Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

End-capped group manipulation of phenothiazine based small molecule non-fullerene acceptors for more efficient organic photovoltaic solar cell: A DFT study

Shahnaz Ahmed[1] and Dhruba Jyoti Kalita [1,*]
[1]Department of Chemistry, Gauhati University
Electronic mail: dhrubajyoti.kalita@gauhati.ac.in

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

1. **Compound S1**

Atoms	Coordinates (Angstrom)		
	X	Y	Z
C	3.648497	1.629254	0.033723
C	2.547198	1.372005	0.861989
C	1.414818	2.166019	0.818012
C	1.308544	3.227950	-0.092698
C	2.387278	3.457100	-0.951361
C	3.533995	2.684028	-0.877234
C	-1.100570	3.411614	0.060264
C	-1.249673	2.369171	0.987470
C	-2.473640	1.752743	1.179802
H	-2.547566	0.947683	1.899561
C	-3.615598	2.170812	0.482994
C	-3.465780	3.223486	-0.423963
C	-2.235263	3.820718	-0.644953
H	2.581564	0.548015	1.563055
H	2.328426	4.234980	-1.702350
H	4.337157	2.882498	-1.577746
H	-4.328414	3.599930	-0.961830
H	-2.164745	4.618062	-1.374006
N	0.149937	4.012442	-0.132316
S	0.125614	1.916684	2.002709
C	0.201499	5.273081	-0.838654
H	-0.608917	5.911562	-0.485073
H	1.144928	5.769776	-0.609590
H	0.115265	5.167398	-1.929501
C	4.876058	0.830394	0.112121
C	6.111874	1.333433	-0.264202
C	4.913540	-0.515140	0.569902
C	7.301986	0.588739	-0.217874
H	6.180907	2.365246	-0.588953

C	6.115531	-1.272091	0.618213
C	7.366541	-0.726923	0.215961
H	8.215364	1.085170	-0.530293
C	8.597971	-1.483630	0.260677
C	8.795763	-2.780122	0.701336
S	10.096800	-0.790874	-0.280934
C	10.126479	-3.201038	0.606435
H	7.981293	-3.383866	1.075862
C	10.981475	-2.242578	0.089838
H	10.477311	-4.181931	0.903312
C	12.376793	-2.408922	-0.116001
H	12.782691	-3.377438	0.170453
N	5.814957	-2.497584	1.080308
N	3.914843	-1.306429	1.003791
N	4.519253	-2.434298	1.284595
C	3.777439	-3.589350	1.739043
H	3.573934	-4.253728	0.896826
H	4.373339	-4.113643	2.483947
H	2.842093	-3.237973	2.167934
C	-4.916850	1.521440	0.676248
C	-5.877810	1.477582	-0.321519
C	-5.308054	0.888696	1.887222
C	-7.137050	0.875990	-0.161916
H	-5.646546	1.905076	-1.290489
C	-6.582138	0.280735	2.053769
C	-7.549313	0.258459	1.010201
H	-7.811824	0.893504	-1.011780
C	-8.850887	-0.357644	1.158037
C	-9.366939	-0.996534	2.273675
S	-9.989765	-0.356585	-0.150513
C	-10.660108	-1.474949	2.067179
H	-8.807337	-1.098601	3.192494
C	-11.169443	-1.218553	0.798946
H	-11.237467	-2.003191	2.816957
N	-4.633223	0.750427	3.043716
N	-6.644963	-0.210491	3.303326
N	-5.473556	0.099272	3.809751
C	-5.149695	-0.210646	5.184414
H	-5.528532	-1.204628	5.415890
H	-4.068002	-0.174301	5.288343
H	-5.612487	0.522330	5.848241
C	-12.477645	-1.640373	0.428935
H	-12.969322	-2.161286	1.249253
C	13.296666	-1.552410	-0.617640
C	14.704244	-1.962383	-0.737021
S	13.085060	0.084990	-1.198360
C	14.796045	0.236731	-1.593448
N	15.456593	-0.914070	-1.284488
C	16.880319	-1.068007	-1.505925

H	17.145279	-2.070525	-1.173347
H	17.109258	-0.941676	-2.565384
H	17.429879	-0.316294	-0.937003
O	15.176409	-3.029677	-0.422900
C	-13.219806	-1.529942	-0.704026
C	-12.845833	-0.892447	-1.963594
S	-14.851332	-2.181289	-0.824883
C	-15.033224	-1.630263	-2.477238
N	-13.896283	-0.991429	-2.882642
C	-13.764018	-0.431003	-4.212287
H	-13.880852	-1.216361	-4.960794
H	-14.533328	0.325324	-4.376226
H	-12.771104	0.011978	-4.272229
O	-11.794190	-0.345852	-2.221981
S	-16.389667	-1.869161	-3.368967
S	15.443277	1.596540	-2.240167

