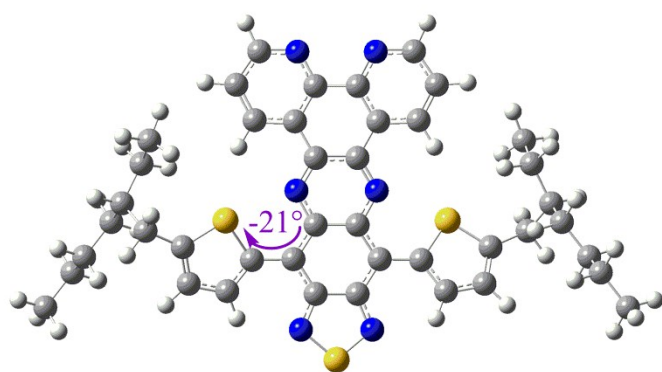


Electronic supplementary information

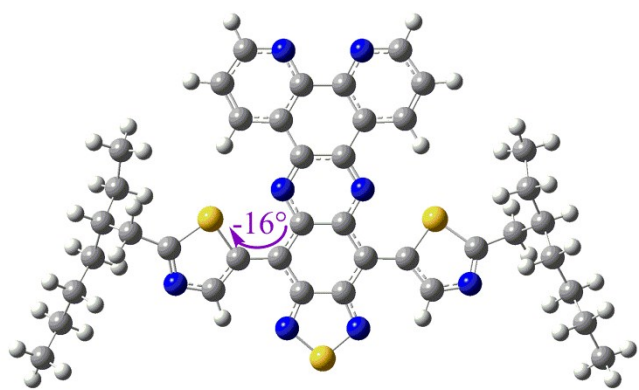
Improving the electron transport performance by changing side chains in sulfur-containing azaacenes: A combined theoretical investigation on free molecule and adsorption system†

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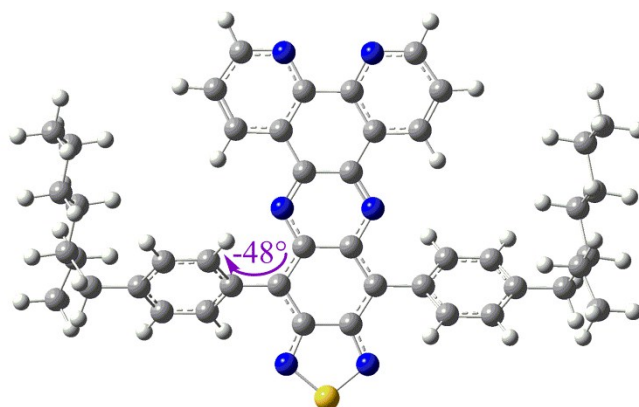
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TDTP



TDTP-I



TDTP-II

Fig. S1 Optimized ground state structures at the B3LYP/6-31G(d,p) level.

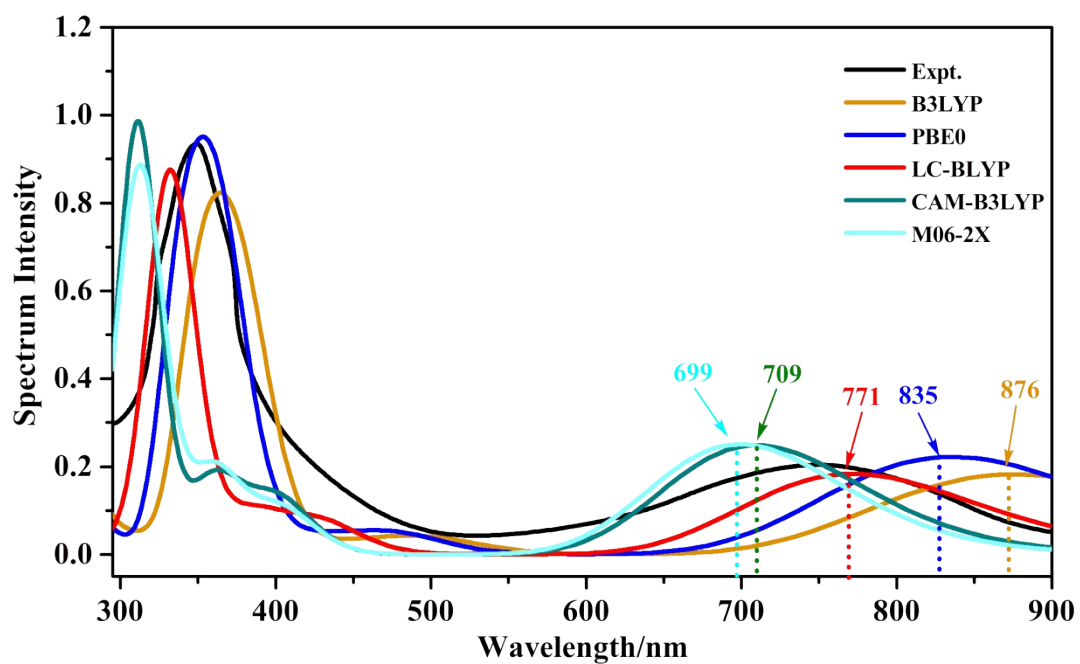


Fig. S2 The simulated absorption spectrum of **TDTP** by means of B3LYP, PBE0, LC-BLYP, CAM-B3LYP, and M06-2X methods in dichloromethane with the 6-31G(d,p) basis set along with the experimental result.⁹ The value of the maximum absorption peak is marked on the chart.

