Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Hopping transport in perylene diimide based organic solar cells : A DFT approach

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Table S1 : Coordinates of the designed compounds studied at B3LYP-D3 level of theory in the angstrom unit.

1. **Compound PDI-DTT-1**

Atoms	Coordinates (Angstroms) X	Y	Z
C	7.396273	-0.929826	-0.656145
C	6.104679	-1.313679	-0.221545
C	5.858864	-2.661580	0.133505
C	6.937065	-3.675349	0.054898
C	8.500565	-1.916902	-0.750353
N	8.192051	-3.236940	-0.385972
C	4.599838	-3.040648	0.564798
C	3.566087	-2.101290	0.642779
C	3.757848	-0.763578	0.291856
C	5.055737	-0.347020	-0.140103
C	5.330670	1.013069	-0.488493
C	7.638038	0.388705	-1.000203
C	6.618545	1.343213	-0.915084
C	2.676050	0.230020	0.353662
C	2.954561	1.595594	0.038783
C	4.257094	2.012386	-0.379483
C	1.899218	2.555177	0.148894
C	2.167679	3.914293	-0.156651
C	4.464015	3.361109	-0.671885
C	3.434237	4.298006	-0.563639
C	0.313508	0.810068	0.772194
C	0.589829	2.166150	0.550067
C	1.372471	-0.119407	0.680527
C	-0.423050	3.219651	0.831141
C	1.118920	4.955660	-0.053817

N	-0.120147	4.530342	0.432598
H	4.433315	-4.076964	0.839147
H	2.598570	-2.441183	0.992485
H	1.111894	-1.156967	0.846958
H	3.606211	5.343390	-0.796322
H	5.438393	3.711978	-0.989525
H	6.858025	2.362406	-1.193427
H	8.632338	0.665885	-1.333816
O	9.622686	-1.603735	-1.125106
O	6.764958	-4.849478	0.355271
O	-1.485418	3.002157	1.396087
O	1.324387	6.124292	-0.356577
C	-1.014564	0.236430	1.052075
C	-1.335270	-0.621402	2.079874
C	-2.672366	-1.090184	2.032816
C	-3.374478	-0.626544	0.938642
S	-2.364719	0.417581	-0.041242
H	-0.635157	-0.866624	2.871458
H	-3.122605	-1.722215	2.789771
C	-4.737529	-0.951568	0.573995
C	-5.409979	-2.121601	0.859301
C	-6.744426	-2.100497	0.383638
C	-7.092322	-0.922166	-0.277177
C	-8.427079	-0.942339	-0.760274
C	-9.085751	-2.134664	-0.462600
C	-10.429216	-2.181730	-0.932379
C	-10.771117	-1.026274	-1.579478
S	-8.065492	-3.263254	0.421794
S	-9.469565	0.145659	-1.632369
S	-5.766180	0.202328	-0.295947
H	-4.941297	-2.958740	1.362461
H	-11.720355	-0.782642	-2.037868
H	-11.103387	-3.019832	-0.800882
C	-1.173296	5.528201	0.654274
H	-2.101455	5.180435	0.196884
H	-1.346140	5.656552	1.726084
H	-0.846097	6.464334	0.207864
C	9.243635	-4.257709	-0.458201
H	10.151311	-3.780096	-0.819588
H	9.403599	-4.690224	0.532355
H	8.931997	-5.056867	-1.134813

2. **Compound PDI-DTT-2**

C	6.140650	-3.295812	-0.022969
C	6.726941	-2.015822	0.125851
C	8.122419	-1.906871	0.336124
C	8.976015	-3.116331	0.406320
C	6.963580	-4.529924	0.037339
N	8.339434	-4.354441	0.251943
C	8.699813	-0.657637	0.478367
C	7.914143	0.498064	0.408326
C	6.534733	0.442060	0.198495
C	5.916329	-0.841027	0.062870
C	4.507267	-0.978011	-0.137620
C	4.777002	-3.404341	-0.234064
C	3.974871	-2.259463	-0.290722
C	5.703400	1.651632	0.105735
C	4.291263	1.516479	-0.078277
C	3.673470	0.231972	-0.177358
C	3.469411	2.684103	-0.166220
C	2.059857	2.579315	-0.330830
C	2.289046	0.171034	-0.277515
C	1.462084	1.312627	-0.339128
C	5.441842	4.074486	0.104029
C	4.073686	3.964250	-0.076564
C	6.244445	2.934918	0.192693
C	3.275068	5.208793	-0.170709
C	1.266207	3.810043	-0.597412
N	1.909946	5.043817	-0.422009
H	9.770449	-0.594214	0.641795
H	8.411640	1.453495	0.523457
H	7.309980	3.074503	0.329135
H	5.874525	5.066580	0.175535
H	2.913708	-2.393799	-0.463754
H	4.345070	-4.392222	-0.353403
O	6.474301	-5.644026	-0.092276
O	10.185114	-3.063629	0.589439
O	3.777904	6.319154	-0.054725
O	0.101626	3.794269	-0.969272
C	0.009505	1.056747	-0.351805
C	-0.666380	0.263089	-1.248441

C	-2.037431	0.135220	-0.903477
C	-2.390300	0.798161	0.261925
C	-3.764044	0.664808	0.637299
C	-4.468748	-0.116440	-0.282433
S	-1.027656	1.617845	0.961602
S	-3.412092	-0.692395	-1.585934
H	-0.196475	-0.174427	-2.121434
C	-5.861571	-0.490538	-0.306633
C	-6.533726	-1.097905	-1.355507
C	-7.884632	-1.368661	-1.048117
C	-8.261262	-0.968840	0.234428
S	-6.935975	-0.241269	1.090425
H	1.782692	-0.786003	-0.275841
C	-9.627419	-1.238296	0.506603
C	-10.278881	-1.844954	-0.567347
S	-9.214722	-2.091898	-1.947332
C	-11.650562	-2.133084	-0.318497
S	-10.713389	-1.014473	1.849266
H	-6.067338	-1.324845	-2.307177
H	-12.997413	-1.833218	1.397032
H	-12.324491	-2.601172	-1.026217
C	-12.021726	-1.741240	0.938584
C	1.078347	6.236347	-0.623653
H	0.757560	6.294872	-1.667079
H	0.188488	6.166017	0.004754
H	1.673513	7.107499	-0.359959
C	9.203649	-5.538203	0.323090
H	9.706908	-5.566439	1.292397
H	8.579626	-6.418574	0.188404
H	9.965997	-5.482648	-0.457575
C	-4.297519	1.279877	1.796472
C	-4.689166	1.826890	2.803118
H	-5.060360	2.302744	3.682399

3. **Compound PDI-DTT-3**

C	-6.328171	-1.993233	-0.069953
C	-6.176083	-0.617133	-0.366217
C	-7.279090	0.116782	-0.864543
C	-8.588782	-0.539128	-1.085909
C	-7.625495	-2.684263	-0.274883

N	-8.677676	-1.902838	-0.777234
C	-7.135459	1.463297	-1.148883
C	-5.910256	2.105595	-0.938501
C	-4.795032	1.425779	-0.444740
C	-4.917916	0.028335	-0.161447
C	-3.814449	-0.738370	0.327078
C	-5.253361	-2.709947	0.427489
C	-4.016154	-2.087527	0.623811
C	-3.509132	2.096454	-0.199057
C	-2.399099	1.327165	0.267750
C	-2.512570	-0.079164	0.503225
C	-1.140000	1.963954	0.503894
C	-0.013748	1.220968	0.952065
C	-1.369619	-0.785772	0.849034
C	-0.113634	-0.174265	1.057258
C	-2.101665	4.086364	-0.180266
C	-1.014926	3.358132	0.274148
C	-3.330958	3.465257	-0.410600
C	0.265963	4.068349	0.501242
C	1.192549	1.955105	1.419095
N	1.300795	3.305226	1.048859
H	-7.991107	2.008493	-1.533172
H	-5.847169	3.161453	-1.172516
H	-4.152347	4.078838	-0.760386
H	-1.973464	5.149221	-0.355015
H	-3.206042	-2.684969	1.025181
H	-5.391043	-3.760474	0.660220
O	-7.776802	-3.872282	-0.022172
O	-9.565495	0.059238	-1.517920
O	0.408573	5.258538	0.249457
O	2.065217	1.455146	2.114013
C	1.010760	-1.063180	1.310265
C	1.126507	-2.222629	2.041508
C	2.469337	-2.662889	1.907982
C	3.093622	-1.756172	1.077959
H	0.348841	-2.672174	2.643174
C	4.430259	-1.641856	0.566836
C	5.440387	-2.580275	0.635662
C	6.637728	-2.106428	0.049319
C	6.540176	-0.814623	-0.471877
S	4.950872	-0.150441	-0.230449
H	-1.400688	-1.865974	0.922916

C	7.752833	-0.376237	-1.064342
C	8.764153	-1.333560	-0.988071
S	8.236773	-2.805947	-0.181273
C	9.994280	-0.917697	-1.571814
S	8.315609	1.063045	-1.866610
H	5.310175	-3.560046	1.079758
H	10.673054	0.916519	-2.582576
H	10.895836	-1.517443	-1.612559
C	9.900188	0.347606	-2.083024
C	2.552185	3.976049	1.418674
H	2.611224	4.091945	2.504559
H	3.394968	3.364106	1.092488
H	2.565437	4.950424	0.935469
C	-9.983636	-2.531932	-1.004123
H	-10.263249	-2.425848	-2.054897
H	-9.902918	-3.581617	-0.731640
H	-10.741932	-2.033030	-0.395860
H	2.930756	-3.518628	2.379373
O	2.202959	-0.795328	0.700516

4. **Compound PDI-DTT-4**

C	1.883754	4.087937	0.000036
C	1.456126	2.735800	0.000014
C	0.067241	2.441050	-0.000034
C	-0.926821	3.537843	-0.000045
C	0.915621	5.208612	-0.000060
N	-0.436620	4.852716	-0.000120
C	-0.351074	1.099192	-0.000083
C	0.629717	0.073599	-0.000081
C	1.990988	0.328852	0.000031
C	2.434904	1.691485	0.000051
C	3.823961	2.022037	0.000120
C	3.236497	4.387340	0.000188
C	4.191316	3.370143	0.000251
C	2.986821	-0.755219	0.000131
C	4.376911	-0.419046	0.000074
C	4.821352	0.940926	0.000027
C	5.346568	-1.468852	0.000060
C	6.729318	-1.163538	-0.000045

C	7.137369	0.158628	-0.000157
C	3.580851	-3.125343	0.000253
C	4.930768	-2.821498	0.000149
C	2.625293	-2.103617	0.000263
C	5.924218	-3.921137	0.000118
C	7.754008	-2.236913	-0.000105
N	7.276641	-3.556975	0.000062
H	1.580563	-2.390501	0.000406
H	3.281366	-4.168082	0.000317
H	8.200246	0.375527	-0.000271
H	3.533932	5.430459	0.000240
O	1.271636	6.380874	-0.000074
O	-2.137597	3.352404	-0.000032
O	5.604277	-5.102725	0.000164
O	8.953158	-1.991933	-0.000271
C	8.242551	-4.661439	-0.000153
H	8.088646	-5.282544	-0.885748
H	8.088663	-5.282832	0.885226
C	-1.448669	5.914488	-0.000128
H	-2.081768	5.818364	-0.885400
H	-0.930059	6.870315	-0.000404
C	6.194598	1.192487	-0.000113
H	6.564147	2.210715	-0.000224
H	5.236299	3.655153	0.000438
C	-4.174251	-0.150655	-0.000105
C	-6.487748	-0.025024	0.000157
C	-6.328831	-1.416557	0.000032
C	-7.569947	-2.102060	-0.000060
C	-8.662136	-1.233439	0.000034
S	-4.651465	-1.864523	-0.000196
S	-8.181082	0.457568	0.000250
S	-8.091562	-3.763282	-0.000130
C	-9.921591	-1.896723	0.000024
H	-10.884555	-1.400074	0.000072
C	-9.767585	-3.256168	-0.000049
H	-10.546362	-4.007346	-0.000084
C	-5.274064	0.693362	0.000072
H	-5.168149	1.771339	0.000142
H	-2.081467	5.818719	0.885398
H	9.242234	-4.233397	-0.000139
H	0.258038	-0.943026	-0.000184
C	-1.702735	0.690145	-0.000136

C	-2.833290	0.233611	-0.000139

5. **Compound PDI-DTT-5**

C	-8.192025	-3.632437	-0.025517
C	-8.915412	-2.425658	-0.179823
C	-10.316045	-2.471143	-0.381992
C	-11.042749	-3.763970	-0.440344
C	-8.883749	-4.942477	-0.073025
N	-10.268636	-4.923969	-0.281289
C	-11.024502	-1.291295	-0.528240
C	-10.367889	-0.057089	-0.470766
C	-8.989368	0.038020	-0.269891
C	-8.235772	-1.169945	-0.129656
C	-6.818959	-1.153095	0.063524
C	-6.823837	-3.593399	0.178020
C	-6.149871	-2.368223	0.222094
C	-8.292728	1.330830	-0.190763
C	-6.873474	1.349908	-0.013320
C	-6.120599	0.140172	0.091570
C	-6.181096	2.599481	0.062941
C	-4.767659	2.648150	0.224390
C	-4.737700	0.229200	0.187196
C	-4.036526	1.453003	0.240043
C	-8.293750	3.767235	-0.207237
C	-6.920802	3.806137	-0.032771
C	-8.969575	2.547535	-0.283808
C	-6.261107	5.130243	0.049388
C	-4.112847	3.959135	0.483853
N	-4.886091	5.115041	0.299863
H	-12.096644	-1.343627	-0.684844
H	-10.966483	0.838185	-0.587921
H	-10.044474	2.570019	-0.415861
H	-8.830565	4.706724	-0.282932
H	-5.079656	-2.384962	0.390110
H	-6.288580	-4.528948	0.301229
O	-8.294734	-6.007128	0.060255
O	-12.252216	-3.822743	-0.617260
O	-6.880619	6.179125	-0.074583
O	-2.954067	4.072735	0.857030

C	-2.565858	1.348460	0.258486
C	-1.822791	0.606448	1.146979
C	-0.442918	0.617419	0.819813
C	-0.136877	1.336124	-0.334602
C	1.235873	1.319469	-0.685411
C	1.991491	0.591171	0.211904
S	-1.573948	2.030623	-1.032343
S	0.995307	-0.077043	1.520732
C	3.414323	0.347996	0.191545
C	4.123600	-0.627707	0.865010
C	5.511304	-0.554567	0.598528
C	5.877454	0.464745	-0.279784
C	7.261560	0.519185	-0.570186
C	7.969302	-0.462606	0.095821
S	4.480591	1.380871	-0.781931
S	6.909599	-1.465624	1.107009
H	-2.258227	0.108429	2.005392
H	1.656299	1.799143	-1.561626
H	3.653458	-1.368120	1.501664
H	7.724516	1.224280	-1.250743
C	9.388555	-0.722525	0.057616
C	10.058640	-1.878067	0.406656
C	11.459400	-1.757756	0.234802
C	11.867925	-0.515243	-0.249549
S	10.508533	0.545689	-0.481927
H	-4.132411	-0.668403	0.188942
C	13.273415	-0.433564	-0.424978
C	13.925715	-1.614447	-0.070833
S	12.810934	-2.856775	0.485620
C	15.339312	-1.560387	-0.232500
S	14.409975	0.768880	-0.967153
H	9.553384	-2.774409	0.747446
H	16.749239	-0.017790	-0.924723
H	16.020450	-2.373804	-0.012098
C	15.740258	-0.341683	-0.706655
C	-4.188204	6.391580	0.493697
H	-3.297956	6.415855	-0.137689
H	-4.875185	7.191788	0.228435
C	-10.931747	-6.232134	-0.328431
H	-10.494158	-6.835262	-1.127307
H	-10.779279	-6.755243	0.618699
H	-11.991229	-6.065658	-0.508303

