Donor Moieties with D-π-A Framing Modulated Electronic and Nonlinear Optical Properties for Non-Fullerene Based Chromophores

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Table S1: Cartesian coordinates of**FH**

Atom	X-axis	Y-axis	Z-axis
C	2.973929	-1.77683	0.000086
C	3.419148	-0.4362	0.00001
C	2.519953	0.629309	-0.000002
C	1.17248	0.32973	0.000063
C	0.726582	-1.00343	0.000153
C	1.626664	-2.06901	0.000167
H	2.873295	1.658646	-0.000044
H	1.278001	-3.10003	0.000252
C	0.000002	1.288082	0.000044
C	-1.17248	0.329729	0.000118
C	-2.51995	0.629305	0.000114
C	-3.41914	-0.43621	0.0002

C	-2.97392	-1.77683	0.000295
C	-1.62665	-2.06902	0.00029
C	-0.72658	-1.00343	0.000195
H	-2.8733	1.658641	0.000062
H	-1.27799	-3.10003	0.000369
C	4.860008	-0.4769	-0.000048
C	4.142395	-2.74917	0.000049
C	5.302874	-1.78834	-0.000034
C	-4.86	-0.47691	0.000216
C	-4.14239	-2.74918	0.000388
C	-5.30287	-1.78835	0.000331
C	7.315871	-0.62787	-0.00014
C	6.683627	-1.87734	-0.00011
H	7.260948	-2.7981	-0.00013
S	6.12313	0.679226	-0.00013
C	-6.68362	-1.87735	0.000351
H	-7.26095	-2.79811	0.000389
C	-7.31587	-0.62788	0.000241
S	-6.12312	0.679212	0.000123
C	-8.72611	-0.5535	0.000144
H	-9.14527	-1.5561	0.000239
C	8.726113	-0.55351	-0.00015
H	9.145269	-1.5561	-0.00029
C	10.59074	2.62904	-0.000082
C	11.64483	1.710581	-0.00021
C	12.95439	2.182676	-0.0004
C	13.16246	3.556834	-0.00047
C	12.10133	4.45789	-0.00033

C	10.79329	3.994143	-0.00013
C	9.635175	0.470649	-0.000021
H	13.80787	1.517026	-0.00049
H	14.18063	3.932786	-0.00062
H	12.30261	5.524381	-0.00038
H	9.940504	4.666109	-0.000008
C	-11.6448	1.71059	0.00002
C	-10.5907	2.629047	0.000184
C	-10.7933	3.994148	0.000344
C	-12.1013	4.457898	0.000342
C	-13.1625	3.556846	0.000186
C	-12.9544	2.182687	0.000024
C	-9.63517	0.470655	-0.000054
H	-9.94049	4.666114	0.000462
H	-12.3026	5.524388	0.00046
H	-14.1806	3.9328	0.000193
H	-13.8079	1.517038	-0.000069
C	9.305874	1.906268	0.000088
O	8.202826	2.411148	0.000318
C	-9.30587	1.906266	0.00012
O	-8.20283	2.411158	0.000237
C	-11.0865	0.341765	-0.00022
C	-11.8398	-0.80677	-0.00063
C	11.08647	0.341756	-0.0001
C	11.83975	-0.80678	-0.000016
C	11.2861	-2.11736	0.000191
N	10.85357	-3.18934	0.000353
C	13.26213	-0.80571	-0.000097

N	14.41696	-0.84148	-0.00015
C	-11.2861	-2.11736	-0.00113
N	-10.8537	-3.18937	-0.00156
C	-13.2621	-0.80568	-0.00062
N	-14.417	-0.84149	-0.00061
C	0.000026	2.159834	1.255513
H	-0.88584	2.804431	1.278604
H	0.000045	1.543733	2.160495
H	0.88589	2.804434	1.278568
C	-0.000025	2.159761	-1.25546
H	0.885833	2.804366	-1.27859
H	-4.1E-05	1.543619	-2.16042
H	-0.88589	2.804361	-1.27856
C	-4.14076	-3.61888	1.256643
H	-5.0278	-4.26219	1.27805
H	-3.25525	-4.26392	1.280312
H	-4.14142	-3.00173	2.160736
C	-4.1408	-3.61904	-1.25576
H	-4.14156	-3.00201	-2.15993
H	-3.25527	-4.26405	-1.2794
H	-5.02782	-4.2624	-1.27702
C	4.140848	-3.61895	1.256242
H	3.255293	-4.26393	1.279971
H	5.027839	-4.26234	1.277502
H	4.14167	-3.00187	2.160378
C	4.140728	-3.61895	-1.25616
H	3.255162	-4.26391	-1.27981
H	4.141483	-3.00185	-2.16029

H	5.027713	-4.26234	-1.27749

Table S2: Cartesian coordinates of**FHD1**

Atom	X-axis	Y-axis	Z-axis
C	2.655593	-1.70776	0.073629
C	3.115453	-0.37432	0.008519
C	2.22596	0.698762	-0.0555
C	0.876895	0.412973	-0.05365
C	0.414834	-0.91464	0.008875
C	1.304753	-1.98664	0.073167
H	2.590062	1.723336	-0.10463
H	0.944792	-3.01266	0.122223
C	-0.28634	1.380832	-0.11243
C	-1.46875	0.435359	-0.07689
C	-2.81523	0.751649	-0.10531
C	-3.72738	-0.29825	-0.06307
C	-3.29673	-1.6429	0.007538
C	-1.95476	-1.95064	0.035974
C	-1.03809	-0.89763	-0.00695
H	-3.15392	1.784625	-0.15975
H	-1.61939	-2.98512	0.090301
C	4.554124	-0.4288	0.026044
C	3.813738	-2.6906	0.138852
C	4.985269	-1.74355	0.102454
C	-5.1708	-0.33299	-0.07889
C	-4.48224	-2.59509	0.042198
C	-5.6313	-1.62184	-0.0239
C	7.009976	-0.60197	0.059367

C	6.363519	-1.84443	0.122639
H	6.932122	-2.769	0.178787
S	5.827636	0.713952	-0.02545
C	-7.03419	-1.71466	-0.03304
H	-7.59665	-2.64049	0.03709
S	-6.45602	0.810836	-0.15564
C	8.418104	-0.54067	0.065609
H	8.82818	-1.54502	0.128545
C	10.31327	2.621205	-0.10032
C	11.35907	1.695564	-0.04342
C	12.67227	2.156716	-0.0568
C	12.89177	3.527726	-0.12749
C	11.83854	4.435781	-0.18467
C	10.52667	3.982554	-0.171
C	9.338702	0.474808	0.010264
H	13.52007	1.485175	-0.01386
H	13.91313	3.894914	-0.13792
H	12.04855	5.499241	-0.23936
H	9.679069	4.659756	-0.21362
C	9.021979	1.909419	-0.0715
O	7.923955	2.424559	-0.10837
C	10.78685	0.333057	0.02325
C	11.53157	-0.82078	0.080176
C	10.96831	-2.12559	0.140076
N	10.52919	-3.19386	0.189067
C	12.9537	-0.83058	0.083566
N	14.10834	-0.87561	0.088068
C	-0.2883	2.311921	1.099876

H	-1.16856	2.964642	1.085036
H	-0.30231	1.738757	2.032581
H	0.603457	2.949125	1.101191
C	-0.26543	2.191724	-1.40755
H	0.626106	2.827556	-1.45222
H	-0.26186	1.532795	-2.28187
H	-1.14608	2.84088	-1.47076
C	-4.50868	-3.39959	1.340654
H	-5.40605	-4.02787	1.384387
H	-3.63296	-4.05506	1.409364
H	-4.51127	-2.7358	2.211089
C	-4.47877	-3.5287	-1.16743
H	-4.45692	-2.95731	-2.10092
H	-3.60483	-4.18993	-1.14739
H	-5.3775	-4.15675	-1.16936
C	3.788152	-3.49508	1.437381
H	2.895508	-4.12902	1.482503
H	4.668325	-4.14494	1.502562
H	3.784154	-2.83264	2.308839
C	3.817478	-3.62394	-1.07114
H	2.92486	-4.25964	-1.07296
H	3.835256	-3.05358	-2.00531
H	4.697538	-4.27699	-1.04942
H	-11.3639	3.398389	0.302983
C	-9.96439	-1.11127	-0.67886
C	-9.06828	-0.18025	-0.13274
C	-9.57092	1.025982	0.373222
C	-10.9257	1.276659	0.326783

C	-11.8103	0.334476	-0.21515
C	-11.3252	-0.86639	-0.71781
H	-9.57179	-2.03152	-1.10145
H	-8.89393	1.749906	0.821572
H	-12.0005	-1.60059	-1.14895
C	-11.6884	2.479034	0.807858
H	-11.5479	2.647394	1.883754
C	-13.1118	2.127692	0.475843
C	-14.2695	2.853964	0.682891
C	-15.486	2.311124	0.282763
C	-15.5402	1.05612	-0.3166
C	-14.3818	0.322132	-0.52624
C	-13.1662	0.862988	-0.12727
H	-14.2334	3.834879	1.149936
H	-16.4031	2.870986	0.438715
H	-16.4992	0.64931	-0.62258
H	-14.4258	-0.65801	-0.99378
C	-7.643	-0.48346	-0.09734

Table S3: Cartesian coordinates of**FHD2**

Atom	X-axis	Y-axis	Z-axis
C	-4.01728	-1.70534	0.0599
C	-4.48162	-0.37471	-0.02767
C	-3.59556	0.700284	-0.10773
C	-2.24559	0.419364	-0.0968
C	-1.77916	-0.90542	-0.00998
C	-2.66555	-1.97944	0.067884

H	-3.9632	1.722628	-0.17418
H	-2.30198	-3.00311	0.135979
C	-1.08517	1.390117	-0.16492
C	0.100309	0.449911	-0.10172
C	1.446022	0.770729	-0.11802
C	2.361445	-0.27456	-0.0427
C	1.934326	-1.61962	0.04485
C	0.593357	-1.93191	0.058542
C	-0.32644	-0.88322	-0.01405
H	1.781907	1.803893	-0.18506
H	0.260621	-2.96646	0.126368
C	-5.91999	-0.43362	-0.00714
C	-5.17207	-2.6909	0.140501
C	-6.34674	-1.74842	0.091768
C	3.804903	-0.30355	-0.02665
C	3.122417	-2.56605	0.118513
C	4.26876	-1.58859	0.070326
C	-8.37525	-0.61384	0.041581
C	-7.72443	-1.85321	0.120032
H	-8.28978	-2.77855	0.193687
S	-7.1974	0.704278	-0.06976
C	5.671828	-1.67695	0.08664
H	6.237135	-2.60304	0.124441
S	5.088292	0.844427	-0.08835
C	-9.78334	-0.55707	0.05695
H	-10.1894	-1.56181	0.136291
C	-11.6899	2.596834	-0.1271
C	-12.7323	1.668882	-0.05065

C	-14.0468	2.126375	-0.05525
C	-14.2708	3.496131	-0.13668
C	-13.2208	4.40648	-0.21309
C	-11.9076	3.956865	-0.2086
C	-10.7079	0.454632	-0.00396
H	-14.8923	1.45298	0.002706
H	-15.2933	3.860403	-0.14014
H	-13.4343	5.468812	-0.27554
H	-11.0623	4.635764	-0.26632
C	-10.3963	1.889049	-0.10453
O	-9.30023	2.406919	-0.15861
C	-12.1553	0.308716	0.023817
C	-12.8961	-0.8467	0.098541
C	-12.3286	-2.14932	0.164984
N	-11.8859	-3.21587	0.219623
C	-14.318	-0.86029	0.11579
N	-15.4725	-0.90845	0.131935
C	-1.09873	2.175622	-1.47574
H	-0.21986	2.826624	-1.54433
H	-1.09287	1.49977	-2.33703
H	-1.99237	2.806831	-1.53974
C	-1.09612	2.344808	1.02891
H	-1.99029	2.978376	1.011374
H	-1.08671	1.790106	1.972766
H	-0.21849	3.000887	1.00801
C	3.151608	-3.51217	-1.08117
H	4.053287	-4.13546	-1.0565
H	2.280494	-4.17743	-1.07377

H	3.148069	-2.95052	-2.02077
C	3.122051	-3.35742	1.425186
H	3.0996	-2.68517	2.288836
H	2.249312	-4.01817	1.479519
H	4.022069	-3.97938	1.496445
C	-5.17378	-3.64141	-1.0562
H	-4.27876	-4.27372	-1.05
H	-6.05144	-4.29728	-1.02432
H	-5.19461	-3.08446	-1.99837
C	-5.14287	-3.47697	1.450167
H	-4.2486	-4.10798	1.503184
H	-5.13958	-2.80236	2.312233
H	-6.02126	-4.12814	1.525559
C	8.607144	-1.00046	0.635412
C	7.701571	-0.14084	0.002937
C	8.218887	0.997651	-0.62319
C	9.574152	1.2643	-0.62528
C	10.46875	0.399655	0.008271
C	9.962039	-0.73861	0.639999
H	8.232239	-1.87132	1.165473
H	7.548419	1.671503	-1.15024
H	10.64642	-1.41071	1.14932
C	6.277862	-0.44535	0.002852
N	11.85156	0.663712	0.012533
H	9.956119	2.146508	-1.13029
C	12.32895	1.982839	0.181501
C	11.71783	2.846234	1.091732
C	13.42382	2.437474	-0.55428

C	12.18933	4.138615	1.252175
H	10.87046	2.493631	1.672038
C	13.89987	3.725657	-0.37303
H	13.89882	1.770904	-1.26785
C	13.28509	4.585685	0.526446
H	11.70303	4.798213	1.964564
H	14.75372	4.063928	-0.95232
H	13.65716	5.596065	0.661314
C	12.76716	-0.40034	-0.16695
C	13.90467	-0.49935	0.633449
C	12.54074	-1.36157	-1.15159
C	14.80212	-1.53726	0.441622
H	14.07909	0.246412	1.40349
C	13.43428	-2.40575	-1.32515
H	11.65679	-1.27955	-1.77745
C	14.57147	-2.49744	-0.53428
H	15.68464	-1.60245	1.07079
H	13.24675	-3.14706	-2.09606
H	15.27401	-3.31203	-0.67736

Table S4: Cartesian coordinates of**FHD3**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	4.75087	-1.67536	-0.15455
C	5.254124	-0.37454	0.06487
C	4.401054	0.713207	0.253748
C	3.043575	0.47587	0.215087
C	2.537469	-0.81875	-0.00365

C	3.391378	-1.90628	-0.18853
H	4.799716	1.712105	0.420931
H	2.996668	-2.90619	-0.35946
C	1.914009	1.470867	0.377637
C	0.700695	0.580631	0.210694
C	-0.6338	0.943043	0.243595
C	-1.58051	-0.05916	0.057026
C	-1.19654	-1.40376	-0.15281
C	0.134006	-1.75753	-0.18335
C	1.085787	-0.75121	-0.00311
H	-0.93833	1.975226	0.406636
H	0.435497	-2.79075	-0.34838
C	6.68982	-0.47206	0.031905
C	5.876708	-2.68061	-0.33774
C	7.078526	-1.78218	-0.1988
C	-3.02325	-0.03573	0.015961
C	-2.41469	-2.29737	-0.3307
C	-3.52849	-1.28894	-0.20717
C	9.138548	-0.71339	-0.05608
C	8.45249	-1.92109	-0.24835
H	8.991198	-2.84966	-0.4185
S	7.998667	0.619116	0.193692
C	-4.93297	-1.32299	-0.26341
H	-5.52933	-2.21947	-0.40218
S	-4.26627	1.149416	0.150899
C	10.54747	-0.6934	-0.08945
H	10.92226	-1.69649	-0.27111
C	12.53746	2.379782	0.361872

C	13.55586	1.442274	0.170228
C	14.88016	1.871041	0.19188
C	15.13543	3.221443	0.403424
C	14.10814	4.14119	0.592087
C	12.7858	3.72022	0.572701
C	11.5008	0.283524	0.049151
H	15.70916	1.189951	0.049743
H	16.16569	3.562597	0.420414
H	14.34679	5.187487	0.754386
H	11.95633	4.405917	0.716031
C	11.22726	1.707535	0.298199
O	10.14636	2.243403	0.428419
C	12.94386	0.109422	-0.02857
C	13.65431	-1.04693	-0.24497
C	13.05388	-2.32205	-0.43516
N	12.58341	-3.36621	-0.59196
C	15.07475	-1.08768	-0.30201
N	16.22696	-1.15681	-0.35467
C	1.93998	2.111292	1.765524
H	1.081069	2.778624	1.89867
H	1.905211	1.347361	2.548938
H	2.852217	2.703067	1.902102
C	1.966786	2.546981	-0.70655
H	2.882736	3.142142	-0.6176
H	1.944816	2.097807	-1.70478
H	1.113267	3.228706	-0.61844
C	-2.49695	-3.35134	0.772563
H	-3.42175	-3.93256	0.677951

