Supplementary Data

Optimizing Hole Transport Efficiency in Perovskite Solar Cells by Structural Modeling of 1,4-Dihydropyrrolo[3,2-b]pyrroles With Various Donors: A DFT Approach

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Table S1: Cartesian coordinate of **PSR** compound

Atoms	X-axis	Y-axis	Z-axis
C	2.106103	-0.25364	0.007555
C	1.198437	-1.29304	0.106394
C	-0.07434	-0.69155	0.062092
C	0.074349	0.691567	-0.06244
C	-1.19843	1.293066	-0.10671
H	1.466231	-2.33339	0.196701
H	-1.46622	2.333418	-0.19694
C	-2.10609	0.253666	-0.00786
C	-4.23558	-0.96846	0.112928
C	-2.07977	-2.19233	0.210411
C	3.541787	-0.25285	-0.00082
C	3.484986	2.21794	-0.21964
C	1.356338	3.380286	-0.31498
C	4.111196	3.466028	-0.33276
C	2.011357	4.587972	-0.42567
H	0.27493	3.357649	-0.3094
C	3.407008	4.65197	-0.43574

H	5.195872	3.516187	-0.34083
H	1.432449	5.504579	-0.50608
C	4.235584	0.968498	-0.11309
C	5.633879	0.924703	-0.11864
C	6.317328	-0.26848	-0.01489
H	6.223101	1.831983	-0.2039
C	4.256935	-1.45395	0.106835
C	5.636387	-1.49198	0.106461
H	3.710689	-2.38861	0.201231
C	-3.54178	0.252888	0.000589
C	-4.25692	1.453986	-0.10702
C	-5.63387	-0.92464	0.118622
C	-5.63637	1.492039	-0.10652
H	-3.71067	2.388644	-0.2015
C	-6.31732	0.268542	0.014937
H	-6.22309	-1.83192	0.203984
C	-3.48498	-2.21791	0.219387
C	-4.11119	-3.466	0.332502
C	-3.40701	-4.65195	0.435361
H	-5.19587	-3.51615	0.34065
C	-1.35634	-3.38028	0.314464
C	-2.01136	-4.58797	0.425153
H	-0.27493	-3.35766	0.308751
H	-1.43245	-5.50459	0.505434
C	-8.52847	0.114266	-1.12376
C	-8.55795	0.583284	1.077445
C	-8.14147	-0.17511	-2.42679
C	-9.87836	0.323802	-0.77364
C	-8.21002	0.839761	2.398489
C	-9.89713	0.624564	0.636636
C	-9.13971	-0.26523	-3.38374
H	-7.09623	-0.32609	-2.68017
C	-10.8621	0.223425	-1.75484
C	-9.23448	1.137734	3.282638
H	-7.17341	0.804504	2.721351
C	-10.908	0.922	1.547688
C	-10.4859	-0.07152	-3.05462
H	-8.87033	-0.49087	-4.41102
H	-11.9076	0.378944	-1.50287
C	-10.5699	1.177759	2.865891
H	-8.99501	1.342936	4.321554
H	-11.9454	0.955086	1.225818
H	-11.241	-0.15146	-3.83011
H	-11.3464	1.412871	3.586793

C	8.558058	-0.58324	-1.07718
C	8.528364	-0.11428	1.124041
C	8.210246	-0.83968	-2.39826
C	9.897181	-0.62462	-0.63623
C	8.141248	0.175075	2.427035
C	9.878279	-0.32389	0.774058
C	9.234778	-1.1377	-3.28231
H	7.173669	-0.80436	-2.72123
C	10.90817	-0.9221	-1.54718
C	9.139391	0.265119	3.384091
H	7.095987	0.326112	2.680313
C	10.86191	-0.22359	1.75536
C	10.57014	-1.17781	-2.86542
H	8.9954	-1.34287	-4.32125
H	11.94547	-0.95526	-1.2252
C	10.48565	0.07134	3.055103
H	8.869921	0.490747	4.411345
H	11.90743	-0.37916	1.503483
H	11.34666	-1.41296	-3.58625
H	11.24065	0.15122	3.830676
C	4.104902	5.971362	-0.55511
H	3.835168	6.637812	0.271405
H	5.191325	5.852872	-0.55058
H	3.82559	6.48416	-1.48198
C	-4.10491	-5.97134	0.554732
H	-3.83529	-6.63774	-0.27186
H	-3.82548	-6.4842	1.48153
H	-5.19133	-5.85283	0.550351
C	-6.39102	2.775682	-0.2366
H	-7.11257	2.729041	-1.06025
H	-6.96364	2.995032	0.672077
H	-5.71302	3.611841	-0.42079
C	6.391036	-2.77563	0.236533
H	6.963634	-2.99496	-0.67217
H	7.112603	-2.729	1.060164
H	5.713036	-3.61179	0.420715
N	-1.4237	-0.9646	0.096212
N	7.738566	-0.25801	-0.00715
N	-7.73856	0.25809	0.007336
N	1.423707	0.964618	-0.09654
C	2.079776	2.192351	-0.21078

Table S2: Cartesian coordinate of **PSD1** compound

Atoms	**X-axis**	**Y-axis**	**Z-axis**
C	-2.11014	0.228617	-0.03631

C	-1.21674	1.267716	0.153578
C	0.064176	0.692463	0.043277
C	-0.06553	-0.67507	-0.20893
C	1.215516	-1.25254	-0.30639
H	-1.49884	2.289683	0.349098
H	1.497654	-2.27732	-0.48679
C	2.10883	-0.21439	-0.11069
C	4.220669	1.015549	0.153062
C	2.048529	2.201761	0.326169
C	-3.54566	0.205849	-0.02765
C	-3.4552	-2.23107	-0.48342
C	-1.31157	-3.34533	-0.71705
C	-4.06493	-3.47107	-0.71429
C	-1.95076	-4.54623	-0.93923
H	-0.2306	-3.30633	-0.72323
C	-3.3454	-4.63012	-0.94134
H	-5.14884	-3.5363	-0.71795
H	-1.36	-5.44146	-1.11629
C	-4.22256	-1.0106	-0.24465
C	-5.62143	-0.99121	-0.21934
C	-6.32155	0.174593	0.008386
H	-6.19788	-1.897	-0.37643
C	-4.27729	1.380094	0.200636
C	-5.65687	1.394106	0.225006
H	-3.7441	2.312039	0.368177
C	3.544293	-0.19703	-0.08681
C	4.276662	-1.37392	-0.29751
C	5.619021	0.985933	0.184924
C	5.656247	-1.39701	-0.2718
H	3.744199	-2.30092	-0.49265
C	6.320001	-0.18453	-0.0162
H	6.194993	1.886422	0.371833
C	3.453063	2.242028	0.358212
C	4.062231	3.48296	0.58557
C	3.342337	4.648438	0.775717
H	5.145981	3.544297	0.613837
C	1.309312	3.369678	0.513424
C	1.947943	4.570994	0.734848
H	0.228576	3.337171	0.481969
H	1.356919	5.472044	0.878318
C	8.569764	0.082782	-1.06201
C	8.526429	-0.57551	1.08768
C	8.236468	0.480481	-2.35187
C	9.906213	-0.14963	-0.6841

C	8.14341	-0.95204	2.370165
C	9.878354	-0.57183	0.693839
C	9.270794	0.653978	-3.25425
H	7.202032	0.64901	-2.63737
C	10.92549	0.039173	-1.61701
C	9.142087	-1.32108	3.253484
H	7.097851	-0.95394	2.665447
C	10.86118	-0.94368	1.610901
C	10.61677	0.442906	-2.90732
H	9.039782	0.965038	-4.27078
H	11.96261	-0.13412	-1.33642
C	10.50189	-1.32167	2.895722
H	8.871216	-1.62112	4.263469
H	11.90971	-0.94129	1.319468
C	-8.58015	0.472085	-1.01782
C	-8.51698	-0.01078	1.177128
C	-8.26022	0.745321	-2.34303
C	-9.91105	0.504658	-0.55884
C	-8.11962	-0.30878	2.475597
C	-9.87061	0.195198	0.848557
C	-9.30133	1.045001	-3.20329
H	-7.2301	0.721641	-2.68739
C	-10.9377	0.805281	-1.45359
C	-9.10736	-0.40764	3.439218
H	-7.0721	-0.45926	2.721002
C	-10.842	0.083204	1.843151
C	-10.642	1.077627	-2.78076
H	-9.0806	1.263004	-4.246
H	-11.9707	0.830213	-1.11204
C	-10.4691	-0.21883	3.144226
H	-8.82586	-0.63994	4.464039
H	-11.892	0.236615	1.601777
C	-4.02608	-5.94141	-1.18503
H	-3.73197	-6.68499	-0.43627
H	-5.11384	-5.84157	-1.15059
H	-3.75612	-6.35143	-2.16436
C	4.022422	5.960269	1.018164
H	3.742387	6.697609	0.257991
H	3.737712	6.379953	1.989223
H	5.110342	5.85741	1.002653
C	6.42914	-2.65431	-0.50841
H	7.165929	-2.52151	-1.3088
H	6.986756	-2.95326	0.386719
H	5.765172	-3.47613	-0.78516

C	-6.43069	2.648241	0.474524
H	-7.0706	2.896025	-0.38013
H	-7.09185	2.540001	1.34194
H	-5.76203	3.492427	0.656323
N	1.409595	0.980002	0.102542
N	-7.74182	0.14102	0.036578
N	7.739891	-0.16086	0.023069
N	-1.41105	-0.96391	-0.2604
C	-2.05045	-2.18474	-0.48776
C	-11.488	-0.34558	4.237191
C	-11.7218	1.406045	-3.76826
C	11.53319	-1.72897	3.905356
C	11.68866	0.65694	-3.93409
H	11.35897	-2.74917	4.265616
H	12.54137	-1.69097	3.484071
H	11.51299	-1.07413	4.783903
H	11.70683	1.695982	-4.28229
H	12.67843	0.422664	-3.53308
H	11.52745	0.028824	-4.8174
H	-12.4986	-0.15709	3.864997
H	-11.4765	-1.34788	4.680295
H	-11.2927	0.36311	5.049913
H	-12.7085	1.401969	-3.29732
H	-11.568	2.394979	-4.21471
H	-11.7419	0.684903	-4.59324

Table S3: Cartesian coordinate of **PSD2** compound

Atoms	**X-axis**	**Y-axis**	**Z-axis**
C	2.099669	0.311236	-0.03388
C	1.163382	1.329795	-0.03397
C	-0.09312	0.691719	-0.03664
C	0.093116	-0.69162	-0.03658
C	-1.16339	-1.3297	-0.0338
H	1.402798	2.381064	-0.02817
H	-1.4028	-2.38097	-0.02791
C	-2.09967	-0.31114	-0.0338
C	-4.26369	0.858552	-0.01492
C	-2.14034	2.143997	-0.02731
C	3.534739	0.347568	-0.03001
C	3.546144	-2.13216	-0.01492
C	1.449613	-3.35581	-0.03361
C	4.205184	-3.3684	-0.00932
C	2.136851	-4.55078	-0.02643
H	0.367969	-3.36144	-0.04567
C	3.533556	-4.57755	-0.014

H	5.290848	-3.38959	-0.00338
H	1.582804	-5.48613	-0.03171
C	4.26368	-0.85847	-0.01495
C	5.658327	-0.77764	0.009219
C	6.322232	0.435059	-0.00324
H	6.265742	-1.67705	0.038055
C	4.222039	1.568223	-0.0525
C	5.60077	1.64383	-0.05139
H	3.6527	2.493221	-0.09625
C	-3.53474	-0.34747	-0.0299
C	-4.22204	-1.56814	-0.0523
C	-5.65834	0.777716	0.00926
C	-5.60076	-1.64376	-0.05119
H	-3.65269	-2.49313	-0.096
C	-6.32224	-0.43498	-0.00313
H	-6.26575	1.67713	0.038028
C	-3.54616	2.132245	-0.01494
C	-4.2052	3.368486	-0.00933
C	-3.53358	4.577638	-0.01406
H	-5.29086	3.389675	-0.00333
C	-1.44963	3.355903	-0.03369
C	-2.13687	4.55087	-0.0265
H	-0.36798	3.361537	-0.04572
H	-1.58283	5.486228	-0.03175
C	-8.40417	-1.04632	1.106495
C	-8.44717	0.166068	-1.04023
C	-7.83931	-0.99142	2.381667
C	-9.60041	-1.74682	0.926919
C	-7.95542	0.088073	-2.34527
C	-9.62417	0.879833	-0.8032
C	-8.45512	-1.62918	3.448682
H	-6.9094	-0.45029	2.530344
C	-10.2163	-2.36499	2.001716
C	-8.62739	0.710455	-3.38543
H	-7.03972	-0.46461	-2.53686
C	-10.2971	1.485486	-1.85243
C	-9.64797	-2.31546	3.269556
H	-7.99913	-1.57815	4.432877
H	-11.1433	-2.90773	1.842628
C	-9.80426	1.408855	-3.14897
H	-8.23042	0.638472	-4.39356
H	-11.21	2.037488	-1.64964
H	-10.1297	-2.80925	4.107079
H	-10.3311	1.890445	-3.9662