6. **Compound PDI-EDOT-1**

C	-6.504146	-0.323741	0.611723
C	-5.277742	-0.881446	0.176092
C	-5.213518	-2.255553	-0.157231
C	-6.414769	-3.116913	-0.055912
C	-7.726788	-1.155595	0.731577
N	-7.597454	-2.510203	0.386409
C	-4.018429	-2.803032	-0.590378
C	-2.869826	-2.010124	-0.685740
C	-2.880841	-0.654565	-0.351382
C	-4.111813	-0.062376	0.071558
C	-4.205168	1.329712	0.388199
C	-6.567896	1.021038	0.933015
C	-5.434164	1.832940	0.819617
C	-1.675472	0.184088	-0.420562
C	-1.775910	1.584470	-0.153100
C	-3.013998	2.179777	0.241702
C	-0.603672	2.393340	-0.286207
C	-0.697978	3.786860	-0.037053
C	-3.048742	3.555113	0.477932
C	-1.907216	4.346621	0.340910
C	0.752653	0.430106	-0.804181
C	0.648602	1.821339	-0.651277
C	-0.424468	-0.346130	-0.702604
C	1.783925	2.725825	-0.975883
C	0.475527	4.680418	-0.170111
N	1.649394	4.081383	-0.632959
H	-3.992204	-3.855752	-0.851336
H	-1.957686	-2.477960	-1.036795
H	-0.301013	-1.416034	-0.813327
H	-1.943973	5.414285	0.528742
H	-3.972170	4.040065	0.770401
H	-5.534971	2.879493	1.080708
H	-7.513939	1.431580	1.269582
O	-8.794787	-0.692783	1.110222
O	-6.402389	-4.307921	-0.339002
O	2.807749	2.357197	-1.533332
O	0.421654	5.876943	0.087568

C	1.997398	-0.327040	-1.004934
C	2.202083	-1.329763	-1.927730
C	3.458438	-1.967340	-1.802571
C	4.220083	-1.481006	-0.754869
S	3.365241	-0.191415	0.074361
H	1.475116	-1.575134	-2.694819
H	3.798152	-2.758716	-2.461991
C	5.529987	-1.918889	-0.337095
C	6.327626	-1.420971	0.670738
C	7.590143	-2.085305	0.799911
C	7.758603	-3.089545	-0.108949
S	6.366515	-3.244741	-1.141981
O	5.954519	-0.394383	1.490217
O	8.517545	-1.714727	1.734224
H	8.613754	-3.740139	-0.220540
C	7.068039	0.187095	2.185131
C	7.952216	-0.903988	2.772976
H	6.641043	0.815609	2.969853
H	7.648043	0.810691	1.491940
H	7.363909	-1.531709	3.456578
H	8.796574	-0.472526	3.316087
C	-8.773673	-3.382007	0.480872
H	-9.607809	-2.783092	0.838792
H	-8.996362	-3.805276	-0.501566
H	-8.565513	-4.204770	1.168916
C	2.818901	4.927678	-0.894526
H	3.697012	4.486738	-0.418678
H	3.005417	4.985116	-1.970218
H	2.612620	5.916611	-0.491678

7. **Compound PDI-EDOT-2**

C	-5.530447	-2.842035	0.118985
C	-5.971839	-1.503636	0.249837
C	-7.344432	-1.237893	0.473005
C	-8.332922	-2.339373	0.578414
C	-6.488498	-3.968432	0.214134
N	-7.832571	-3.643516	0.438600
C	-7.775725	0.071441	0.596430
C	-6.867982	1.131199	0.492529

C	-5.506331	0.918735	0.267468
C	-5.036774	-0.427679	0.155471
C	-3.653994	-0.723064	-0.052989
C	-4.190651	-3.105392	-0.106621
C	-3.267544	-2.057648	-0.192240
C	-4.547687	2.026750	0.136217
C	-3.159678	1.735039	-0.042315
C	-2.692296	0.387672	-0.115155
C	-2.205121	2.796902	-0.151862
C	-0.809005	2.532832	-0.302951
C	-1.328836	0.168095	-0.217474
C	-0.359324	1.197048	-0.296608
C	-4.026650	4.399688	0.057435
C	-2.676646	4.135321	-0.107675
C	-4.949850	3.362141	0.181410
C	-1.762058	5.288853	-0.246425
C	0.112332	3.678169	-0.550285
N	-0.422441	4.975609	-0.477176
H	-8.829921	0.258099	0.771476
H	-7.254996	2.137885	0.594136
H	-5.994163	3.620402	0.307397
H	-4.346054	5.435803	0.086889
H	-0.953725	-0.846280	-0.191361
H	-2.230760	-2.311124	-0.378712
H	-3.873287	-4.137266	-0.213684
O	-6.147976	-5.139243	0.105661
O	-9.522514	-2.130001	0.776256
O	-2.151192	6.448937	-0.180319
O	1.299274	3.562024	-0.822364
C	1.041932	0.751607	-0.320959
C	2.108014	1.197429	0.425823
C	3.270992	0.421957	0.212031
C	3.107322	-0.611868	-0.699273
C	4.280733	-1.386089	-0.944567
C	5.362865	-0.927529	-0.181785
S	1.486149	-0.656119	-1.316135
S	4.905001	0.468128	0.819764
H	2.047399	2.053354	1.083584
C	6.707668	-1.441051	-0.125274
C	7.758838	-0.959386	0.637775
C	8.978152	-1.687662	0.487883
C	8.864635	-2.731540	-0.384554

O	7.657213	0.126583	1.457647
O	10.117321	-1.359853	1.170952
S	7.263634	-2.844493	-1.046628
H	9.636875	-3.429783	-0.674276
H	8.586578	-0.518894	3.200616
H	10.898305	0.046947	2.410158
H	10.208003	0.701128	0.896704
C	8.737156	0.217598	2.400409
C	10.067829	-0.030649	1.704290
H	8.688857	1.225529	2.818305
C	0.530059	6.070307	-0.696527
H	1.344670	5.997910	0.027577
H	0.957178	5.992453	-1.699087
H	-0.007851	7.008042	-0.579369
C	-8.763072	-4.774129	0.530610
H	-8.726698	-5.354417	-0.394369
H	-8.467649	-5.426301	1.356015
H	-9.761268	-4.375223	0.695183
C	4.291130	-2.472648	-1.853533
C	4.223601	-3.386851	-2.644935
H	4.194646	-4.196117	-3.338726

8. **Compound PDI-EDOT-3**

C	-6.359241	0.466583	0.579610
C	-5.293727	-0.380839	0.190181
C	-5.544279	-1.752804	-0.052348
C	-6.907758	-2.312263	0.097333
C	-7.736596	-0.058421	0.746876
N	-7.919218	-1.426828	0.491542
C	-4.507734	-2.582745	-0.442920
C	-3.211008	-2.077276	-0.583239
C	-2.912185	-0.736221	-0.334897
C	-3.973933	0.145632	0.040024
C	-3.748772	1.541554	0.261712
C	-6.115778	1.809633	0.809171
C	-4.829601	2.336296	0.648613
C	-1.549088	-0.199056	-0.451451
C	-1.333113	1.206757	-0.288518
C	-2.398309	2.090061	0.064516

C	-0.013952	1.725357	-0.478158
C	0.218055	3.114775	-0.310444
C	-2.116872	3.450286	0.216155
C	-0.827324	3.954757	0.036213
C	0.864092	-0.520072	-0.821105
C	1.067802	0.867992	-0.813162
C	-0.448823	-1.017290	-0.665010
C	2.343547	1.473753	-1.276180
C	1.569915	3.696560	-0.483864
N	2.560323	2.822128	-0.936502
H	-4.722837	-3.628367	-0.636466
H	-2.431259	-2.758537	-0.903148
H	-0.563770	-2.094745	-0.665604
H	-0.619075	5.011289	0.167352
H	-2.903143	4.147351	0.479466
H	-4.690598	3.394367	0.835141
H	-6.942470	2.444065	1.110676
O	-8.669436	0.656762	1.088572
O	-7.166960	-3.491393	-0.106612
O	3.175963	0.881535	-1.944930
O	1.811014	4.879474	-0.271636
C	1.946086	-1.485010	-0.893893
C	2.069560	-2.724825	-1.478258
C	3.387519	-3.175562	-1.206804
C	3.987821	-2.189394	-0.449609
H	1.318828	-3.223965	-2.075135
H	3.850167	-4.093455	-1.541075
C	5.291252	-2.048570	0.134113
C	5.869755	-0.922465	0.685851
C	7.209387	-1.147067	1.148436
C	7.645501	-2.424209	0.940252
S	6.417720	-3.396219	0.184614
O	5.254538	0.288637	0.796194
O	7.960680	-0.158689	1.720375
H	8.609050	-2.838960	1.198104
C	6.175831	1.354261	1.068491
C	7.161238	0.949438	2.154900
H	5.566786	2.204867	1.383555
H	6.717760	1.615986	0.149538
H	6.617531	0.679874	3.070928
H	7.858712	1.761249	2.374855
C	-9.260318	-2.003081	0.638242

H	-9.935580	-1.208063	0.945746
H	-9.580108	-2.434767	-0.313165
H	-9.237038	-2.800032	1.385319
C	3.874638	3.376254	-1.272148
H	4.631149	2.619416	-1.065735
H	3.924103	3.635931	-2.334402
H	4.028779	4.271532	-0.672258
O	3.105479	-1.174989	-0.242572

9. **Compound PDI-EDOT-4**

C	4.170521	-2.330302	0.000979
C	4.406989	-0.934872	0.001726
C	5.738096	-0.451731	0.001386
C	6.893453	-1.382230	-0.000094
C	5.298289	-3.290827	-0.000464
N	6.591641	-2.753502	-0.001063
C	5.969985	0.912584	0.002370
C	4.900568	1.814761	0.003566
C	3.571800	1.386515	0.003692
C	3.308647	-0.020326	0.002791
C	1.974465	-0.535254	0.002935
C	2.871547	-2.807436	0.001594
C	1.791155	-1.919342	0.002584
C	2.441547	2.328293	0.004527
C	1.108535	1.818410	0.003834
C	0.845729	0.409283	0.003132
C	0.001180	2.724545	0.003764
C	-1.336547	2.249425	0.002266
C	-0.469598	-0.022085	0.002208
C	-1.577741	0.865904	0.001344
C	1.548468	4.596150	0.006271
C	0.246671	4.121134	0.005182
C	2.628885	3.713360	0.005799
C	-0.862308	5.103697	0.005704
C	-2.466423	3.202973	0.001782
N	-2.155337	4.572074	0.004618
H	6.995460	1.266454	0.002138
H	5.133647	2.872606	0.004304
H	3.627674	4.132395	0.006459

H	1.705470	5.669409	0.007424
H	-0.706934	-1.078177	0.001528
H	0.792040	-2.338018	0.003079
H	2.711299	-3.880428	0.001210
O	5.135785	-4.504492	-0.001110
O	8.050958	-0.984223	-0.000592
O	-0.664144	6.312941	0.007167
O	-3.640586	2.855163	-0.000694
C	-2.858004	0.271042	-0.000273
C	-3.875743	-0.401298	-0.003045
C	-5.090102	-1.082011	-0.006851
C	-5.299324	-2.451415	-0.011598
C	-6.681104	-2.814426	-0.019728
C	-7.518380	-1.731638	-0.029490
S	-6.641294	-0.235763	-0.024942
O	-4.295514	-3.367606	0.003221
O	-7.094182	-4.118293	-0.025464
C	-4.750191	-4.689573	-0.331764
C	-6.052376	-5.011936	0.388821
H	-3.952013	-5.370263	-0.026583
H	-4.894442	-4.761060	-1.417935
H	-5.907364	-4.935953	1.475386
H	-6.395872	-6.018865	0.140184
H	-8.599164	-1.750070	-0.032427
C	-3.300256	5.489082	0.004994
H	-3.912200	5.312472	-0.882748
H	-3.917317	5.304783	0.887550
H	-2.914419	6.505811	0.010306
C	7.693207	-3.722421	-0.002713
H	8.628562	-3.167708	-0.003943
H	7.623184	-4.358773	0.882719
H	7.620604	-4.358547	-0.888081

10. **Compound PDI-EDOT-5**

C	-7.206497	3.567960	0.029954
C	-7.916219	2.346644	-0.059750
C	-9.325078	2.365280	-0.199888
C	-10.074543	3.644719	-0.260717
C	-7.920817	4.865437	-0.021224

N	-9.312955	4.820241	-0.168992
C	-10.019946	1.171179	-0.282004
C	-9.341282	-0.050810	-0.221381
C	-7.953698	-0.119401	-0.080972
C	-7.214446	1.103222	-0.007303
C	-5.790230	1.112872	0.121552
C	-5.830135	3.554960	0.173254
C	-7.233134	-1.398882	-0.000021
C	-5.807382	-1.391886	0.111062
C	-5.070105	-0.168463	0.149424
C	-5.091533	-2.628215	0.186162
C	-3.671299	-2.651229	0.280167
C	-3.683202	-0.233905	0.178898
C	-2.959109	-1.445134	0.226696
C	-7.195577	-3.834368	0.046999
C	-5.815385	-3.847873	0.157153
C	-7.894041	-2.627694	-0.029231
C	-5.131320	-5.159219	0.242417
C	-2.984963	-3.944089	0.547238
N	-3.747129	-5.116463	0.429591
H	-11.098757	1.202915	-0.391217
H	-9.929612	-0.958032	-0.287486
H	-8.973463	-2.669783	-0.109529
H	-7.719829	-4.783603	0.021155
H	-5.305228	4.501439	0.248199
O	-7.344407	5.942353	0.058601
O	-11.291596	3.680651	-0.384418
O	-5.738798	-6.220395	0.174078
O	-1.809777	-4.030569	0.873389
C	-1.492717	-1.317548	0.161233
C	0.642158	-0.518232	0.566515
C	0.899309	-1.284020	-0.569478
C	2.254962	-1.280512	-0.982121
C	3.046522	-0.507432	-0.155878
S	-0.557688	-2.041890	-1.149616
S	2.100990	0.243058	1.146552
C	4.466413	-0.266723	-0.247915
C	5.322673	0.187395	0.736232
C	6.656103	0.297949	0.274787
C	6.835201	-0.071720	-1.057438
C	8.169203	0.025120	-1.515016
C	9.027780	0.472468	-0.526962

S	5.320689	-0.551881	-1.779053
S	8.167907	0.780029	0.999303
H	2.647536	-1.838208	-1.824315
H	4.997532	0.404335	1.747322
H	8.495607	-0.218704	-2.519368
C	10.450195	0.683045	-0.636914
C	11.340412	1.118916	0.321962
C	12.695735	1.204666	-0.134036
C	12.844327	0.831679	-1.438305
S	11.319651	0.368572	-2.138283
O	10.975109	1.456120	1.594246
O	13.716909	1.604192	0.683050
C	12.093611	1.511130	2.492476
C	13.244729	2.278387	1.857184
H	13.756047	0.808723	-2.017225
H	12.413399	0.491029	2.743694
H	11.733979	2.012329	3.393913
H	12.916286	3.294094	1.596786
H	14.097449	2.338255	2.537861
C	-9.998577	6.116393	-0.222589
H	-9.818068	6.666106	0.704388
H	-9.602164	6.705407	-1.052854
H	-11.061422	5.929150	-0.356327
C	-3.020820	-6.376468	0.626049
H	-3.704348	-7.193807	0.408273
H	-2.156184	-6.402251	-0.039875
H	-2.661932	-6.443297	1.656508
C	-5.134797	2.341869	0.218620
H	-4.058531	2.379283	0.337577
C	-0.716488	-0.520588	0.971360
H	-1.114240	0.009245	1.829102
H	-3.093739	0.672640	0.125702