H	-1.65224	-4.04715	0.711022
H	-2.48588	-2.88262	1.761743
C	-2.41949	-2.96133	-1.70683
H	-2.35792	-2.21145	-2.50192
H	-1.57003	-3.64578	-1.8118
H	-3.33956	-3.5401	-1.84993
C	5.850721	-3.7492	0.754542
H	4.936142	-4.34907	0.687061
H	6.707441	-4.42511	0.651154
H	5.890199	-3.29375	1.749211
C	5.825119	-3.3272	-1.72141
H	4.913511	-3.92411	-1.83662
H	5.840762	-2.56757	-2.50938
H	6.684792	-3.99147	-1.86623
C	-7.82315	-0.49732	-0.82859
C	-6.90788	0.278976	-0.10715
C	-7.40176	1.395753	0.573759
C	-8.74329	1.725506	0.536814
C	-9.64473	0.949212	-0.19246
C	-9.16316	-0.1725	-0.87147
H	-7.46522	-1.34889	-1.39995
H	-6.72607	2.002687	1.170822
H	-9.85376	-0.77813	-1.45078
C	-5.49761	-0.0816	-0.08517
N	-11.0104	1.289812	-0.2547
H	-9.10747	2.591399	1.081492
C	-11.4059	2.641664	-0.36351
C	-10.7098	3.516942	-1.19916

C	-12.5048	3.116245	0.352824
C	-11.1033	4.840122	-1.30477
H	-9.85936	3.147784	-1.76461
C	-12.9023	4.437734	0.225666
H	-13.044	2.44067	1.010244
C	-12.2033	5.308468	-0.59814
H	-10.5524	5.508992	-1.95909
H	-13.7602	4.792161	0.789016
H	-12.5129	6.34445	-0.68963
C	-11.9956	0.281072	-0.1522
C	-13.1109	0.311711	-1.02691
C	-11.8836	-0.73236	0.768134
C	-14.0714	-0.65412	-0.95608
H	-13.1825	1.115685	-1.75331
C	-12.8562	-1.75218	0.84973
H	-11.0318	-0.75694	1.443621
C	-13.9786	-1.71338	-0.02276
H	-14.9224	-0.62865	-1.63215
C	-14.9567	-2.72722	0.070131
C	-12.7623	-2.80428	1.790188
H	-11.9056	-2.82941	2.458922
C	-14.8375	-3.73371	0.989867
H	-15.596	-4.50755	1.053921
C	-13.729	-3.76985	1.859488
H	-13.6448	-4.57116	2.587198
H	-15.8096	-2.69114	-0.60323

Table S5: Cartesian coordinates of**FHD4**

Atom	X-axis	Y-axis	Z-axis
C	-3.30215	1.577006	-0.15461
C	-3.83129	0.271801	-0.05518
C	-3.00144	-0.84891	-0.02581
C	-1.64094	-0.63879	-0.09926
C	-1.10865	0.659798	-0.20071
C	-1.93959	1.779812	-0.22842
H	-3.41899	-1.85109	0.051737
H	-1.52556	2.783477	-0.30708
C	-0.53442	-1.67247	-0.08962
C	0.695762	-0.79719	-0.19907
C	2.020585	-1.19196	-0.23979
C	2.988076	-0.19844	-0.3487
C	2.634653	1.168563	-0.41483
C	1.313166	1.554739	-0.37126
C	0.340336	0.558316	-0.26297
H	2.301487	-2.24232	-0.19089
H	1.034615	2.606167	-0.42182
C	-5.26359	0.406128	-0.00355
C	-4.4065	2.623111	-0.1657
C	-5.62549	1.742295	-0.06551
C	4.42916	-0.25134	-0.42182
C	3.870515	2.047138	-0.53733
C	4.961428	1.00623	-0.52793
C	-7.70523	0.711604	0.076224
C	-6.99582	1.917216	-0.0199
H	-7.51603	2.871124	-0.05177
S	-6.59268	-0.66616	0.110013

C	6.364624	1.011729	-0.61682
H	6.977001	1.899534	-0.74103
C	6.899538	-0.25402	-0.57668
S	5.644334	-1.47162	-0.41521
C	-9.11408	0.728027	0.130225
H	-9.46793	1.753924	0.087947
C	-11.1613	-2.33549	0.299966
C	-12.1624	-1.36022	0.287879
C	-13.4952	-1.76158	0.307972
C	-13.7763	-3.12302	0.339144
C	-12.7658	-4.08021	0.353122
C	-11.435	-3.68716	0.333844
C	-10.0854	-0.23705	0.214146
H	-14.3114	-1.05121	0.298091
H	-14.8133	-3.44297	0.352684
H	-13.0246	-5.13391	0.37788
H	-10.6181	-4.40225	0.342465
C	-9.83867	-1.68698	0.261859
O	-8.76747	-2.25726	0.266182
C	-11.5256	-0.02528	0.249354
C	-12.2143	1.1639	0.257917
C	-11.5889	2.441276	0.233985
N	-11.0975	3.487435	0.214403
C	-13.6338	1.240643	0.298378
N	-14.7846	1.339591	0.330544
C	-0.53375	-2.4676	1.215637
H	0.308059	-3.16877	1.239797
H	-0.45002	-1.80126	2.080235

H	-1.45832	-3.04732	1.316663
C	-0.64969	-2.61545	-1.28715
H	-1.57623	-3.19836	-1.23424
H	-0.64944	-2.05567	-2.22803
H	0.190169	-3.31914	-1.30628
C	3.998549	2.996453	0.652997
H	4.932653	3.567008	0.588906
H	3.167328	3.71052	0.671674
H	3.998064	2.442533	1.597164
C	3.864099	2.831743	-1.8484
H	3.767876	2.158651	-2.7062
H	3.029807	3.542076	-1.87188
H	4.795209	3.399775	-1.95986
C	-4.29668	3.558718	1.037485
H	-3.37028	4.142196	0.991288
H	-5.13832	4.260606	1.054637
H	-4.30073	2.993948	1.97518
C	-4.40209	3.421706	-1.46818
H	-3.4781	4.003194	-1.56273
H	-4.48088	2.758247	-2.33526
H	-5.24563	4.121109	-1.49165
C	14.41252	0.463149	2.626423
C	13.29474	0.971264	1.978258
C	12.74546	0.310177	0.880549
C	13.3331	-0.89315	0.47057
C	14.42518	-1.41467	1.144715
C	14.98173	-0.73027	2.216443
C	11.00885	-1.32093	-0.77854

C	10.63853	-0.07511	-0.25303
C	9.285228	0.23467	-0.17097
H	8.971511	1.163204	0.293376
C	8.302852	-0.64375	-0.64244
C	8.697205	-1.87684	-1.15988
C	10.03966	-2.21388	-1.20456
H	14.82833	1.005444	3.469708
H	12.84752	1.891358	2.337424
H	14.84854	-2.35776	0.81121
H	15.84902	-1.13382	2.728097
H	7.956137	-2.56889	-1.54792
H	10.34814	-3.17627	-1.60228
N	11.6311	0.816276	0.186104
C	11.26033	2.194248	0.407183
H	10.62236	2.529231	-0.41384
H	10.72487	2.361641	1.355552
H	12.16065	2.812726	0.405746
S	12.72645	-1.70036	-0.98953

Table S6: Cartesian coordinates of**FHD5**

Atom	X-axis	Y-axis	Z-axis
C	-3.08057	1.57221	-0.19492
C	-3.61136	0.26601	-0.1187
C	-2.7829	-0.85622	-0.11488
C	-1.4224	-0.64648	-0.18765
C	-0.88833	0.653326	-0.26412
C	-1.71797	1.774646	-0.2689
H	-3.20148	-1.85922	-0.05552

H	-1.30279	2.779187	-0.32786
C	-0.31703	-1.68137	-0.19837
C	0.914557	-0.80538	-0.2842
C	2.239439	-1.20071	-0.32177
C	3.209016	-0.2063	-0.40109
C	2.856647	1.162079	-0.44379
C	1.535284	1.548613	-0.40592
C	0.560553	0.551282	-0.32446
H	2.51878	-2.25212	-0.28978
H	1.258605	2.601311	-0.43707
C	-5.04289	0.401613	-0.05379
C	-4.18323	2.619972	-0.18027
C	-5.40296	1.739445	-0.08694
C	4.651136	-0.25827	-0.45223
C	4.094301	2.042108	-0.52954
C	5.18486	1.001042	-0.52138
C	-7.48305	0.710011	0.059333
C	-6.77224	1.915923	-0.02278
H	-7.2908	2.871238	-0.02927
S	-6.37284	-0.67024	0.054257
C	6.590084	1.009396	-0.5771
H	7.204818	1.899555	-0.66902
C	7.12517	-0.25622	-0.54825
S	5.868491	-1.47771	-0.43992
C	-8.89053	0.728239	0.13753
H	-9.24276	1.755479	0.120742
C	-10.9423	-2.33355	0.284758
C	-11.9407	-1.35587	0.314964

C	-13.2739	-1.7543	0.354056
C	-13.5582	-3.11542	0.361598
C	-12.5505	-4.0751	0.333406
C	-11.2192	-3.68494	0.2949
C	-9.8625	-0.23639	0.221611
H	-14.0881	-1.04192	0.376636
H	-14.5957	-3.43308	0.389822
H	-12.8117	-5.12846	0.340758
H	-10.4044	-4.40206	0.270686
C	-9.61888	-1.68747	0.232704
O	-8.54956	-2.26043	0.201123
C	-11.3009	-0.02203	0.292435
C	-11.9854	1.168501	0.344327
C	-11.3565	2.444314	0.336464
N	-10.8624	3.489391	0.330367
C	-13.4034	1.248147	0.419554
N	-14.5527	1.349621	0.481018
C	-0.32162	-2.50706	1.087598
H	0.519599	-3.2093	1.098648
H	-0.24096	-1.8614	1.968017
H	-1.24673	-3.08867	1.171431
C	-0.42954	-2.5956	-1.41839
H	-1.35596	-3.17997	-1.38128
H	-0.42768	-2.01327	-2.34547
H	0.411002	-3.29795	-1.45271
C	4.202782	2.968104	0.680938
H	5.137318	3.54034	0.642658
H	3.370799	3.681305	0.701085

H	4.18817	2.395394	1.613731
C	4.109443	2.85173	-1.82516
H	4.029986	2.194897	-2.69717
H	3.274015	3.560764	-1.84994
H	5.041244	3.423387	-1.90919
C	-4.0646	3.535063	1.037736
H	-3.13862	4.119444	0.994959
H	-4.90604	4.236551	1.072697
H	-4.06213	2.954481	1.965727
C	-4.18567	3.440408	-1.46911
H	-3.26084	4.021201	-1.55975
H	-4.27153	2.791823	-2.34669
H	-5.02773	4.141964	-1.47527
C	15.12353	0.072757	2.069504
C	13.92231	0.705942	1.76537
C	13.04325	0.149825	0.843044
C	13.38454	-1.07774	0.263561
C	14.56565	-1.71403	0.574516
C	15.45122	-1.13165	1.475681
C	11.23125	-1.31545	-0.60304
C	10.84048	-0.08933	-0.04737
C	9.488487	0.218554	-0.01706
H	9.151515	1.125182	0.473304
C	8.531104	-0.64229	-0.57369
C	8.953397	-1.84402	-1.13428
C	10.3002	-2.18153	-1.13128
H	15.79866	0.532621	2.783673
H	13.67261	1.639676	2.256836

H	14.7786	-2.66147	0.090245
H	16.38667	-1.62748	1.711241
H	8.233796	-2.51418	-1.59383
H	10.65395	-3.11276	-1.56111
O	12.55353	-1.6667	-0.65743
N	11.83765	0.747287	0.457732
C	11.50878	2.073384	0.90788
H	10.78144	2.517455	0.224127
H	11.09073	2.094438	1.92656
H	12.40455	2.698109	0.886019

Table S7: Cartesian coordinates of**FHD6**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	2.734173	1.538168	-0.07177
C	3.293149	0.244226	0.011405
C	2.488367	-0.89415	0.061144
C	1.122699	-0.7132	0.02539
C	0.559859	0.574406	-0.05708
C	1.366027	1.711894	-0.10586
H	2.929178	-1.88734	0.1246
H	0.928467	2.706459	-0.17143
C	0.038947	-1.7699	0.059854
C	-1.21193	-0.92066	-0.0142
C	-2.52823	-1.34512	-0.02444
C	-3.52061	-0.37329	-0.10234
C	-3.19828	1.001917	-0.16732
C	-1.8854	1.417428	-0.15598

C	-0.88748	0.442332	-0.07971
H	-2.78381	-2.40191	0.024713
H	-1.63257	2.475414	-0.20659
C	4.722705	0.407548	0.021794
C	3.816279	2.606528	-0.11413
C	5.055884	1.751002	-0.05073
C	-4.96119	-0.45755	-0.13771
C	-4.45625	1.853414	-0.24838
C	-5.52348	0.788862	-0.21811
C	7.159454	0.762038	0.027749
C	6.422696	1.953227	-0.04776
H	6.922455	2.917137	-0.09989
S	6.075903	-0.6376	0.097847
C	-6.92884	0.764653	-0.26998
H	-7.565	1.638592	-0.3703
C	-7.43526	-0.5121	-0.22784
S	-6.15101	-1.70367	-0.11067
C	8.568046	0.805677	0.026494
H	8.899863	1.837863	-0.03525
C	10.67917	-2.21596	0.179116
C	11.66049	-1.22373	0.105217
C	13.00047	-1.60071	0.094241
C	13.30783	-2.95544	0.156477
C	12.31673	-3.92965	0.231059
C	10.97877	-3.56093	0.243351
C	9.560878	-0.14043	0.078812
H	13.80292	-0.87738	0.037469
H	14.35064	-3.2562	0.146691

H	12.59578	-4.97739	0.278335
H	10.17577	-4.28946	0.300021
C	9.343964	-1.59274	0.168858
O	8.285312	-2.18353	0.224801
C	10.99693	0.09783	0.047524
C	11.66296	1.298159	-0.02212
C	11.01349	2.562419	-0.07375
N	10.50297	3.598716	-0.11638
C	13.08114	1.401091	-0.04869
N	14.23011	1.521521	-0.0725
C	0.143332	-2.70643	-1.14368
H	-0.6825	-3.42681	-1.14463
H	0.108085	-2.14355	-2.08204
H	1.082589	-3.27056	-1.11608
C	0.08861	-2.56925	1.361749
H	1.025865	-3.13265	1.435629
H	0.016447	-1.9071	2.230613
H	-0.73957	-3.28549	1.406594
C	-4.50322	2.649018	-1.55203
H	-5.44854	3.198725	-1.63166
H	-3.68423	3.37627	-1.59377
H	-4.41876	1.984747	-2.41795
C	-4.57154	2.789895	0.953348
H	-4.53442	2.227717	1.891912
H	-3.75486	3.52093	0.95657
H	-5.51895	3.340781	0.919361
C	3.758261	3.406309	-1.4147
H	2.821724	3.971514	-1.4808

H	4.588171	4.120701	-1.46248
H	3.822832	2.745133	-2.2847
C	3.722283	3.538788	1.09296
H	2.78263	4.102319	1.074393
H	3.765557	2.973491	2.029349
H	4.549047	4.258343	1.08642
C	-13.5592	0.353587	0.324599
C	-13.7506	-0.73539	-0.73416
C	-11.5327	-1.6648	-0.36018
C	-11.1704	-0.42986	0.216487
C	-9.81616	-0.08517	0.252712
H	-9.50149	0.847627	0.706857
C	-8.83256	-0.93322	-0.26543
C	-9.20958	-2.14874	-0.83279
C	-10.5529	-2.49162	-0.87489
H	-8.46383	-2.80537	-1.26988
H	-10.8547	-3.43462	-1.32576
N	-12.149	0.374963	0.781831
C	-11.7282	1.518808	1.551232
H	-10.9516	1.228056	2.2657
H	-11.3332	2.342655	0.933358
H	-12.5677	1.909814	2.129244
C	-12.9857	-2.00242	-0.39954
H	-13.3177	-2.39903	0.571863
H	-13.1774	-2.78676	-1.13973
C	-13.9297	1.693459	-0.31127
H	-14.9274	1.62909	-0.75957
H	-13.9487	2.51097	0.41598

H	-13.2164	1.950635	-1.10232
C	-14.4753	0.073562	1.514004
H	-14.3348	0.803637	2.31718
H	-15.5254	0.125695	1.204179
H	-14.2866	-0.91967	1.932334
H	-13.3942	-0.36268	-1.70458
H	-14.8263	-0.92105	-0.83789

Table S8: Summarized structural parameters of compound **FH**, bond length (Å) and bond angles.