C	8.404151	1.046427	1.106399
C	8.447172	-0.16621	-1.04017
C	7.839232	0.991732	2.381555
C	9.600488	1.746759	0.926804
C	7.955514	-0.08834	-2.34526
C	9.624062	-0.88009	-0.80297
C	8.455111	1.629484	3.448533
H	6.909235	0.450758	2.530253
C	10.21645	2.364928	2.001568
C	8.627463	-0.71097	-3.38529
H	7.039889	0.464429	-2.53698
C	10.29693	-1.48599	-1.85206
C	9.648069	2.315573	3.269395
H	7.99908	1.578618	4.432718
H	11.14356	2.907529	1.842467
C	9.804226	-1.40948	-3.14865
H	8.230556	-0.63907	-4.39345
H	11.20976	-2.03808	-1.64914
H	10.12982	2.809354	4.106897
H	10.33106	-1.89127	-3.96577
C	4.267325	-5.88299	-0.00628
H	4.004369	-6.49034	-0.87922
H	5.350144	-5.73479	-0.01348
H	4.014398	-6.47408	0.880813
C	-4.26735	5.883077	-0.00652
H	-4.01275	6.475241	0.879373
H	-4.00605	6.489378	-0.88069
H	-5.35017	5.734859	-0.01155
C	-6.30279	-2.96111	-0.13445
H	-6.77459	-3.23222	0.818223
H	-7.10439	-2.93088	-0.88157
H	-5.60486	-3.75691	-0.40485
C	6.302815	2.961167	-0.13474
H	6.774471	3.232399	0.817968
H	7.104513	2.930829	-0.88175
H	5.604928	3.756942	-0.40534
N	-1.45038	0.929696	-0.03394
N	7.743935	0.451528	0.013856
N	-7.74394	-0.45144	0.01394
N	1.450373	-0.9296	-0.03388
C	2.140328	-2.1439	-0.02724
H	-10.0365	-1.8136	-0.06552
H	-10.0068	0.959248	0.209738
H	10.00667	-0.95941	0.210001

H	10.03657	1.813408	-0.06563

Table S4: Cartesian coordinate of **PSD3** compound

Atoms	X-axis	Y-axis	Z-axis
C	2.101409	0.301775	-0.06517
C	1.169605	1.324467	-0.06598
C	-0.08992	0.691992	-0.07066
C	0.089929	-0.69199	-0.07061
C	-1.1696	-1.32447	-0.06589
H	1.41372	2.374639	-0.05788
H	-1.41372	-2.37464	-0.05772
C	-2.1014	-0.30177	-0.06516
C	-4.26022	0.877985	-0.03967
C	-2.13061	2.153367	-0.0615
C	3.53662	0.331145	-0.05698
C	3.536502	-2.14832	-0.04434
C	1.434117	-3.36195	-0.0744
C	4.189375	-3.38785	-0.04015
C	2.115437	-4.56031	-0.06837
H	0.352522	-3.3622	-0.0919
C	3.511919	-4.59378	-0.05061
H	5.274917	-3.41416	-0.03117
H	1.55692	-5.49297	-0.07924
C	4.260227	-0.87798	-0.03962
C	5.655112	-0.80381	-0.00794
C	6.32622	0.405598	-0.01663
H	6.257453	-1.70653	0.024519
C	4.230184	1.548353	-0.07705
C	5.60908	1.617506	-0.06995
H	3.665499	2.476075	-0.12486
C	-3.53662	-0.33114	-0.05696
C	-4.23018	-1.54835	-0.07694
C	-5.65511	0.803814	-0.00797
C	-5.60908	-1.6175	-0.06983
H	-3.6655	-2.47608	-0.12471
C	-6.32622	-0.40559	-0.01658
H	-6.25745	1.706537	0.024441
C	-3.5365	2.148322	-0.04449
C	-4.18937	3.387853	-0.0404
C	-3.51191	4.593777	-0.05095
H	-5.27491	3.414158	-0.03141
C	-1.43411	3.361953	-0.07466
C	-2.11543	4.56031	-0.06872
H	-0.35252	3.362202	-0.09218
H	-1.55692	5.492968	-0.07967

C	-8.40443	-1.01925	1.100364
C	-8.45651	0.241516	-1.01546
C	-7.83933	-0.98831	2.373775
C	-9.60614	-1.71055	0.920678
C	-8.00302	0.176108	-2.33377
C	-9.60444	0.986094	-0.74136
C	-8.45766	-1.63792	3.433091
H	-6.9028	-0.46061	2.530529
C	-10.22	-2.33642	1.989697
C	-8.68151	0.838959	-3.34324
H	-7.10697	-0.3959	-2.56038
C	-10.2824	1.62901	-1.76421
C	-9.66012	-2.317	3.26827
H	-7.99432	-1.60663	4.416602
H	-11.1518	-2.87405	1.826895
C	-9.83796	1.571432	-3.08355
H	-8.30792	0.778383	-4.36301
H	-11.173	2.20761	-1.52855
C	8.40443	1.019354	1.100248
C	8.456508	-0.24161	-1.01546
C	7.839347	0.988509	2.37366
C	9.606146	1.71065	0.920496
C	8.002983	-0.17637	-2.33377
C	9.604453	-0.98614	-0.7413
C	8.457681	1.638204	3.432927
H	6.902822	0.460804	2.530466
C	10.22004	2.336607	1.989458
C	8.681465	-0.83933	-3.34318
H	7.10692	0.395596	-2.56043
C	10.28244	-1.62917	-1.76409
C	9.660128	2.317278	3.268041
H	7.994362	1.60697	4.416446
H	11.15185	2.874215	1.826613
C	9.83793	-1.57175	-3.08343
H	8.307848	-0.77888	-4.36294
H	11.17298	-2.20773	-1.52837
C	4.239545	-5.90269	-0.04258
H	3.963146	-6.51503	-0.90779
H	5.322901	-5.75969	-0.06362
H	3.994804	-6.48627	0.851838
C	-4.23954	5.902689	-0.04299
H	-3.99507	6.486164	0.851574
H	-3.96288	6.515129	-0.90804
H	-5.32289	5.759692	-0.06436

C	-6.31682	-2.93159	-0.1552
H	-6.78693	-3.20466	0.797742
H	-7.12104	-2.89373	-0.89924
H	-5.62325	-3.72918	-0.4318
C	6.316822	2.931589	-0.15539
H	6.786933	3.204705	0.797542
H	7.121051	2.893679	-0.89943
H	5.623263	3.72916	-0.43203
N	-1.44626	0.936028	-0.06694
N	7.745853	0.417067	0.009796
N	-7.74585	-0.41705	0.009866
N	1.446265	-0.93603	-0.06687
C	2.130617	-2.15337	-0.06134
H	-10.0476	-1.76486	-0.07042
H	-9.96126	1.062455	0.28151
H	9.961296	-1.06238	0.281569
H	10.04762	1.76487	-0.07061
C	-10.3456	-2.99151	4.416687
H	-11.2054	-2.40774	4.766405
H	-10.725	-3.97834	4.132007
H	-9.66945	-3.12037	5.266318
C	10.3456	2.991974	4.416352
H	11.20637	2.409058	4.765143
H	10.72367	3.979425	4.131945
H	9.669878	3.119593	5.266509
C	10.58952	-2.25274	-4.18594
H	11.33742	-1.58482	-4.63023
H	11.12223	-3.13575	-3.82051
H	9.919738	-2.56809	-4.99143
C	-10.5896	2.252298	-4.18613
H	-11.3376	1.584378	-4.63024
H	-11.1222	3.135423	-3.82081
H	-9.91981	2.567447	-4.99172

Table S5: Cartesian coordinate of **PSD4** compound

Atoms	**X-axis**	**Y-axis**	**Z-axis**
C	2.041749	0.337619	-0.07173
C	1.101961	1.34795	-0.17309
C	-0.15251	0.710742	-0.09081
C	0.038837	-0.66377	0.060184
C	-1.21511	-1.30071	0.148079
H	1.338364	2.393737	-0.28745
H	-1.45107	-2.34562	0.270714
C	-2.15506	-0.29086	0.045597
C	-4.32376	0.862905	-0.07325

C	-2.20595	2.147852	-0.23483
C	3.476764	0.375771	-0.08561
C	3.496219	-2.0893	0.171932
C	1.402785	-3.31039	0.320206
C	4.157989	-3.31865	0.289257
C	2.092891	-4.49832	0.434219
H	0.321155	-3.31742	0.331794
C	3.489501	-4.52259	0.41992
H	5.243599	-3.33882	0.27675
H	1.541277	-5.42967	0.535536
C	4.209029	-0.8201	0.034674
C	5.603567	-0.73258	0.021588
C	6.285038	0.47025	-0.09617
H	6.19903	-1.63406	0.128414
C	4.165013	1.586948	-0.22365
C	5.544305	1.666675	-0.2294
H	3.593507	2.504129	-0.34359
C	-3.58979	-0.32991	0.065566
C	-4.27524	-1.54193	0.21013
C	-5.71852	0.77377	-0.05563
C	-5.65406	-1.6214	0.23633
H	-3.70219	-2.46218	0.293004
C	-6.39576	-0.426	0.10401
H	-6.31634	1.675007	-0.15198
C	-3.61198	2.131089	-0.22476
C	-4.27516	3.357679	-0.36123
C	-3.60802	4.561048	-0.50352
H	-5.36089	3.37597	-0.35595
C	-1.51975	3.353842	-0.37757
C	-2.2113	4.539086	-0.50959
H	-0.43804	3.362273	-0.38482
H	-1.66076	5.470093	-0.61949
C	4.226754	-5.82028	0.543298
H	3.952482	-6.50986	-0.26257
H	5.308985	-5.67232	0.505281
H	3.988699	-6.32294	1.487197
C	-4.34672	5.855856	-0.6468
H	-4.07993	6.55462	0.153646
H	-4.10228	6.348728	-1.59421
H	-5.42893	5.706275	-0.61534
C	-6.31177	-2.9629	0.360296
H	-6.66465	-3.15468	1.379777
H	-7.18163	-3.04893	-0.29798
H	-5.60817	-3.75959	0.10549

C	6.20116	3.001465	-0.41647
H	6.543097	3.427653	0.533374
H	7.077601	2.93344	-1.06791
H	5.49975	3.714818	-0.85698
N	-1.51068	0.943673	-0.10168
N	1.396764	-0.89722	0.070384
C	2.090392	-2.10387	0.18883
C	7.764349	0.444313	-0.09537
C	8.516877	1.220807	0.788043
C	8.457069	-0.40814	-0.95794
C	9.897672	1.142777	0.819461
H	8.009918	1.869827	1.496509
C	9.839093	-0.47679	-0.95072
H	7.898333	-1.01145	-1.66887
C	10.58102	0.29459	-0.0547
H	10.45839	1.736347	1.535254
H	10.35463	-1.13231	-1.64618
C	-7.8762	-0.40863	0.108387
C	-8.6143	-0.9396	1.168193
C	-8.57909	0.182	-0.94314
C	-9.99694	-0.89411	1.174178
H	-8.09568	-1.38819	2.010848
C	-9.96252	0.240519	-0.94215
H	-8.02741	0.603994	-1.77913
C	-10.6887	-0.30341	0.116215
H	-10.5535	-1.31388	2.007072
H	-10.4898	0.707817	-1.7686
N	11.98772	0.215303	-0.02909
N	-12.1016	-0.25344	0.126161
C	12.63666	-1.02849	-0.21044
C	13.77501	-1.11616	-1.01243
C	12.15497	-2.17948	0.41417
C	14.42012	-2.33154	-1.17897
H	14.15007	-0.22269	-1.50309
C	12.79582	-3.39435	0.228541
H	11.27423	-2.11436	1.046229
C	13.93308	-3.47813	-0.56465
H	15.30482	-2.38419	-1.80619
H	12.40968	-4.28154	0.721199
H	14.43625	-4.42961	-0.70245
C	12.76224	1.375043	0.210921
C	12.46473	2.572218	-0.44054
C	13.83609	1.332562	1.100196
C	13.22299	3.706415	-0.196

H	11.63407	2.605701	-1.1395
C	14.60004	2.466798	1.326659
H	14.06655	0.402538	1.611769
C	14.29636	3.660449	0.684643
H	12.9804	4.631472	-0.71011
H	15.43269	2.419345	2.021873
H	14.8922	4.548493	0.868698
C	-12.8327	-0.50861	-1.05571
C	-12.4447	-1.54077	-1.91189
C	-13.9529	0.257818	-1.37913
C	-13.1613	-1.79257	-3.07053
H	-11.5783	-2.14512	-1.6602
C	-14.6734	-0.01224	-2.53251
H	-14.2551	1.066969	-0.72081
C	-14.2816	-1.03424	-3.38704
H	-12.8479	-2.59978	-3.72553
H	-15.5428	0.592916	-2.77061
H	-14.8444	-1.23857	-4.2919
C	-12.7748	0.12678	1.308696
C	-13.905	-0.60587	1.730895
C	-12.3035	1.244151	2.034795
C	-14.6365	-0.28063	2.875429
H	-14.2077	-1.46295	1.134921
C	-13.084	1.454234	3.14341
H	-11.4494	1.819846	1.693165
C	-14.0603	0.792032	3.5267
H	-15.5043	-0.85004	3.188422