11. **Compound PDI-BDT-1**

C	5.823009	-2.722130	0.107239
C	6.097726	-1.381401	-0.253613
C	7.395795	-1.028558	-0.695117
C	8.477146	-2.040789	-0.790288
C	6.877682	-3.760438	0.027590

N	8.140454	-3.352143	-0.419983
C	7.665970	0.282804	-1.045248
C	6.668407	1.260225	-0.960484
C	5.375045	0.960797	-0.527849
C	5.071324	-0.390917	-0.171208
C	3.766640	-0.776032	0.269415
C	4.557436	-3.071212	0.544535
C	3.545731	-2.108205	0.624238
C	4.324057	1.984086	-0.421498
C	3.015028	1.599370	0.007667
C	2.708722	0.242815	0.335315
C	1.982105	2.583257	0.116890
C	0.667280	2.226882	0.530677
C	1.401253	-0.073785	0.680255
C	0.364661	0.880113	0.772236
C	3.550655	4.285723	-0.619699
C	2.278599	3.933485	-0.201658
C	4.558746	3.325397	-0.726404
C	1.254382	4.998903	-0.100086
C	-0.323241	3.303892	0.802356
N	0.008486	4.605017	0.395765
H	8.664954	0.536242	-1.383699
H	6.929713	2.272618	-1.243929
H	5.538545	3.652081	-1.053003
H	3.744359	5.325135	-0.861839
H	1.119428	-1.102858	0.863570
H	2.572028	-2.425564	0.977849
H	4.368226	-4.102710	0.822292
O	6.680158	-4.929256	0.332728
O	9.604399	-1.754164	-1.170785
O	1.484280	6.160477	-0.412213
O	-1.391553	3.113356	1.365980
C	-0.972299	0.339097	1.077567
C	-1.299057	-0.482688	2.131626
C	-2.640479	-0.941295	2.098855
C	-3.343134	-0.496439	0.997826
S	-2.324506	0.507084	-0.015628
H	-0.597831	-0.718121	2.925015
H	-3.085661	-1.560522	2.869913
C	-4.716281	-0.769547	0.632893
C	-5.522762	-0.072259	-0.224751
C	-6.841108	-0.618452	-0.360810

C	-7.022967	-1.782819	0.445930
S	-5.550401	-2.174897	1.328026
C	-7.903602	-0.147176	-1.144975
C	-9.104871	-0.844539	-1.107159
C	-9.285428	-2.009214	-0.301805
C	-8.223482	-2.478120	0.485306
C	-10.613322	-2.550791	-0.433814
C	-11.395307	-1.841610	-1.286808
S	-10.577580	-0.460677	-1.995165
H	-5.199551	0.830025	-0.733429
H	-7.780959	0.738865	-1.760844
H	-8.346762	-3.361732	1.104690
H	-10.951208	-3.435103	0.095763
H	-12.424888	-2.040365	-1.555709
C	9.168235	-4.396870	-0.493349
H	10.084692	-3.941343	-0.860991
H	9.323298	-4.829135	0.498101
H	8.834989	-5.191267	-1.165230
C	-1.020816	5.627961	0.614742
H	-1.956447	5.302701	0.155881
H	-1.192488	5.760720	1.686167
H	-0.670357	6.555619	0.168350

12. **Compound PDI-BDT-2**

C	6.034048	-3.408924	-0.028732
C	6.667605	-2.146174	0.063177
C	8.072178	-2.079295	0.224884
C	8.886541	-3.314997	0.304293
C	6.817049	-4.668385	0.039933
N	8.204252	-4.534306	0.205634
C	8.695504	-0.847058	0.310585
C	7.947187	0.332534	0.229558
C	6.560576	0.317909	0.065402
C	5.895073	-0.946549	-0.008136
C	4.476000	-1.040712	-0.154903
C	4.661190	-3.476461	-0.191732
C	3.896089	-2.306742	-0.253756
C	5.767733	1.551953	-0.041195
C	4.345694	1.460105	-0.166588

C	3.681890	0.195405	-0.198073
C	3.560448	2.651967	-0.262118
C	2.142602	2.590803	-0.365133
C	2.293121	0.179231	-0.237475
C	1.503214	1.346302	-0.304312
C	5.587682	3.981020	-0.120505
C	4.210331	3.912617	-0.241969
C	6.354610	2.817744	-0.022458
C	3.450171	5.180208	-0.347257
C	1.379042	3.838753	-0.639322
N	2.070733	5.054415	-0.536180
H	9.772438	-0.815771	0.437954
H	8.479774	1.273335	0.299466
H	7.428967	2.924518	0.066167
H	6.056033	4.959227	-0.102193
H	2.825701	-2.408978	-0.387570
H	4.192844	-4.451870	-0.268858
O	6.286905	-5.768155	-0.042596
O	10.101903	-3.298774	0.448426
O	3.994103	6.275683	-0.291253
O	0.198718	3.850459	-0.957914
C	0.043271	1.140410	-0.247724
C	-0.695575	0.343809	-1.089966
C	-2.053191	0.268074	-0.680653
C	-2.331921	0.973676	0.480051
C	-3.689415	0.889247	0.922912
C	-4.456285	0.103307	0.060235
S	-0.915062	1.770662	1.093579
S	-3.479614	-0.538088	-1.273245
H	-0.278463	-0.133350	-1.968993
C	-5.860533	-0.234743	0.112480
C	-6.598391	-0.813440	-0.891470
C	-7.960185	-1.075939	-0.545984
C	-8.255795	-0.666795	0.788790
C	-9.518869	-0.817029	1.346123
C	-10.524655	-1.395896	0.559443
C	-10.228116	-1.804808	-0.776787
C	-8.966726	-1.651806	-1.336533
C	-11.896926	-1.660180	0.907389
C	-12.601454	-2.233834	-0.100843
S	-6.844302	0.031422	1.571342
S	-11.651396	-2.497569	-1.552036

H	-6.189169	-1.042333	-1.869944
H	-12.321355	-1.423666	1.877202
H	-13.643176	-2.528155	-0.091445
H	-9.730768	-0.499609	2.363061
H	-8.754832	-1.965913	-2.354360
C	1.271289	6.267740	-0.743724
H	0.903534	6.300001	-1.772654
H	0.410449	6.252047	-0.072558
H	1.907514	7.125996	-0.540592
C	9.030310	-5.744639	0.283107
H	9.558361	-5.767354	1.239347
H	8.373939	-6.606267	0.186486
H	9.772724	-5.732953	-0.518308
H	1.755862	-0.759116	-0.180852
C	-4.145943	1.554719	2.087969
C	-4.460396	2.147048	3.095637
H	-4.768753	2.661849	3.977216

13. **Compound PDI-BDT-3**

C	6.334100	-2.027285	-0.109091
C	6.208408	-0.651828	-0.418490
C	7.321557	0.052867	-0.937078
C	8.620486	-0.625849	-1.169460
C	7.616640	-2.738296	-0.322999
N	8.679647	-1.990398	-0.844997
C	7.200592	1.399326	-1.233514
C	5.991329	2.068735	-1.015737
C	4.868244	1.417503	-0.502004
C	4.966079	0.021043	-0.205969
C	3.852963	-0.718162	0.303020
C	5.251815	-2.718074	0.407275
C	4.029676	-2.068415	0.610801
C	3.599675	2.117138	-0.247733
C	2.479394	1.375635	0.239808
C	2.567240	-0.030080	0.488003
C	1.236528	2.040443	0.485066
C	0.099638	1.324731	0.952099
C	1.414550	-0.709033	0.856303
C	0.173445	-0.070797	1.073115

C	2.235404	4.136261	-0.228967
C	1.139377	3.435312	0.245631
C	3.448010	3.487246	-0.469831
C	-0.120415	4.176804	0.487005
C	-1.089056	2.086880	1.419427
N	-1.164503	3.441171	1.054838
H	8.061820	1.923937	-1.633324
H	5.947626	3.123238	-1.260084
H	4.277675	4.080197	-0.835220
H	2.127960	5.200327	-0.410135
H	1.425096	-1.788529	0.943076
H	3.211927	-2.645171	1.026645
H	5.371869	-3.768892	0.648801
O	7.766908	-3.925347	-0.064351
O	9.592623	-0.034182	-1.619654
O	-0.238904	5.368565	0.230387
O	-1.975573	1.606821	2.110717
C	-0.960953	-0.941003	1.355599
C	-1.071352	-2.087576	2.107082
C	-2.414415	-2.531287	1.982188
C	-3.042183	-1.637615	1.143468
H	-0.289845	-2.528100	2.710249
H	-2.873127	-3.384445	2.461685
C	-4.381740	-1.521228	0.636769
C	-4.912781	-0.462430	-0.047095
C	-6.287742	-0.644476	-0.405727
C	-6.796454	-1.902775	0.041484
S	-5.552102	-2.826899	0.880977
C	-7.131906	0.235222	-1.098815
C	-8.444569	-0.159055	-1.326051
C	-8.951301	-1.416751	-0.879334
C	-8.107658	-2.296373	-0.184949
C	-10.335738	-1.592582	-1.234130
C	-10.851023	-0.533662	-1.909017
S	-9.692886	0.758559	-2.165292
H	-4.338809	0.429950	-0.267651
H	-6.759730	1.195518	-1.443251
H	-8.479915	-3.255813	0.162176
H	-10.905978	-2.481221	-0.985688
H	-11.860197	-0.419951	-2.283879
C	9.938631	-2.715222	-1.051417
H	10.661977	-2.019822	-1.470653

H	10.294238	-3.112397	-0.097583
H	9.770318	-3.554275	-1.730485
C	-2.391576	4.144513	1.444451
H	-3.256956	3.574124	1.101866
H	-2.446735	4.229021	2.533236
H	-2.370385	5.132163	0.989451
O	-2.154120	-0.679690	0.747129

14. **Compound PDI-BDT-4**

C	5.011284	-2.880811	0.000098
C	5.424178	-1.527253	0.000004
C	6.806235	-1.219056	-0.000124
C	7.833219	-2.290288	-0.000129
C	6.007157	-3.978382	0.000042
N	7.358703	-3.611410	-0.000117
C	7.211448	0.103993	-0.000243
C	6.266482	1.135834	-0.000229
C	4.893745	0.881410	-0.000067
C	4.452284	-0.479551	0.000033
C	3.062982	-0.818877	0.000136
C	3.662084	-3.187663	0.000207
C	2.704313	-2.167989	0.000216
C	3.893974	1.960314	-0.000008
C	2.505169	1.625932	0.000058
C	2.064935	0.262924	0.000134
C	1.524040	2.667860	0.000066
C	0.135159	2.371783	0.000103
C	0.703622	0.005657	0.000190
C	-0.278571	1.028916	0.000171
C	3.300498	4.324386	0.000005
C	1.949595	4.020190	0.000027
C	4.257986	3.309044	-0.000014
C	0.973745	5.131786	0.000010
C	-0.869656	3.463504	0.000103
N	-0.376226	4.780270	-0.000050
H	8.273845	0.323212	-0.000348
H	6.633964	2.154822	-0.000355
H	5.302328	3.596461	-0.000037
H	3.594171	5.368692	-0.000001

H	0.333313	-1.011401	0.000256
H	1.660115	-2.456851	0.000278
H	3.365061	-4.231104	0.000271
O	5.689440	-5.160580	0.000098
O	9.031778	-2.042692	-0.000118
O	1.308370	6.310447	0.000016
O	-2.075080	3.252696	0.000210
C	-1.631011	0.615022	0.000156
C	-2.750032	0.132708	0.000087
C	-4.098113	-0.242763	0.000076
C	-4.633496	-1.507278	0.000159
C	-6.062725	-1.525884	0.000064
C	-6.615231	-0.206079	-0.000081
C	-7.986828	0.016914	-0.000192
C	-8.839783	-1.094847	-0.000153
C	-8.286023	-2.412596	-0.000003
C	-6.917412	-2.639997	0.000100
C	-10.279480	-1.120845	-0.000248
C	-10.789087	-2.378804	-0.000188
S	-5.354459	1.018146	-0.000107
S	-9.560282	-3.630308	0.000040
H	-4.018509	-2.400205	0.000272
H	-8.395562	1.023108	-0.000315
H	-6.508285	-3.646020	0.000207
H	-10.891156	-0.225171	-0.000383
H	-11.833122	-2.665110	-0.000242
C	-1.332157	5.893656	-0.000088
H	-2.336057	5.476393	-0.000173
H	-1.171088	6.513160	0.885355
H	-1.170937	6.513191	-0.885485
C	8.327059	-4.713769	-0.000173
H	9.325792	-4.283525	-0.000332
H	8.174644	-5.335285	0.885374
H	8.174404	-5.335387	-0.885611

15. **Compound PDI-BDT-5**

C	-8.140451	3.714287	-0.037817
C	-8.885888	2.519187	0.101736
C	-10.288168	2.587203	0.285028

C	-10.993874	3.891810	0.339624
C	-8.810925	5.035520	0.005229
N	-10.198459	5.039366	0.196127
C	-11.018133	1.418755	0.416304
C	-10.381569	0.173937	0.361432
C	-9.002283	0.056681	0.178509
C	-8.226636	1.252524	0.055871
C	-6.807511	1.212901	-0.115330
C	-6.770433	3.653216	-0.222811
C	-6.116190	2.417144	-0.260993
C	-8.326480	-1.247220	0.100989
C	-6.904698	-1.289104	-0.050089
C	-6.130053	-0.091564	-0.134195
C	-6.231853	-2.549676	-0.120008
C	-4.816316	-2.621035	-0.251179
C	-4.747067	-0.202990	-0.200514
C	-4.065393	-1.438125	-0.243846
C	-8.368904	-3.683284	0.098678
C	-6.993478	-3.744241	-0.047861
C	-9.025514	-2.452871	0.171100
C	-6.354556	-5.078686	-0.125647
C	-4.177283	-3.941267	-0.502421
N	-4.974237	-5.085010	-0.345975
H	-12.091251	1.488334	0.558899
H	-10.996540	-0.711679	0.466668
H	-10.103138	-2.457999	0.281000
H	-8.922891	-4.614044	0.156210
H	-5.043562	2.416532	-0.413942
H	-6.218114	4.580109	-0.335636
O	-8.202641	6.090607	-0.116847
O	-12.204414	3.970016	0.500897
O	-6.994121	-6.117787	-0.023055
O	-3.011386	-4.072210	-0.846880
C	-2.593157	-1.358489	-0.226768
C	-1.815748	-0.625253	-1.092802
C	-0.445906	-0.654232	-0.726340
C	-0.181995	-1.379869	0.434197
C	1.184241	-1.404400	0.808944
C	1.975706	-0.693124	-0.070842
S	-1.646606	-2.058902	1.088137
S	1.018965	0.031272	-1.378919
C	3.404778	-0.493666	-0.025187