Bond Lengths		**Bond Angles**	
DFT		**DFT**	
C1-C2	1.413	C2-C1-C6	120.6
C1-C6	1.379	C2-C1-C15	111.4
C1-C15	1.52	C1-C2-C3	121.5
C2-C3	1.394	C1-C2-C14	106.8
C2-C14	1.441	C6-C1-C15	128
C3-C4	1.38	C1-C6-C5	118
C4-C5	1.406	C1-C15-C16	100.6
C4-C7	1.514	C1-C15-C62	111.3
C5-C6	1.395	C1-C15-C63	111.3
C5-C13	1.453	C3-C2-C14	131.8
C7-C8	1.514	C2-C3-C4	117.6
C7-C58	1.528	C2-C14-C16	110.3
C7-C59	1.528	C2-C14-S22	135.9
C8-C9	1.38	C3-C4-C5	121
C8-C13	1.406	C3-C4-C7	128.2
C9-C10	1.394	C5-C4-C7	110.8
C10-C11	1.413	C4-C5-C6	121.3
C10-C17	1.441	C4-C5-C13	108.5
C11-C12	1.379	C4-C7-C8	101.5
C11-C18	1.52	C4-C7-C58	111.2
C12-C13	1.395	C4-C7-C59	111.2
C14-C16	1.384	C6-C5-C13	130.2
C14-S22	1.712	C5-C13-C8	108.5
C15-C16	1.507	C5-C13-C12	130.2
C15-C62	1.528	C8-C7-C58	111.2
C15-C63	1.528	C8-C7-C59	111.2

C16-C21	1.384	C7-C8-C9	128.2
C17-C19	1.384	C7-C8-C13	110.8
C17-S25	1.712	C58-C7-C59	110.5
C18-C19	1.507	C9-C8-C13	121
C18-C60	1.528	C8-C9-C10	117.6
C18-C61	1.528	C8-C13-C12	121.3
C19-C23	1.384	C9-C10-C11	121.5
C20-C21	1.4	C9-C10-C17	131.8
C20-S22	1.769	C11-C10-C17	106.8
C20-C27	1.412	C10-C11-C12	120.6
C23-C24	1.4	C10-C11-C18	111.4
C24-S25	1.769	C10-C17-C19	110.3
C24-C26	1.412	C10-C17-C25	135.9
C26-C41	1.369	C12-C11-C18	128
C27-C34	1.369	C11-C12-C13	118
C28-C29	1.398	C11-C18-C19	100.6
C28-C33	1.38	C11-C18-C60	111.3
C28-C42	1.474	C11-C18-C61	111.3
C29-C30	1.392	C16-C14-S22	113.8
C29-C48	1.478	C14-C16-C15	111
C30-C31	1.39	C14-C16-C21	112.3
C31-C32	1.392	C14-S22-C20	89.9
C32-C33	1.388	C16-C15-C62	111.3
C34-C42	1.473	C16-C15-C63	111.3
C34-C48	1.457	C15-C16-C21	136.7
C35-C36	1.398	C62-C15-C63	110.6
C35-C40	1.392	C16-C21-C20	113.2
C35-C46	1.478	C19-C17-S25	113.8
C36-C37	1.38	C17-C19-C18	111
C36-C44	1.474	C17-C19-C23	112.3
C37-C38	1.388	C17-S25-C24	89.9
C38-C39	1.392	C19-C18-C60	111.3
C39-C40	1.39	C19-C18-C61	111.3
C41-C44	1.473	C18-C19-C23	136.7
C41-C46	1.457	C60-C18-C61	110.6
C42-O43	1.213	C19-C23-C24	113.2
C44-O45	1.213	C21-C20-S22	110.8
C46-C47	1.374	C21-C20-C27	119.9
C47-C54	1.423	S22-C20-C27	129.4
C47-C56	1.422	C20-C27-C34	134.6
C48-C49	1.374	C23-C24-S25	110.8
C49-C50	1.423	C23-C24-C26	119.9

C49-C52	1.422	S25-C24-C26	129.4
C50-N51	1.156	C24-C26-C41	134.6
C52-N53	1.155	C26-C41-C44	125.5
C54-N55	1.156	C26-C41-C46	126.5
C56-N57	1.155	C27-C34-C42	125.5

Table S8 continued……

Bond	Angles
C27-C34-C48	126.5
C29-C28-C33	122.6
C29-C28-C42	109.6
C28-C29-C30	119.1
C28-C29-C48	108.9
C33-C28-C42	127.8
C28-C33-C32	118
C28-C42-C34	106.4
C28-C42-O43	126
C30-C29-C48	132
C29-C30-C31	118.4
C29-C48-C34	107.1
C29-C48-C49	124.5
C30-C31-C32	121.7
C31-C32-C33	120.1
C42-C34-C48	108
C34-C42-O43	127.5
C34-C48-C49	128.3
C36-C35-C40	119.1
C36-C35-C46	108.9
C35-C36-C37	122.6
C35-C36-C44	109.6
C40-C35-C46	132
C35-C40-C39	118.4
C35-C46-C41	107.1
C35-C46-C47	124.5
C37-C36-C44	127.8
C36-C37-C38	118
C36-C44-C41	106.4
C36-C44-O45	126
C37-C38-C39	120.1
C38-C39-C40	121.7
C44-C41-C46	108
C41-C44-O45	127.5
C41-C46-C47	128.3

C46-C47-C54	123.8
C46-C47-C56	123.2
C54-C47-C56	112.9
C47-C54-N55	179.1
C47-C56-N57	178.2
C48-C49-C50	123.8
C48-C49-C52	123.2
C50-C49-C52	112.9
C49-C50-N51	179.1
C49-C52-N53	178.2

Table S9: Summarized structural parameters of compound**FHD1**, bond length (Å) and bond angles.

Bond Lengths		**Bond Angles**	
DFT		**DFT**	
C1-C2	1.412	C2-C1-C6	120.7
C1-C6	1.379	C2-C1-C15	111.4
C1-C15	1.52	C1-C2-C3	121.4
C2-C3	1.395	C1-C2-C14	106.8
C2-C1	1.44	C6-C1-C15	128
C3-C4	1.379	C1-C6-C5	118
C4-C5	1.407	C1-C15-C16	100.7
C4-C7	1.514	C1-C15-C45	111.4
C5-C6	1.395	C1-C15-C46	111.3
C5-C13	1.453	C3-C2-C14	131.8
C7-C8	1.514	C2-C3-C4	117.7
C7-C41	1.529	C2-C14-C16	110.3
C7-C42	1.528	C2-C14-S22	135.9
C8-C9	1.383	C3-C4-C5	121.1
C8-C13	1.403	C3-C4-C7	128.2
C9-C10	1.391	C5-C4-C7	110.6
C10-C11	1.414	C4-C5-C6	121.2
C10-C17	1.444	C4-C5-C13	108.5
C11-C12	1.377	C4-C7-C8	101.5
C11-C18	1.521	C4-C7-C41	111.1
C12-C13	1.397	C4-C7-C42	111.2
C14-C16	1.386	C6-C5-C13	130.4
C14-S22	1.712	C5-C13-C8	108.6
C15-C16	1.507	C5-C13-C12	130.3
C15-C45	1.528	C8-C7-C41	111.1
C15-C46	1.528	C8-C7-C42	111.2
C16-C21	1.382	C7-C8-C9	128.1

C17-C19	1.37	C7-C8-C13	110.8
C17-S24	1.722	C41-C7-C42	110.4
C18-C19	1.507	C9-C8-C13	121.1
C18-C43	1.528	C8-C9-C10	117.7
C18-C44	1.528	C8-C13-C12	121.1
C19-C23	1.406	C9-C10-C11	121.3
C20-C21	1.402	C9-C10-C17	132.3
C20-S22	1.771	C11-C10-C17	106.4
C20-C25	1.409	C10-C11-C12	120.7
C23-C60	1.375	C10-C11-C18	111
S24-C60	1.757	C10-C17-C19	111
C25-C32	1.372	C10-C17-S24	136.9
C26-C27	1.398	C12-C11-C18	128.3
C26-C31	1.38	C11-C12-C13	118.1
C26-C33	1.475	C11-C18-C19	100.9
C27-C28	1.392	C11-C18-C43	111.3
C27-C35	1.479	C11-C18-C44	111.3
C28-C29	1.39	C16-C14-S22	113.8
C29-C30	1.392	C14-C16-C15	110.8
C30-C31	1.388	C14-C16-C21	112.4
C32-C33	1.471	C14-S22-C20	90
C32-C35	1.455	C16-C15-C45	111.4
C33-O34	1.213	C16-C15-C46	111.3
C35-C36	1.374	C15-C16-C21	136.8
C36-C37	1.422	C45-C15-C46	110.6
C36-C39	1.422	C16-C21-C20	113.2
C37-N38	1.156	C19-C17-S24	112.1
C39-N40	1.156	C17-C19-C18	110.7
C47-C48	1.403	C17-C19-C23	113.4
C47-C52	1.383	C17-C24-C60	90.8
C48-C49	1.401	C19-C18-C43	111.4
C48-C60	1.458	C19-C18-C44	111.2
C49-C50	1.379	C18-C19-C23	135.9
C50-C51	1.401	C43-C18-C44	110.6
C50-C53	1.503	C19-C23-C60	112.5
C51-C52	1.389	C21-C20-S22	110.7
C51-C59	1.458	C21-C20-C25	119.9
C53-C54	1.503	S22-C20-C25	129.4
C54-C55	1.382	C20-C25-C32	134.6
C54-C59	1.402	C23-C60-S24	111.2
C55-C56	1.391	C23-C60-C48	128.3
C56-C57	1.392	S24-C60-C48	120.4

C57-C58	1.387	C25-C32-C33	125.4
C58-C59	1.389	C25-C32-C35	126.5

Table S9 continued……

Bond Angles	
C27-C26-C31	122.7
C27-C26-C33	109.6
C26-C27-C28	119.1
C26-C27-C35	108.8
C31-C26-C33	127.8
C26-C31-C30	118
C26-C33-C32	106.5
C26-C33-O34	125.9
C28-C27-C35	132.1
C27-C28-C29	118.4
C27-C35-C32	107.1
C27-C35-C36	124.4
C28-C29-C30	121.7
C29-C30-C31	120.1
C33-C32-C35	108
C32-C33-O34	127.6
C32-C35-C36	128.4
C35-C36-C37	123.9
C35-C36-C39	123.2
C37-C36-C39	112.9
C36-C37-N38	179
C36-C39-N40	178.2
C48-C47-C52	121.5
C47-C48-C49	118.9
C47-C48-C60	119.7
C47-C52-C51	119.1
C49-C48-C60	121.4
C48-C49-C50	119.8
C49-C50-C51	120.7
C49-C50-C53	129.3
C51-C50-C53	110
C50-C51-C52	120
C50-C51-C59	108.7
C50-C53-C54	102.9
C52-C51-C59	131.3
C51-C59-C54	108.5
C51-C59-C58	131
C53-C54-C55	129.6

C53-C54-C59	110
C55-C54-C59	120.4
C54-C55-C56	119
C54-C59-C58	120.6
C55-C56-C57	120.7
C56-C57-C58	120.6
C57-C58-C59	118.8

Table S10: Summarized structural parameters of compound**FHD2**, bond length (Å) and bond angles.

Bond Lengths		**Bond Angles**	
DFT		**DFT**	
C1-C2	1.412	C1-C2-C3	121.4
C2-C3	1.395	C2-C1-C6	120.7
C3-C4	1.379	C1-C2-C14	106.8
C4-C5	1.407	C2-C1-C15	111.4
C5-C6	1.395	C2-C3-C4	117.7
C1-C6	1.379	C3-C2-C14	131.8
C4-C7	1.514	C3-C4-C5	121.1
C7-C8	1.514	C3-C4-C7	128.3
C8-C9	1.384	C4-C5-C6	121.2
C9-C10	1.392	C5-C4-C7	110.6
C10-C11	1.414	C4-C5-C13	108.5
C11-C12	1.377	C5-C6-C1	118.0
C8-C13	1.403	C6-C5-C13	130.3
C5-C13	1.453	C6-C1-C15	128.0
C12-C13	1.397	C4-C7-C8	101.5
C2-C14	1.440	C4-C7-C41	111.2
C1-C15	1.520	C4-C7-C42	111.1
C14-C16	1.386	C7-C8-C9	128.1
C15-C16	1.507	C7-C8-C13	110.8
C10-C17	1.444	C8-C7-C41	111.2
C11-C18	1.521	C8-C7-C42	111.1
C17-C19	1.370	C8-C9-C10	117.7
C18-C19	1.507	C9-C8-C13	121.1
C16-C21	1.382	C9-C10-C11	121.3
C20-C21	1.402	C9-C10-C17	132.3
C14-S22	1.712	C10-C11-C12	120.7
C20-S22	1.771	C11-C10-C17	106.4
C19-C23	1.406	C10-C11-C18	111.0
C17-S24	1.723	C11-C12-C13	118.1
C20-C25	1.409	C12-C11-C18	128.3
C26-C27	1.398	C8-C13-C5	108.6
C27-C28	1.392	C8-C13-C12	121.1
C28-C29	1.390	C5-C13-C12	130.3
C29-C30	1.392	C2-C14-C16	110.3
C30-C31	1.388	C2-C14-S22	135.9
C26-C31	1.380	C1-C15-C16	100.7
C25-C32	1.372	C1-C15-C45	111.3

C26-C33	1.475	C1-C15-C46	111.4
C32-C33	1.471	C14-C16-C15	110.8
C33-O34	1.213	C14-C16-C21	112.4
C27-C35	1.479	C16-C14-S22	113.8
C32-C35	1.455	C15-C16-C21	136.8
C35-C36	1.375	C16-C15-C45	111.3
C36-C37	1.422	C16-C15-C46	111.4
C37-N38	1.156	C10-C17-C19	111.0
C36-C39	1.422	C10-C17-S24	137.0
C39-N40	1.156	C11-C18-C19	100.9
C7-C41	1.528	C11-C18-C43	111.2
C7-C42	1.529	C11-C18-N44	111.3
C18-C43	1.528	C17-C19-C18	110.7
C18-C44	1.528	C17-C19-C23	113.4
C15-C45	1.528	C19-C17-C24	112.0
C15-C46	1.528	C18-C19-C23	135.9
C47-C48	1.400	C19-C18-C43	111.2
C48-C49	1.398	C19-C18-N44	111.3
C49-C50	1.381	C16-C21-C20	113.2
C50-C51	1.396	C21-C20-S22	110.7
C47-C52	1.380	C21-C20-C25	119.9
C51-C52	1.397	C14-S22-C20	90.0
C24-C53	1.757	S22-C20-C25	129.4
C48-C53	1.456	C19-C23-C53	112.5
C23-C53	1.375	C17-C24-C53	90.8
C51-N54	1.408	C20-C25-C32	134.6
N54-C55	1.413	C26-C27-C28	119.1
C55-C56	1.396	C27-C26-C31	122.7
C55-C57	1.395	C27-C26-C33	109.6
C56-C58	1.385	C26-C27-C35	108.8
C57-C59	1.385	C27-C28-C29	118.4
C59-C60	1.388	C28-27-C35	132.1
C58-C60	1.388	C28-C29-C30	121.7
N54-C61	1.415	C29-C30-C31	120.1
C61-C62	1.394	C30-C31-C26	118.0
C61-C63	1.395	C31-C26-C33	127.8
C62-C64	1.385	C25-C32-C33	125.4
C63-C65	1.385	C25-C32-C35	126.6
C65-C66	1.388	C26-C33-C32	106.4
C64-C66	1.388	C26-C33-O34	125.9

Table S10 continued….

