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Supporting Information

Molecular engineering on the core part of D-π-A-π-D based small acceptor molecules for efficient organic solar cells: A DFT approach

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Table S1 : Calculated energies of HOMO, LUMO, Δ_{H-L}, and λ_{max} values of the reference compound using various functionals .

Functional	**HOMO (eV)**	**LUMO (eV)**	**Δ_{H-L} (eV)**	**λ_{max} (nm)**
Experimental	-5.32	-3.50	1.82	555
B3LYP	-4.98	-2.27	2.71	538
B3LYP-D3	-4.97	-2.30	2.67	546
B3PW91	-5.10	-2.37	2.73	533
CAM-B3LYP	-6.24	-1.16	5.08	394
HSEH1PBE	-4.83	-2.59	2.24	557
PBEPBE	-4.34	-2.89	1.45	781
WB97XD	-6.86	-0.61	6.25	385

Table S2 : Coordinates of the designed compounds studied at HSEH1PBE/6-31G(d) level of theory in the angstrom unit.

1. **Compound C1**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	18.759430	-1.766546	1.208941
C	17.671886	-1.093364	1.726746
C	16.421234	-1.139189	1.096920
C	18.590653	-2.516317	0.039628
C	16.256208	-1.873418	-0.100499

C	17.368542	-2.576475	-0.606348
C	15.301718	-0.422596	1.710462
C	14.003767	-0.607064	1.038726
C	13.899670	-1.362820	-0.153148
C	12.881601	-0.034196	1.626362
C	11.610404	-0.181667	1.071126
C	11.498095	-0.981866	-0.090641
C	12.621080	-1.552373	-0.679925
C	10.186104	-1.256880	-0.698838
C	9.039591	-0.712258	0.034989
C	9.219141	0.087933	1.187339
C	8.061874	0.533067	1.859332
C	6.804923	0.218028	1.386381
C	6.613361	-0.547746	0.218358
C	7.756089	-0.999746	-0.432036
C	5.279927	-0.871998	-0.279874
C	4.917596	-1.864194	-1.161108
C	3.533256	-1.881462	-1.443737
C	2.814866	-0.899582	-0.782932
C	1.367818	-0.715559	-0.783022
C	0.734404	0.567761	-0.743678
C	-0.698114	0.683946	-0.753696
C	-1.538310	-0.485996	-0.842899
C	0.531318	-1.815320	-0.774831
C	-0.885205	-1.708635	-0.810246
C	-2.987892	-0.388319	-0.949404
C	-3.733593	0.658755	-1.457887
C	-5.124490	0.446335	-1.409499
C	0.933135	2.852047	-0.621197
C	-0.482889	2.967232	-0.558619
C	1.765585	4.045613	-0.605923
C	1.164006	5.320143	-0.485045
C	-0.292182	5.435501	-0.356135
C	-1.100459	4.275399	-0.391550
C	-0.934441	6.675601	-0.192023
C	-2.309069	6.766239	-0.067483
C	-3.097513	5.611516	-0.097859
C	-2.493748	4.379457	-0.256751
C	3.159307	3.928788	-0.724065
C	2.008220	6.444738	-0.490219
N	15.032900	-1.899597	-0.749404
N	10.485722	0.411539	1.632637

N	1.506672	1.658511	-0.697053
N	-1.257454	1.894301	-0.642273
S	-4.060826	-1.657769	-0.410588
S	3.892011	0.070024	0.175143
O	15.419019	0.261270	2.724152
O	10.066479	-1.917438	-1.727368
H	17.737628	-0.507125	2.638357
H	17.275435	-3.197823	-1.488850
H	19.427344	-3.074328	-0.372025
H	19.724863	-1.727174	1.703416
H	12.425459	-2.168839	-1.549855
H	13.066228	0.503805	2.549353
H	7.698113	-1.588449	-1.342550
H	8.138783	1.094530	2.782590
H	5.623617	-2.566104	-1.590673
H	3.082884	-2.552544	-2.169646
H	-3.273876	1.548706	-1.863863
H	-5.850364	1.150654	-1.801414
H	3.581551	2.934028	-0.821595
H	1.587136	7.440633	-0.407051
H	-0.350932	7.588898	-0.155050
H	-2.773195	7.740322	0.059904
H	-4.176232	5.681312	0.008419
H	-3.077242	3.464672	-0.269405
C	-5.476504	-0.764640	-0.855317
H	5.941104	0.556668	1.953120
C	3.963878	5.051510	-0.723378
H	5.041267	4.951005	-0.818887
C	3.380690	6.317263	-0.606419
H	4.003568	7.207548	-0.609673
C	10.652699	1.379137	2.701215
H	9.864137	2.130023	2.640298
C	14.927126	-2.497350	-2.066955
H	15.850159	-2.323647	-2.621766
H	14.730906	-3.575739	-2.021902
O	0.962166	-3.102584	-0.731592
O	-1.585681	-2.860537	-0.810429
H	10.631312	0.912191	3.693477
H	14.122863	-2.014160	-2.621697
H	11.602665	1.898459	2.574669
H	1.920156	-3.100398	-0.549667
H	-0.946221	-3.590947	-0.755003