C	4.245598	-0.100158	-1.048360
C	5.592755	-0.013763	-0.624201
C	5.797955	-0.341572	0.715649
C	7.146359	-0.263719	1.136784
C	7.987806	0.128511	0.113891
S	4.289805	-0.748728	1.492022
S	7.100340	0.393266	-1.400867
H	-2.220673	-0.118269	-1.960833
H	1.581915	-1.938125	1.664265
H	3.900232	0.090736	-2.057749
H	7.492253	-0.467624	2.143410
C	9.417518	0.326342	0.163574
C	10.229375	0.911251	-0.771702
C	11.613794	0.948130	-0.405002
C	11.843310	0.360947	0.876258
C	13.107171	0.288845	1.444215
C	14.187971	0.815093	0.720995
C	13.959483	1.403080	-0.559463
C	12.693387	1.476214	-1.127447
C	15.579201	0.858887	1.089753
C	16.361586	1.444331	0.147717
S	10.340382	-0.231019	1.577036
S	15.466852	1.987357	-1.260009
H	9.855719	1.326533	-1.701971
H	15.959970	0.463551	2.025333
H	17.432404	1.598708	0.184411
H	13.265564	-0.160546	2.420224
H	12.533977	1.927349	-2.102410
C	-4.293451	-6.371802	-0.532784
H	-3.951564	-6.465567	-1.566836
H	-3.420902	-6.417160	0.121761
H	-5.000864	-7.162230	-0.293156
C	-10.840260	6.358222	0.240553
H	-10.399742	6.952052	1.044724
H	-10.670989	6.881067	-0.703901
H	-11.903913	6.208885	0.410589
H	-4.127265	0.684519	-0.183999

16. **Compound PDI-BITHN-1**

C	3.490422	3.940652	-0.278001

C	3.008430	2.652713	0.070684
C	1.649672	2.486867	0.463148
C	0.818351	3.696468	0.706017
C	2.619660	5.137088	-0.220887
N	1.328638	4.929801	0.272466
C	1.158656	1.195982	0.712357
C	2.064348	0.112180	0.679668
C	3.412473	0.245917	0.376970
C	3.901641	1.537086	0.008382
C	5.253017	1.726897	-0.417766
C	4.804168	4.105739	-0.684185
C	5.672875	3.015124	-0.752941
C	4.332151	-0.900601	0.388232
C	5.674380	-0.714390	-0.067805
C	6.152381	0.565647	-0.491664
C	6.560350	-1.834680	-0.096490
C	7.887239	-1.682274	-0.566207
C	8.322648	-0.440179	-0.994285
C	4.821972	-3.255916	0.811692
C	6.116493	-3.103581	0.346609
C	3.944249	-2.166579	0.831119
C	7.025696	-4.273721	0.326874
C	8.823749	-2.832519	-0.609687
N	8.324466	-4.062642	-0.153424
H	2.942300	-2.328403	1.210712
H	4.504502	-4.234105	1.157140
H	9.340513	-0.341700	-1.356267
H	5.140025	5.102642	-0.948614
O	3.007015	6.247525	-0.562797
O	-0.267060	3.671712	1.269896
O	6.682467	-5.385667	0.706713
O	9.971749	-2.721783	-1.019080
C	9.205984	-5.235525	-0.166654
H	8.767549	-6.016560	-0.792361
H	9.309617	-5.627282	0.848009
C	0.448754	6.088998	0.459866
H	-0.516749	5.889599	-0.009371
H	0.930651	6.951555	0.005459
C	7.466265	0.665600	-0.953432
H	7.854523	1.617245	-1.295900
H	6.692329	3.196005	-1.071415
C	-4.121295	0.383146	0.423141

C	-6.271005	0.887175	-0.450061
C	-6.483901	-0.438645	-0.038784
S	-5.024155	-1.082590	0.662794
C	-4.930502	1.360192	-0.176216
H	0.282020	6.261660	1.526309
H	10.171675	-4.925908	-0.559311
H	1.644099	-0.868246	0.865681
C	-4.589892	2.710878	-0.492464
C	-7.196679	1.754819	-1.104738
C	-5.518378	3.520232	-1.093795
C	-6.820927	3.034275	-1.420928
H	-3.607539	3.093647	-0.237319
H	-5.263250	4.550005	-1.328147
H	-7.522034	3.693943	-1.924552
H	-8.185959	1.389361	-1.358181
C	-7.698607	-1.221829	-0.064328
C	-10.079294	-1.996701	0.234221
C	-7.877718	-2.578235	-0.377225
C	-9.248853	-3.017325	-0.201292
C	-6.911841	-3.511056	-0.864424
C	-9.600903	-4.373197	-0.486940
C	-7.290113	-4.801409	-1.129714
C	-8.638921	-5.238540	-0.932398
S	-9.220103	-0.528716	0.446285
H	-11.143824	-2.044174	0.421573
H	-5.890358	-3.188355	-1.035814
H	-6.557301	-5.509691	-1.506310
H	-8.896173	-6.271206	-1.151439
H	-10.628582	-4.697608	-0.347937
C	-0.248737	0.843554	0.956399
C	-2.731927	0.435823	0.815602
C	-0.731292	0.034037	1.962248
C	-2.129123	-0.181914	1.896280
S	-1.530739	1.286542	-0.140991
H	-0.097877	-0.347513	2.756087
H	-2.692017	-0.742725	2.634236

17. **Compound PDI-BITHN-2**

C	-11.031048	0.965253	0.594127

S	-9.947898	-1.430456	0.154880
S	-9.441709	1.513289	0.060967
C	-8.744709	-0.126147	-0.032880
C	-7.428698	-0.354994	-0.234789
S	-6.228887	0.941884	-0.461118
C	-5.075821	-1.442707	-0.126072
C	-4.813202	-0.115437	-0.168823
H	-4.320690	-2.206998	0.023321
S	-6.721085	-1.990385	-0.319614
C	-3.241577	1.837499	0.253678
C	-1.869865	2.125332	0.316160
C	-3.515021	0.507026	-0.041557
C	-1.061912	1.017599	0.071703
H	-1.467493	3.102610	0.545428
S	-2.042861	-0.405463	-0.266525
C	0.357969	0.944674	0.069219
C	1.238010	-0.123683	-0.042033
N	1.183857	2.060365	0.309310
C	2.590491	0.345734	-0.018274
C	2.589654	1.795985	0.088681
O	3.448357	2.649490	0.033547
C	1.236978	-1.575097	-0.040053
C	3.469593	-0.721832	0.027240
N	2.644911	-1.852829	0.171179
O	0.382690	-2.427353	-0.161360
C	4.897045	-0.787536	0.054402
C	5.700997	-1.915825	0.222580
S	5.873366	0.649869	-0.130858
C	7.072820	-1.632765	0.205514
H	5.292332	-2.907961	0.356020
C	7.352598	-0.280653	0.017204
H	7.838482	-2.387477	0.328291
C	8.596335	0.431734	-0.068859
C	9.877297	-0.036321	0.031988
H	8.494530	1.507457	-0.202838
C	11.067837	0.882249	-0.006441
O	10.922456	2.036074	-0.711896
H	10.160854	1.976014	-1.311315
O	12.094734	0.637041	0.573407
C	10.182700	-1.405247	0.293466
N	10.406684	-2.531135	0.486704
H	-4.017757	2.569835	0.444400

C	-11.257257	-0.351686	0.636386
H	-11.759740	1.728419	0.840964
H	-12.195883	-0.811843	0.921992
F	0.745209	3.308609	-0.100759
F	3.092481	-3.067010	-0.322055

18. **Compound PDI-BITHN-3**

C	2.496544	3.652650	-0.256194
C	2.353567	2.311384	0.182554
C	1.111694	1.873271	0.721123
C	0.081863	2.886613	1.057319
C	1.386260	4.625678	-0.145498
N	0.237246	4.169243	0.508078
C	0.941559	0.513814	1.034339
C	2.060404	-0.346264	0.945880
C	3.311586	0.069371	0.516463
C	3.463738	1.417507	0.061030
C	4.689800	1.876651	-0.509052
C	3.694992	4.080603	-0.805008
C	4.775629	3.206618	-0.928582
C	4.462810	-0.843052	0.469154
C	5.679774	-0.390143	-0.129569
C	5.816117	0.939855	-0.639373
C	6.788129	-1.287644	-0.215378
C	7.997179	-0.871443	-0.823666
C	8.100607	0.412261	-1.330717
C	5.507676	-3.005647	0.914148
C	6.684396	-2.597670	0.310281
C	4.414304	-2.136723	0.992224
C	7.825843	-3.538884	0.230363
C	9.158948	-1.788019	-0.929711
N	8.991889	-3.073709	-0.390862
H	3.516379	-2.493070	1.483357
H	5.452760	-4.009421	1.322119
H	9.032066	0.713915	-1.797855
H	3.770690	5.110473	-1.137059
O	1.469762	5.770586	-0.573349
O	-0.873194	2.668994	1.792674
O	7.778327	-4.677743	0.677274
O	10.210128	-1.449149	-1.457240

C	10.106731	-4.024653	-0.464963
H	9.787128	-4.921385	-1.000884
H	10.407552	-4.317491	0.543905
C	-0.843370	5.123181	0.782126
H	-1.800699	4.678012	0.504104
H	-0.649301	6.022840	0.202580
C	7.025515	1.302744	-1.235447
H	7.156768	2.297744	-1.643320
H	5.693245	3.589407	-1.358554
C	-3.801483	-0.198495	0.657259
C	-5.651636	0.799730	-0.439896
C	-6.220625	-0.433199	-0.077457
S	-5.047591	-1.402839	0.776065
C	-4.277382	0.941196	-0.012364
H	-0.874906	5.357838	1.849601
H	10.929315	-3.538487	-0.984212
H	1.889618	-1.389917	1.179566
C	-3.580179	2.157664	-0.275846
C	-6.262021	1.856329	-1.180599
C	-4.215127	3.159398	-0.964514
C	-5.553473	3.001965	-1.435886
H	-2.570388	2.280450	0.091576
H	-3.690614	4.090286	-1.164277
H	-6.013605	3.804639	-2.005462
H	-7.275624	1.738958	-1.548067
C	-7.573244	-0.907327	-0.253423
C	-10.087802	-1.088663	-0.254545
C	-8.031161	-2.191377	-0.591460
C	-9.478197	-2.288186	-0.587808
C	-7.265177	-3.338525	-0.961449
C	-10.107129	-3.528068	-0.920251
C	-7.906019	-4.508423	-1.277196
C	-9.333417	-4.608181	-1.248321
S	-8.936595	0.139463	0.066885
H	-11.147603	-0.877995	-0.199232
H	-6.183326	-3.273113	-1.005958
H	-7.323449	-5.379235	-1.564887
H	-9.801583	-5.555271	-1.501909
H	-11.191570	-3.594885	-0.909861
C	-0.323712	-0.112425	1.379313
C	-2.500611	-0.460027	1.195371
C	-0.632705	-1.157436	2.223172

C	-2.027890	-1.372717	2.120595
H	0.060005	-1.670912	2.875343
H	-2.626134	-2.082660	2.674093
O	-1.457966	0.293917	0.735184

19. **Compound PDI-BITHN-4**

C	-3.060400	4.110982	-0.155571
C	-2.468598	2.825617	-0.063026
C	-1.054442	2.707009	-0.008397
C	-0.207642	3.915370	-0.041588
C	-2.239413	5.341522	-0.189867
N	-0.853701	5.157043	-0.128615
C	-0.471729	1.427589	0.071288
C	-1.322830	0.290260	0.115059
C	-2.703095	0.374553	0.075440
C	-3.311632	1.669260	-0.030918
C	-4.727810	1.821361	-0.106889
C	-4.439798	4.238057	-0.217173
C	-5.260531	3.111469	-0.194467
C	-3.557913	-0.822092	0.136687
C	-4.975974	-0.665522	0.039118
C	-5.582177	0.623998	-0.092752
C	-5.808226	-1.826774	0.075202
C	-7.214496	-1.700705	-0.033640
C	-7.779079	-0.445174	-0.174112
C	-3.857968	-3.239332	0.327734
C	-5.231706	-3.110997	0.220211
C	-3.035929	-2.108503	0.285480
C	-6.081421	-4.323978	0.261886
C	-8.098032	-2.892008	-0.001037
N	-7.464712	-4.136174	0.147151
H	-1.966640	-2.258129	0.375082
H	-3.434929	-4.231617	0.443576
H	-8.857586	-0.365763	-0.259817
H	-4.862629	5.234608	-0.285380
O	-2.734761	6.459732	-0.267038
O	1.018036	3.885438	0.004099
O	-5.621560	-5.451503	0.389258
O	-9.315052	-2.803298	-0.097160

C	-8.286722	-5.350597	0.189531
H	-8.122992	-5.871181	1.136110
H	-7.995000	-6.019193	-0.623889
C	0.019620	6.334912	-0.157174
H	0.628707	6.362555	0.749540
H	-0.612221	7.217587	-0.222937
C	-6.972077	0.697498	-0.201682
H	-7.461798	1.657193	-0.313650
H	-6.332045	3.261663	-0.244005
C	3.450162	0.589077	0.144317
C	5.793285	0.968191	0.074035
C	5.770238	-0.440685	0.153665
S	4.127335	-1.015681	0.234107
C	4.477418	1.552045	0.074824
H	0.689644	6.274914	-1.018241
H	-9.328397	-5.054883	0.089034
H	-0.829712	-0.671228	0.179318
C	0.913370	1.179692	0.106562
C	2.083726	0.825654	0.127434
C	4.308378	2.960454	-0.008560
C	6.925079	1.826910	-0.048814
C	5.426588	3.752923	-0.100289
C	6.734934	3.184367	-0.130045
H	3.305742	3.376674	-0.001660
H	5.317953	4.832079	-0.164453
H	7.594765	3.841045	-0.229645
H	7.922996	1.405450	-0.097095
C	6.873984	-1.365256	0.244157
C	9.010996	-2.511115	0.928948
C	7.019540	-2.642097	-0.326566
C	8.251035	-3.294332	0.073547
C	6.155466	-3.310496	-1.245658
C	8.560952	-4.596990	-0.425678
C	6.490316	-4.557955	-1.706060
C	7.693051	-5.210137	-1.288267
S	8.253261	-1.011154	1.258974
H	9.973149	-2.748402	1.363297
H	5.249131	-2.823195	-1.588147
H	5.835468	-5.063021	-2.410608
H	7.918297	-6.200373	-1.674179
H	9.483187	-5.080614	-0.115933

20. **Compound PDI-BITHN-5**

C	-9.295640	3.463087	-0.629550
C	-9.983718	2.259120	-0.343799
C	-11.390006	2.278384	-0.184412
C	-12.149917	3.544666	-0.306277
C	-10.023323	4.749929	-0.765375
N	-11.414710	4.703383	-0.587134
C	-12.066190	1.102814	0.089863
C	-11.369892	-0.105829	0.200784
C	-9.983853	-0.176398	0.046544
C	-9.263987	1.031431	-0.218372
C	-7.841806	1.041048	-0.364252
C	-7.921091	3.444995	-0.791786
C	-7.207433	2.248807	-0.660768
C	-9.245261	-1.444810	0.139280
C	-7.819846	-1.433188	0.021591
C	-7.101557	-0.217896	-0.198355
C	-7.085695	-2.656678	0.124273
C	-5.665070	-2.670563	0.037572
C	-5.713399	-0.264673	-0.215067
C	-4.972192	-1.458537	-0.082753
C	-9.171452	-3.862297	0.433739
C	-7.791052	-3.870686	0.326514
C	-9.887698	-2.667002	0.341311
C	-7.086959	-5.170307	0.427876
C	-4.955732	-3.976829	-0.031862
N	-5.702269	-5.132849	0.240944
H	-13.143515	1.138407	0.212758
H	-11.942510	-1.000361	0.414205
H	-10.966548	-2.713312	0.427025
H	-9.681816	-4.806170	0.592453
H	-6.133700	2.281396	-0.802469
H	-7.411163	4.374952	-1.019486
O	-9.446598	5.799298	-1.017757
O	-13.365162	3.603317	-0.171950
O	-7.678809	-6.220485	0.643002
O	-3.774060	-4.088696	-0.325510
C	-3.507162	-1.302330	-0.030907
C	-2.731793	-0.645151	-0.957699

