Supporting information material

(Total 29 pages)

for

Which One Among Aspartyl Protease, Metallopeptidase, and Artificial Metallopeptidase is the Most Efficient Catalyst in Peptide Hydrolysis?

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(a) Figures 1-5.

(b) Details of the MD simulations.

(c) Tables **S1-S21**: Cartesian coordinates (in Å) of all the optimized structures.

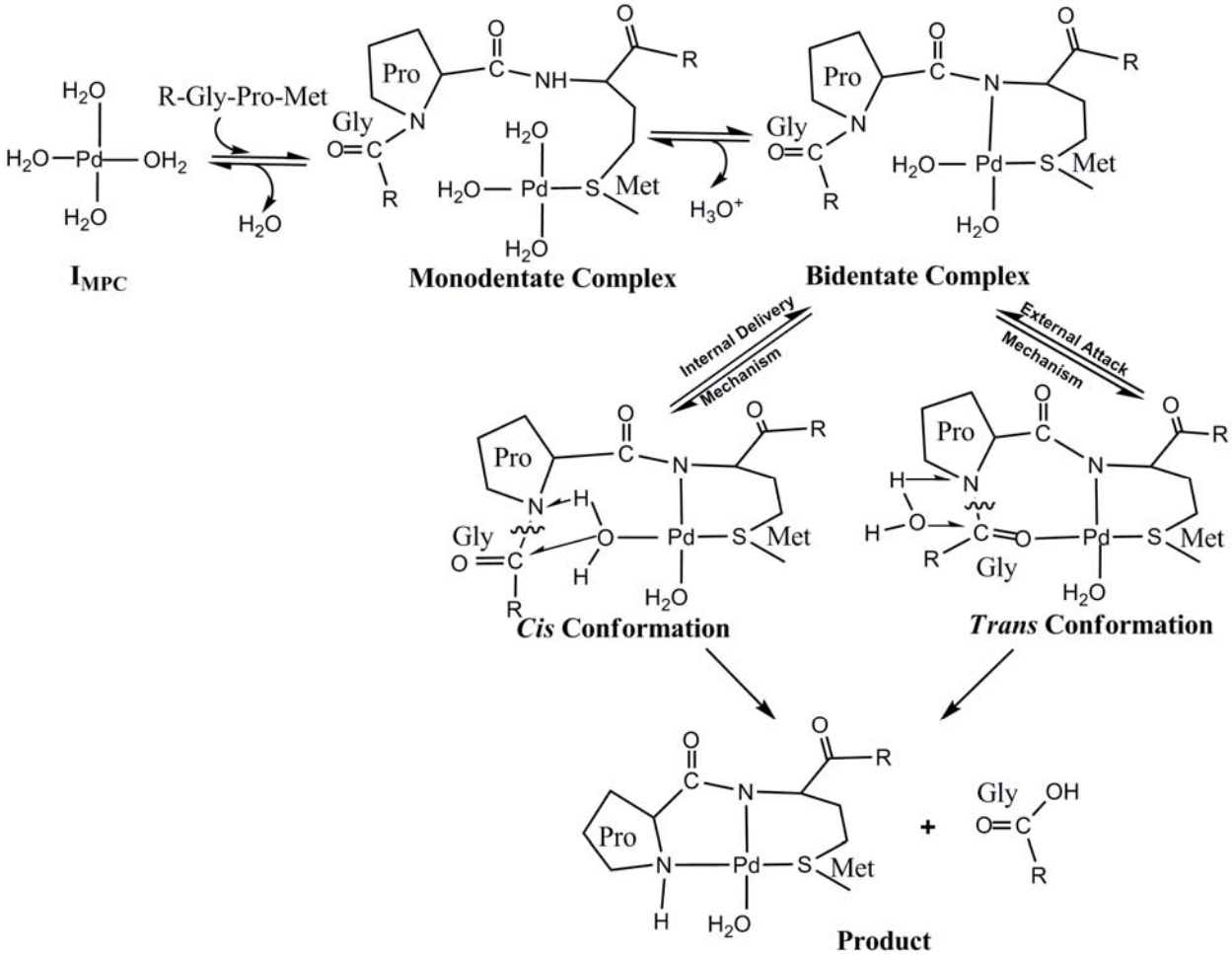

Fig. 1: Experimentally suggested mechanism utilized by $[Pd(H_2O)_4]^{2+}$ for the hydrolysis of Gly-Pro bond of the Gly-Pro-Met sequence. The arrows describe the movement of atoms.

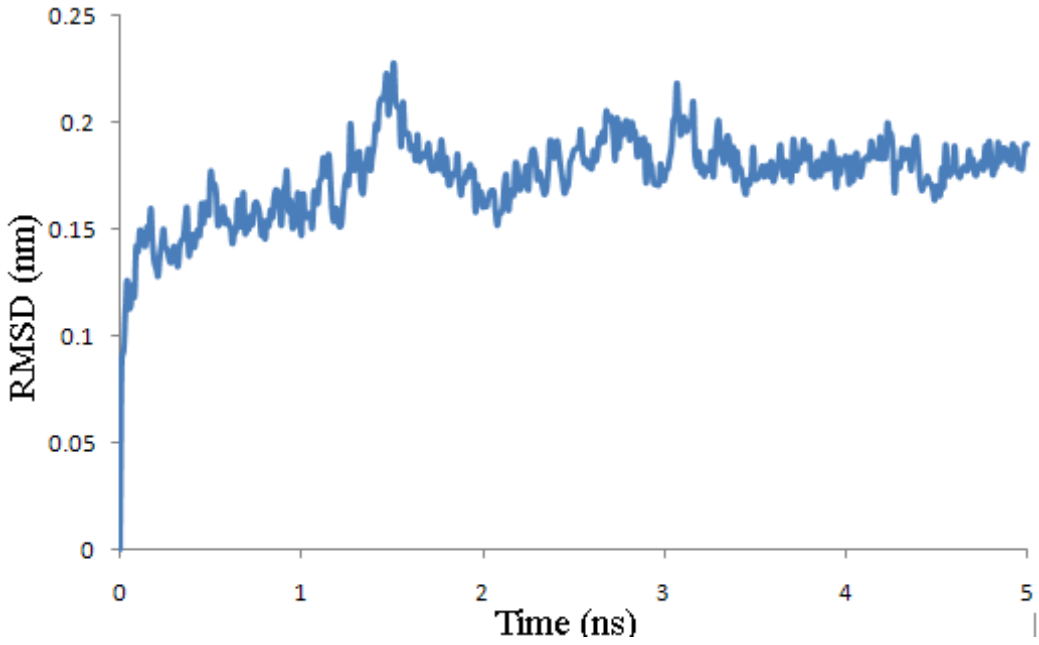

Fig. 2.a: The root-mean-square-deviation (rmsd) of the BACE2-substrate MD simulation.

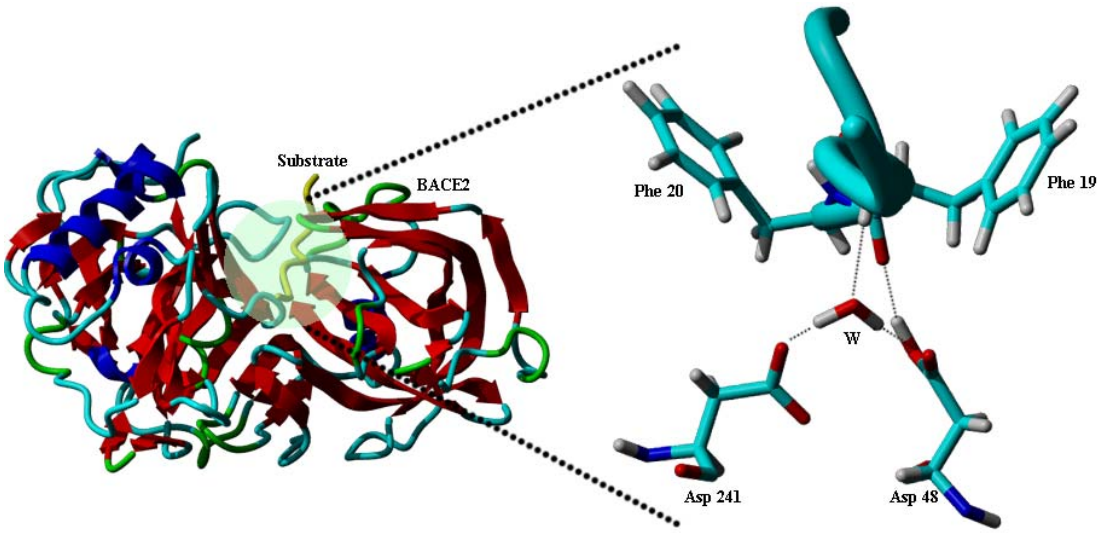

Fig. 2.b: The most representative structure derived from the 5ns MD simulation of the BACE2-substrate complex.

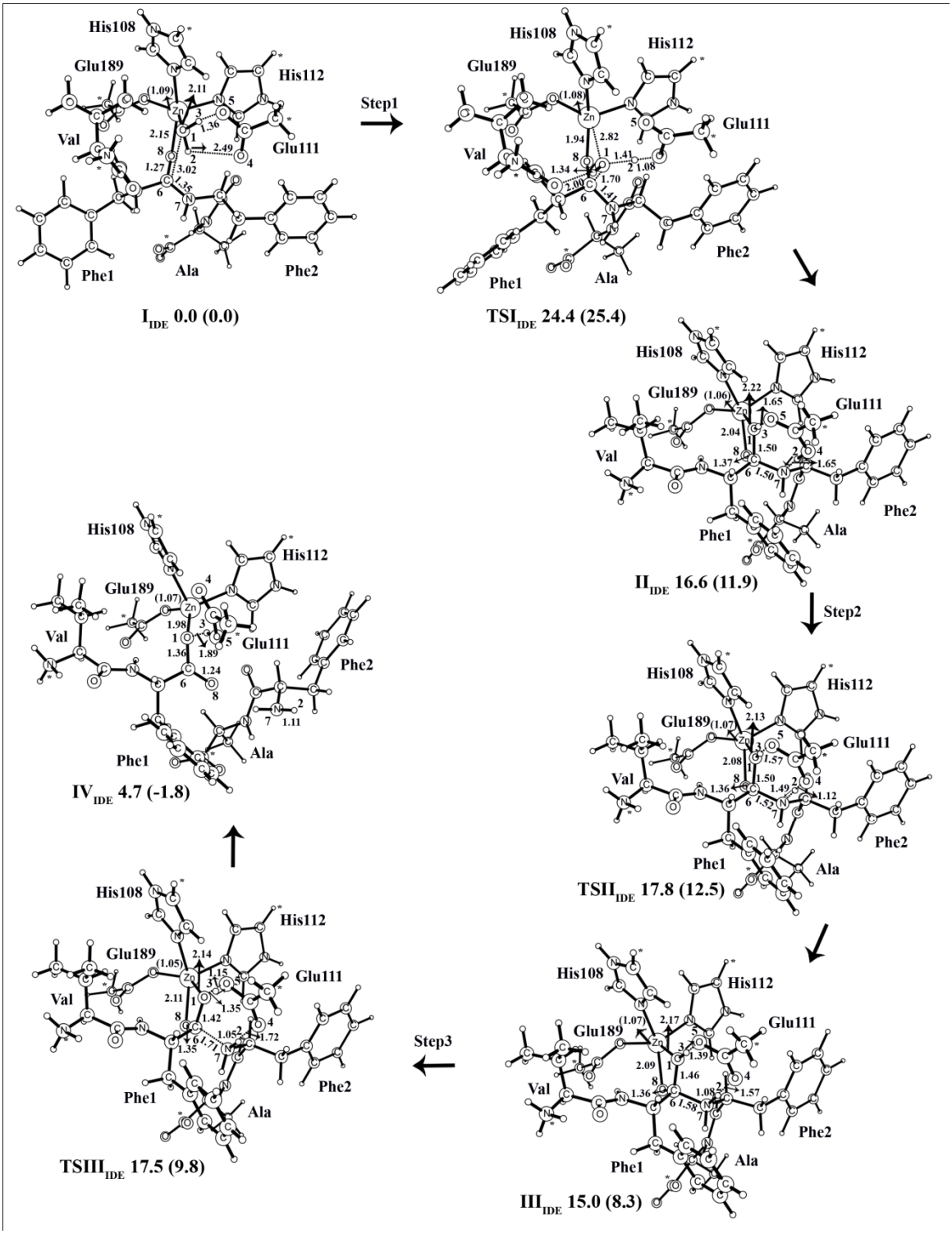

Fig. 3: Structures (in Å) and energies (in kcal/mol) of the reactant, intermediates, transition states (optimized), and the product for peptide hydrolysis catalyzed by IDE. Stars indicate the atoms fixed to their crystallographic positions during optimizations.