Bond Angles	
C32-C33-O34	127.6
C33-C32-C35	108.0
C27-C35-C32	107.1
C27-C35-C36	124.4
C32-C35-C36	128.4
C35-C36-C37	123.9
C35-C36-C39	123.2
C36-C37-N38	179.0

C37-C36-C39	112.9
C36-C39-N40	178.2
C41-C7-C42	110.4
C43-C18-C44	110.5
C45-C15-C46	110.6
C47-C48-C49	117.6
C48-C47-C52	121.3
C47-C48-C53	120.3
C48-C49-C50	121.4
C49-C48-C53	122.1
C49-C50-C51	120.6
C50-C51-C52	118.5
C50-C51-N54	121.0
C47-C52-C51	120.6
C52-C51-N54	120.5
S24-C53-C48	120.6
S24-C53-C23	111.2
C48-C53-C23	128.2
C51-N54-C55	120.5
C51-N54-C61	119.6
N54-C55-C56	120.5
N54-C55-C57	120.4
C55-N54-C61	119.9
C56-C55-C57	119.1
C55-C56-C58	120.3
C55-C57-C59	120.2
C56-C58-C60	120.6
C57-C59-C60	120.6
C59-C60-C58	119.3
N54-C61-C62	120.6
N54-C61-C63	120.2
C62-C61-C63	119.3
C61-C62-C64	120.1
C61-C63-C65	120.2
C62-C64-C66	120.5
C63-C65-C66	120.5
C65-C66-C64	119.4

Table S11: Summarized structural parameters of compound**FHD3**, bond length (Å) and bond angles.

Bond Lengths		**Bond Angles**	
DFT		**DFT**	
C1-C2	1.412	C1-C2-C3	121.4
C2-C3	1.395	C2-C1-C6	120.6
C3-C4	1.379	C1-C2-C14	106.8
C4-C5	1.407	C2-C1-C15	111.3
C1-C6	1.379	C2-C3-C4	117.6
C5-C6	1.395	C3-C2-C14	131.7
C4-C7	1.514	C3-C4-C5	121.1
C7-C8	1.514	C3-C4-C7	128.2
C8-C9	1.383	C4-C5-C6	121.2

C9-C10	1.391	C5-C4-C7	110.7
C10-C11	1.414	C4-C5-C13	108.4
C11-C12	1.377	C1-C6-C5	118.0
C8-C13	1.403	C6-C1-C15	128.0
C5-C13	1.453	C6-C5-C13	130.4
C12-C13	1.397	C4-C7-C8	101.5
C2-C14	1.439	C4-C7-C41	111.1
C1-C15	1.520	C4-C7-C42	111.1
C14-C16	1.386	C7-C8-C9	128.1
C15-C16	1.507	C7-C8-C13	110.8
C10-C17	1.444	C8-C7-C41	111.1
C11-C18	1.521	C8-C7-C42	111.3
C17-C19	1.370	C8-C9-C10	117.7
C18-C19	1.508	C9-C8-C13	121.1
C20-C21	1.402	C9-C10-C11	121.3
C16-C21	1.382	C9-C10-C17	132.2
C20-S22	1.771	C10-C11-C12	120.7
C14-S22	1.712	C11-C10-C17	106.4
C19-C23	1.406	C10-C11-C18	111.0
C17-S24	1.723	C11-C12-C13	118.1
C20-C25	1.409	C12-C11-C18	128.3
C26-C27	1.397	C8-C13-C5	108.6
C27-C28	1.392	C8-C13-C12	121.1
C28-C29	1.391	C5-C13-C12	130.3
C29-C30	1.392	C2-C14-C16	110.3
C30-C31	1.388	C2-C14-S22	135.8
C26-C31	1.379	C1-C15-C16	100.7
C25-C32	1.372	C1-C15-C45	111.3
C26-C33	1.474	C1-C15-C46	111.3
C32-C33	1.471	C14-C16-C15	110.8
C33-O34	1.213	C14-C16-C21	112.3
C27-C35	1.480	C16-C14-S22	113.8
C32-C35	1.456	C15-C16-C21	136.9
C35-C36	1.374	C16-C15-C45	111.4
C36-C37	1.422	C16-C15-C46	111.3
C37-N38	1.156	C10-C17-C19	111.0
C36-C39	1.422	C10-C17-S24	136.9
C39-N40	1.155	C11-C18-C19	100.9
C7-C41	1.529	C11-C18-C43	111.3
C7-C42	1.528	C11-C18-C44	111.3
C18-C43	1.528	C17-C19-C18	110.7
C18-C44	1.528	C17-C19-C23	113.4
C15-C45	1.528	C19-C17-S24	112.1
C15-C46	1.528	C18-C19-C23	135.9
C47-C48	1.400	C19-C18-C43	111.3
C48-C49	1.398	C19-C18-C44	111.2
C49- C50	1.382	C20-C21-C16	113.3
C50-C51	1.395	C21-C20-S22	110.6
C47-C52	1.379	C21-C20-C25	119.9
C51-C52	1.397	C20-S22-C14	90.0
C24-C53	1.757	C22-C20-C25	129.5

C48-C53	1.456	C19-C23-C53	112.5
C23-C53	1.375	C17-S24-C53	90.8
C51-N54	1.409	C20-C25-C32	134.6
N54-C55	1.413	C26-C27-C28	119.0
C55-C56	1.396	C27-C26-C31	122.8
C55-C57	1.395	C27-C26-C33	109.6
C56-C58	1.384	C26-C27-C35	108.7
C57-C59	1.386	C27-C28-C29	118.4
C58-C60	1.389	C28-C27-C35	132.3
C59-C60	1.388	C28-C29-C30	121.8
N54-C61	1.414	C29-C30-C31	120.1
C61-C62	1.418	C30-C31-C26	117.9
C61-C63	1.374	C31-C26-C33	127.6
C62-C64	1.364	C25-C32-C33	125.2
C63-C65	1.412	C25-C32-C35	126.7
C64-C66	1.415	C26-C33-C32	106.5
C65-C66	1.422	C26-C33-O34	125.9
C66-C67	1.412	C32-C33-O34	127.7
C65-C68	1.414	C33-C32-C35	108.0
C67-C69	1.369	C27-C35-C32	107.2
C68-C70	1.368	C27-C35-C36	124.4
C69-C70	1.409	C32-C35-C36	128.4

Table S11 continued….

Bond Angles	
C35-C36-C37	123.9
C35-C36-C39	123.1
C36-C37-C38	179.0
C37-C36-C39	113.0
C36-C39-N40	178.2
C41-C7-C42	110.4
C43-C18-C44	110.5
C45-C15-C46	110.5
C47-C48-C49	117.6
C48-C47-C52	121.4
C47-C48-C53	120.2
C48-C49-C50	121.4
C49-C48-C53	122.2
C49-C50-C51	120.6
C50-C51-C52	118.6
C50-C51-N54	121.0
C47-C52-C51	120.6
C52-C51-N54	120.5
C24-C53-C48	120.5
C24-C53-C23	111.2
C48-C53-C23	128.3
C51-N54-C55	120.4
C51-N54-C61	120.0
N54-C55-C56	120.4
N54-C55-C57	120.4
C55-N54-C61	119.6

C56-C55-C57	119.1
C55-C56-C58	120.2
C55-C57-C59	120.2
C56-C58-C60	120.6
C57-C59-C60	120.6
C58-C60-C59	119.3
N54-C61-C62	119.2
N54-C61-C63	121.2
C62-C61-C63	119.6
C61-C62-C64	120.4
C61-C63-C65	121.0
C62-C64-C66	121.2
C63-C65-C66	119.2
C63-C65-C68	122.0
C64-C66-C65	118.5
C64-C66-C67	122.4
C65-C66-C67	119.1
C66-C65-C68	118.7
C66-C67-C69	120.8
C65-C68-C70	120.8
C67-C69-C70	120.1
C68-C70-C69	120.4

Table S12: Summarized structural parameters of compound**FHD4**, bond length (Å) and bond angles.

Bond Lengths		**Bond Angles**	
DFT		**DFT**	
C1-C2	1.412	C1-C2-C3	121.4
C2-C3	1.395	C2-C1-C6	120.7
C3-C4	1.379	C1-C2-C14	106.8
C4-C5	1.407	C2-C1-C15	111.4
C1-C6	1.38	C2-C3-C4	117.6
C5-C6	1.395	C3-C2-C14	131.8
C4-C7	1.514	C3-C4-C5	121.2
C7-C8	1.514	C3-C4-C7	128.1
C8-C9	1.383	C4-C5-C6	121.1
C9-C10	1.391	C5-C4-C7	110.7
C10-C11	1.413	C4-C5-C13	108.4
C11-C12	1.377	C1-C6-C5	118
C5-C13	1.454	C6-C1-C15	128
C12-C13	1.397	C6-C5-C13	130.5
C8-C13	1.403	C4-C7-C8	101.5
C2-C14	1.44	C4-C7-C42	111.2
C1-C15	1.521	C4-C7-C43	111.2
C15-C16	1.507	C7-C8-C9	128
C14-C16	1.386	C7-C8-C13	110.9

C10-C17	1.444	C8-C7-C42	111.2
C11-C18	1.521	C8-C7-C43	111.2
C18-C19	1.508	C8-C9-C10	117.7
C17-C19	1.37	C9-C8-C13	121.1
C16-C21	1.382	C9-C10-C11	121.4
C20-C21	1.402	C9-C10-C17	132.2
C20-S22	1.771	C10-C11-C12	120.6
C14-S22	1.711	C11-C10-C17	106.4
C19-C23	1.406	C10-C11-C18	111
C23-C24	1.375	C11-C12-C13	118.1
C17-S25	1.722	C12-C11-C18	128.3
C24-S25	1.756	C5-C13-C12	130.4
C20-C26	1.41	C5-C13-C8	108.5
C27-C28	1.398	C12-C13-C8	121.1
C28-C29	1.392	C2-C14-C16	110.4
C29-C30	1.391	C2-C14-S22	135.8
C30-C31	1.392	C1-C15-C16	100.6
C27-C32	1.38	C1-C15-C46	111.3
C31-C32	1.388	C1-C15-C47	111.3
C26-C33	1.372	C15-C16-C14	110.8
C33-C34	1.472	C15-C16-C21	136.9
C27-C34	1.474	C16-C15-C46	111.3
C34-O35	1.214	C16-C15-C47	111.4
C33-C36	1.456	C14-C16-C21	112.3
C28-C36	1.48	C16-C14-S22	113.8
C36-C37	1.374	C10-C17-C19	111
C37-C38	1.422	C10-C17-S25	136.9
C38-N39	1.156	C11-C18-C19	100.9
C37-C40	1.422	C11-C18-C44	111.4
C40-N41	1.155	C11-C18-C45	111.2
C7-C42	1.528	C18-C19-C17	110.7
C7-C43	1.529	C18-C19-C23	136
C18-C44	1.528	C19-C18-C44	111.3
C18-C45	1.528	C19-C18-C45	111.3
C15-C46	1.528	C17-C19-C23	113.3
C15-C47	1.528	C19-C17-S25	112.1
C48-C49	1.388	C16-C21-C20	113.3
C49-C50	1.394	C21-C20-S22	110.6
C50-C51	1.401	C21-C20-C26	119.9
C51-C52	1.385	C20-S22-C14	90
C48-C53	1.384	S22-C20-C26	129.5
C52-C53	1.388	C19-C23-C24	112.5
C54-C55	1.402	C23-C24-S25	111.3

C55-C56	1.391	C23-C24-C57	128.3
C24-C57	1.458	C17-S25-C24	90.7
C56-C57	1.4	S25-C24-C57	120.4
C57-C58	1.394	C20-C26-C33	134.6
C58-C59	1.385	C27-C28-C29	119
C54-C59	1.385	C28-C27-C32	122.8
C55-N60	1.404	C28-C27-C34	109.6
C50-N60	1.407	C27-C28-C36	108.8
N60-C61	1.444	C28-C29-C30	118.4
C51-S62	1.775	C29-C28-C36	132.3
C54-S62	1.772	C29-C30-C31	121.8

Table S12 continued….

Bond Angles	
C30-C31-C32	120.1
C27-C32-C31	117.9
C32-C27-C34	127.6
C26-C33-C34	125.2
C26-C33-C36	126.8
C33-C34-C27	106.5
C33-C34-O35	127.7
C34-C33-36C	108
C27-C34-O35	125.8
C33-C36-C28	107.2
C33-C36-C37	128.4
C28-C36-C37	124.4
C36-C37-C38	123.8
C36-C37-C40	123.2
C37-C38-N39	179.1
C38-C37-C40	113
C37-C40-N41	178.2
C42-C7-C43	110.4
C44-C18-C45	110.5
C46-C15-C47	110.5
C48-C49-C50	120.7
C49-C48-C53	120.5
C49-C50-C51	118.2
C49-C50-N60	122
C50-C51-C52	120.8
C51-C50-N60	119.8
C50-C51-S62	119.2
C51-C52-C53	120.4
C52-C51-S62	119.9

C48-C53-C52	119.3
C54-C55-C56	118.5
C55-C54-C59	120.2
C54-C55-N60	119.6
C55-C54-S62	119.4
C55-C56-C57	121.6
C56-C55-N60	121.9
C24-C57-C56	119.5
C24-C57-C58	121.7
C56-C57-C58	118.8
C57-C58-C59	120.1
C58-C59-C54	120.8
C59-C54-S62	120.2
C55-N60-C50	119.1
C55-N60-C61	118.2
C50-N60-C61	118.1
C51-S62-C54	97.8

Table S13: Summarized structural parameters of compound**FHD5**, bond length (Å) and bond angles.

Bond Lengths		**Bond Angles**	
DFT		**DFT**	
C1-C2	1.412	C1-C2-C3	121.4
C2-C3	1.395	C2-C1-C6	120.7
C3-C4	1.378	C1-C2-C14	106.8
C4-C5	1.407	C2-C1-C15	111.4
C1-C6	1.38	C2-C3-C4	117.6
C5-C6	1.395	C3-C2-C14	131.8
C4-C7	1.514	C3-C4-C5	121.2
C7-C8	1.514	C3-C4-C7	128.1
C8-C9	1.383	C4-C5-C6	121.1
C9-C10	1.391	C5-C4-C7	110.7
C10-C11	1.414	C4-C5-C13	108.4
C11-C12	1.377	C1-C6-C5	118
C5-C13	1.454	C6-C1-C15	128
C12-C13	1.397	C6-C5-C13	130.5
C8-C13	1.403	C4-C7-C8	101.5
C2-C14	1.439	C4-C7-C42	111.2
C1-C15	1.521	C4-C7-C43	111.1
C15-C16	1.507	C7-C8-C9	128
C14-C16	1.386	C7-C8-C13	110.9
C10-C17	1.444	C8-C7-C42	111.3
C11-C18	1.521	C8-C7-C43	111.1

C18-C19	1.508	C8-C9-C10	117.7
C17-C19	1.369	C9-C8-C13	121.2
C20-C21	1.402	C9-C10-C11	121.3
C16-C21	1.382	C9-C10-C17	132.3
C20-S22	1.771	C10-C11-C12	120.7
C14-S22	1.712	C11-C10-C17	106.4
C19-C23	1.406	C10-C11-C18	111
C23-C24	1.374	C11-C12-C13	118.1
C17-S25	1.723	C12-C11-C18	128.3
C24-S25	1.756	C5-C13-C12	130.4
C20-C26	1.41	C5-C13-C8	108.6
C27-C28	1.398	C12-C13-C8	121.1
C28-C29	1.392	C2-C14-C16	110.4
C29-C30	1.391	C2-C14-S22	135.8
C30-C31	1.392	C1-C15-C16	100.7
C27-C32	1.379	C1-C15-C46	111.3
C31-C32	1.388	C1-C15-C47	111.3
C26-C33	1.372	C15-C16-C14	110.8
C33-C34	1.471	C15-C16-C21	136.9
C27-C34	1.474	C6-C15-C46	111.3
C34-O35	1.214	C16-C15-C47	111.4
C33-C36	1.456	C14-C16-C21	112.3
C28-C36	1.48	C16-C14-S22	113.8
C36-C37	1.374	C10-C17-C19	111
C37-C38	1.422	C10-C17-S25	137
C38-N39	1.156	C11-C18-C19	100.9
C37-C40	1.422	C11-C18-C44	111.3
C40-N41	1.155	C11-C18-C45	111.3
C7-C42	1.528	C18-C19-C17	110.7
C7-C43	1.529	C18-C19-C23	135.9
C18-C44	1.528	C19-C18-C44	111.3
C18-C45	1.528	C19-C18-C45	111.3
C15-C46	1.528	C17-C19-C23	113.4
C15-C47	1.528	C19-C17-S25	112.1
C48-C49	1.392	C20-C21-C16	113.3
C49-C50	1.39	C21-C20-S22	110.6
C50-C51	1.4	C21-C20-C26	119.9
C51-C52	1.377	C20-S22-C14	90
C48-C53	1.382	S22-C20-C26	129.5
C52-C53	1.391	C19-C23-C24	112.5
C54-C55	1.402	C23-C24-S25	111.3
C55-C56	1.387	C23-C24-C57	128.2
C24-C57	1.458	C17-S25-C24	90.7

C56-C57	1.403	S25-C24-C57	120.5
C57-C58	1.392	C20-C26-C33	134.6
C54-C59	1.377	C27-C28-C29	119
C58-C59	1.388	C28-C27-C32	122.8
C54-O60	1.369	C28-C27-C34	109.6
C51-O60	1.373	C27-C28-C36	108.7
C55-N61	1.396	C28-C29-C30	118.4
C50-N61	1.4	C29-C28-C36	132.3
N61-C62	1.439	C29-C30-C31	121.8

Table S13 continued….