C	-6.815388	-1.308667	-0.658876
C	-7.045452	-2.691426	-0.506948
C	-7.929364	-0.477481	-0.605373
C	-9.222629	-0.976839	-0.438688
C	-9.442013	-2.368500	-0.315605
C	-8.311829	-3.210908	-0.334465
C	-10.335004	-0.024859	-0.375346
C	-11.650466	-0.625247	-0.097709
C	-11.803452	-2.027266	0.022446
C	-12.733870	0.231250	0.065386
C	-14.010750	-0.250996	0.355178
C	-14.151534	-1.648300	0.529427
C	-13.069322	-2.505141	0.363485
C	-15.443717	-2.238819	0.917227
C	-16.510866	-1.271011	1.178933
C	-16.311719	0.114890	0.978539
C	-17.370428	0.990173	1.296243
C	-18.576706	0.495050	1.758787
C	-18.781483	-0.878592	1.930249
C	-17.744667	-1.743396	1.645130
N	-10.721192	-2.874873	-0.176731
N	-15.107618	0.590814	0.488557
O	-10.187161	1.186311	-0.518060
O	-15.596916	-3.452021	1.035975
C	-10.940020	-4.307892	-0.232916
H	-10.233576	-4.757770	-0.931845
H	-10.830221	-4.785591	0.748495
H	-11.941303	-4.508025	-0.613957
C	-14.983016	1.985841	0.110864
H	-14.694930	2.623871	0.955578
H	-14.235874	2.083623	-0.676719
H	-15.930577	2.339351	-0.298397
H	-7.834303	0.601881	-0.674171
H	-6.203813	-3.379027	-0.531368
H	-8.414994	-4.280019	-0.193135
H	-12.505395	1.287433	-0.021137
H	-13.278002	-3.553344	0.544876
H	-17.244177	2.062926	1.213490
H	-19.371107	1.195989	2.000835
H	-19.734025	-1.252531	2.292279
H	-17.838811	-2.817712	1.771904

2. **Compound C2**

Atoms	Coordinates (Angstroms) X	Y	Z
C	18.789230	-0.406099	2.184184
C	17.878239	0.457658	1.611466
C	16.583844	0.035170	1.281361
C	18.393460	-1.722204	2.447500
C	16.191740	-1.302263	1.521086
C	17.123142	-2.168448	2.128856
C	15.657686	1.006905	0.697678
C	14.290855	0.505122	0.475026
C	13.955370	-0.843257	0.744050
C	13.336675	1.404679	0.012675
C	12.013274	1.020186	-0.201977
C	11.665236	-0.313140	0.120134
C	12.619846	-1.213673	0.579121
C	10.275610	-0.784087	0.006113
C	9.306209	0.243403	-0.387438
C	9.719632	1.558206	-0.707069
C	8.715865	2.495619	-1.030365
C	7.387912	2.126349	-1.063841
C	6.965783	0.812930	-0.769916
C	7.955692	-0.102513	-0.424528
C	5.563996	0.421964	-0.807886
C	5.030314	-0.852144	-0.845772
C	3.628628	-0.882417	-0.869349
C	3.050322	0.379326	-0.852656
C	-3.050354	-0.379775	-0.852852
C	-3.628642	0.881968	-0.870029
C	-5.030322	0.851735	-0.846447
N	14.925341	-1.740229	1.170005
N	11.056372	1.901676	-0.694080
S	-4.294429	-1.604855	-0.796196
S	4.294372	1.604446	-0.796492
O	15.977813	2.163335	0.434515
O	9.955101	-1.944476	0.247418
H	18.122412	1.493732	1.397072
H	16.848566	-3.184981	2.383410
H	19.086633	-2.412497	2.920619

H	19.789819	-0.070566	2.437926
H	12.244815	-2.201349	0.821964
H	13.692483	2.417511	-0.138438
H	7.715964	-1.125294	-0.150524
H	8.967715	3.528882	-1.235753
H	5.644057	-1.745346	-0.876233
H	3.025240	-1.786479	-0.902561
H	-3.025236	1.786007	-0.903574
H	-5.644045	1.744938	-0.877248
C	-5.564029	-0.422354	-0.808036
H	6.651552	2.880399	-1.330646
C	11.476349	3.199741	-1.189493
H	10.825020	3.507390	-2.008381
C	14.603022	-3.152509	1.250657
H	15.485076	-3.743152	0.999021
H	14.246616	-3.443317	2.246533
H	11.461404	3.968350	-0.407221
H	13.835208	-3.393169	0.515658
H	12.485858	3.124480	-1.593354
C	-6.965823	-0.813241	-0.769917
C	-7.388043	-2.126665	-1.063676
C	-7.955664	0.102311	-0.424603
C	-9.306201	-0.243512	-0.387420
C	-9.719708	-1.558324	-0.706894
C	-8.716022	-2.495848	-1.030120
C	-10.275534	0.784064	0.006070
C	-11.665184	0.313212	0.120170
C	-12.013310	-1.020120	-0.201812
C	-12.619717	1.213868	0.579093
C	-13.955267	0.843572	0.744055
C	-14.290838	-0.504819	0.475182
C	-13.336731	-1.404499	0.012919
C	-15.657709	-1.006485	0.697865
C	-16.583830	-0.034614	1.281380
C	-16.191638	1.302817	1.520958
C	-17.122985	2.169137	2.128610
C	-18.393357	1.723028	2.447237
C	-18.789221	0.406927	2.184050
C	-17.878263	-0.456976	1.611498
N	-11.056472	-1.901719	-0.693838
N	-14.925186	1.740650	1.169901
O	-9.954938	1.944443	0.247310