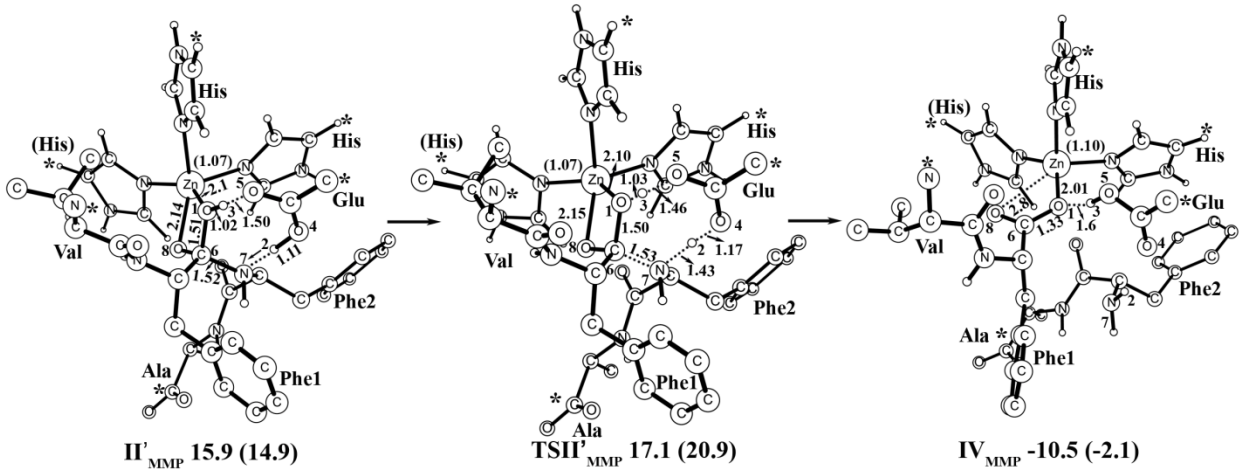

Fig. 4: Structures (in Å) and energies (in kcal/mol) of the intermediate (**II'$_{MMP}$**), transition state (**TSII'$_{MMP}$**), and the product (**IV$_{MMP}$**) in the concerted mechanism for peptide hydrolysis catalyzed by MMP. Stars indicate the atoms fixed to their crystallographic positions during optimizations and the non-critical hydrogen atoms have been omitted in the figure.

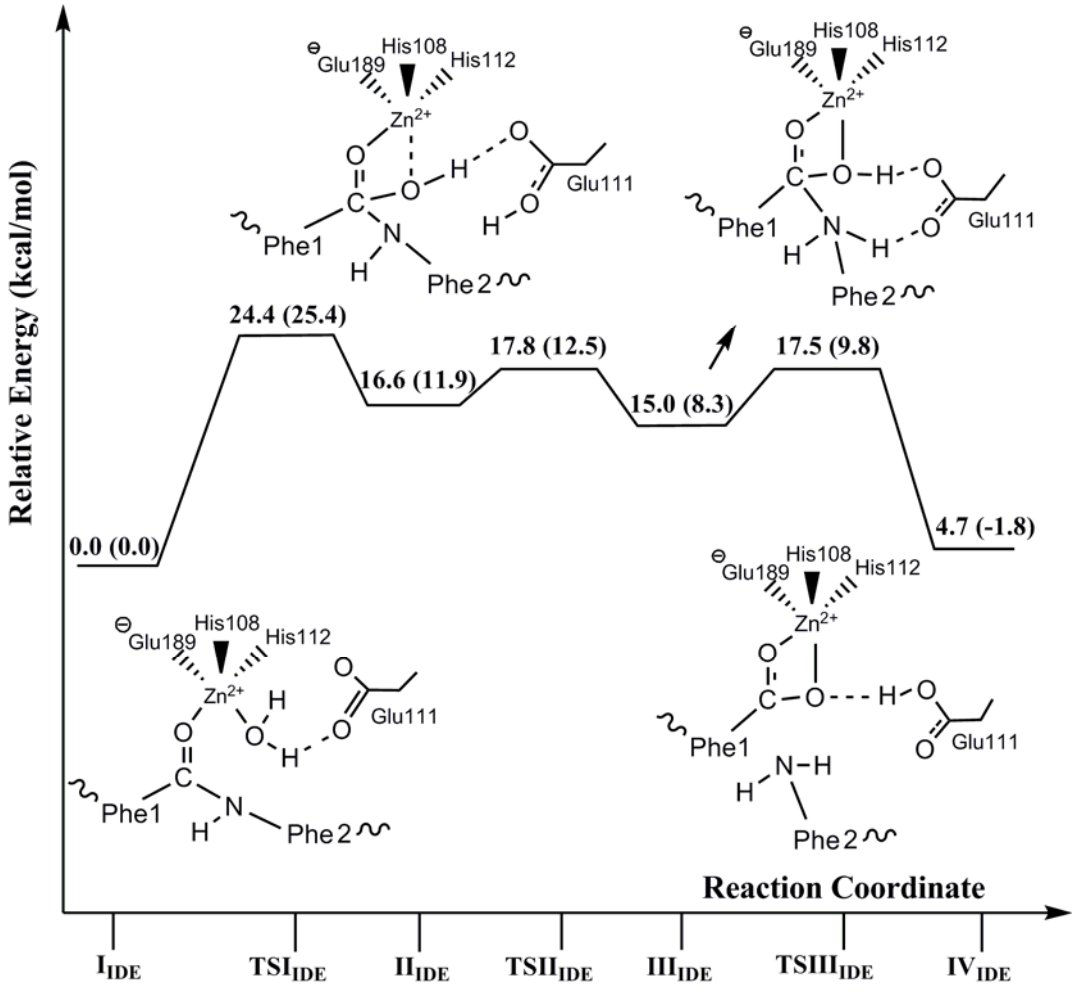

Fig. 5: Potential energy diagram for peptide hydrolysis catalyzed by IDE.

MD simulation:

All molecular dynamics (MD) simulations were performed using GROMACS software package [1-2], utilizing the GROMOS force field 53A5[3] force field and SPC[4] water model. Enzyme substrate complex was then placed in the center of a box with dimensions 7.2 x 5.4 x 6.8 nm. The box contained 6842 number of water molecules. Some water molecules were replaced by sodium ions, to neutralize the systems. All starting structures were further energy minimized with a steepest descent method for 3000 steps. The results of these minimizations produced the initial structures for the position restrained MD simulation. The structure was subjected to 200ps of position restrained MD simulation, where the protein was kept fixed and the water molecules were allowed to settle around the protein molecule. The MD simulations were then carried out with a constant number of particles (N), pressure (P) and temperature (T) i.e. NPT ensemble. The SETTLE algorithm was used to constrain the bond length and angle of the water molecules [5], while the LINCS algorithm is used to constrain the bond length of the proteins [6]. The long range electrostatic interactions were calculated by the particle-mesh Ewald (PME) method [7-8]. A constant pressure of 1 bar was applied with a coupling constant of 1.0 ps; protein, water molecules and ions were coupled separately to a bath at 300 K with a coupling constant of 0.1 ps. The PBC were applied and the equation of motion was integrated at time-steps of 2 fs. The tools available in GROMACS program package and the YASARA program [9] have been utilized to analyze the different MD trajectories. The PyMol [10]and VMD [11] software was also extensively used for visualizations and for the preparation of structural diagrams presented in this study

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(11) Humphrey, W., Dalke, A., and Schulten, K. *J. Molec. Graphics* **1996**, *14*, 33.

Table S1: Structure I_{BACE2}

C	1.952955	-5.544828	2.037075
H	2.978825	-5.780843	1.734961
H	1.295001	-6.395701	1.844849
C	1.454028	-4.299355	1.318000
O	2.296761	-3.346039	1.184109
O	0.257448	-4.287348	0.945625
H	-0.120776	-3.032979	0.011378
C	0.135649	-0.428737	5.780732
H	0.336352	-1.464321	6.074592
H	-0.945892	-0.274061	5.852782
C	0.595977	-0.202992	4.345312
O	1.436837	0.619519	4.020048
O	-0.035412	-1.023300	3.507220
N	4.464340	2.757491	-1.602116
H	4.957593	3.639525	-1.456519
H	5.135172	1.981138	-1.727902
H	3.833872	2.752656	-2.457479
C	3.453254	2.426192	-0.516569
H	3.967300	1.846198	0.253604
C	2.478367	1.546521	-1.337023
O	2.374371	1.821905	-2.550804
C	2.811637	3.694069	0.078334
H	2.361425	4.252491	-0.755453
C	1.687354	3.300619	1.055969
H	1.254350	4.205400	1.494257
H	2.056152	2.676969	1.880352
H	0.879079	2.753828	0.563027
C	3.851199	4.585044	0.778892
H	3.362308	5.474359	1.188597
H	4.646621	4.949550	0.111613
H	4.327005	4.054045	1.612077
N	1.922371	0.538656	-0.702080
H	2.024751	0.402834	0.305668
C	1.218890	-0.577935	-1.328246
H	0.660794	-0.205253	-2.188127
C	0.211686	-1.081734	-0.241643
O	-0.278498	-2.299898	-0.667048
C	2.220541	-1.702588	-1.783665
H	2.104313	-2.553773	-1.109996
H	1.912061	-2.036546	-2.778628
C	3.673439	-1.276343	-1.797725
C	4.254155	-0.662146	-2.916582
H	3.659917	-0.532976	-3.817246
C	4.464256	-1.444648	-0.645657
H	4.037052	-1.967058	0.208451
C	5.572465	-0.191722	-2.881554
H	6.009940	0.255787	-3.772501
C	5.774976	-0.965568	-0.600577
H	6.368377	-1.107415	0.299536
C	6.335380	-0.325363	-1.713953
H	7.368136	0.016750	-1.689169
N	-0.790200	-0.041657	-0.049795
H	-0.893915	0.465569	-0.934092
C	-2.143361	-0.545207	0.203515
H	-2.082414	-1.593811	0.503732
C	-2.918565	-0.491788	-1.139999
O	-2.420774	0.084341	-2.120437
C	-2.865175	0.207616	1.355255
H	-3.791224	-0.331734	1.587068
H	-2.216485	0.123779	2.234570
C	-3.201249	1.658665	1.091974
C	-4.450587	2.013071	0.557501
H	-5.182321	1.233752	0.343938
C	-2.282049	2.676407	1.384745
H	-1.321682	2.406991	1.817866
C	-4.758548	3.352492	0.310966
H	-5.730685	3.608202	-0.104011
C	-2.592686	4.015456	1.140860
H	-1.868955	4.792930	1.381576
C	-3.833192	4.358341	0.598920
H	-4.079575	5.401334	0.409663
N	-4.108638	-1.101433	-1.132787
H	-4.579679	-1.290813	-0.238857
C	-5.148944	-0.904682	-2.136574
H	-5.013428	0.085895	-2.589597
C	-6.516296	-0.899153	-1.354185
O	-6.412599	-0.912614	-0.087238
O	-7.541041	-0.865316	-2.061029
C	-5.117992	-1.958242	-3.244650
H	-5.984790	-1.805693	-3.893871
H	-5.180037	-2.967679	-2.819417
H	-4.194618	-1.888562	-3.832443
O	0.937568	-1.182540	0.992425
H	0.302439	-0.930596	2.566014
H	1.485069	-2.055142	1.025749
H	0.656804	0.258091	6.449590
H	1.967973	-5.352969	3.117608

Table S2: Structure TSI_{BACE2}

C	1.592656	-3.904383	4.694591
H	2.658158	-3.956457	4.925875
H	1.155303	-4.907715	4.689481
C	1.377034	-3.230009	3.357459
O	2.305883	-2.689674	2.747180
O	0.130065	-3.276682	2.969833
H	-0.026413	-2.792326	2.040682
C	-0.595622	2.299721	5.155550
H	-0.427132	1.572459	5.955903
H	-1.672407	2.317791	4.952988
C	0.148056	1.880805	3.890958
O	0.851395	2.650839	3.248272
O	-0.084246	0.615063	3.590718
N	4.609241	1.595177	-2.314996
H	5.184203	2.414663	-2.514208
H	5.204466	0.782071	-2.086187
H	3.988128	1.299934	-3.128003
C	3.550782	1.823846	-1.247547
H	3.983460	1.556804	-0.280820
C	2.495719	0.781747	-1.707071
O	2.426912	0.583605	-2.939694
C	3.054483	3.281874	-1.248373
H	2.727021	3.512041	-2.273270
C	1.839200	3.430079	-0.313166
H	1.530017	4.479894	-0.283685
H	2.055460	3.119108	0.716246
H	0.982552	2.845829	-0.657315
C	4.171565	4.259820	-0.845279
H	3.797729	5.287934	-0.879166
H	5.051834	4.226124	-1.505031
H	4.511839	4.063535	0.178455
N	1.857029	0.156398	-0.745951
H	1.957068	0.366178	0.270703
C	1.074869	-1.072784	-0.863357
H	0.497663	-1.047832	-1.791110
C	0.063195	-1.075881	0.337551
O	-0.308110	-2.231615	0.737299
C	1.989168	-2.344356	-0.817518
H	1.970817	-2.725939	0.205991
H	1.521182	-3.108372	-1.445517
C	3.420060	-2.111335	-1.245908
C	3.830092	-2.237799	-2.582226
H	3.105100	-2.546440	-3.330611
C	4.377180	-1.709129	-0.298168
H	4.082496	-1.642993	0.746396
C	5.140871	-1.952084	-2.968365
H	5.433568	-2.066875	-4.009511
C	5.689478	-1.409640	-0.677447
H	6.415659	-1.116789	0.078012
C	6.078064	-1.522636	-2.019867
H	7.107724	-1.327348	-2.313304
N	-0.886122	-0.031173	0.200978
H	-0.807656	0.427007	-0.706252
C	-2.288035	-0.377298	0.385580
H	-2.328380	-1.302150	0.964823
C	-2.915309	-0.641604	-1.008807
O	-2.314575	-0.279880	-2.035839
C	-3.044505	0.716699	1.188490
H	-4.065761	0.361988	1.373308
H	-2.539839	0.794238	2.157876
C	-3.096087	2.077466	0.526959
C	-4.141628	2.407138	-0.348598
H	-4.917173	1.671719	-0.547471
C	-2.102669	3.039261	0.768184
H	-1.282190	2.805216	1.441409
C	-4.195611	3.657949	-0.964725
H	-5.016316	3.889058	-1.639902
C	-2.157499	4.293132	0.154903
H	-1.383714	5.028768	0.367207
C	-3.203824	4.608355	-0.714299
H	-3.248973	5.586633	-1.188639
N	-4.097433	-1.258619	-0.979936
H	-4.608445	-1.472871	-0.111007
C	-4.985710	-1.549860	-2.097909
H	-5.155836	-0.630889	-2.676138
C	-6.364565	-1.988631	-1.455503
O	-6.399326	-1.956280	-0.191059
O	-7.249211	-2.309732	-2.273714
C	-4.436788	-2.623963	-3.039768
H	-5.202492	-2.847245	-3.788201
H	-4.220534	-3.544613	-2.483197
H	-3.515967	-2.289548	-3.530392
O	1.153934	-0.387953	1.570508
H	0.404851	0.305811	2.721827
H	1.616802	-1.164378	1.952402
H	-0.269959	3.293312	5.469564
H	1.077588	-3.330331	5.473163