Bond Angles	
C30-C31-C32	120.1
C27-C32-C31	117.9
C32-C27-C34	127.6
C26-C33-C34	125.2
C26-C33-C36	126.8
C33-C34-C27	106.5
C33-C34-O35	127.7
C34-C33-C36	108
C27-C34-O35	125.8
C33-C36-C28	107.2
C33-C36-C37	128.4
C28-C36-C37	124.4
C36-C37-C38	123.8
C36-C37-C40	123.2
C37-C38-N39	179.1
C38-C37-C40	113
C37-C40-N41	178.2
C42-C7-C43	110.4
C44-C18-C45	110.5
C46-C15-C47	110.5
C48-C49-C50	120.6
C49-C48-C53	120.5
C49-C50-C51	118.1
C49-C50-N61	123.8
C50-C51-C52	121.4
C50-C51-O60	120.4
C51-C50-N61	118.1
C51-C52-C53	119.9
C52-C51-O60	118.2
C48-C53-C52	119.5
C54-C55-C56	118.3

C55-C54-C59	120.9
C55-C54-O60	120.6
C54-C55-N61	117.9
C55-C56-C57	121.4
C56-C55-N61	123.7
C24-C57-C56	119.3
C24-C57-C58	121.9
C56-C57-C58	118.9
C57-C58-C59	120.2
C54-C59-C58	120.3
C59-C54-O60	118.5
C54-O60-C51	116.6
C55-N61-C50	117.3
C55-N61-C62	120.2
C50-N61-C62	120.3

Table S14: Summarized structural parameters of compound**FHD6**, bond length (Å) and bond angles.

Bond Lengths		**Bond Angles**	
DFT		**DFT**	
C1-C2	1.412	C1-C2-C3	121.4
C2-C3	1.395	C2-C1-C6	120.6
C3-C4	1.378	C1-C2-C14	106.8
C4-C5	1.408	C2-C1-C15	111.3
C5-C6	1.395	C2-C3-C4	117.6
C1-C6	1.38	C3-C2-C14	131.7
C4-C7	1.514	C3-C4-C5	121.2
C7-C8	1.514	C3-C4-C7	128.1
C8-C9	1.383	C4-C5-C6	121.1
C9-C10	1.391	C5-C4-C7	110.7
C10-C11	1.414	C4-C5-C13	108.4
C11-C12	1.377	C5-C6-C1	118
C12-C13	1.397	C6-C5-C13	130.5
C5-C13	1.454	C6-C1-C15	128
C8-C13	1.403	C4-C7-C8	101.5
C2-C14	1.439	C4-C7-C42	111.2
C1-C15	1.521	C4-C7-C43	111.2
C15-C16	1.508	C7-C8-C9	127.9
C14-C16	1.386	C7-C8-C13	110.9
C10-C17	1.443	C8-C7-C42	111.2
C11-C18	1.521	C8-C7-C43	111.2
C17-C19	1.37	C8-C9-C10	117.7
C18-C19	1.508	C9-C8-C13	121.2

C16-C21	1.382	C9-C10-C11	121.3
C20-C21	1.403	C9-C10-C17	132.3
C14-S22	1.712	C10-C11-C12	120.7
C20-S22	1.771	C11-C10-C17	106.4
C19-C23	1.407	C10-C11-C18	111
C23-C24	1.374	C11-C12-C13	118.1
C24-S25	1.756	C12-C11-C18	128.3
C17-S25	1.723	C12-C13-C5	130.4
C20-C26	1.409	C12-C13-C8	121
C27-C28	1.397	C5-C13-C8	108.5
C28-C29	1.392	C2-C14-C16	110.4
C29-C30	1.391	C2-C14-S22	135.8
C30-C31	1.392	C1-C15-C16	100.7
C31-C32	1.388	C1-C15-C46	111.4
C27-C32	1.379	C1-C15-C47	111.3
C26-C33	1.372	C15-C16-C14	110.8
C27-C34	1.474	C15-C16-C21	136.9
C33-C34	1.471	C16-C15-C46	111.4
C34-O35	1.214	C16-C15-C47	111.3
C28-C36	1.48	C14-C16-C21	112.3
C33-C36	1.456	C16-C14-S22	113.8
C36-C37	1.374	C10-C17-C19	111
C37-C38	1.422	C10-C17-S25	137
C38-N39	1.156	C11-C18-C19	100.9
C37-C40	1.422	C11-C18-C44	111.2
C40-N41	1.156	C11-C18-C45	111.3
C7-C42	1.529	C17-C19-C18	110.7
C7-C43	1.529	C17-C19-C23	113.4
C18-C44	1.528	C19-C17-S25	112.1
C18-C45	1.528	C18-C19-C23	135.9
C15-C46	1.528	C19-C18-C44	111.3
C15-C47	1.528	C19-C18-C45	111.3
C48-C49	1.531	C16-C21-C20	113.3
C50-C51	1.41	C21-C20-S22	110.6
C51-C52	1.398	C21-C20-C26	119.9
C24-C53	1.46	C14-S22-C20	90
C52-C53	1.398	S22-C20-C26	129.5
C53-C54	1.393	C19-C23-C24	112.5
C50-C55	1.382	C23-C24-S25	111.3
C54-C55	1.387	C23-C24-C53	128.3
C51-N56	1.387	C24-S25-C17	90.8
C48-N56	1.483	S25-C24-C53	120.4
N56-C57	1.441	C20-C26-C33	134.6

C49-C58	1.517	C27-C28-C29	119
C50-C58	1.492	C28-C27-C32	122.8
C48-C59	1.529	C28-C27-C34	109.6
C48-C60	1.527	C27-C28-C36	108.7

Table S14 continued….

Bond Angles	
C28-C29-C30	118.4
C29-C28-C36	132.3
C29-C30-C31	121.8
C30-C31-C32	120.1
C31-C32-C27	117.9
C32-C27-C34	127.6
C26-C33-C34	125.2
C26-C33-C36	126.9
C27-C34-C33	106.5
C27-C34-O35	125.7
C33-C34-O35	127.7
C34-C33-C36	108
C28-C36-C33	107.2
C28-C36-C37	124.4
C33-C36-C37	128.5
C36-C37-C38	123.8
C36-C37-C40	123.2
C37-C38-N39	179
C38-C37-C40	113
C37-C40-N41	178.2
C42-C7-C43	110.4
C44-C18-C45	110.5
C46-C15-C47	110.5
C49-C48-N56	110
C48-C49-C58	112.2
C49-C48-C59	107.8
C49-C48-C60	109.5
C50-C51-C52	118.4
C51-C50-C55	119.6
C50-C51-N56	119.6
C51-C50-C58	117.3
C51-C52-C53	121.5
C52-C51-N56	122
C24-C53-C52	119.3
C24-C53-C54	121.4
C52-C53-C54	119.3

C53-C54-C55	119.3
C50-C55-C54	121.8
C55-C50-C58	123.1
C51-N56-C48	122.5
C51-N56-C57	118.2
C48-N56-C57	117
N56-C48-C59	110.3
N56-C48-C60	109.5
C49-C58-C50	107.9
C59-C48-C60	109.8

Table S15: E_{HOMO}, E_{LUMO} and energy gap (LUMO+1, HOMO-1, LUMO+2 and HOMO-2) of investigated compounds in *eV*.

Compounds	LUMO+1	HOMO-1	Band Gap	LUMO+2	HOMO-2	Band Gap
FH	-3.143	-6.564	3.421	-2.631	-7.345	4.714
FHD1	-2.557	-6.242	3.685	-1.850	-6.809	4.959
FHD2	-2.554	-5.923	3.369	-1.785	-6.484	4.699
FHD3	-2.554	-5.900	3.346	-1.789	-6.454	4.665
FHD4	-2.559	-5.894	3.335	-1.819	-6.428	4.609
FHD5	-2.555	-5.806	3.251	-1.764	-6.415	4.651
FHD6	-2.549	-5.800	3.251	-1.719	-6.354	4.635

E= energy, ΔE (e*V*)= E_{LUMO}-E_{HOMO}; HOMO= highest occupied molecular orbital; LUMO= lowest unoccupied molecular orbital, MO, molecular orbital

Table S16: Natural bond orbital (NBO) analysis of investigated compound **FH**

Donor(i)	Type	Acceptor(j)	Type	E(2)[a] [kJ/mol]	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C28-C30	π	C32-C53	π*	31.51	0.31	0.089
C14-C15	π	C12-C13	π*	27.02	0.29	0.08
C32-C53	π	C62-C63	π*	26.77	0.30	0.08
C18-C20	π	C24-C25	π*	25.12	0.29	0.078
C32-C53	π	C60-O61	π*	23.63	0.31	0.078
C50-C51	π	C47-C52	π*	22.46	0.29	0.073
C10-C11	π	C14-C15	π*	21.21	0.30	0.073
C12-C13	π	C14-C15	π*	20.89	0.30	0.071
C14-C15	π	C10-C11	π*	20.35	0.30	0.072
C12-C13	π	C10-C11	π*	19.24	0.30	0.070
C47-C52	π	C62-C63	π*	18.74	0.29	0.067
C24-C25	π	C18-C20	π*	17.83	0.31	0.067
C21-C23	π	C12-C13	π*	14.60	0.32	0.062
C32-C53	π	C28-C30	π*	11.17	0.29	0.053

C64-C65	π	C37-C38	π*	8.80	0.33	0.050
C64-C65	π	C34-C42	π*	7.85	0.33	0.046
C60-O61	π	C32-C53	π*	3.64	0.43	0.038
C34-C42	π	C34-C42	π*	2.70	0.31	0.026
C64-C65	π	C64-C65	π*	1.94	0.32	0.023
C70-N71	π	C72-N73	π*	0.74	0.47	0.017
C32-H33	σ	C30-S31	σ*	10.29	0.71	0.076
C63-C72	σ	C72-N73	σ*	8.15	1.61	0.103
C66-N67	σ	C65-C66	σ*	7.89	1.57	0.100
C32-H33	σ	C53-C60	σ*	6.95	0.99	0.074
C65-C66	σ	C64-C65	σ*	6.14	1.34	0.081
C36-C41	σ	C36-C37	σ*	5.99	1.30	0.079
C14-C15	σ	C13-C22	σ*	4.96	1.14	0.067
C11-H16	σ	C12-C13	σ*	4.69	1.08	0.064
C63-C70	σ	C47-C62	σ*	3.99	1.22	0.062
C86-H87	σ	C22-C82	σ*	3.67	0.89	0.051
C53-C62	σ	C60-O61	σ*	3.02	1.28	0.056
C40-C41	σ	C39-C40	σ*	2.95	1.3	0.055
C60-O61	σ	C47-C48	σ*	0.65	1.68	0.030
C30-S31	σ	C30-C32	σ*	0.51	1.21	0.022
S31	LP(2)	C28-C30	π*	22.51	0.26	0.069
O59	LP(2)	C36-C58	σ*	20.97	0.76	0.114
O61	LP(2)	C53-C60	σ*	19.03	0.75	0.108
N69	LP(1)	C65-C68	σ*	12.61	1.04	0.102
S31	LP(1)	C21-C23	σ*	3.28	1.23	0.057
S31	LP(1)	C28-C30	σ*	2.19	1.21	0.046
O59	LP(1)	C36-C58	σ*	1.66	1.18	0.040
O61	LP(1)	C21-S31	σ*	1.30	0.95	0.032
S31	LP(1)	C12-C21	σ*	1.05	1.18	0.032

Table S17: Natural bond orbital (NBO) analysis of investigated compound **FHD1**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a] [kcal/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C24-C25	π	C31-C39	π*	32.47	0.31	0.09
C5-C6	π	C1-C2	π*	27.78	0.29	0.081
C18-C20	π	C24-C25	π*	25.86	0.28	0.078
C31-C39	π	C44-O45	π*	24.01	0.31	0.078
C81-C82	π	C77-C78	π*	23.56	0.29	0.074
C79-C80	π	C77-C78	π*	22.67	0.30	0.074
C89-C90	π	C91-C92	π*	21.99	0.30	0.072
C88-C93	π	C81-C82	π*	20.94	0.29	0.07
C5-C6	π	C3-C4	π*	19.79	0.30	0.071
C34-C35	π	C46-C47	π*	18.69	0.29	0.066

C24-C25	π	C18-C20	π*	17.77	0.3	0.067
C18-C20	π	C1-C2	π*	14.44	0.32	0.062
C77-C78	π	C28-C98	π*	12.97	0.28	0.055
C31-C39	π	C24-C25	π*	11.25	0.29	0.053
C28-C98	π	C77-C78	π*	10.7	0.32	0.055
C46-C47	π	C34-C35	π*	8.77	0.33	0.05
C46-C47	π	C31-C39	π*	7.81	0.33	0.046
C44-O45	π	C31-C39	π*	3.61	0.43	0.038
C18-C20	π	C18-C20	π*	1.15	0.3	0.017
C50-N51	π	C48-N49	π*	0.77	0.47	0.017
C31-H32	σ	C24-S27	σ*	10.41	0.71	0.077
C47-C50	σ	C50-N51	σ*	8.15	1.61	0.103
C48-N49	σ	C47-C48	σ*	7.89	1.57	0.100
C31-H32	σ	C39-C44	σ*	6.88	0.99	0.074
C46-C47	σ	C47-C50	σ*	6.14	1.27	0.079
C28-H29	σ	S30-C98	σ*	5.95	0.73	0.059
C31-C39	σ	C39-C46	σ*	5.35	1.24	0.073
C10-C11	σ	C11-C12	σ*	4.98	1.30	0.072
C23-C28	σ	C21-C23	σ*	4.48	1.28	0.068
C22-C23	σ	C13-C14	σ*	4.21	1.24	0.065
C22-C23	σ	C21-C23	σ*	3.98	1.21	0.062
C68-H69	σ	C19-C20	σ*	3.75	0.94	0.054
C5-C15	σ	C4-C5	σ*	3.38	1.23	0.058
C80-C86	σ	C80-C81	σ*	2.13	1.21	0.045
C14-H17	σ	C13-C14	σ*	1.66	1.14	0.039
C22-C60	σ	C21-C23	σ*	0.93	1.20	0.030
C12-C13	σ	C22-C64	σ*	0.84	1.06	0.027
C86-H87	σ	C86-C88	σ*	0.51	0.94	0.020
S27	LP(2)	C18-C20	π*	29.92	0.28	0.082
S30	LP(2)	C21-C23	π*	24.58	0.29	0.076
S27	LP(2)	C24-C25	π*	22.09	0.26	0.068
O45	LP(2)	C33-C44	σ*	20.99	0.76	0.114
O45	LP(2)	C39-C44	σ*	18.93	0.76	0.108
N51	LP(1)	C47-C50	σ*	12.61	1.04	0.102
N49	LP(1)	C47-C48	σ*	12.58	1.04	0.102
O45	LP(1)	C39-C44	σ*	3.38	1.18	0.057
S30	LP(1)	C28-C98	σ*	2.58	1.24	0.051
S30	LP(1)	C21-C23	σ*	2.51	1.24	0.050
S27	LP(1)	C24-C25	σ*	2.17	1.20	0.046
O45	LP(1)	C33-C44	σ*	1.65	1.18	0.040
S27	LP(1)	C2-C18	σ*	1.05	1.19	0.032
S30	LP(1)	C12-C21	σ*	0.95	1.18	0.030

