Supporting Information

Enhancing Photovoltaic Properties of Organic Solar Cells through Core Alteration of Methyl-Substituted Bithiophene-Based Small Molecule Acceptors

Smiti Rani Bora[1] and Dhruba Jyoti Kalita[1,*]
Department of Chemistry, Gauhati University, Guwahati-781014, India
E-mail: dhrubajyoti.kalita@gauhati.ac.in

Table S1 : Coordinates of the investigated compounds studied at HSEH1PBE/6-31G(d,p) level of theory in the angstrom unit.

1. **Compound C1**

Atoms	Coordinates (Angstroms) X	Y	Z
C	-10.841947	-0.688548	0.008619
C	-9.708774	0.208561	0.003542
C	-7.429416	1.268108	0.052414
C	-0.323447	-0.613853	-0.115692
C	0.331958	0.606262	0.023975
C	7.436443	-1.276760	-0.107065
C	9.702912	-0.203541	0.061894
C	10.837651	0.690968	0.056588
C	13.172975	1.555349	-0.013919
S	-12.295663	-0.198711	-0.821376
S	-8.082545	-0.325245	0.312691
S	-0.808684	1.897724	0.195241
S	0.817563	-1.905174	-0.287117
S	8.085242	0.328129	-0.291365
S	12.431295	0.012776	-0.147495
C	-13.114238	-1.638294	-0.368425
H	-14.139163	-1.798945	-0.672468
C	-12.309537	-2.458068	0.366280
H	-12.631832	-3.419004	0.752499
C	-11.004838	-1.933470	0.592208
C	-9.708646	1.558571	-0.273561

H	-10.619808	2.107534	-0.489124
C	-8.433435	2.171716	-0.255605
C	-1.730121	-0.526197	-0.073447
H	-2.409754	-1.366980	-0.145640
C	1.738566	0.519031	-0.019161
H	2.418295	1.359925	0.050457
C	8.438008	-2.185738	0.194555
C	9.705972	-1.563940	0.283360
H	10.609259	-2.108370	0.539703
C	10.903207	2.066658	0.201550
C	12.245698	2.539938	0.160449
H	12.503065	3.588250	0.266474
H	-9.462729	-2.013835	2.103254
H	-10.426828	-3.487973	1.943870
C	-8.223219	3.622588	-0.558399
H	-7.257408	3.792008	-1.042628
H	-9.009733	3.994606	-1.220434
C	8.226126	-3.645002	0.451795
H	7.251590	-3.830505	0.912356
H	9.001061	-4.034856	1.117139
C	9.731971	2.980922	0.394203
H	9.178313	3.137596	-0.539049
H	9.022640	2.587300	1.128925
C	-9.967682	-2.668108	1.385640
H	-9.193328	-3.103285	0.742976
H	-8.248182	4.234881	0.351167
H	8.269313	-4.230088	-0.474793
H	10.068355	3.960801	0.742484
H	14.248309	1.648243	-0.075178
C	-2.157159	0.773802	0.097686
C	2.165627	-0.780879	-0.190736
C	-6.011061	1.501514	0.175858
C	-3.506055	1.264800	0.194072
C	3.515014	-1.270553	-0.287285
C	6.019682	-1.507404	-0.249229
S	-4.858920	0.257387	-0.234068
S	4.862904	-0.275346	0.183469
C	-5.350470	2.640157	0.589911
H	-5.869777	3.528388	0.926741
C	-3.946560	2.507813	0.596792

H	-3.271894	3.292478	0.921505
C	3.960020	-2.501571	-0.720298
H	3.288833	-3.276132	-1.075057
C	5.363965	-2.633975	-0.702700
H	5.887211	-3.511802	-1.060068

2. **Compound C2**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	14.021857	0.894088	0.592915
C	12.922191	-0.024144	0.406019
C	10.694479	-1.128455	0.028141
C	-10.696971	1.125648	0.096113
C	-12.913473	-0.002938	0.454324
C	-14.023413	-0.924743	0.539803
C	-16.335753	-1.844848	0.652187
S	15.483436	0.304889	1.342056
S	11.314422	0.498076	-0.006893
S	-11.321265	-0.493028	-0.043906
S	-15.643864	-0.285871	0.455865
C	16.249110	1.835065	1.199552
H	17.261541	1.970093	1.553705
C	15.423862	2.752080	0.619443
H	15.712051	3.781646	0.436916
C	14.145118	2.234597	0.265934
C	12.941126	-1.395711	0.542803
H	13.843975	-1.943454	0.793888
C	11.695046	-2.034228	0.338778
C	-11.688627	2.007975	0.491845
C	-12.929502	1.355262	0.686585
H	-13.819406	1.875691	1.026126
C	-14.044235	-2.300493	0.694660
C	-15.374209	-2.805976	0.758495
H	-15.597279	-3.859479	0.888382
H	-17.410051	-1.963768	0.674380
C	-12.839554	-3.185096	0.800940
H	-12.360803	-3.341878	-0.172857
H	-12.081914	-2.765330	1.469890