O	-15.977900	-2.162931	0.434847
C	-11.476488	-3.199805	-1.189167
H	-10.825356	-3.507373	-2.008254
H	-11.461248	-3.968440	-0.406927
H	-12.486117	-3.124622	-1.592731
C	-14.602818	3.152926	1.250447
H	-14.246714	3.443860	2.246392
H	-13.834768	3.393449	0.515653
H	-15.484773	3.743577	0.998452
H	-7.715871	1.125113	-0.150734
H	-6.651748	-2.880795	-1.330432
H	-8.967979	-3.529108	-1.235382
H	-12.244570	2.201527	0.821831
H	-13.692639	-2.417317	-0.138062
H	-16.848338	3.185675	2.383072
H	-19.086513	2.413448	2.920198
H	-19.789863	0.071520	2.437748
H	-18.122484	-1.493065	1.397226
C	0.395649	-1.750825	-0.872739
C	0.626498	-0.328844	-0.876522
C	-0.626530	0.328358	-0.876671
C	-1.641825	-0.625363	-0.866450
C	1.641788	0.624891	-0.866410
C	-0.395691	1.750342	-0.873212
N	1.024791	1.865347	-0.865641
N	-1.024837	-1.865825	-0.865352
O	-1.135990	2.726671	-0.878590
O	1.135945	-2.727160	-0.877759
C	1.631428	3.172679	-0.866656
H	2.254470	3.327050	-1.753513
H	0.804215	3.886256	-0.882509
H	2.229942	3.340974	0.034547
C	-1.631463	-3.173162	-0.866266
H	-2.254741	-3.327474	-1.752960
H	-0.804249	-3.886731	-0.882363
H	-2.229741	-3.341528	0.035088

3. **Compound C3**

Atoms	Coordinates (Angstroms)		
	X	Y	Z

C	-21.788275	0.509627	0.661989
C	-20.773730	-0.416273	0.529149
C	-19.449023	-0.016636	0.309263
C	-21.470148	1.870217	0.586821
C	-19.130579	1.357372	0.205575
C	-20.171705	2.294199	0.366187
C	-18.415010	-1.047482	0.200545
C	-17.039541	-0.535959	0.072094
C	-16.782599	0.853075	-0.014736
C	-16.001332	-1.460782	0.062868
C	-14.667687	-1.061753	-0.028715
C	-14.408038	0.329231	-0.058420
C	-15.446471	1.253896	-0.052409
C	-13.029473	0.844516	-0.070933
C	-11.986917	-0.181311	0.027594
C	-12.310642	-1.558117	0.039853
C	-11.248588	-2.476469	0.174812
C	-9.942996	-2.039623	0.264906
C	-9.606439	-0.671288	0.223403
C	-10.656627	0.232550	0.104365
C	-8.227734	-0.207838	0.318793
C	-7.768636	1.025306	0.722738
C	-6.362999	1.142472	0.695902
C	-5.723314	-0.001632	0.271544
C	5.751673	-0.132170	-0.674505
C	6.406505	-1.255156	-1.130414
C	7.810701	-1.116252	-1.157364
N	-17.830171	1.763879	-0.042457
N	-13.622211	-1.976871	-0.072950
S	6.901673	1.102097	-0.250516
S	-6.890436	-1.231230	-0.119724
O	-18.661676	-2.250277	0.239877
O	-12.779665	2.045524	-0.131268
H	-20.956684	-1.484728	0.592158
H	-19.965668	3.357628	0.350381
H	-22.249574	2.616915	0.712832
H	-22.811934	0.192054	0.833495
H	-15.139746	2.293659	-0.050813
H	-16.304947	-2.497065	0.158892
H	-10.481942	1.302886	0.051602
H	-11.442192	-3.539438	0.252773