Table S18: Natural bond orbital (NBO) analysis of investigated compound **FHD2**

Donor(i)	Type	Acceptor(j)	Type	E(2)[a] [kcal/mol]	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C24-C25	π	C31-C39	π*	32.52	0.31	0.090
C31-C39	π	C46-C47	π*	27.44	0.30	0.081
C18-C20	π	C24-C25	π*	25.90	0.28	0.078
C31-C39	π	C44-O45	π*	24.03	0.31	0.078
C2-C3	π	C4-C5	π*	23.88	0.31	0.076
C1-C6	π	C4-C5	π*	22.94	0.31	0.076
C102-C106	π	C99-C100	π*	21.84	0.29	0.072
C13-C14	π	C10-C15	π*	20.85	0.31	0.073
C10-C15	π	C13-C14	π*	19.73	0.30	0.071
C34-C35	π	C46-C47	π*	18.68	0.29	0.066
C24-C25	π	C18-C20	π*	17.77	0.30	0.067
C21-C23	π	C28-C85	π*	16.39	0.31	0.065
C4-C5	π	C10-C15	π*	15.96	0.30	0.062
C28-C85	π	C77-C78	π*	11.41	0.32	0.057
C46-C47	π	C34-C35	π*	8.77	0.33	0.050
C46-C47	π	C31-C39	π*	7.81	0.33	0.046
C44-O45	π	C33-C38	π*	4.02	0.44	0.041
C46-C47	π	C46-C47	π*	2.01	0.32	0.023
C18-C20	π	C18-C20	π*	1.15	0.30	0.017
C50-N51	π	C48-N49	π*	0.77	0.47	0.017
C31-H32	σ	C24-S27	σ*	10.42	0.71	0.077
C47-C50	σ	C50-N51	σ*	8.15	1.61	0.103
C24-C25	σ	C19-C20	σ*	7.21	1.16	0.082
C31-H32	σ	C39-C44	σ*	6.88	0.99	0.074
C28-H29	σ	S30-C85	σ*	5.94	0.73	0.059
C21-C23	σ	C11-C12	σ*	5.06	1.30	0.072
C5-C6	σ	C1-C19	σ*	4.96	1.14	0.067
C18-S27	σ	C24-C31	σ*	3.85	1.26	0.062
C101-C104	σ	C104-C106	σ*	3.47	1.30	0.060
C1-C2	σ	C6-H8	σ*	2.89	1.08	0.050
C77-C85	σ	C78-C79	σ*	1.99	1.30	0.046
C22-C23	σ	C64-H66	σ*	1.51	1.01	0.035
C81-H84	σ	C80-N86	σ*	0.93	0.95	0.027
C38-H43	σ	C37-H42	σ*	0.74	0.94	0.024
S30-C85	σ	C22-C23	σ*	0.52	1.11	0.022
S27	LP(2)	C18-C20	π*	29.93	0.28	0.082
S30	LP(2)	C21-C23	π*	24.42	0.29	0.075
S27	LP(2)	C24-C25	π*	22.07	0.26	0.068
O45	LP(2)	C33-C44	σ*	20.99	0.76	0.114
O45	LP(2)	C39-C44	σ*	18.92	0.76	0.108

N49	LP(1)	C47-C48	σ*	12.58	1.04	0.102
N86	LP(1)	C99-C101	σ*	3.44	0.85	0.051
N86	LP(1)	C80-C81	σ*	2.97	0.84	0.048
S30	LP(1)	C28-C85	σ*	2.58	1.24	0.051
S27	LP(1)	C24-C25	σ*	2.17	1.20	0.046
O45	LP(1)	C33-C44	σ*	1.65	1.18	0.040
S27	LP(1)	C2-C18	σ*	1.05	1.19	0.032
S30	LP(1)	C12-C21	σ*	0.95	1.18	0.030

Table S19: Natural bond orbital (NBO) analysis of investigated compound **FHD3**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a] [kcal/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C24-C25	π	C31-C39	π*	32.54	0.31	0.09
C31-C39	π	C46-C47	π*	27.35	0.30	0.081
C18-C20	π	C24-C25	π*	25.94	0.28	0.079
C31-C39	π	C44-O45	π*	24.08	0.31	0.079
C2-C3	π	C4-C5	π*	23.91	0.31	0.076
C89-C91	π	C88-C90	π*	22.95	0.29	0.075
C33-C38	π	C34-C35	π*	21.95	0.30	0.073
C13-C14	π	C10-C15	π*	20.86	0.31	0.073
C10-C15	π	C13-C14	π*	19.75	0.30	0.071
C100-C102	π	C99-C101	π*	18.94	0.31	0.070
C104-C106	π	C100-C102	π*	17.96	0.29	0.069
C99-C101	π	C100-C102	π*	16.61	0.32	0.066
C4-C5	π	C10-C15	π*	15.94	0.30	0.062
C77-C78	π	C28-C85	π*	14.82	0.29	0.058
C11-C12	π	C21-C23	π*	13.59	0.30	0.057
C28-C85	π	C77-C78	π*	11.67	0.32	0.057
C46-C47	π	C34-C35	π*	8.76	0.33	0.05
C46-C47	π	C31-C39	π*	7.82	0.33	0.046
C44-O45	π	C33-C38	π*	4.02	0.44	0.041
C44-O45	π	C31-C39	π*	0.74	0.43	0.038
C31-H32	σ	C24-S27	σ*	10.44	0.71	0.077
C47-C50	σ	C50-N51	σ*	8.14	1.61	0.103
C48-N49	σ	C47-C48	σ*	7.91	1.57	0.100
C31-H32	σ	C39-C44	σ*	6.84	0.99	0.074
C28-H29	σ	S30-C85	σ*	5.94	0.73	0.059
C5-C6	σ	C1-C19	σ*	4.97	1.14	0.067
C24-C31	σ	C24-C25	σ*	3.99	1.28	0.064
C47-C48	σ	C47-C50	σ*	2.56	1.26	0.051
C104-C109	σ	C99-C101	σ*	2.09	1.30	0.047
N86-C99	σ	C79-C80	σ*	1.95	1.36	0.046
C9-C10	σ	C9-C56	σ*	1.77	1.01	0.038

C9-C10	σ	C52-H55	σ*	1.49	1.01	0.035
C111-H112	σ	C108-C111	σ*	0.99	1.14	0.03
C44-O45	σ	C39-C46	σ*	0.73	1.60	0.031
C113-H114	σ	C111-C113	σ*	0.50	1.08	0.021
S27	LP(2)	C18-C20	π*	29.96	0.28	0.082
S30	LP(2)	C21-C23	π*	24.46	0.29	0.075
S30	LP(2)	C28-C85	π*	24.21	0.28	0.074
S27	LP(2)	C24-C25	π*	22.07	0.26	0.068
O45	LP(2)	C33-C44	σ*	20.95	0.76	0.114
N86	LP(1)	C99-C101	π*	19.20	0.30	0.069
O45	LP(2)	C39-C44	σ*	18.91	0.76	0.108
N51	LP(1)	C47-C50	σ*	12.6	1.04	0.102
N49	LP(1)	C47-C48	σ*	12.57	1.04	0.102
N86	LP(1)	C99-C100	σ*	3.44	0.82	0.051
N86	LP(1)	C88-C90	σ*	2.79	0.85	0.046
S27	LP(1)	C24-C25	σ*	2.16	1.20	0.046
O45	LP(1)	C33-C44	σ*	1.65	1.18	0.040
S27	LP(1)	C2-C18	σ*	1.05	1.19	0.032
S30	LP(1)	C12-C21	σ*	0.94	1.18	0.030

Table S20: Natural bond orbital (NBO) analysis of investigated compound **FHD4**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a] [kcal/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C24-C25	π	C32-C40	π*	32.42	0.31	0.090
C5-C6	π	C1-C2	π*	27.71	0.29	0.081
C11-C12	π	C10-C15	π*	25.61	0.31	0.08
C81-C82	π	C77-C78	π*	24.25	0.30	0.076
C84-C85	π	C87-C88	π*	22.92	0.31	0.076
C37-C38	π	C34-C39	π*	21.57	0.30	0.073
C13-C14	π	C10-C15	π*	20.95	0.31	0.073
C5-C6	π	C3-C4	π*	19.82	0.30	0.071
C35-C36	π	C47-C48	π*	18.62	0.29	0.066
C24-C25	π	C18-C20	π*	17.73	0.30	0.067
C21-C23	π	C28-C30	π*	16.74	0.31	0.066
C5-C6	π	C10-C15	π*	13.91	0.31	0.058
C28-C30	π	C87-C88	π*	11.75	0.32	0.058
C47-C48	π	C35-C36	π*	8.78	0.33	0.050
C47-C48	π	C32-C40	π*	7.82	0.33	0.046
C45-O46	π	C34-C39	π*	4.03	0.44	0.041
C32-C40	π	C32-C40	π*	2.82	0.31	0.027
C47-C48	π	C47-C48	π*	1.99	0.32	0.023
C28-C30	π	C87-C88	σ*	0.74	0.86	0.023
C32-H33	σ	C24-S27	σ*	10.42	0.71	0.077

C48-C51	σ	C51-N52	σ*	8.15	1.61	0.103
C1-C2	σ	C18-S27	σ*	7.31	0.91	0.073
C32-H33	σ	C40-C45	σ*	6.83	0.99	0.074
C28-H29	σ	C30-S31	σ*	5.95	0.73	0.059
C83-C84	σ	C83-C89	σ*	4.94	1.31	0.072
C23-C28	σ	C21-C23	σ*	4.48	1.28	0.068
C35-C47	σ	C35-C36	σ*	3.94	1.25	0.063
C4-C5	σ	C5-C15	σ*	3.26	1.20	0.056
C34-C35	σ	C36-H41	σ*	2.90	1.12	0.051
C78-C79	σ	C77-H90	σ*	1.99	1.14	0.043
C9-C10	σ	C53-H56	σ*	1.49	1.01	0.035
C88-H94	σ	C87-C88	σ*	0.96	1.10	0.029
C82-H93	σ	C77-H90	σ*	0.76	0.94	0.024
C84-N96	σ	C97-H100	σ*	0.50	1.17	0.022
S27	LP(1)	C2-C18	σ*	29.96	1.19	0.032
S27	LP(1)	C18-C20	σ*	29.1	1.23	0.057
S27	LP(1)	C24-C25	σ*	27.95	1.20	0.046
S27	LP(2)	C24-C25	π*	24.08	0.26	0.068
S31	LP(1)	C12-C21	σ*	22.11	1.18	0.03
S31	LP(1)	C21-C23	σ*	20.92	1.25	0.050
S31	LP(1)	C28-C30	σ*	18.9	1.24	0.051
O46	LP(1)	C18-S27	σ*	12.57	0.95	0.032
O46	LP(1)	C34-C45	σ*	11.89	1.18	0.040
O46	LP(1)	C40-C45	σ*	8.27	1.18	0.057
N50	LP(1)	C48-C49	σ*	3.32	1.04	0.102
N52	LP(1)	C48-C51	σ*	2.59	1.04	0.102
N96	LP(1)	C84-C85	π*	1.91	0.31	0.086
S101	LP(2)	C83-C84	σ*	0.94	0.82	0.026
S101	LP(2)	C83-C89	π*	0.89	0.29	0.057

Table S21: Natural bond orbital (NBO) analysis of investigated compound **FHD5**

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)[a] [kcal/mol]**	**E(J)E(i)[b](a.u)**	**F(I,j)[c](a.u)**
C24-C25	π	C32-C40	π*	32.48	0.31	0.090
C32-C40	π	C47-C48	π*	27.26	0.3	0.081
C18-C20	π	C24-C25	π*	25.92	0.28	0.078
C32-C40	π	C45-O46	π*	24.07	0.31	0.079
C2-C3	π	C4-C5	π*	23.95	0.31	0.076
C1-C6	π	C4-C5	π*	22.92	0.31	0.076
C37-C38	π	C34-C39	π*	21.56	0.3	0.073
C79-C80	π	C77-C78	π*	20.97	0.31	0.072
C10-C15	π	C13-C14	π*	19.76	0.30	0.071
C87-C88	π	C84-C85	π*	18.92	0.29	0.067

C21-C23	π	C28-C30	π*	16.45	0.31	0.065
C11-C12	π	C21-C23	π*	13.56	0.30	0.057
C87-C88	π	C28-C30	π*	12.99	0.29	0.055
C32-C40	π	C24-C25	π*	11.24	0.29	0.053
C47-C48	π	C35-C36	π*	8.78	0.33	0.050
C47-C48	π	C32-C40	π*	7.81	0.33	0.046
C45-O46	π	C32-C40	π*	3.59	0.43	0.038
C32-C40	π	C32-C40	π*	2.83	0.31	0.027
C47-C48	π	C47-C48	π*	1.99	0.32	0.023
C49-N50	π	C51-N52	π*	0.73	0.47	0.017
C32-H33	σ	C24-S27	σ*	10.43	0.71	0.077
C48-C51	σ	C51-N52	σ*	8.15	1.61	0.103
C12-C13	σ	C21-S31	σ*	7.64	0.89	0.074
C32-H33	σ	C40-C45	σ*	6.82	0.99	0.074
C28-C30	σ	C22-C23	σ*	6.64	1.18	0.079
C34-C39	σ	C34-C35	σ*	6.02	1.30	0.079
C83-C89	σ	C83-C84	σ*	5.71	1.28	0.076
C2-C3	σ	C3-C4	σ*	4.88	1.32	0.072
C36-H41	σ	C34-C35	σ*	4.47	1.10	0.063
C22-C23	σ	C21-C23	σ*	3.99	1.21	0.062
C10-C15	σ	C5-C15	σ*	3.41	1.20	0.057
C1-C2	σ	C6-H8	σ*	2.89	1.08	0.050
C19-C73	σ	C19-C20	σ*	2.09	1.06	0.042
C1-C6	σ	C19-C20	σ*	0.69	1.16	0.025
C19-C73	σ	C73-H76	σ*	0.60	1.01	0.022
N97	LP(1)	C84-C85	π*	36.44	0.3	0.096
N97	LP(1)	C79-C80	π*	32.65	0.3	0.092
S27	LP(2)	C18-C20	π*	29.98	0.28	0.082
S31	LP(2)	C21-C23	π*	24.47	0.29	0.075
O96	LP(2)	C83-C89	π*	22.03	0.39	0.087
O46	LP(2)	C34-C45	σ*	20.93	0.76	0.114
O46	LP(2)	C40-C45	σ*	18.89	0.76	0.108
N50	LP(1)	C48-C49	σ*	12.57	1.04	0.102
N97	LP(1)	C98-H100	σ*	8.27	0.64	0.070
S27	LP(1)	C18-C20	σ*	3.32	1.23	0.057
O46	LP(2)	C18-S27	σ*	2.24	0.53	0.031
N97	LP(1)	C98-H99	σ*	1.97	0.65	0.034
O46	LP(1)	C34-C45	σ*	1.64	1.18	0.040
S31	LP(1)	C12-C21	σ*	0.95	1.18	0.030
O96	LP(2)	C80-C81	σ*	0.68	0.95	0.024

Table S22: Natural bond orbital (NBO) analysis of investigated compound **FHD6**

Donor(i)	Type	Acceptor(j)	Type	E(2)[a] [kcal/mol]	E(J)E(i)[b](a.u)	F(I,j)[c](a.u)
C24-C25	π	C32-C40	π*	32.62	0.31	0.09
C5-C6	π	C1-C2	π*	27.82	0.29	0.081
C18-C20	π	C24-C25	π*	26.04	0.28	0.079
C11-C12	π	C10-C15	π*	25.83	0.31	0.08
C32-C40	π	C45-O46	π*	24.13	0.31	0.079
C83-C84	π	C79-C85	π*	23.62	0.31	0.076
C10-C15	π	C5-C6	π*	22.65	0.29	0.073
C34-C39	π	C35-C36	π*	21.93	0.30	0.073
C13-C14	π	C10-C15	π*	20.76	0.31	0.073
C1-C2	π	C3-C4	π*	19.33	0.30	0.070
C35-C36	π	C47-C48	π*	18.61	0.29	0.066
C24-C25	π	C18-C20	π*	17.75	0.30	0.067
C83-C84	π	C80-C81	π*	16.73	0.29	0.064
C5-C6	π	C10-C15	π*	13.84	0.31	0.058
C32-C40	π	C24-C25	π*	11.26	0.29	0.053
C28-C30	π	C83-C84	π*	10.88	0.33	0.056
C47-C48	π	C35-C36	π*	8.78	0.33	0.050
C45-O46	π	C34-C39	π*	4.03	0.44	0.041
C18-C20	π	C18-C20	π*	1.16	0.3	0.017
C51-N52	π	C49-N50	π*	0.76	0.47	0.017
C32-H33	σ	C24-S27	σ*	10.45	0.71	0.077
C48-C51	σ	C51-N52	σ*	8.14	1.61	0.103
C48-C49	σ	C49-N50	σ*	8.09	1.61	0.102
C12-C13	σ	C21-S31	σ*	7.63	0.89	0.074
C32-H33	σ	C40-C45	σ*	6.81	0.99	0.074
C28-H29	σ	C30-S31	σ*	5.98	0.73	0.059
C21-C23	σ	C12-C21	σ*	4.87	1.23	0.069
C48-C49	σ	C35-C47	σ*	3.97	1.22	0.062
C38-C39	σ	C37-C38	σ*	2.97	1.30	0.055
C5-C6	σ	C4-C9	σ*	2.21	1.15	0.045
C35-C47	σ	C40-C47	σ*	1.92	1.16	0.042
C4-C5	σ	C9-C53	σ*	0.91	1.07	0.028
C2-C18	σ	C18-S27	σ*	0.76	0.93	0.024
C22-C65	σ	C65-H68	σ*	0.61	1.01	0.022
C96-H99	σ	C77-N88	σ*	0.51	0.84	0.019
N88	LP(1)	C80-C81	π*	41.21	0.29	0.102
S27	LP(2)	C18-C20	π*	30.02	0.28	0.082
S31	LP(2)	C21-C23	π*	24.47	0.29	0.075
S27	LP(2)	C24-C25	π*	22.04	0.26	0.068
O46	LP(2)	C34-C45	σ*	20.91	0.76	0.114
O46	LP(2)	C40-C45	σ*	18.88	0.76	0.108
N50	LP(1)	C48-C49	σ*	12.57	1.04	0.102

N88	LP(1)	C89-H91	σ*	8.86	0.63	0.071
N88	LP(1)	C77-C96	σ*	5.36	0.65	0.056
O46	LP(1)	C40-C45	σ*	3.41	1.18	0.057
S31	LP(1)	C21-C23	σ*	2.51	1.24	0.050
O46	LP(1)	C18-S27	σ*	1.33	0.95	0.032
N88	LP(1)	C80-C81	σ*	0.98	0.84	0.027
N88	LP(1)	C100-H102	σ*	0.66	0.65	0.02
N88	LP(1)	C79-C80	σ*	0.51	0.83	0.019

$E^{(2)}$ means energy of hyper conjugative interaction (stabilization energy in kcal/mol); Energy difference between donor & acceptor *i* &*j* NBO orbitals.; F(*i;j*) is the Fock matrix element between *i*& *j* NBO orbitals.