H	-13.122581	-4.167594	1.187224
C	-11.488959	3.470316	0.741851
H	-10.475598	3.678065	1.096655
H	-11.647143	4.062302	-0.167682
H	-12.197816	3.832831	1.491223
C	11.505740	-3.512900	0.475195
H	10.501706	-3.752761	0.835954
H	11.644686	-4.030429	-0.481679
H	12.232761	-3.930082	1.177227
C	13.090627	3.074352	-0.387452
H	12.681054	2.594271	-1.282393
H	12.249607	3.272718	0.287235
H	13.505573	4.040084	-0.686539
C	9.300871	-1.380417	-0.252663
C	6.797902	-1.208743	-0.474284
C	5.407416	-0.771269	-0.452032
C	3.054609	-1.309415	-0.480290
C	2.744586	0.062762	-0.431453
C	1.299492	0.203128	-0.428787
C	0.724836	-1.085139	-0.472526
C	-1.302598	-0.178971	-0.444402
C	-0.727929	1.109282	-0.400260
C	-2.747713	-0.038585	-0.440936
C	-3.057638	1.333834	-0.399093
C	-5.410514	0.795388	-0.412056
C	-6.800904	1.233756	-0.406134
C	-9.303071	1.392543	-0.169745
S	8.073127	-0.221233	0.176233
S	-8.076302	0.205788	0.178378
N	-0.581195	-1.306827	-0.480969
N	0.578095	1.330945	-0.391088
C	8.721481	-2.482585	-0.847080
H	9.300503	-3.312101	-1.233384
C	7.318268	-2.385261	-0.965391
H	6.706469	-3.140336	-1.445709
C	5.075287	0.596292	-0.403480
H	5.873199	1.333771	-0.398720
C	3.755119	1.020082	-0.389034
H	3.506932	2.076190	-0.354773
C	4.372022	-1.725278	-0.483428

H	4.618134	-2.783602	-0.485542
C	1.792647	-2.158629	-0.506725
C	-1.795697	2.182743	-0.364025
C	-3.758371	-0.996425	-0.464951
H	-3.510263	-2.052499	-0.500856
C	-5.078528	-0.572416	-0.454099
H	-5.876482	-1.308437	-0.500338
C	-4.375036	1.749179	-0.377622
H	-4.621036	2.805305	-0.309198
C	-7.320820	2.440382	-0.818011
H	-6.708866	3.225208	-1.247757
C	-8.723861	2.530889	-0.691404
H	-9.303142	3.384480	-1.020752
C	1.682930	-3.068367	0.724161
H	0.712449	-3.572920	0.726401
H	2.471029	-3.827909	0.711659
H	1.776454	-2.493492	1.649732
C	1.683011	-2.988289	-1.792980
H	1.778621	-2.356137	-2.680264
H	2.469885	-3.748488	-1.827416
H	0.711838	-3.490276	-1.828710
C	-1.689783	3.004770	0.927584
H	-0.719169	3.507476	0.968360
H	-2.477515	3.763860	0.965554
H	-1.786665	2.366981	1.810624
C	-1.682261	3.099743	-1.589025
H	-1.774810	2.530867	-2.518452
H	-2.469273	3.860403	-1.572755
H	-0.711093	3.602950	-1.586438

3. **Compound C3**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	14.919160	0.253474	-0.492156
C	13.584603	0.142262	0.056369
C	11.106122	0.062522	0.451993
C	-11.111655	0.056755	0.458612
C	-13.583084	-0.163946	0.081675