Table S6: Cartesian coordinate of **PSD5** compound

Atoms	**X-axis**	**Y-axis**	**Z-axis**
C	2.106633	0.249532	-0.00173
C	1.200852	1.29524	-0.0018
C	-0.07306	0.694489	-0.00221
C	0.073058	-0.69447	-0.00223
C	-1.20085	-1.29522	-0.00185
H	1.470514	2.339012	-0.00139
H	-1.47052	-2.33899	-0.00147
C	-2.10663	-0.24951	-0.00174
C	-4.23396	0.982628	-0.00101
C	-2.07571	2.206125	-0.00251
C	3.54233	0.24508	-0.00113
C	3.480937	-2.23509	-0.00191
C	1.35002	-3.39726	-0.00421
C	4.104804	-3.48944	-0.00261
C	2.002783	-4.61122	-0.00492

H	0.268648	-3.37249	-0.00543
C	3.398335	-4.67853	-0.00394
H	5.18941	-3.54166	-0.00229
H	1.422196	-5.53027	-0.00651
C	4.233954	-0.98261	-0.00103
C	5.632623	-0.94093	-0.00017
C	6.319727	0.254085	0.000465
H	6.220805	-1.85318	0.000025
C	4.260298	1.44944	-0.0005
C	5.640001	1.484013	0.000277
H	3.715867	2.389999	-0.00061
C	-3.54233	-0.24506	-0.00115
C	-4.2603	-1.44942	-0.00056
C	-5.63263	0.940946	-0.00015
C	-5.64	-1.48399	0.000217
H	-3.71587	-2.38998	-0.0007
C	-6.31973	-0.25406	0.000447
H	-6.22081	1.853195	0.000074
C	-3.48094	2.235114	-0.00186
C	-4.10481	3.489455	-0.00253
C	-3.39834	4.67855	-0.00381
H	-5.18941	3.541682	-0.00221
C	-1.35002	3.397278	-0.00411
C	-2.00278	4.611241	-0.00479
H	-0.26865	3.372506	-0.00532
H	-1.4222	5.53029	-0.00635
C	-8.44747	-0.3366	1.209134
C	-8.44899	-0.3365	-1.20558
C	-7.81324	-0.35577	2.447282
C	-9.84445	-0.42143	1.180993
C	-7.81629	-0.35565	-2.44451
C	-9.84593	-0.4213	-1.17572
C	-8.54993	-0.45414	3.623424
H	-6.7306	-0.28826	2.48689
C	-10.5749	-0.52272	2.346803
C	-8.55443	-0.45388	-3.61975
H	-6.7337	-0.28824	-2.48546
C	-10.5778	-0.52243	-2.34063
C	-9.9303	-0.53779	3.579443
H	-8.02907	-0.46426	4.575191
H	-11.6555	-0.58565	2.266582
C	-9.93475	-0.53744	-3.57407
H	-8.03474	-0.46398	-4.57215
H	-11.6583	-0.58532	-2.25907

H	-10.511	-0.61484	4.492167
H	-10.5165	-0.61436	-4.48608
C	8.447482	0.336538	1.209139
C	8.448973	0.336556	-1.20557
C	7.813266	0.355651	2.447293
C	9.844458	0.421345	1.180989
C	7.816271	0.35577	-2.4445
C	9.845915	0.421326	-1.17572
C	8.549961	0.45394	3.623434
H	6.730623	0.288167	2.486907
C	10.5749	0.522547	2.346799
C	8.5544	0.454028	-3.61974
H	6.733672	0.288381	-2.48544
C	10.57779	0.522485	-2.34063
C	9.930333	0.53757	3.579446
H	8.029114	0.46402	4.575207
H	11.65552	0.585457	2.266571
C	9.934725	0.537549	-3.57407
H	8.034704	0.464177	-4.57214
H	11.65831	0.585347	-2.25908
H	10.511	0.614555	4.492169
H	10.51651	0.614496	-4.48609
C	4.093886	-6.00455	-0.00305
H	3.80487	-6.60356	-0.87344
H	5.180385	-5.88795	-0.02042
H	3.832023	-6.588	0.88644
C	-4.09389	6.00457	-0.00289
H	-3.83206	6.587977	0.886642
H	-3.80483	6.603622	-0.87324
H	-5.18039	5.887967	-0.02031
C	-6.39604	-2.77324	0.000901
H	-7.04386	-2.85329	0.881424
H	-7.04555	-2.85328	-0.87837
H	-5.71491	-3.62706	0.000263
C	6.396037	2.773263	0.000993
H	7.043891	2.853274	0.881497
H	7.045517	2.853335	-0.8783
H	5.714913	3.62708	0.00041
N	-1.42196	0.971935	-0.00205
N	7.745787	0.234224	0.001351
N	-7.74579	-0.2342	0.001345
N	1.42196	-0.97192	-0.00208
C	2.075713	-2.20611	-0.00257
O	10.54759	0.392058	0.00307

O	-10.5476	-0.39209	0.003081

Table S7: Cartesian coordinate of **PSD6** compound

Atoms	X-axis	Y-axis	Z-axis
C	2.10523	0.264133	-0.26218
C	1.192993	1.304185	-0.27036
C	-0.07729	0.695408	-0.28798
C	0.077236	-0.69232	-0.28826
C	-1.19303	-1.30112	-0.27049
H	1.455652	2.349637	-0.25078
H	-1.45567	-2.34658	-0.25122
C	-2.10527	-0.26108	-0.26165
C	-4.23856	0.959276	-0.18973
C	-2.08905	2.194521	-0.28423
C	3.540487	0.26762	-0.21808
C	3.493429	-2.21284	-0.23683
C	1.370979	-3.38576	-0.34603
C	4.124261	-3.4637	-0.24238
C	2.030468	-4.59611	-0.34976
H	0.290676	-3.36549	-0.39773
C	3.425299	-4.65611	-0.2954
H	5.208567	-3.51027	-0.20714
H	1.45604	-5.51777	-0.3984
C	4.238494	-0.95633	-0.19127
C	5.634979	-0.90701	-0.12197
C	6.315788	0.291089	-0.08451
H	6.226712	-1.81665	-0.09002
C	4.251794	1.475411	-0.18705
C	5.630021	1.516437	-0.12068
H	3.703136	2.413274	-0.21179
C	-3.54051	-0.26463	-0.21714
C	-4.25172	-1.47248	-0.18629
C	-5.63504	0.909867	-0.12011
C	-5.62992	-1.51359	-0.11955
H	-3.70302	-2.4103	-0.21145
C	-6.31575	-0.2883	-0.08285
H	-6.22682	1.819459	-0.08772
C	-3.49354	2.215817	-0.23501
C	-4.12441	3.466667	-0.23989
C	-3.4255	4.659116	-0.29258
H	-5.20871	3.513184	-0.20436
C	-1.37115	3.388859	-0.34423
C	-2.03068	4.599184	-0.34729
H	-0.29085	3.368649	-0.39619
H	-1.45629	5.520884	-0.39567

C	-8.34697	-0.30807	1.268758
C	-8.50169	-0.31829	-1.17284
C	-7.59523	-0.33975	2.43574
C	-9.75319	-0.30279	1.357742
C	-7.90343	-0.35806	-2.42505
C	-9.90791	-0.3157	-1.08315
C	-8.20753	-0.35979	3.687888
H	-6.51228	-0.34162	2.366093
C	-10.3503	-0.322	2.611364
C	-8.66917	-0.39195	-3.58949
H	-6.82033	-0.35604	-2.49218
C	-10.6587	-0.351	-2.25077
C	-9.58364	-0.34934	3.775197
H	-7.59327	-0.38166	4.581997
H	-11.4327	-0.31281	2.680473
C	-10.0453	-0.38778	-3.50194
H	-8.17295	-0.42	-4.55396
H	-11.7412	-0.34634	-2.18217
H	-10.0796	-0.36197	4.740207
H	-10.6592	-0.41252	-4.39628
C	8.347418	0.310343	1.266509
C	8.50145	0.320856	-1.1751
C	7.59608	0.343978	2.433689
C	9.753656	0.30251	1.355105
C	7.902895	0.362976	-2.42709
C	9.907688	0.31573	-1.08579
C	8.208777	0.363517	3.685652
H	6.51311	0.347646	2.364353
C	10.35112	0.321305	2.608521
C	8.668366	0.396806	-3.5917
H	6.819766	0.362777	-2.49391
C	10.65821	0.351201	-2.2536
C	9.584898	0.350624	3.77257
H	7.594823	0.386899	4.579928
H	11.43356	0.310005	2.67718
C	10.04456	0.390321	-3.50453
H	8.171932	0.426636	-4.55601
H	11.74078	0.344597	-2.18544
H	10.08112	0.362787	4.73744
H	10.65826	0.415004	-4.39902
C	4.128268	-5.97829	-0.29766
H	3.869815	-6.56255	-1.18747
H	5.214098	-5.85562	-0.27905
H	3.842587	-6.57962	0.572419

C	-4.12851	5.981272	-0.2941
H	-3.84259	6.582266	0.576141
H	-3.87034	6.565905	-1.18375
H	-5.21433	5.858564	-0.27521
C	-6.38013	-2.80534	-0.08018
H	-6.98131	-2.88539	0.832798
H	-7.07444	-2.88547	-0.92442
H	-5.69748	-3.65731	-0.11607
C	6.380286	2.808155	-0.0812
H	6.981563	2.888067	0.831721
H	7.074508	2.88838	-0.9255
H	5.697658	3.660148	-0.1169
N	-1.42798	0.964393	-0.27724
N	7.73902	0.27818	0.002129
N	-7.73896	-0.27572	0.004189
N	1.42792	-0.96132	-0.27803
C	2.088937	-2.19147	-0.2857
N	-10.5144	-0.26972	0.180397
N	10.51442	0.266941	0.177577
C	-11.9366	-0.21606	0.270266
C	-12.6781	-1.38791	0.341877
C	-12.5816	1.012801	0.292758
C	-14.06	-1.32588	0.435325
H	-12.1601	-2.34328	0.328961
C	-13.964	1.066269	0.385408
H	-11.9885	1.92183	0.240735
C	-14.7241	-0.10015	0.455686
H	-14.6377	-2.2449	0.496305
H	-14.4658	2.030518	0.40707
C	11.93656	0.20963	0.266857
C	12.68133	1.379822	0.334988
C	12.57888	-1.02052	0.279445
C	14.06361	1.314458	0.41756
H	12.16596	2.336538	0.31925
C	13.96205	-1.07732	0.361162
H	11.98404	-1.9279	0.219533
C	14.72483	0.086881	0.4347
H	14.64461	2.232139	0.466946
H	14.46235	-2.04252	0.36607
C	-16.2188	-0.03947	0.526407
C	16.21631	0.022932	0.553952
H	-16.6284	-0.89554	1.069856
H	-16.5592	0.875697	1.018706
H	-16.6588	-0.05156	-0.47764

H	16.61449	-0.89381	0.110552
H	16.69318	0.8772	0.06508
H	16.52557	0.03749	1.605592

Table S8: Cartesian coordinate of **PSD7** compound

Atoms	X-axis	Y-axis	Z-axis
C	-2.10172	-0.28866	-0.15754
C	-1.17671	-1.31727	-0.16422
C	0.085956	-0.69281	-0.17778
C	-0.08596	0.692891	-0.17772
C	1.176703	1.317353	-0.16411
H	-1.42663	-2.36593	-0.14899
H	1.426624	2.366006	-0.14878
C	2.101716	0.288737	-0.15752
C	4.251309	-0.90459	-0.09655
C	2.116558	-2.16707	-0.17094
C	-3.53718	-0.31086	-0.12365
C	-3.52144	2.170749	-0.12884
C	-1.41342	3.370802	-0.2174
C	-4.16785	3.413571	-0.12835
C	-2.08803	4.572837	-0.21543
H	-0.33264	3.364582	-0.26177
C	-3.48371	4.615053	-0.16844
H	-5.25282	3.446656	-0.09848
H	-1.52486	5.50191	-0.25336
C	-4.25131	0.904665	-0.09646
C	-5.64641	0.837338	-0.04068
C	-6.3138	-0.37012	-0.01849
H	-6.24818	1.741076	-0.00944
C	-4.23357	-1.52631	-0.10688
C	-5.61294	-1.58422	-0.05573
H	-3.67366	-2.45738	-0.13292
C	3.537174	0.310937	-0.12363
C	4.233571	1.526383	-0.10675
C	5.646406	-0.83727	-0.04077
C	5.612933	1.584297	-0.0556
H	3.673659	2.457461	-0.13271
C	6.313795	0.370189	-0.01847
H	6.248174	-1.74101	-0.0096
C	3.521435	-2.17067	-0.12905
C	4.167851	-3.41349	-0.12866
C	3.483712	-4.61497	-0.16885
H	5.252819	-3.44658	-0.09879
C	1.41342	-3.37072	-0.2177
C	2.088028	-4.57275	-0.21583

