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Supporting Information

Terminal Group Engineering in Small Molecule Acceptors: A First Principles Approach to Improving Organic Solar Cell Performance

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Table S1 : Coordinates of the designed compounds in the angstrom unit.

1. Compound A1

Atoms	Coordinates (Angstroms) X	Y	Z
S	-3.588501	1.634208	0.113986
C	-4.956817	0.507436	-0.016645
C	-2.418626	0.332632	-0.180872
C	-4.475088	-0.818936	-0.291725
C	-3.119238	-0.903951	-0.377660
C	-1.044983	0.484486	-0.212981
C	-0.217820	1.632838	-0.073440
C	1.135967	1.417278	-0.172506
C	1.541992	0.071759	-0.392730
S	0.039935	-0.923948	-0.469995
S	4.327830	0.380791	-0.476885
C	2.786984	-0.497127	-0.527997
C	3.018755	-1.915165	-0.736950
C	4.302980	-2.285788	-0.843711
C	5.321967	-1.181172	-0.734360
C	-0.449876	3.088209	0.158423
C	1.841350	2.721408	-0.019204
N	0.825759	3.666523	0.178177
C	1.056291	5.085679	0.381120
H	0.579361	5.665451	-0.413253
H	0.645306	5.401491	1.343129
H	2.134060	5.248983	0.364840
O	3.030789	2.971814	-0.053490
O	-1.485768	3.706097	0.306493
H	-5.139248	-1.656203	-0.447933
H	-2.594991	-1.827965	-0.594355

H	2.193334	-2.617234	-0.788814
H	4.647419	-3.304236	-0.980279
C	-6.246722	0.979024	0.063735
C	-7.474419	0.237501	0.085168
C	-7.772882	-0.990726	0.604482
C	-9.162132	-1.597588	0.432956
C	-9.180380	-2.648162	-0.595393
C	-6.865150	-1.765308	1.380931
N	-6.165519	-2.424842	2.040284
N	-9.172707	-3.469135	-1.415540
H	-6.374858	2.059582	0.061348
H	-8.324331	0.772164	-0.340498
H	-9.875395	-0.818587	0.142726
H	-9.517470	-2.030616	1.375167
C	6.220038	-1.055409	-1.948911
C	7.485938	-1.210227	-1.534573
C	7.416395	-1.432704	-0.072882
C	8.647381	-1.655480	0.770238
C	8.375986	-1.923626	2.183437
N	6.222529	-1.415530	0.408379
N	8.208220	-2.145382	3.308805
H	5.848812	-0.869831	-2.947990
H	8.391970	-1.180316	-2.127882
H	9.224589	-2.491972	0.354465
H	9.297748	-0.773552	0.693183

2. Compound A2

S	4.008123	-0.515321	-0.070960
C	5.176257	-1.846867	-0.112476
C	2.641259	-1.646159	-0.054352
C	4.482679	-3.106047	-0.112426
C	3.125111	-2.991936	-0.077336
C	1.306909	-1.266611	-0.027972
C	0.688923	0.007828	-0.015172
C	-0.689963	0.007134	0.011983
C	-1.306633	-1.267736	0.025511
S	0.000540	-2.493931	-0.002874
S	-4.007317	-0.516287	0.071107
C	-2.640870	-1.647527	0.053629
C	-3.124917	-2.993155	0.077463
C	-4.482519	-3.106885	0.113123
C	-5.175824	-1.847525	0.112796
C	1.163454	1.422003	-0.025760
C	-1.164432	1.421313	0.029080

N	-0.001343	2.199635	0.005301
C	-0.008479	3.653374	-0.003560
H	0.970758	3.997616	0.329814
H	-0.204811	4.036042	-1.009317
H	-0.789031	4.009449	0.670457
O	-2.295058	1.866149	0.063029
O	2.295526	1.863600	-0.051677
H	5.017864	-4.047384	-0.131693
H	2.455434	-3.844302	-0.065036
H	-2.455378	-3.845636	0.065422
H	-5.017946	-4.048069	0.133232
C	6.556883	-1.704149	-0.082072
C	7.336764	-0.456927	-0.083857
C	6.862127	0.732638	-0.675666
C	7.615923	1.898262	-0.642511
C	8.862820	1.879392	-0.021296
C	9.377692	0.716527	0.551087
C	8.617994	-0.443022	0.511620
N	7.917215	-3.907599	0.089645
C	7.306077	-2.918350	0.009871
H	5.915857	0.745126	-1.201750
H	7.259855	2.813088	-1.098553
H	10.354556	0.738069	1.017000
H	9.012422	-1.350545	0.955676
N	9.661172	3.113311	0.019921
O	9.177213	4.123927	-0.490672
O	10.764690	3.061068	0.563264
C	-6.556434	-1.704537	0.082578
C	-7.305682	-2.918719	-0.009050
C	-7.336166	-0.457230	0.083958
C	-6.860902	0.732884	0.674198
C	-7.614563	1.898583	0.640455
C	-8.861955	1.879277	0.020258
C	-9.377440	0.715912	-0.550559
C	-8.617883	-0.443698	-0.510533
N	-7.916755	-3.908032	-0.088476
H	-5.914230	0.745879	1.199528
H	-7.257954	2.813842	1.095198
H	-10.354666	0.737123	-1.015726
H	-9.012797	-1.351574	-0.953423
N	-9.660171	3.113270	-0.021564
O	-10.763952	3.060721	-0.564345
O	-9.175861	4.124223	0.488018