H	-8.429556	1.815637	1.060907
H	-5.827784	2.034044	1.005890
H	5.883338	-2.145164	-1.464503
H	8.481247	-1.888304	-1.518108
C	8.253327	0.112195	-0.721188
H	-9.157670	-2.779406	0.399604
C	-13.919310	-3.387902	-0.236250
H	-13.126793	-3.863538	-0.815424
C	-17.554209	3.158311	-0.331971
H	-18.385224	3.585202	-0.895513
H	-17.394116	3.750371	0.577622
H	-14.024407	-3.905531	0.725067
H	-16.667697	3.230241	-0.961714
H	-14.843708	-3.500949	-0.802425
C	9.623126	0.600337	-0.620563
C	9.922025	1.976486	-0.554513
C	10.699300	-0.279890	-0.575860
C	12.019465	0.165405	-0.494424
C	12.307520	1.549610	-0.451733
C	11.216899	2.443260	-0.466372
C	13.089533	-0.835301	-0.434557
C	14.441350	-0.286281	-0.238622
C	14.661861	1.110871	-0.190642
C	15.490620	-1.184218	-0.075454
C	16.797989	-0.748968	0.146523
C	17.006921	0.646714	0.252078
C	15.959103	1.544666	0.083420
C	18.337046	1.193895	0.570175
C	19.367814	0.190518	0.842437
C	19.100543	-1.191963	0.710376
C	20.128648	-2.100766	1.033559
C	21.370161	-1.642280	1.437111
C	21.641433	-0.273503	1.541495
C	20.635929	0.625311	1.249537
N	13.612094	1.999367	-0.391159
N	17.860284	-1.633041	0.280292
O	12.878490	-2.042498	-0.515289
O	18.547255	2.402848	0.627759
C	13.895653	3.416276	-0.524244
H	13.179635	3.869358	-1.211123
H	13.855299	3.941534	0.437884
H	14.886275	3.548882	-0.958935

C	17.661949	-3.036027	-0.030511
H	17.381001	-3.624203	0.851905
H	16.880874	-3.134192	-0.784301
H	18.576808	-3.447686	-0.459392
H	10.554786	-1.355964	-0.584246
H	9.112850	2.702272	-0.578317
H	11.374876	3.511851	-0.386217
H	15.212245	-2.231566	-0.103547
H	16.220709	2.589190	0.208971
H	19.952007	-3.169129	1.002026
H	22.139905	-2.367949	1.685703
H	22.620848	0.071284	1.857782
H	20.782550	1.698541	1.325317
C	-4.309589	-0.242794	0.128877
C	-3.649640	-1.430170	-0.045353
C	-2.235728	-1.286433	-0.147463
C	-1.826101	0.050764	-0.042737
C	-1.252208	-2.292706	-0.324521
C	0.070456	-1.950795	-0.393214
C	0.495013	-0.596945	-0.288451
C	-0.467913	0.442422	-0.107250
C	1.853263	-0.204163	-0.353574
C	2.260366	1.133839	-0.247373
C	-0.045303	1.796722	-0.001634
C	1.276736	2.139653	-0.069541
C	3.673182	1.281216	-0.350892
C	4.336181	0.096082	-0.527998
S	-3.191776	1.108416	0.161716
S	3.222227	-1.258167	-0.561035
H	-4.157789	-2.388523	-0.082023
H	4.178686	2.240989	-0.315685
H	-1.557743	-3.332080	-0.405532
H	0.820324	-2.725576	-0.530610
H	-0.796162	2.570472	0.136064
H	1.582127	3.178990	0.012296

4. **Compound C4**

Atoms	Coordinates (Angstroms)		
	X	Y	Z

C	18.853124	-1.216067	0.618110
C	17.869268	-0.254496	0.509953
C	16.529412	-0.605577	0.299280
C	18.487858	-2.563826	0.527549
C	16.163157	-1.966305	0.179119
C	17.173426	-2.940120	0.315493
C	15.530075	0.461457	0.217620
C	14.136843	-0.000797	0.095923
C	13.831821	-1.378661	-0.010072
C	13.130619	0.958636	0.111801
C	11.783246	0.606850	0.025856
C	11.476109	-0.773913	-0.025747
C	12.482614	-1.733162	-0.043083
C	10.080709	-1.242007	-0.041140
C	9.073789	-0.183651	0.075894
C	9.444343	1.180622	0.115290
C	8.414542	2.131608	0.271986
C	7.094509	1.738832	0.349980
C	6.709500	0.384025	0.275609
C	7.729484	-0.552404	0.142421
C	5.313609	-0.029301	0.344467
C	4.811885	-1.267968	0.684539
C	3.408733	-1.327271	0.644603
C	2.803819	-0.139382	0.272304
C	-2.959679	0.638621	-0.330293
C	-3.715120	1.775604	-0.539381
C	-5.099307	1.526474	-0.636992
N	14.847361	-2.324374	-0.061388
N	10.769464	1.557267	0.006697
S	-4.008757	-0.756376	-0.245650
S	4.023187	1.071304	-0.023881
O	15.818558	1.654336	0.272623
O	9.791138	-2.433152	-0.120356
H	18.089089	0.806121	0.586206
H	16.931028	-3.995583	0.287513
H	19.242534	-3.338418	0.634492
H	19.888820	-0.935968	0.782530
H	12.140656	-2.761777	-0.056944
H	13.470396	1.982254	0.221465
H	7.518875	-1.614963	0.068461
H	8.644826	3.185144	0.374736
H	5.438451	-2.101245	0.982984