Table S23: Wave length, excitation energy and oscillator strength of investigated compound **FH**

NO	λ (nm)	E(eV)	*f*	MO contributions
1	650.460	1.906	3.249	H→L (92%), H-1→L+1 (6%)
2	553.205	2.241	0.031	H-1→L (12%), H→L+1 (86%),
3	461.131	2.689	0.022	H-1→L (82%), H→L+1 (12%), H-2→L+1 (2%)
4	458.352	2.705	0.109	H→L+2 (84%), H-1→L+1 (4%), H-1→L+3 (9%)
5	442.548	2.802	0.085	H-1→L+2 (11%), H→L+3 (83%),
6	420.628	2.948	0.234	H-1→L+1 (85%), H-2→L (3%), H→L (7%), H→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S24: Wave length, excitation energy and oscillator strength of investigated compound **FHD1**

λ_{max}(nm)	E(eV)	f_{os}	MO transition
661.955	1.873	1.978	H→L (88%), H-1→L (8%)
495.422	2.503	0.216	H-1→L (84%), H-2→L (6%), H→L (9%)
485.927	2.552	0.374	H-1→L+1 (10%), H→L+1 (84%)
414.621	2.990	0.940	H→L+2 (85%), H-1→L+1 (7%)
394.264	3.145	0.111	H-1→L+1 (69%), H→L+1 (14%), H-2→L+1 (6%), H→L+2 (6%)
386.943	3.204	0.052	H-2→L (85%), H-5→L (3%), H-1→L (7%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S25: Wave length, excitation energy and oscillator strength of investigated compound **FHD2**

λ_{max}(nm)	E(eV)	f_{os}	MO transition

683.221	1.815	1.712	H-1→L (13%), H→L (83%),
546.643	2.268	0.481	H-1→L (72%), H→L (16%),
496.831	2.496	0.297	H-1→L+1 (13%), H→L+1 (79%)
443.609	2.795	0.042	H-2→L (83%), H-1→L (12%),
427.281	2.902	0.213	H-1→L+1 (50%), H→L+2 (26%)
421.056	2.945	0.875	H-1→L+1 (17%), H→L+2 (60%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S26: Wave length, excitation energy and oscillator strength of investigated compound**FHD3**

λ_{max}**(nm)**	***E*(*eV*)**	f_{os}	**MO transition**
683.899	1.812	1.703	H-1→L (14%), H→L (82%)
550.674	2.251	0.490	H-2→L (10%), H-1→L (72%)
497.090	2.494	0.307	H-1→L+1 (13%), H→L+1 (78%)
447.920	2.768	0.050	H-2→L(80%), H-1→L (13%)
429.859	2.884	0.271	H-2→L+1 (10%), H-1→L+1 (44%)
423.979	2.924	0.781	H-1→L+1 (23%), H→L+1 (15%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S27: Wave length, excitation energy and oscillator strength of investigated compound **FHD4**

λ_{max}**(nm)**	***E*(*eV*)**	f_{os}	**MO transition**
661.602	1.874	1.862	H-1→L (16%), H→L (78%)
536.751	2.309	0.272	H-1→L (69%), H→L (21%)
485.946	2.551	0.309	H-1→L+1 (16%), H→L+1 (73%)
455.172	2.723	0.077	H-2→L (81%), H-1→L (14%)
420.699	2.947	0.110	H-2→L+1 (11%), H-1→L+1 (51%)
411.279	3.014	0.707	H-1→L+1 (12%), H→L+1 (11%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S28: Wave length, excitation energy and oscillator strength of investigated compound **FHD5**

λ_{max}**(nm)**	***E*(*eV*)**	f_{os}	**MO transition**
676.068	1.833	1.600	H-1→L (20%), H→L (75%)
569.179	2.178	0.490	H-1→L (68%), H→L (24%)
493.273	2.513	0.252	H-1→L+1 (19%), H→L+1 (72%)
461.268	2.687	0.102	H-2→L (85%), H-1→L (11%)
437.596	2.833	0.045	H-2→L+1 (10%), H-1→L+1 (63%)
414.649	2.990	0.669	H→L+2 (84%), H-1→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S29: Wave length, excitation energy and oscillator strength of investigated compound **FHD6**

λ_{max}(nm)	E(eV)	f_{os}	MO transition
669.244	1.852	1.816	H-1→L (13%), H→L (80%)
544.938	2.275	0.210	H-1→L (74%), H→L (18%)
489.263	2.534	0.265	H-1→L+1 (13%), H→L+1 (76%)
473.584	2.618	0.155	H-2→L (83%), H-1→L (12%)
422.333	2.935	0.020	H-2→L+1 (10%), H-1→L+1 (67%)
400.712	3.094	0.744	H→L+2 (84%), H-1→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S30: Dipole polarizability and major contributing tensors (Debye) of the studied compounds **D1, D3, D4, D5, D6** and **D7.**

Dipole Moment	R	D1	D2	D3	D4	D5	D6
μ_x	0.0004	-10.4100	-11.3337	11.0320	9.2847	10.1613	-13.2380
μ_y	6.5575	3.0371	-2.3342	-2.4484	0.8777	0.7817	-1.4817
μ_z	0.0014	0.2302	-0.1856	0.3255	-0.6963	-0.4821	0.3501
μ_{total}	6.5575	10.8464	11.5731	11.3051	9.3521	10.2027	13.3253
Polarizability							
α_{xx}	4.511×10^{-22}	3.931×10^{-22}	4.069×10^{-22}	4.040×10^{-22}	3.898×10^{-22}	3.877×10^{-22}	3.652×10^{-22}
α_{yy}	1.723×10^{-22}	1.516×10^{-22}	1.697×10^{-22}	1.754×10^{-22}	1.526×10^{-22}	1.500×10^{-22}	1.416×10^{-22}
α_{zz}	5.755×10^{-23}	6.170×10^{-23}	7.456×10^{-23}	7.411×10^{-23}	7.335×10^{-23}	6.773×10^{-23}	5.916×10^{-23}
α_{total}	**2.270×10^{-22}**	**2.021×10^{-22}**	**2.170×10^{-22}**	**2.178×10^{-22}**	**2.053×10^{-22}**	**2.018×10^{-22}**	**1.886×10^{-22}**
2nd Hyper pol.							
γ_X	3.095×10^{-32}	3.233×10^{-32}	4.259×10^{-32}	4.085×10^{-32}	3.120×10^{-32}	3.448×10^{-32}	2.884×10^{-32}
γ_Y	1.452×10^{-34}	1.102×10^{-34}	1.467×10^{-34}	1.760×10^{-34}	7.352×10^{-35}	6.825×10^{-35}	7.584×10^{-35}
γ_Z	6.125×10^{-36}	7.847×10^{-36}	7.996×10^{-36}	7.900×10^{-36}	5.474×10^{-35}	5.649×10^{-35}	9.571×10^{-36}
Average<γ>	**3.111×10^{-32}**	**3.245×10^{-32}**	**4.275×10^{-32}**	**4.103×10^{-32}**	**3.133×10^{-32}**	**3.460×10^{-32}**	**2.893×10^{-32}**
Magnitude of γ	**3.096×10^{-32}**	**3.233×10^{-32}**	**4.259×10^{32}**	**4.085×10^{-32}**	**3.120×10^{-32}**	**3.448×10^{-32}**	**2.884×10^{-32}**

Table S31:The computed first hyperpolarizability (β_{tot}) and major contributing tensors (*esu*) of entitled compounds.

Polarizability	R	D1	D2	D3	D4	D5	D6
β_{xxx}	5.841×10^{-32}	-2.641×10^{-27}	-3.188×10^{-27}	3.051×10^{-27}	2.602×10^{-27}	2.797×10^{-27}	-2.615×10^{-27}
β_{xxy}	-1.852×10^{-28}	-1.286×10^{-28}	9.338×10^{-29}	-4.590×10^{-30}	5.908×10^{-30}	1.368×10^{-29}	-6.488×10^{-29}
β_{xyy}	-8.261×10^{-34}	2.358×10^{-29}	3.620×10^{-29}	-4.896×10^{-29}	-2.677×10^{-29}	-2.691×10^{-29}	2.343×10^{-29}
β_{yyy}	1.611×10^{-29}	6.575×10^{-30}	1.288×10^{-30}	-4.203×10^{-30}	2.501×10^{-30}	2.632×10^{-30}	-1.051×10^{-30}
β_{xxz}	6.396×10^{-32}	-1.276×10^{-29}	-4.660×10^{-30}	-1.518×10^{-31}	1.014×10^{-28}	1.100×10^{-28}	-2.940×10^{-29}
β_{yyz}	-1.918×10^{-33}	9.455×10^{-32}	-6.408×10^{-31}	-1.194×10^{-30}	-1.780×10^{-30}	-1.926×10^{-30}	1.039×10^{-30}
β_{xzz}	-5.946×10^{-35}	1.026×10^{-30}	2.210×10^{-30}	-3.013×10^{-30}	-8.959×10^{-31}	3.562×10^{-30}	-1.889×10^{-31}
β_{yzz}	2.111×10^{-31}	1.450×10^{-31}	-1.199×10^{-31}	1.290×10^{-31}	-5.052×10^{-32}	2.730×10^{-32}	8.169×10^{-31}
β_{zzz}	-3.321×10^{-34}	-3.454×10^{-31}	-7.702×10^{-33}	-2.314×10^{-31}	1.881×10^{-30}	9.462×10^{-31}	-1.133×10^{-31}
β_{total}	1.689×10^{-27}	2.620×10^{-27}	3.150×10^{-27}	3.000×10^{-27}	2.576×10^{-27}	2.776×10^{-27}	2.592×10^{-27}

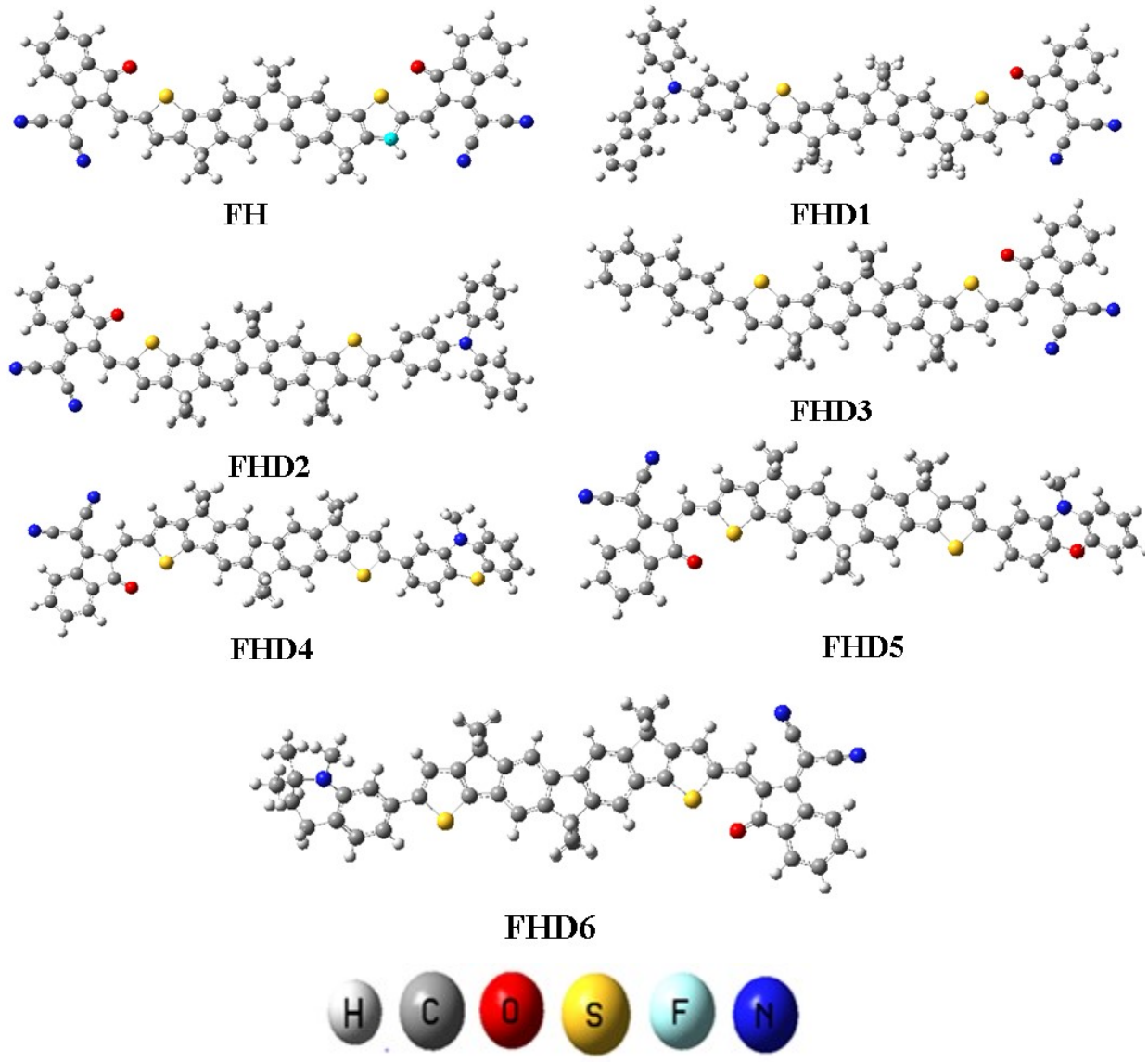

Figure S1: The optimized structures of entitled compounds (**FH** and **FHD1-FHD6**)