Table S3: Structure II_{BACE2}

C	1.952955	-5.544828	2.037075
H	2.978825	-5.780843	1.734961
H	1.295001	-6.395701	1.844849
C	1.454028	-4.299355	1.318000
O	2.296761	-3.346039	1.184109
O	0.257448	-4.287348	0.945625
H	-0.120776	-3.032979	0.011378
C	0.135649	-0.428737	5.780732
H	0.336352	-1.464321	6.074592
H	-0.945892	-0.274061	5.852782
C	0.595977	-0.202992	4.345312
O	1.436837	0.619519	4.020048
O	-0.035412	-1.023300	3.507220
N	4.464340	2.757491	-1.602116
H	4.957593	3.639525	-1.456519
H	5.135172	1.981138	-1.727902
H	3.833872	2.752656	-2.457479
C	3.453254	2.426192	-0.516569
H	3.967300	1.846198	0.253604
C	2.478367	1.546521	-1.337023
O	2.374371	1.821905	-2.550804
C	2.811637	3.694069	0.078334
H	2.361425	4.252491	-0.755453
C	1.687354	3.300619	1.055969
H	1.254350	4.205400	1.494257
H	2.056152	2.676969	1.880352
H	0.879079	2.753828	0.563027
C	3.851199	4.585044	0.778892
H	3.362308	5.474359	1.188597
H	4.646621	4.949550	0.111613
H	4.327005	4.054045	1.612077
N	1.922371	0.538656	-0.702080
H	2.024751	0.402834	0.305668
C	1.218890	-0.577935	-1.328246
H	0.660794	-0.205253	-2.188127
C	0.211686	-1.081734	-0.241643
O	-0.278498	-2.299898	-0.667048
C	2.220541	-1.702588	-1.783665
H	2.104313	-2.553773	-1.109996
H	1.912061	-2.036546	-2.778628
C	3.673439	-1.276343	-1.797725
C	4.254155	-0.662146	-2.916582
H	3.659917	-0.532976	-3.817246
C	4.464256	-1.444648	-0.645657
H	4.037052	-1.967058	0.208451
C	5.572465	-0.191722	-2.881554
H	6.009940	0.255787	-3.772501
C	5.774976	-0.965568	-0.600577
H	6.368377	-1.107415	0.299536
C	6.335380	-0.325363	-1.713953
H	7.368136	0.016750	-1.689169
N	-0.790200	-0.041657	-0.049795
H	-0.893915	0.465569	-0.934092
C	-2.143361	-0.545207	0.203515
H	-2.082414	-1.593811	0.503732
C	-2.918565	-0.491788	-1.139999
O	-2.420774	0.084341	-2.120437
C	-2.865175	0.207616	1.355255
H	-3.791224	-0.331734	1.587068
H	-2.216485	0.123779	2.234570
C	-3.201249	1.658665	1.091974
C	-4.450587	2.013071	0.557501
H	-5.182321	1.233752	0.343938
C	-2.282049	2.676407	1.384745
H	-1.321682	2.406991	1.817866
C	-4.758548	3.352492	0.310966
H	-5.730685	3.608202	-0.104011
C	-2.592686	4.015456	1.140860
H	-1.868955	4.792930	1.381576
C	-3.833192	4.358341	0.598920
H	-4.079575	5.401334	0.409663
N	-4.108638	-1.101433	-1.132787
H	-4.579679	-1.290813	-0.238857
C	-5.148944	-0.904682	-2.136574
H	-5.013428	0.085895	-2.589597
C	-6.516296	-0.899153	-1.354185
O	-6.412599	-0.912614	-0.087238
O	-7.541041	-0.865316	-2.061029
C	-5.117992	-1.958242	-3.244650
H	-5.984790	-1.805693	-3.893871
H	-5.180037	-2.967679	-2.819417
H	-4.194618	-1.888562	-3.832443
O	0.937568	-1.182540	0.992425
H	0.302439	-0.930596	2.566014
H	1.485069	-2.055142	1.025749
H	0.656804	0.258091	6.449590
H	1.967973	-5.352969	3.117608

Table S4: Structure $TSII_{BACE2}$

C	1.606638	-0.394009	5.888066
H	2.661152	-0.280519	6.149167
H	1.160081	-1.230419	6.432630
C	1.452553	-0.581361	4.388019
O	2.367300	-0.192154	3.627653
O	0.345570	-1.115745	4.007267
H	0.285553	-1.266879	2.814928
C	-0.536940	4.871308	2.545393
H	-0.635820	4.498370	3.570754
H	-1.531781	5.208658	2.228435
C	-0.057306	3.730354	1.606657
O	0.888431	3.940901	0.825584
O	-0.746524	2.654218	1.733629
N	5.046395	0.068889	-2.854533
H	5.756932	0.645612	-3.307068
H	5.477667	-0.618719	-2.214728
H	4.453155	-0.484344	-3.531570
C	3.967156	0.873697	-2.126651
H	4.306707	1.020704	-1.098523
C	2.772162	-0.123505	-2.183804
O	2.740330	-0.898647	-3.158558
C	3.722904	2.229412	-2.820256
H	3.577355	2.021105	-3.891746
C	2.437184	2.899485	-2.292751
H	2.337519	3.889762	-2.748924
H	2.415816	3.041575	-1.204380
H	1.548871	2.322591	-2.562156
C	4.934926	3.161442	-2.650548
H	4.770863	4.093739	-3.199547
H	5.877610	2.735351	-3.026922
H	5.081641	3.418181	-1.595153
N	1.960766	-0.069887	-1.141817
H	2.182623	0.581647	-0.379437
C	1.061171	-1.120253	-0.628411
H	0.204341	-1.259876	-1.291718
C	0.526546	-0.562883	0.768509
O	0.242182	-1.535730	1.609092
C	1.800582	-2.486337	-0.496335
H	1.254352	-3.039783	0.273113
H	1.686466	-3.022209	-1.443301
C	3.277700	-2.405837	-0.157590
C	4.241176	-2.783976	-1.107204
H	3.908107	-3.179383	-2.063597
C	3.731326	-1.925249	1.082066
H	3.018027	-1.641973	1.847957
C	5.612835	-2.650811	-0.849086
H	6.339070	-2.997311	-1.584122
C	5.096126	-1.781899	1.341113
H	5.409962	-1.392508	2.305828
C	6.045425	-2.133693	0.377982
H	7.107635	-2.033900	0.589130
N	-0.796640	0.332397	0.424897
H	-0.835601	0.483620	-0.591262
C	-2.111599	-0.287316	0.780281
H	-1.910147	-0.948821	1.625469
C	-2.593655	-1.130226	-0.426906
O	-1.982174	-1.059117	-1.508930
C	-3.170708	0.767161	1.219830
H	-3.946755	0.216940	1.763348
H	-2.684569	1.444739	1.928336
C	-3.826735	1.565246	0.104303
C	-5.061450	1.161598	-0.428888
H	-5.551760	0.264836	-0.051772
C	-3.219460	2.726291	-0.398002
H	-2.281091	3.054672	0.039565
C	-5.662391	1.897427	-1.452664
H	-6.616611	1.566545	-1.855927
C	-3.823866	3.458315	-1.421616
H	-3.339673	4.357989	-1.796601
C	-5.046528	3.045284	-1.954824
H	-5.518167	3.616377	-2.752286
N	-3.680001	-1.874404	-0.200048
H	-4.268491	-1.731454	0.633512
C	-4.525667	-2.508821	-1.217816
H	-4.560610	-1.853299	-2.097174
C	-5.994852	-2.587608	-0.609366
O	-6.127836	-2.014746	0.515676
O	-6.829505	-3.186479	-1.308109
C	-4.010074	-3.883301	-1.644432
H	-4.742608	-4.330193	-2.322302
H	-3.901437	-4.541889	-0.773650
H	-3.037469	-3.807688	-2.145555
O	1.430153	0.408063	1.224418
H	-0.651910	1.306905	0.923731
H	1.757008	0.189952	2.147323
H	0.153392	5.719987	2.520973
H	1.074462	0.518217	6.183556

Table S5: Structure III_{BACE2}

C	1.601660	3.917423	4.742545
H	2.521132	3.991627	5.325697
H	0.747694	3.761887	5.410511
C	1.701187	2.767562	3.758824
O	2.688767	2.050370	3.675030
O	0.600407	2.654972	3.032995
H	0.660069	1.876562	2.381983
C	-0.722989	5.244084	-1.284723
H	-1.149627	5.585160	-0.334940
H	-1.513375	5.182256	-2.033928
C	-0.090956	3.877240	-1.088745
O	0.983529	3.937312	-0.301355
O	-0.522322	2.852677	-1.590004
N	6.054382	-2.001532	-1.443037
H	6.974181	-2.013705	-1.886175
H	6.141920	-1.969409	-0.410003
H	5.479564	-2.859829	-1.647825
C	5.128193	-0.907483	-1.952039
H	5.368021	0.010336	-1.409389
C	3.749350	-1.499150	-1.527057
O	3.648498	-2.738192	-1.624913
C	5.292334	-0.723704	-3.472416
H	5.077501	-1.696146	-3.938433
C	4.257163	0.291618	-3.986379
H	4.357493	0.408291	-5.070042
H	4.407115	1.277190	-3.528941
H	3.232932	-0.025916	-3.774837
C	6.714746	-0.281687	-3.857374
H	6.783182	-0.145082	-4.941292
H	7.493253	-1.011352	-3.591531
H	6.972553	0.673794	-3.384760
N	2.886796	-0.633558	-1.033680
H	3.088164	0.378960	-1.016643
C	1.751270	-0.862202	-0.122020
H	0.839325	-1.159435	-0.660781
C	1.455040	0.552173	0.478313
O	0.640823	0.582940	1.422832
C	2.069847	-1.912686	0.971554
H	1.287066	-1.783975	1.725591
H	1.966623	-2.916494	0.550146
C	3.449043	-1.757321	1.588751
C	4.432072	-2.742036	1.397825
H	4.170106	-3.648181	0.857267
C	3.795118	-0.615265	2.329856
H	3.060597	0.155133	2.547454
C	5.735968	-2.574591	1.887171
H	6.466575	-3.374760	1.769036
C	5.092802	-0.444073	2.817822
H	5.319037	0.454082	3.385695
C	6.074339	-1.411234	2.590186
H	7.080292	-1.280245	2.982679
N	-1.626511	-0.660239	-1.043900
H	-2.068698	-1.045552	-1.880200
C	-2.643595	-0.690163	0.014125
H	-2.160498	-0.973152	0.959960
C	-3.682578	-1.789540	-0.337229
O	-3.661766	-2.336266	-1.446851
C	-3.332981	0.684752	0.293094
H	-3.856797	0.614375	1.253684
H	-2.525647	1.415975	0.432256
C	-4.305936	1.176037	-0.760286
C	-5.678160	0.899064	-0.638072
H	-6.043463	0.334659	0.220021
C	-3.865180	1.917407	-1.867449
H	-2.812415	2.172451	-1.961612
C	-6.578264	1.341782	-1.609025
H	-7.635930	1.114747	-1.496250
C	-4.769440	2.357378	-2.836944
H	-4.407923	2.932324	-3.687968
C	-6.129587	2.069327	-2.713388
H	-6.834648	2.413385	-3.467934
N	-4.568008	-2.081328	0.637404
H	-4.722715	-1.428425	1.413271
C	-5.811047	-2.828049	0.427004
H	-6.154088	-2.644641	-0.599750
C	-6.900410	-2.231997	1.413331
O	-6.537879	-1.187298	2.036991
O	-7.983047	-2.845717	1.452175
C	-5.631479	-4.335522	0.614882
H	-6.610508	-4.816165	0.532916
H	-5.224074	-4.554560	1.610370
H	-4.948511	-4.749651	-0.136958
O	2.084305	1.517937	-0.053352
H	-1.334629	0.295888	-1.237097
H	1.349677	3.009633	-0.156929
H	0.033547	5.975759	-1.586496
H	1.423615	4.854065	4.203442