C	-1.376713	-0.559955	-0.547512
C	-1.124045	-1.120530	0.703521
C	0.227147	-1.031509	1.121046
C	1.018578	-0.399880	0.182480
S	-2.579815	-1.784891	1.391403
S	0.079851	0.109014	-1.235454
C	2.435767	-0.131813	0.244061
C	3.300195	0.136980	-0.798955
C	4.625671	0.348922	-0.349885
C	4.791403	0.238809	1.031101
C	6.123706	0.406525	1.478212
C	6.993638	0.663479	0.434367
S	3.270441	-0.113514	1.810905
S	6.145165	0.700989	-1.128364
H	-3.126249	-0.272002	-1.895628
H	0.616848	-1.434388	2.048585
H	2.987740	0.153114	-1.836636
H	6.455565	0.297719	2.502954
C	8.417386	0.888865	0.511082
C	10.931737	0.833786	0.126336
H	-5.138169	0.649163	-0.294469
C	12.239932	0.652327	-0.461230
C	12.781035	-0.475316	-1.097855
C	14.107407	-0.233766	-1.632858
S	13.374310	1.979546	-0.547536
H	15.501232	1.493347	-1.660122
C	14.547507	1.058304	-1.392292
C	-4.955028	-6.396006	0.229331
H	-4.564313	-6.587572	-0.773367
H	-4.110642	-6.323114	0.917641
H	-5.634844	-7.189334	0.531141
C	-12.187117	5.945658	-0.702841
H	-12.733324	6.123821	0.226293
H	-11.491081	6.757087	-0.902104
H	-12.912630	5.852984	-1.514679
C	9.138648	1.553524	1.514622
C	10.569433	1.506693	1.304230
C	12.210685	-1.778271	-1.230695
C	14.802910	-1.286425	-2.305356
C	12.911281	-2.761538	-1.879152
C	14.210263	-2.513804	-2.427367
C	8.621390	2.260083	2.641385

C	11.434922	2.095002	2.275539
C	9.485538	2.839039	3.534236
C	10.900031	2.736481	3.362318
H	12.509741	2.019585	2.150628
H	7.547969	2.352141	2.766781
H	9.093966	3.385346	4.387890
H	11.557525	3.180047	4.104792
H	11.234253	-1.985058	-0.805704
H	15.793832	-1.097307	-2.709054
H	12.480089	-3.754145	-1.975326
H	14.730075	-3.319969	-2.937694
S	9.504303	0.257720	-0.691657

21. **Compound PDI-BTAC-1**

C	-9.442778	-1.778130	0.192591
C	-8.054902	-1.953702	-0.025347
C	-7.538125	-3.256323	-0.224082
C	-8.432573	-4.437799	-0.207222
C	-10.369443	-2.936995	0.218982
N	-9.795391	-4.201377	0.013475
C	-6.183230	-3.432586	-0.443559
C	-5.319907	-2.331854	-0.460552
C	-5.781746	-1.029950	-0.257569
C	-7.180942	-0.823660	-0.046615
C	-7.727265	0.485497	0.138924
C	-9.949004	-0.504278	0.383622
C	-9.101274	0.608436	0.355070
C	-4.883287	0.133674	-0.257149
C	-5.429411	1.445500	-0.109249
C	-6.831037	1.650461	0.087829
C	-4.543985	2.567838	-0.161068
C	-5.078090	3.874551	-0.020034
C	-7.301192	2.956965	0.226112
C	-6.437275	4.052840	0.174495
C	-2.613410	1.095256	-0.395023
C	-3.142513	2.392034	-0.341633
C	-3.505276	0.000860	-0.365344
C	-2.289589	3.588641	-0.579335
C	-4.214407	5.077111	-0.074067

N	-2.863418	4.848242	-0.347043
H	-5.807533	-4.438049	-0.601247
H	-4.268026	-2.516281	-0.643534
H	-3.053847	-0.982610	-0.396672
H	-6.813694	5.064020	0.285694
H	-8.356834	3.149121	0.374847
H	-9.545963	1.584520	0.507273
H	-11.014201	-0.386981	0.552127
O	-11.571299	-2.804683	0.408259
O	-8.024841	-5.579549	-0.376472
O	-1.134457	3.528036	-0.974800
O	-4.655190	6.207837	0.090080
C	-1.180968	0.748164	-0.432306
C	-0.574125	-0.117901	-1.312016
C	0.792964	-0.360707	-1.017078
C	1.236652	0.293160	0.111631
S	-0.055656	1.249868	0.805559
H	-1.098712	-0.553193	-2.156129
H	1.424870	-1.023117	-1.598045
C	2.577804	0.259611	0.706326
C	3.696723	0.057477	-0.112373
C	4.981014	0.003696	0.436909
C	2.770806	0.422858	2.097076
C	5.139223	0.171665	1.830411
C	4.039422	0.386091	2.662528
C	6.250141	-0.194743	-0.244623
C	7.337539	-0.172379	0.649720
C	8.655108	-0.360574	0.208118
C	8.898898	-0.546487	-1.165893
C	6.494459	-0.415327	-1.605240
C	7.803032	-0.584244	-2.043148
N	9.727570	-0.372536	1.102059
C	10.886474	-1.093812	0.781920
C	11.206429	-1.297468	-0.574877
C	10.361251	-0.576551	-1.633862
C	11.698526	-1.608300	1.799619
C	12.833247	-2.347820	1.478908
C	13.149941	-2.588942	0.141895
C	12.338121	-2.064729	-0.866260
H	3.568100	-0.031221	-1.186666
H	1.908910	0.560817	2.743525
H	4.166221	0.512082	3.733522

H	5.671630	-0.447558	-2.312993
H	7.975486	-0.740623	-3.101565
H	11.428263	-1.437289	2.839759
H	13.458279	-2.745302	2.273812
H	14.026887	-3.174226	-0.118833
H	12.606765	-2.253020	-1.899955
H	9.489600	-0.361418	2.085409
C	10.511534	-1.214666	-3.024342
C	10.858861	0.896340	-1.713745
H	10.169630	-2.254968	-3.030274
H	11.555280	-1.189803	-3.350095
H	9.942769	-0.655632	-3.772853
H	11.910123	0.923528	-2.023068
H	10.260686	1.458910	-2.439959
H	10.774634	1.392616	-0.742243
S	6.831284	0.092523	2.329816
C	-1.970913	6.000901	-0.516781
H	-1.076155	5.856694	0.091672
H	-1.664253	6.084540	-1.562775
H	-2.512699	6.891825	-0.207867
C	-10.662359	-5.385115	0.024025
H	-10.578801	-5.907995	-0.931562
H	-10.343547	-6.066479	0.816479
H	-11.683818	-5.052105	0.192328

22. **Compound PDI-BTAC-2**

C	-7.898509	-3.607172	0.072179
C	-8.590106	-2.392609	-0.151154
C	-10.000330	-2.404285	-0.276602
C	-10.770838	-3.668762	-0.175185
C	-8.633444	-4.889996	0.178243
N	-10.026993	-4.837974	0.047581
C	-10.677115	-1.217557	-0.497708
C	-9.977624	-0.010417	-0.602527
C	-8.587337	0.050572	-0.488242
C	-7.868621	-1.163382	-0.250633
C	-6.445242	-1.179018	-0.113194
C	-6.519791	-3.602122	0.189988
C	-5.806053	-2.402468	0.096583
C	-7.842410	1.312781	-0.609931

C	-6.419269	1.301045	-0.464438
C	-5.708244	0.090041	-0.201265
C	-5.681110	2.520770	-0.583840
C	-4.265703	2.540206	-0.436246
C	-4.334049	0.159929	-0.008573
C	-3.593646	1.356883	-0.106047
C	-7.755928	3.720125	-0.977505
C	-6.377866	3.728275	-0.846171
C	-8.476882	2.529450	-0.862874
C	-5.666997	5.021075	-0.985647
C	-3.520956	3.792669	-0.740505
N	-4.272467	4.964514	-0.914117
H	-11.757674	-1.243704	-0.589548
H	-10.551930	0.891220	-0.777891
H	-9.552998	2.574723	-0.978101
H	-8.261015	4.660265	-1.171327
H	-4.727472	-2.447117	0.188538
H	-6.007633	-4.544020	0.355729
O	-8.072089	-5.960450	0.370954
O	-11.989832	-3.697445	-0.279391
O	-6.259295	6.076742	-1.170214
O	-2.305045	3.843914	-0.855642
C	-2.153531	1.250337	0.199092
C	-1.257074	0.416581	-0.424138
C	0.025614	0.477246	0.184747
C	0.088530	1.322723	1.282341
C	1.371682	1.386846	1.916174
C	2.295542	0.570889	1.268718
S	-1.443640	2.086807	1.581996
S	1.569594	-0.278384	-0.098863
H	-1.510512	-0.180398	-1.292413
C	3.712413	0.353358	1.579686
C	4.155294	0.323301	2.923106
C	4.646013	0.155240	0.552628
C	5.490998	0.109087	3.236834
C	5.993412	-0.069519	0.848271
C	6.404291	-0.088418	2.199169
C	7.097646	-0.290833	-0.070713
C	8.316087	-0.477416	0.605020
C	9.520983	-0.713867	-0.082327
C	9.503063	-0.758899	-1.487529
C	7.084172	-0.336830	-1.470874

C	8.274850	-0.565970	-2.145576
C	10.782571	-1.005775	-2.305065
C	12.009926	-1.204013	-1.400399
C	11.922899	-1.143392	0.002480
N	10.701432	-0.894849	0.616378
C	13.063610	-1.329863	0.800462
C	14.299553	-1.575757	0.215792
C	14.409217	-1.637457	-1.174774
C	13.270664	-1.451692	-1.957258
H	3.435840	0.459887	3.721719
H	5.811990	0.085922	4.273891
H	4.327692	0.199451	-0.484838
H	6.158167	-0.194252	-2.019299
H	8.255719	-0.597269	-3.230402
H	10.678713	-0.884013	1.624914
H	13.367168	-1.501084	-3.038153
H	15.368913	-1.827635	-1.645931
H	15.173469	-1.718023	0.845535
H	12.968522	-1.278703	1.883343
C	11.031806	0.216783	-3.227294
C	10.587640	-2.277370	-3.172514
H	11.171661	1.124459	-2.631672
H	11.927125	0.069219	-3.840262
H	10.186908	0.379621	-3.904657
H	9.732383	-2.169156	-3.847694
H	11.472424	-2.472996	-3.787171
H	10.413097	-3.151813	-2.537635
S	8.136377	-0.378234	2.368274
C	-3.501925	6.193674	-1.137083
H	-2.769977	6.310465	-0.335669
H	-2.963724	6.129322	-2.086444
H	-4.199645	7.027719	-1.151983
C	-10.733894	-6.119123	0.157398
H	-10.371669	-6.804490	-0.612483
H	-10.534562	-6.565100	1.134733
H	-11.797143	-5.928166	0.032447
H	-3.773719	-0.726557	0.260303
C	1.634759	2.231976	3.026265
C	1.799000	2.967458	3.973201
H	1.962428	3.623233	4.798060

23. **Compound PDI-BTAC-3**

C	-9.367453	-1.235109	0.960753
C	-8.117257	-1.579234	0.392109
C	-7.895274	-2.902063	-0.059592
C	-8.954941	-3.931163	0.057262
C	-10.451327	-2.239083	1.098763
N	-10.167339	-3.533409	0.634867
C	-6.678428	-3.240680	-0.625152
C	-5.662034	-2.286499	-0.740719
C	-5.828656	-0.974458	-0.293530
C	-7.086619	-0.596999	0.271746
C	-7.340377	0.740121	0.713222
C	-9.586859	0.060079	1.396301
C	-8.586992	1.030820	1.270878
C	-4.761500	0.032263	-0.389565
C	-5.026963	1.380372	0.007702
C	-6.290763	1.758742	0.556682
C	-3.994194	2.358284	-0.148986
C	-4.248216	3.697101	0.245528
C	-6.485691	3.089957	0.930270
C	-5.478103	4.043985	0.779971
C	-2.443363	0.658568	-0.954182
C	-2.721259	2.007715	-0.681311
C	-3.482028	-0.290072	-0.815713
C	-1.775017	3.095063	-1.048764
C	-3.220621	4.754399	0.106677
N	-2.037077	4.374928	-0.532050
H	-6.531695	-4.257095	-0.974935
H	-4.729497	-2.592239	-1.200205
H	-3.223069	-1.322261	-1.016107
H	-5.637468	5.074289	1.079349
H	-7.432405	3.411525	1.347029
H	-8.808561	2.031054	1.622961
H	-10.549145	0.306633	1.832194
O	-11.537424	-1.961300	1.589861
O	-8.803467	-5.084355	-0.324850
O	-0.808297	2.940869	-1.781988
O	-3.400040	5.900052	0.501601
C	-1.138566	0.129485	-1.325657
C	-0.772403	-0.900325	-2.161890

C	0.644191	-0.987618	-2.107309
C	1.062910	-0.017130	-1.225462
H	-1.440230	-1.487162	-2.777225
H	1.280235	-1.652037	-2.674357
C	2.369340	0.426438	-0.765594
C	3.486429	-0.408110	-0.889502
C	4.744342	0.032443	-0.469920
C	2.518735	1.716757	-0.207765
C	4.864921	1.323987	0.091377
C	3.758972	2.167183	0.223551
C	6.015208	-0.673058	-0.515511
C	7.067136	0.103091	0.007541
C	8.379229	-0.387171	0.073243
C	8.656986	-1.674842	-0.422981
C	6.290249	-1.966002	-0.976233
C	7.595004	-2.443615	-0.925988
N	9.412655	0.371693	0.625771
C	10.513562	-0.277267	1.202805
C	10.865061	-1.560295	0.739053
C	10.127585	-2.112785	-0.488726
C	11.237053	0.342164	2.228751
C	12.312019	-0.316324	2.818842
C	12.656387	-1.600469	2.396570
C	11.933833	-2.206821	1.366794
H	3.374127	-1.407263	-1.300384
H	1.650032	2.363311	-0.144968
H	3.865058	3.161668	0.646413
H	5.494551	-2.588495	-1.374339
H	7.792054	-3.442295	-1.297960
H	10.944572	1.333583	2.568813
H	12.868408	0.169593	3.615609
H	13.486751	-2.127011	2.857894
H	12.223766	-3.200972	1.044485
H	9.139902	1.234095	1.079196
C	10.271711	-3.638402	-0.609991
C	10.757391	-1.457810	-1.752600
H	9.837475	-4.154811	0.252526
H	11.324928	-3.921654	-0.690848
H	9.784014	-4.004493	-1.517962
H	11.818083	-1.724146	-1.827118
H	10.240869	-1.803167	-2.655732
H	10.680033	-0.367267	-1.708925