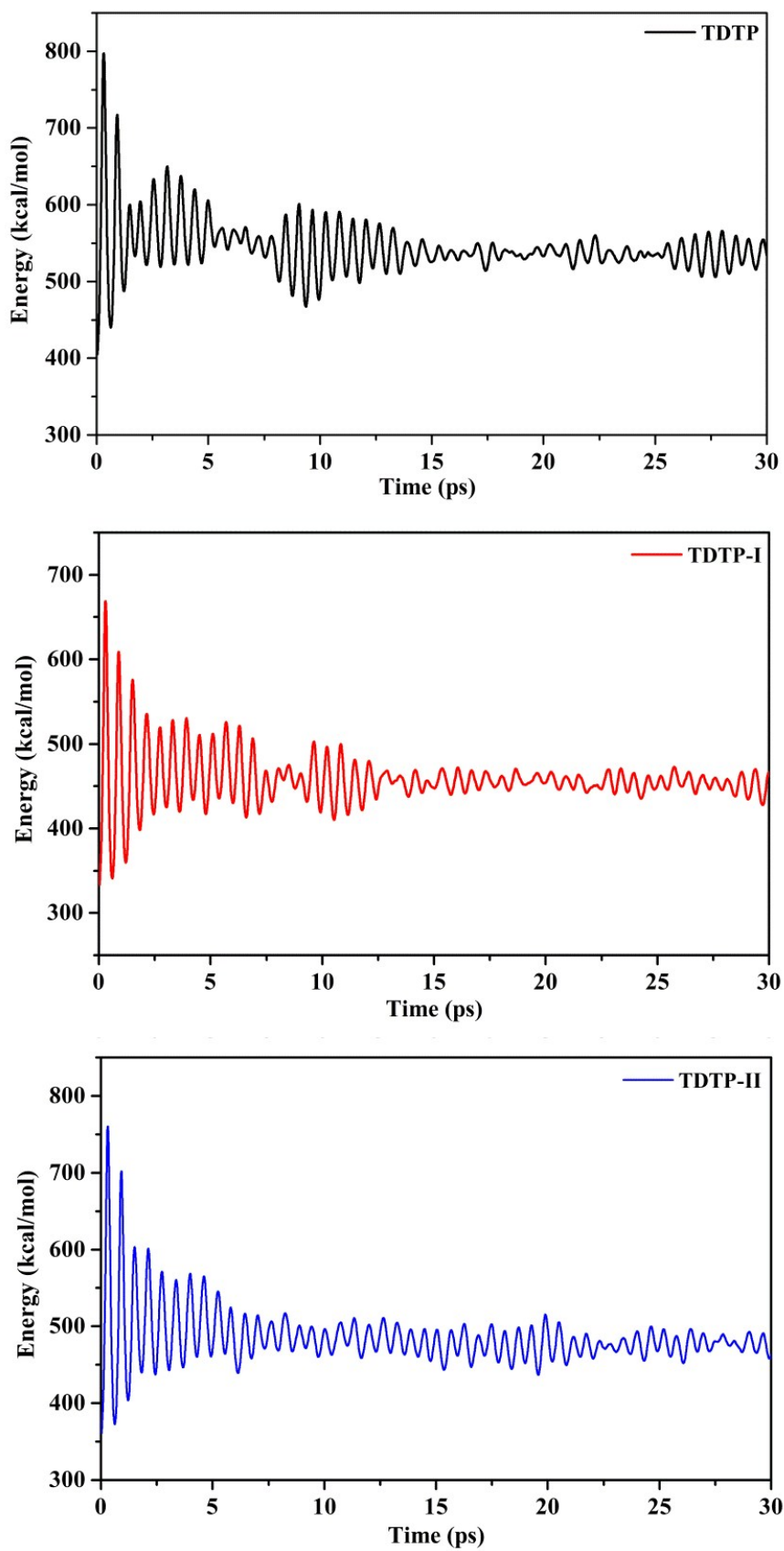


Fig. S3 Evolutions of the total energy as a function of the simulation time.

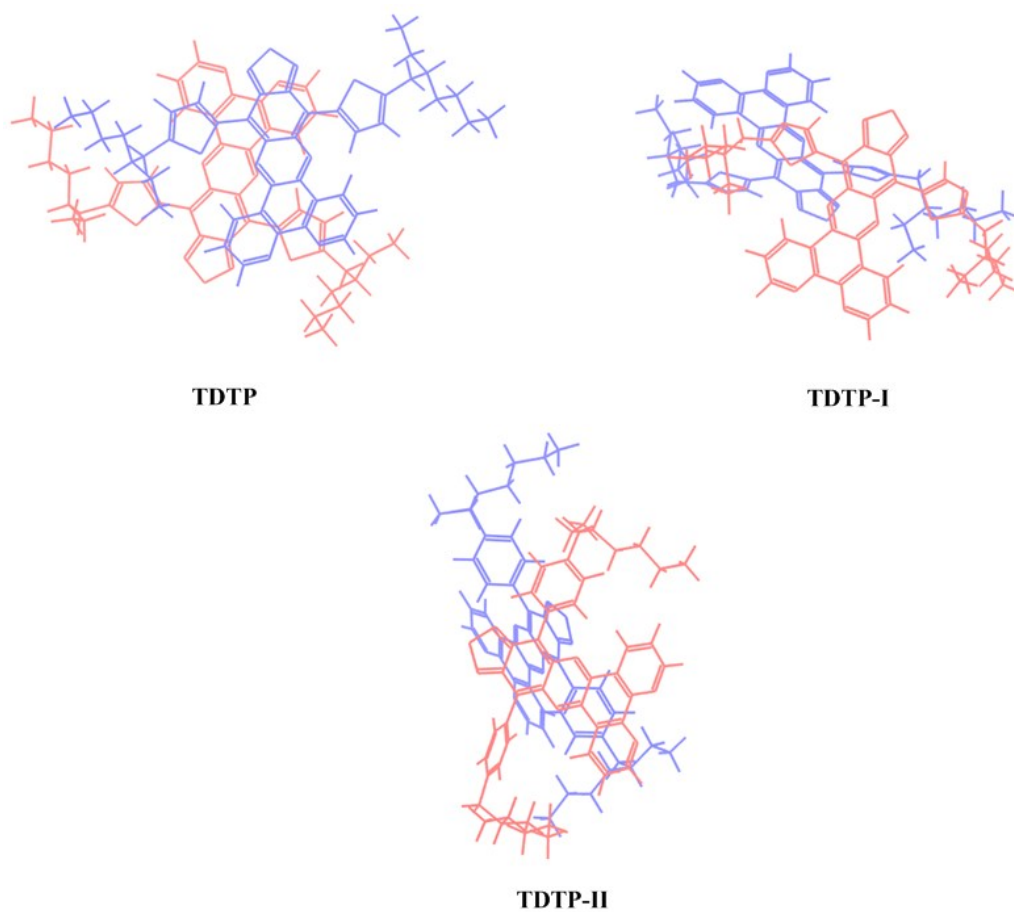


Fig. S4 Optimized dimers at the M06-2X/6-31G(d,p) level.

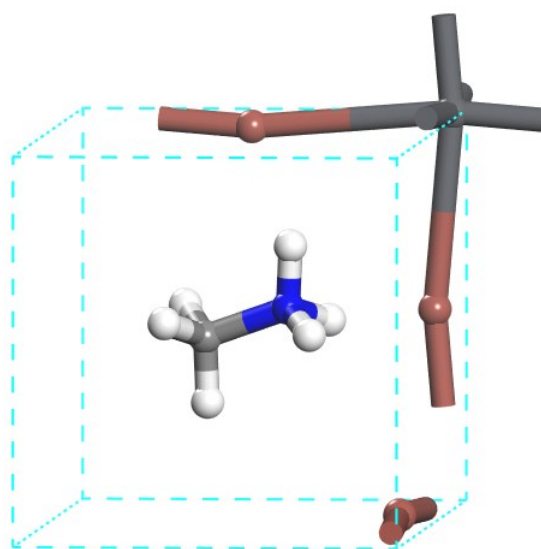


Fig. S5 The optimized crystal structure of $\text{CH}_3\text{NH}_3\text{PbI}_3$.