H	0.332638	-3.36449	-0.26207
H	1.524857	-5.50182	-0.25385
C	8.35975	0.248697	1.302778
C	8.485198	0.212469	-1.12436
C	7.59917	0.011118	2.451799
C	9.758411	0.343727	1.398663
C	7.846841	-0.05816	-2.33849
C	9.886609	0.305295	-1.0777
C	8.215424	-0.17707	3.677751
H	6.51808	-0.03705	2.382673
C	10.34793	0.123199	2.63891
C	8.586005	-0.28226	-3.48809
H	6.764282	-0.10357	-2.38013
C	10.60054	0.048219	-2.24326
C	9.596689	-0.14128	3.775725
H	7.605135	-0.36262	4.556326
H	11.42716	0.178482	2.732787
C	9.970081	-0.24989	-3.44343
H	8.069315	-0.49315	-4.41938
H	11.68387	0.101004	-2.22663
H	10.08947	-0.3008	4.729181
H	10.55836	-0.43747	-4.33568
C	-8.35977	-0.24888	1.302771
C	-8.48519	-0.21227	-1.12436
C	-7.59922	-0.01144	2.451843
C	-9.75843	-0.34403	1.398621
C	-7.84684	0.05861	-2.33844
C	-9.8866	-0.30521	-1.07773
C	-8.21551	0.176506	3.677816
H	-6.51814	0.036817	2.382741
C	-10.348	-0.12375	2.638898
C	-8.58601	0.282846	-3.48801
H	-6.76429	0.104115	-2.38006
C	-10.6005	-0.048	-2.24325
C	-9.59677	0.140601	3.775765
H	-7.60525	0.361951	4.55643
H	-11.4272	-0.17914	2.732755
C	-9.97009	0.25036	-3.44337
H	-8.06933	0.493935	-4.41926
H	-11.6839	-0.10088	-2.22665
H	-10.0896	0.299919	4.729241
H	-10.5584	0.43804	-4.33559
C	-4.20321	5.928288	-0.16244
H	-3.93202	6.532325	-1.035

H	-5.28754	5.791999	-0.17058
H	-3.94507	6.516565	0.725067
C	4.203212	-5.9282	-0.16297
H	3.945062	-6.51657	0.724479
H	3.932032	-6.53216	-1.03559
H	5.287541	-5.79191	-0.17109
C	6.346235	2.886088	-0.03572
H	6.953619	2.983395	0.871853
H	7.032813	2.96517	-0.88677
H	5.652687	3.729086	-0.07537
C	-6.34625	-2.88601	-0.03596
H	-6.95364	-2.98339	0.871601
H	-7.03282	-2.96502	-0.88702
H	-5.6527	-3.72901	-0.07568
N	1.439968	-0.9451	-0.16904
N	-7.74133	-0.39229	0.05147
N	7.741328	0.392339	0.051496
N	-1.43997	0.945178	-0.16896
C	-2.11656	2.167149	-0.17074
C	-10.5499	-0.81835	0.190348
C	10.5499	0.81816	0.190477
C	-10.476	-2.3576	0.161513
H	-10.9256	-2.77495	1.070328
H	-11.0183	-2.74536	-0.70904
H	-9.43991	-2.70645	0.101716
C	-12.019	-0.41915	0.272919
H	-12.4877	-0.84093	1.165851
H	-12.1441	0.668923	0.295234
H	-12.5791	-0.81593	-0.5778
C	10.47622	2.357428	0.161894
H	10.92589	2.774573	1.07079
H	11.0186	2.745266	-0.70858
H	9.440172	2.706398	0.102131
C	12.01896	0.418791	0.273013
H	12.48774	0.840331	1.166052
H	12.14399	-0.6693	0.295105
H	12.57919	0.815693	-0.57761

Table S9: Calculated energies **(*E*)** and energy gap **(Δ*E*)** of **HOMO-1, LUMO+1, HOMO-2** and **LUMO+2** for **PSR** and **PSD1-PSD7**.

Compounds	HOMO-1	LUMO+1	Δ*E*	HOMO-2	LUMO+2	Δ*E*
PSR	-6.096	-1.321	4.775	-6.155	-1.272	4.883
PSD1	-5.942	-1.304	4.638	-5.943	-1.252	4.691
PSD2	-5.755	-1.247	4.508	-5.827	-1.204	4.623
PSD3	-5.577	-1.216	4.361	-5.718	-1.166	4.552
PSD4	-5.669	-1.576	4.093	-5.779	-1.179	4.6

PSD5	-5.430	-1.339	4.091	-5.430	-1.296	4.134
PSD6	-4.902	-1.287	3.615	-5.293	-1.239	4.054
PSD7	-5.740	-1.305	4.435	-5.740	-1.270	4.474

E= energy, $\Delta E(eV) = E_{LUMO} - E_{HOMO}$; **HOMO**= highest occupied molecular orbital; **LUMO**= lowest unoccupied molecular orbital; **MO**= molecular orbital; Units in ***eV***

Uv solvent tables (In Gaseous phase)

Table S10: Wavelength, excitation energy and oscillator strength of investigated compound **PSR** at **M06/6-311g(d,p)**.

NO	DFT λ(nm)	*E* (*eV*)	f_{os}	MO contributions
1	422.3	2.936	0.788	H→L (94%) H→L+2 (4%)
2	391.8	3.165	0.000	H→L+1 (97%)
3	383.1	3.236	0.366	H→L+2 (87%) H-3→L (5%) H→L (4%)
4	337.8	3.670	0.435	H-3→L (36%) H-1→L (41%) H→L+6 (12%) H→L+2 (6%)
5	330.4	3.753	0.000	H-2→L (90%) H-1→L+5 (5%)
6	329.1	3.767	0.020	H-3→L (37%) H-1→L (49%) H-2→L+5 (5%) H→L+6 (5%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S11: Wavelength, excitation energy and oscillator strength of investigated compound **PSD1** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	*E* (*eV*)	f_{os}	MO contributions
1	422.2	2.936	0.811	H→L (94%) H→L+2 (3%)
2	391.5	3.167	0.000	H→L+1 (97%)
3	382.5	3.241	0.390	H→L+2 (88%) H-3→L (6%) H→L (3%)
4	345.4	3.589	0.036	H-2→L (89%) H-2→L+5 (2%) H-1→L+5 (3%)
5	345.2	3.591	0.000	H-1→L (91%) H-2→L+5 (3%) H-1→L+5 (2%)
6	336.1	3.688	0.447	H-3→L (71%) H→L+6 (16%) H→L+2 (6%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S12: Wavelength, excitation energy and oscillator strength of investigated compound **PSD2** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	*E* (*eV*)	f_{os}	MO contributions
1	437.9	2.831	0.986	H→L (94%) H→L+2 (2%)
2	408.4	3.036	0.000	H→L+1 (96%)
3	400.6	3.095	0.435	H→L+2 (91%) H→L (2%)
4	348.2	3.561	0.311	H-2→L (81%) H-3→L (2%) H-1→L+3 (2%) H→L+6 (5%)
5	346.2	3.581	0.001	H-1→L (67%) H→L+3 (14%) H-2→L+1 (4%) H-2→L+3 (3%) H-1→L+2 (6%)
6	340.2	3.645	0.001	H-2→L+1 (28%) H-1→L (24%) H-1→L+2 (12%) H→L+3 (29%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S13: Wavelength, excitation energy and oscillator strength of investigated compound **PSD3** at **M06/6-311g(d,p)**.

NO	DFT λ (*nm*)	*E* (*eV*)	f_{os}	MO contributions

1	441.8	2.807	1.043	H→L (95%)
2	411.7	3.012	0.000	H→L+1 (95%)
3	403.5	3.073	0.462	H→L+2 (91%) H-1→L+1 (2%)
4	355.3	3.490	0.001	H-1→L (85%) H-2→L+3 (3%) H-1→L+2 (3%) H→L+3 (5%)
5	351.7	3.525	0.257	H-2→L (82%) H-3→L (3%) H-1→L+1 (3%) H-1→L+3 (2%) H→L+6 (2%)
6	346.1	3.582	0.001	H-2→L+1 (35%) H-1→L+2 (28%) H→L+3 (25%) H-1→L (6%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S14: Wavelength, excitation energy and oscillator strength of investigated compound **PSD4** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	470.6	2.635	0.051	H-2→L (43%) H→L (42%) H-17→L (3%) H-3→L (7%)
2	438.5	2.828	0.634	H-2→L (20%) H→L (28%) H→L+1 (43%) H-3→L (4%)
3	435.0	2.850	0.695	H-2→L (12%) H→L (30%) H→L+1 (51%) H-3→L (2%)
4	399.0	3.107	0.010	H→L+2 (94%)
5	391.4	3.168	0.481	H→L+3 (89%) H-3→L+1 (3%) H→L+1 (2%)
6	352.8	3.515	0.036	H-1→L (86%) H-3→L (3%) H-2→L (5%) H-1→L+1 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S15: Wavelength, excitation energy and oscillator strength of investigated compound **PSD5** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	422.0	2.938	0.762	H-2→L (93%) H-2→L+2 (4%)
2	411.3	3.015	0.000	H→L (90%) H-1→L+3 (6%)
3	411.3	3.015	0.000	H-1→L (90%) H→L+3 (6%)
4	392.8	3.157	0.000	H-2→L+1 (97%)
5	389.3	3.185	0.000	H-1→L+1 (43%) H→L+2 (43%) H-1→L+2 (3%) H→L+1 (5%)
6	389.2	3.185	0.001	H-1→L+2 (43%) H→L+1 (43%) H-1→L+1 (5%) H→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S16: Wavelength, excitation energy and oscillator strength of investigated compound **PSD6** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	474.8	2.612	0.000	H→L (92%) H→L+5 (4%)
2	474.8	2.612	0.000	H-1→L (92%) H-1→L+5 (4%)
3	447.1	2.773	0.001	H→L+1 (45%) H→L+2 (45%) H-1→L+1 (4%)
4	447.0	2.774	0.002	H-1→L+1 (45%) H-1→L+2 (45%) H→L+1 (4%)
5	421.7	2.940	0.823	H-2→L (93%) H-2→L+2 (4%)
6	397.9	3.115	0.009	H→L+3 (55%) H→L+4 (20%) H-1→L+4 (9%) H→L+9 (5%) H→L+10 (6%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S17: Wavelength, excitation energy and oscillator strength of investigated compound **PSD7** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	420.5	2.949	0.816	H→L (93%) H→L+2 (4%)
2	393.4	3.152	0.000	H→L+1 (97%)
3	386.0	3.212	0.384	H→L+2 (88%) H-3→L (5%) H→L (4%)
4	366.3	3.385	0.000	H-1→L (87%) H-2→L+3 (8%) H-1→L+2 (3%)
5	366.3	3.385	0.000	H-2→L (87%) H-2→L+2 (3%) H-1→L+3 (8%)
6	350.7	3.535	0.000	H-2→L+2 (42%) H-1→L+1 (46%) H-2→L (3%) H-2→L+1 (3%) H-1→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

UV solvent tables (In Chloroform)

Table S18: Wavelength, excitation energy and oscillator strength of investigated compound **PSR** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	428.8	2.892	1.064	H→L (97%)
2	387.8	3.198	0.000	H→L+1 (97%)
3	381.6	3.249	0.316	H→L+2 (91%) H-1→L (4%)
4	339.9	3.648	0.634	H-1→L (76%) H-3→L (6%) H→L+2 (6%) H→L+6 (9%)
5	325.6	3.808	0.000	H-1→L+1 (28%) H→L+5 (54%) H-6→L (7%) H-3→L+1 (4%)
6	322.4	3.845	0.000	H-2→L (88%) H-3→L+5 (5%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S19: Wavelength, excitation energy and oscillator strength of investigated compound **PSD1** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	428.5	2.893	1.081	H→L (97%)
2	387.5	3.200	0.000	H→L+1 (97%)
3	381.1	3.254	0.334	H→L+2 (91%) H-3→L (5%)
4	340.5	3.641	0.488	H-3→L (45%) H-1→L (37%) H-2→L (3%) H→L+2 (4%) H→L+6 (6%)
5	337.6	3.672	0.000	H-2→L (83%) H-2→L+5 (5%) H-1→L (9%)
6	336.1	3.689	0.175	H-3→L (36%) H-1→L (46%) H-2→L (5%) H-1→L+5 (3%) H→L+6 (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S20: Wavelength, excitation energy and oscillator strength of investigated compound **PSD2** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	444.3	2.790	1.317	H→L (97%)
2	403.9	3.069	0.000	H→L+1 (95%)
3	398.6	3.110	0.364	H→L+2 (93%) H-1→L+1 (2%)
4	350.9	3.533	0.001	H-1→L (73%) H→L+3 (13%) H-2→L+3 (3%) H-1→L+2 (4%)