H	2.850768	-2.219638	0.904877
H	-3.262648	2.753762	-0.628840
H	-5.832870	2.302218	-0.827512
C	-5.437084	0.198241	-0.505645
H	6.335405	2.502661	0.498669
C	11.113290	2.960423	-0.130110
H	10.332377	3.474772	-0.691540
C	14.519885	-3.703921	-0.368138
H	15.333241	-4.153818	-0.939400
H	14.340082	-4.301399	0.534220
H	11.244462	3.453595	0.840829
H	13.629802	-3.735203	-0.996339
H	12.036029	3.054319	-0.702599
C	-6.759382	-0.410745	-0.563995
C	-6.938431	-1.781213	-0.843067
C	-7.908470	0.341381	-0.341120
C	-9.186082	-0.215439	-0.415468
C	-9.353237	-1.585315	-0.725972
C	-8.189098	-2.357645	-0.917885
C	-10.339546	0.648472	-0.145864
C	-11.641628	-0.038397	-0.143919
C	-11.741406	-1.414996	-0.457000
C	-12.767344	0.702932	0.198128
C	-14.036407	0.124334	0.249903
C	-14.126505	-1.263730	-0.010283
C	-13.001789	-2.004277	-0.355727
C	-15.410901	-1.975786	0.101920
C	-16.529696	-1.158944	0.575568
C	-16.379835	0.227591	0.810613
C	-17.489184	0.939795	1.310257
C	-18.694923	0.297806	1.530444
C	-18.849383	-1.068661	1.271613
C	-17.764028	-1.781090	0.804143
N	-10.614725	-2.138582	-0.829425
N	-15.173226	0.859265	0.559515
O	-10.233150	1.849804	0.086072
O	-15.517646	-3.171706	-0.157959
C	-10.772176	-3.492987	-1.325983
H	-10.004698	-3.699808	-2.072884
H	-10.708525	-4.240715	-0.525931
H	-11.737816	-3.587381	-1.822607
C	-15.088263	2.305892	0.623915

H	-14.869015	2.667376	1.636252
H	-14.307896	2.654290	-0.052606
H	-16.028182	2.742254	0.283027
H	-7.856610	1.394310	-0.081181
H	-6.068748	-2.410796	-1.013800
H	-8.255205	-3.422334	-1.106223
H	-12.579713	1.741603	0.445514
H	-13.175318	-3.063303	-0.509373
H	-17.404875	1.990783	1.559113
H	-19.529431	0.873073	1.922314
H	-19.801960	-1.558338	1.447624
H	-17.819039	-2.845870	0.598513
C	1.382389	0.096133	0.112038
C	0.827409	1.401565	-0.132400
C	-0.615903	1.605199	-0.278755
C	-1.526260	0.489028	-0.185828
C	0.458242	-0.930518	0.179745
C	-0.929747	-0.738608	0.041668
N	1.573999	2.485619	-0.242925
N	-0.991336	2.853942	-0.500966
H	0.477889	3.847824	-0.540264
H	0.805136	-1.946471	0.337586
H	-1.557875	-1.622652	0.115416

5. **Compound C5**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-18.932223	-0.740772	-0.142969
C	-17.908932	0.183905	-0.188917
C	-16.582550	-0.185908	0.069614
C	-18.621690	-2.072063	0.155931
C	-16.271102	-1.525611	0.398591
C	-17.321763	-2.465495	0.419914
C	-15.539485	0.837822	-0.019372
C	-14.164745	0.340628	0.160785
C	-13.915248	-1.015850	0.477835
C	-13.119877	1.240795	-0.015185
C	-11.787171	0.846588	0.107646
C	-11.536299	-0.521246	0.370605

C	-12.581588	-1.420349	0.551558
C	-10.160690	-1.042734	0.433111
C	-9.115094	-0.064214	0.119669
C	-9.430851	1.292920	-0.122493
C	-8.370178	2.159637	-0.457235
C	-7.072083	1.697082	-0.520033
C	-6.740109	0.353051	-0.251417
C	-7.790745	-0.501843	0.065811
C	-5.367258	-0.132111	-0.320276
C	-4.931174	-1.428985	-0.487467
C	-3.529907	-1.547051	-0.517982
C	-2.862432	-0.345158	-0.374214
C	2.931111	0.429322	-0.333462
C	3.659068	1.601616	-0.358265
C	5.054702	1.399536	-0.355199
N	-14.968425	-1.897041	0.685261
N	-10.734982	1.742149	-0.037570
S	4.011840	-0.938973	-0.290196
S	-4.015169	0.949620	-0.195304
O	-15.779764	2.019408	-0.254570
O	-9.918176	-2.217216	0.698552
H	-18.086260	1.227995	-0.428758
H	-17.122279	-3.513052	0.610645
H	-19.408436	-2.821498	0.173409
H	-19.957066	-0.446537	-0.346205
H	-12.283560	-2.448676	0.721811
H	-13.416967	2.249248	-0.279905
H	-7.620679	-1.548885	0.297486
H	-8.561194	3.194563	-0.714250
H	-5.605576	-2.268577	-0.615160
H	-3.020595	-2.493034	-0.663194
H	3.181721	2.573134	-0.387943
H	5.775213	2.208979	-0.399058
C	5.424692	0.073489	-0.325092
H	-6.289121	2.392052	-0.812961
C	-11.016821	3.163463	-0.108845
H	-10.198692	3.721240	0.348651
C	-14.693933	-3.224075	1.202829
H	-15.518284	-3.544505	1.841555
H	-14.548464	-3.962376	0.404495
H	-11.157760	3.509617	-1.140205
H	-13.798745	-3.193791	1.823902