S	6.524114	1.698001	0.564030
C	-1.034365	5.403981	-0.826863
H	-0.050654	5.051387	-0.510059
H	-0.998812	5.595374	-1.902617
H	-1.314137	6.307038	-0.289214
C	-11.200559	-4.569373	0.744505
H	-11.455638	-4.940751	-0.251012
H	-10.818357	-5.405666	1.334422
H	-12.070950	-4.126567	1.222970
O	-0.023057	0.647730	-0.737479

24. **Compound PDI-BTAC-4**

C	6.060875	-3.561801	0.000869
C	6.839451	-2.381483	-0.057605
C	8.250661	-2.478073	-0.120694
C	8.931567	-3.796592	-0.128373
C	6.704661	-4.896577	-0.001894
N	8.103259	-4.928439	-0.068715
C	9.012918	-1.324527	-0.176535
C	8.399297	-0.067084	-0.169643
C	7.012213	0.078513	-0.107762
C	6.204510	-1.101160	-0.052802
C	4.777505	-1.032168	0.007216
C	4.681448	-3.472968	0.062790
C	4.052140	-2.223628	0.065266
C	6.359384	1.396749	-0.096926
C	4.934007	1.470688	-0.043139
C	4.126936	0.288108	0.005073
C	4.287775	2.748229	-0.037621
C	2.871897	2.855958	0.010344
C	2.749443	0.426575	0.047780
C	2.095709	1.684712	0.050709
C	6.460523	3.830916	-0.130532
C	5.079246	3.924287	-0.081932
C	7.090692	2.586208	-0.138084
C	4.467465	5.272832	-0.078254
C	2.228280	4.191749	0.015978
N	3.071097	5.313608	-0.028019
H	10.092799	-1.415606	-0.224936

H	9.039405	0.805590	-0.214829
H	8.172924	2.565156	-0.176439
H	7.038313	4.748284	-0.162997
H	2.106793	-0.443775	0.080124
H	2.970135	-2.203475	0.114882
H	4.102067	-4.389028	0.108625
O	6.066342	-5.939879	0.050331
O	10.149837	-3.899607	-0.183776
O	5.139589	6.296430	-0.116533
O	1.016332	4.363426	0.056957
C	0.681942	1.676802	0.093163
C	-0.530459	1.583117	0.126812
C	-1.942807	1.719604	0.161000
C	-2.486681	3.030136	0.165216
C	-3.859031	3.225798	0.195146
C	-4.696867	2.105946	0.219065
C	-2.795628	0.606549	0.187836
C	-4.180433	0.789072	0.217245
C	-5.229003	-0.218361	0.245618
C	-6.512680	0.359357	0.269031
C	-7.673154	-0.427508	0.279777
C	-5.112701	-1.613155	0.230675
C	-7.550390	-1.829986	0.299032
C	-6.264212	-2.391848	0.259855
C	-8.832026	-2.656708	0.479811
C	-9.975676	-1.971140	-0.280220
C	-10.019352	-0.563261	-0.286533
C	-11.106113	0.122577	-0.841679
C	-12.158944	-0.586299	-1.412949
C	-12.120492	-1.980348	-1.445464
C	-11.035530	-2.655460	-0.882287
N	-8.944372	0.148820	0.265302
H	-1.801881	3.872027	0.143424
H	-4.272110	4.229926	0.197884
H	-2.373332	-0.393448	0.184900
H	-8.980108	1.150485	0.127076
H	-4.134156	-2.082802	0.202079
H	-6.155861	-3.470169	0.260958
H	-11.028706	-3.739594	-0.906427
H	-12.931826	-2.542591	-1.898382
H	-12.998895	-0.047777	-1.842982
H	-11.114434	1.210715	-0.834551

C	-9.192648	-2.638813	1.993971
C	-8.643155	-4.118614	0.043028
H	-8.386400	-3.094238	2.580746
H	-9.557716	-4.693900	0.212470
H	-8.376824	-4.192128	-1.016590
H	-9.339741	-1.614655	2.349954
H	-10.118272	-3.199337	2.168631
H	-7.861023	-4.603410	0.634247
S	-6.459344	2.132990	0.259024
C	2.400988	6.618571	-0.020691
H	1.736657	6.695241	-0.884708
H	1.797667	6.716361	0.884915
H	3.168291	7.388326	-0.056409
C	8.719207	-6.260116	-0.072680
H	8.447454	-6.792923	0.841762
H	8.347831	-6.832679	-0.925832
H	9.797213	-6.131586	-0.135816

25. **Compound PDI-BTAC-5**

C	-10.524395	3.632518	0.497167
C	-11.242465	2.414695	0.421391
C	-12.657544	2.437955	0.398853
C	-13.395988	3.721807	0.447527
C	-11.229164	4.937937	0.552643
N	-12.631549	4.893276	0.520287
C	-13.362882	1.249642	0.329958
C	-12.686226	0.025642	0.288274
C	-11.292000	-0.048756	0.310372
C	-10.543934	1.169468	0.369200
C	-9.114186	1.172819	0.379853
C	-9.140717	3.611478	0.525202
C	-8.448714	2.396954	0.467912
C	-10.572173	-1.330905	0.280655
C	-9.141788	-1.329336	0.271050
C	-8.399112	-0.109036	0.298421
C	-8.427874	-2.568601	0.233946
C	-7.005166	-2.596273	0.204511
C	-7.014108	-0.176644	0.213923
C	-6.295790	-1.389558	0.149304

C	-10.540575	-3.766661	0.226117
C	-9.156290	-3.785667	0.216272
C	-11.237819	-2.557116	0.258577
C	-8.472773	-5.099868	0.187329
C	-6.301265	-3.900489	0.340791
N	-7.076940	-5.065882	0.249249
H	-14.446952	1.287756	0.311408
H	-13.281348	-0.878067	0.236383
H	-12.320301	-2.595304	0.268787
H	-11.069334	-4.713546	0.206940
H	-7.366161	2.429718	0.497890
H	-8.606601	4.553331	0.590984
O	-10.625408	6.000079	0.622038
O	-14.618269	3.783986	0.426346
O	-9.088610	-6.156779	0.131200
O	-5.099047	-4.001572	0.539180
C	-4.836642	-1.264569	-0.025189
C	-3.981439	-0.560619	0.789214
C	-2.660025	-0.537291	0.272592
C	-2.514572	-1.191675	-0.949200
C	-1.197306	-1.166578	-1.472206
C	-0.324789	-0.490456	-0.643907
S	-4.030867	-1.869501	-1.474541
S	-1.142178	0.142661	0.798501
H	-4.295706	-0.112105	1.724410
H	-0.886170	-1.645331	-2.393317
C	1.089797	-0.264168	-0.830434
C	2.043852	0.014742	0.127131
C	3.333577	0.171316	-0.438213
C	3.379301	0.012781	-1.821877
C	4.675185	0.141938	-2.382963
C	5.631898	0.403759	-1.426687
S	1.790557	-0.321671	-2.460243
S	4.923847	0.502151	0.195654
H	1.818841	0.073698	1.185689
H	4.909535	0.016410	-3.433200
C	7.069682	0.601695	-1.631328
C	7.534194	1.159206	-2.845922
C	8.004289	0.243491	-0.650888
C	8.889230	1.343788	-3.086797
C	9.372757	0.430839	-0.868437
C	9.803443	0.981352	-2.095426

C	10.482033	0.117533	0.017942
C	11.724745	0.441872	-0.559511
C	12.929567	0.238340	0.128195
C	12.897737	-0.334847	1.413514
C	10.453296	-0.418408	1.310910
C	11.650303	-0.637376	1.983193
C	14.239197	-0.701581	2.064707
C	15.276142	0.370151	1.701085
C	15.229445	0.928102	0.408313
N	14.157168	0.596805	-0.432438
C	16.224904	1.807426	-0.034008
C	17.273386	2.155878	0.812595
C	17.321014	1.639713	2.107663
C	16.327498	0.757292	2.537123
H	6.813880	1.472518	-3.595015
H	9.225604	1.776677	-4.024127
H	7.668656	-0.207875	0.278451
H	9.507062	-0.666307	1.782223
H	11.610747	-1.064541	2.978413
H	14.116347	1.120197	-1.297431
H	16.387213	0.357812	3.543580
H	18.128932	1.913639	2.779810
H	18.041892	2.839831	0.463133
H	16.165009	2.225214	-1.037015
C	14.712122	-2.047300	1.441514
C	14.112117	-0.889244	3.585243
H	14.821117	-1.960122	0.356279
H	15.681948	-2.337481	1.862006
H	13.983440	-2.838900	1.651436
H	13.408369	-1.692629	3.820935
H	15.071663	-1.183669	4.019503
H	13.773418	0.027988	4.078323
S	11.560213	1.128588	-2.187462
C	-6.340580	-6.333518	0.320406
H	-5.553263	-6.336928	-0.435894
H	-5.872585	-6.437327	1.302793
H	-7.048053	-7.141400	0.148873
C	-13.383385	6.152553	0.567839
H	-12.667696	6.969803	0.617421
H	-14.007846	6.239752	-0.324376
H	-14.035590	6.157316	1.444424
H	-6.425473	0.730276	0.157322

Table S2: Energies of HOMO, LUMO, Δ_{H-L}, and λ_{max} values of the reference compound PDI-DTT (bay-substituted).

Functional	**HOMO (eV)**	**LUMO (eV)**	**Δ_{H-L} (eV)**	**λ_{max} (nm)**
Experimental	-5.70	-3.80	1.90	490
B3LYP	-5.62	-3.43	2.19	669
B3LYP-D3	-5.58	-3.44	2.14	681
B3PW91	-5.74	-3.55	2.19	668
CAM-B3LYP	-6.90	-2.42	4.48	443
HSEH1PBE	-5.51	-3.73	1.78	675
PBEPBE	-5.00	-3.91	1.09	923
WB97XD	-7.40	-1.93	5.47	440

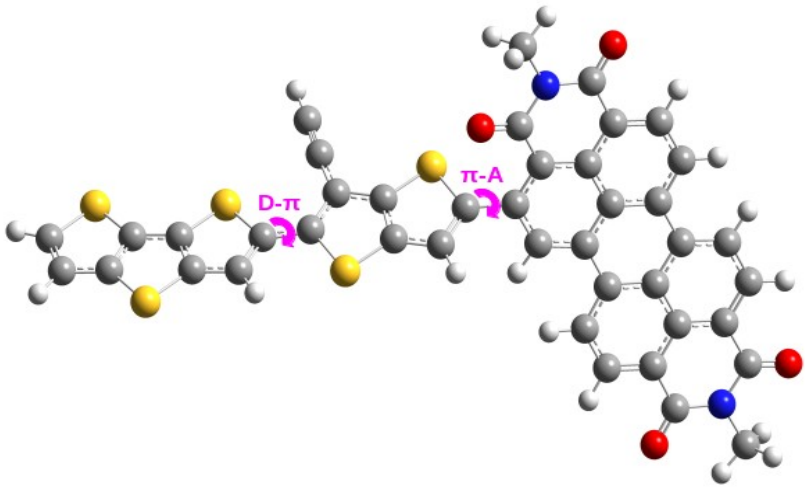


Fig. S1 : Representation of dihedral angles in a monomer.

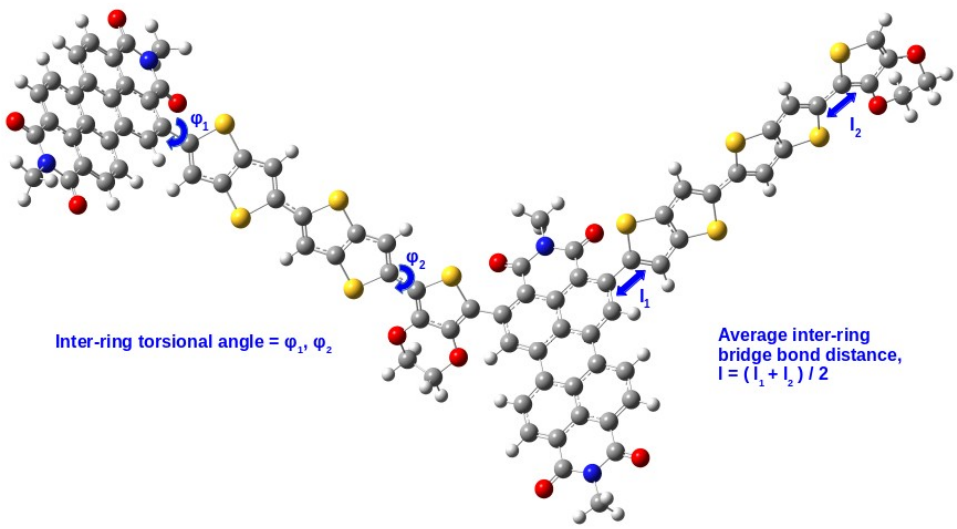
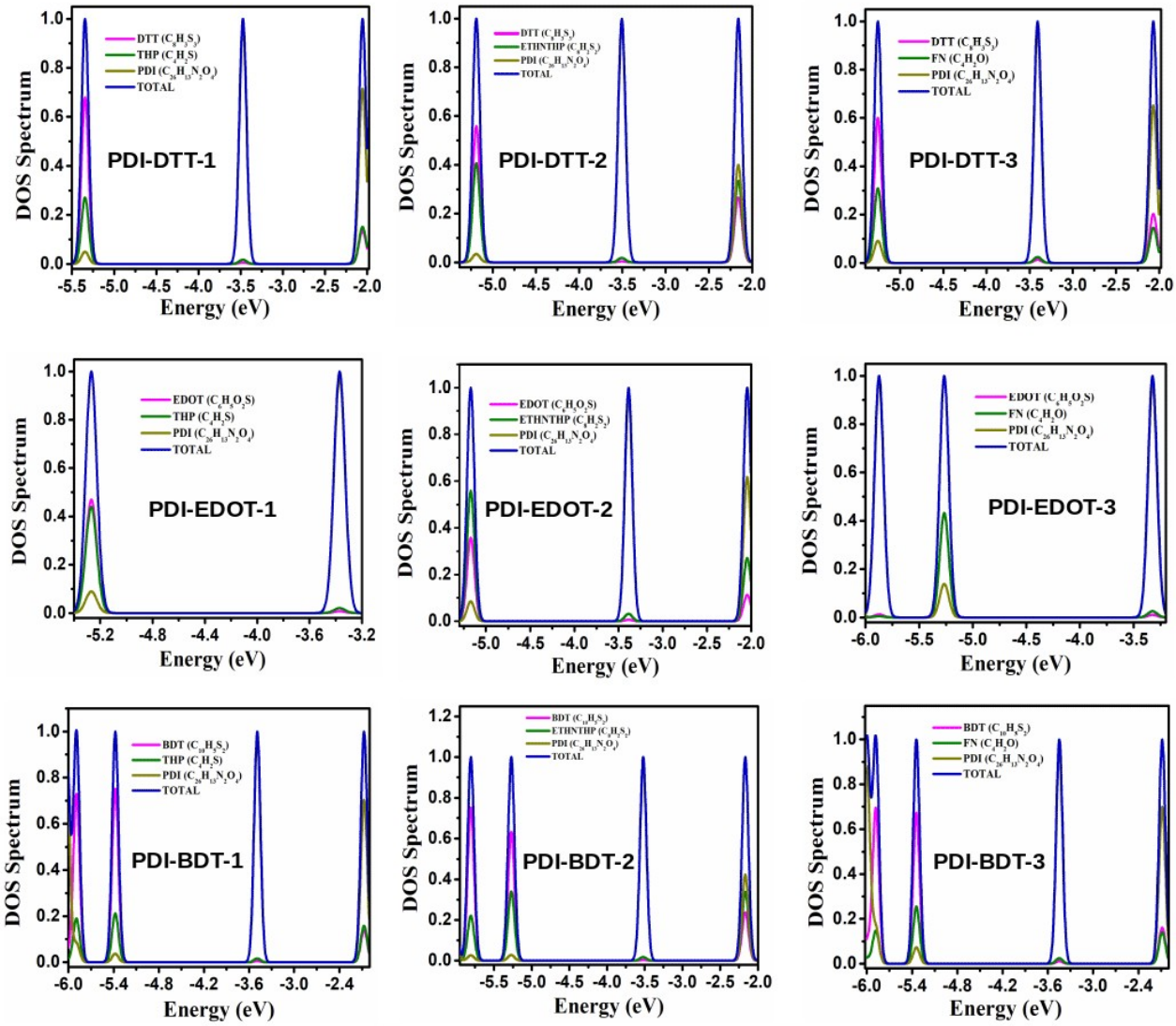


Fig. S2 : Representation of dihedral angle, inter-ring torsional angle, inter-ring bridge bond distance.