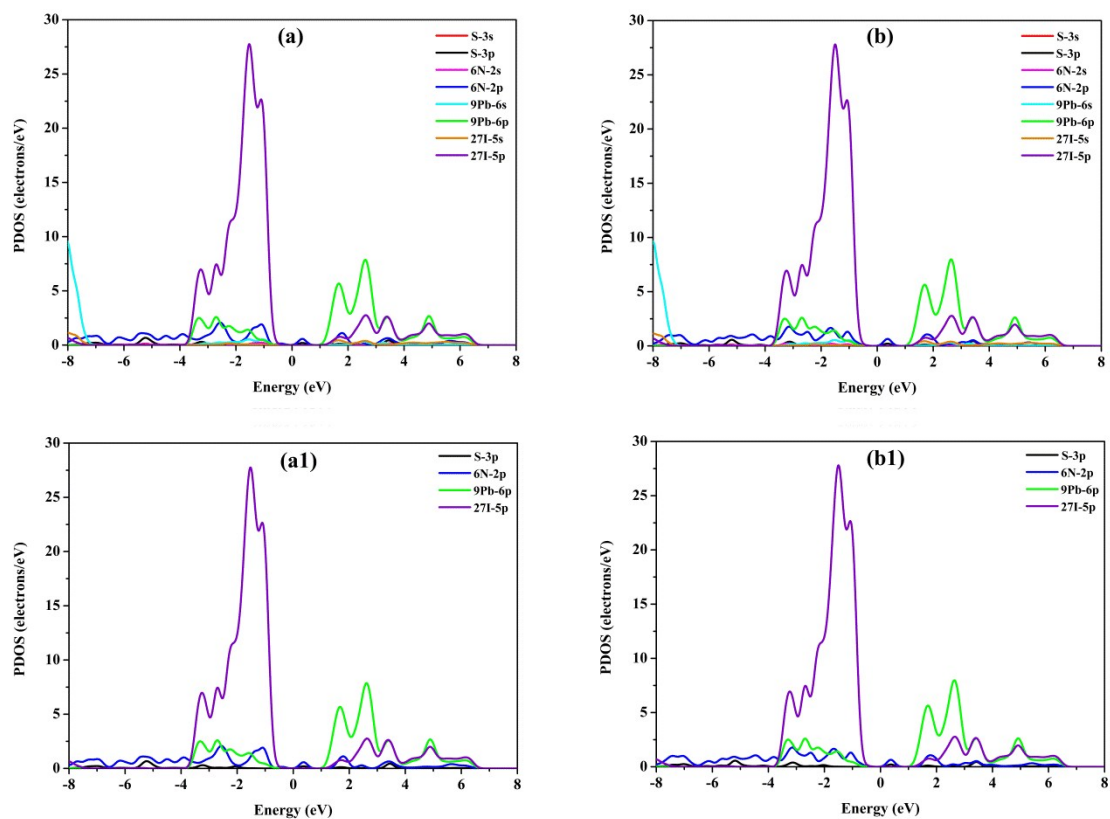


Fig. S6 The PDOS of s and p orbitals of S, N, Pb and I of **TDTP** ((a), (a1)) and **TDTP-II** ((b), (b1)) absorbed on the $\text{CH}_3\text{NH}_3\text{PbI}_3$ (110) facet. (Note: the six nitrogen atoms and one sulfur atom represent the atoms in the backbone of the investigated molecules, and the nine lead atoms and twenty-seven iodine atoms of methylammonium iodide monolayer are closest and directly opposite to the two ETMs.)

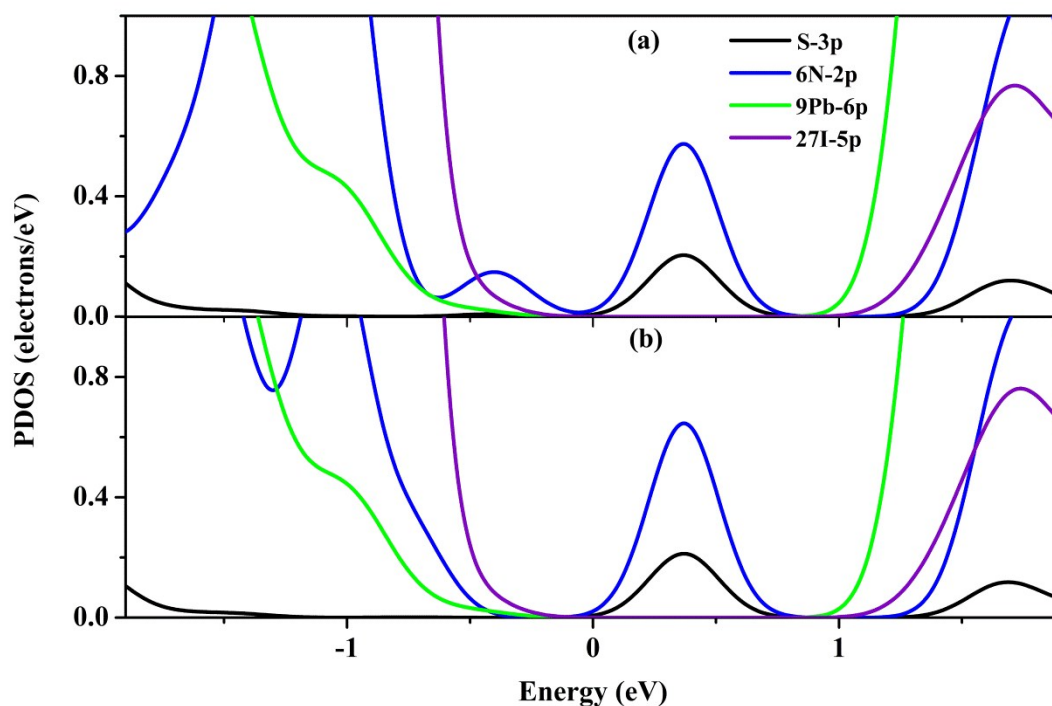


Fig. S7 The zoomed PDOS of p orbitals of S, N, Pb and I of **TDTP** (a) and **TDTP-II** (b) absorbed on the $\text{CH}_3\text{NH}_3\text{PbI}_3$ (110) facet.

The optimized geometries of the ground state in Cartesian coordinates:

TDTP

6	0.736496	4.346099	0.069366
6	1.441848	3.119269	0.101356
6	0.722089	1.849762	0.007249
6	-0.721953	1.849789	-0.007243
6	-1.441663	3.119328	-0.101317
6	-0.736262	4.346129	-0.069290
7	1.357267	5.536271	0.159568
6	2.679960	5.545923	0.288250
6	3.469778	4.387967	0.337994
6	2.838897	3.159720	0.243620
6	-2.838709	3.159840	-0.243586
6	-3.469540	4.388115	-0.337926
6	-2.679677	5.546038	-0.288145