C	-14.912834	-0.339028	-0.463233
C	-17.374020	-0.168351	-0.802345
S	16.205079	0.799800	0.551496
S	12.156997	0.161623	-0.933199
S	-12.150176	-0.331176	-0.883855
S	-16.232336	0.529393	0.273684
C	17.372143	0.640922	-0.697863
H	18.409307	0.878445	-0.506477
C	16.801985	0.207715	-1.858146
H	17.362921	0.041265	-2.771522
C	15.398781	-0.018595	-1.761478
C	13.229706	0.063668	1.384735
H	13.964354	0.038324	2.183301
C	11.834161	0.016327	1.624526
C	-11.849426	0.324465	1.595208
C	-13.242077	0.192512	1.367083
H	-13.983187	0.325487	2.148686
C	-15.361092	-1.118798	-1.514531
C	-16.770617	-1.008428	-1.691179
H	-17.312108	-1.553095	-2.457208
H	-18.422726	0.081270	-0.720251
C	-14.506236	-1.999497	-2.374254
H	-14.014957	-1.434049	-3.174798
H	-13.718779	-2.491985	-1.796651
H	-15.114707	-2.774414	-2.848231
C	-11.270842	0.667976	2.932757
H	-10.280490	0.225317	3.064373
H	-11.158562	1.751323	3.042411
H	-11.918072	0.306005	3.736520
C	11.244110	-0.059128	2.998759
H	10.264639	0.423785	3.038268
H	11.105028	-1.100193	3.307034
H	11.897686	0.431669	3.725280
C	14.579173	-0.505711	-2.917247
H	13.882873	-1.295859	-2.619402
H	13.982957	0.299194	-3.362923
H	15.227170	-0.905225	-3.701709
C	9.657169	-0.027775	0.285095
C	8.884129	0.869709	-0.444016
C	7.454196	0.784610	-0.601536

C	6.708020	-0.243687	0.004372
C	8.905413	-1.084098	0.850899
C	7.491466	-1.191624	0.715139
C	5.262839	-0.378873	-0.040801
C	3.144359	-1.333622	0.062554
C	2.802630	-0.003522	-0.050497
C	1.370022	0.168934	-0.063116
C	0.810842	-1.127703	0.051435
C	-1.370641	-0.168466	-0.023387
C	-0.811397	1.128103	-0.139147
C	-2.803156	0.004517	-0.031364
C	-3.144825	1.334193	-0.149005
C	-5.264143	0.376996	-0.080738
C	-6.709501	0.254018	-0.013894
C	-7.457141	-0.871166	-0.411117
C	-8.888013	-0.920981	-0.246860
C	-9.661718	0.103556	0.288957
C	-7.493789	1.323643	0.495633
C	-8.908587	1.247695	0.642295
S	9.526661	2.275331	-1.270167
S	4.183761	1.010619	-0.142797
N	9.340148	-2.134776	1.577478
N	7.100034	-2.303748	1.374852
N	-7.102952	2.542947	0.926902
N	-9.344206	2.420904	1.146853
S	-4.184574	-1.009322	0.058848
S	-9.530610	-2.460783	-0.783774
N	-8.233625	3.109670	1.286631
N	8.229790	-2.785856	1.844100
C	-8.261768	4.477794	1.749750
H	-9.109324	4.592306	2.423652
H	-7.324891	4.683189	2.265501
H	-8.373303	5.158678	0.901805
C	8.258171	-4.035478	2.568331
H	9.086191	-4.002303	3.274829
H	7.308259	-4.149155	3.088386
H	8.401911	-4.868205	1.874833
C	-4.533074	1.551697	-0.170004
H	-5.018931	2.516426	-0.236380
C	-1.901843	2.193407	-0.227674

C	1.901352	-2.193205	0.137157
C	1.828113	-2.961005	1.464572
H	2.659421	-3.669202	1.542277
H	1.878975	-2.277050	2.315779
H	0.893604	-3.527575	1.532949
C	1.819162	-3.166977	-1.046905
H	0.881742	-3.732025	-1.017905
H	1.868540	-2.631482	-1.998660
H	2.646620	-3.883099	-1.011513
C	-1.819361	3.170980	0.953283
H	-1.868208	2.638110	1.906482
H	-0.882166	3.736293	0.921928
H	-2.647622	3.886019	0.916162
C	-1.828950	2.956925	-1.557531
H	-1.880416	2.270633	-2.406884
H	-2.659494	3.665865	-1.637063
H	-0.894238	3.522849	-1.628266
C	0.560513	1.305794	-0.158795
H	0.999953	2.296290	-0.246167
C	-0.561082	-1.305293	0.072640
H	-1.000489	-2.295769	0.160402
C	4.532881	-1.551353	0.076727
H	5.019190	-2.512881	0.178713
C	6.972782	1.857166	-1.434354
H	5.940039	1.968313	-1.736409
C	7.945646	2.702282	-1.841654
H	7.832633	3.568405	-2.480231
C	-7.948729	-2.994778	-1.252738
H	-7.835043	-3.969433	-1.708620
C	-6.975820	-2.087303	-1.015697
H	-5.942828	-2.257566	-1.287527