H	-11.917217	3.384099	0.464583
C	6.766401	-0.494851	-0.312525
C	7.014896	-1.830042	-0.691845
C	7.868572	0.267368	0.061070
C	9.163643	-0.253111	0.069292
C	9.394794	-1.603821	-0.280662
C	8.282270	-2.374125	-0.677441
C	10.267656	0.632103	0.451796
C	11.607545	0.030432	0.352240
C	11.773641	-1.326224	-0.015618
C	12.705604	0.843864	0.609610
C	14.011601	0.361312	0.515840
C	14.177903	-0.979940	0.095992
C	13.080181	-1.794058	-0.159310
C	15.520268	-1.550749	-0.108467
C	16.625959	-0.608476	0.074316
C	16.396467	0.719762	0.502578
C	17.505408	1.583596	0.610094
C	18.781583	1.126136	0.333708
C	19.010284	-0.196197	-0.062955
C	17.929969	-1.044621	-0.194357
N	10.668098	-2.138643	-0.236257
N	15.115886	1.153340	0.801678
O	10.098160	1.796695	0.803481
O	15.687124	-2.723375	-0.434490
C	10.860377	-3.564200	-0.426951
H	10.009011	-4.106310	-0.013435
H	10.979130	-3.830393	-1.484410
H	11.744861	-3.888069	0.121355
C	14.919724	2.451834	1.418036
H	14.837571	3.257789	0.678269
H	14.013630	2.433706	2.023498
H	15.751664	2.666210	2.090522
H	7.764027	1.301251	0.375765
H	6.190325	-2.451299	-1.032480
H	8.408358	-3.394857	-1.017559
H	12.471030	1.872736	0.857584
H	13.317336	-2.795695	-0.499483
H	17.370977	2.624288	0.879135
H	19.615013	1.818187	0.419767
H	20.017388	-0.541428	-0.274437
H	18.043127	-2.076695	-0.512317

C	-1.429103	-0.128445	-0.355322
C	-0.824031	1.158037	-0.324461
C	0.584454	1.347550	-0.316449
C	1.494939	0.252213	-0.339433
C	-0.515709	-1.178025	-0.370976
C	0.877228	-0.994069	-0.367429
N	-1.407992	2.369451	-0.290688
N	0.822642	2.672598	-0.277744
H	-0.883572	-2.198971	-0.381925
H	1.496733	-1.887118	-0.387023
N	-0.385205	3.195239	-0.260122
C	-0.579307	4.626456	-0.279444
H	-0.579905	4.990896	-1.310718
H	-1.538323	4.844376	0.189217
H	0.236879	5.090707	0.273669