3. Compound A3

S	-4.013765	-0.629773	-0.000140
C	-5.187023	-1.962753	-0.000179
C	-2.642549	-1.757934	0.000272
C	-4.483511	-3.218132	-0.000308
C	-3.126251	-3.106077	-0.000043
C	-1.309846	-1.376626	0.000969
C	-0.690975	-0.102687	0.001077
C	0.689552	-0.101805	0.000832
C	1.310073	-1.375203	0.000603
S	0.000691	-2.604773	0.002580
S	4.014394	-0.628251	-0.000825
C	2.642881	-1.756100	-0.000250
C	3.126499	-3.104337	-0.000471
C	4.483703	-3.216653	-0.000635
C	5.187440	-1.961409	-0.000513
C	-1.165599	1.310092	-0.002231
C	1.163901	1.310995	-0.003011
N	-0.002051	2.089262	-0.006452
C	-0.010165	3.541662	0.001685
H	-0.785632	3.899758	-0.677549
H	-0.213401	3.925878	1.005740
H	0.971766	3.884980	-0.324890
O	2.295199	1.757299	-0.007481
O	-2.295485	1.760094	-0.005690
H	-5.018613	-4.161184	-0.000632
H	-2.453171	-3.955793	-0.000115
H	2.453362	-3.954002	-0.000537
H	5.018615	-4.159810	-0.000872
C	-6.555880	-1.867897	-0.000123
C	-7.443686	-0.727802	0.000240
C	-7.028205	0.626574	0.001065
C	-7.952803	1.659927	0.001490
C	-9.315438	1.358507	0.001064
C	-9.769859	0.038264	0.000263
C	-8.838108	-0.985558	-0.000119
H	-5.977295	0.885333	0.001506
H	-7.638435	2.695880	0.002179
H	-10.834293	-0.158585	-0.000023
H	-9.184193	-2.014988	-0.000723
N	-10.291764	2.451066	0.001499
O	-9.861628	3.606307	0.002134
O	-11.487813	2.151051	0.001204
C	6.556330	-1.866923	-0.000227
C	7.444514	-0.727140	0.000192

C	7.029475	0.627369	0.000792
C	7.954396	1.660425	0.001325
C	9.316942	1.358583	0.001255
C	9.770931	0.038197	0.000669
C	8.838859	-0.985331	0.000157
H	5.978631	0.886392	0.000978
H	7.640388	2.696486	0.001839
H	10.835302	-0.158997	0.000633
H	9.184616	-2.014871	-0.000281
N	10.293590	2.450828	0.001827
O	11.489552	2.150460	0.001824
O	9.863807	3.606211	0.002281
H	-7.061741	-2.831688	-0.000252
H	7.061895	-2.830870	-0.000150

4. Compound A4

S	-4.016268	-0.452722	-0.001639
C	-5.188984	-1.787467	-0.001219
C	-2.643120	-1.579474	-0.000869
C	-4.483267	-3.041731	-0.001119
C	-3.126305	-2.928152	-0.000886
C	-1.310958	-1.198063	0.000037
C	-0.689746	0.075182	0.000316
C	0.691093	0.074162	0.001100
C	1.310421	-1.199689	0.001094
S	-0.000904	-2.428252	0.002077
S	4.015257	-0.454365	0.000722
C	2.642496	-1.581523	0.000676
C	3.125806	-2.930081	0.000242
C	4.482839	-3.043317	0.000226
C	5.188241	-1.788848	0.000699
C	-1.164023	1.487437	-0.003649
C	1.165701	1.486437	-0.001937
N	0.002283	2.265947	-0.006630
C	0.011607	3.717877	0.000762
H	-0.981765	4.060298	-0.290196
H	0.251354	4.101903	0.996796
H	0.761294	4.078008	-0.706119
O	2.295219	1.938026	-0.004580
O	-2.295159	1.934760	-0.008250
H	-5.017076	-3.985569	-0.001138
H	-2.452388	-3.777205	-0.000657
H	2.451975	-3.779209	-0.000174
H	5.016907	-3.987011	-0.000212

C	-6.557243	-1.693423	-0.000889
C	-7.446386	-0.553482	-0.000112
C	-7.033346	0.800533	-0.000111
C	-7.959216	1.832329	0.001133
C	-9.337711	1.553776	0.002318
C	-9.770530	0.214968	0.002176
C	-8.839908	-0.809538	0.000992
H	-5.982407	1.059813	-0.001163
H	-7.622027	2.863262	0.001215
H	-10.832396	-0.006233	0.003036
H	-9.186446	-1.839028	0.000958
C	6.556489	-1.694436	0.000545
C	7.445287	-0.554233	0.000837
C	7.031871	0.799666	0.002291
C	7.957476	1.831734	0.002517
C	9.336039	1.553539	0.001274
C	9.769233	0.214844	-0.000181
C	8.838901	-0.809928	-0.000365
H	5.980871	1.058722	0.003432
H	7.619972	2.862563	0.003713
H	10.831161	-0.006054	-0.001125
H	9.185724	-1.839320	-0.001483
H	-7.062870	-2.657466	-0.000691
H	7.062388	-2.658338	0.000216
C	-10.290634	2.620793	0.003673
C	10.288681	2.620772	0.001524
N	-11.067465	3.487675	0.004787
N	11.065334	3.487811	0.001714