4. **Compound C4**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-13.992000	-0.046955	-0.620260
C	-12.783801	0.682117	-0.311671
C	-10.418485	1.460139	0.040937

C	10.418585	-1.455840	0.211496
C	12.783695	-0.677806	-0.129449
C	13.994756	0.011325	-0.511879
C	16.387880	0.502734	-0.999282
S	-15.492561	0.485946	0.092728
S	-11.193312	0.070643	-0.665823
S	11.198978	-0.108691	-0.566048
S	15.492475	-0.882093	-0.522235
C	-16.381799	-0.750048	-0.700304
H	-17.450613	-0.826316	-0.557170
C	-15.569613	-1.537141	-1.461610
H	-15.930715	-2.377238	-2.044843
C	-14.198918	-1.152748	-1.428828
C	-12.678649	1.906907	0.312270
H	-13.547358	2.479353	0.621581
C	-11.355168	2.358757	0.525270
C	11.350212	-2.316086	0.769938
C	12.675141	-1.863115	0.565329
H	13.540926	-2.390171	0.953322
C	14.204850	1.327930	-0.886540
C	15.578175	1.588365	-1.158588
H	15.943426	2.564809	-1.457885
H	17.457922	0.436351	-1.138235
C	-13.140739	-1.881554	-2.199091
H	-12.522069	-1.199314	-2.791534
H	-12.466398	-2.440005	-1.539355
H	-13.597174	-2.599644	-2.884785
C	-11.035964	3.648126	1.214897
H	-10.106668	3.573593	1.786902
H	-10.918049	4.472250	0.501139
H	-11.840351	3.926175	1.900993
C	11.022078	-3.555724	1.541688
H	10.082811	-3.445353	2.091378
H	10.917292	-4.426866	0.883929
H	11.815333	-3.784090	2.258393
C	13.147635	2.384136	-0.993280
H	12.528153	2.252751	-1.888276
H	12.474702	2.377771	-0.130096
H	13.605218	3.374706	-1.055608
C	-8.980638	1.561801	0.055727

C	-6.544734	1.215372	0.098416
C	-5.200338	0.711586	0.120189
C	-3.349707	-0.670789	0.154314
C	-2.744144	0.568189	0.138723
C	-1.307348	0.442420	0.156889
C	-1.020866	-0.943151	0.200884
C	1.306705	-0.436892	0.184335
C	1.020200	0.948660	0.140232
C	2.743554	-0.562684	0.200040
C	3.349093	0.676274	0.182485
C	5.199827	-0.706124	0.210688
C	6.544417	-1.209720	0.226480
C	8.980485	-1.555874	0.223185
S	-7.942968	0.160971	0.132212
S	-3.877818	1.858797	0.110742
S	3.877347	-1.853300	0.223983
S	7.942125	-0.153746	0.212261
N	-6.842060	2.490786	0.051367
N	6.842538	-2.485442	0.251882
C	2.309466	1.784245	0.130803
C	-2.310147	-1.778749	0.207970
C	8.183338	-2.681224	0.244196
H	8.568797	-3.692951	0.221742
C	4.752540	0.602500	0.184080
H	5.421111	1.456047	0.162183
C	0.286824	-1.393247	0.210657
H	0.514580	-2.454912	0.234136
C	-0.287479	1.398773	0.130767
H	-0.515247	2.460418	0.106585
C	-4.753147	-0.597031	0.149244
H	-5.421793	-1.450563	0.169087
C	-8.182484	2.686308	0.022511
H	-8.566272	3.695672	-0.058025
C	-2.517151	-2.571818	1.503459
C	-3.511383	-3.555314	1.561557
C	-1.809807	-2.287163	2.671119
C	-3.779796	-4.231780	2.743858
H	-4.073675	-3.801539	0.664891
C	-2.082225	-2.969339	3.853885
H	-1.039015	-1.523226	2.662112

