472507
1	1.143588	-2.450459	0.779905
6	2.856928	1.252241	0.538421
1	3.175075	2.266216	0.809381
6	2.999339	-1.738265	-0.037363
1	3.693305	-1.873895	0.799313
1	2.978331	-2.694240	-0.569572
6	3.895880	0.679143	-0.424917
1	4.053248	1.381290	-1.250420
1	4.847086	0.627268	0.115074
1	-3.452351	1.674154	0.195738
1	-3.264901	-1.644576	1.864098
1	2.884050	0.683044	1.474030
6	-3.573137	0.040308	-1.215178
1	-2.997343	-0.323494	-2.070166
1	-4.562429	0.277885	-1.615345
6	-3.737329	-1.068971	-0.144596
1	-3.593713	-2.049473	-0.612034
1	-4.775629	-1.052392	0.198973
6	3.576899	-0.700802	-1.009993
1	2.906201	-0.587849	-1.864192
1	4.500814	-1.112876	-1.427544

CSC-adduct:

6	-0.011498	-1.954392	-0.073041
6	-1.213934	-1.692576	0.429988
1	0.155876	-2.887734	-0.605971
1	-2.020266	-2.410732	0.305174
6	1.201905	-1.070948	0.100222
6	-1.493782	-0.414092	1.178093
1	1.842415	-1.625887	0.795739
1	-1.140156	-0.559399	2.208708
6	0.871334	0.298898	0.782736
6	-0.609749	0.715883	0.613264
1	-0.769723	1.591364	1.258088
1	1.012498	0.150651	1.861636
6	-2.985939	-0.066843	1.308550
1	-3.411181	-0.664398	2.121229
6	-0.924432	1.148038	-0.827647
1	-0.329661	2.040081	-1.043996
1	-0.585593	0.373736	-1.524211
6	-2.389831	1.457615	-1.156703
6	1.821406	1.425941	0.362863
1	1.790396	1.550550	-0.723346

1	1.446528	2.366152	0.782899
6	1.995214	-0.965612	-1.218209
1	1.983572	-1.955507	-1.682928
6	3.279347	1.245166	0.791875
1	3.853916	2.084662	0.386541
1	3.355437	1.316273	1.881909
6	3.474586	-0.501559	-1.082866
1	3.661244	0.325512	-1.775740
1	-2.407608	1.976537	-2.119219
1	1.459383	-0.310668	-1.909277
1	-3.053502	0.974754	1.640110
1	-2.808555	2.159725	-0.425484
6	-3.869500	-0.268509	0.070244
1	-4.809307	0.263949	0.248123
1	-4.139396	-1.325017	-0.021945
6	-3.263208	0.201044	-1.258086
1	-2.652052	-0.600975	-1.684596
1	-4.078315	0.372556	-1.966603
1	4.127734	-1.315535	-1.407207
6	3.918656	-0.069340	0.319320
1	3.706610	-0.868120	1.034334
1	5.006256	0.045188	0.322418

TCT:

6	1.969293	-1.601910	-0.632196
6	1.245437	-2.885045	-0.557981
1	2.012253	-1.141530	-1.618436
1	1.555128	-3.645003	-1.272457
6	2.574880	-1.006882	0.394802
6	0.223496	-3.167566	0.253664
1	2.559921	-1.516889	1.356417
6	-1.361041	2.133820	0.658969
6	-2.269796	1.847242	-0.268983
1	-0.228777	-4.154551	0.167724
1	-1.402460	1.599412	1.609939
1	-2.222193	2.366765	-1.226762
6	-0.260927	3.147411	0.524674
1	-0.342458	3.865850	1.347507
1	-0.391876	3.711470	-0.404799
6	1.141262	2.520261	0.551299
1	1.887633	3.311638	0.686104
1	1.216783	1.865655	1.427227
6	3.320579	0.302215	0.346709
1	3.197860	0.808644	1.309318
1	4.393749	0.088569	0.272415
6	2.918027	1.251910	-0.785564
1	3.581905	2.122577	-0.752820
1	3.100479	0.771478	-1.751632
6	-0.454228	-2.231449	1.212486
1	0.124641	-1.311427	1.318247
6	-3.362398	0.828284	-0.111675
1	-4.319976	1.277622	-0.394335

1	-3.448333	0.551875	0.942760
6	-1.868376	-1.859879	0.737582
1	-2.504382	-2.752158	0.701744
1	-2.309482	-1.193532	1.484813
1	-0.511994	-2.697178	2.201801
6	-1.850896	-1.182060	-0.635246
1	-1.005433	-0.486040	-0.673303
1	-1.656315	-1.935880	-1.403075
6	-3.136391	-0.426706	-0.974953
1	-3.108964	-0.125994	-2.027802
1	-3.997888	-1.094689	-0.864247
6	1.465608	1.737018	-0.720551
1	0.778652	0.890643	-0.809187
1	1.274355	2.382684	-1.585377