5. Compound A5

S	4.019475	0.295903	0.165101
C	5.181463	1.638972	0.038619
C	2.643242	1.414914	0.092437
C	4.469973	2.892781	-0.039368
C	3.118033	2.768085	-0.015446
C	1.312848	1.040272	0.131438
C	0.687994	-0.229534	0.237854
C	-0.690361	-0.228172	0.237197
C	-1.312486	1.042484	0.130480
S	0.001109	2.268021	0.034947
S	-4.018481	0.298238	0.163850
C	-2.642755	1.417740	0.091141
C	-3.117560	2.770713	-0.017772

C	-4.469584	2.894982	-0.042360
C	-5.180762	1.641011	0.036228
C	1.163520	-1.635944	0.368406
C	-1.166222	-1.634717	0.367459
N	-0.003432	-2.412337	0.429104
C	-0.016592	-3.857342	0.561971
H	1.018790	-4.198184	0.541676
H	-0.486179	-4.150541	1.504840
H	-0.575014	-4.305802	-0.263268
O	-2.294894	-2.083253	0.423459
O	2.294627	-2.078088	0.424392
H	4.999279	3.835708	-0.118463
H	2.435414	3.608448	-0.071708
H	-2.434993	3.611110	-0.074270
H	-4.999156	3.837694	-0.122269
C	6.538593	1.524392	0.088567
C	7.341320	0.302341	0.175651
C	7.191438	-0.806885	-0.697803
C	7.970057	-1.964262	-0.522491
C	8.918191	-2.029317	0.491560
C	9.113154	-0.924147	1.325865
C	8.342101	0.221388	1.161418
H	7.832136	-2.796726	-1.204195
H	9.863660	-0.959437	2.109691
H	8.486689	1.070271	1.823169
C	-6.537880	1.526078	0.086241
C	-7.339935	0.303713	0.174745
C	-7.189031	-0.806492	-0.697389
C	-7.966568	-1.964361	-0.520657
C	-8.914478	-2.029117	0.493623
C	-9.110257	-0.923219	1.326753
C	-8.340358	0.222883	1.160866
H	-7.827831	-2.797576	-1.201275
H	-9.860535	-0.958363	2.110807
H	-8.485717	1.072384	1.821653
H	7.091990	2.459474	0.155271
H	-7.091630	2.460972	0.152633
H	9.513608	-2.927338	0.619856
H	-9.508996	-2.927560	0.623097
C	6.331816	-0.747897	-1.843448
C	-6.329183	-0.748048	-1.842880
N	5.676228	-0.722160	-2.804015
N	-5.673001	-0.722388	-2.803069

6. Compound A6

S	-4.019218	-0.797427	-0.030902
C	-5.189707	-2.135962	-0.045454
C	-2.642913	-1.921457	-0.024201
C	-4.479682	-3.388609	-0.045627
C	-3.123680	-3.271804	-0.033510
C	-1.311782	-1.539484	-0.011850
C	-0.689166	-0.266384	-0.006508
C	0.691650	-0.267867	0.004543
C	1.311451	-1.541850	0.010795
S	-0.001117	-2.770661	-0.000289
S	4.018172	-0.799870	0.030052
C	2.642442	-1.924479	0.023548
C	3.123378	-3.274638	0.033546
C	4.479494	-3.390936	0.046023
C	5.189061	-2.138023	0.045560
C	-1.163516	1.145351	-0.010699
C	1.166408	1.143958	0.007769
N	0.003570	1.924150	-0.001665
C	0.017107	3.375646	-0.003455
H	-1.019207	3.713794	0.010497
H	0.544450	3.750079	0.877485
H	0.519071	3.750455	-0.899210
O	2.295294	1.597443	0.016652
O	-2.294890	1.592354	-0.019342
H	-5.011149	-4.333804	-0.054134
H	-2.447593	-4.119137	-0.031520
H	2.447423	-4.122084	0.031795
H	5.011326	-4.335923	0.055108
C	-6.556659	-2.045959	-0.053596
C	-7.452166	-0.907718	-0.048949
C	-7.045168	0.446602	-0.041931
C	-7.980337	1.473471	-0.033266
C	-9.347705	1.185216	-0.034501
C	-9.776814	-0.145283	-0.045261
C	-8.843025	-1.170163	-0.053262
H	-7.650087	2.506437	-0.033594
H	-10.838025	-0.368075	-0.055166
H	-9.185345	-2.201143	-0.064811
C	6.555986	-2.047403	0.054263
C	7.450944	-0.908728	0.049779
C	7.043350	0.445419	0.042570
C	7.978093	1.472680	0.034211
C	9.345585	1.185000	0.035883