C	-3.066992	-3.954858	3.914374
H	-4.558057	-4.991301	2.758816
H	-1.514209	-2.726845	4.748844
C	-2.315177	-2.675023	-1.034761
C	-1.712440	-3.936421	-1.003514
C	-2.835126	-2.227147	-2.250108
C	-1.637320	-4.720078	-2.148711
H	-1.308097	-4.315255	-0.069149
C	-2.759417	-3.016534	-3.392905
H	-3.301775	-1.248184	-2.305984
C	-2.162493	-4.277943	-3.365406
H	-1.162131	-5.696825	-2.095266
H	-3.173848	-2.642024	-4.325952
C	2.316873	2.680687	1.373390
C	1.712807	3.941473	1.343462
C	2.840639	2.233720	2.587453
C	1.640125	4.725432	2.488624
H	1.305496	4.319649	0.410119
C	2.767347	3.023380	3.730205
H	3.308450	1.255259	2.642287
C	2.169155	4.284231	3.703966
H	1.163871	5.701715	2.436186
H	3.184820	2.649615	4.662195
C	2.513915	2.577223	-1.165181
C	3.506541	3.562183	-1.224836
C	1.805744	2.290896	-2.331987
C	3.772486	4.238609	-2.407778
H	4.069487	3.809646	-0.328922
C	2.075708	2.972958	-3.515317
H	1.036238	1.525683	-2.321824
C	3.058783	3.960131	-3.577311
H	4.549443	4.999451	-2.423929
H	1.507104	2.729097	-4.409528
C	3.326884	4.717823	-4.846709
H	2.983749	4.162188	-5.723551
H	2.809015	5.684360	-4.848024
H	4.394216	4.923259	-4.972007
C	2.121223	5.149936	4.931031
H	1.220964	5.771020	4.947191
H	2.135273	4.549426	5.844783

H	2.983182	5.826626	4.972142
C	-3.338337	-4.712402	5.183167
H	-4.407296	-4.907167	5.311791
H	-2.830518	-5.684238	5.180645
H	-2.986524	-4.162084	6.059905
C	-2.111684	-5.143298	-4.592602
H	-2.127808	-4.542699	-5.506247
H	-1.209283	-5.761279	-4.608914
H	-2.971261	-5.823011	-4.633717

5. **Compound C5**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-14.602549	0.041977	1.603495
C	-13.362688	-0.545408	1.144951
C	-10.993777	-1.030957	0.466850
C	11.116358	1.048032	0.382902
C	13.493866	0.561629	1.018068
C	14.725241	0.005866	1.537503
C	17.041873	-0.194185	2.428394
S	-16.106313	-0.660658	1.067444
S	-11.838595	0.284931	1.232127
S	11.963978	-0.239502	1.190684
S	16.002875	1.101276	1.992167
C	-17.030111	0.462439	1.980377
H	-18.110030	0.414053	1.968605
C	-16.227704	1.338522	2.649114
H	-16.609651	2.130602	3.284084
C	-14.835531	1.115706	2.445891
C	-13.188170	-1.775784	0.550179
H	-14.008982	-2.467726	0.390349
C	-11.856813	-2.065219	0.162822
C	11.981959	2.060486	0.017115
C	13.320601	1.769615	0.380068
H	14.152117	2.425667	0.143583
C	15.104945	-1.308606	1.742926
C	16.432840	-1.401468	2.250993
H	16.915569	-2.348885	2.465455

H	18.040005	0.007285	2.791710
C	14.262566	-2.515405	1.461032
H	13.556458	-2.718768	2.274676
H	13.675566	-2.399532	0.545415
H	14.893302	-3.401211	1.348479
C	11.587376	3.302558	-0.719908
H	10.719629	3.126771	-1.360497
H	11.318616	4.101834	-0.021843
H	12.410461	3.655513	-1.347352
C	-11.462379	-3.342088	-0.512188
H	-10.598267	-3.196275	-1.164922
H	-11.188122	-4.104567	0.223843
H	-12.287477	-3.728206	-1.117177
C	-13.781974	1.961052	3.093866
H	-12.999949	1.353217	3.560332
H	-13.288941	2.623358	2.372649
H	-14.224525	2.591682	3.869065
C	-9.546103	-0.974860	0.279094
C	-8.870276	0.059562	-0.360986
C	-7.438586	0.118103	-0.534133
C	-6.587454	-0.881730	-0.017566
C	-8.688776	-1.989909	0.764579
C	-7.271212	-1.949152	0.621183
C	-5.139410	-0.874978	-0.082275
C	-2.941900	-1.633643	-0.063248
C	-2.727689	-0.271795	-0.102925
C	-1.318190	0.033989	-0.121367
C	-0.639187	-1.209453	-0.089114
C	1.441259	-0.046439	-0.127744
C	0.762038	1.196980	-0.161491
C	2.850719	0.260101	-0.135051
C	3.064646	1.621818	-0.172688
C	5.263229	0.865104	-0.159304
C	6.711579	0.875839	-0.097328
C	7.562706	-0.147208	-0.565780
C	8.994442	-0.083306	-0.395362
C	9.669749	0.981190	0.195161
C	7.395321	1.972950	0.488008
C	8.812828	2.019552	0.629283
S	-9.666368	1.421187	-1.120721