TCT-TS-cbc:

6	-0.905910	-1.835618	0.549475
6	0.270586	-1.861416	1.303924
1	-1.792607	-2.233185	1.035595
1	0.181006	-2.186039	2.336817
6	-1.080338	-1.129806	-0.623065
6	1.452313	-1.232316	0.939271
1	-0.248276	-0.975893	-1.287894
6	-0.309462	1.012322	0.244181
6	0.816431	0.821783	1.033779
1	2.201614	-1.193533	1.729478
1	-0.165813	1.408363	-0.758098
1	0.614337	0.756123	2.101135
6	-1.649954	1.343722	0.874400
1	-1.505596	2.192189	1.553734
1	-1.973974	0.513050	1.513143
6	-2.726803	1.711943	-0.166231
1	-3.087436	2.727159	0.019235
1	-2.257983	1.745994	-1.154337
6	-2.444699	-1.042884	-1.283482
1	-2.409838	-0.323141	-2.106853
1	-2.628365	-2.016479	-1.754643
6	-3.622049	-0.710654	-0.351083
1	-4.520210	-1.225143	-0.702586
1	-3.423709	-1.115622	0.643425
6	2.083196	-1.301876	-0.446500
1	1.530135	-0.716161	-1.178969
6	2.150094	1.518243	0.758340
1	2.026537	2.541381	1.129259
6	3.551509	-0.843119	-0.472389
1	4.146272	-1.536726	-1.071529
1	2.006437	-2.343267	-0.776034
1	3.962678	-0.903041	0.539613
1	2.929911	1.075091	1.386581
6	3.754733	0.575444	-1.034086
1	4.708120	0.964624	-0.663181
1	3.850553	0.523804	-2.123342

6	2.634956	1.571467	-0.700261
1	1.792605	1.412911	-1.377308
1	2.998829	2.576992	-0.925489
6	-3.943728	0.786260	-0.235656
1	-4.546689	1.090065	-1.098261
1	-4.573784	0.939519	0.646805

TCT-TS-cbb:

6	1.045046	-1.553745	-0.427514
6	-0.073216	-1.579413	-1.261740
1	1.989163	-1.852734	-0.870208
1	0.121343	-1.769093	-2.314875
6	1.080947	-0.853340	0.770486
6	-1.343034	-1.130732	-0.934510
1	0.190837	-0.821971	1.385043
6	0.521016	1.111176	0.073771
6	-0.832460	1.100463	-0.244772
1	-1.986897	-0.991872	-1.801634
1	0.766315	1.448972	1.079137
1	-1.125101	1.344078	-1.261734
6	1.546195	1.430332	-0.985474
1	1.282857	2.406683	-1.409222
1	1.438985	0.711491	-1.808847
6	3.012248	1.489667	-0.525031
1	3.541784	2.153926	-1.213402
1	3.071081	1.972389	0.458368
6	2.356399	-0.652301	1.552347
1	2.295087	0.309789	2.072698
1	2.403814	-1.404686	2.349230
6	3.668876	-0.709585	0.763555
1	4.463965	-0.406907	1.451835
1	3.888754	-1.748562	0.497841
6	-2.136545	-1.492081	0.303530
1	-1.698844	-1.113034	1.223101
6	-1.812519	1.426290	0.862850
1	-1.532486	2.400732	1.280252
1	-1.671073	0.723548	1.692431
6	-3.609318	-1.054248	0.199275
1	-4.130927	-1.761178	-0.454674
1	-4.079652	-1.143330	1.184592
1	-2.107580	-2.583139	0.404515
6	-3.843987	0.353293	-0.355744
1	-3.427186	0.422510	-1.364432
1	-4.922030	0.501008	-0.473911
6	-3.296510	1.504215	0.487734
1	-3.470103	2.436779	-0.059690
1	-3.876313	1.582260	1.413773
6	3.767583	0.151771	-0.511754
1	3.440126	-0.421095	-1.383198
1	4.829754	0.352868	-0.679034

TCT-TS-bbc:

6	-0.736619	2.031538	-0.901350
6	0.609896	2.004045	-1.263098
1	-1.422251	2.478608	-1.620069
1	0.868457	2.403522	-2.239290
6	-1.315981	1.323440	0.133763
6	1.557998	1.220819	-0.613998
1	-0.782199	1.098827	1.043706
6	-0.381145	-0.917467	-0.465398
6	0.789199	-0.673691	-1.174789
1	2.527238	1.176184	-1.109410
1	-0.248284	-1.357645	0.521618
1	0.640629	-0.443557	-2.229110
6	-1.692279	-1.260196	-1.141281
1	-1.516361	-2.067607	-1.863934
1	-2.045989	-0.416451	-1.740041
6	-2.775300	-1.767723	-0.162603
1	-3.753520	-1.719258	-0.654240
1	-2.579594	-2.829820	0.016813
6	-2.823430	1.269076	0.187222
1	-3.196821	2.283613	0.374313
6	1.641956	1.090590	0.897635
1	0.970487	0.311903	1.261717
6	2.052173	-1.511486	-0.966402
1	1.788231	-2.525996	-1.287025
6	3.049593	0.775856	1.401609
1	2.990286	0.621206	2.483416
1	1.291161	2.025722	1.347951
1	3.706044	1.637883	1.247628
1	2.815628	-1.168694	-1.672708
6	3.680362	-0.461887	0.746948
1	4.187419	-0.175684	-0.180427
1	4.467248	-0.833877	1.408672
6	2.708729	-1.608585	0.421491
1	1.954495	-1.714787	1.209104
1	3.277677	-2.541966	0.432190
1	-3.202494	1.001326	-0.805895
6	-3.430804	0.329119	1.227187
1	-3.291235	0.751802	2.227892
1	-4.511905	0.289339	1.057973
6	-2.862758	-1.090860	1.211914
1	-1.874919	-1.085518	1.678869
1	-3.488982	-1.714614	1.857176

TCT-TS-bbb:

6	0.865177	1.888446	0.383234
6	-0.326362	1.894463	1.104050
1	1.721957	2.377132	0.842270
1	-0.272672	2.271187	2.122434
6	1.121112	1.041746	-0.687062
6	-1.488918	1.229088	0.739455
1	0.314424	0.773336	-1.355766
6	0.670128	-0.866083	0.316417
6	-0.702898	-0.952536	0.526364
1	-2.208386	1.151598	1.552621
1	1.029565	-1.354029	-0.583073
1	-1.058989	-1.052953	1.547531
6	1.621958	-0.858020	1.483525
1	1.621204	-1.868233	1.913802
1	1.215247	-0.198707	2.259907
6	3.066883	-0.454387	1.171448
1	3.153905	0.633980	1.172976
1	3.700797	-0.800168	1.993291
6	2.496660	1.009829	-1.327389
1	2.410222	1.439799	-2.331503
6	-2.172414	1.292922	-0.611956
1	-1.611450	0.801624	-1.402358
6	-1.523859	-1.613450	-0.564207
1	-1.109257	-2.614538	-0.731423
1	-1.355889	-1.087415	-1.511041
6	-3.605954	0.732946	-0.564387
1	-4.255209	1.486427	-0.106012
1	-3.970376	0.595786	-1.588123
1	-2.220066	2.347012	-0.908110
6	-3.779900	-0.570468	0.220538
1	-3.492325	-0.409713	1.263039
1	-4.846358	-0.815183	0.247228
6	-3.027768	-1.786838	-0.319250
1	-3.173418	-2.610916	0.387277
1	-3.487063	-2.109061	-1.260069
1	3.169425	1.669096	-0.769710
6	3.142608	-0.376935	-1.462779
1	2.437177	-1.044639	-1.963965
1	3.990105	-0.288817	-2.147864
6	3.652907	-1.003092	-0.138300
1	3.506534	-2.088493	-0.171255
1	4.734734	-0.849901	-0.090307

CAC-adduct:

6	0.949573	-1.403801	0.864762
6	-0.076690	-1.817189	0.124307
1	1.602371	-2.138105	1.331452
1	-0.239425	-2.884638	-0.009799
6	1.240244	0.054149	1.107130
6	-1.087020	-0.909806	-0.538388
1	0.698636	0.340324	2.019038
6	0.625459	0.909464	-0.015801

6	-0.879563	0.577451	-0.144823
1	-0.957830	-1.001218	-1.625997
1	0.706655	1.957533	0.303357
1	-1.254538	1.196482	-0.965021
6	1.289098	0.804325	-1.398652
1	0.829411	1.576144	-2.026420
1	1.032938	-0.154991	-1.859521
6	2.813495	0.941221	-1.468083
1	3.083885	1.092298	-2.517007
1	3.150241	1.837935	-0.934530
6	2.713827	0.359980	1.426872
1	2.840054	1.447030	1.380321
1	2.902854	0.085637	2.469905
6	3.786594	-0.320108	0.568360
1	4.738468	0.176113	0.783469
1	3.910917	-1.357898	0.892574
6	-2.495581	-1.439245	-0.217682
1	-2.620985	-1.468976	0.869703
6	-1.661074	0.945448	1.126652
1	-1.241630	1.875914	1.522403
1	-1.472157	0.183702	1.889009
6	-3.662444	-0.669122	-0.840931
1	-3.616201	-0.753145	-1.931751
1	-4.583647	-1.175123	-0.535227
1	-2.550063	-2.480657	-0.551607
6	-3.755342	0.816233	-0.441927
1	-3.250315	1.439471	-1.182894
1	-4.804587	1.123390	-0.470421
6	-3.197354	1.126849	0.951391
1	-3.460733	2.159202	1.195451
1	-3.722396	0.504773	1.683385
6	3.537030	-0.305927	-0.945651
1	2.938320	-1.180290	-1.220940
1	4.498244	-0.420432	-1.454153