7	-1.356985	5.536329	-0.159459
7	1.390348	0.717415	-0.051421
7	-1.390254	0.717463	0.051393
6	-0.727135	-0.469841	0.066956
6	0.727183	-0.469863	-0.067017
6	1.493426	-1.658049	-0.190014
6	0.726013	-2.863191	-0.101389
6	-0.726030	-2.863169	0.101262
6	-1.493408	-1.658012	0.189927
7	1.235934	-4.104659	-0.183632
16	-0.000056	-5.151588	-0.000114
7	-1.236000	-4.104619	0.183478
6	-5.121980	-2.510170	0.635388
6	-3.789020	-2.764620	0.239431
6	-2.931643	-1.686349	0.404423
16	-3.847733	-0.320228	1.053168
6	-5.329373	-1.239919	1.121200
6	-6.616549	-0.676770	1.663547
6	-7.431077	0.277124	0.738402
6	-6.756893	1.646329	0.515062
6	-6.484671	2.456023	1.788100
6	-7.800670	-0.369824	-0.610610
6	-8.743224	-1.577778	-0.525057
6	-9.148724	-2.122250	-1.901015
6	-10.086724	-3.330274	-1.822314
6	5.329391	-1.239851	-1.121237
16	3.847720	-0.320210	-1.053207
6	2.931663	-1.686373	-0.404507
6	3.789075	-2.764616	-0.239509
6	5.122030	-2.510116	-0.635450
6	6.616557	-0.676665	-1.663570
6	7.431151	0.277104	-0.738354
6	7.800529	-0.369918	0.610682
6	6.757174	1.646419	-0.515069

6	6.485156	2.456135	-1.788137
6	8.742792	-1.578101	0.525179
6	9.148095	-2.122667	1.901157
6	10.085804	-3.330921	1.822505
1	3.144680	6.528062	0.361753
1	4.546118	4.460460	0.455649
1	3.389744	2.227321	0.282429
1	-3.389593	2.227465	-0.282426
1	-4.545877	4.460653	-0.455583
1	-3.144357	6.528197	-0.361621
1	-5.909661	-3.254151	0.582972
1	-3.450569	-3.717327	-0.138385
1	-7.251295	-1.532579	1.916448
1	-6.423781	-0.162214	2.611653
1	-8.368559	0.469954	1.283179
1	-7.411271	2.233615	-0.142135
1	-5.821937	1.505509	-0.042037
1	-6.110555	3.455215	1.542986
1	-7.398164	2.581584	2.381075
1	-5.734369	1.983918	2.430020
1	-6.880630	-0.661193	-1.134691
1	-8.277597	0.396228	-1.237189
1	-8.273935	-2.387426	0.049173
1	-9.647993	-1.295945	0.033180
1	-9.630266	-1.321515	-2.478619
1	-8.244113	-2.396168	-2.460362
1	-10.357417	-3.692830	-2.819247
1	-9.618844	-4.161716	-1.282802
1	-11.015164	-3.078522	-1.297101
1	3.450656	-3.717335	0.138303
1	5.909737	-3.254071	-0.583035
1	6.423784	-0.162019	-2.611626
1	7.251271	-1.532470	-1.916562
1	8.368708	0.469786	-1.283057

1	8.277607	0.396024	1.237279
1	6.880395	-0.661066	1.134722
1	5.822164	1.505756	0.041978
1	7.411607	2.233610	0.142156
1	6.111174	3.455388	-1.543063
1	7.398708	2.581551	-2.381053
1	5.734826	1.984134	-2.430101
1	8.273332	-2.387638	-0.049072
1	9.647655	-1.296490	-0.033018
1	8.243392	-2.396364	2.460463
1	9.629805	-1.322048	2.478781
1	10.356361	-3.693540	2.819451
1	9.617746	-4.162250	1.282972
1	11.014330	-3.079398	1.297335

TDTP-I

6	0.739223	4.697153	0.025559
6	1.446310	3.471002	0.029098
6	0.723214	2.200212	-0.016777
6	-0.723005	2.200269	0.016737
6	-1.445995	3.471124	-0.029088
6	-0.738804	4.697215	-0.025498
7	1.362118	5.888618	0.066297
6	2.690039	5.901980	0.113873
6	3.483161	4.745520	0.129598
6	2.849554	3.516031	0.089670
6	-2.849235	3.516276	-0.089663
6	-3.482736	4.745821	-0.129540
6	-2.689516	5.902213	-0.113766
7	-1.361597	5.888735	-0.066188
7	1.388975	1.066451	-0.080361
7	-1.388856	1.066556	0.080281
6	-0.726474	-0.121749	0.069684
6	0.726500	-0.121800	-0.069804

6	1.491484	-1.311949	-0.178340
6	0.725863	-2.516338	-0.093061
6	-0.725993	-2.516289	0.092872
6	-1.491535	-1.311855	0.178191
7	1.237567	-3.757613	-0.166806
16	-0.000149	-4.804124	-0.000131
7	-1.237789	-3.757529	0.166572
7	-5.107350	-2.214480	0.547160
6	-3.792513	-2.419942	0.248365
6	-2.932531	-1.337699	0.369275
16	-3.897087	0.037287	0.897312
6	-5.325941	-0.976483	0.919257
6	-6.675225	-0.447350	1.315021
6	-7.637150	-0.088639	0.142392
6	-7.138543	1.098671	-0.705871
6	-6.998821	2.426495	0.047552
6	-7.974854	-1.292030	-0.760083
6	-8.615055	-2.492375	-0.051174
6	-9.097098	-3.572909	-1.028247
6	-9.727377	-4.780598	-0.328474
6	5.325912	-0.976644	-0.919314
16	3.897066	0.037138	-0.897411
6	2.932481	-1.337841	-0.369410
6	3.792449	-2.420094	-0.248479
7	5.107297	-2.214641	-0.547230
6	6.675215	-0.447514	-1.315014
6	7.637080	-0.088809	-0.142335
6	7.974632	-1.292178	0.760225
6	7.138487	1.098575	0.705833
6	6.998892	2.426368	-0.047670
6	8.614771	-2.492618	0.051421
6	9.096652	-3.573144	1.028581
6	9.726876	-4.780922	0.328915
1	3.156208	6.885547	0.146147

1	4.564721	4.818986	0.175700
1	3.407198	2.587769	0.109444
1	-3.406958	2.588064	-0.109478
1	-4.564290	4.819381	-0.175642
1	-3.155601	6.885821	-0.146001
1	-3.471473	-3.404382	-0.056045
1	-7.148707	-1.216005	1.933251
1	-6.548166	0.432142	1.953826
1	-8.571274	0.229610	0.630937
1	-6.180674	0.837683	-1.174266
1	-7.846693	1.238838	-1.532178
1	-6.740266	3.236634	-0.642800
1	-7.936697	2.703568	0.542780
1	-6.218842	2.390943	0.815622
1	-8.660849	-0.935446	-1.541195
1	-7.067129	-1.626584	-1.277406
1	-7.890456	-2.940796	0.638452
1	-9.466201	-2.151740	0.557496
1	-9.822212	-3.134477	-1.727842
1	-8.248385	-3.906903	-1.639886
1	-10.060843	-5.533676	-1.050025
1	-9.012815	-5.261880	0.348643
1	-10.597791	-4.483813	0.268090
1	3.471395	-3.404528	0.055934
1	6.548193	0.431979	-1.953825
1	7.148724	-1.216172	-1.933219
1	8.571260	0.229355	-0.630828
1	7.066847	-1.626629	1.277511
1	8.660609	-0.935610	1.541359
1	7.846590	1.238744	1.532180
1	6.180571	0.837668	1.174178
1	6.740324	3.236556	0.642621
1	7.936820	2.703366	-0.542840
1	6.218970	2.390815	-0.815798