Table S6: Structure I_{MMP}

C	0.5059	-6.07007	0.33347
H	0.67502	-6.96726	-0.24485
N	-0.03589	-6.04725	1.62289
H	-0.29915	-6.8535	2.17557
C	0.74199	-4.75173	-0.00207
H	1.1528	-4.37747	-0.93114
C	-0.11455	-4.73649	2.02907
H	-0.49812	-4.43562	2.99074
N	0.34425	-3.91825	1.06589
C	3.41983	-2.85302	-3.8194
H	4.09751	-3.4613	-3.20737
H	3.94162	-1.95702	-4.16374
H	3.12611	-3.46295	-4.68104
C	2.1936	-2.49299	-3.00634
O	1.97121	-1.24242	-2.69659
O	1.41726	-3.46571	-2.6161
C	4.78987	-2.28888	1.30398
H	5.72083	-2.83245	1.35199
N	4.70024	-0.9067	1.48124
H	5.47154	-0.26228	1.60604
C	3.49613	-2.71866	1.08347
H	3.1443	-3.71894	0.89669
C	3.39313	-0.52546	1.36555
H	3.05876	0.51115	1.44104
N	2.62847	-1.61077	1.12113
Zn	0.55127	-1.70193	0.86157
N	-4.63193	-3.12052	-2.00939
H	-4.25093	-3.95737	-1.55466
H	-3.97378	-2.80359	-2.80363
H	-5.57624	-3.31215	-2.3557
C	-4.56725	-1.89161	-1.08132
H	-5.50409	-1.33677	-1.21616
C	-3.41996	-1.04682	-1.72412
O	-3.02567	-1.43042	-2.8753
C	-4.3993	-2.28181	0.40649
H	-4.3003	-1.33181	0.95075
C	-5.665	-2.98745	0.9473
H	-5.5595	-3.17919	2.02081
H	-5.83363	-3.96101	0.46371
H	-6.56459	-2.37459	0.80875
C	-3.11793	-3.10748	0.65681
H	-2.93344	-3.17916	1.73347
H	-2.23559	-2.65418	0.19247
H	-3.20922	-4.14291	0.29084
N	-2.97598	0.03334	-1.07097
H	-3.38438	0.29082	-0.1785
C	-2.04398	1.00656	-1.66084
H	-1.83694	0.64052	-2.67191
C	-0.70245	1.00327	-0.89677
O	-0.53003	0.38764	0.20486
C	-2.66763	2.47381	-1.74508
H	-2.05122	3.17198	-1.16738
H	-2.62378	2.77398	-2.80004
C	-4.10147	2.59933	-1.24223
C	-4.35682	3.34089	-0.06561
H	-3.52428	3.84675	0.42807
C	-5.18758	2.02866	-1.94926
H	-5.00583	1.51115	-2.89239
C	-5.67887	3.47682	0.40753
H	-5.86672	4.06751	1.30078
C	-6.50525	2.17024	-1.47642
H	-7.3369	1.75863	-2.04505
C	-6.7528	2.88887	-0.28736
H	-7.77171	3.0154	0.07129
N	0.28674	1.70266	-1.49949
H	0.10042	2.14453	-2.39486
C	1.66216	1.79941	-0.96121
H	1.99232	0.79391	-0.6913
C	1.72561	2.6671	0.32413
O	2.47688	2.29761	1.28606
C	2.59899	2.33506	-2.08385
H	2.37622	1.75293	-2.98805
H	2.35743	3.38853	-2.27734
C	4.07419	2.18003	-1.74722
C	4.71703	0.94198	-1.97518
H	4.14242	0.11711	-2.39387
C	4.82031	3.25133	-1.21382
H	4.33669	4.20948	-1.03478
C	6.08279	0.78281	-1.67545
H	6.57435	-0.16663	-1.87887
C	6.18581	3.09335	-0.91058
H	6.7505	3.92995	-0.50659
C	6.82248	1.85829	-1.14152
H	7.88283	1.7428	-0.92791
N	0.98278	3.78858	0.3121
H	0.19869	3.88508	-0.34689
C	0.75773	4.70714	1.44748
H	0.94255	4.16359	2.38277
C	-0.76925	5.10292	1.40407
O	-1.1947	5.86676	2.31741
O	-1.44638	4.53603	0.42801
C	1.67223	5.94607	1.40272
H	1.39575	6.61621	2.22316
H	1.54321	6.49168	0.45946
H	2.7271	5.66271	1.50734
O	0.13048	-1.85206	-1.09953
H	0.27383	-2.72264	-1.59737
H	0.77159	-1.28977	-1.70551
N	-0.05392	-1.02624	2.74626
C	0.28794	-1.61126	3.97786
C	-0.53626	0.20005	3.02437
C	-0.00035	-0.72528	4.99833
H	0.7515	-2.58173	4.04482
H	-0.84982	0.92152	2.28907
H	0.13035	-0.79955	6.06521
H	-0.80388	1.26945	4.83149
N	-0.52177	0.40984	4.37478

Table S7: Structure TSI_{MMP}

C	0.57565	-5.88851	-0.13162
H	0.70439	-6.79263	-0.72324
N	0.55602	-5.90137	1.26937
H	0.64622	-6.72066	1.85727
C	0.43713	-4.55682	-0.49644
H	0.40631	-4.12251	-1.48827
C	0.41792	-4.61223	1.71379
H	0.37579	-4.33745	2.75535
N	0.346	-3.76471	0.66882
C	2.20332	-2.58975	-4.88585
H	3.21087	-2.24671	-4.62423
H	1.87142	-1.98304	-5.73693
H	2.23259	-3.64073	-5.17968
C	1.27806	-2.39297	-3.72865
O	1.24903	-1.12092	-3.27811
O	0.59272	-3.31492	-3.2134
C	4.88971	-2.05422	-0.12806
H	5.81428	-2.4385	-0.52967
N	4.82728	-0.84367	0.56396
H	5.58417	-0.17753	0.67152
C	3.59326	-2.53671	-0.15451
H	3.21837	-3.44416	-0.59911
C	3.53591	-0.60866	0.93312
H	3.18923	0.30962	1.41022
N	2.75099	-1.62367	0.50494
Zn	0.67238	-1.63146	0.84531
N	-5.03993	-3.18456	-0.96666
H	-5.08299	-4.04209	-0.40664
H	-4.14731	-3.16125	-1.57381
H	-5.87631	-3.12105	-1.5561
C	-4.83698	-1.93735	-0.0942
H	-5.68063	-1.26038	-0.27012
C	-3.55363	-1.3205	-0.70334
O	-2.97102	-2.0178	-1.6198
C	-4.75327	-2.28075	1.41958
H	-4.52465	-1.32851	1.91909
C	-6.12061	-2.77134	1.95203
H	-6.07137	-2.91021	3.03735
H	-6.41333	-3.74099	1.52197
H	-6.92181	-2.0503	1.74715
C	-3.61199	-3.27092	1.74904
H	-3.5305	-3.37911	2.83594
H	-2.64142	-2.92894	1.37328
H	-3.80056	-4.2797	1.34915
N	-3.16115	-0.11302	-0.32548
H	-3.65921	0.37916	0.41165
C	-2.17271	0.70534	-1.07613
H	-2.30035	0.44456	-2.13616
C	-0.6896	0.3542	-0.67279
O	-0.45695	0.04018	0.62825
C	-2.50926	2.19208	-0.8479
H	-2.21236	2.50221	0.1603
H	-1.86167	2.79408	-1.49166
C	-3.95767	2.60678	-1.1048
C	-4.39119	3.82446	-0.52684
H	-3.67478	4.4054	0.05511
C	-4.8493	1.89281	-1.93926
H	-4.52334	0.9877	-2.45239
C	-5.69693	4.29351	-0.75594
H	-6.01141	5.23451	-0.31158
C	-6.15576	2.36912	-2.17262
H	-6.8239	1.82367	-2.8367
C	-6.58728	3.56656	-1.57262
H	-7.5924	3.93922	-1.75504
N	0.18301	1.31325	-1.24658
H	0.01074	1.57028	-2.21265
C	1.54374	1.54436	-0.74278
H	2.02839	0.59386	-0.5185
C	1.54269	2.37308	0.57047
O	2.25652	1.99474	1.56698
C	2.38365	2.24401	-1.85984
H	2.15484	1.73403	-2.80523
H	2.05511	3.28734	-1.94871
C	3.88524	2.16857	-1.62222
C	4.665	1.2353	-2.34213
H	4.18061	0.58982	-3.0725
C	4.53188	3.01238	-0.69027
H	3.95567	3.74945	-0.13745
C	6.05478	1.13933	-2.13535
H	6.64245	0.43325	-2.7184
C	5.91885	2.91411	-0.47381
H	6.40061	3.57966	0.23833
C	6.68764	1.97609	-1.19427
H	7.76422	1.92327	-1.0482
N	0.79874	3.48728	0.5443
H	0.06669	3.62455	-0.16917
C	0.61452	4.47666	1.6218
H	0.49581	3.95253	2.58136
C	-0.74973	5.21644	1.31679
O	-1.06575	6.16723	2.09206
O	-1.42225	4.7127	0.31352
C	1.79216	5.46203	1.73978
H	1.53904	6.21742	2.49042
H	1.96115	5.97777	0.78583
H	2.71425	4.94641	2.03831
O	-0.37512	-1.07408	-1.41506
H	-1.18503	-1.60042	-1.6411
H	0.57727	-1.02851	-2.46982
N	0.77355	-1.2553	2.92304
C	1.50162	-1.84716	3.96704
C	0.43761	-0.01829	3.33985
C	1.59463	-0.95636	5.01832
H	1.93642	-2.83046	3.887
H	-0.07811	0.70786	2.7333
H	2.07528	-1.03595	5.97842
H	0.84138	1.06221	5.11257
N	0.91359	0.19014	4.60301

Table S8: Structure II_{MMP}

C	1.63533	-5.83063	0.61247
H	2.02116	-6.75899	0.20493
N	1.23789	-5.6869	1.94852
H	1.26033	-6.40977	2.65699
C	1.45231	-4.58907	0.02883
H	1.64482	-4.26406	-0.98324
C	0.83975	-4.38942	2.14365
H	0.48831	-4.0029	3.08701
N	0.95838	-3.69189	0.99783
C	3.64442	-2.65596	-4.01035
H	4.41446	-1.88991	-3.86337
H	3.41732	-2.68005	-5.08259
H	4.02075	-3.62966	-3.6909
C	2.40272	-2.2965	-3.23514
O	1.89495	-1.08673	-3.53337
O	1.87884	-3.06003	-2.38243
C	5.22323	-1.3144	0.9436
H	6.26169	-1.59683	0.8954
N	4.81374	-0.0327	1.31609
H	5.41532	0.7681	1.47223
C	4.06195	-2.02226	0.69546
H	3.94746	-3.04438	0.37408
C	3.45204	0.02349	1.29041
H	2.85042	0.91019	1.50489
N	2.95937	-1.17718	0.91242
Zn	0.9157	-1.555	0.84829
N	-4.04846	-4.20478	-1.44145
H	-3.82859	-4.93379	-0.75512
H	-3.17101	-3.9517	-2.02831
H	-4.81846	-4.5172	-2.04022
C	-4.32533	-2.8509	-0.76685
H	-5.28259	-2.47893	-1.15037
C	-3.17258	-1.95614	-1.3188
O	-2.36872	-2.5453	-2.13671
C	-4.3993	-2.96407	0.78044
H	-4.57748	-1.94038	1.13867
C	-5.61035	-3.82281	1.21629
H	-5.7161	-3.79465	2.30601
H	-5.49504	-4.88075	0.93614
H	-6.54983	-3.45442	0.785
C	-3.07517	-3.45761	1.40724
H	-3.16144	-3.43736	2.49924
H	-2.22731	-2.82491	1.1238
H	-2.83848	-4.49755	1.13032
N	-3.12938	-0.68552	-0.94717
H	-3.86228	-0.34534	-0.32451
C	-2.26717	0.42743	-1.47079
H	-2.45669	0.50477	-2.55042
C	-0.70389	0.13633	-1.31223
O	-0.39931	-0.47254	-0.12028
C	-2.71553	1.71734	-0.753
H	-2.35798	1.68183	0.28631
H	-2.20223	2.57928	-1.19233
C	-4.2162	2.02371	-0.75915
C	-4.68962	3.01527	0.13424
H	-3.99467	3.55147	0.77953
C	-5.13232	1.44535	-1.67135
H	-4.7897	0.74111	-2.42876
C	-6.04573	3.38301	0.13738
H	-6.38081	4.16207	0.81695
C	-6.49231	1.81875	-1.66874
H	-7.17638	1.37968	-2.39232
C	-6.95659	2.78065	-0.75462
H	-8.00236	3.07842	-0.75498
N	0.0132	1.36233	-1.58783
H	-0.13465	1.72747	-2.5236
C	1.28709	1.71119	-0.94556
H	1.77663	0.80094	-0.59217
C	1.07038	2.60083	0.31096
O	1.53716	2.22712	1.44831
C	2.23614	2.39157	-1.9836
H	2.22339	1.76981	-2.88756
H	1.82629	3.37613	-2.24698
C	3.67283	2.52848	-1.49736
C	4.6715	1.66221	-1.99752
H	4.40064	0.91545	-2.74167
C	4.0449	3.50948	-0.54928
H	3.29748	4.20021	-0.16718
C	6.00692	1.76756	-1.5633
H	6.76621	1.1089	-1.97967
C	5.37629	3.61222	-0.10474
H	5.64592	4.38391	0.61249
C	6.36473	2.74155	-0.60942
H	7.40001	2.84526	-0.29181
N	0.3818	3.73663	0.12495
H	-0.15586	3.90607	-0.7405
C	-0.15329	4.62478	1.1813
H	-0.16844	4.0824	2.13224
C	-1.63479	4.93889	0.74128
O	-2.46352	5.22176	1.67133
O	-1.85269	4.79057	-0.53297
C	0.67546	5.91478	1.34179
H	0.20532	6.55441	2.09754
H	0.70976	6.47083	0.39673
H	1.7022	5.68961	1.6597
O	-0.35695	-0.7807	-2.48927
H	-0.91039	-1.60307	-2.46925
H	0.96607	-0.89537	-3.07092
N	0.34132	-0.8432	2.73942
C	0.85393	-1.04415	4.03194
C	-0.38301	0.29099	2.78653
C	0.42226	-0.02104	4.85515
H	1.50852	-1.86652	4.27271
H	-0.86196	0.74009	1.93438
H	0.60881	0.18293	5.89645
H	-0.7748	1.69179	4.31953
N	-0.36197	0.807	4.04877