TCC:

6	-0.301518	2.511221	-0.868343
6	1.108310	2.276335	-1.205090
1	-0.810167	3.280226	-1.447694
1	1.375699	2.498327	-2.235822
6	-1.001918	1.819460	0.033703
6	2.088903	1.842854	-0.401769
1	-0.500954	1.012654	0.555026
6	-0.770642	-1.472056	-1.081079
6	0.542499	-1.376430	-1.288455
1	3.072135	1.724749	-0.851715
1	0.882634	-0.674548	-2.047610
1	-1.413132	-0.855267	-1.703465
6	-2.465461	1.970336	0.318329
1	-2.618718	2.226734	1.374130
1	-2.878484	2.789414	-0.276721
6	2.007800	1.574338	1.075600

1	1.187162	2.160034	1.499886
1	2.932668	1.940745	1.535742
6	1.633317	-2.188503	-0.642683
1	1.271220	-2.683982	0.264524
1	1.885080	-2.995222	-1.341644
6	-1.466385	-2.376997	-0.094430
1	-1.559171	-3.381816	-0.524439
6	-2.860562	-1.889714	0.326908
1	-3.274915	-2.619897	1.026820
1	-3.525973	-1.888776	-0.543935
6	-3.209129	0.659532	0.009809
1	-4.288741	0.832968	0.045216
1	-2.979805	0.378096	-1.020638
6	1.836221	0.103065	1.500863
1	1.754998	0.095762	2.592414
1	-0.848582	-2.488207	0.804360
1	0.892349	-0.296776	1.117050
6	2.978569	-0.833764	1.091881
1	3.936539	-0.321304	1.239922
6	2.918757	-1.396161	-0.333849
1	3.029155	-0.597116	-1.071983
1	3.782269	-2.054960	-0.462718
1	2.984230	-1.688704	1.777153
6	-2.851542	-0.490991	0.971310
1	-1.860941	-0.324295	1.407762
1	-3.549880	-0.463998	1.812148

TCC-TS-cbc:

6	-0.611179	2.412928	-0.360041
6	0.757133	2.563472	-0.584585
1	-1.263536	3.118635	-0.871585
1	1.035486	3.288103	-1.346268
6	-1.221319	1.278558	0.150572
6	1.731018	1.657313	-0.183346
1	-0.732129	0.664281	0.892494
6	-0.371558	-0.303800	-1.278251
6	0.989786	-0.039313	-1.461648
1	2.697268	1.770762	-0.677970
1	1.199193	0.644898	-2.274818
1	-1.041525	0.192209	-1.973183
6	-2.723278	1.153091	0.036882
1	-3.177736	2.135214	0.202699
1	-2.976176	0.887062	-0.996968
6	1.895560	1.214286	1.256797
1	0.936169	1.158939	1.771587
1	2.425942	2.052143	1.728922
6	2.136099	-1.029412	-1.307158
1	2.147233	-1.647565	-2.215432
6	-0.881851	-1.656216	-0.816352
1	-0.682790	-2.355273	-1.641634
6	-2.361786	-1.788508	-0.431919
1	-2.601393	-2.854735	-0.457320

6	2.701942	-0.055142	1.535841
1	2.993420	-0.029749	2.589281
1	-0.299730	-2.028798	0.024959
1	-2.999075	-1.322238	-1.191525
6	-3.362551	0.139842	0.984495
1	-4.417714	0.033531	0.712897
1	3.637236	-0.037965	0.963206
1	3.066030	-0.453722	-1.344241
6	1.929154	-1.350128	1.260100
1	2.162241	-2.093558	2.027883
1	0.860281	-1.133731	1.363944
6	2.212026	-1.979069	-0.103982
1	1.553616	-2.837629	-0.252477
1	3.228714	-2.387515	-0.087106
1	-3.343521	0.530964	2.006669
6	-2.697726	-1.241439	0.968503
1	-1.777227	-1.213273	1.562259
1	-3.359100	-1.939771	1.488268

TCC-TS-cbb:

6	-0.702488	2.334414	-0.459801
6	0.669587	2.504432	-0.610957
1	-1.349496	3.011063	-1.014929
1	0.995253	3.224533	-1.357391
6	-1.299278	1.196581	0.067631
6	1.614997	1.618830	-0.107993
1	-0.818808	0.636135	0.858255
6	-0.392077	-0.379321	-1.258425
6	0.988094	-0.144480	-1.386179
1	2.613640	1.758488	-0.511863
1	1.266998	0.511007	-2.200951
1	-1.029187	0.080595	-2.006286
6	-2.798358	1.051310	-0.065591
1	-3.263422	2.035307	0.051386
1	-3.032103	0.740290	-1.091192
6	1.603595	1.161517	1.344256
1	0.730436	1.596311	1.836330
1	2.475574	1.637803	1.811665
6	2.017213	-1.251889	-1.156186
1	1.541013	-2.141708	-0.738157
1	2.359814	-1.546072	-2.154998
6	-0.902367	-1.726693	-0.770741
1	-0.681820	-2.443658	-1.574049
6	-2.383333	-1.882437	-0.402296
1	-2.591138	-2.955522	-0.392143
6	1.669405	-0.332378	1.653876
1	1.563740	-0.464413	2.735654
1	-0.323032	-2.073405	0.088759
1	0.809140	-0.828133	1.197825
6	2.959414	-1.020527	1.206807
1	3.804779	-0.601285	1.763363
6	3.250510	-0.945804	-0.297871

1	3.670820	0.023598	-0.571138
1	4.026503	-1.681977	-0.529169
1	-3.021761	-1.464331	-1.188223
6	-3.442562	0.075163	0.916468
1	-4.491534	-0.057300	0.632715
1	-3.445220	0.512610	1.919820
1	2.897174	-2.076869	1.491950
6	-2.758219	-1.294933	0.970505
1	-1.851346	-1.230710	1.582340
1	-3.420814	-1.985073	1.499398

TCC-TS-bbc:

6	-0.663644	2.132262	-0.326045
6	0.507357	2.270070	-1.080036
1	-1.541202	2.701115	-0.625498
1	0.423506	2.799534	-2.026189
6	-0.822061	1.074771	0.553897
6	1.662448	1.523157	-0.854020
1	0.070475	0.648891	0.976747
6	-0.513456	-0.590693	-0.922011
6	0.801336	-0.517452	-1.381931
1	2.387746	1.534900	-1.667903
1	0.894552	-0.113326	-2.382584
1	-1.218400	-0.118478	-1.588800
6	-2.050723	0.814453	1.393900
1	-1.880707	-0.091427	1.983051
1	-2.139919	1.622659	2.129970
6	2.348597	1.492786	0.507418
1	1.647910	1.790919	1.289234
1	3.073099	2.315591	0.444704
6	1.901450	-1.519905	-1.099861
1	1.711391	-2.392828	-1.740672
6	-1.108217	-1.683447	-0.060545
1	-0.739925	-2.657597	-0.403241
6	-2.661207	-1.730372	-0.100359
1	-3.025101	-2.144957	0.846043
1	-2.951674	-2.449221	-0.871993
6	-3.388388	0.666996	0.667241
1	-4.147324	0.453029	1.427130
1	-3.677359	1.619116	0.210878
6	3.130527	0.257257	0.971488
1	3.731763	0.577278	1.827065
1	-0.755947	-1.593234	0.972288
1	3.849083	-0.044222	0.201177
1	2.841512	-1.097376	-1.467977
6	2.120182	-2.030598	0.325147
1	3.033696	-2.635234	0.309682
1	1.315625	-2.709217	0.617646
6	2.270872	-0.944436	1.393611
1	1.283040	-0.593458	1.706148
1	2.705483	-1.407074	2.284147
6	-3.424841	-0.430540	-0.407036

1	-3.081381	-0.020294	-1.358268
1	-4.471338	-0.700940	-0.577935

TCC-TS-bbb:

6	-0.623062	2.197798	-0.557520
6	0.645740	2.216309	-1.129644
1	-1.409127	2.783341	-1.030917
1	0.750268	2.691006	-2.102014
6	-1.010090	1.245140	0.377248
6	1.697579	1.433368	-0.664501
1	-0.273559	0.830186	1.047439
6	-0.563835	-0.587696	-0.776392
6	0.781489	-0.582272	-1.178945
1	2.551074	1.384899	-1.335301
1	0.952760	-0.244487	-2.193871
1	-1.264257	-0.223884	-1.517679
6	-2.437172	1.239530	0.894576
1	-2.459181	0.837482	1.911894
1	-2.747615	2.285653	0.978634
6	2.084545	1.405337	0.811649
1	1.385853	2.043763	1.357496
1	3.058410	1.908567	0.871699
6	1.756972	-1.676460	-0.765057
1	1.373025	-2.232140	0.094015
1	1.779368	-2.388669	-1.598776
6	-1.153862	-1.639164	0.152671
1	-0.591613	-2.570962	0.048599
6	-2.620455	-1.949497	-0.176206
1	-2.857630	-2.951977	0.192494
1	-2.726204	-1.993716	-1.266383
6	-3.500207	0.499401	0.059574
1	-4.461945	0.983372	0.252295
1	-3.301466	0.635303	-1.009561
6	2.216329	0.067325	1.538388
1	2.390608	0.272676	2.599334
1	-1.063738	-1.354800	1.209839
1	1.267532	-0.476057	1.481838
6	3.344555	-0.826104	1.025008
1	4.305960	-0.322065	1.169798
6	3.194958	-1.254847	-0.440028
1	3.514507	-0.461161	-1.118525
1	3.867931	-2.097282	-0.623208
1	3.371677	-1.729018	1.645203
6	-3.661668	-0.988329	0.396042
1	-3.679007	-1.089189	1.488201
1	-4.644531	-1.319869	0.046283