1	7.890178	-2.941010	-0.638231
1	9.465988	-2.152092	-0.557211
1	8.247868	-3.907032	1.640179
1	9.821756	-3.134738	1.728204
1	10.060227	-5.533993	1.050528
1	9.012319	-5.262178	-0.348227
1	10.597356	-4.484243	-0.267605

TDTP-II

6	0.738901	-4.120413	-0.047517
6	1.443460	-2.894031	-0.083432
6	0.723702	-1.620688	-0.027164
6	-0.723717	-1.620689	0.027170
6	-1.443474	-2.894033	0.083437
6	-0.738913	-4.120414	0.047521
7	1.365224	-5.310313	-0.094613
6	2.691881	-5.318071	-0.177411
6	3.481814	-4.159391	-0.217868
6	2.844952	-2.931591	-0.170428
6	-2.844966	-2.931595	0.170433
6	-3.481825	-4.159395	0.217871
6	-2.691891	-5.318074	0.177415
7	-1.365235	-5.310315	0.094616
7	1.400973	-0.496006	-0.022672
7	-1.400989	-0.496008	0.022678
6	-0.731034	0.693983	-0.014204
6	0.731016	0.693984	0.014209
6	1.485887	1.885913	0.049397
6	0.730633	3.088344	0.024458
6	-0.730655	3.088343	-0.024454
6	-1.485906	1.885911	-0.049393
7	1.256548	4.330685	0.051274
16	-0.000012	5.369199	0.000000
7	-1.256570	4.330684	-0.051269

6	-2.964597	1.902430	-0.105105
6	2.964578	1.902434	0.105108
6	-3.709900	2.742612	0.738772
6	-5.101242	2.754685	0.689357
6	-5.810770	1.943017	-0.207532
6	-5.060665	1.126323	-1.067837
6	-3.670486	1.097273	-1.015792
6	-7.325001	1.954814	-0.255388
6	-8.047107	0.921797	0.664568
6	-7.795512	1.173666	2.166026
6	-8.369210	2.487721	2.708560
6	-7.728707	-0.542907	0.299305
6	-8.245020	-1.005144	-1.070102
6	-7.955806	-2.484488	-1.356920
6	-8.482922	-2.952690	-2.716528
6	3.709879	2.742615	-0.738773
6	5.101221	2.754691	-0.689359
6	5.810751	1.943026	0.207530
6	5.060649	1.126333	1.067839
6	3.670470	1.097280	1.015795
6	7.324982	1.954828	0.255383
6	8.047090	0.921819	-0.664581
6	7.795447	1.173667	-2.166034
6	8.369085	2.487739	-2.708592
6	7.728738	-0.542890	-0.299295
6	8.245116	-1.005106	1.070095
6	7.955947	-2.484454	1.356935
6	8.483132	-2.952635	2.716524
1	3.161015	-6.300141	-0.214865
1	4.562503	-4.232130	-0.286398
1	3.392209	-1.995686	-0.198436
1	-3.392224	-1.995690	0.198441
1	-4.562514	-4.232136	0.286401
1	-3.161024	-6.300145	0.214868

1	-3.195203	3.387516	1.441551
1	-5.645321	3.417189	1.356900
1	-5.573051	0.511280	-1.802607
1	-3.122255	0.459644	-1.699264
1	-7.682601	2.956359	0.007102
1	-7.649782	1.782928	-1.287352
1	-9.123728	1.073055	0.488089
1	-8.244167	0.344493	2.728192
1	-6.718211	1.126654	2.369773
1	-8.212727	2.563575	3.789530
1	-7.905925	3.368296	2.252401
1	-9.447979	2.553318	2.525279
1	-6.644483	-0.707241	0.358842
1	-8.173456	-1.189530	1.067963
1	-9.329690	-0.832944	-1.125144
1	-7.804726	-0.398060	-1.872209
1	-6.871516	-2.656340	-1.305964
1	-8.397616	-3.099740	-0.561231
1	-8.260799	-4.010561	-2.890255
1	-9.569286	-2.825746	-2.784903
1	-8.032681	-2.380197	-3.535445
1	3.195179	3.387517	-1.441552
1	5.645298	3.417195	-1.356904
1	5.573036	0.511292	1.802609
1	3.122241	0.459651	1.699269
1	7.649768	1.782941	1.287346
1	7.682577	2.956375	-0.007105
1	9.123712	1.073106	-0.488131
1	6.718142	1.126617	-2.369752
1	8.244117	0.344506	-2.728205
1	8.212571	2.563580	-3.789559
1	7.905781	3.368301	-2.252427
1	9.447857	2.553375	-2.525340
1	8.173472	-1.189508	-1.067966

1	6.644516	-0.707250	-0.358788
1	9.329785	-0.832881	1.125091
1	7.804842	-0.398026	1.872215
1	8.397738	-3.099702	0.561231
1	6.871660	-2.656331	1.306026
1	8.261040	-4.010510	2.890267
1	9.569495	-2.825665	2.784852
1	8.032912	-2.380146	3.535456

dimer-TDTP

6	-0.700970	4.129740	-2.673668
6	-1.748444	3.196807	-2.577153
6	-1.465876	1.758188	-2.542347
6	-0.091403	1.309438	-2.577635
6	0.987856	2.284794	-2.756601
6	0.701102	3.662349	-2.804631
7	-0.909501	5.452923	-2.639774
6	-2.157953	5.882525	-2.527610
6	-3.271470	5.038666	-2.441854
6	-3.058401	3.674632	-2.458775
6	2.319968	1.876166	-2.879919
6	3.303622	2.836289	-3.033003
6	2.915478	4.178568	-3.055992
7	1.655804	4.588512	-2.952072
7	-2.448285	0.906973	-2.463750
7	0.202073	0.046474	-2.470143
6	-0.795096	-0.875053	-2.335446
6	-2.183761	-0.430762	-2.367754
6	-3.271893	-1.322740	-2.273257
6	-2.898814	-2.695133	-2.178174
6	-1.516675	-3.137388	-2.183455
6	-0.421260	-2.229403	-2.218480
7	-3.759693	-3.718348	-2.098718
16	-2.892193	-5.077675	-2.054477