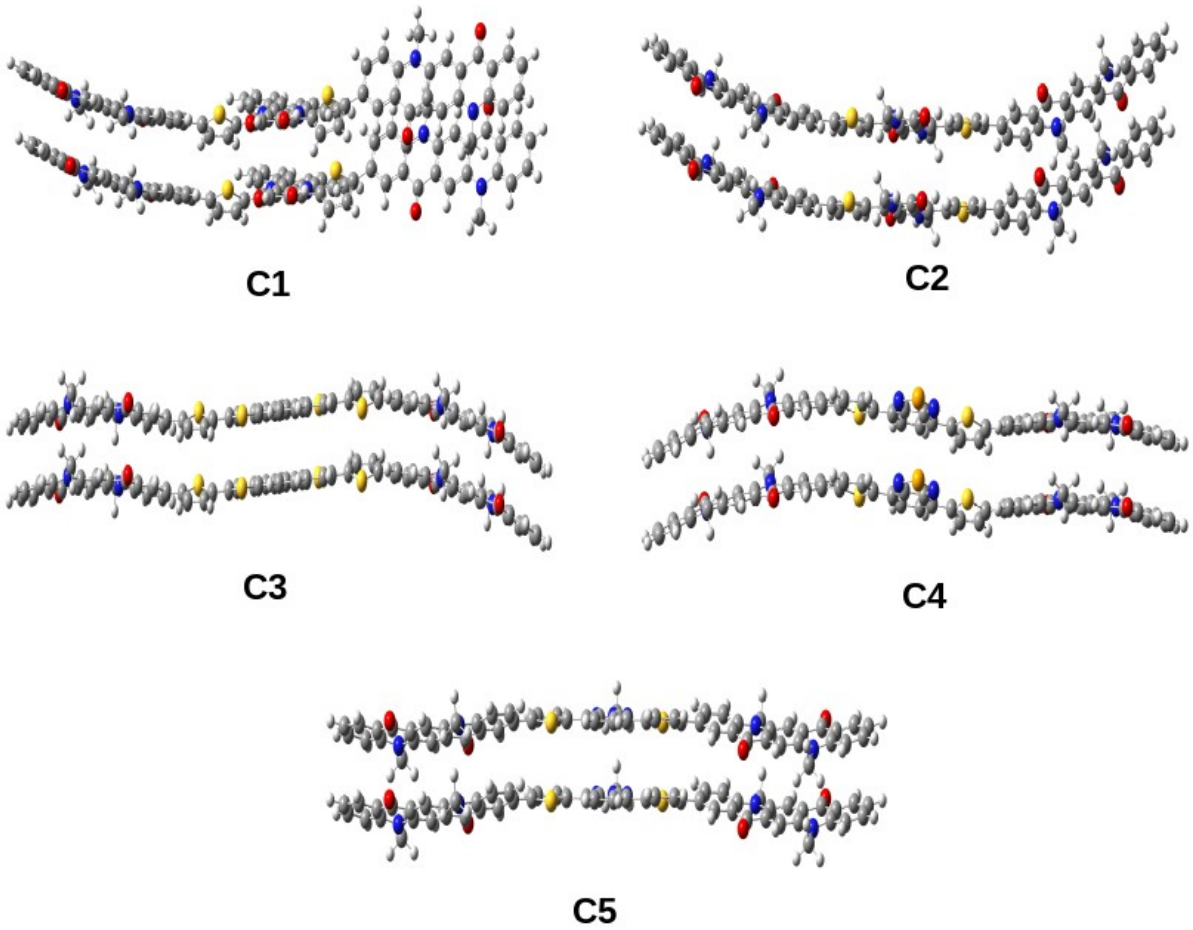

Fig. S1 : Optimized structures of the studied compounds in the π-stacked orientation.

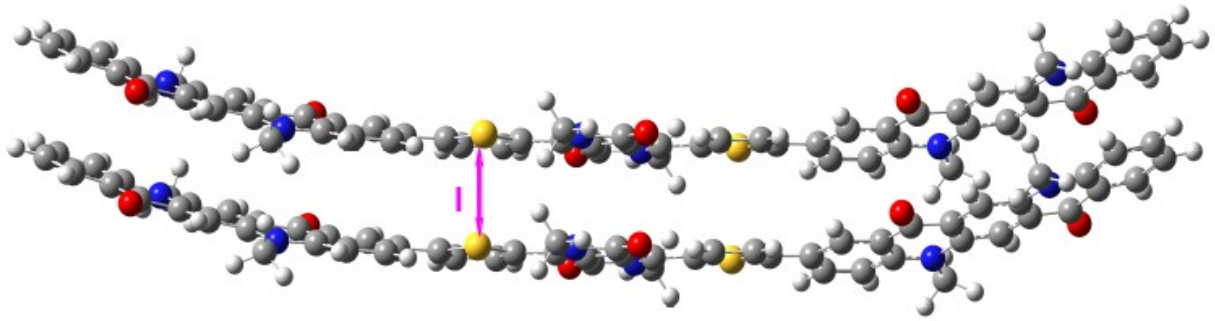

Fig. S2 : Representative structure of two stacked molecules along with distance l.