TSC-adduct:

6	-0.539554	2.127388	0.401645
6	0.587778	2.161769	-0.304808
1	-0.990346	3.060478	0.732112
1	1.030406	3.125340	-0.548774
6	-1.234089	0.844961	0.789346
6	1.349269	0.945746	-0.779004
1	-0.895793	0.581701	1.801253
6	-0.772248	-0.264802	-0.163158
6	0.765724	-0.355083	-0.183096
1	1.244229	0.889270	-1.872536
1	1.005045	-1.174050	-0.867650
1	-1.053824	0.054043	-1.175384
6	-2.769129	1.001047	0.880168
1	-3.141336	0.388314	1.708032
1	-2.986581	2.036897	1.157840
6	2.841084	1.147259	-0.472711
1	2.953860	1.345391	0.598943
1	3.175331	2.057821	-0.980771
6	1.357027	-0.689972	1.194880
1	1.300017	0.204197	1.823478
1	0.711109	-1.434272	1.670548
6	-1.467065	-1.611481	0.094753
1	-0.765862	-2.426358	-0.116125
6	-2.706017	-1.798249	-0.788656
1	-3.053122	-2.833775	-0.718120
1	-2.404065	-1.645239	-1.831678
6	-3.577046	0.626786	-0.370935
1	-4.532741	1.157085	-0.330067
1	-3.072881	0.979662	-1.277480
6	3.765550	-0.004222	-0.876545
1	3.730324	-0.136190	-1.963003
1	-1.741986	-1.708604	1.152308
1	4.788813	0.304303	-0.641071
6	3.482870	-1.353404	-0.182029
1	2.869113	-1.989803	-0.823228
6	2.818820	-1.224974	1.193633
1	2.835360	-2.209354	1.668082
1	3.443760	-0.582648	1.821999
1	4.428101	-1.889359	-0.059664
6	-3.885113	-0.875363	-0.466064
1	-4.324959	-1.185545	0.489873
1	-4.659142	-1.033757	-1.223428

CCC:

6	-1.074089	2.109147	-1.397128
6	-0.256488	3.019399	-0.573507
1	-0.913719	2.194277	-2.470077
1	-0.292156	4.060708	-0.890064

6	-2.051074	1.297480	-0.986727
6	0.533699	2.725908	0.460525
6	0.072923	-2.297653	-1.020818
6	1.301162	-1.788679	-1.093324
1	1.055864	3.553759	0.938172
1	-2.597364	0.760215	-1.760033
1	1.644271	-1.401281	-2.051247
1	-0.533968	-2.294770	-1.922135
6	-2.549391	1.094372	0.421357
1	-1.716917	1.087069	1.126915
1	-3.165547	1.956642	0.702477
6	-0.558731	-2.864092	0.225835
1	-1.159001	-3.741575	-0.038800
1	0.216567	-3.210354	0.913666
6	-1.457533	-1.836635	0.935066
1	-1.793632	-2.238105	1.897152
1	-0.854071	-0.952031	1.157813
6	-3.391170	-0.182115	0.566133
1	-4.311517	-0.060244	-0.015292
1	-3.697171	-0.295516	1.611387
6	2.297146	-1.735393	0.038772
1	2.729752	-2.733550	0.178207
1	1.784635	-1.495729	0.977163
6	0.841393	1.374292	1.033208
1	0.387957	1.296902	2.030382
1	0.398573	0.593941	0.406062
6	2.994784	0.729965	-0.196499
1	3.865552	1.351389	-0.419819
6	2.359279	1.150847	1.142958
1	2.562170	0.386648	1.899791
1	2.822466	2.069697	1.514583
1	2.277091	0.908316	-1.006179
6	-2.675131	-1.449997	0.094013
1	-3.380580	-2.287663	0.089372
1	-2.362931	-1.307797	-0.944559
6	3.433828	-0.738475	-0.204643
1	4.199178	-0.877744	0.566180
1	3.910849	-0.973432	-1.162443

CCC-TS-cbc:

6	0.820205	2.529272	0.587973
6	-0.566755	2.578482	0.468574
1	1.221248	3.239517	1.308662
1	-1.037902	3.349058	1.074138
6	1.685660	1.485398	0.261173
6	-1.423914	1.587886	0.013414
6	0.713539	-0.037772	1.586364
6	-0.689990	-0.067526	1.519747
1	-2.453950	1.754103	0.327990
1	2.626371	1.552969	0.812079
1	-1.180263	0.593830	2.220443
1	1.117313	0.590540	2.369507

6	1.971184	0.888117	-1.110293
1	1.086260	0.554318	-1.644112
1	2.355637	1.735228	-1.691057
6	1.559485	-1.269541	1.310581
1	2.612015	-1.024411	1.478037
1	1.309380	-2.016997	2.074306
6	1.380655	-1.887665	-0.086495
1	1.210842	-2.965389	-0.006480
1	0.473403	-1.480644	-0.532245
6	3.055901	-0.201461	-1.102123
1	3.732393	-0.010043	-0.262759
1	3.670233	-0.099744	-2.000872
6	-1.465089	-1.372243	1.302300
1	-2.221693	-1.386042	2.094277
1	-0.793628	-2.208906	1.528022
6	-1.351557	0.769913	-1.256315
1	-1.012035	1.411526	-2.077459
1	-0.631256	-0.037382	-1.172529
6	-2.714230	0.168524	-1.598063
1	-2.621633	-0.419577	-2.517004
1	-3.430787	0.969872	-1.806240
6	-2.219448	-1.755174	0.009519
1	-1.525421	-1.996781	-0.800935
1	-2.728102	-2.695044	0.242447
6	2.549709	-1.647992	-1.044465
1	2.237018	-1.959335	-2.046764
1	3.388130	-2.297088	-0.770406
6	-3.251742	-0.731705	-0.481690
1	-4.142331	-1.248188	-0.849407
1	-3.582928	-0.124463	0.367162

CCC-TS-cbb:

6	-0.658241	2.370436	-0.874124
6	0.735881	2.380587	-0.863829
1	-1.108661	3.000737	-1.636470
1	1.166603	3.003625	-1.645182
6	-1.485526	1.391443	-0.333091
6	1.644171	1.494411	-0.295410
6	-0.733066	-0.287005	-1.456454
6	0.594003	-0.556357	-1.103929
1	2.604274	1.558336	-0.810373
1	-2.508121	1.442162	-0.707319
1	1.350269	-0.333009	-1.845577
1	-0.840102	0.238111	-2.399069
6	-1.409398	0.844659	1.080168
1	-0.741029	-0.006994	1.133210
1	-0.994893	1.611475	1.741572
6	-1.855959	-1.312422	-1.266130
1	-2.696005	-0.987610	-1.888388
1	-1.490191	-2.239854	-1.726052
6	-2.449784	-1.695007	0.105028
1	-3.000658	-2.624417	-0.065918

1	-1.668374	-1.944690	0.828735
6	-2.770734	0.388534	1.600943
1	-3.442232	1.246067	1.708983
1	-2.629772	-0.028255	2.603329
6	0.942739	-1.637329	-0.109740
1	0.355698	-2.535917	-0.348215
1	0.630564	-1.364839	0.903876
6	1.872785	0.991384	1.112115
1	2.024785	1.872306	1.748146
1	1.022671	0.475549	1.539374
6	3.408409	-0.870925	0.074517
1	4.407262	-1.293814	0.220764
6	3.147745	0.122982	1.214625
1	3.134463	-0.412121	2.170291
1	4.010368	0.796314	1.255245
1	3.459960	-0.328670	-0.873379
6	-3.426221	-0.668936	0.702314
1	-4.188833	-1.193050	1.284716
1	-3.963762	-0.185542	-0.120185
6	2.421507	-2.031687	-0.064473
1	2.563176	-2.729035	0.768033
1	2.672674	-2.585487	-0.975342

CCC-TS-bbc:

6	-0.826981	2.540666	-0.456806
6	0.562543	2.592732	-0.561861
1	-1.344322	3.218644	-1.133334
1	0.925057	3.344281	-1.259037
6	-1.604793	1.519792	0.072849
6	1.486654	1.592504	-0.262453
6	-0.710321	-0.104771	-1.438163
6	0.679435	0.005524	-1.577987
1	2.442773	1.758949	-0.759859
1	-2.624079	1.519733	-0.309822
1	0.998503	0.660593	-2.378802
1	-1.281980	0.533641	-2.101495
6	-1.547721	0.973106	1.482308
1	-0.643861	1.315373	1.985700
1	-2.376900	1.469449	2.005723
6	-1.444668	-1.406586	-1.170661
1	-1.543734	-1.891116	-2.152290
1	-0.865399	-2.104443	-0.565538
6	-2.906734	-1.182332	0.958096
1	-2.975734	-2.209280	1.331532
6	1.633462	-1.173992	-1.403576
1	2.643507	-0.841050	-1.664782
1	1.358133	-1.901071	-2.178348
6	1.689082	0.834097	1.036270
1	1.716419	1.579598	1.838556
1	0.845689	0.184185	1.258669
6	3.002811	0.027245	1.044474
1	3.542221	0.210071	1.976958