7	-1.403135	-4.468212	-2.122269
6	3.282940	-2.753403	-1.855937
6	2.095764	-1.985050	-1.798428
6	0.956899	-2.692846	-2.140463
16	1.393081	-4.346418	-2.503675
6	3.069184	-4.050518	-2.251322
6	4.060249	-5.164238	-2.441631
6	4.552922	-5.807751	-1.126319
6	5.371928	-4.829130	-0.279555
6	6.597871	-4.240165	-0.974291
6	3.374429	-6.388584	-0.334211
6	3.763600	-7.293812	0.832487
6	2.544199	-7.790306	1.605804
6	2.930467	-8.607830	2.834901
6	-7.168507	-0.783353	-1.921595
16	-5.934876	-1.962379	-1.653153
6	-4.675378	-0.913845	-2.273781
6	-5.238408	0.276409	-2.690778
6	-6.640201	0.343998	-2.493885
6	-8.613516	-1.071550	-1.612432
6	-9.042934	-0.811144	-0.147827
6	-8.851521	0.671306	0.203482
6	-8.312864	-1.791612	0.782103
6	-8.764666	-1.840074	2.241762
6	-9.717917	1.213227	1.340800
6	-9.431311	2.684700	1.633811
6	-10.262952	3.226282	2.792093
1	-2.289313	6.962364	-2.499365
1	-4.268096	5.454639	-2.344792
1	-3.868117	2.962306	-2.339718
1	2.550498	0.815379	-2.857812
1	4.350966	2.565636	-3.112976
1	3.664564	4.960528	-3.158092
1	4.265237	-2.354977	-1.624440

1	2.067447	-0.941016	-1.521483
1	3.605623	-5.946617	-3.059595
1	4.913153	-4.779487	-3.010615
1	5.215489	-6.636271	-1.422281
1	5.703461	-5.346991	0.626281
1	4.709792	-4.021233	0.058095
1	6.330253	-3.595078	-1.816950
1	7.184163	-3.635628	-0.276057
1	7.250043	-5.030806	-1.360713
1	2.728647	-6.957175	-1.019633
1	2.754834	-5.568287	0.054312
1	4.353588	-8.146746	0.465849
1	4.409970	-6.746951	1.530193
1	1.952829	-6.917859	1.906198
1	1.914379	-8.394453	0.939147
1	2.049697	-8.968313	3.373304
1	3.537215	-9.478251	2.562583
1	3.517096	-7.998088	3.530626
1	-4.652555	1.061482	-3.142130
1	-7.248806	1.193016	-2.785877
1	-8.839753	-2.113022	-1.869168
1	-9.221334	-0.444139	-2.273703
1	-10.119473	-1.037191	-0.102519
1	-7.792428	0.850216	0.426560
1	-9.066487	1.273819	-0.691299
1	-8.422407	-2.796825	0.353014
1	-7.240128	-1.567492	0.747183
1	-8.414138	-0.975686	2.812776
1	-9.856017	-1.878975	2.324086
1	-8.360608	-2.730875	2.731108
1	-10.778713	1.091282	1.080370
1	-9.564678	0.637636	2.259764
1	-9.614618	3.279154	0.729532
1	-8.363052	2.798026	1.865412

1	-10.043245	4.278621	2.991513
1	-11.333582	3.139595	2.581116
1	-10.059696	2.662797	3.709401
6	1.110723	-3.508235	1.562212
6	0.362847	-2.368951	1.211816
6	1.011703	-1.061417	1.107197
6	2.445332	-0.971392	1.268043
6	3.183583	-2.128460	1.779376
6	2.537394	-3.366836	1.944180
7	0.573217	-4.733648	1.604693
6	-0.717995	-4.860811	1.329886
6	-1.557967	-3.785328	1.019804
6	-1.002491	-2.522185	0.946468
6	4.522469	-2.010565	2.170766
6	5.147672	-3.105936	2.734692
6	4.411402	-4.288370	2.872424
7	3.152751	-4.430898	2.479428
7	0.305477	0.009504	0.874079
7	3.081325	0.134277	1.005789
6	2.376654	1.252051	0.660270
6	0.925176	1.215888	0.721266
6	0.117826	2.368049	0.624367
6	0.850010	3.576606	0.410040
6	2.291726	3.588147	0.228681
6	3.089467	2.416005	0.313414
7	0.323045	4.805834	0.304655
16	1.523747	5.830302	0.000976
7	2.773732	4.819053	0.002994
6	6.641157	1.681107	-0.624391
6	5.292364	1.340185	-0.362097
6	4.515849	2.414179	0.026744
16	5.486933	3.867867	0.032308
6	6.912120	3.011636	-0.436376
6	8.232256	3.708940	-0.605405

6	9.108117	3.759040	0.668874
6	8.467663	4.569604	1.801963
6	8.093991	5.999633	1.414921
6	9.490131	2.344295	1.119054
6	10.530491	2.284646	2.236833
6	11.007532	0.860095	2.515135
6	12.032491	0.792019	3.643413
6	-3.784248	1.768299	0.801468
16	-2.295964	0.895430	0.848286
6	-1.337182	2.358267	0.723594
6	-2.181078	3.453057	0.696976
6	-3.555271	3.117093	0.739039
6	-5.108504	1.064112	0.817596
6	-5.622013	0.661947	2.216145
6	-5.862911	1.897173	3.093830
6	-4.723925	-0.366643	2.915737
6	-4.503345	-1.657684	2.127043
6	-6.876308	1.668196	4.213559
6	-7.194066	2.937191	5.001993
6	-8.141104	2.681507	6.170587
1	-1.112980	-5.874275	1.360265
1	-2.614425	-3.944885	0.821752
1	-1.592304	-1.651626	0.674500
1	5.023013	-1.055567	2.042734
1	6.177474	-3.059731	3.070973
1	4.871070	-5.167919	3.320603
1	7.392694	0.971046	-0.952321
1	4.889460	0.342842	-0.467752
1	8.791397	3.175772	-1.382964
1	8.072810	4.725230	-0.980228
1	10.033136	4.278333	0.373458
1	9.172876	4.608898	2.639015
1	7.580900	4.037386	2.170576
1	8.948686	6.518627	0.967155

1	7.270405	6.031642	0.695617
1	7.777905	6.570108	2.291664
1	9.880062	1.794207	0.249864
1	8.584246	1.810093	1.436105
1	11.394263	2.910667	1.971175
1	10.118050	2.704531	3.162495
1	10.140693	0.234461	2.762820
1	11.437510	0.438770	1.597761
1	12.364900	-0.233343	3.824949
1	12.915161	1.393293	3.403959
1	11.612237	1.178760	4.577019
1	-1.816873	4.465780	0.609687
1	-4.354583	3.849446	0.693965
1	-5.072798	0.183953	0.165115
1	-5.839060	1.744398	0.362774
1	-6.598074	0.182420	2.045745
1	-4.908415	2.241641	3.515087
1	-6.222795	2.722453	2.462203
1	-3.756366	0.098075	3.141259
1	-5.174205	-0.619094	3.883206
1	-4.026250	-1.475575	1.155695
1	-3.860372	-2.345331	2.684210
1	-5.452958	-2.167162	1.929247
1	-7.809481	1.277305	3.777989
1	-6.512409	0.895325	4.903271
1	-7.633571	3.678334	4.320661
1	-6.259593	3.376320	5.373198
1	-9.079956	2.236145	5.825178
1	-7.694035	1.987059	6.888854
1	-8.384613	3.604665	6.702586
dimer-TDTP-I			
6	3.994449	-1.677025	-4.605539
6	4.603608	-1.453581	-3.356614