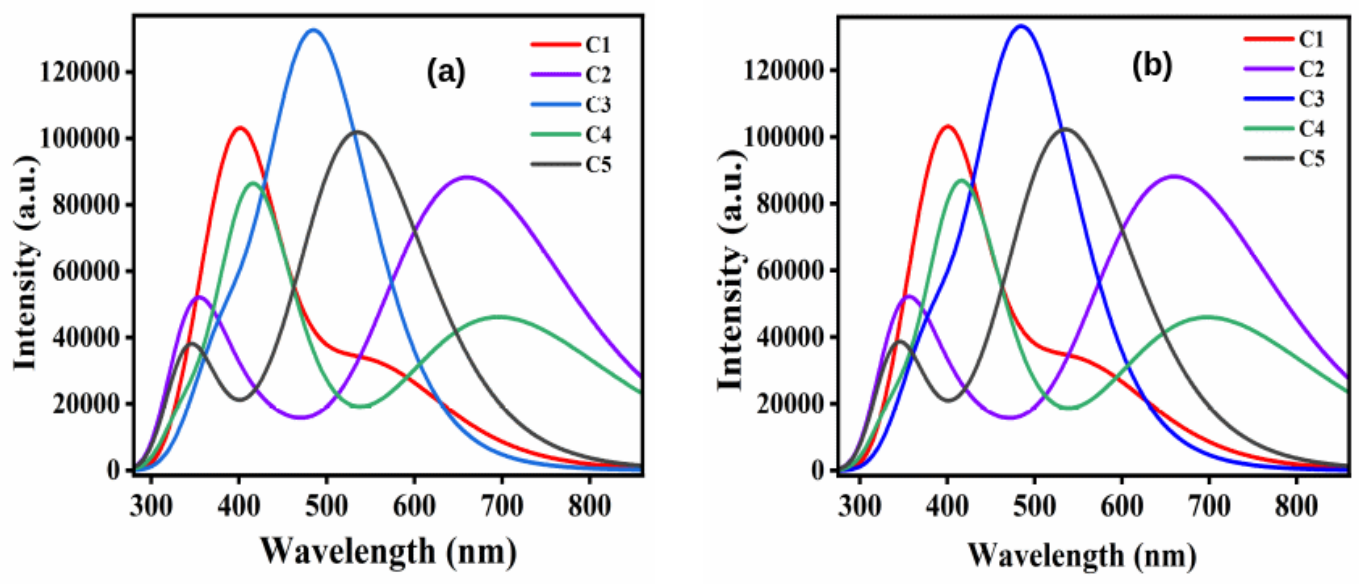

Fig. S3 : Absorption spectra of the studied compounds in (a) DCM phase and (b) ethanol phase.

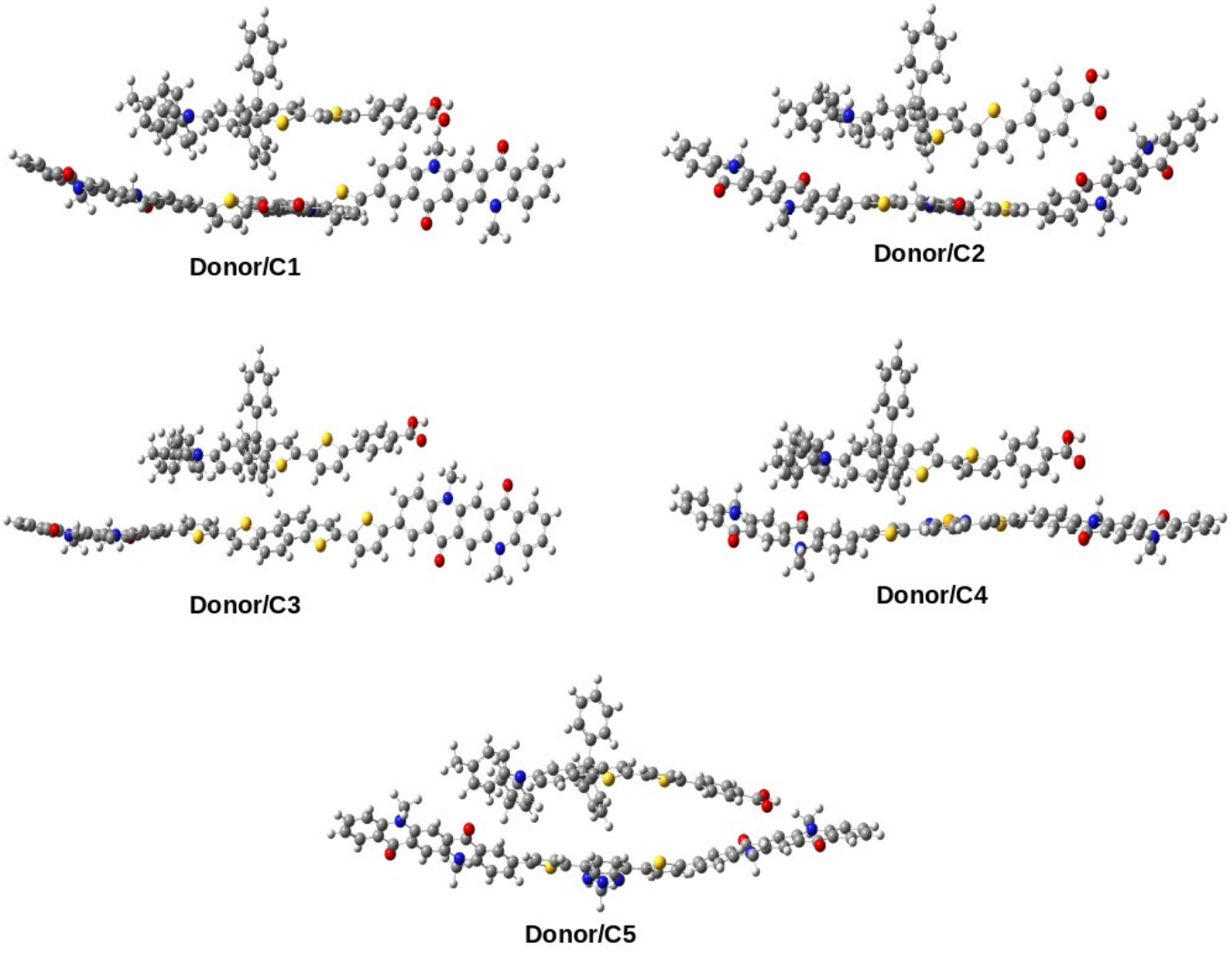

Fig. S4 : Optimized structures of the A1/C1-C5 molecules.