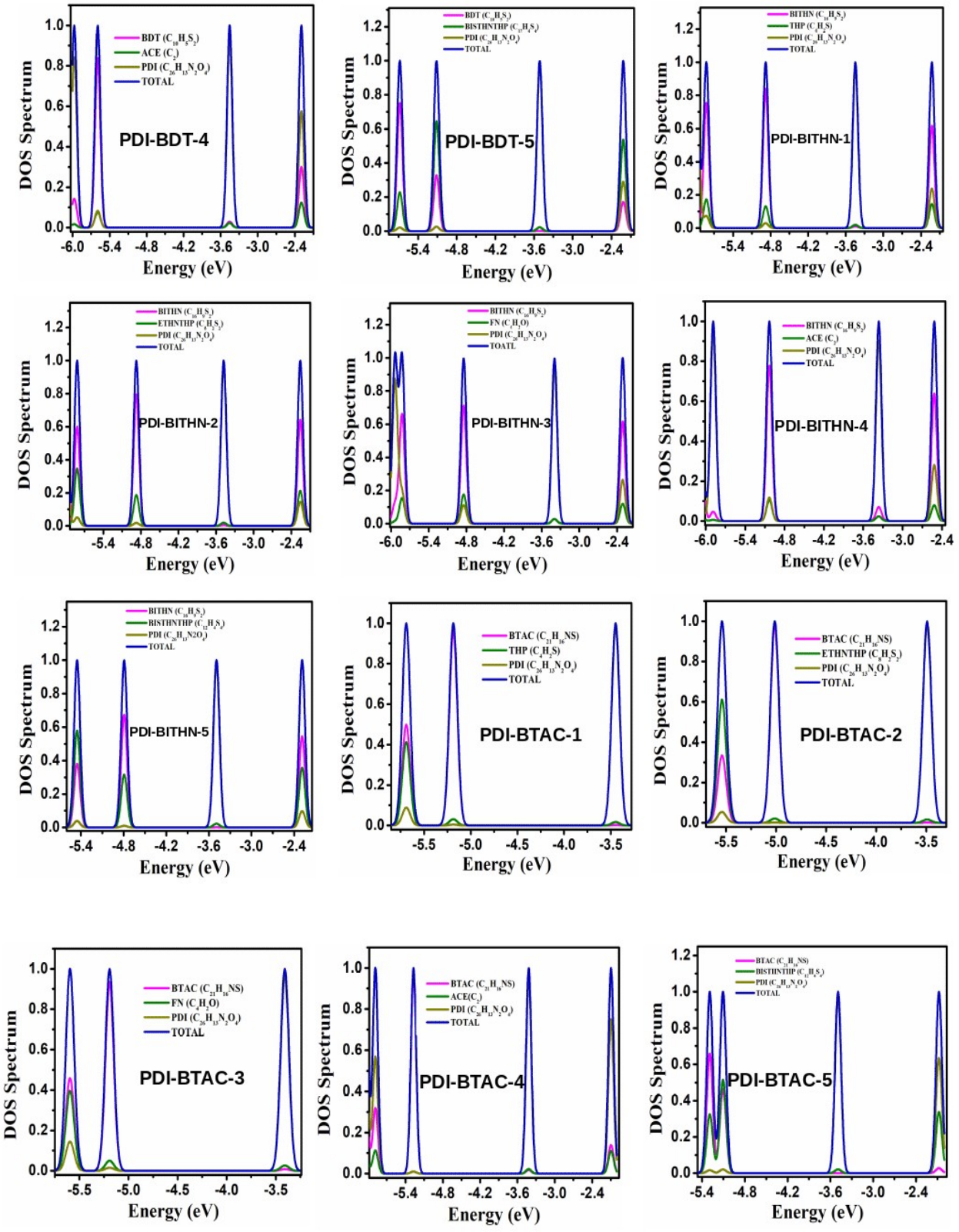


Fig. S3 : PDOS spectra of the studied compounds.

Table S3: Spectral data of designed compounds obtained from PDOS spectra.

Compounds	Groups	Contribution to HOMO (%)	Contribution to LUMO (%)
PDI-DTT-1	Donor Bridging unit Acceptor	68 27 5	1 2 97
PDI-DTT-2	Donor Bridging unit Acceptor	56 41 3	0 2 98
PDI-DTT-3	Donor Bridging unit Acceptor	60 31 9	1 2 97
PDI-DTT-4	Donor Bridging unit Acceptor	67 15 18	3 2 44
PDI-DTT-5	Donor Bridging unit Acceptor	35 63 2	0 2 98
PDI-EDOT-1	Donor Bridging unit Acceptor	47 44 9	1 2 97
PDI-EDOT-2	Donor Bridging unit Acceptor	36 56 8	1 2 97
PDI-EDOT-3	Donor Bridging unit Acceptor	43 43 14	1 3 96
PDI-EDOT-4	Donor Bridging unit Acceptor	45 21 34	2 3 95
PDI-EDOT-5	Donor Bridging unit Acceptor	24 73 3	0 3 97
PDI-BDT-1	Donor Bridging unit	75 21	1 2

	Acceptor	4	97
PDI-BDT-2	Donor Bridging unit Acceptor	63 34 3	0 2 98
PDI-BDT-3	Donor Bridging unit Acceptor	67 26 7	1 3 96
PDI-BDT-4	Donor Bridging unit Acceptor	84 8 8	3 2 95
PDI-BDT-5	Donor Bridging unit Acceptor	33 64 3	0 2 98
PDI-BITHN-1	Donor Bridging unit Acceptor	84 13 3	1 2 97
PDI-BITHN-2	Donor Bridging unit Acceptor	80 18 2	0 98 2
PDI-BITHN-3	Donor Bridging unit Acceptor	71 18 11	3 3 94
PDI-BITHN-4	Donor Bridging unit Acceptor	78 10 12	7 2 91
PDI-BITHN-5	Donor Bridging unit Acceptor	67 32 1	0 2 98
PDI-BTAC-1	Donor Bridging unit Acceptor	97 3 0	0 2 98
PDI-BTAC-2	Donor Bridging unit Acceptor	98 2 0	0 2 98
PDI-BTAC-3	Donor Bridging unit Acceptor	93 5 2	1 3 96

PDI-BTAC-4	Donor Bridging unit Acceptor	98 1 1	2 2 96
PDI-BTAC-5	Donor Bridging unit Acceptor	46 52 2	0 2 98

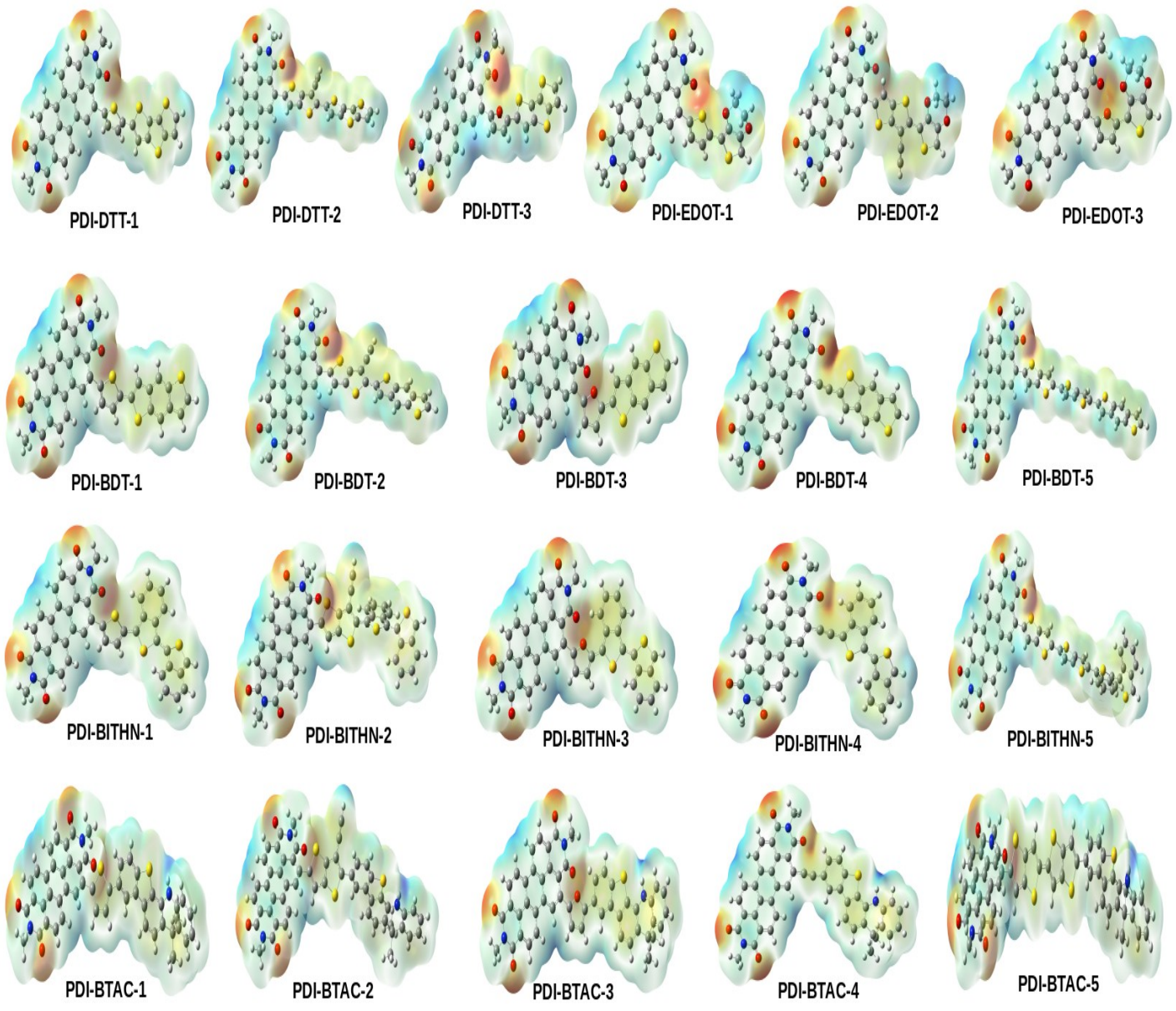


Fig. S4 : MEPS contour plot of the studied compounds.

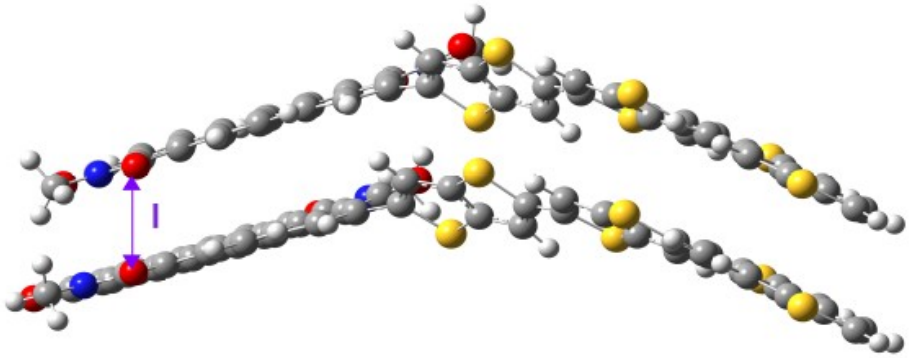
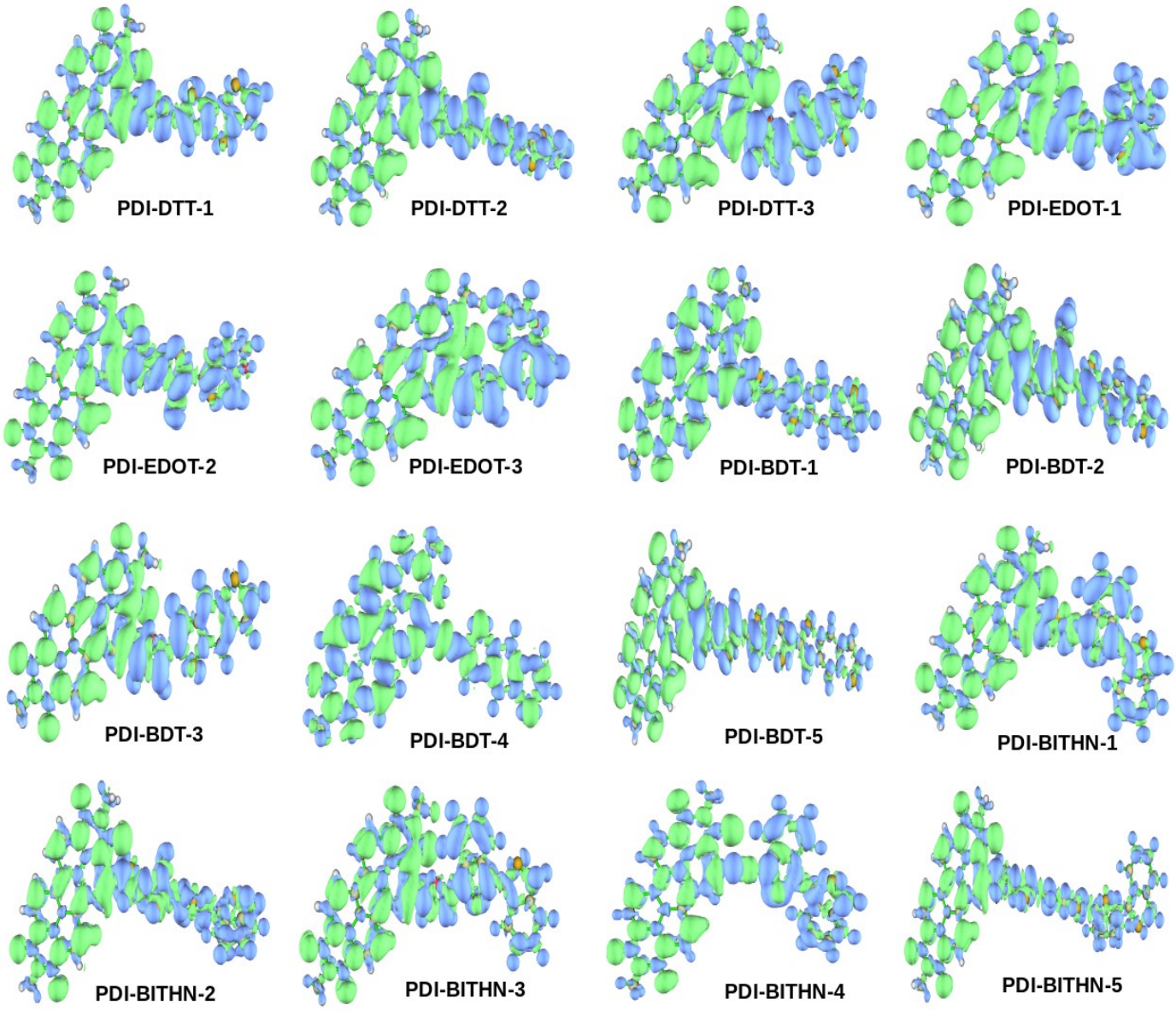


Fig. S5 : Representative structure of two stacked monomers along with distance l.