6	3.878590	-1.726743	-2.112753
6	2.522052	-2.235257	-2.181621
6	1.904551	-2.475503	-3.487766
6	2.611330	-2.210509	-4.673448
7	4.618111	-1.425304	-5.763613
6	5.851986	-0.944159	-5.716222
6	6.547956	-0.690527	-4.528235
6	5.912693	-0.956155	-3.331435
6	0.600057	-2.976016	-3.580693
6	0.061545	-3.195208	-4.832775
6	0.848750	-2.898820	-5.952495
7	2.083075	-2.420422	-5.886296
7	4.456072	-1.505820	-0.964728
7	1.842951	-2.488601	-1.100113
6	2.415411	-2.258184	0.117599
6	3.770853	-1.747695	0.192601
6	4.409109	-1.470195	1.413321
6	3.613479	-1.689619	2.573827
6	2.268307	-2.230935	2.495902
6	1.658351	-2.551121	1.257110
7	3.980403	-1.411488	3.830193
16	2.731831	-1.778703	4.782495
7	1.676464	-2.331668	3.693817
7	-1.452070	-4.521678	1.829519
6	-0.163115	-4.120450	2.043433
6	0.327019	-3.146672	1.212797
16	-0.924942	-2.705049	0.092773
6	-1.996905	-3.851598	0.854459
6	-3.406322	-4.061668	0.385918
6	-3.547839	-5.007216	-0.828867
6	-2.915903	-4.454969	-2.114296
6	-3.365075	-3.042133	-2.485517
6	-3.013921	-6.401855	-0.481602
6	-3.274040	-7.466893	-1.546149

6	-2.896955	-8.870146	-1.074490
6	-3.124983	-9.930905	-2.147714
6	8.150279	-0.372040	1.292207
16	7.000117	-1.202878	0.294638
6	5.774525	-0.966718	1.513653
6	6.355408	-0.289809	2.563948
7	7.669121	0.057314	2.426064
6	9.556344	-0.103807	0.847208
6	9.690310	0.998422	-0.230190
6	8.998297	2.284135	0.240623
6	9.206987	0.573520	-1.626921
6	9.716469	-0.789772	-2.092776
6	9.259764	3.513753	-0.626334
6	8.557125	4.757227	-0.084818
6	8.849968	6.014271	-0.897736
1	6.322281	-0.747401	-6.677442
1	7.556210	-0.291785	-4.554817
1	6.392028	-0.783793	-2.372724
1	0.048264	-3.179851	-2.667698
1	-0.940998	-3.590865	-4.954232
1	0.454183	-3.058913	-6.953691
1	0.412157	-4.571378	2.843012
1	-3.947587	-4.492416	1.235645
1	-3.869453	-3.093187	0.162891
1	-4.630643	-5.091771	-1.007179
1	-1.821623	-4.492711	-2.021648
1	-3.172819	-5.130659	-2.937384
1	-2.985561	-2.752298	-3.469338
1	-4.457988	-2.975996	-2.516607
1	-3.010812	-2.290688	-1.772841
1	-1.934647	-6.336607	-0.287340
1	-3.467260	-6.723380	0.465392
1	-4.336034	-7.453157	-1.831349
1	-2.707208	-7.239456	-2.457927

1	-1.843838	-8.873523	-0.766780
1	-3.478429	-9.117423	-0.177942
1	-2.851782	-10.928155	-1.793545
1	-4.176433	-9.958816	-2.451030
1	-2.529040	-9.716833	-3.040632
1	5.837066	-0.033303	3.476683
1	10.025970	-1.029583	0.499739
1	10.090602	0.217145	1.745900
1	10.769956	1.195917	-0.310153
1	9.308177	2.498500	1.272521
1	7.913524	2.107161	0.288618
1	9.536370	1.334980	-2.342153
1	8.109119	0.593354	-1.655167
1	9.485036	-0.957722	-3.148053
1	10.803204	-0.864584	-1.976522
1	9.265370	-1.614142	-1.531162
1	10.341522	3.698779	-0.690329
1	8.913442	3.337050	-1.652834
1	8.853105	4.914946	0.961119
1	7.474940	4.568037	-0.069994
1	9.923178	6.228846	-0.911510
1	8.521480	5.895551	-1.935086
1	8.340343	6.888025	-0.481315
6	-4.051101	-2.492037	3.273044
6	-3.023343	-1.565111	3.022385
6	-3.239832	-0.451706	2.098047
6	-4.539538	-0.266870	1.484049
6	-5.603472	-1.237551	1.755116
6	-5.367670	-2.334100	2.605764
7	-3.895028	-3.533441	4.097680
6	-2.721090	-3.677765	4.697742
6	-1.638860	-2.807846	4.523179
6	-1.791752	-1.736962	3.665988
6	-6.868260	-1.104510	1.168939

6	-7.827439	-2.063121	1.428775
6	-7.484478	-3.129322	2.268363
7	-6.298969	-3.266765	2.845615
7	-2.258117	0.366135	1.847916
7	-4.773045	0.752952	0.705776
6	-3.778079	1.654681	0.454092
6	-2.458151	1.426626	1.015293
6	-1.368841	2.273668	0.750064
6	-1.677278	3.426397	-0.017868
6	-3.005625	3.678255	-0.548068
6	-4.085144	2.771795	-0.342808
7	-0.798667	4.383966	-0.342779
16	-1.592920	5.475786	-1.222468
7	-3.063699	4.817586	-1.252495
7	-7.158759	4.167325	-1.942650
6	-5.910336	4.205315	-1.389789
6	-5.394832	3.011687	-0.935038
16	-6.578697	1.770157	-1.240443
6	-7.631948	2.951615	-1.948203
6	-8.996584	2.588268	-2.452425
6	-10.099479	2.610463	-1.366717
6	-9.906050	1.480911	-0.344206
6	-11.127110	1.231071	0.539225
6	-10.217237	3.979565	-0.687233
6	-10.423805	5.153603	-1.643501
6	-10.757628	6.450415	-0.908438
6	-10.903868	7.638990	-1.854087
6	2.327310	1.939887	1.930566
16	1.206811	3.188693	1.492346
6	-0.016671	1.978441	1.201439
6	0.538607	0.744280	1.446809
7	1.843042	0.729664	1.843462
6	3.760470	2.195515	2.283711
6	4.653398	2.613524	1.084746