Table S9: Structure II'$_{MMP}$

C	-4.71971	-3.03033	-1.86886
H	-5.36488	-3.21266	-2.71852
N	-4.76512	-3.81561	-0.71306
H	-5.37125	-4.61207	-0.55931
C	-3.73275	-2.08324	-1.63852
H	-3.36898	-1.31104	-2.29884
C	-3.82683	-3.34068	0.1687
H	-3.62231	-3.78831	1.12811
N	-3.18441	-2.28539	-0.3593
C	-0.28394	-1.2327	-5.45754
H	0.09413	-2.25589	-5.34561
H	0.40682	-0.70321	-6.12331
H	-1.2857	-1.24406	-5.88838
C	-0.32441	-0.54938	-4.10348
O	0.82775	-0.42752	-3.43602
O	-1.43472	-0.14053	-3.62753
C	0.68223	-4.74182	-1.2153
H	0.89922	-5.50656	-1.94009
N	1.55517	-4.39623	-0.1822
H	2.4974	-4.74871	-0.0493
C	-0.40691	-3.90348	-1.08259
H	-1.29347	-3.85142	-1.6922
C	1.00029	-3.37562	0.53693
H	1.48821	-2.82674	1.33599
N	-0.1972	-3.04616	0.00973
Zn	-1.37269	-1.36366	0.48921
N	-5.39767	3.30688	-0.82932
H	-5.95516	2.46018	-0.98298
H	-4.71143	3.47276	-1.67085
H	-6.01937	4.10571	-0.67705
C	-4.3704	3.11481	0.29027
H	-4.30438	4.06786	0.82946
C	-3.06143	2.95219	-0.53846
O	-3.15657	3.30707	-1.77249
C	-4.7487	1.98847	1.28055
H	-3.8801	1.86977	1.94387
C	-5.94987	2.40756	2.16111
H	-6.15409	1.63721	2.91286
H	-6.86878	2.53139	1.56955
H	-5.75645	3.34626	2.69553
C	-4.99879	0.63721	0.57561
H	-5.09332	-0.15472	1.32549
H	-4.1806	0.36028	-0.09666
H	-5.94177	0.63119	0.00556
N	-1.95273	2.50835	0.03375
H	-1.91104	2.09612	0.96862
C	-0.6835	2.37013	-0.70829
H	-0.91955	2.49254	-1.76782
C	-0.24058	0.89381	-0.43504
O	-0.38283	0.49764	0.86691
C	0.30472	3.48329	-0.25013
H	-0.30061	4.38822	-0.09477
H	0.73643	3.22949	0.72597
C	1.41864	3.82617	-1.2444
C	2.71112	4.13311	-0.75541
H	2.91948	4.09243	0.31535
C	1.16565	3.93335	-2.63376
H	0.17	3.74444	-3.03269
C	3.72781	4.52389	-1.64961
H	4.71233	4.76552	-1.25709
C	2.18597	4.32167	-3.5211
H	1.97543	4.40592	-4.58481
C	3.47396	4.61515	-3.03122
H	4.26215	4.9209	-3.71502
N	1.12365	0.66453	-1.05881
H	1.5801	1.56959	-1.23613
C	2.06576	-0.23549	-0.28513
H	1.64048	-1.2337	-0.36516
C	2.22825	-0.01762	1.26406
O	1.92613	-1.01406	2.02388
C	3.45175	-0.24346	-1.01075
H	3.2812	-0.06675	-2.07952
H	4.06837	0.58199	-0.63507
C	4.16445	-1.57993	-0.8434
C	4.14133	-2.52431	-1.89467
H	3.65412	-2.26551	-2.83297
C	4.82219	-1.9229	0.36009
H	4.86809	-1.20514	1.1747
C	4.75134	-3.78584	-1.74799
H	4.75084	-4.48835	-2.57886
C	5.42679	-3.18453	0.51333
H	5.93899	-3.42647	1.44132
C	5.3912	-4.12425	-0.53797
H	5.88509	-5.08703	-0.42807
N	2.78524	1.10261	1.74989
H	2.96345	1.97557	1.22491
C	3.06136	1.36453	3.19216
H	2.15645	1.13334	3.77098
C	3.35145	2.92258	3.35424
O	3.60315	3.33239	4.52297
O	3.26638	3.57526	2.225
C	4.23589	0.52554	3.73152
H	4.42182	0.82382	4.7684
H	5.14974	0.72837	3.15758
H	4.01438	-0.54792	3.69255
O	-1.22703	-0.02119	-1.12545
H	-1.35976	0.06191	-2.13675
H	0.90116	0.06657	-2.44092
N	-1.78683	-1.49696	2.54017
C	-0.77059	-1.21604	3.38103
C	-2.92252	-1.72367	3.32953
H	0.25104	-0.99347	3.07552
C	-2.58554	-1.57552	4.66149
H	-3.88362	-1.96625	2.90578
H	-0.65705	-1.07809	5.49096
H	-3.17951	-1.66886	5.55342
N	-1.22513	-1.25846	4.67196

Table S10: Structure $TSII_{MMP}$

C	-4.73717	-3.01705	-1.85644
H	-5.38055	-3.20039	-2.7071
N	-4.81414	-3.77539	-0.68424
H	-5.44269	-4.55188	-0.51912
C	-3.72466	-2.09414	-1.64003
H	-3.32988	-1.35213	-2.31766
C	-3.8697	-3.30794	0.19466
H	-3.68574	-3.74125	1.16474
N	-3.19326	-2.283	-0.35074
C	-0.29872	-1.23628	-5.45585
H	0.12091	-2.24696	-5.38451
H	0.35668	-0.66033	-6.11867
H	-1.30807	-1.27598	-5.86704
C	-0.33453	-0.59797	-4.07699
O	0.80565	-0.40855	-3.4308
O	-1.47133	-0.27776	-3.56933
C	0.66903	-4.73971	-1.2008
H	0.88034	-5.50289	-1.92824
N	1.54248	-4.40493	-0.16455
H	2.47979	-4.76846	-0.02863
C	-0.4132	-3.89285	-1.06891
H	-1.29738	-3.83101	-1.68083
C	0.99446	-3.38139	0.55578
H	1.48551	-2.83889	1.35641
N	-0.19831	-3.04033	0.02591
Zn	-1.37802	-1.36454	0.49761
N	-5.40057	3.32414	-0.835
H	-5.96883	2.48344	-0.98184
H	-4.72168	3.47887	-1.68258
H	-6.01187	4.13051	-0.68037
C	-4.368	3.12314	0.27753
H	-4.29326	4.07304	0.82103
C	-3.06473	2.95383	-0.55898
O	-3.16287	3.30581	-1.79277
C	-4.74839	1.99372	1.264
H	-3.87723	1.86547	1.92207
C	-5.94237	2.41572	2.15289
H	-6.14767	1.64271	2.90164
H	-6.86352	2.54832	1.56673
H	-5.74047	3.35042	2.69117
C	-5.01059	0.64805	0.55258
H	-5.10809	-0.14714	1.29863
H	-4.19716	0.36885	-0.12452
H	-5.95579	0.65148	-0.01384
N	-1.95513	2.51013	0.01236
H	-1.91293	2.10947	0.95181
C	-0.68775	2.36234	-0.73156
H	-0.92564	2.47479	-1.79181
C	-0.25401	0.88582	-0.4447
O	-0.37248	0.51036	0.86253
C	0.3045	3.47453	-0.28132
H	-0.29495	4.3858	-0.14146
H	0.72752	3.23013	0.70114
C	1.42912	3.7971	-1.27038
C	2.71914	4.10162	-0.77295
H	2.91727	4.07348	0.30031
C	1.18987	3.88824	-2.66328
H	0.19731	3.69951	-3.06976
C	3.74672	4.47466	-1.66221
H	4.72888	4.71531	-1.26325
C	2.22117	4.25868	-3.54557
H	2.02137	4.32934	-4.61228
C	3.5063	4.55031	-3.0472
H	4.30277	4.84248	-3.72731
N	1.12718	0.65583	-1.07821
H	1.57888	1.56443	-1.25417
C	2.07411	-0.23775	-0.29626
H	1.64748	-1.23566	-0.37273
C	2.23099	-0.00872	1.25028
O	1.92336	-0.99903	2.01394
C	3.45822	-0.24679	-1.02566
H	3.28312	-0.08954	-2.09687
H	4.06904	0.58958	-0.66503
C	4.18166	-1.57463	-0.83797
C	4.15413	-2.54046	-1.86942
H	3.65562	-2.30449	-2.80793
C	4.85529	-1.88684	0.36481
H	4.90345	-1.15186	1.16382
C	4.77616	-3.79367	-1.70344
H	4.77274	-4.51321	-2.51959
C	5.47246	-3.13982	0.53705
H	5.99659	-3.35859	1.46408
C	5.4329	-4.10108	-0.49419
H	5.93532	-5.05762	-0.36968
N	2.79098	1.11264	1.73174
H	2.97397	1.97717	1.19776
C	3.06107	1.37889	3.17473
H	2.15335	1.14757	3.74882
C	3.35164	2.93593	3.34173
O	3.58854	3.34117	4.51586
O	3.28017	3.59179	2.21476
C	4.23218	0.53862	3.71993
H	4.41124	0.83527	4.75841
H	5.14982	0.74265	3.15247
H	4.01096	-0.53482	3.67788
O	-1.22081	-0.03362	-1.11796
H	-1.35598	-0.01488	-2.15031
H	0.9145	0.09349	-2.32666
N	-1.79151	-1.46556	2.54673
C	-0.77626	-1.18259	3.38769
C	-2.92719	-1.69262	3.3358
H	0.24516	-0.96116	3.08327
C	-2.59088	-1.54379	4.66761
H	-3.88821	-1.93499	2.91205
H	-0.66339	-1.04438	5.49769
H	-3.18513	-1.63859	5.5588
N	-1.23099	-1.2253	4.67847

Table S11: Structure III_{MMP}

C	-4.67484	-3.12046	-1.83837
H	-5.3214	-3.32634	-2.68302
N	-4.75073	-3.84917	-0.64711
H	-5.37967	-4.62069	-0.46192
C	-3.6545	-2.19894	-1.64983
H	-3.24553	-1.48511	-2.34937
C	-3.80337	-3.36214	0.21794
H	-3.61933	-3.7719	1.19817
N	-3.12572	-2.35227	-0.35392
C	-0.33665	-1.1942	-5.48384
H	0.07656	-2.21078	-5.47843
H	0.26687	-0.60026	-6.17781
H	-1.37639	-1.22458	-5.81439
C	-0.24319	-0.60859	-4.08901
O	0.86494	-0.25846	-3.55534
O	-1.39522	-0.49375	-3.43651
C	0.79962	-4.68706	-1.22434
H	1.01937	-5.42431	-1.9759
N	1.66382	-4.3689	-0.17488
H	2.60612	-4.72219	-0.04525
C	-0.29459	-3.8596	-1.07478
H	-1.17421	-3.789	-1.69196
C	1.09678	-3.37276	0.57068
H	1.57609	-2.84753	1.38863
N	-0.09783	-3.03583	0.04445
Zn	-1.32805	-1.39216	0.48205
N	-5.5337	3.19182	-0.80068
H	-6.10158	2.34772	-0.92922
H	-4.88184	3.34341	-1.66622
H	-6.14478	3.99613	-0.63369
C	-4.47249	2.99941	0.28651
H	-4.39127	3.94868	0.83014
C	-3.18552	2.83908	-0.57863
O	-3.31538	3.16489	-1.81595
C	-4.82494	1.86576	1.2782
H	-3.93997	1.74264	1.91842
C	-6.00416	2.27735	2.1914
H	-6.18964	1.50084	2.94167
H	-6.93771	2.40544	1.62405
H	-5.79815	3.21189	2.72847
C	-5.09143	0.51982	0.56893
H	-5.17054	-0.27741	1.31499
H	-4.28853	0.24702	-0.12285
H	-6.04617	0.51809	0.01879
N	-2.05542	2.43895	-0.01549
H	-1.98389	2.07533	0.93792
C	-0.78244	2.33013	-0.75921
H	-1.02191	2.38006	-1.82365
C	-0.28209	0.88521	-0.40429
O	-0.36054	0.57155	0.91486
C	0.1365	3.52066	-0.35274
H	-0.51394	4.40469	-0.28876
H	0.5414	3.36077	0.65493
C	1.27003	3.83549	-1.33287
C	2.5502	4.17486	-0.83308
H	2.73764	4.19355	0.24163
C	1.04262	3.87603	-2.73001
H	0.05715	3.65216	-3.13594
C	3.58129	4.5355	-1.72499
H	4.5545	4.80822	-1.32486
C	2.07668	4.23202	-3.61365
H	1.88761	4.26124	-4.68409
C	3.3526	4.56114	-3.11313
H	4.15038	4.84412	-3.79552
N	1.21354	0.77265	-0.98451
H	1.63559	1.71396	-1.03557
C	2.13752	-0.17973	-0.23525
H	1.66834	-1.15513	-0.34175
C	2.27816	0.04506	1.30123
O	1.99533	-0.95219	2.06249
C	3.52076	-0.2045	-0.96706
H	3.35017	-0.03561	-2.03761
H	4.14163	0.62036	-0.59711
C	4.22923	-1.54254	-0.79313
C	4.24068	-2.47248	-1.85697
H	3.77639	-2.20614	-2.80468
C	4.85783	-1.89448	0.42321
H	4.87764	-1.18703	1.24797
C	4.85889	-3.72996	-1.71055
H	4.88554	-4.42162	-2.5498
C	5.46934	-3.15269	0.57588
H	5.95958	-3.40251	1.5135
C	5.47015	-4.07816	-0.4887
H	5.96981	-5.03783	-0.37845
N	2.80204	1.18809	1.76159
H	2.95406	2.05596	1.21579
C	3.03587	1.51384	3.19423
H	2.12455	1.27984	3.76142
C	3.27162	3.08433	3.27997
O	3.46941	3.56525	4.43178
O	3.20598	3.67594	2.11624
C	4.22331	0.73829	3.7953
H	4.37658	1.08759	4.82143
H	5.14291	0.94381	3.23215
H	4.03608	-0.34264	3.80061
O	-1.0709	-0.10418	-1.10485
H	-1.23049	-0.19448	-2.31297
H	1.11186	0.39985	-1.98378
N	-1.73451	-1.47067	2.53523
C	-0.71815	-1.17222	3.36865
C	-2.85641	-1.73346	3.33326
H	0.29534	-0.92637	3.05879
C	-2.50957	-1.58773	4.66255
H	-3.81644	-1.99164	2.91685
H	-0.58625	-1.05121	5.47826
H	-3.0879	-1.70365	5.56093
N	-1.15742	-1.23879	4.66319