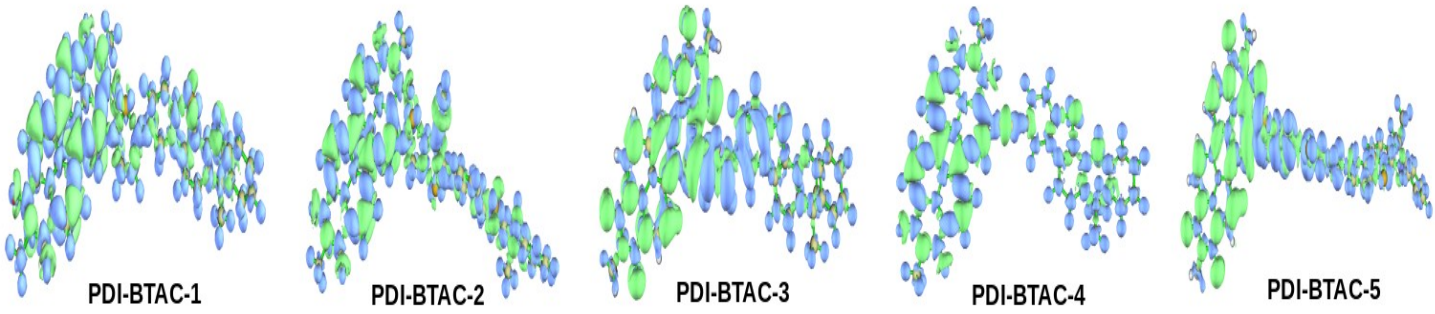


Fig. S6 : Electron density difference (EDD) maps for the studied compounds.

Table S4 : Absorption properties of the studied dimers in the chloroform solvent (ε= 4.7113) at the CAM-B3LYP/6-31G(d) level of theory.

Compounds	**λ_{max} (nm)**	**E_g (eV)**	**f_{osc}**	**Configuration**	**Orbital Contribution (%)**	**n_λ**
PDI-DTT-1	481.27	2.576	1.81	H-3 → L	46	0.9845
PDI-DTT-2	490.75	2.526	1.39	H → L	66	0.9593
PDI-DTT-3	516.93	2.398	0.76	H → L	62	0.8262
PDI-DTT-4	490.69	2.527	2.20	H → L	53	0.9937
PDI-DTT-5	502.74	2.466	1.82	H → L	56	0.9848
PDI-EDOT-1	521.06	2.337	1.23	H-1 → L	31	0.9411
PDI-EDOT-2	546.33	2.256	0.98	H → L	58	0.8953
PDI-EDOT-3	531.74	2.217	1.36	H → L	55	0.9563
PDI-EDOT-4	482.96	2.567	1.54	H-1 → L	30	0.9711
PDI-EDOT-5	535.10	2.317	1.15	H → L	51	0.9292
PDI-BDT-1	480.72	2.579	0.62	H-3 → L	72	0.7601
PDI-BDT-2	481.08	2.577	0.66	H-3 → L	75	0.7812
PDI-BDT-3	489.45	2.533	0.70	H → L	39	0.8005
PDI-BDT-4	478.57	2.591	1.33	H-3 → L	78	0.9532
PDI-BDT-5	485.12	2.556	1.86	H → L	48	0.9862
PDI-BITHN-1	608.16	2.039	0.97	H → L	64	0.8928
PDI-BITHN-2	606.98	2.043	0.74	H → L	70	0.8180

PDI-BITHN-3	647.73	1.914	1.33	H → L	70	0.9532
PDI-BITHN-4	650.20	1.907	2.22	H → L	67	0.9940
PDI-BITHN-5	623.09	1.990	1.03	H → L	68	0.9067
PDI-BTAC-1	478.63	2.590	0.18	H-3 → L	31	0.3393
PDI-BTAC-2	487.21	2.481	0.54	H-3 → L	56	0.7116
PDI-BTAC-3	479.56	2.585	0.72	H-4 → L	41	0.8094
PDI-BTAC-4	475.84	2.606	0.90	H-3 → L	32	0.8741
PDI-BTAC-5	498.42	2.420	0.82	H-3 → L	34	0.8486

Table S5 : Absorption properties of the studied monomers in the gas phase.

Compounds	**λ_{max} (nm)**	**E_g (eV)**	**f_{osc}**	**Configuration**	**Orbital Contribution (%)**
PDI-DTT-1	458	2.703	0.16	H → L	73
PDI-DTT-2	477	2.598	0.28	H → L	82
PDI-DTT-3	491	2.521	0.26	H → L	85
PDI-DTT-4	454	2.729	0.44	H → L	59
PDI-DTT-5	485	2.554	0.46	H → L	71
PDI-EDOT-1	483	2.563	0.16	H → L	88
PDI-EDOT-2	501	2.474	0.32	H → L	84
PDI-EDOT-3	495	2.501	0.17	H → L	90
PDI-EDOT-4	452	2.741	0.63	H → L	63
PDI-EDOT-5	504	2.460	0.35	H → L	79
PDI-BDT-1	455	2.725	0.44	H-1 → L	65
PDI-BDT-2	461	2.685	0.25	H → L	76
PDI-BDT-3	480	2.579	0.22	H → L	79
PDI-BDT-4	452	2.740	0.73	H-1 → L	84
PDI-BDT-5	481	2.576	0.49	H → L	70
PDI-BITHN-1	536	2.312	0.33	H → L	82
PDI-BITHN-2	509	2.433	0.40	H → L	76

PDI-BITHN-3	591	2.095	0.48	H → L	83
PDI-BITHN-4	569	2.178	0.87	H → L	79
PDI-BITHN-5	504	2.459	0.79	H → L	54
PDI-BTAC-1	453	2.732	0.78	H -2 → L	75
PDI-BTAC-2	454	2.730	0.77	H -2 → L	90
PDI-BTAC-3	467	2.653	0.19	H-1 → L	54
PDI-BTAC-4	451	2.744	0.72	H-1 → L	82
PDI-BTAC-5	478	2.590	0.33	H → L	62

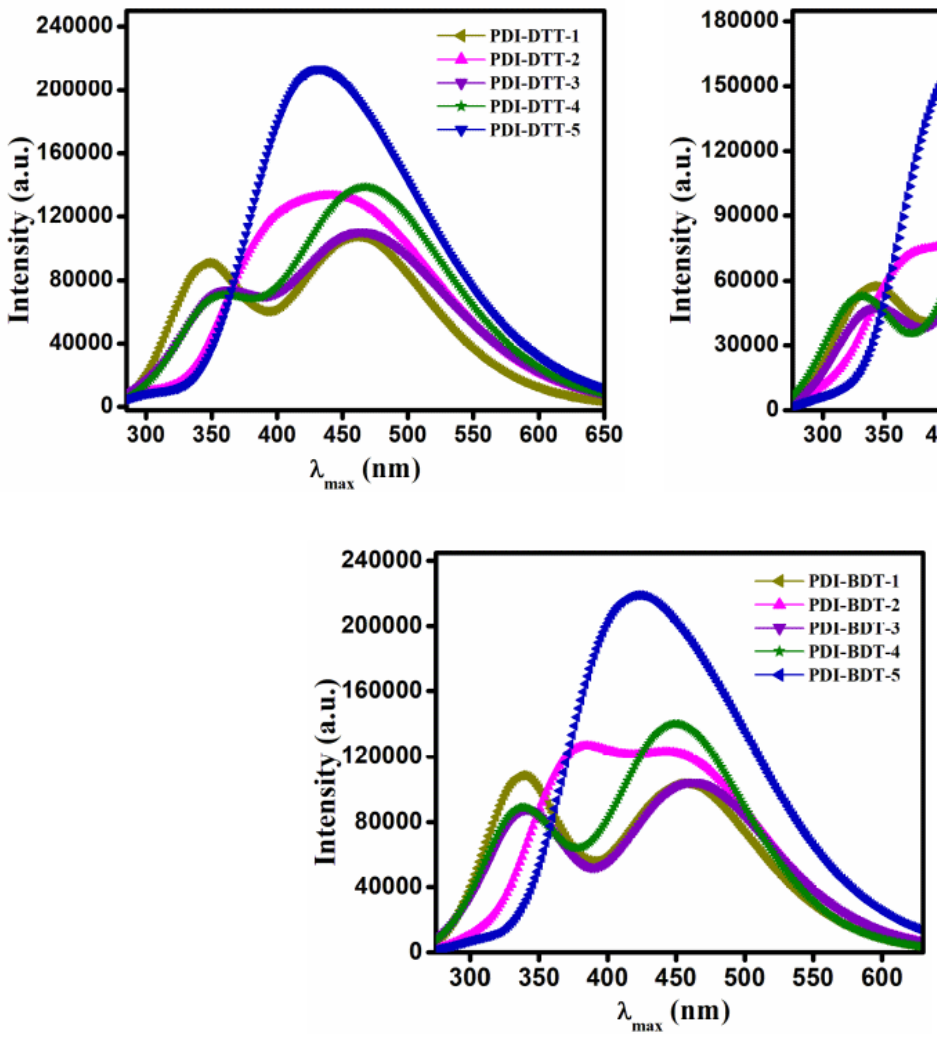


Fig. S7 : Absorption spectra of the PDI-DTT, PDI-EDOT and PDI-BDT groups of dimers.

Table S6 : Energies of planarized and neutral geometries obtained for distortion energy calculation.

Compounds	**$E_{planarized}$ (eV)**	**$E_{neutral}$ (eV)**	**ΔE_{dis} (eV)**
PDI-DTT-1	-94210.760	-94212.104	1.344
PDI-DTT-2	-109191.902	-109193.417	1.515
PDI-DTT-3	-85423.169	-85423.586	0.417
PDI-DTT-4	-81268.726	-81268.798	0.072
PDI-DTT-5	-135045.168	-135046.359	1.191
PDI-EDOT-1	-74592.161	-74593.822	1.661
PDI-EDOT-2	-89573.245	-89575.094	1.849
PDI-EDOT-3	-65804.673	-65805.217	0.544
PDI-EDOT-4	-61650.326	-61650.447	0.121
PDI-EDOT-5	-115426.944	-115428.025	1.081
PDI-BDT-1	-85482.792	-85484.301	1.509
PDI-BDT-2	-100463.371	-100465.537	2.166
PDI-BDT-3	-76695.265	-76695.736	0.471
PDI-BDT-4	-72540.8823	-72540.8828	0.0005
PDI-BDT-5	-126316.889	-126318.506	1.617
PDI-BITHN-1	-91766.066	-91771.182	5.116
PDI-BITHN-2	-106746.143	-106752.397	6.254
PDI-BITHN-3	-82978.496	-82982.720	4.224
PDI-BITHN-4	-78824.256	-78827.995	3.739
PDI-BITHN-5	-132596.950	-132605.350	8.400
PDI-BTAC-1	-87725.292	-87727.183	1.891
PDI-BTAC-2	-102706.728	-102708.443	1.715
PDI-BTAC-3	-78938.130	-78938.682	0.552
PDI-BTAC-4	-74783.799	-74783.817	0.018
PDI-BTAC-5	-128559.976	-128561.399	1.423

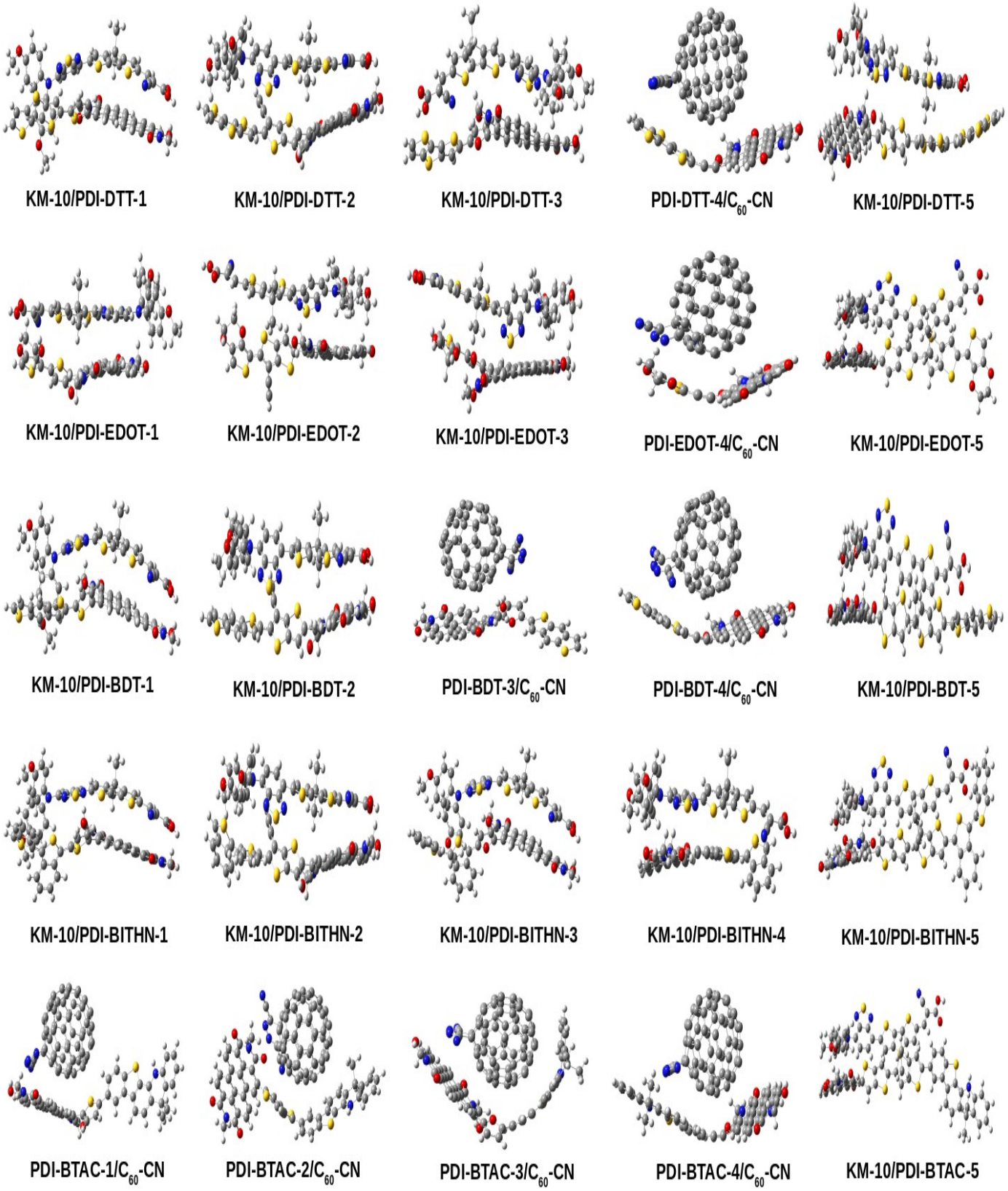


Fig. S8 : Optimized structures of the designed D/A complexes.