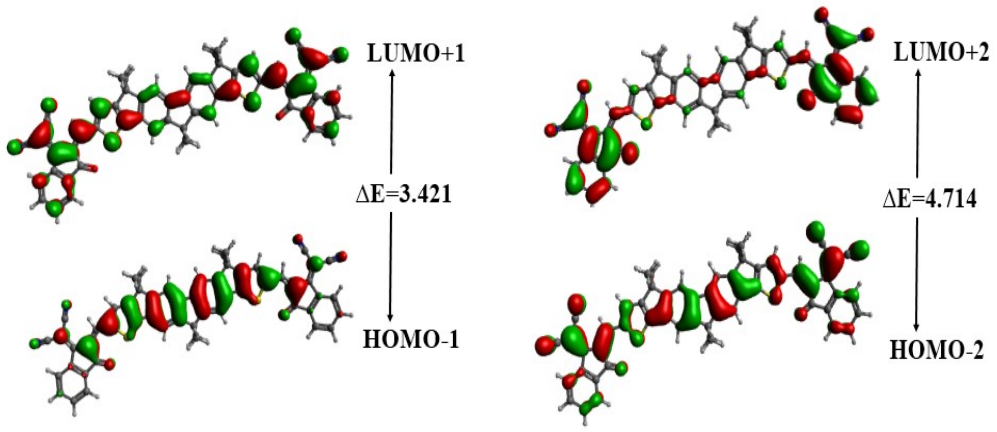

Figure S2: Frontier molecular orbitals of **FH**

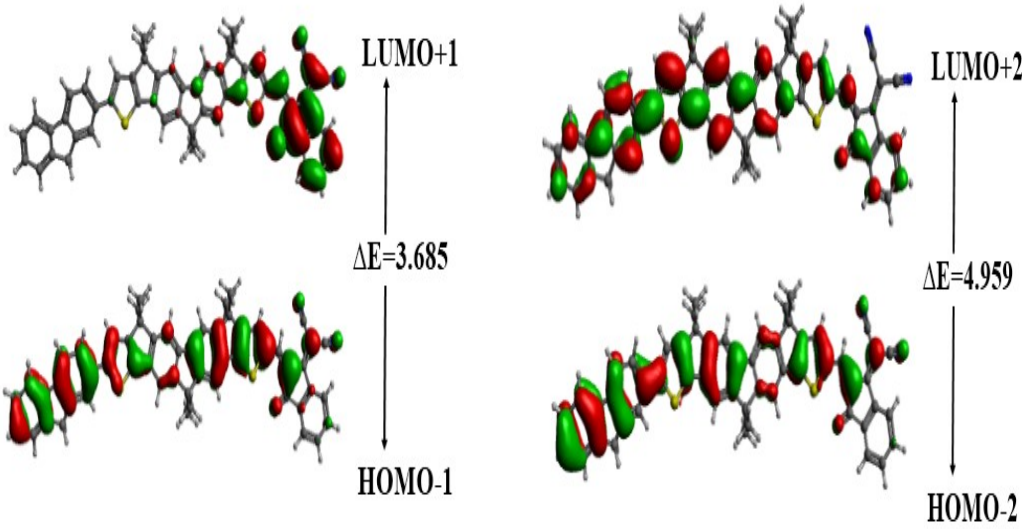

Figure S3: Frontier molecular orbitals of **FHD1**

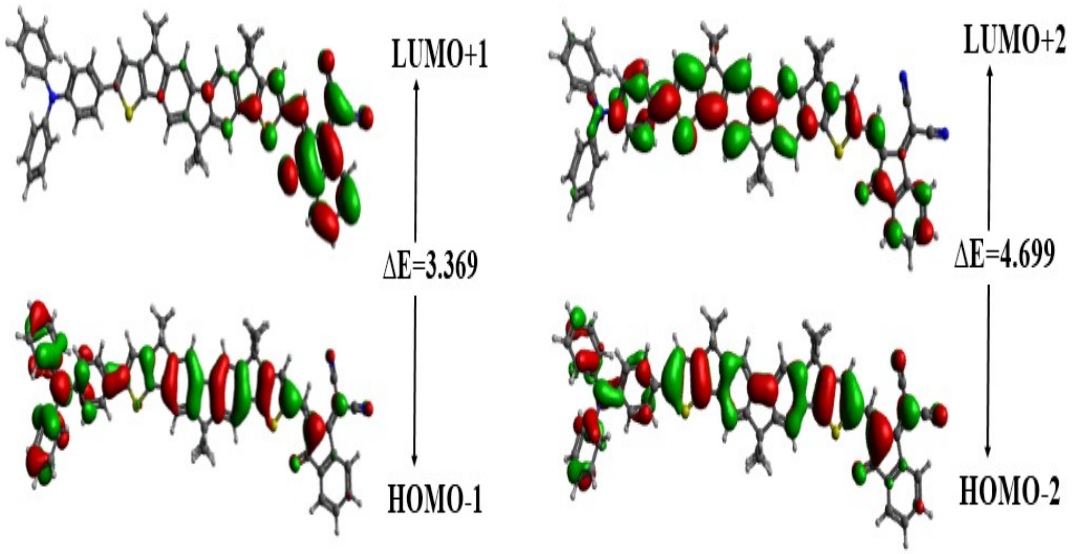

Figure S3: Frontier molecular orbitals of **FHD2**

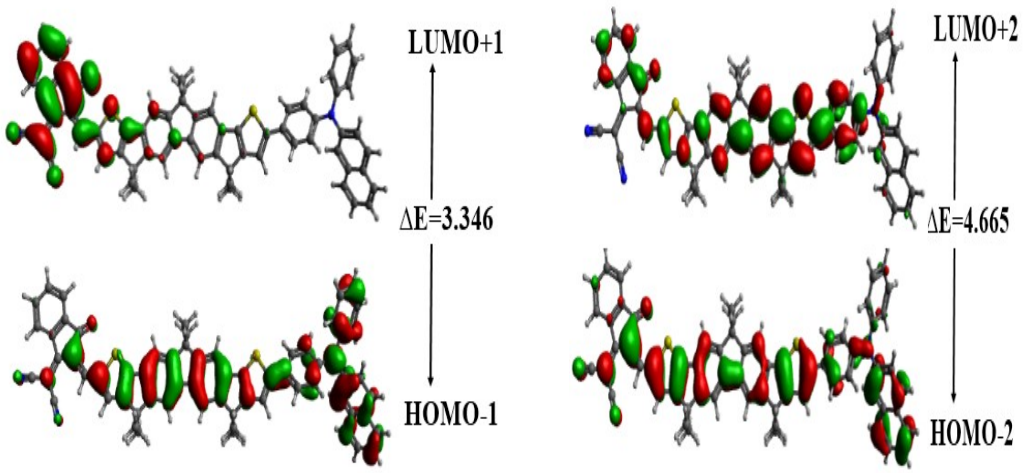

Figure S4: Frontier molecular orbitals of **FHD3**

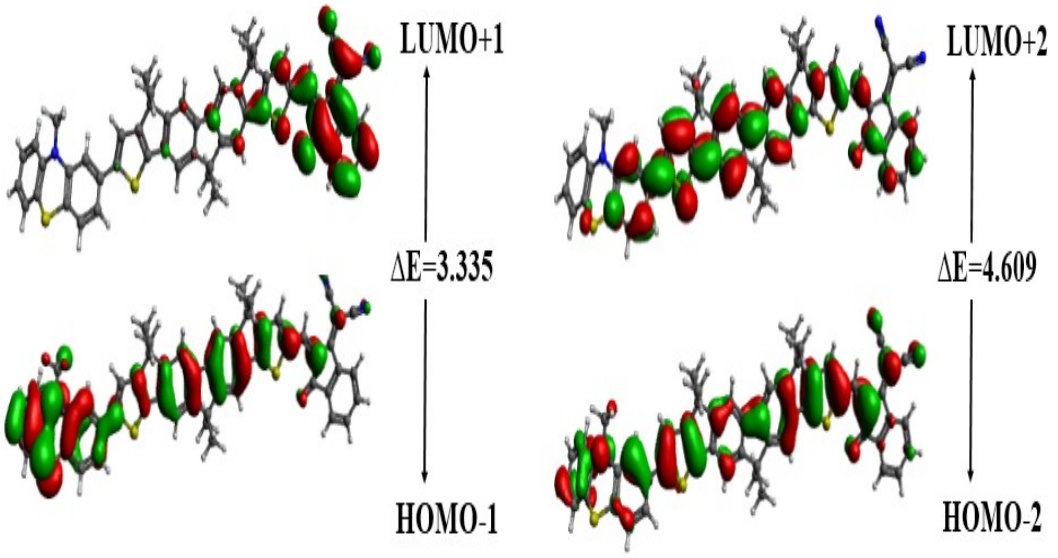

Figure S5: Frontier molecular orbitals of **FHD4**

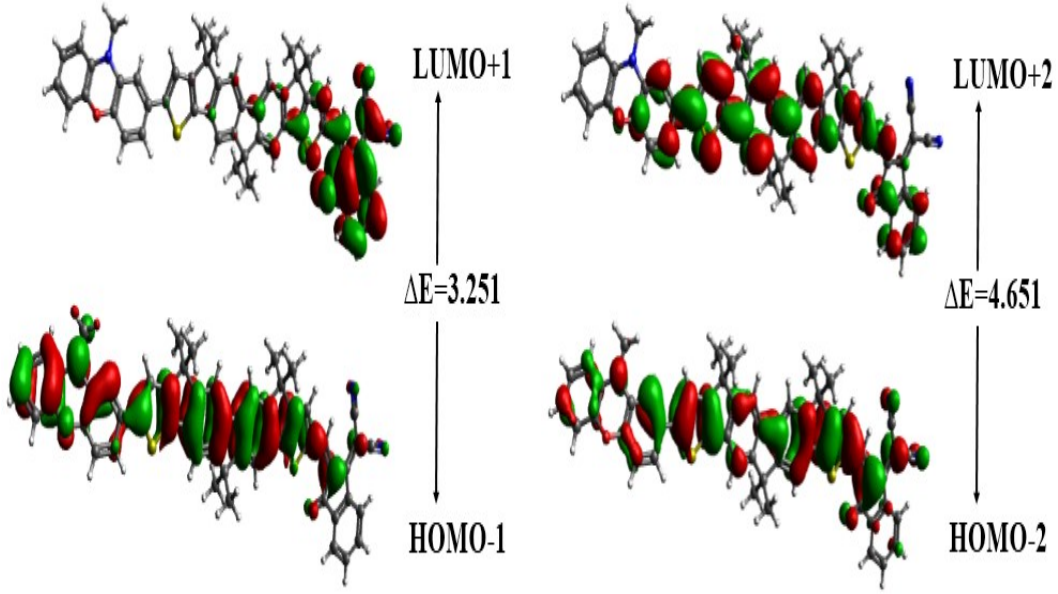

Figure S6: Frontier molecular orbitals of **FHD5**

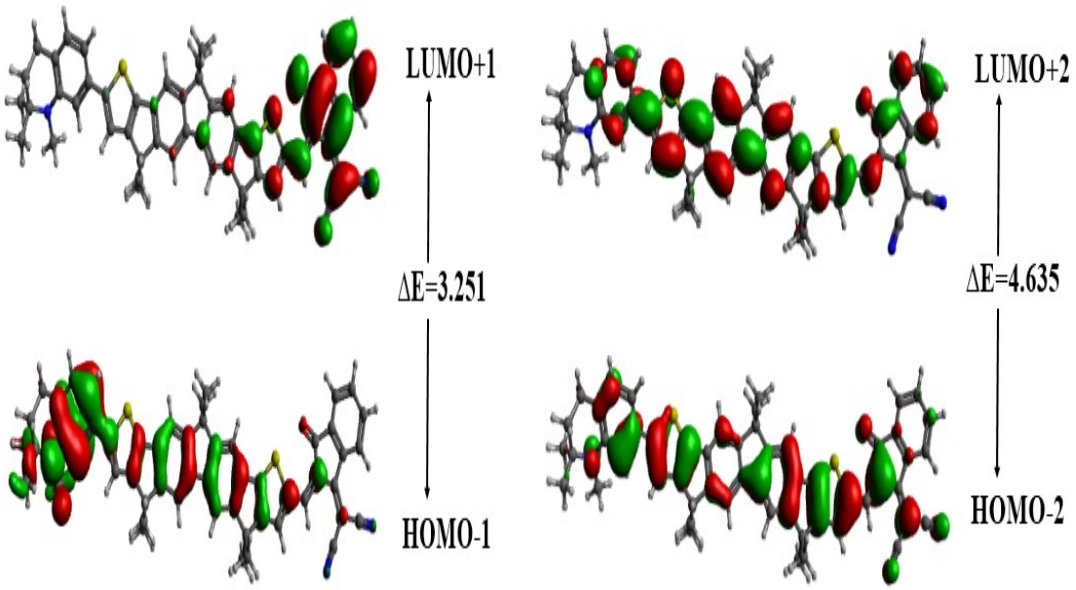

Figure S7: Frontier molecular orbitals of **FHD6**

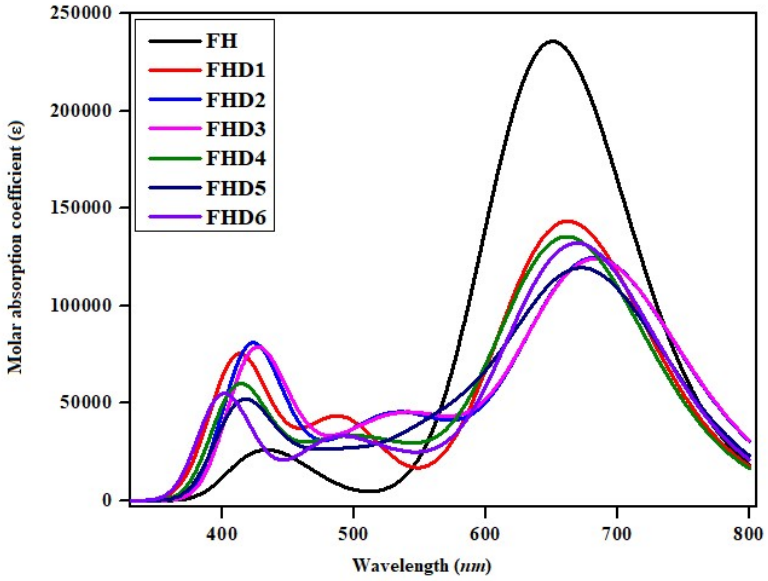

Figure S8: Simulated absorption spectra of studied compounds

The designed compounds and their IUPAC names are: *(Z)*-2-(2-((9-(9H-fluoren-2-yl)-4,4,7,7,12,12-hexamethyl-7,12-dihydro-4H-thieno[2",3":1',2']indeno[5',6':5,6]-s-indaceno[1,2-b]thien-2-yl)methylene)-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (**FHD1**), *(Z)*-2-(2-

((9-(4-(diphenylamino)phenyl)-4,4,7,7,12,12-hexamethyl-7,7a,10a,12-tetrahydro-4H-thieno[2",3":1',2']indeno[5',6':5,6]-s-indaceno[1,2-b]thien-2-yl)methylene)-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (**FHD2**), *(Z)*-2-(2-((4,4,7,7,12,12-hexamethyl-9-(1,2,2-trimethyl-1,2,3,4-tetrahydroquinolin-7-yl)-7,7a,10a,12-tetrahydro-4H-thieno[2",3":1',2']indeno[5',6':5,6]-s-indaceno[1,2-b]thien-2-yl)methylene)-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (**FHD3**), *(Z)*-2-(2-((4,4,7,7,12,12-hexamethyl-9-(10-methyl-10H-phenothiazin-2-yl)-7,7a,10a,12-tetrahydro-4H-thieno[2",3":1',2']indeno[5',6':5,6]-s-indaceno[1,2-b]thien-2-yl)methylene)-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (**FHD4**), *(Z)*-2-(2-((4,4,7,7,12,12-hexamethyl-9-(10-methyl-10H-phenoxazin-2-yl)-7,7a,10a,12-tetrahydro-4H-thieno[2",3":1',2']indeno[5',6':5,6]-s-indaceno[1,2-b]thien-2-yl)methylene)-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (**FHD5**) and *(Z)*-2-(2-((4,4,7,7,12,12-hexamethyl-9-(4-(naphthalen-2-yl(phenyl)amino)phenyl)-7,7a,10a,12-tetrahydro-4H-thieno[2",3":1',2']indeno[5',6':5,6]-s-indaceno[1,2-b]thien-2-yl)methylene)-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (**FHD6**).

$$IP = -E_{HOMO} \tag{S1}$$

$$EA = -E_{LUMO} \tag{S2}$$

$$X = \frac{[IP + EA]}{2} = -\frac{[E_{LUMO} + E_{HOMO}]}{2} \tag{S3}$$

$$\eta = \frac{[IP - EA]}{2} = -\frac{[E_{LUMO} - E_{HOMO}]}{2} \tag{S4}$$

$$\mu = \frac{E_{HOMO} + E_{LUMO}}{2} \tag{S5}$$

$$\sigma = \frac{1}{2\eta} \tag{S6}$$

$$\omega = \frac{\mu^2}{2\eta} \tag{S7}$$