Table S12: Structure $TSIII_{MMP}$

C	-4.61618	-3.2091	-1.85142
H	-5.26121	-3.43258	-2.69255
N	-4.68068	-3.93075	-0.65508
H	-5.29682	-4.71142	-0.46516
C	-3.61407	-2.26649	-1.66802
H	-3.21817	-1.54898	-2.37208
C	-3.74086	-3.4242	0.20606
H	-3.54923	-3.82617	1.18797
N	-3.079	-2.40739	-0.37253
C	-0.32441	-1.20215	-5.50175
H	-0.68216	-2.2366	-5.43525
H	0.64769	-1.18001	-5.99839
H	-1.05633	-0.63774	-6.08986
C	-0.22372	-0.60938	-4.11025
O	0.86964	-0.22983	-3.58494
O	-1.39167	-0.52216	-3.46168
C	0.88712	-4.67798	-1.25101
H	1.12	-5.41021	-2.00258
N	1.7528	-4.33718	-0.21056
H	2.70682	-4.66346	-0.09175
C	-0.22596	-3.87808	-1.09314
H	-1.11237	-3.83058	-1.70271
C	1.16922	-3.35418	0.53803
H	1.6443	-2.82066	1.35276
N	-0.03885	-3.0476	0.02299
Zn	-1.29427	-1.43027	0.47571
N	-5.59341	3.07788	-0.80096
H	-6.15454	2.22546	-0.89971
H	-4.93421	3.20283	-1.66763
H	-6.21107	3.88407	-0.67236
C	-4.53773	2.94123	0.30037
H	-4.49676	3.90111	0.82926
C	-3.23522	2.80395	-0.54694
O	-3.36597	3.07394	-1.79653
C	-4.85781	1.81032	1.30762
H	-3.97969	1.73814	1.965
C	-6.06958	2.1857	2.19334
H	-6.23516	1.41446	2.95364
H	-6.99774	2.26486	1.60854
H	-5.91275	3.13692	2.71753
C	-5.04994	0.43996	0.62108
H	-5.10951	-0.34381	1.38317
H	-4.22196	0.18836	-0.04947
H	-5.99172	0.38384	0.05216
N	-2.09584	2.46764	0.04303
H	-2.03553	2.16073	1.01464
C	-0.8081	2.36191	-0.68522
H	-1.04169	2.40224	-1.75074
C	-0.31464	0.9224	-0.31966
O	-0.35745	0.60092	0.98064
C	0.10351	3.5562	-0.27841
H	-0.55864	4.42431	-0.14808
H	0.56303	3.36911	0.70081
C	1.17931	3.93421	-1.30158
C	2.47446	4.28377	-0.85017
H	2.71215	4.25708	0.21444
C	0.88479	4.02085	-2.68398
H	-0.11336	3.7913	-3.05362
C	3.45469	4.6982	-1.77543
H	4.44154	4.9737	-1.41214
C	1.86815	4.43161	-3.6011
H	1.62776	4.49514	-4.65974
C	3.15994	4.76938	-3.14935
H	3.91903	5.09216	-3.85774
N	1.28829	0.84645	-0.93874
H	1.69868	1.79179	-0.94369
C	2.18176	-0.14339	-0.22316
H	1.68896	-1.10504	-0.35192
C	2.32222	0.06176	1.31278
O	2.04856	-0.94084	2.07095
C	3.57042	-0.19436	-0.94715
H	3.40679	0.00297	-2.01384
H	4.20995	0.60713	-0.55744
C	4.24637	-1.55236	-0.80254
C	4.27526	-2.4409	-1.90101
H	3.83989	-2.13205	-2.84935
C	4.83586	-1.96136	0.41608
H	4.84404	-1.28708	1.26818
C	4.8712	-3.71238	-1.78724
H	4.91034	-4.37147	-2.65172
C	5.42387	-3.23437	0.53653
H	5.88547	-3.52712	1.47633
C	5.44212	-4.11787	-0.5635
H	5.92661	-5.08781	-0.47812
N	2.82561	1.21258	1.77196
H	2.95458	2.08814	1.22757
C	3.05163	1.5551	3.19925
H	2.15408	1.29262	3.77557
C	3.22166	3.13295	3.25966
O	3.41773	3.64112	4.39946
O	3.10841	3.70492	2.08803
C	4.273	0.83464	3.80027
H	4.42007	1.20034	4.82171
H	5.17938	1.06821	3.22705
H	4.12823	-0.25277	3.81894
O	-1.03809	-0.07899	-1.03924
H	-1.21649	-0.18907	-2.32222
H	1.16944	0.52266	-1.93271
N	-1.6863	-1.54331	2.5239
C	-0.67187	-1.23783	3.35763
C	-2.80713	-1.80938	3.3221
H	0.33948	-0.98017	3.05106
C	-2.46137	-1.66123	4.65131
H	-3.76556	-2.07431	2.90633
H	-0.54128	-1.11384	5.46651
H	-3.04023	-1.77837	5.54851
N	-1.11162	-1.3049	4.65167

Table S13: Structure IV_{MMP}

C	0.70787	-5.98421	1.04485
H	1.06553	-6.70027	1.76674
N	0.03366	-6.37346	-0.11657
H	-0.17419	-7.32547	-0.39131
C	0.74744	-4.60051	1.01511
H	1.15416	-3.91062	1.7388
C	-0.32657	-5.24613	-0.80443
H	-0.89518	-5.25596	-1.72053
N	0.10104	-4.15266	-0.15035
C	-0.10324	-2.00257	5.48211
H	-0.56452	-2.98642	5.34159
H	-0.63185	-1.44939	6.26072
H	0.93717	-2.16454	5.78735
C	-0.13688	-1.22025	4.18186
O	-0.64021	-0.08815	4.03116
O	0.4644	-1.89788	3.15003
C	-4.0326	-2.7829	1.55291
H	-4.64231	-3.2046	2.32139
N	-4.44569	-1.75361	0.70952
H	-5.33113	-1.25337	0.74801
C	-2.73387	-3.07289	1.20026
H	-2.0647	-3.80175	1.62545
C	-3.40849	-1.42805	-0.11623
H	-3.3981	-0.59803	-0.81272
N	-2.35213	-2.21666	0.15926
Zn	-0.45928	-2.14978	-0.58842
N	5.93098	-2.36919	-0.14215
H	5.95692	-2.72029	-1.10504
H	5.01376	-2.66923	0.35637
H	6.75598	-2.6966	0.36813
C	5.7705	-0.84084	-0.11766
H	6.53174	-0.42896	0.55483
C	4.35806	-0.68658	0.51016
O	3.79553	-1.77103	0.90344
C	5.92987	-0.21803	-1.53325
H	5.7146	0.85257	-1.40799
C	7.39078	-0.33967	-2.02778
H	7.51	0.21296	-2.9659
H	7.67838	-1.38141	-2.23719
H	8.10691	0.07594	-1.30702
C	4.9142	-0.78851	-2.55155
H	5.01664	-0.24877	-3.49956
H	3.87746	-0.68461	-2.21075
H	5.10386	-1.85098	-2.78197
N	3.78324	0.51127	0.57903
H	4.26939	1.35614	0.29012
C	2.35354	0.65549	0.95964
H	2.2369	0.38926	2.01545
C	1.54591	-0.34426	0.11067
O	1.80967	-0.5342	-1.10813
C	1.8733	2.10148	0.70211
H	1.88033	2.30037	-0.37737
H	0.81636	2.14692	1.01107
C	2.66213	3.19215	1.42708
C	2.48522	4.53224	0.99904
H	1.80417	4.76927	0.18042
C	3.50587	2.93472	2.53261
H	3.63468	1.92142	2.90922
C	3.1583	5.57655	1.65836
H	3.0084	6.59846	1.31911
C	4.17599	3.98606	3.19018
H	4.8131	3.77109	4.04568
C	4.00872	5.31117	2.75149
H	4.52249	6.12493	3.25778
N	-1.21903	2.37645	1.73303
H	-1.23235	3.37565	1.9276
C	-2.32204	1.87521	0.8959
H	-2.41046	0.80522	1.10115
C	-2.03052	1.99938	-0.62178
O	-2.33639	1.02352	-1.41393
C	-3.69262	2.5778	1.2554
H	-3.6884	2.69383	2.34591
H	-3.67725	3.58733	0.82118
C	-4.95698	1.83968	0.84737
C	-5.73655	1.18525	1.83019
H	-5.42839	1.23405	2.87269
C	-5.39806	1.78998	-0.49705
H	-4.83127	2.30304	-1.26844
C	-6.91153	0.48549	1.48527
H	-7.51127	0.01675	2.26234
C	-6.56785	1.09079	-0.84785
H	-6.89649	1.07653	-1.8842
C	-7.32944	0.43036	0.13925
H	-8.24568	-0.08858	-0.13141
N	-1.51059	3.15104	-1.05656
H	-1.01191	3.82009	-0.44239
C	-1.26112	3.53362	-2.46406
H	-0.74023	2.71173	-2.97747
C	-0.25398	4.75509	-2.41986
O	-0.02578	5.34426	-3.51835
O	0.24726	4.9696	-1.23273
C	-2.55352	3.87322	-3.22772
H	-2.27812	4.25525	-4.21604
H	-3.11066	4.66319	-2.70865
H	-3.20183	2.99368	-3.33985
O	0.55199	-0.99525	0.71342
H	0.48146	-1.40052	2.25745
H	-1.047	1.8127	2.56535
N	-0.56674	-2.0055	-2.61884
C	-1.08826	-0.9669	-3.29994
C	0.01871	-2.86747	-3.55446
H	-1.59435	-0.1131	-2.85079
C	-0.1508	-2.34034	-4.8167
H	0.53507	-3.76858	-3.26741
H	-1.12645	-0.49591	-5.36448
H	0.15478	-2.72228	-5.77337
N	-0.8502	-1.14418	-4.63715

Table S14: Structure II_{MPC-T}

N	-0.781957	1.149652	0.499188
C	0.581313	1.627209	0.829586
C	1.294252	0.516342	1.641763
O	1.413252	0.645479	2.907931
C	-1.141628	0.243793	-0.401586
N	1.676369	-0.576277	0.941338
Pd	1.795912	-0.501067	-1.063579
O	1.877948	-0.525905	-3.183569
C	2.310881	-1.780938	1.545943
C	1.633322	-2.436894	2.797227
C	3.824868	-1.538157	1.791860
C	4.631107	-1.652102	0.481635
S	4.147461	-0.427697	-0.822332
C	4.859135	-1.248512	-2.294016
O	1.400271	-3.653798	2.760866
O	-0.266436	-1.677252	-3.516223
O	-0.333848	-0.407751	-1.191258
H	2.210113	-2.572571	0.797083
H	3.984862	-0.572339	2.284470
H	4.217007	-2.311927	2.464445
H	5.696425	-1.473099	0.669402
H	4.513405	-2.654927	0.054103
H	4.451980	-2.254468	-2.420759
H	4.610614	-0.650442	-3.172407
H	5.946802	-1.288792	-2.175026
H	-0.679858	-1.398723	-2.660309
H	-0.667066	-2.442001	-3.961037
H	1.051039	-1.064502	-3.519571
H	2.023435	0.304329	-3.673450
H	1.123256	1.785427	-0.112117
C	-2.653719	-0.043086	-0.490670
H	-2.917675	-0.004532	-1.558246
O	1.423002	-1.681909	3.898750
H	1.511165	-0.683710	3.721386
H	-1.609412	1.548098	0.975742
C	0.503413	2.958174	1.610605
H	0.029807	2.769685	2.580198
H	1.534076	3.261076	1.831811
C	-0.226606	4.051027	0.841763
C	-1.483627	4.520956	1.279157
C	0.342216	4.620731	-0.320257
C	-2.162576	5.530962	0.569243
H	-1.923342	4.118421	2.190417
C	-0.332224	5.628109	-1.032627
H	1.328042	4.298806	-0.656187
C	-1.590612	6.084597	-0.591235
H	-3.122872	5.892982	0.927875
H	0.124378	6.067796	-1.915946
H	-2.107861	6.870937	-1.134711
N	-3.384351	0.959119	0.298968
H	-4.118378	0.564174	0.883291
H	-3.726280	1.757504	-0.231740
C	-2.927291	-1.491766	0.034486
H	-2.307420	-2.187041	-0.545130
H	-2.587529	-1.555211	1.076600
C	-4.397366	-1.874645	-0.058415
C	-5.024297	-2.036078	-1.314946
C	-5.159972	-2.075077	1.112381
C	-6.383022	-2.385330	-1.399388
H	-4.451398	-1.900832	-2.232260
C	-6.522172	-2.426050	1.031252
H	-4.687390	-1.980887	2.088887
C	-7.137378	-2.579449	-0.224411
H	-6.851928	-2.512757	-2.371784
H	-7.094566	-2.585417	1.941241
H	-8.186810	-2.854048	-0.288847