5	350.7	3.535	0.401	H-2→L (84%) H-3→L (2%) H-1→L+3 (3%) H→L+6 (3%)
6	339.9	3.648	0.002	H-2→L+1 (31%) H-1→L (16%) H-1→L+2 (16%) H→L+3 (30%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S21: Wavelength, excitation energy and oscillator strength of investigated compound **PSD3** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	448.4	2.765	1.374	H→L (96%)
2	407.7	3.041	0.000	H→L+1 (94%) H-1→L+2 (2%)
3	402.2	3.083	0.381	H→L+2 (92%) H-1→L+1 (3%)
4	362.2	3.423	0.001	H-1→L (84%) H-2→L+3 (3%) H-1→L+2 (3%) H→L+3 (7%)
5	355.3	3.490	0.305	H-2→L (85%) H-3→L (3%) H-1→L+1 (3%) H-1→L+3 (3%)
6	346.9	3.574	0.001	H-2→L+1 (36%) H-1→L+2 (31%) H→L+3 (21%) H-1→L (7%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S22: Wavelength, excitation energy and oscillator strength of investigated compound **PSD4** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	476.8	2.601	0.054	H-2→L (60%) H→L (25%) H-17→L (3%) H-3→L (4%) H-1→L (4%)
2	442.3	2.803	1.554	H→L+1 (89%) H-2→L (3%) H→L (4%)
3	430.8	2.878	0.076	H-2→L (19%) H→L (71%) H→L+1 (6%)
4	393.3	3.152	0.002	H→L+2 (95%)
5	387.8	3.197	0.431	H→L+3 (91%) H-3→L+1 (3%)
6	355.6	3.486	0.057	H-1→L (83%) H-2→L (5%) H-1→L+1 (6%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S23: Wavelength, excitation energy and oscillator strength of investigated compound **PSD5** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	428.3	2.895	1.035	H→L (97%)
2	398.3	3.113	0.000	H-1→L (89%) H-2→L+3 (7%) H-1→L+2 (2%)
3	398.3	3.113	0.000	H-2→L (89%) H-2→L+2 (2%) H-1→L+3 (7%)
4	388.9	3.188	0.000	H→L+1 (97%)
5	383.1	3.236	0.317	H→L+2 (91%) H-3→L (5%)
6	375.9	3.298	0.000	H-2→L+1 (40%) H-1→L+2 (41%) H-2→L+2 (5%) H-2→L+3 (2%) H-1→L+1 (7%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S24: Wavelength, excitation energy and oscillator strength of investigated compound **PSD6** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	461.6	2.686	0.0002	H→L (91%) H→L+3 (3%)
2	461.6	2.686	0.0001	H-1→L (91%) H-1→L+3 (3%)
3	433.5	2.860	0.003	H→L+1 (44%) H→L+2 (45%) H-1→L+1 (4%) H→L+3 (3%)

4	433.4	2.861	0.004	H-1→L+1 (44%) H-1→L+2 (45%) H-1→L+3 (2%) H→L+1 (4%)
5	427.5	2.900	1.092	H-2→L (97%)
6	392.5	3.159	0.016	H-1→L+4 (14%) H→L+3 (23%) H→L+4 (26%) H→L+5 (16%) H-1→L+9 (2%) H→L+1 (2%) H→L+9 (5%) H→L+10 (7%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S25: Wavelength, excitation energy and oscillator strength of investigated compound **PSD7** at **M06/6-311g(d,p)**.

NO	DFT λ (nm)	E (eV)	f_{os}	MO contributions
1	426.4	2.907	1.103	H→L (97%)
2	389.3	3.185	0.000	H→L+1 (97%)
3	384.4	3.225	0.315	H→L+2 (92%) H-3→L (4%)
4	359.4	3.449	0.000	H-1→L (87%) H-2→L+3 (8%) H-1→L+2 (3%)
5	359.4	3.449	0.000	H-2→L (87%) H-2→L+2 (3%) H-1→L+3 (8%)
6	342.	3.620	0.000	H-2→L+1 (32%) H-2→L+2 (15%) H-1→L+1 (17%) H-1→L+2 (30%) H-1→L (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (nm)

Table S26: Natural bond orbital (NBO) analysis of **PSR** by using **M06/6-311 G(d,p).**

Donor(i)	Type	Acceptor(j)	Type	$E^{(2)}$ [$kcal/mol$]	$E(j)$-$E(i)$ [$a.u$]	$F(i,j)$ [$a.u$]
C11 - C24	π	C22-C25	π^*	27.45	0.29	0.08
C27 - C28	π	C30-C32	π^*	27.45	0.29	0.08
C22 - C25	π	C20-C21	π^*	26.52	0.3	0.079
C30 - C32	π	C9-C29	π^*	26.52	0.3	0.079
C15 - C17	π	C12-C14	π^*	24.77	0.29	0.076
C36 - C39	π	C34-C35	π^*	24.77	0.29	0.076
C51 - C57	π	C47-C53	π^*	23.77	0.3	0.076
C48 - C54	π	C45-C50	π^*	23.72	0.3	0.076
C10 - C38	π	C36-C39	π^*	22.64	0.31	0.075
C13 - C102	π	C15-C17	π^*	22.64	0.31	0.075
C22 - C25	π	C11-C24	π^*	20.63	0.3	0.07
C62 - C65	π	C64-C68	π^*	19.37	0.29	0.068
C11 - C24	π	C1-C2	π^*	18.99	0.29	0.066
C5 - C8	π	C27-C28	π^*	13.63	0.31	0.061
C62 - C65	π	C62-C65	π^*	0.72	0.29	0.013
C5 - C8	σ	C4-N101	σ^*	10.32	1.15	0.097
C44 - C48	σ	C42-N100	σ^*	6.4	1.15	0.077
C3 - C4	σ	C10-N98	σ^*	6.17	1.09	0.073
C3 - C4	σ	N101-C102	σ^*	6.17	1.09	0.073
C10 - C38	σ	C10-C34	σ^*	5.98	1.28	0.078
C63 - C67	σ	C22-N99	σ^*	5.05	1.08	0.066

C90 - H93	σ	C30-C32	σ^*	4.99	1.08	0.066
C68 - H75	σ	C70-C74	σ^*	4.02	1.11	0.06
C13 - H16	σ	C15-C17	σ^*	3.99	1.12	0.06
C43 - C46	σ	C43-N100	σ^*	3.02	1.17	0.053
C8 - C27	σ	C9-C29	σ^*	2.83	1.27	0.054
C12 - C102	σ	C20-C21	σ^*	2.72	1.28	0.053
C63 - C67	σ	C73-H79	σ^*	2.63	1.09	0.048
C2 - H6	σ	C3-C4	σ^*	1.99	1.09	0.042
C30 - C32	σ	C43-N100	σ^*	1.06	1.15	0.031
C2 - C3	σ	C1-N101	σ^*	0.99	1.11	0.03
N100	LP(1)	C43-C46	π^*	40.78	0.31	0.102
N99	LP(1)	C63-C66	π^*	40.65	0.31	0.102
N100	LP(1)	C42-C44	π^*	40.65	0.31	0.102
N98	LP(1)	C5-C8	π^*	38.38	0.31	0.098
N101	LP(1)	C1-C2	π^*	38.38	0.31	0.098
N98	LP(1)	C10-C38	π^*	37.95	0.31	0.096
N101	LP(1)	C13-C102	π^*	37.95	0.31	0.096
N98	LP(1)	C3-C4	π^*	36.14	0.31	0.096
N101	LP(1)	C3-C4	π^*	36.14	0.31	0.096
N99	LP(1)	C62-C65	π^*	36.03	0.31	0.097
N100	LP(1)	C30-C32	σ^*	6.51	0.85	0.072
N99	LP(1)	C22-C25	σ^*	6.51	0.85	0.072
N100	LP(1)	C29-C32	σ^*	5.44	0.87	0.067
N99	LP(1)	C21-C22	σ^*	5.44	0.87	0.067

Table S27: Natural bond orbital (NBO) analysis of **PSD1** by using **M06/6-311 G(d,p).**

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*$^{(2)}$ [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C9 - C27	π	C29-C32	π^*	22.88	0.29	0.074
C11 - C20	π	C21-C22	π^*	22.84	0.29	0.074
C38 - C39	π	C10-C34	π^*	21.73	0.3	0.074
C44 - C48	π	C42-C45	π^*	21.43	0.3	0.075
C68 - C72	π	C60-C63	π^*	20.05	0.29	0.071
C71 - C75	π	C61-C65	π^*	20.05	0.29	0.071
C42 - C45	π	C44-C48	π^*	19.86	0.29	0.069
C9 - C27	π	C28-C30	π^*	17.75	0.3	0.067
C21 - C22	π	C11-C20	π^*	17.35	0.31	0.068
C11 - C20	π	C12-C98	π^*	15.75	0.29	0.061
C9 - C27	π	C10-C34	π^*	15.74	0.29	0.061
C12 - C98	π	C11-C20	π^*	14.62	0.3	0.06
C61 - C65	π	C61-C65	π^*	0.6	0.29	0.012

C42 - C45	π	C42-C45	π^*	0.59	0.29	0.012
C5 - C8	σ	C4-N97	σ^*	10.32	1.15	0.097
C44 - C48	σ	C42-N96	σ^*	6.35	1.15	0.077
C3 - C4	σ	C10-N94	σ^*	6.17	1.09	0.073
C10 - C38	σ	C10-C34	σ^*	5.98	1.28	0.078
C29 - H33	σ	C30-C32	σ^*	5.27	1.1	0.068
C63 - C65	σ	C65-C71	σ^*	5.18	1.25	0.072
C45 - C47	σ	C47-C53	σ^*	5.17	1.25	0.072
C45 - C50	σ	C42-C45	σ^*	5.15	1.26	0.072
C86 - H89	σ	C30-C32	σ^*	4.99	1.08	0.066
C90 - H93	σ	C22-C25	σ^*	4.99	1.08	0.066
C71 - H77	σ	C61-C65	σ^*	4.76	1.08	0.064
C29 - C32	σ	C9-C29	σ^*	4.69	1.3	0.07
C20 - C 21	σ	C21-C22	σ^*	4.55	1.31	0.069
C44 - C48	σ	C42-C44	σ^*	4.39	1.3	0.067
C38 - H40	σ	C36-C39	σ^*	3.99	1.12	0.06
C10 - C38	σ	C38-C39	σ^*	3.96	1.32	0.065
C36 - C39	σ	C35-H37	σ^*	2.87	1.12	0.051
C42 - N96	σ	C32-N96	σ^*	2.87	1.2	0.053
C43 - N96	σ	C43-C47	σ^*	1.67	1.35	0.042
C46 - H52	σ	C43-C46	σ^*	0.88	1.11	0.028
C61 - N95	σ	C21-C22	σ^*	0.54	1.39	0.025
N94	LP(1)	C5-C8	π^*	38.37	0.31	0.098
N94	LP(1)	C10-C34	π^*	37.35	0.31	0.096
N94	LP(1)	C3-C4	π^*	36.15	0.31	0.096
N95	LP(1)	C60-C63	π^*	35.34	0.31	0.097
N95	LP(1)	C61-C65	π^*	35.3	0.31	0.097
N96	LP(1)	C43-C47	π^*	35.39	0.31	0.097
N96	LP(1)	C42-C45	π^*	35.32	0.31	0.097
N97	LP(1)	C1-C2	π^*	38.36	0.31	0.098
N97	LP(1)	C12-C98	π^*	37.35	0.31	0.096
N97	LP(1)	C3-C4	π^*	36.14	0.31	0.096
N95	LP(1)	C22-C25	σ^*	6.7	0.85	0.073
N96	LP(1)	C30-C32	σ^*	6.62	0.85	0.072
N95	LP(1)	C21-C22	σ^*	5.51	0.87	0.067
N96	LP(1)	C29-C32	σ^*	5.48	0.87	0.067

Table S28: Natural bond orbital (NBO) analysis of **PSD2** by using **M06/6-311 G(d,p).**

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	$E^{(2)}$ **[*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C63 - C66	π	C71-C77	π^*	24.02	0.3	0.076

C68 - C74	π	C65-C70	π^*	24.02	0.3	0.075
C42 - C44	π	C48-C54	π^*	23.92	0.3	0.076
C62 - C64	π	C68-C74	π^*	23.92	0.3	0.076
C11 - C20	π	C21-C22	π^*	22.39	0.29	0.073
C14 - C17	π	C13-C15	π^*	21.97	0.3	0.072
C38 - C39	π	C35-C36	π^*	20.05	0.31	0.071
C43 - C46	π	C47-C53	π^*	19.85	0.3	0.07
C21 - C22	π	C11-C20	π^*	18.76	0.31	0.071
C11 - C20	π	C24-C25	π^*	18.44	0.3	0.069
C10 - C34	π	C9-C29	π^*	17.2	0.3	0.065
C11 - C20	π	C12-C102	π^*	15.66	0.29	0.06
C12 - C102	π	C11-C20	π^*	14.55	0.3	0.06
C62 - C64	π	C21-C22	π^*	0.78	0.3	0.014
C5 - C8	σ	C4-N101	σ^*	10.32	1.15	0.097
C1 - C2	σ	C3-N98	σ^*	10.31	1.15	0.097
C2 - C3	σ	C1-C11	σ^*	6.2	1.23	0.078
C3 - C4	σ	N101-C102	σ^*	6.17	1.09	0.073
C10 - C38	σ	C10-C34	σ^*	5.96	1.28	0.078
C22 - C25	σ	C21-C22	σ^*	5.07	1.3	0.073
C20 - C21	σ	C11-C20	σ^*	4.98	1.27	0.071
C9 - C29	σ	C9-C27	σ^*	4.98	1.27	0.071
C24 - C25	σ	C22-N99	σ^*	4.65	1.13	0.065
C38 - H40	σ	C36-C39	σ^*	3.99	1.12	0.06
C42 - C45	σ	C45-C50	σ^*	3.99	1.31	0.065
C3 - N98	σ	C2-C3	σ^*	3.54	1.36	0.062
C73 - C77	σ	C67-C73	σ^*	3.5	1.3	0.06
C44 - C48	σ	C48-C54	σ^*	3.49	1.3	0.06
C17 - C82	σ	C15-C17	σ^*	2.59	1.23	0.051
C22 - C25	σ	C24-H26	σ^*	2.59	1.11	0.048
C32 - N100	σ	C9-C29	σ^*	1.91	1.35	0.045
C42 - N100	σ	C43-C46	σ^*	1.89	1.36	0.045
C4 - C5	σ	C3-N98	σ^*	0.61	1.13	0.023
C22 - N99	σ	C63-C66	π^*	0.59	0.8	0.021
C32	LP(1)	C9-C29	π^*	75.45	0.16	0.115
C32	LP(1)	C28-C30	π^*	61.37	0.17	0.111
N98	LP(1)	C5-C8	π^*	38.49	0.31	0.098
N101	LP(1)	C1-C2	π^*	38.49	0.31	0.098
N98	LP(1)	C10-C34	π^*	37.48	0.31	0.096
N101	LP(1)	C12-C102	π^*	37.48	0.31	0.096
N98	LP(1)	C3-C4	π^*	35.93	0.31	0.096
N101	LP(1)	C3-C4	π^*	35.93	0.31	0.096