2. **Compound S2**

C	3.643972	1.747319	-0.037972
C	2.541087	1.519160	0.796982
C	1.408402	2.310077	0.722323
C	1.302897	3.338085	-0.226854
C	2.383835	3.538115	-1.090233
C	3.531111	2.769631	-0.985687
C	-1.106764	3.524769	-0.083481
C	-1.255990	2.518285	0.882785
C	-2.480091	1.910387	1.098785
H	-2.554345	1.133950	1.849295
C	-3.621793	2.301297	0.385769
C	-3.471580	3.317661	-0.561885
C	-2.241197	3.906206	-0.804771
H	2.574631	0.721056	1.527371
H	2.325832	4.288678	-1.868507
H	4.335779	2.944061	-1.690809
H	-4.333747	3.672561	-1.114942
H	-2.170342	4.674344	-1.564457
N	0.143264	4.118115	-0.298800
S	0.118768	2.104179	1.914632
C	0.194304	5.352909	-1.049950
H	-0.617955	6.002200	-0.721353
H	1.136271	5.859287	-0.836704
H	0.110764	5.207793	-2.136381
C	4.870200	0.950849	0.070555
C	6.107201	1.437608	-0.325074
C	4.905562	-0.376417	0.579266
C	7.295733	0.694059	-0.250019
H	6.177523	2.456059	-0.689236

C	6.106190	-1.132830	0.656363
C	7.358375	-0.604872	0.234253
H	8.209786	1.176740	-0.581357
C	8.587536	-1.359994	0.308270
C	8.779759	-2.644458	0.790575
S	10.090053	-0.687159	-0.246577
C	10.106922	-3.070847	0.715240
H	7.961433	-3.233537	1.179668
C	10.971443	-2.130200	0.172604
H	10.454265	-4.042841	1.043540
C	12.360767	-2.322926	-0.013175
H	12.744045	-3.289716	0.308082
N	5.803732	-2.339338	1.164260
N	3.905606	-1.149274	1.042609
N	4.508033	-2.266495	1.365914
C	3.764233	-3.402841	1.862711
H	3.542045	-4.087666	1.041844
H	4.368413	-3.911444	2.611643
H	2.838447	-3.032974	2.296865
C	-4.922615	1.660362	0.604305
C	-5.884668	1.579158	-0.390966
C	-5.312607	1.073410	1.838482
C	-7.142246	0.982476	-0.208521
H	-5.654147	1.970537	-1.375208
C	-6.585763	0.470970	2.028664
C	-7.553235	0.407914	0.986627
H	-7.817206	0.966770	-1.058237
C	-8.850989	-0.206240	1.157513
C	-9.364330	-0.805056	2.299218
S	-9.990748	-0.262110	-0.150144
C	-10.650393	-1.296942	2.111059
H	-8.804346	-0.868565	3.221408
C	-11.169233	-1.096017	0.830400
H	-11.223739	-1.799770	2.881015
N	-4.637306	0.980338	2.999253
N	-6.647738	0.027986	3.295937
N	-5.476542	0.358327	3.789936
C	-5.151500	0.100051	5.175114
H	-5.511293	-0.893072	5.438833
H	-4.071100	0.161128	5.280182
H	-5.630968	0.845379	5.812694
C	-12.472454	-1.559306	0.518962
H	-12.902126	-2.038864	1.398144
C	13.306522	-1.495807	-0.532799
C	14.707379	-1.865108	-0.652409
S	13.051552	0.125624	-1.149669
C	14.741759	0.310869	-1.556306
N	15.428474	-0.831681	-1.219843
C	16.856736	-0.957576	-1.446691

H	17.044965	-1.812191	-2.098179
H	17.202952	-0.035227	-1.907778
H	17.361107	-1.127794	-0.494265
C	-13.323652	-1.575378	-0.552724
C	-13.219934	-1.078928	-1.902110
S	-14.901234	-2.344685	-0.329781
C	-15.387716	-2.017567	-1.963189
N	-14.373270	-1.353840	-2.615526
C	-14.501062	-0.949557	-4.002928
H	-15.477004	-1.278823	-4.353549
H	-14.409424	0.135387	-4.076590
H	-13.702889	-1.407082	-4.589619
S	-16.850995	-2.461938	-2.568274
S	15.337231	1.680673	-2.237546
S	15.390357	-3.298633	-0.192932
S	-11.936239	-0.281069	-2.573089

3. **Compound S3**

C	-3.66055600	2.45414200	-0.55643100
C	-2.51162100	1.98359300	-1.20697300
C	-1.29181700	2.61901100	-1.05906300
C	-1.15404000	3.73789000	-0.22323400
C	-2.29527700	4.19785600	0.43975700
C	-3.52155300	3.57774300	0.26316600
C	1.25923800	3.59550800	-0.05895300
C	1.37396700	2.45559700	-0.86960800
C	2.51484400	1.67333800	-0.84552400
H	2.55555400	0.78673100	-1.46536200
C	3.61848800	2.02301700	-0.05542100
C	3.50006300	3.16014600	0.74932300
C	2.34234800	3.92017000	0.76293400
H	-2.57668800	1.12075000	-1.85717500
H	-2.23260200	5.05390800	1.09964400
H	-4.38907400	3.99291800	0.76332300
H	4.30850400	3.43510500	1.41725700
H	2.27876700	4.76469700	1.43756200
N	0.08975300	4.36367200	-0.07817300
S	0.08882300	2.08803600	-2.02641900
C	0.12847300	5.68495100	0.50891500
H	1.06327700	6.17071500	0.22740900
H	-0.69260600	6.27755800	0.10413400
H	0.05114400	5.67845300	1.60530500
C	-4.95709600	1.78776600	-0.71205600
C	-5.92997100	1.81551900	0.27629800
C	-5.32993600	1.06243200	-1.87570300
C	-7.18326400	1.19694800	0.14753600
H	-5.71123600	2.31520100	1.21298000