C	9.775274	-0.145307	0.046790
C	8.841923	-1.170581	0.054551
H	7.647365	2.505489	0.034481
H	10.836571	-0.367655	0.057010
H	9.184687	-2.201411	0.066243
H	-7.059399	-3.011615	-0.061847
H	7.059179	-3.012820	0.062984
H	-5.995285	0.710550	-0.045484
H	5.993389	0.709055	0.045806
C	-10.353809	2.297875	0.043972
F	-9.901865	3.429859	-0.541447
F	-10.649642	2.612046	1.328552
F	-11.520380	1.964534	-0.554861
C	10.351186	2.298181	-0.042066
F	9.898485	3.429784	0.543509
F	11.517693	1.965178	0.557128
F	10.647462	2.612724	-1.326464

7. Compound A7

S	4.009505	-0.310066	-0.053721
C	5.178571	-1.641721	-0.079197
C	2.642124	-1.440312	-0.080064
C	4.484592	-2.900115	-0.107397
C	3.126439	-2.785788	-0.104094
C	1.307657	-1.060226	-0.079409
C	0.689341	0.213898	-0.068545
C	-0.690328	0.213157	-0.068810
C	-1.307257	-1.061418	-0.079826
S	0.000675	-2.287717	-0.091934
S	-4.008687	-0.311162	-0.054356
C	-2.641648	-1.441791	-0.080738
C	-3.126144	-2.787132	-0.104992
C	-4.484354	-2.901105	-0.108421
C	-5.178052	-1.642542	-0.080022
C	1.163859	1.627666	-0.067060
C	-1.164978	1.626949	-0.067897
N	-0.001598	2.405402	-0.062804
C	-0.008873	3.858809	-0.072287
H	0.966162	4.202749	0.273502
H	-0.192143	4.241434	-1.080618
H	-0.797649	4.215961	0.591614
O	-2.295763	2.073206	-0.069094

O	2.295957	2.070484	-0.067183
H	5.019746	-3.841572	-0.122388
H	2.456526	-3.637985	-0.115321
H	-2.456356	-3.639431	-0.116309
H	-5.019745	-3.842425	-0.123619
C	6.557973	-1.499003	-0.015843
C	7.338650	-0.252546	0.007594
C	6.877448	0.943141	-0.580650
C	7.632617	2.106102	-0.523685
C	8.882066	2.106136	0.117805
C	9.367628	0.915260	0.685921
C	8.609171	-0.243231	0.624099
H	5.939955	0.962386	-1.122288
H	7.264625	3.015774	-0.985259
H	10.336002	0.908347	1.174056
H	8.996007	-1.154919	1.066725
C	-6.557432	-1.499511	-0.016727
C	-7.337869	-0.252920	0.007275
C	-6.876162	0.943227	-0.579657
C	-7.631126	2.106292	-0.521994
C	-8.880893	2.105984	0.118869
C	-9.366970	0.914677	0.685653
C	-8.608707	-0.243899	0.623159
H	-5.938411	0.962881	-1.120818
H	-7.262666	3.016315	-0.982496
H	-10.335588	0.907504	1.173300
H	-8.995952	-1.155891	1.064795
C	9.659518	3.306873	0.181413
C	-9.658159	3.306803	0.183207
N	10.290021	4.283354	0.233304
N	-10.288549	4.283325	0.235697
C	7.304624	-2.714144	0.084189
C	-7.304331	-2.714557	0.082759
N	7.914854	-3.703408	0.171257
N	-7.914721	-3.703761	0.169365

8. Compound A8

S	-4.006766	-0.079449	-0.190790
C	-5.163192	-1.419048	-0.198469
C	-2.638711	-1.206584	-0.125265
C	-4.472612	-2.681312	-0.177849
C	-3.118462	-2.559268	-0.134329
C	-1.307113	-0.831129	-0.068511

C	-0.686982	0.444346	-0.039618
C	0.688218	0.443237	0.039826
C	1.306230	-0.832901	0.068843
S	-0.001256	-2.059549	0.001890
S	4.005552	-0.081412	0.190263
C	2.637787	-1.208853	0.123818
C	3.117588	-2.561475	0.130437
C	4.471800	-2.683306	0.173165
C	5.162132	-1.420912	0.196134
C	-1.160923	1.858055	-0.082098
C	1.162690	1.857095	0.075281
N	0.002808	2.635936	-0.006709
C	0.014060	4.088482	-0.003571
H	-0.988768	4.427673	-0.263821
H	0.286097	4.470490	0.984338
H	0.738765	4.451539	-0.735150
O	2.289689	2.304156	0.158433
O	-2.289618	2.299446	-0.171112
H	-5.010719	-3.621376	-0.184076
H	-2.442589	-3.406338	-0.103242
H	2.441738	-3.408515	0.097909
H	5.010073	-3.623286	0.177642
C	-6.529035	-1.241907	-0.263016
C	-7.215053	0.074979	-0.226082
C	-7.076951	0.963779	0.868301
C	-7.723909	2.210453	0.853339
C	-8.521882	2.573186	-0.226555
C	-8.691452	1.687614	-1.293468
C	-8.047929	0.452553	-1.288310
H	-7.603696	2.875794	1.701361
H	-9.322351	1.960572	-2.133461
H	-8.177657	-0.233383	-2.119241
C	6.527946	-1.243829	0.261723
C	7.213725	0.073304	0.228870
C	7.076393	0.965277	-0.862968
C	7.722573	2.212291	-0.843454
C	8.518877	2.572310	0.238564
C	8.687583	1.683703	1.303093
C	8.044882	0.448251	1.293380
H	7.603135	2.880034	-1.689692
H	9.317101	1.954618	2.144781
H	8.173915	-0.240074	2.122444
H	-9.018980	3.537678	-0.230150
H	9.015334	3.537112	0.245711
C	-6.333620	0.594287	2.037769