S	-4.197189	0.612479	-0.117999
N	-9.009202	-3.104650	1.453926
N	-6.766366	-3.047514	1.226048
N	6.891119	3.100539	1.036952
N	9.134042	3.167329	1.261917
S	4.321542	-0.622912	-0.106405
S	9.789924	-1.478508	-1.090725
N	7.963569	3.735090	1.452386
N	-7.838204	-3.661277	1.672822
C	7.854940	4.984968	2.169517
H	8.759599	5.562718	1.986847
H	6.975174	5.513194	1.805321
H	7.751810	4.792617	3.240499
C	-7.729228	-4.873593	2.451670
H	-8.612433	-5.482450	2.264028
H	-6.824287	-5.395350	2.144818
H	-7.671715	-4.629449	3.515493
C	4.424920	1.969928	-0.178512
H	4.817232	2.978580	-0.185644
C	1.746280	2.363348	-0.196576
C	-1.623632	-2.375718	-0.052112
C	-1.472464	-3.271529	-1.289841
H	-2.231683	-4.060350	-1.285231
H	-1.584992	-2.691781	-2.209756
H	-0.487845	-3.750232	-1.302488
C	-1.457023	-3.204659	1.229401
H	-0.472269	-3.682537	1.255451
H	-1.558341	-2.576404	2.118188
H	-2.216480	-3.991857	1.276582
C	1.587470	3.186527	-1.482939
H	1.695602	2.554911	-2.368583
H	0.602248	3.662643	-1.518020
H	2.345550	3.975210	-1.528023
C	1.586990	3.264784	1.036018
H	1.692797	2.689041	1.959212
H	2.347403	4.052365	1.033158
H	0.602816	3.744431	1.039321
C	-0.620369	1.245975	-0.158454
H	-1.151976	2.193922	-0.184471
C	0.743295	-1.258387	-0.092090

H	1.274742	-2.206502	-0.066801
C	-4.302003	-1.980484	-0.043353
H	-4.695120	-2.987546	0.006947
C	-7.074843	1.263566	-1.312537
H	-6.070368	1.515310	-1.626311
C	-8.132767	2.031712	-1.681545
C	8.257384	-2.109113	-1.624842
C	7.197152	-1.326480	-1.292281
H	6.189098	-1.579750	-1.591261
O	9.259727	-4.003562	-2.628383
O	-6.970020	3.694634	-2.909248
C	8.255877	-3.370912	-2.375234
C	-8.018746	3.251607	-2.493318
O	7.015062	-3.734554	-2.737814
O	-9.221424	3.810387	-2.707375
C	6.917809	-4.953033	-3.494547
H	5.899444	-5.304261	-3.313682
H	7.628898	-5.677024	-3.088199
C	-9.230006	5.008639	-3.500679
H	-10.138237	5.531841	-3.193946
H	-8.356377	5.609704	-3.235251
C	7.170493	-4.708248	-4.966239
H	8.198510	-4.375906	-5.126994
H	7.017810	-5.634402	-5.528716
H	6.486034	-3.951113	-5.358281
C	-9.242582	4.686795	-4.979143
H	-9.328722	5.610219	-5.559900
H	-8.316594	4.185053	-5.269001
H	-10.089885	4.042762	-5.229262

Table S2 : The reference compound's HOMO and LUMO energies, as well as their Δ_{H-L} and λ_{max} values using different functionals. (Dyes Pigm. 2018, 155, 126-134 for reference compound)

Functional	**HOMO (eV)**	**LUMO (eV)**	**Δ_{H-L} (eV)**	**λ_{max} (nm)**
Experimental	-5.29	-3.38	1.91	523
B3LYP	-4.90	-1.97	2.93	478
CAM-B3LYP	-6.38	-0.80	5.58	353
B3PW91	-5.04	-2.03	3.01	464
HSEH1PBE	-4.79	-2.25	2.54	483
PBEPBE	-4.19	-2.62	1.57	684
WB97XD	-6.93	-0.19	6.74	346