C	-6.59892300	0.43776600	-2.01216400
C	-7.57851300	0.49058200	-0.98085500
H	-7.86819100	1.27247700	0.98597100
C	-8.87371300	-0.14218500	-1.09555900
C	-9.35974500	-0.87952600	-2.16926100
S	-10.03601800	-0.03914600	0.18502900
C	-10.64756600	-1.34931100	-1.95037800
H	-8.77879100	-1.05251300	-3.06365100
C	-11.19043800	-0.99196000	-0.71355200
H	-11.20845400	-1.94535600	-2.66095700
C	-12.49631900	-1.40753300	-0.36435700
H	-12.92766100	-1.99157300	-1.17033000
N	-6.64743000	-0.13675800	-3.22590600
N	-4.64319800	0.84969800	-3.01383100
N	-5.47513500	0.14975900	-3.74397200
C	-5.09834000	-0.33722600	-5.05268000
H	-4.78370900	-1.38043000	-4.98347500
H	-5.95941700	-0.25782700	-5.71382600
H	-4.27641600	0.27708600	-5.41213400
C	4.85428500	1.23492200	-0.06587800
C	6.09291700	1.79758200	0.20410200
C	4.89544400	-0.15773000	-0.34434000
C	7.28982100	1.06473400	0.22059600
H	6.15466300	2.86415900	0.38729600
C	6.10401500	-0.90483400	-0.32425600
C	7.35886700	-0.29830300	-0.03508800
H	8.20567400	1.60527400	0.43688100
C	8.60213600	-1.03662800	-0.01388200
C	8.78017800	-2.39722000	-0.23757100
S	10.10612400	-0.24315300	0.31731400
C	10.11078200	-2.78111400	-0.13935500
H	7.95688900	-3.06038900	-0.46094800
C	10.99202500	-1.73896400	0.15928700
H	10.46467700	-3.79629600	-0.27704000
N	3.89205100	-1.00754300	-0.63188300
N	5.80231600	-2.18470400	-0.60032300
N	4.49928300	-2.16034700	-0.76414100
C	3.77056900	-3.35424500	-1.13213200
H	4.18625800	-4.19730700	-0.58331600
H	2.72613100	-3.19999600	-0.87217800
H	3.86690900	-3.53113900	-2.20522100
C	12.37708200	-1.99430000	0.28796900
H	12.57711500	-3.04797600	0.12508000
C	-13.29086200	-1.22822700	0.74015600
C	-14.64154500	-1.74217600	0.93410300
C	-12.91739900	-0.47214200	1.95107500
C	-15.09240100	-1.29714200	2.27100100
C	-14.07124000	-0.54743400	2.86697100
C	-16.28296900	-1.49622700	2.96870100

C	-14.19284200	0.00913300	4.12666300
C	-16.40939200	-0.93763200	4.23737900
H	-17.10250500	-2.06698800	2.55565500
C	-15.38228300	-0.19297800	4.81641400
H	-13.37259300	0.58206500	4.54473600
H	-17.33270900	-1.08832500	4.78594600
H	-15.51634400	0.22711800	5.80719800
O	-11.87050400	0.10480800	2.16785200
C	-15.39721400	-2.50153000	0.06908400
C	-16.71249900	-2.94896200	0.36816300
C	-14.95340400	-2.92314500	-1.21349700
N	-14.62336100	-3.28253200	-2.26179200
N	-17.78360400	-3.33315600	0.57098600
C	13.46948500	-1.21069400	0.56379200
C	14.85619300	-1.65190700	0.65883400
C	13.44076600	0.24359200	0.81189200
C	15.67686900	-0.45808700	0.95876300
C	14.83637800	0.65786700	1.04910800
C	17.04803300	-0.29085700	1.14914100
C	15.30949000	1.92800900	1.32117300
C	17.52857900	0.98652700	1.42275800
H	17.74173900	-1.11753200	1.09019900
C	16.67714300	2.08752100	1.50975700
H	14.61684000	2.76019100	1.38090500
H	18.59401900	1.12395700	1.57146200
H	17.08741700	3.06803900	1.72496900
O	12.46880000	0.97231600	0.82153200
C	15.35782600	-2.92538400	0.50972800
C	14.55930700	-4.06606800	0.22535800
C	16.73901800	-3.23892200	0.62711800
N	13.93882200	-5.01399800	-0.00577000
N	17.85233700	-3.53711500	0.71428800