Table S15: Structure II_{MPC-C}

N	1.185931	0.769400	-0.512979
C	-0.266826	0.905029	-0.670034
C	-0.841745	-0.420370	-1.211068
O	-0.468362	-0.797193	-2.376906
C	1.822975	0.375336	0.599371
N	-1.686195	-1.146158	-0.432859
Pd	-2.527164	-0.411026	1.230128
O	-3.197178	0.275697	3.132475
C	-2.378089	-2.384114	-0.905429
C	-1.501196	-3.558457	-1.461445
C	-3.530379	-2.016670	-1.878117
C	-4.717173	-1.364532	-1.135662
S	-4.265829	0.203325	-0.252084
C	-5.773290	0.458903	0.751726
O	-1.663468	-4.685950	-0.973115
O	-0.884984	-0.865125	2.464968
O	1.250043	0.030858	1.694683
H	-2.818617	-2.837100	-0.011789
H	-3.162489	-1.373769	-2.685376
H	-3.919323	-2.931424	-2.343843
H	-5.504080	-1.086060	-1.846693
H	-5.137145	-2.057927	-0.397216
H	-5.965939	-0.390229	1.413653
H	-5.640597	1.375876	1.333567
H	-6.625003	0.599208	0.078159
H	0.043222	-0.431237	2.126389
H	-0.769415	-1.811221	2.683023
H	-4.022735	0.575745	3.548565
H	-2.441401	0.156054	3.744749
H	-0.691809	1.123935	0.315778
C	3.355395	0.328819	0.498947
H	3.738785	0.800248	1.415613
O	-0.676878	-3.313107	-2.502187
H	-0.553656	-2.317491	-2.683051
H	1.835912	1.004375	-1.275984
C	-0.602550	2.063617	-1.650727
H	-0.214878	1.794856	-2.640045
H	-1.696806	2.111615	-1.742051
C	-0.049767	3.406393	-1.196322
C	0.991034	4.034615	-1.912700
C	-0.569826	4.051002	-0.051535
C	1.505927	5.276712	-1.492752
H	1.389919	3.563140	-2.809268
C	-0.058026	5.289952	0.372684
H	-1.388392	3.592999	0.504372
C	0.984869	5.906497	-0.347030
H	2.300705	5.753556	-2.060850
H	-0.472274	5.778396	1.251247
H	1.377422	6.867434	-0.024984
N	3.799066	1.019202	-0.725189
H	4.559757	0.542970	-1.205973
H	4.010546	2.006864	-0.596603
C	3.804728	-1.169731	0.500777
H	3.388433	-1.633462	1.402583
H	3.354142	-1.670191	-0.366893
C	5.317479	-1.325467	0.465448
C	6.100021	-0.998995	1.596493
C	5.967076	-1.792120	-0.698110
C	7.499069	-1.131043	1.562769
H	5.615397	-0.655453	2.509611
C	7.369268	-1.926166	-0.734989
H	5.377693	-2.074759	-1.569366
C	8.138904	-1.593085	0.394552
H	8.088631	-0.883863	2.442123
H	7.854233	-2.294857	-1.635273
H	9.220276	-1.699547	0.370086

Table S16: Structure TS(II-III)$_{MPC}$

N	-0.393550	0.867988	0.555298
C	0.683502	1.710751	-0.099991
C	2.026315	1.418247	0.625158
O	2.671338	2.391702	1.141713
C	-1.179611	-0.148730	-0.367252
N	2.409749	0.115611	0.734770
Pd	1.716083	-1.250385	-0.576036
O	0.661098	-2.389512	-2.044265
C	3.648966	-0.305740	1.453508
C	3.802767	0.144800	2.943958
C	4.918168	0.038950	0.628168
C	5.078217	-0.880809	-0.600912
S	3.680057	-0.730879	-1.806032
C	4.027982	-2.159665	-2.892649
O	3.958634	-0.719000	3.816181
O	-0.045411	-1.468325	0.555073
O	-0.861765	-0.258924	-1.575944
H	3.577722	-1.393331	1.545415
H	4.912449	1.094641	0.334683
H	5.806923	-0.116581	1.253522
H	5.983448	-0.613111	-1.158764
H	5.152105	-1.930125	-0.290816
H	4.026913	-3.099850	-2.333799
H	3.262981	-2.182077	-3.673706
H	5.004231	-2.013696	-3.366075
H	0.022401	0.176192	1.215969
H	-0.314080	-2.408886	0.623943
H	0.811709	-3.149387	-2.629861
H	-0.114800	-1.808514	-2.252237
H	0.743463	1.359794	-1.138266
C	-2.640504	-0.314023	0.140658
H	-3.232752	0.093012	-0.689639
O	3.857816	1.474263	3.211458
H	3.557750	2.045053	2.433454
H	-1.162945	1.376621	1.051437
C	0.324860	3.215309	-0.060084
H	0.476406	3.588531	0.958088
H	1.063996	3.735442	-0.681305
C	-1.091386	3.515218	-0.536483
C	-2.026187	4.097005	0.348593
C	-1.495948	3.239325	-1.863133
C	-3.336121	4.394963	-0.077310
H	-1.724057	4.344170	1.364872
C	-2.802622	3.533587	-2.291549
H	-0.789602	2.806338	-2.569346
C	-3.728827	4.110808	-1.398968
H	-4.036292	4.862007	0.610747
H	-3.094234	3.328885	-3.318566
H	-4.734173	4.351387	-1.734691
N	-2.874208	0.517300	1.337252
H	-3.025485	-0.010447	2.195213
H	-3.597375	1.222630	1.213840
C	-3.041854	-1.805937	0.319347
H	-2.704464	-2.357416	-0.568853
H	-2.505007	-2.210474	1.187727
C	-4.541508	-1.979854	0.514648
C	-5.433868	-1.775164	-0.562080
C	-5.066777	-2.335545	1.774960
C	-6.820735	-1.917404	-0.380376
H	-5.047629	-1.518765	-1.548261
C	-6.455843	-2.477791	1.961048
H	-4.393446	-2.520026	2.611196
C	-7.336293	-2.266293	0.884166
H	-7.496380	-1.764309	-1.218029
H	-6.846235	-2.756886	2.936256
H	-8.408022	-2.378977	1.024484

Table S17: Structure III_{MPC}

N	-0.160624	1.223095	-0.732011
C	-0.603097	2.076638	0.425992
C	-2.129716	1.911628	0.543629
O	-2.808434	2.809736	1.148288
C	3.608505	0.119672	-1.104328
N	-2.616717	0.787106	-0.038428
Pd	-1.179243	-0.569129	-0.467024
O	0.458615	-1.897184	-0.775731
C	-4.035131	0.352082	-0.107852
C	-5.226739	1.375626	-0.209472
C	-4.364007	-0.674146	1.025132
C	-4.152242	-2.133551	0.573083
S	-2.411377	-2.546351	0.089123
C	-2.664713	-3.407725	-1.508312
O	-6.212106	0.984965	-0.857363
O	4.697758	0.712448	-0.549189
O	2.500238	0.675109	-1.177321
H	-4.126917	-0.166663	-1.067068
H	-3.776717	-0.441370	1.921157
H	-5.421914	-0.593233	1.301663
H	-4.416347	-2.828228	1.377636
H	-4.791171	-2.345111	-0.291447
H	-3.227452	-2.785655	-2.209556
H	-1.676056	-3.625430	-1.921050
H	-3.199186	-4.345798	-1.328969
H	-0.489161	1.628416	-1.614950
H	4.515714	1.639813	-0.235786
H	0.654470	-2.466838	-0.003416
H	1.330122	-1.771508	-1.353528
H	-0.150357	1.641120	1.325465
C	3.894308	-1.272773	-1.657856
H	4.678028	-1.140304	-2.421038
O	-5.200795	2.542018	0.455383
H	-4.295597	2.766491	0.882090
H	0.860353	1.096084	-0.784839
C	-0.155055	3.553425	0.310637
H	-0.577622	3.994472	-0.601981
H	-0.613331	4.087309	1.152056
C	1.363187	3.693393	0.321097
C	2.058868	4.160692	-0.815273
C	2.108618	3.342145	1.470811
C	3.463233	4.263201	-0.813221
H	1.502545	4.461333	-1.700869
C	3.512016	3.438829	1.480226
H	1.592093	3.019374	2.373615
C	4.199309	3.892473	0.331797
H	3.979326	4.646634	-1.689810
H	4.065686	3.196368	2.384247
H	5.279313	4.022400	0.353820
N	2.632071	-1.795197	-2.266450
H	2.755473	-2.765868	-2.566128
H	2.350747	-1.231403	-3.073918
C	4.478768	-2.250207	-0.588837
H	4.782586	-3.162589	-1.118763
H	5.394472	-1.786945	-0.205879
C	3.535031	-2.598835	0.552783
C	2.819625	-3.817675	0.550760
C	3.367205	-1.718411	1.646426
C	1.935490	-4.139016	1.601301
H	2.972000	-4.533861	-0.255151
C	2.487792	-2.035643	2.698015
H	3.943811	-0.796904	1.689895
C	1.761889	-3.243283	2.675741
H	1.410084	-5.090527	1.596116
H	2.383540	-1.356715	3.540432
H	1.094489	-3.496302	3.495096

Table S18: Structure III_{DPC}

N	-2.15091	2.53756	-0.51158
C	-3.10575	1.47143	-0.1554
C	-4.47568	1.53308	-0.95063
C	-2.45188	0.09996	-0.38721
O	-1.42193	-0.03053	-1.14786
N	-3.02997	-0.96328	0.21323
C	-2.72058	-2.38768	-0.00695
C	-1.22652	-2.71673	0.09689
O	-0.40271	-2.02909	0.76434
O	-0.79814	-3.81063	-0.53497
Pd	2.59523	-0.12345	-1.29884
Pd	3.3876	0.70251	1.21328
O	0.85086	-0.0645	-0.17129
N	3.27279	-2.07715	-0.92723
C	2.78004	-2.94933	0.21184
C	2.73467	-2.25878	1.602
N	3.87165	-1.28866	1.90849
C	4.15704	-1.1324	3.41842
C	3.573	0.16607	3.99531
N	4.03903	1.31293	3.12375
C	3.4974	2.70305	3.4077
C	2.31612	3.02209	2.48287
N	2.66748	2.71017	1.02443
C	1.44063	2.9241	0.15152
C	1.65794	2.93545	-1.37943
N	2.59977	1.88095	-1.91856
C	2.59799	1.72589	-3.43637
C	3.79252	0.83382	-3.84022
N	3.93081	-0.36924	-2.89712
C	3.45395	-1.71503	-3.44472
C	3.26078	-2.76094	-2.29598
H	-0.02592	0.17585	-0.6966
H	0.53496	-0.89116	0.33386
H	2.29528	-3.25892	-2.41182
H	4.04166	-3.53065	-2.31677
H	5.24674	-1.13892	3.54249
H	3.76257	-1.99559	3.9646
H	1.79177	-1.72954	1.74028
H	2.75264	-3.07032	2.34162
H	3.43342	-3.83297	0.24867
H	1.76472	-3.28761	-0.01734
H	4.16963	-2.08107	-4.19063
H	2.50313	-1.53348	-3.95375
H	3.67654	0.48906	-4.87295
H	4.72907	1.40029	-3.78904
H	1.63823	1.28739	-3.72643
H	2.68443	2.70436	-3.92721
H	0.67423	2.78469	-1.83381
H	2.03512	3.91152	-1.71749
H	1.00171	3.8995	0.40605
H	0.71572	2.15855	0.42282
H	1.4386	2.41797	2.73418
H	2.0374	4.07934	2.5844
H	4.31673	3.41446	3.2548
H	3.18623	2.78461	4.45601
H	2.47886	0.15865	4.00577
H	3.92193	0.30189	5.02836
H	4.25664	-1.86473	-0.71892
H	4.91686	-0.44446	-2.62141
H	3.55017	2.16101	-1.64112
H	3.42654	3.34353	0.737
H	5.06601	1.34442	3.13524
H	4.74204	-1.646	1.4977
H	-3.05233	-2.67409	-1.01394
H	-3.33141	1.56964	0.91401
H	-4.25886	1.40653	-2.01948
H	-2.44854	3.43972	-0.1377
H	-3.86764	-0.81021	0.777
H	-1.45599	-4.49854	-0.99381
O	-2.25375	-5.55362	-1.55987
H	-2.36827	-6.40621	-1.09501
H	-2.52071	-5.62674	-2.49655
C	-3.51698	-3.25106	1.04489
H	-3.37018	-4.30466	0.78199
H	-3.07379	-3.08933	2.03488
C	-5.00178	-2.91681	1.07091
C	-5.56109	-2.2423	2.18116
C	-5.8473	-3.30049	0.00022
C	-6.94161	-1.96234	2.22461
H	-4.93772	-1.98955	3.03799
C	-7.22253	-3.01838	0.04072
H	-5.44087	-3.84865	-0.84892
C	-7.77419	-2.34702	1.15321
H	-7.37052	-1.47478	3.09556
H	-7.86847	-3.33564	-0.77291
H	-8.84122	-2.14801	1.19381
H	-5.0987	0.68005	-0.6444
C	-5.24212	2.82181	-0.71819
C	-5.82008	3.09608	0.55549
C	-5.43098	3.75338	-1.77272
C	-6.56472	4.26236	0.76583
H	-5.71421	2.37866	1.36801
C	-6.17851	4.92226	-1.56741
H	-5.02124	3.54518	-2.75862
C	-6.74859	5.18438	-0.29555
H	-7.01926	4.45759	1.73255
H	-6.33712	5.62159	-2.38299
H	-7.33752	6.0838	-0.13903
H	-2.02549	2.60368	-1.52306