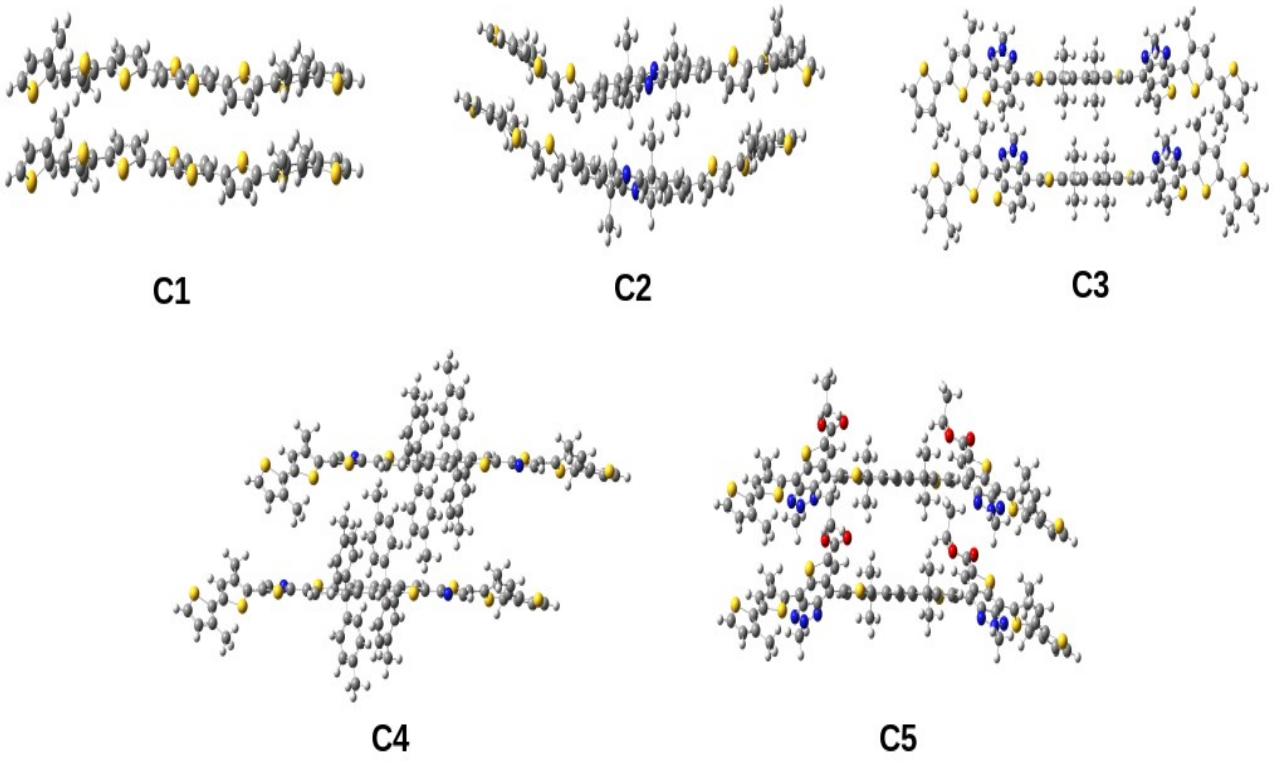

Fig. S1 : Investigated compounds' optimized structures in the π-stacked arrangement.

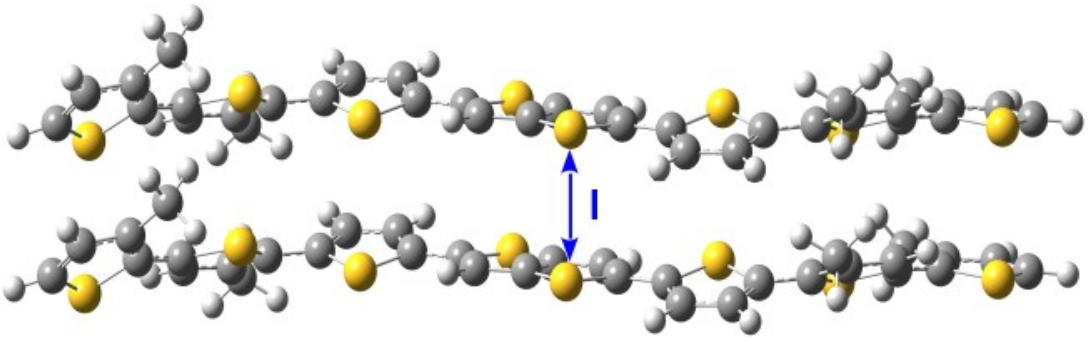

Fig. S2 : A typical configuration of two stacked molecules at a spacing l.