4. **Compound S4**

C	-3.66650600	2.25976500	-1.16652200
C	-2.51368600	1.70195900	-1.73648600
C	-1.29272300	2.34823400	-1.66307800
C	-1.15907500	3.57049300	-0.98634700
C	-2.30486000	4.12065400	-0.40496800
C	-3.53133100	3.48508900	-0.50755000
C	1.25007400	3.44319300	-0.77112300
C	1.36935000	2.20265300	-1.41681000
C	2.50514800	1.42677000	-1.27009300
H	2.54951500	0.46460100	-1.76403400
C	3.59918500	1.87596900	-0.51738600
C	3.47535300	3.11235200	0.12410200
C	2.32277600	3.87225100	0.01585400
H	-2.57620000	0.75875300	-2.26388200

H	-2.24487900	5.05869100	0.13224900
H	-4.40226900	3.96640900	-0.07761100
H	4.27501300	3.47195800	0.76160800
H	2.25384400	4.80105900	0.56791000
N	0.08590800	4.20593400	-0.91280700
S	0.09761000	1.68652500	-2.53119100
C	0.12407000	5.59539300	-0.51136500
H	1.06599100	6.03412700	-0.84196000
H	-0.68707100	6.13044200	-1.00624100
H	0.03039200	5.73892200	0.57426600
C	-4.96369800	1.58099600	-1.23692300
C	-5.94214700	1.75082400	-0.26803600
C	-5.33235800	0.69862900	-2.28806000
C	-7.19652200	1.12431700	-0.31560000
H	-5.72679500	2.37664500	0.59041700
C	-6.60295100	0.06452000	-2.34234800
C	-7.58837400	0.26707400	-1.33574700
H	-7.88477100	1.31815600	0.50080500
C	-8.88621900	-0.36870000	-1.36587300
C	-9.36145800	-1.27777800	-2.30509100
S	-10.06853200	-0.03751300	-0.14451800
C	-10.65599900	-1.69595900	-2.03045000
H	-8.76770400	-1.60536000	-3.14633800
C	-11.21619000	-1.12623000	-0.88342300
H	-11.20999100	-2.40360100	-2.63637100
C	-12.53075200	-1.46391000	-0.49038100
H	-12.95663600	-2.17782000	-1.18740000
N	-6.64728800	-0.67582100	-3.46262200
N	-4.64035200	0.32459200	-3.38054700
N	-5.47088400	-0.46904600	-4.00909300
C	-5.08743200	-1.13960100	-5.23198900
H	-4.72912500	-2.14606000	-5.00647200
H	-5.95885800	-1.19741500	-5.88132300
H	-4.29494600	-0.55849600	-5.69751600
C	4.82981100	1.08840500	-0.40333600
C	6.06622800	1.67559000	-0.17653500
C	4.86894200	-0.32811500	-0.51020400
C	7.25803900	0.94659900	-0.04656600
H	6.13100400	2.75621400	-0.12306600
C	6.07278500	-1.07089100	-0.37552300
C	7.32472500	-0.43774000	-0.13536700
H	8.17239100	1.50663300	0.12101600
C	8.56282400	-1.17164200	-0.00091800
C	8.74099400	-2.54874100	-0.08145900
S	10.05966600	-0.35162200	0.29428100
C	10.06567700	-2.92317800	0.09338800
H	7.92098400	-3.22913500	-0.26066000
C	10.94328000	-1.85750200	0.31227300
H	10.41851200	-3.94767500	0.06749500

N	3.86716800	-1.20394200	-0.71318400
N	5.77000300	-2.37382400	-0.50100300
N	4.47068200	-2.36588400	-0.69306800
C	3.74286700	-3.59421000	-0.92480400
H	4.12168400	-4.35642400	-0.24613700
H	2.69046900	-3.39681600	-0.73633700
H	3.88445800	-3.91919700	-1.95739100
C	12.32116400	-2.10044600	0.50847200
H	12.52266600	-3.16520900	0.45865300
C	-13.34180900	-1.08378500	0.55089700
C	-14.70219400	-1.54097700	0.80538800
C	-12.98033300	-0.12685500	1.61215700
C	-15.17369000	-0.85407300	2.02649100
C	-14.15450800	-0.02162700	2.49864000
C	-16.38423700	-0.90891500	2.71680400
C	-14.28544600	0.76136300	3.63094500
C	-16.51740400	-0.12630500	3.84844500
H	-17.22234200	-1.52483500	2.42072700
C	-15.48752400	0.69968700	4.30568000
H	-13.47991100	1.39856200	3.97661500
O	-11.93200400	0.47007100	1.75104900
C	-15.45285300	-2.43940800	0.08131900
C	-16.77880700	-2.80524500	0.43704000
C	-14.99197500	-3.09669200	-1.09111500
N	-14.64669300	-3.64720900	-2.04737600
N	-17.85851200	-3.12390700	0.69894700
C	13.40887100	-1.29437700	0.73941100
C	14.78800100	-1.72850200	0.92325700
C	13.37974400	0.17585600	0.84076100
C	15.60432100	-0.51449900	1.13478500
C	14.76962000	0.60595500	1.08453500
C	16.96954500	-0.33886200	1.35822700
C	15.23397900	1.89851500	1.24643900
C	17.43563900	0.95236900	1.52030600
H	17.68314000	-1.14961800	1.41169900
C	16.58655500	2.06059500	1.46639000
H	14.56616100	2.75088200	1.20296100
O	12.41687100	0.90962300	0.74567800
C	15.29062400	-3.00998900	0.91307900
C	14.49903100	-4.17264700	0.71135600
C	16.66731800	-3.30397000	1.10541800
N	13.88315500	-5.13778200	0.55027600
N	17.78001300	-3.57688400	1.25820600
F	17.11100700	3.27051300	1.63149400
F	18.73001900	1.16502600	1.73494000
F	-17.65485400	-0.14793800	4.53579700
F	-15.69249100	1.42218100	5.40209600