C	6.334700	0.598662	-2.034349
N	-5.750143	0.311763	3.003250
N	5.752450	0.318024	-3.001142
C	-7.354534	-2.388257	-0.439916
N	-8.036280	-3.321658	-0.598249
C	7.353425	-2.390476	0.436786
N	8.035171	-3.324128	0.593606

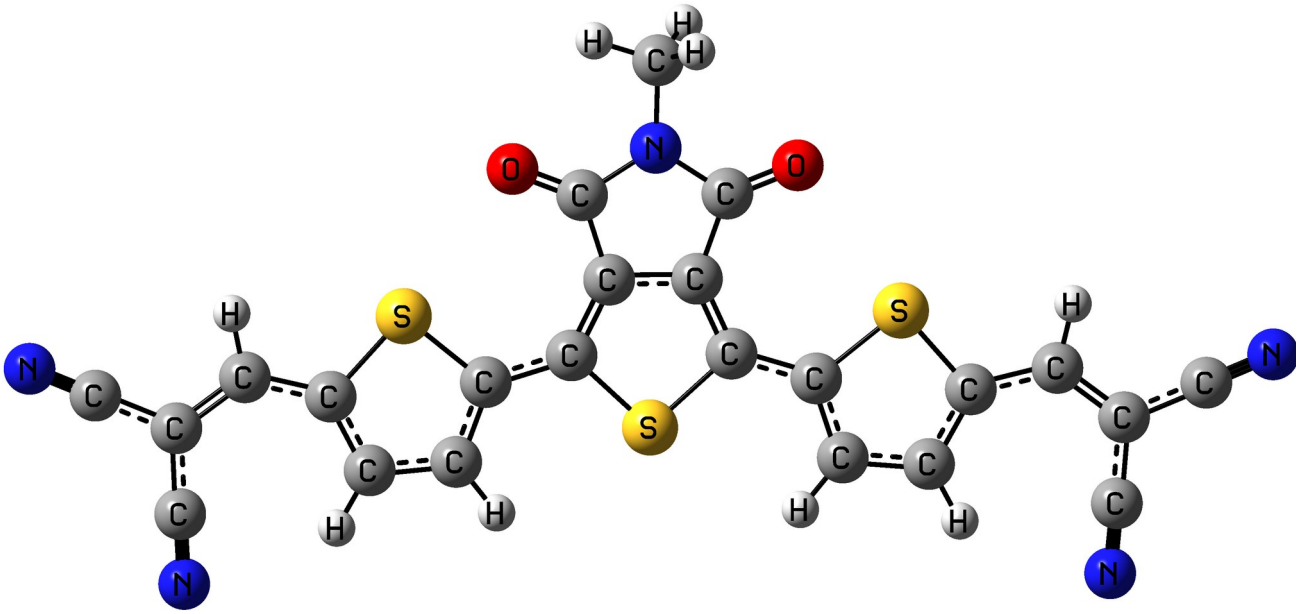

Fig. S1: Optimized structure of the test compound

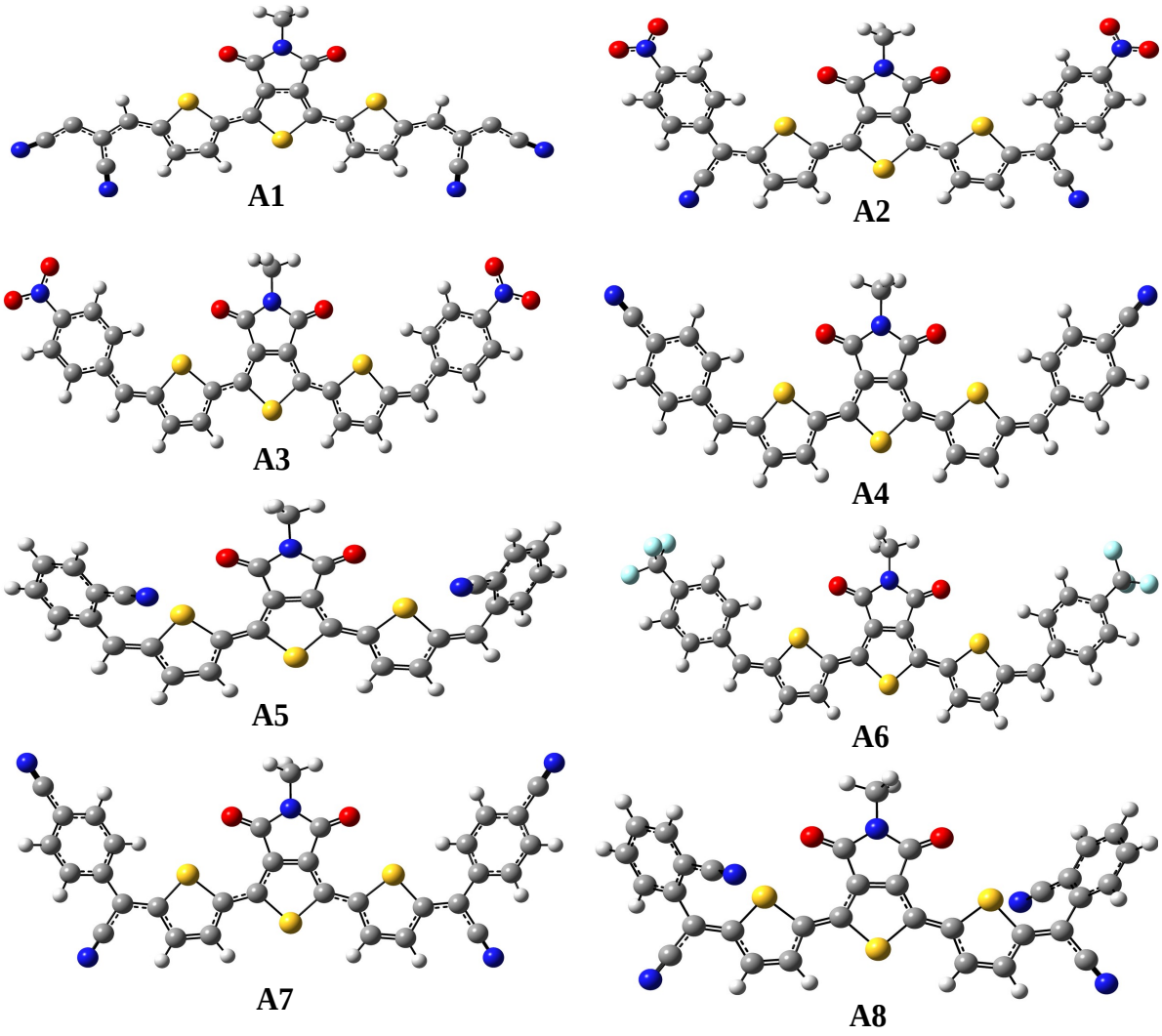

Fig. S2: Optimized structures of the studied compounds.

Table S2: Energies of HOMO, LUMO, Δ_{H-L}, and λ_{max} values of the test compound with different functional along with 6-31G (d,p) basis set.

Functional	**HOMO (eV)**	**LUMO (eV)**	**Δ_{H-L} (eV)**	**λ_{max} (nm)**
Experimental	-6.34	-3.75	2.59	477
B3LYP	-6.45	-3.84	2.61	542
B3LYP-D3	-6.44	-3.84	2.60	544
B3PW91	-6.58	-3.94	2.64	538
CAM-B3LYP	-7.65	-2.70	4.95	422
PBEPBE	-5.86	-4.33	1.53	617
wB97XD	-8.23	-2.19	6.04	414

Table S3: Validation of basis set.

Compound	**6-311G (d,p)**	**6-31G (d,p)**	**reported value**
TPD-T-CN	420 nm	422 nm	477 nm

We have also validated the basis sets used in our calculations. To further evaluate the reliability of the employed basis sets, we conducted additional test calculations using the reference compound TPD-T-CN with both double-zeta and triple-zeta basis sets (6-31G (d,p) and 6-311G (d,p), respectively) with CAM-B3LYP functional. The results of these tests have presented in Table S3. From this Table, it is evident that the double-zeta basis set shows a closer match with the reported results, affirming its appropriateness for our calculations. We are confident that this selected basis set offers a reasonable compromise between computational cost and accuracy for the systems under investigation.