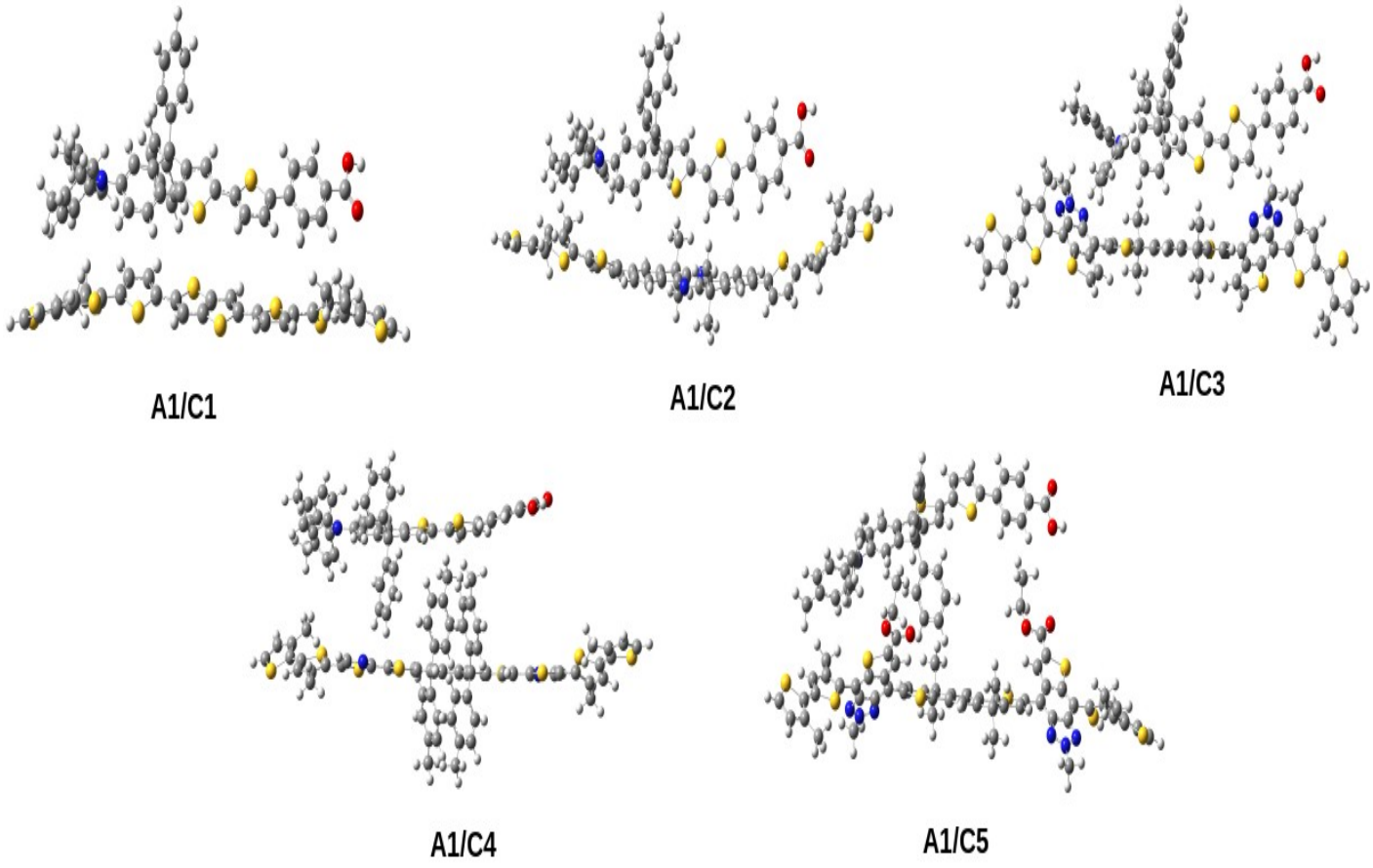

Fig. S3 : The A1/C1-C5 complexes' optimized structures.