5. **Compound S5**

C	3.64520000	2.31147300	-0.19397500
C	2.49790800	2.07796900	0.57622900
C	1.27609700	2.62684300	0.22833900
C	1.13555700	3.40792100	-0.92883200
C	2.27529400	3.62876800	-1.70615500
C	3.50366600	3.10535900	-1.33510200
C	-1.27380800	3.19720200	-1.04746100
C	-1.38813000	2.38921600	0.09388700
C	-2.52239300	1.62955900	0.32194600
H	-2.56358100	0.99816700	1.20045500
C	-3.61806300	1.68196200	-0.55017200
C	-3.49759100	2.48515700	-1.68778100
C	-2.34713200	3.21382200	-1.94203600
H	2.56552500	1.47579900	1.47320800
H	2.20987000	4.22126900	-2.61004800
H	4.37139000	3.33584900	-1.94269900
H	-4.29927900	2.50884300	-2.41728400
H	-2.28079200	3.78614600	-2.85878000
N	-0.11186100	3.94642000	-1.27011000
S	-0.10769900	2.43819300	1.31272200
C	-0.15569000	4.99489400	-2.26459600
H	-1.09843300	5.53468400	-2.16897000
H	0.65552200	5.69881300	-2.07482100
H	-0.06582500	4.62431500	-3.29589500
C	4.94401400	1.73101400	0.16550600
C	5.90559000	1.42061800	-0.78216800
C	5.33004200	1.43787200	1.50145200
C	7.16278900	0.87774500	-0.46529600
H	5.67670500	1.57670000	-1.83039700
C	6.60168300	0.89294800	1.82650300
C	7.57101300	0.59239100	0.82890300
H	7.83844000	0.66559300	-1.28788000
C	8.86651300	0.03130400	1.14321800
C	9.38971200	-0.28761100	2.37897700
S	10.01548500	-0.33936200	-0.11405200
C	10.68819400	-0.81896600	2.31372200
H	8.83124200	-0.13252400	3.29131500
C	11.18750100	-0.91918300	1.03158800
H	11.25992500	-1.12751400	3.18080400
C	12.47405000	-1.42260400	0.66015200
C	12.96659100	-1.52967100	-0.59324100
H	13.08642100	-1.74204300	1.50038700
N	6.66447100	0.75751600	3.16227600
N	4.65531400	1.61874300	2.65205300
N	5.49692300	1.20264000	3.56644700
C	5.13153600	1.17872700	4.96507500
H	4.79916500	0.17706900	5.24546300

H	6.00320500	1.45391000	5.55611700
H	4.32423400	1.89247500	5.11076100
C	-4.84918800	0.92769200	-0.29007400
C	-6.08766700	1.35563000	-0.73942800
C	-4.88424200	-0.29714700	0.42976200
C	-7.28045700	0.64264500	-0.52819900
H	-6.15529800	2.30276500	-1.26271400
C	-6.08747600	-1.02300300	0.64237500
C	-7.34288600	-0.56169900	0.15623400
H	-8.19713200	1.07273000	-0.91919200
C	-8.57609700	-1.28795000	0.36545000
C	-8.76846800	-2.48858600	1.01652400
S	-10.09317600	-0.67596100	-0.23586100
C	-10.10948400	-2.90601900	1.03035200
H	-7.94793100	-3.03261800	1.46270600
C	-10.97176100	-2.03801100	0.39301200
H	-10.45304500	-3.82268000	1.49465600
N	-3.88001600	-0.99397000	0.99316600
N	-5.78210300	-2.13785800	1.32820500
N	-4.48194700	-2.04657300	1.49006800
C	-3.75043300	-3.04014200	2.24361400
H	-4.19953100	-4.01349100	2.05619900
H	-2.71574400	-3.01983000	1.90922200
H	-3.80109200	-2.81033400	3.31002600
C	-12.38612400	-2.19954900	0.25089500
C	-13.23534500	-1.35032100	-0.36771900
H	-12.77786300	-3.10909300	0.70069800
C	16.28653700	-2.79268300	-2.17917200
C	16.41618500	-2.93791300	-0.81505300
C	15.28088500	-2.51611800	-0.10939300
C	14.26836300	-2.04338200	-0.92498800
S	14.74203600	-2.12684800	-2.58967100
H	17.31120800	-3.33805800	-0.35725500
H	15.20193500	-2.55475200	0.96899000
C	17.23128600	-3.11585200	-3.16993500
N	18.00694800	-3.38112200	-3.98577100
C	-14.65470200	-1.54763400	-0.49001300
C	-15.45792200	-2.58511300	-0.05157300
C	-16.81352500	-2.41304700	-0.36385500
C	-17.06422200	-1.24205700	-1.04550800
S	-15.60468600	-0.34655800	-1.30089100
H	-15.07429000	-3.44590800	0.47989700
H	-17.59730000	-3.11341000	-0.10703100
C	-18.30524800	-0.76610800	-1.50585200
N	-19.32485700	-0.37325200	-1.88488400
H	-12.83539800	-0.44203200	-0.81258900
H	12.34735400	-1.21023100	-1.42828900