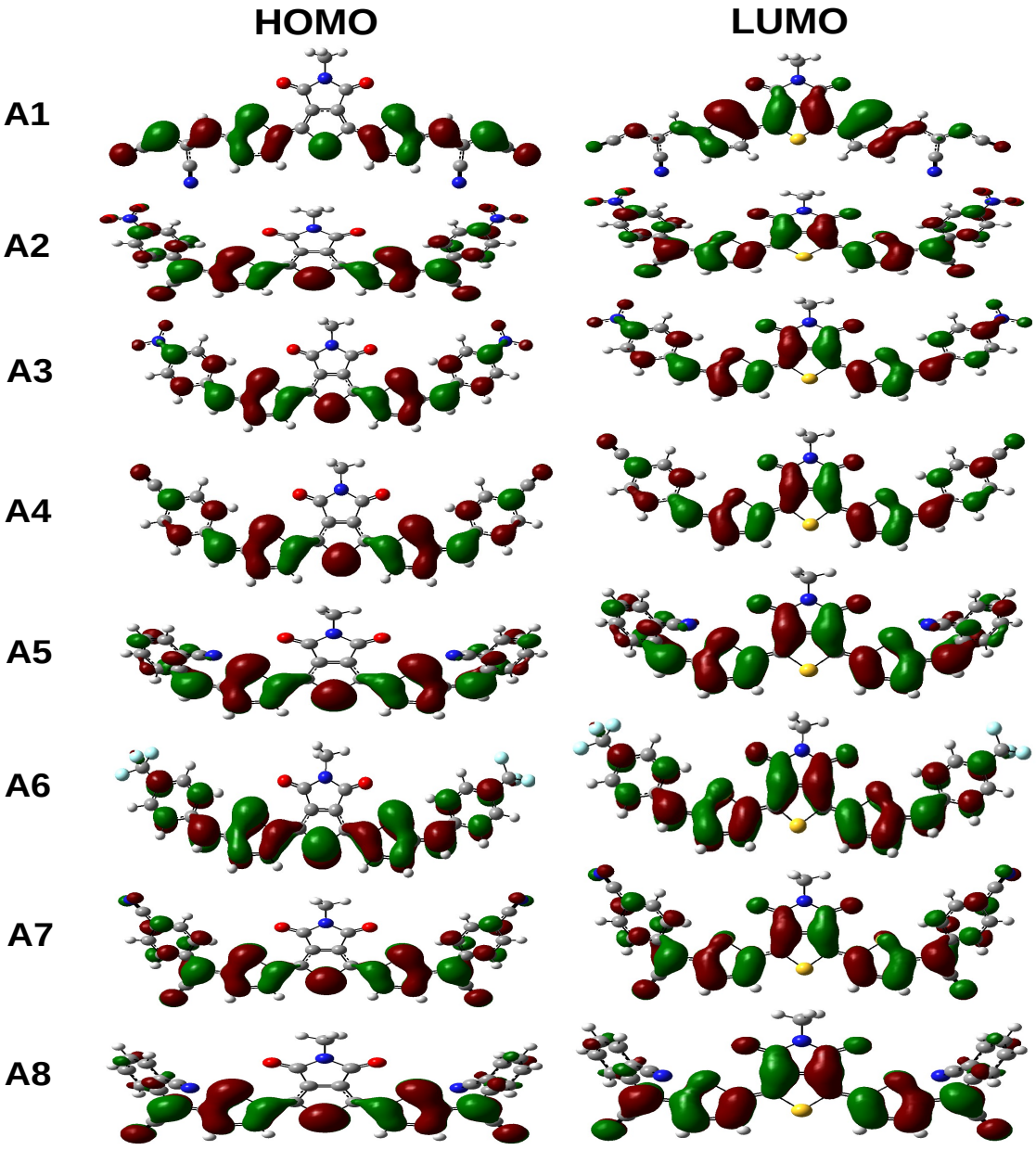

Fig. S3 : FMO diagram of the studied compounds in the solvent phase.