Table S19: Structure IV_{DPC}

N	-3.11081	2.53929	0.4713
C	-4.20237	1.59836	0.20273
C	-5.39296	2.18035	-0.67094
C	-3.63238	0.36302	-0.49819
O	-2.57253	0.42421	-1.2316
N	-4.28525	-0.8096	-0.3632
C	-3.95597	-2.05502	-1.07466
C	-2.45672	-2.34676	-1.08119
O	-1.65316	-2.1088	-0.1453
O	-1.95811	-2.98517	-2.17935
Pd	2.96917	-1.0431	1.05571
Pd	4.11866	0.89885	-0.73593
O	2.1136	0.64739	0.13072
N	3.8167	-0.08422	2.75115
C	3.76406	1.40228	3.09951
C	3.9921	2.4727	1.9749
N	4.9141	2.11218	0.82175
C	5.53529	3.33813	0.10403
C	5.52769	3.19331	-1.44124
N	5.67553	1.733	-1.84729
C	5.42896	1.39743	-3.3199
C	4.00005	0.8578	-3.54498
N	3.67819	-0.19388	-2.48148
C	2.27584	-0.76149	-2.57368
C	2.0016	-2.12971	-1.88108
N	2.62793	-2.41403	-0.51966
C	1.93642	-3.55378	0.23524
C	2.79245	-3.96533	1.45742
N	3.42799	-2.74962	2.14632
C	2.89219	-2.35885	3.51773
C	3.46632	-0.9816	3.96018
H	0.58876	0.35272	-0.27714
H	1.98338	1.37514	0.77484
H	2.71552	-0.46878	4.56698
H	4.36525	-1.09791	4.57744
H	6.55484	3.4676	0.48563
H	4.96955	4.23346	0.37686
H	3.04549	2.80392	1.53713
H	4.40358	3.34966	2.49272
H	4.50557	1.56261	3.89411
H	2.78214	1.60537	3.53765
H	3.14391	-3.12999	4.25681
H	1.80267	-2.31103	3.43398
H	2.17292	-4.51565	2.17274
H	3.60721	-4.63103	1.15201
H	0.94335	-3.19951	0.52518
H	1.79951	-4.42079	-0.42493
H	0.91548	-2.20157	-1.77099
H	2.31397	-2.95086	-2.54011
H	2.03146	-0.91708	-3.63417
H	1.60317	0.00419	-2.19391
H	3.24926	1.65008	-3.46224
H	3.92278	0.42438	-4.55104
H	6.17355	0.64862	-3.61249
H	5.59583	2.28294	-3.94355
H	4.58304	3.55223	-1.86069
H	6.33814	3.79298	-1.87617
H	4.79971	-0.28685	2.52757
H	4.43846	-2.92007	2.2176
H	3.59721	-2.71203	-0.69564
H	4.36942	-0.95057	-2.56957
H	6.6089	1.39456	-1.58555
H	5.70369	1.57176	1.1947
H	-4.2979	-1.96707	-2.11627
H	-4.62199	1.2835	1.16647
H	-4.98019	2.51175	-1.63245
H	-3.30548	3.15904	1.25468
H	-5.15715	-0.84978	0.16886
H	-2.59279	-3.16007	-2.91062
C	-4.72414	-3.26211	-0.40299
H	-4.55502	-4.15377	-1.01939
H	-4.28	-3.44659	0.58239
C	-6.21269	-2.97256	-0.27436
C	-6.76416	-2.63135	0.98302
C	-7.06134	-3.04799	-1.40234
C	-8.14453	-2.37404	1.10953
H	-6.13653	-2.62897	1.87398
C	-8.43716	-2.7876	-1.27594
H	-6.66479	-3.34402	-2.37306
C	-8.98115	-2.44748	-0.01994
H	-8.56702	-2.14523	2.08395
H	-9.0867	-2.86878	-2.14275
H	-10.04739	-2.26532	0.07824
H	-6.10529	1.36976	-0.8815
C	-6.10998	3.3209	0.0256
C	-7.00244	3.05129	1.10092
C	-5.92103	4.66242	-0.38792
C	-7.68434	4.09264	1.74387
H	-7.18514	2.02299	1.41035
C	-6.60381	5.70879	0.25205
H	-5.26756	4.88351	-1.22897
C	-7.48697	5.42884	1.32367
H	-8.37754	3.87784	2.5517
H	-6.47036	6.73369	-0.08165
H	-8.0233	6.23796	1.81119
H	-2.81946	3.06634	-0.35071
O	-0.35999	0.02785	-0.44841
H	-0.67646	-0.89743	-0.1825
H	-1.25229	0.52667	-0.80489

Table S20: Structure TS(IV-V)$_{DPC}$

N	0.87587	1.61973	0.31755
C	2.10617	0.95449	-0.28692
C	3.39539	1.71907	0.13521
C	2.05084	-0.50793	0.21669
O	1.84203	-0.76861	1.4354
N	3.31199	-1.36416	-0.45116
C	3.7617	-2.56429	0.36407
C	2.70795	-3.67305	0.27301
O	1.62995	-3.52881	-0.35051
O	2.93493	-4.83055	0.91032
Pd	-2.62183	-0.34851	-1.40679
Pd	-2.54939	0.14636	1.44026
O	-1.09403	0.13611	-0.09897
N	-3.36907	1.57312	-1.89212
C	-2.89722	2.91248	-1.34206
C	-2.40633	3.00225	0.13609
N	-3.12731	2.17198	1.18663
C	-3.08807	2.78521	2.60265
C	-3.01727	1.69987	3.71838
N	-3.5674	0.36564	3.22877
C	-3.25442	-0.85243	4.10918
C	-2.09444	-1.6824	3.51842
N	-2.33467	-1.85358	2.01803
C	-1.2889	-2.67898	1.30057
C	-1.68587	-3.25582	-0.09567
N	-2.56328	-2.44201	-1.04871
C	-2.51498	-2.96568	-2.48737
C	-3.68227	-2.35577	-3.29818
N	-3.89799	-0.87549	-2.95488
C	-3.51128	0.14565	-4.01743
C	-3.54105	1.58619	-3.42439
H	-0.17567	-0.68645	-0.43236
H	-0.22783	0.99731	0.05143
H	-2.72153	2.16492	-3.85718
H	-4.47734	2.1028	-3.66837
H	-3.96783	3.42764	2.72372
H	-2.20459	3.42495	2.67723
H	-1.35422	2.73828	0.2022
H	-2.49929	4.06302	0.40633
H	-3.71885	3.62608	-1.4974
H	-2.06107	3.25187	-1.9607
H	-4.18906	0.07109	-4.87689
H	-2.50363	-0.10957	-4.35713
H	-3.48872	-2.46688	-4.36994
H	-4.61746	-2.88371	-3.08095
H	-1.5422	-2.68883	-2.90282
H	-2.5929	-4.06097	-2.50352
H	-0.75105	-3.49623	-0.60832
H	-2.20828	-4.21235	0.04843
H	-1.06164	-3.56025	1.91783
H	-0.38162	-2.07683	1.26093
H	-1.12489	-1.1918	3.6447
H	-2.04785	-2.66025	4.01591
H	-4.16743	-1.45564	4.16887
H	-3.01122	-0.52956	5.12716
H	-1.9801	1.52594	4.01914
H	-3.57291	2.02971	4.60527
H	-4.31233	1.43508	-1.5061
H	-4.8909	-0.75215	-2.72275
H	-3.5303	-2.5652	-0.71941
H	-3.25382	-2.30302	1.90662
H	-4.58691	0.43488	3.12638
H	-4.11907	2.11189	0.92462
H	3.79711	-2.21848	1.40506
H	1.98192	0.98719	-1.37323
H	3.59655	1.53125	1.19793
H	0.91012	2.60655	0.02523
H	4.15086	-0.75273	-0.50807
H	3.80929	-4.9809	1.33652
C	5.19888	-3.00277	-0.09611
H	5.5691	-3.75445	0.61374
H	5.14098	-3.48875	-1.07852
C	6.15497	-1.81459	-0.13654
C	6.50249	-1.22115	-1.37462
C	6.72424	-1.30936	1.05616
C	7.41052	-0.14317	-1.41808
H	6.13442	-1.64389	-2.30921
C	7.62865	-0.23275	1.01062
H	6.50795	-1.7819	2.01355
C	7.97148	0.35343	-0.22571
H	7.70526	0.2795	-2.37443
H	8.08966	0.12658	1.92613
H	8.69247	1.16499	-0.26056
H	4.24952	1.32379	-0.4343
C	3.27947	3.21907	-0.12909
C	3.25585	3.71423	-1.45508
C	3.22764	4.13497	0.94643
C	3.18562	5.09863	-1.69948
H	3.34998	3.03134	-2.29951
C	3.15978	5.52166	0.70157
H	3.29942	3.77745	1.97273
C	3.1359	6.0054	-0.62075
H	3.20504	5.47222	-2.71953
H	3.15828	6.21983	1.53401
H	3.11179	7.07487	-0.80902
H	0.98904	1.59019	1.34096
O	0.83514	-1.14695	-0.78043
H	3.05669	-1.63625	-1.41086
H	0.97963	-2.14604	-0.73582

Table S21: Structure V_{DPC}

N	0.31422	2.48525	-1.22393
C	-0.69785	3.14507	-0.27414
C	-0.80522	4.66291	-0.57804
C	-2.05054	2.4186	-0.35078
O	-3.12301	3.05348	-0.42523
N	-7.27523	0.32691	-2.02317
C	-6.74909	-0.05018	-0.73622
C	-5.41899	0.69361	-0.56066
O	-4.30714	0.10554	-0.41149
O	-5.55602	2.02321	-0.59411
Pd	2.86002	-0.29883	1.09914
Pd	2.82895	-2.48444	-0.59592
O	1.28162	0.20642	-0.20881
N	4.46046	0.53487	-0.00051
C	4.38476	0.89056	-1.46748
C	3.66432	-0.16027	-2.34711
N	4.09875	-1.59813	-2.10215
C	3.98913	-2.52362	-3.33125
C	2.84359	-3.55068	-3.22528
N	2.90316	-4.21453	-1.87061
C	1.78112	-5.14585	-1.47375
C	0.69086	-4.39862	-0.69229
N	1.28921	-3.58324	0.45695
C	0.20445	-2.76427	1.12398
C	0.55658	-2.11492	2.4818
N	1.92988	-1.49666	2.569
C	2.16887	-0.6768	3.83283
C	3.68354	-0.40176	3.97799
N	4.32533	-0.07578	2.62964
C	4.73157	1.37175	2.39359
C	5.08108	1.6133	0.89132
H	0.43078	-0.19458	0.06999
H	0.7573	1.5688	-0.82332
H	4.68848	2.58566	0.58262
H	6.16614	1.62489	0.73009
H	4.94892	-3.04494	-3.43039
H	3.85368	-1.92337	-4.2374
H	2.5881	-0.11594	-2.1706
H	3.87083	0.11015	-3.39186
H	5.40943	1.06066	-1.83037
H	3.8461	1.83789	-1.56265
H	5.58378	1.63671	3.03193
H	3.88277	1.99456	2.69065
H	3.84751	0.41897	4.68393
H	4.19145	-1.28376	4.3838
H	1.59168	0.24808	3.74308
H	1.80804	-1.216	4.7192
H	-0.1867	-1.33628	2.68169
H	0.47148	-2.8557	3.29074
H	-0.67081	-3.40579	1.30705
H	-0.10303	-2.01217	0.39224
H	0.15326	-3.69678	-1.33896
H	-0.03944	-5.12069	-0.30218
H	2.21658	-5.94246	-0.85995
H	1.33845	-5.62318	-2.35715
H	1.8644	-3.07377	-3.33291
H	2.9494	-4.29186	-4.03022
H	5.08134	-0.28192	0.06099
H	5.14485	-0.68171	2.51074
H	2.60123	-2.27595	2.57575
H	1.70483	-4.24095	1.13018
H	3.80107	-4.70011	-1.76712
H	5.08648	-1.61557	-1.82636
H	-6.52966	-1.12101	-0.72814
H	-0.29479	2.99291	0.73457
H	-1.29344	4.80513	-1.54993
H	1.04913	3.20221	-1.37789
H	-7.8075	-0.34672	-2.56031
H	-4.69913	2.55602	-0.52776
C	-7.68999	0.29206	0.53068
H	-7.08213	0.09694	1.42529
H	-7.90046	1.3651	0.4791
C	-8.95017	-0.51748	0.5758
C	-10.15049	-0.03306	-0.01915
C	-8.97051	-1.78996	1.23828
C	-11.33015	-0.77779	0.05665
H	-10.1551	0.93573	-0.51167
C	-10.14808	-2.53776	1.31541
H	-8.06271	-2.16257	1.7084
C	-11.33602	-2.03931	0.72365
H	-12.24915	-0.40005	-0.38128
H	-10.16376	-3.49161	1.83336
H	-12.25582	-2.61529	0.77946
H	-1.48009	5.10206	0.16448
C	0.56079	5.33683	-0.54376
C	1.13193	5.74253	0.68609
C	1.27195	5.58614	-1.74337
C	2.38394	6.38458	0.7153
H	0.57036	5.62072	1.61162
C	2.52833	6.22903	-1.71392
H	0.80898	5.3748	-2.70751
C	3.08752	6.62497	-0.48456
H	2.78712	6.74397	1.65852
H	3.03862	6.46335	-2.64419
H	4.03263	7.16046	-0.46403
H	-0.11957	2.28074	-2.13298
O	-1.97025	1.07142	-0.32873
H	-7.43735	1.30817	-2.22386
H	-2.93253	0.61735	-0.3655