Table S2: Calculated values of HOMO and LUMO energies, Δ_{H-L} and Λ_{max} values of the reference compound obtained using various functionals.

Functionals	E_{HOMO} (eV)	E_{LUMO} (eV)	Δ_{H-L} (eV)	Λ_{max} (nm)
Experimental	-5.70	-3.57	2.13	509
B3LYP	-5.87	-3.53	2.34	-
PBEPBE	-5.31	-4.06	1.25	-
HSEH1PBE	-5.70	-3.77	1.93	-
MPW1PW91	-6.08	-3.44	2.63	-
CAM-B3LYP	-7.05	-2.41	2.64	478.91
M06-2X-D3	-	-	-	481.58
ωB97XD	-	-	-	464.60

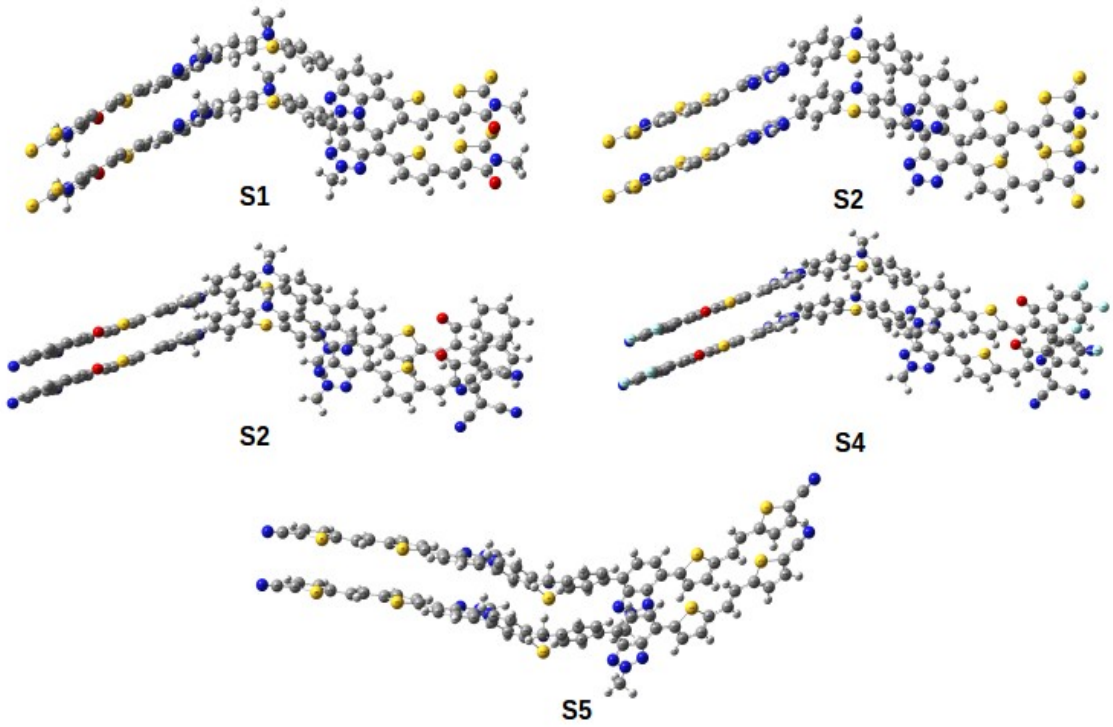

Fig. S1: Optimized structures of the studied compounds in the π-stacked orientation.