N99	LP(1)	C62-C64	π^*	24.95	0.3	0.079
N100	LP(1)	C42-C44	π^*	24.95	0.3	0.079
N99	LP(1)	C63-C66	π^*	23.68	0.3	0.077
N100	LP(1)	C43-C46	π^*	23.68	0.3	0.077
N99	LP(1)	C21-C22	π^*	7.42	0.3	0.043
N99	LP(1)	C22-C25	σ^*	5.28	0.84	0.063
N99	LP(1)	C21-C22	σ^*	5.19	0.87	0.064
N100	LP(1)	C30-C32	σ^*	5.17	0.84	0.062
N100	LP(1)	C29-C32	σ^*	5.16	0.87	0.063
C32	LP(1)	C42-N100	σ^*	3.82	0.56	0.056
C32	LP(1)	C43-N100	σ^*	3.69	0.55	0.055
N99	LP(1)	C63-C67	σ^*	2.68	0.85	0.045
N100	LP(1)	C43-C47	σ^*	2.68	0.85	0.045
N99	LP(1)	C62-C65	σ^*	2.45	0.84	0.043
N100	LP(1)	C42-C45	σ^*	2.45	0.84	0.043
N99	LP(1)	C63-C66	σ^*	2.36	0.85	0.042
N100	LP(1)	C43-C46	σ^*	2.36	0.85	0.042
N99	LP(1)	C62-C64	σ^*	2.29	0.85	0.042

Table S29: Natural bond orbital (NBO) analysis of **PSD3** by using **M06/6-311 G(d,p).**

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*$^{(2)}$ [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C51 - C57	π	C47-C53	π^*	23.16	0.29	0.074
C71 - C75	π	C64-C69	π^*	23.12	0.29	0.074
C51 - C57	π	C43-C46	π^*	22.89	0.29	0.073
C71 - C75	π	C61-C65	π^*	22.85	0.29	0.073
C35 - C36	π	C38-C39	π^*	21.98	0.3	0.072
C42 - C44	π	C48-C54	π^*	21.96	0.31	0.074
C64 - C69	π	C71-C75	π^*	20.88	0.31	0.072
C47 - C53	π	C51-C57	π^*	20.77	0.31	0.072
C12 - C98	π	C13-C15	π^*	19.85	0.3	0.07
C10 - C34	π	C35-C36	π^*	19.82	0.31	0.072
C29 - C32	π	C9-C27	π^*	18.99	0.31	0.071
C9 - C27	π	C28-C30	π^*	18.49	0.3	0.069
C12 - C98	π	C20-C21	π^*	17.18	0.3	0.065
C9 - C27	π	C10-C34	π^*	15.66	0.29	0.06
C10 - C34	π	C9-C27	π^*	14.52	0.31	0.06
C42 - C44	π	C29-C32	π^*	0.77	0.3	0.014
C5 - C8	σ	C4-N97	σ^*	10.31	1.15	0.097
C2 - C3	σ	C1-C11	σ^*	6.2	1.23	0.078
C5 - C8	σ	C8-C27	σ^*	5.91	1.25	0.077

C1 - N97	σ	C4-C5	σ^*	5.79	1.33	0.078
C60 - C62	σ	C60-C63	σ^*	4.89	1.29	0.071
C90 - H93	σ	C22-C25	σ^*	4.88	1.08	0.065
C3 - C4	σ	C2-H6	σ^*	4.47	1.08	0.063
C3 - C4	σ	C5-H7	σ^*	4.47	1.08	0.063
C64 - H70	σ	C69-C75	σ^*	4.03	1.11	0.06
C71 - C75	σ	C65-C71	σ^*	3.99	1.3	0.064
C51 - C57	σ	C46-C51	σ^*	3.98	1.3	0.064
C9 - C34	σ	C10-C38	σ^*	2.8	1.24	0.053
C50 - C54	σ	C48-H55	σ^*	2.79	1.12	0.05
C42 - N96	σ	C43-C46	σ^*	1.9	1.36	0.045
C22 -N95	σ	C22-C25	σ^*	1.89	1.35	0.045
C69 - H76	σ	C69-C75	σ^*	0.94	1.11	0.029
C53 - H59	σ	C53-C57	σ^*	0.93	1.11	0.029
C22	LP(1)	C20-C21	π^*	75.52	0.16	0.115
C22	LP(1)	C24-C25	π^*	61.36	0.17	0.111
N94	LP(1)	C5-C8	π^*	38.51	0.31	0.098
N97	LP(1)	C1-C2	π^*	38.51	0.31	0.098
N94	LP(1)	C10-C34	π^*	37.51	0.31	0.096
N97	LP(1)	C12-C98	π^*	37.51	0.31	0.096
N94	LP(1)	C3-C4	π^*	35.89	0.31	0.096
N97	LP(1)	C3-C4	π^*	35.89	0.31	0.096
N95	LP(1)	C60-C62	π^*	24.1	0.3	0.078
N96	LP(1)	C42-C44	π^*	24.1	0.3	0.078
N95	LP(1)	C61-C65	π^*	22.55	0.3	0.076
N96	LP(1)	C43-C46	π^*	22.24	0.3	0.075
N96	LP(1)	C29-C32	π^*	8.29	0.3	0.045
N96	LP(1)	C29-C32	σ^*	5.2	0.86	0.064
N95	LP(1)	C21-C22	σ^*	5.17	0.86	0.063
N96	LP(1)	C30-C32	σ^*	5.15	0.84	0.062
N95	LP(1)	C22-C25	σ^*	5.03	0.84	0.061
C22	LP(1)	C60-N95	σ^*	3.8	0.56	0.056
C22	LP(1)	C61-N95	σ^*	3.53	0.55	0.053
N96	LP(1)	C43-C47	σ^*	2.9	0.85	0.047
N95	LP(1)	C61-C65	σ^*	2.78	0.85	0.046
N95	LP(1)	C61-C64	σ^*	2.58	0.85	0.044
N95	LP(1)	C60-C63	σ^*	2.51	0.84	0.044
N96	LP(1)	C42-C45	σ^*	2.51	0.84	0.044
N96	LP(1)	C43-C46	σ^*	2.49	0.85	0.044
N95	LP(1)	C60-C62	σ^*	2.43	0.85	0.043
N96	LP(1)	C42-C44	σ^*	2.43	0.85	0.043

Table S30: Natural bond orbital (NBO) analysis of **PSD4** by using **M06/6-311 G(d,p).**

Donor(*i*)	Type	Acceptor(*j*)	Type	$E^{(2)}$ [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i*,*j*) [*a.u*]
C22 - C25	π	C20-C21	π^*	25.03	0.29	0.076
C36 - C39	π	C34-C35	π^*	24.48	0.29	0.076
C95 - C97	π	C94-C96	π^*	23.03	0.29	0.075
C61 - C63	π	C62-C64	π^*	22.83	0.3	0.074
C11 - C24	π	C20-C21	π^*	21.09	0.29	0.07
C106 - C108	π	C110-C112	π^*	20.04	0.3	0.07
C105 - C107	π	C106-C108	π^*	19.99	0.3	0.07
C9 - C27	π	C34-C35	π^*	18.03	0.29	0.065
C20 - C21	π	C12-C60	π^*	17.7	0.29	0.065
C34 - C35	π	C9-C27	π^*	16.8	0.3	0.064
C5 - C8	π	C9-C27	π^*	14.88	0.31	0.065
C1 - C2	π	C11-C24	π^*	13.27	0.31	0.061
C29 - C32	π	C71-C73	π^*	6.2	0.3	0.039
C61 - C63	π	C22-C25	π^*	6.04	0.3	0.039
C22 - C25	π	C61-C63	π^*	5.93	0.29	0.037
C116 - C118	π	C76-C78	π^*	0.57	0.31	0.012
C5 - C8	σ	C4-N59	σ^*	10.32	1.15	0.097
C2 - C3	σ	C1-C11	σ^*	6.2	1.23	0.078
C3 - C4	σ	N59-C60	σ^*	6.17	1.09	0.073
C10 - C38	σ	C10-C34	σ^*	5.96	1.28	0.078
C28 - H31	σ	C30-C32	σ^*	5.02	1.09	0.066
C11 - C20	σ	C11-C24	σ^*	4.94	1.27	0.071
C38 - H40	σ	C36-C39	σ^*	3.99	1.12	0.06
C64 - C68	σ	N81-C83	σ^*	3.02	1.13	0.052
C105 - C107	σ	C78-N82	σ^*	2.98	1.13	0.052
C30 - C 50	σ	C28-C30	σ^*	2.93	1.26	0.054
N59 - C60	σ	C13-C60	σ^*	2.01	1.39	0.047
C3 - N58	σ	C10-C34	σ^*	1.99	1.37	0.047
C36 - C46	σ	C46-H49	σ^*	0.63	1.03	0.023
C117 - H120	σ	C117-C119	σ^*	0.55	1.08	0.022
N59	LP(1)	C1-C2	π^*	38.53	0.31	0.098
N58	LP(1)	C5-C8	π^*	38.5	0.31	0.098
N58	LP(1)	C10-C38	π^*	38.12	0.3	0.096
N59	LP(1)	C12-C60	π^*	37.36	0.31	0.096
N59	LP(1)	C3-C4	π^*	35.97	0.31	0.096
N58	LP(1)	C3-C4	π^*	35.94	0.31	0.096

N81	LP(1)	C66-C68	π^*	23.27	0.3	0.076
N82	LP(1)	C105-C107	π^*	21.71	0.3	0.074
N81	LP(1)	C83-C84	π^*	19.04	0.3	0.069
N82	LP(1)	C76-C78	π^*	18.68	0.3	0.069
N82	LP(1)	C116-C118	π^*	18.54	0.28	0.066
N81	LP(1)	C94-C96	π^*	18.29	0.3	0.068
N82	LP(1)	C116-C118	σ^*	3.81	0.8	0.053
N82	LP(1)	C116-C117	σ^*	3.64	0.82	0.052
N81	LP(1)	C94-C95	σ^*	3.38	0.85	0.051
N82	LP(1)	C76-C78	σ^*	3.36	0.85	0.051
N81	LP(1)	C83-C85	σ^*	3.35	0.85	0.051
N81	LP(1)	C94-C96	σ^*	3.35	0.85	0.051
N82	LP(1)	C74-C78	σ^*	3.24	0.85	0.05
N81	LP(1)	C83-C84	σ^*	3.12	0.85	0.049
N82	LP(1)	C105-C107	σ^*	2.78	0.85	0.046
N81	LP(1)	C64-C68	σ^*	2.76	0.84	0.046
N82	LP(1)	C105-C106	σ^*	2.7	0.85	0.045
N81	LP(1)	C66-C68	σ^*	2.55	0.84	0.044

Table S31: Natural bond orbital (NBO) analysis of **PSD5** by using **M06/6-311 G(d,p).**

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*$^{(2)}$ [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C11 - C20	π	C21-C22	π^*	22.92	0.29	0.074
C9 - C27	π	C29-C32	π^*	22.92	0.29	0.074
C14 - C17	π	C13-C15	π^*	21.95	0.3	0.072
C35 - C36	π	C38-C39	π^*	21.95	0.3	0.072
C42 - C44	π	C45-C50	π^*	20.85	0.3	0.072
C43 - C46	π	C47-C53	π^*	20.85	0.3	0.072
C3 - C4	π	C1-C2	π^*	19.89	0.29	0.069
C3 - C4	π	C5-C8	π^*	19.89	0.29	0.069
C11 - C20	π	C24-C25	π^*	17.74	0.31	0.067
C9 - C27	π	C28-C30	π^*	17.74	0.31	0.067
C11 - C20	π	C12-C102	π^*	15.69	0.29	0.061
C9 - C27	π	C10-C34	π^*	15.69	0.29	0.061
C5 - C8	π	C9-C27	π^*	15.28	0.31	0.065
C10 - C34	π	C9-C27	π^*	14.66	0.3	0.06
C12 - C102	π	C11-C20	π^*	14.66	0.3	0.06
C5 - C8	σ	C4-N101	σ^*	10.32	1.15	0.097
C2 - C3	σ	C1-C11	σ^*	6.21	1.23	0.078
C13 - C102	σ	C12-C102	σ^*	5.98	1.28	0.078
C1 - C2	σ	C1-C11	σ^*	5.9	1.25	0.077