1	3.652568	0.408623	0.251462
6	1.689802	-1.908912	-0.050856
1	0.751202	-1.776517	0.481061
1	1.775418	-2.984166	-0.231717
6	-1.716849	-0.532149	1.670245
1	-0.801833	-1.037545	1.356661
1	-1.814430	-0.729208	2.742809
1	-3.833634	-0.687170	1.268349
6	-2.852590	-1.243567	-0.582654
1	-3.471613	-2.087509	-0.900262
1	-3.311775	-0.357249	-1.027031
6	2.833989	-1.489942	0.875009
1	2.658605	-1.949584	1.853103
1	3.776474	-1.907720	0.506348

CCC-TS-bbb:

6	-0.776702	2.291864	-1.038225
6	0.611929	2.312237	-0.977126
1	-1.200285	2.803749	-1.899558
1	1.081379	2.897219	-1.764420
6	-1.615450	1.400515	-0.376729
6	1.479296	1.428910	-0.336843
6	-0.759626	-0.456309	-1.317998
6	0.637440	-0.563124	-1.196674
1	2.475195	1.512385	-0.763872
1	-2.604812	1.334512	-0.823042
1	1.235148	-0.274188	-2.053489
1	-1.107693	-0.016627	-2.246235
6	-1.670602	1.240163	1.128337
1	-0.770073	1.649022	1.583543
1	-2.485812	1.903754	1.448990
6	-1.664653	-1.598523	-0.856959
1	-1.729427	-2.276927	-1.717771
1	-1.193102	-2.181780	-0.064934
6	-3.189654	-0.845105	1.072525
1	-3.364341	-1.757572	1.651694
6	1.220035	-1.666834	-0.336626
1	0.836720	-2.622728	-0.717947
1	0.829332	-1.597594	0.684182
6	1.550401	0.917165	1.083842
1	1.464223	1.771346	1.765730
1	0.717450	0.262021	1.324533
6	3.526650	-0.585180	0.229525
6	2.893976	0.207205	1.381096
1	2.758871	-0.452655	2.244892
1	3.620955	0.965377	1.688901
1	4.512583	-0.926934	0.559000
6	-1.963837	-0.152445	1.675351
1	-1.085065	-0.789468	1.537005
1	-2.110781	-0.072397	2.757113
1	-4.073753	-0.216586	1.226047
6	-3.086624	-1.240733	-0.416028

1	-3.484324	-0.459504	-1.066210
1	-3.731083	-2.109703	-0.576082
1	3.725210	0.083410	-0.609782
6	2.742126	-1.804318	-0.268146
1	3.123193	-2.087547	-1.255054
1	2.952057	-2.653514	0.390844

CSC-adduct:

6	-0.487846	2.334525	0.029207
6	0.827428	2.288238	-0.154747
1	-0.939084	3.251913	0.400714
1	1.419742	3.175837	0.058185
6	-1.433526	1.187976	-0.224305
6	1.590731	1.077114	-0.629823
6	-0.702886	0.087856	-1.028498
6	0.733214	-0.203006	-0.527066
1	1.832569	1.229916	-1.692199
1	-2.238215	1.577486	-0.865256
1	1.132504	-0.915160	-1.254722
1	-0.534207	0.546251	-2.011875
6	-2.095827	0.760479	1.105619
1	-1.484492	-0.002450	1.587929
1	-2.093852	1.615672	1.788576
6	-1.503979	-1.205977	-1.322340
1	-2.039892	-1.059675	-2.266806
1	-0.779485	-2.004875	-1.517610
6	-2.550867	-1.728904	-0.325597
1	-2.916118	-2.679257	-0.725899
1	-2.107613	-1.964365	0.647065
6	-3.535564	0.259127	0.970326
1	-4.203795	1.109063	0.797412
1	-3.836336	-0.178586	1.927666
6	0.826824	-0.862770	0.858645
1	0.012502	-1.585652	0.949248
1	0.648059	-0.102223	1.623884
6	2.918913	0.990861	0.133746
1	3.473950	1.917992	-0.043916
1	2.704737	0.973207	1.208065
6	3.215107	-1.586646	0.052376
1	4.021429	-2.270615	0.330849
6	3.819265	-0.193466	-0.225884
1	4.742075	-0.088338	0.352823
1	4.111231	-0.122699	-1.278885
1	2.783167	-2.003759	-0.860017
6	-3.737042	-0.773214	-0.145975
1	-4.649056	-1.339567	0.060396
1	-3.910193	-0.261342	-1.098861
6	2.164886	-1.599353	1.167956
1	2.613802	-1.173976	2.070923
1	1.943598	-2.641830	1.410473