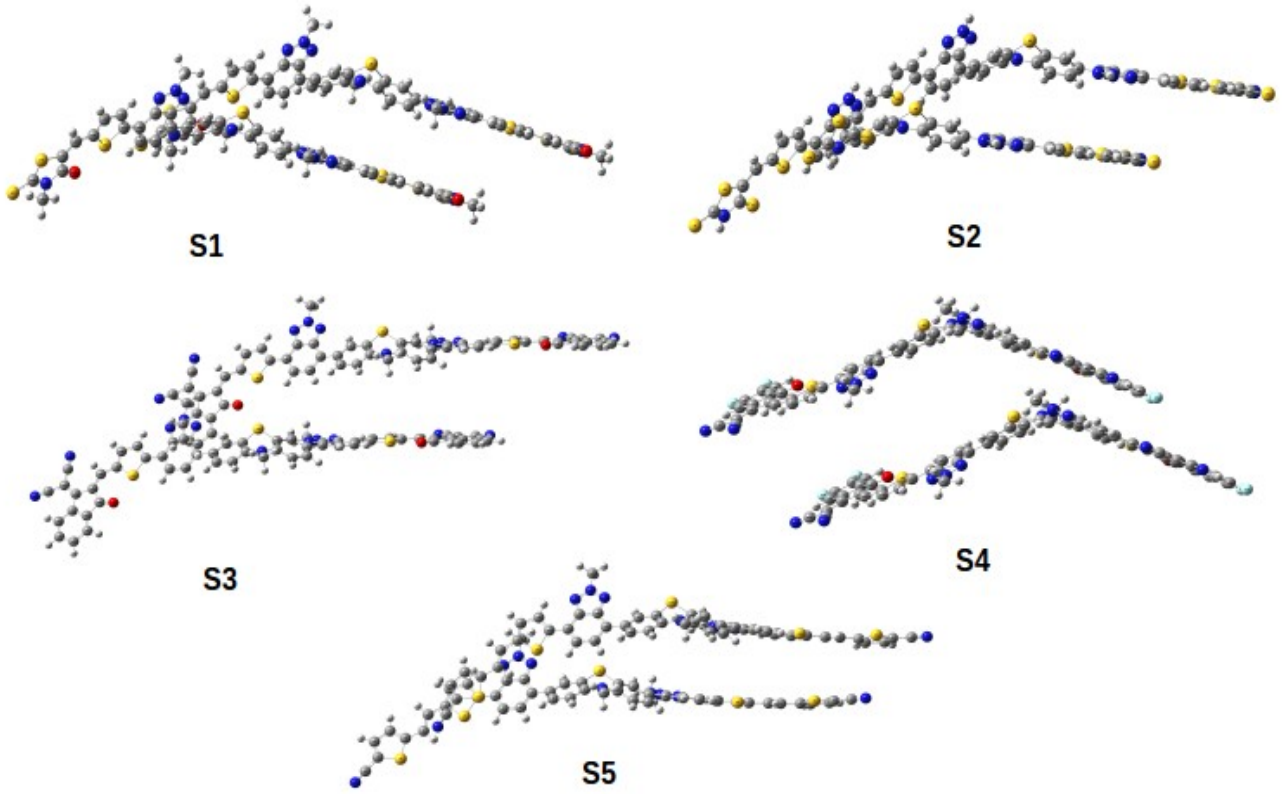

Fig. S2: Optimized structures of the studied compounds in the shifted π-stacked orientation.

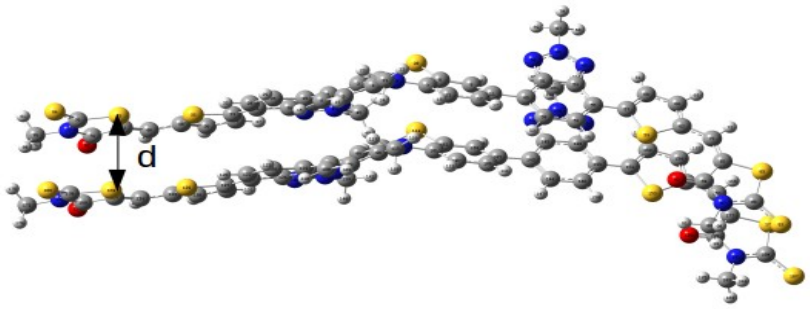

Fig. S3: Optimized structure of two stacked molecules along with the space distance, d.