C28 - C30	σ	C30-C32	σ^*	4.88	1.29	0.071
C24 - H26	σ	C11-C20	σ^*	4.87	1.09	0.065
C77 - H81	σ	C67-C73	σ^*	3.98	1.11	0.059
C10 - C38	σ	C38-C39	σ^*	3.97	1.32	0.065
C8 - C27	σ	C9-C29	σ^*	2.83	1.27	0.054
C30 - C32	σ	C30-C90	σ^*	2.71	1.15	0.05
C4 - N101	σ	C12-C102	σ^*	1.98	1.38	0.047
C66 - H72	σ	C66-C71	σ^*	1.01	1.11	0.03
C14 - H18	σ	C12-C14	σ^*	0.99	1.1	0.029
C10 - N98	σ	C3-C4	σ^*	0.78	1.37	0.029
C63 - N99	σ	C22-C25	σ^*	0.56	1.37	0.025
N98	LP(1)	C5-C8	π^*	38.37	0.31	0.098
N101	LP(1)	C1-C2	π^*	38.37	0.31	0.098
N98	LP(1)	C10-C34	π^*	37.38	0.31	0.096
N101	LP(1)	C12-C102	π^*	37.38	0.31	0.096
N99	LP(1)	C62-C64	π^*	36.63	0.3	0.097
N99	LP(1)	C63-C66	π^*	36.63	0.3	0.097
N100	LP(1)	C42-C44	π^*	36.63	0.3	0.097
N100	LP(1)	C43-C46	π^*	36.63	0.3	0.097
N98	LP(1)	C3-C4	π^*	36.14	0.31	0.096
N101	LP(1)	C3-C4	π^*	36.14	0.31	0.096
O103	LP(2)	C65-C70	π^*	24.13	0.38	0.09
O103	LP(2)	C67-C73	π^*	24.13	0.38	0.09
O104	LP(2)	C45-C50	π^*	24.13	0.38	0.09
O104	LP(2)	C47-C53	π^*	24.13	0.38	0.09
N99	LP(1)	C22-C25	σ^*	6.93	0.85	0.073
N100	LP(1)	C30-C32	σ^*	6.93	0.85	0.073
O103	LP(1)	C62-C65	σ^*	6.62	1.12	0.077
O103	LP(1)	C63-C67	σ^*	6.62	1.12	0.077
O104	LP(1)	C42-C45	σ^*	6.62	1.12	0.077
O104	LP(1)	C43-C47	σ^*	6.62	1.12	0.077
N99	LP(1)	C21-C22	σ^*	5.64	0.88	0.067
N100	LP(1)	C29-C32	σ^*	5.64	0.88	0.067
O103	LP(1)	C65-C70	σ^*	0.69	1.15	0.025
O103	LP(1)	C67-C73	σ^*	0.69	1.15	0.025
O104	LP(1)	C45-C50	σ^*	0.69	1.15	0.025
O104	LP(1)	C47-C53	σ^*	0.69	1.15	0.025

Table S32: Natural bond orbital (NBO) analysis of **PSD6** by using **M06/6-311 G(d,p).**

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*$^{(2)}$ [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**

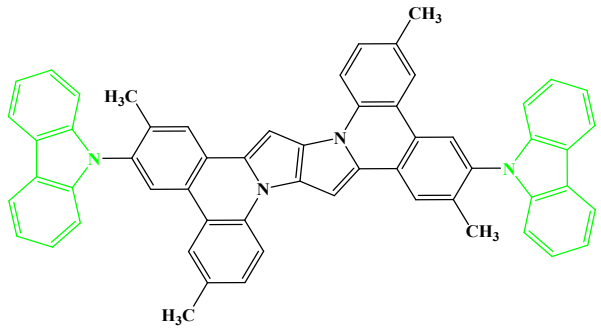
C120 - C122	π	C115-C117	π^*	25.39	0.29	0.077
C106 - C108	π	C110-C112	π^*	23.58	0.31	0.076
C9 - C27	π	C29-C32	π^*	22.67	0.29	0.074
C28 - C30	π	C9-C27	π^*	22.24	0.3	0.075
C14 - C17	π	C13-C15	π^*	21.95	0.3	0.072
C110 - C112	π	C106-C108	π^*	20.94	0.29	0.071
C45 - C50	π	C48-C54	π^*	20.68	0.31	0.073
C67 - C73	π	C63-C66	π^*	19.95	0.3	0.071
C45 - C50	π	C42-C44	π^*	19.94	0.3	0.071
C11 - C20	π	C24-C25	π^*	17.78	0.31	0.068
C29 - C32	π	C9-C27	π^*	17.62	0.31	0.069
C11 - C20	π	C12-C102	π^*	15.71	0.29	0.061
C5 - C8	π	C9-C27	π^*	15.18	0.31	0.065
C10 - C34	π	C9-C27	π^*	14.62	0.3	0.06
C12 - C102	π	C11-C20	π^*	14.62	0.3	0.06
C5 - C8	σ	C4-N101	σ^*	10.31	1.15	0.097
C2 - C3	σ	C1-C11	σ^*	6.21	1.23	0.078
C3 - C4	σ	N101-C102	σ^*	6.17	1.09	0.073
C63 - C66	σ	C63-C67	σ^*	6.01	1.27	0.078
C13 - C102	σ	C12-C102	σ^*	5.98	1.28	0.078
C30 - C32	σ	C29-C32	σ^*	5.16	1.31	0.074
C21 - C22	σ	C20-C21	σ^*	4.99	1.3	0.072
C115 - C116	σ	C116-C118	σ^*	4.01	1.31	0.065
C13 - H16	σ	C15-C17	σ^*	3.99	1.12	0.06
C30 - C90	σ	C27-C28	σ^*	3.01	1.22	0.054
C12 - C20	σ	C11-C24	σ^*	2.98	1.24	0.054
C9 - C34	σ	C29-C32	σ^*	2.01	1.27	0.045
C2 - H6	σ	C3-C4	σ^*	1.99	1.09	0.042
C53 - H59	σ	C47-N103	σ^*	0.99	0.94	0.027
C125 - H129	σ	C108-C112	σ^*	0.53	1.09	0.021
N98	LP(1)	C5-C8	π^*	38.38	0.31	0.098
N101	LP(1)	C1-C2	π^*	38.38	0.31	0.098
N103	LP(1)	C45-C50	π^*	37.55	0.3	0.098
N103	LP(1)	C47-C53	π^*	37.55	0.3	0.098
N104	LP(1)	C65-C70	π^*	37.55	0.3	0.098
N104	LP(1)	C67-C73	π^*	37.54	0.3	0.098
N98	LP(1)	C10-C34	π^*	37.36	0.31	0.096
N101	LP(1)	C12-C102	π^*	37.36	0.31	0.096
N99	LP(1)	C63-C66	π^*	37.06	0.3	0.098
N100	LP(1)	C43-C46	π^*	37.06	0.3	0.098
N99	LP(1)	C62-C64	π^*	37.01	0.3	0.097

N100	LP(1)	C42-C44	π^*	37.01	0.3	0.097
N101	LP(1)	C3-C4	π^*	36.1	0.31	0.096
N98	LP(1)	C3-C4	π^*	36.09	0.31	0.096
N99	LP(1)	C22-C25	σ^*	6.7	0.85	0.072
N100	LP(1)	C30-C32	σ^*	6.7	0.85	0.072
N104	LP(1)	C115-C116	σ^*	6.52	0.85	0.071
N103	LP(1)	C105-C106	σ^*	6.51	0.86	0.071
N103	LP(1)	C105-C107	σ^*	6.37	0.86	0.07
N104	LP(1)	C115-C117	σ^*	6.36	0.86	0.07
N99	LP(1)	C21-C22	σ^*	6.01	0.87	0.069
N100	LP(1)	C29-C32	σ^*	6.01	0.87	0.069

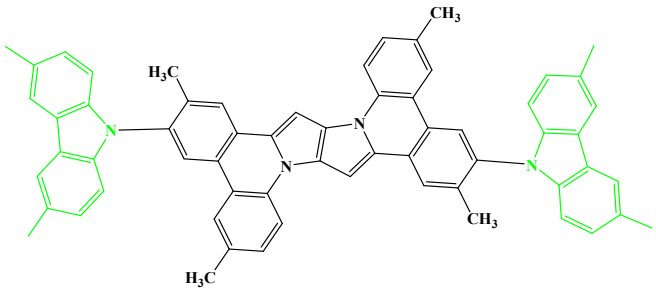
Table S33: Natural bond orbital (NBO) analysis of **PSD7** by using **M06/6-311 G(d,p).**

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*$^{(2)}$ [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C62 - C64	π	C68-C74	π^*	24.35	0.3	0.077
C48 - C54	π	C45-C50	π^*	23.65	0.3	0.076
C11 - C20	π	C21-C22	π^*	22.97	0.29	0.074
C28 - C30	π	C9-C27	π^*	22.59	0.3	0.076
C14 - C17	π	C13-C15	π^*	21.96	0.3	0.072
C24 - C25	π	C21-C22	π^*	20.98	0.29	0.07
C38 - C39	π	C35-C36	π^*	20.05	0.31	0.071
C42 - C44	π	C45-C50	π^*	19.93	0.31	0.07
C12 - C102	π	C13-C15	π^*	19.71	0.3	0.07
C11 - C20	π	C24-C25	π^*	17.96	0.31	0.068
C9 - C27	π	C28-C30	π^*	17.96	0.31	0.068
C11 - C20	π	C12-C102	π^*	15.71	0.29	0.061
C5 - C8	π	C9-C27	π^*	15.15	0.31	0.065
C10 - C34	π	C9-C27	π^*	14.6	0.3	0.06
C12 - C102	π	C11-C20	π^*	14.6	0.3	0.06
C5 - C8	σ	C4-N101	σ^*	10.32	1.15	0.097
C42 - C44	σ	C42-C45	σ^*	6.43	1.28	0.081
C10 - C38	σ	C10-C34	σ^*	5.98	1.28	0.078
C24 - C25	σ	C22-C25	σ^*	4.99	1.3	0.072
C73 - C77	σ	C67-C103	σ^*	4.02	1.14	0.061
C13 - H16	σ	C15-C17	σ^*	3.99	1.12	0.06
C36 - C39	σ	C38-C39	σ^*	3.8	1.3	0.063
C10 - C34	σ	C9-C34	σ^*	3.77	1.22	0.061
N101 - C102	σ	C4-N101	σ^*	3.04	1.26	0.056
C1 - N101	σ	C4-N101	σ^*	2.98	1.23	0.054
C3 - N98	σ	C3-C4	σ^*	2.02	1.36	0.047

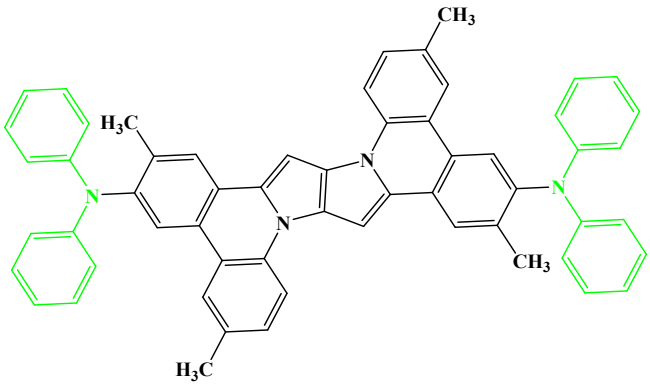
C5 - H7	σ	C3-C4	σ^*	1.99	1.09	0.042
C66 - H72	σ	C66-C71	σ^*	1.07	1.12	0.031
C28 - H31	σ	C27-C28	σ^*	0.93	1.09	0.028
C15 - H19	σ	C13-C15	σ^*	0.92	1.12	0.029
N98	LP(1)	C5-C8	π^*	38.4	0.31	0.098
N101	LP(1)	C1-C2	π^*	38.4	0.31	0.098
N98	LP(1)	C10-C34	π^*	37.34	0.31	0.096
N101	LP(1)	C12-C102	π^*	37.34	0.31	0.096
N98	LP(1)	C3-C4	π^*	36.09	0.31	0.096
N101	LP(1)	C3-C4	π^*	36.09	0.31	0.096
N99	LP(1)	C63-C66	π^*	35.01	0.31	0.095
N100	LP(1)	C43-C46	π^*	35.01	0.31	0.095
N99	LP(1)	C62-C64	π^*	34.98	0.31	0.095
N100	LP(1)	C42-C44	π^*	34.98	0.31	0.095
N99	LP(1)	C21-C22	σ^*	6.63	0.87	0.073
N100	LP(1)	C29-C32	σ^*	6.63	0.87	0.073
N99	LP(1)	C22-C25	σ^*	5.5	0.86	0.065
N100	LP(1)	C30-C32	σ^*	5.5	0.86	0.065