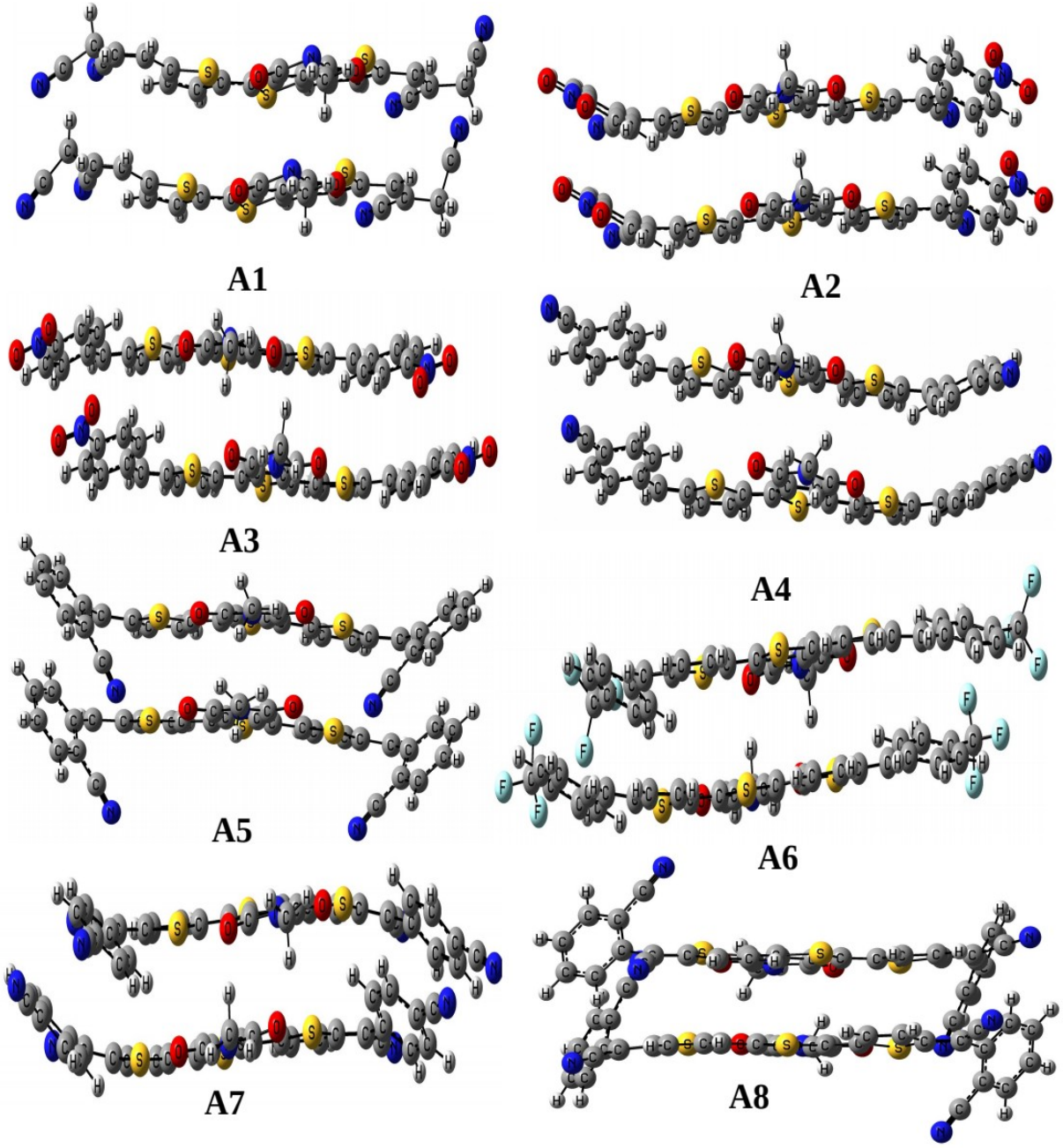

Fig. S4: Optimized structure of two stacked compounds.

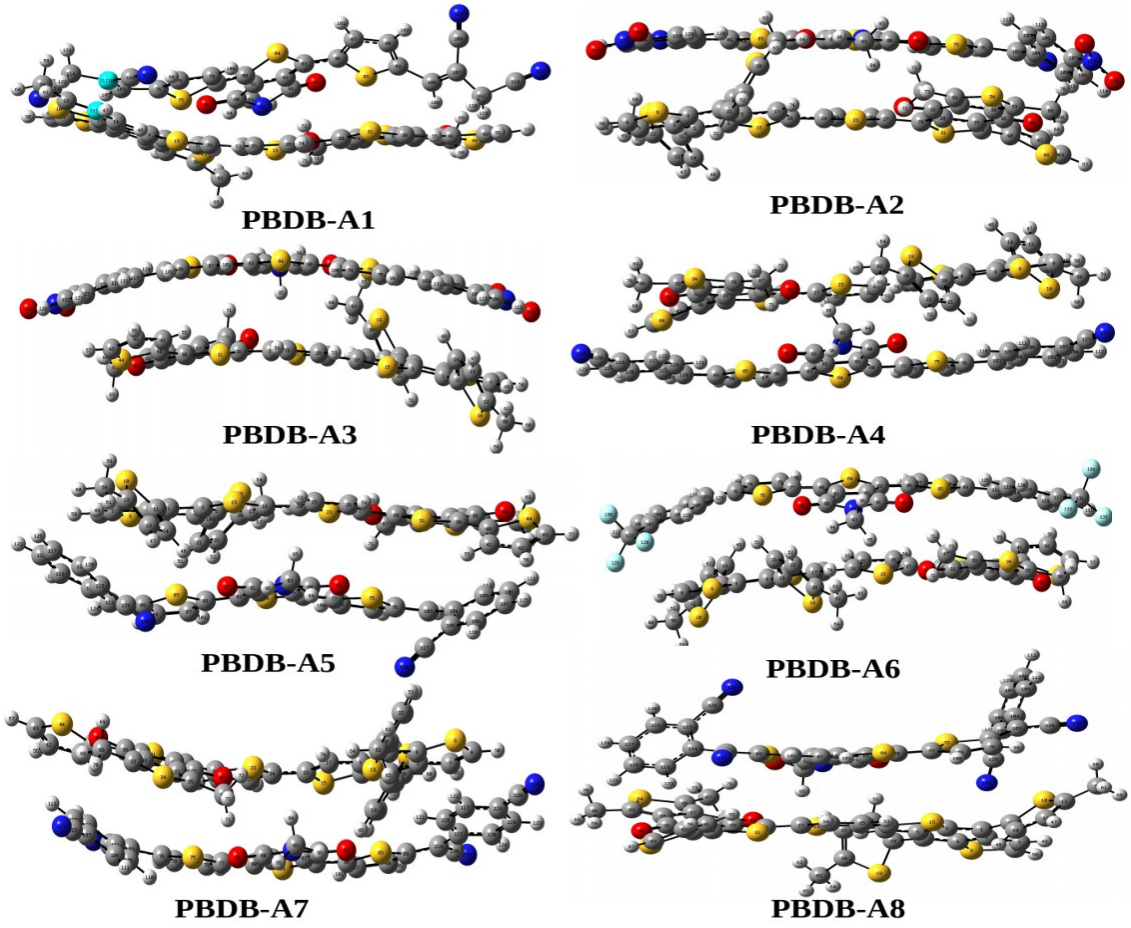

Fig. S5: Optimized structure of D/A blends.