6	4.721551	4.136313	0.920419
6	4.215646	1.925833	-0.216412
6	5.322657	1.851282	-1.262372
6	5.553767	4.845674	1.987251
6	5.735548	6.334976	1.702451
6	6.646154	7.020209	2.716752
1	-2.628376	-4.539205	5.355486
1	-0.691776	-2.988731	5.018617
1	-0.983032	-1.037839	3.474746
1	-7.066284	-0.252897	0.526275
1	-8.819539	-2.000124	0.995449
1	-8.211772	-3.909315	2.484642
1	-5.385861	5.148093	-1.333665
1	-9.241040	3.301955	-3.243829
1	-8.967817	1.591412	-2.906390
1	-11.041550	2.415389	-1.901543
1	-9.659357	0.554248	-0.882019
1	-9.039725	1.711115	0.288550
1	-10.962265	0.376395	1.200899
1	-11.352376	2.093504	1.171330
1	-12.013240	1.019849	-0.067999
1	-11.056701	3.948451	0.018548
1	-9.313355	4.161298	-0.088753
1	-9.513482	5.306547	-2.234987
1	-11.233604	4.917976	-2.349970
1	-11.683529	6.316364	-0.334576
1	-9.967727	6.656590	-0.175261
1	-11.151683	8.556327	-1.313642
1	-9.974336	7.813098	-2.404622
1	-11.695012	7.458526	-2.588968
1	0.008496	-0.191698	1.329589
1	4.117260	1.244503	2.688493
1	3.830913	2.941014	3.083172
1	5.667631	2.257493	1.327605

1	3.702179	4.550978	0.898777
1	5.151829	4.368227	-0.063280
1	3.347467	2.459899	-0.625741
1	3.870697	0.910819	0.009156
1	4.947557	1.445194	-2.206432
1	5.763925	2.832380	-1.472709
1	6.122926	1.192105	-0.910359
1	5.098130	4.722958	2.978887
1	6.541465	4.366524	2.045991
1	4.753665	6.824662	1.688938
1	6.151961	6.457265	0.693470
1	7.645319	6.571954	2.704401
1	6.754702	8.087280	2.505954
1	6.249803	6.916428	3.731757

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6	2.828196	-0.873303	3.753262
6	2.084995	-1.850737	3.071377
6	2.477205	-2.283239	1.727886
6	3.660925	-1.714203	1.113239
6	4.453363	-0.730085	1.856018
6	4.054691	-0.308535	3.136473
7	2.471159	-0.415845	4.961958
6	1.380132	-0.918081	5.522236
6	0.586124	-1.912481	4.937592
6	0.950783	-2.386327	3.693200
6	5.612702	-0.180796	1.297322
6	6.327416	0.746820	2.029819
6	5.850266	1.094690	3.297837
7	4.747672	0.595480	3.840907
7	1.748613	-3.160088	1.102744
7	4.029511	-2.053279	-0.086808
6	3.271653	-2.950642	-0.791525
6	2.100330	-3.543014	-0.165989

6	1.285312	-4.467821	-0.828980
6	1.674855	-4.795827	-2.150626
6	2.850989	-4.214124	-2.771534
6	3.664393	-3.267146	-2.097927
7	1.030777	-5.655778	-2.956833
16	1.851578	-5.690976	-4.344093
7	3.042898	-4.653396	-4.026668
6	4.844036	-2.660193	-2.748255
6	0.058061	-5.018883	-0.217824
6	5.755704	-3.454191	-3.452131
6	6.888170	-2.889819	-4.028283
6	7.143324	-1.519605	-3.933946
6	6.203858	-0.725044	-3.267665
6	5.077522	-1.280445	-2.677962
6	8.410465	-0.915056	-4.486846
6	9.600715	-0.950053	-3.492687
6	10.107800	-2.375920	-3.237170
6	10.640877	-3.095770	-4.474164
6	9.265112	-0.272988	-2.158430
6	8.985273	1.228527	-2.232008
6	8.366749	1.759537	-0.940287
6	8.147952	3.269177	-0.949684
6	-1.158869	-4.962258	-0.906997
6	-2.343101	-5.347186	-0.285787
6	-2.348032	-5.827837	1.026756
6	-1.119272	-5.926315	1.691846
6	0.063430	-5.522955	1.087734
6	-3.630794	-6.230555	1.714510
6	-4.337146	-5.095024	2.497430
6	-4.934078	-4.049241	1.544357
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6	-1.969881	-4.776310	5.613389

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1	1.117395	-0.513990	6.497784
1	-0.289588	-2.291881	5.452628
1	0.387174	-3.163744	3.183018
1	5.920744	-0.502618	0.306081
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1	5.580385	-4.521054	-3.537365
1	7.589323	-3.527255	-4.561277
1	6.359447	0.349610	-3.208886
1	4.366691	-0.644285	-2.162608
1	8.700593	-1.438405	-5.403814
1	8.216647	0.122844	-4.775981
1	10.418767	-0.387318	-3.968704
1	10.910090	-2.318250	-2.491624
1	9.305659	-2.965260	-2.774117
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1	11.093796	-4.052969	-4.203121
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1	9.097884	3.801969	-1.055297
1	7.507400	3.563690	-1.786910
1	-1.181315	-4.579327	-1.921917
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7	-1.461363	3.682831	-0.151053
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6	-9.582303	-1.113983	-1.116979
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6	1.260295	2.947933	0.424548
6	3.863873	3.886857	3.044547
6	3.450963	5.214076	3.730281
6	2.466034	4.941503	4.876289
6	2.252090	6.127652	5.815280
6	2.895241	6.249543	2.745560
6	3.888379	6.734326	1.689906
6	3.240809	7.644896	0.648863
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1	-6.396064	0.184608	-4.176093
1	-6.911460	-2.378357	-0.780862
1	-4.875699	-1.443444	0.231814
1	-8.069982	-1.587340	-4.222263
1	-8.231033	-2.719259	-2.887509
1	-10.237282	-1.382918	-3.140014
1	-10.219855	1.068338	-2.513945
1	-8.468130	1.035372	-2.577880
1	-8.574768	0.450103	-5.033336
1	-10.335473	0.380567	-4.936713
1	-9.494009	1.917476	-4.704707
1	-9.314597	-2.146923	-0.859537
1	-8.879634	-0.470557	-0.567663
1	-11.353935	0.127321	-0.996952
1	-11.680032	-1.596044	-1.076792
1	-10.545373	-0.074931	1.324133
1	-12.191281	-0.661017	1.153781
1	-11.280103	-3.044841	1.043176
1	-9.671771	-2.402784	1.399333
1	-10.967223	-2.234551	2.584249
1	0.276968	0.889348	2.937988
1	2.245000	1.920800	4.013576
1	2.982703	4.218931	0.469589
1	0.994244	3.229203	-0.588310
1	4.674459	4.074885	2.330753
1	4.265132	3.222760	3.817512
1	4.369674	5.629127	4.173986

1	2.839060	4.090349	5.460074
1	1.504015	4.622383	4.455437
1	1.630163	5.840967	6.667273
1	3.206850	6.493340	6.207661
1	1.754331	6.963537	5.316976
1	2.543530	7.125236	3.304531
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1	4.712139	7.268523	2.183361
1	4.350710	5.884777	1.170876
1	2.749765	8.484560	1.158844
1	2.445363	7.086024	0.136082
1	3.751546	8.811630	-1.121698
1	5.020661	8.765817	0.109516
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