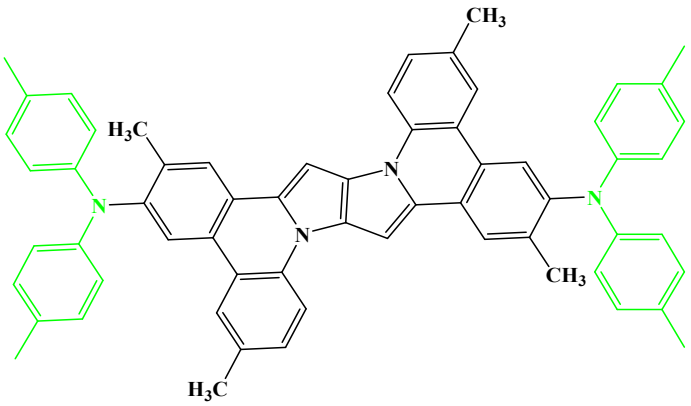
PSR



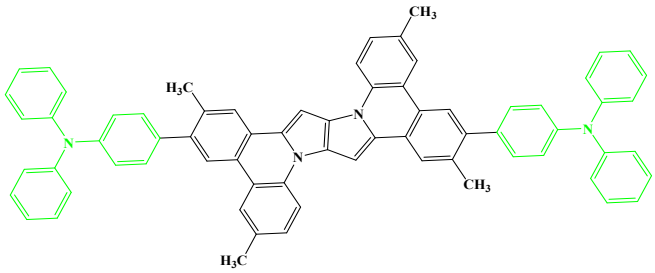
PSD1



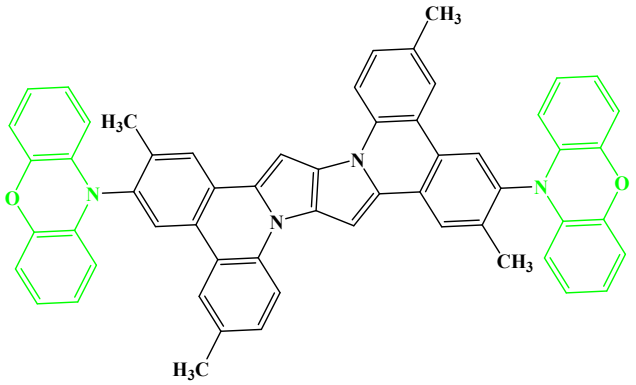
PSD2



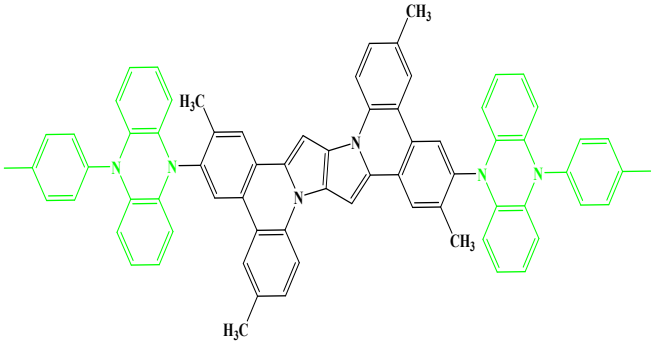
PSD3



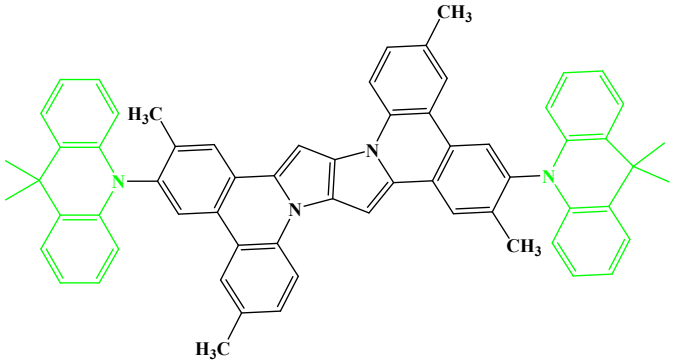
PSD4



PSD5

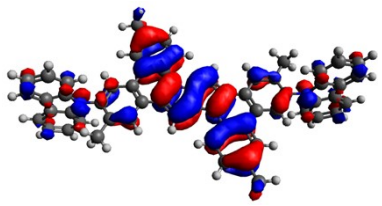


PSD6

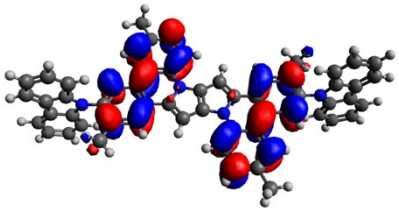


PSD7

Figure S1: Chemdraw structures of designed compounds **PSR** and **PSD1-PSD7**.



HOMO-1



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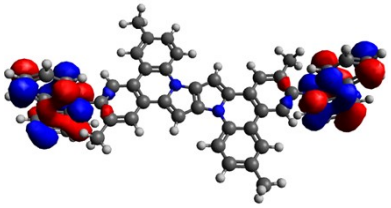

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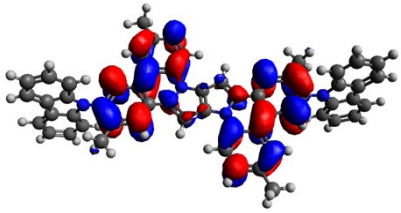
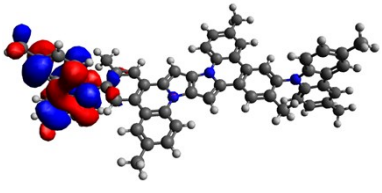


LUMO+2

PSR



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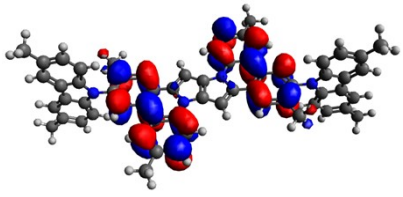
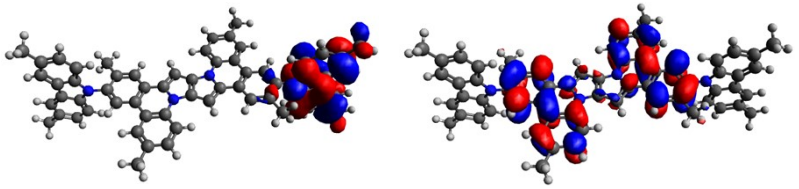
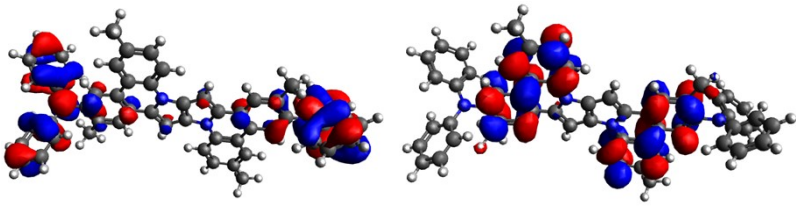


LUMO+1

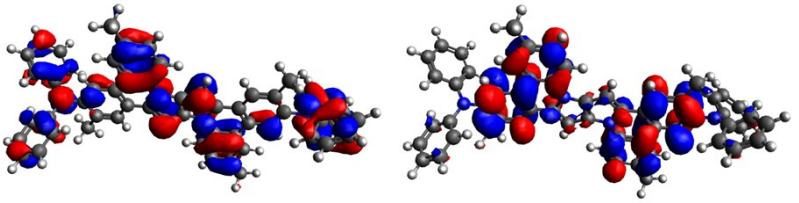


HOMO-2 LUMO+2

PSD1

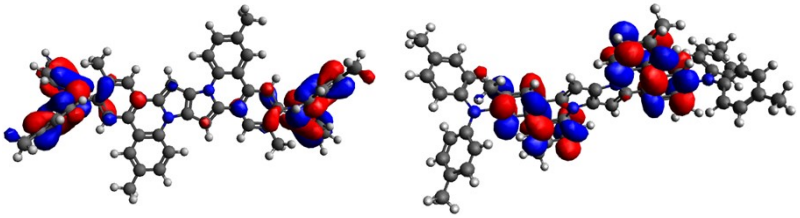


HOMO-1 LUMO+1

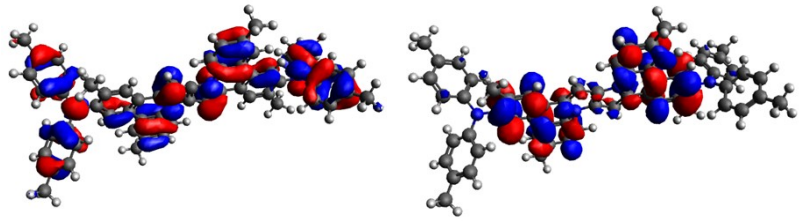


HOMO-2 LUMO+2

PSD2

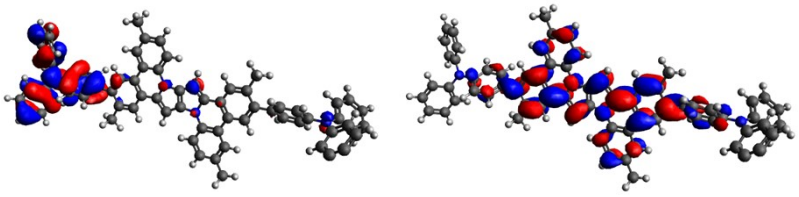


HOMO-1 LUMO+1

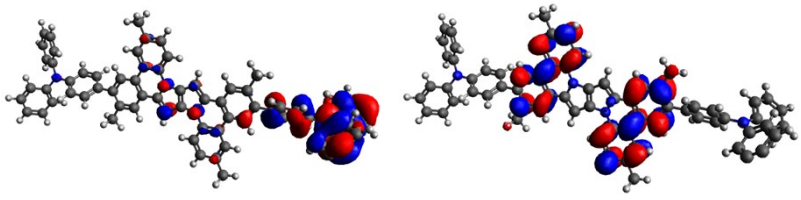


HOMO-2 LUMO+2

PSD3



HOMO-1 LUMO+1



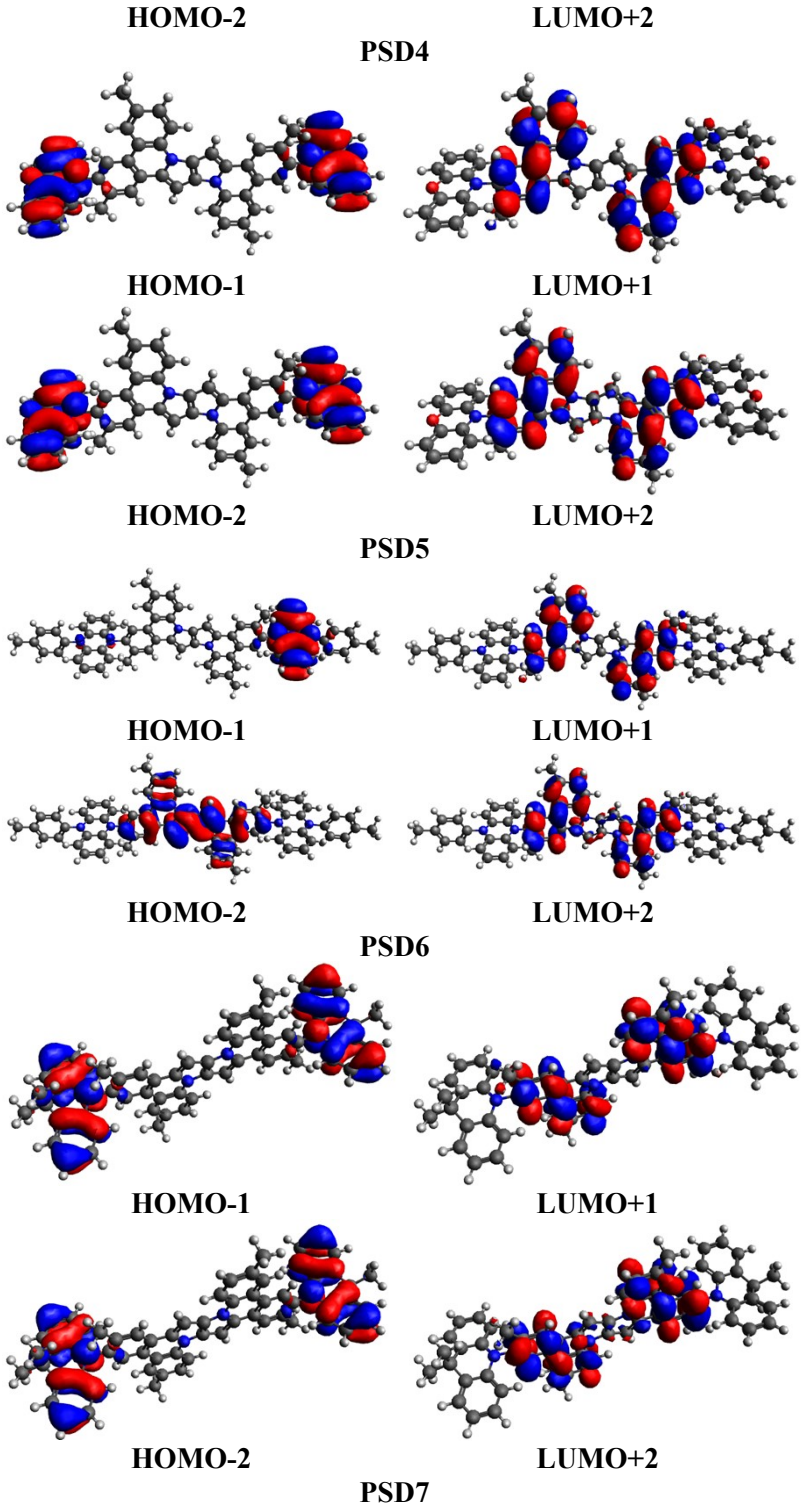


Figure S2: HOMO-1, LUMO+1, HOMO-2 and LUMO+2 of **PSR** &**PSD1**-**PSD7**.