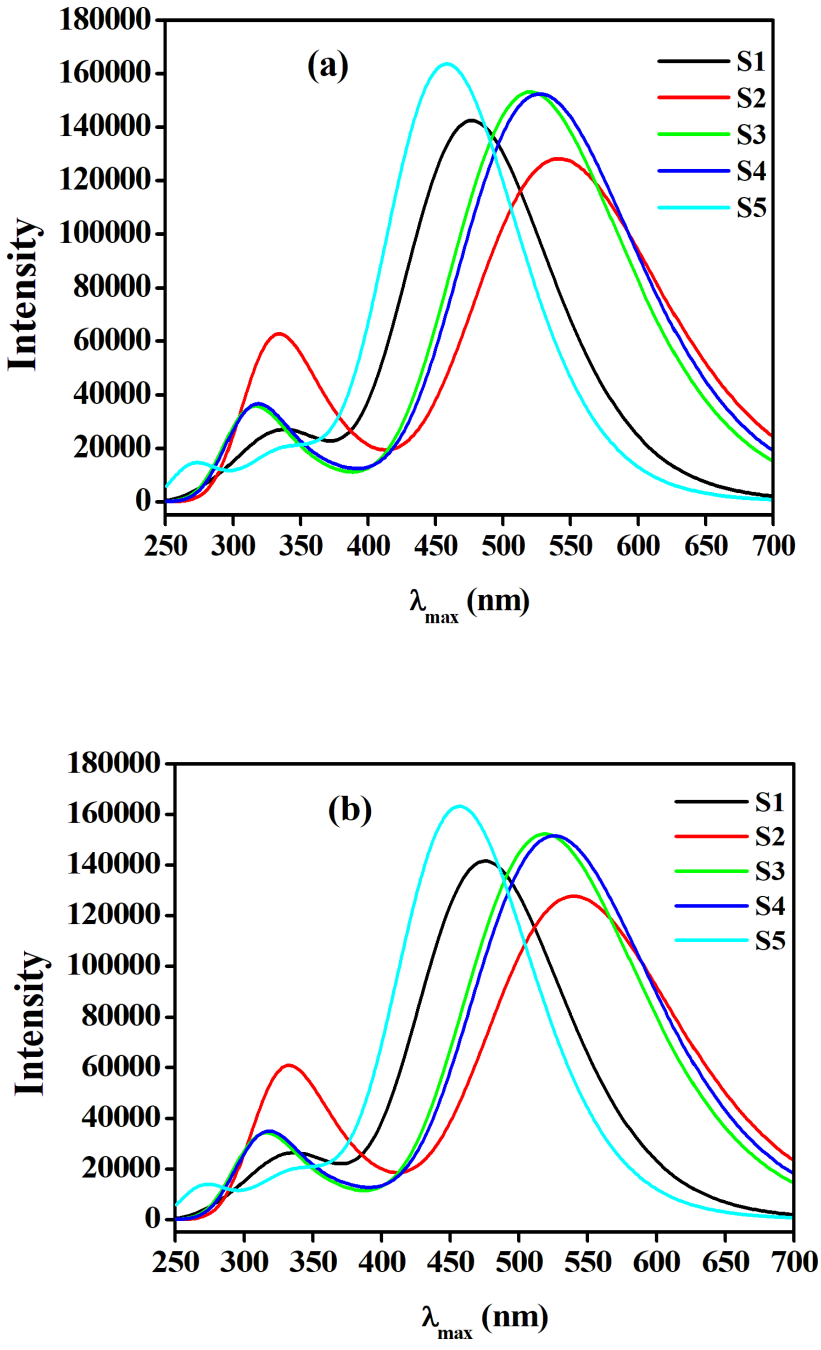

Fig. S4: Uv-visible spectra of the studied compounds (a) in DCM phase and (b) in ethanol phase.

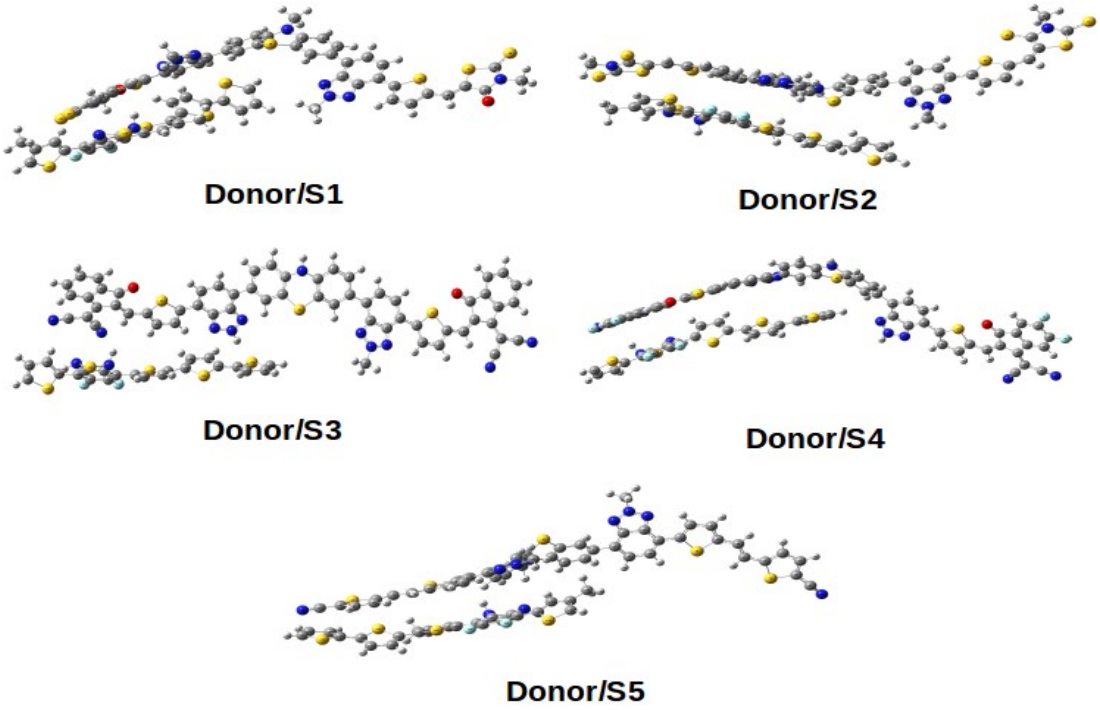

Fig. S5: Optimized structures of the PffBT4T-2OD/S1-S5 molecules.