Enhancing Photovoltaic Properties of Phenylsulfonyl Carbazole-based Materials by Incorporating Thiophene Ring and End-capped Acceptors for Organic Solar Cells: A DFT Approach

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Table S1: Cartesian coordinates of **PSCR** compound.

Atom	X-axis	Y-axis	Z-axis
C	2.672155	1.824776	-0.36842
C	2.997374	3.144175	-0.73497
C	4.313293	3.547302	-0.91584
C	5.311877	2.617237	-0.69562
C	5.025326	1.297092	-0.31885
C	3.694231	0.904964	-0.16828
C	0.720668	3.010619	-0.64502
H	4.549292	4.557292	-1.22511
H	6.346875	2.926618	-0.8091
H	3.470332	-0.12682	0.07613
C	1.226964	1.732895	-0.31249
C	0.375949	0.661022	-0.02986
C	-0.63622	3.285393	-0.71858
C	-0.99458	0.922619	-0.08323
H	-1.03412	4.24783	-1.00983
C	-1.44701	2.212918	-0.42314
O	-2.80675	2.282465	-0.4452
C	-3.25825	1.038818	-0.12455
C	-2.2031	0.148451	0.118915

C	-2.53159	-1.16259	0.46646
C	-4.58864	0.700288	-0.04077
C	-3.86033	-1.52851	0.554535
H	-1.7682	-1.90721	0.659556
C	-4.90115	-0.61603	0.306935
H	-5.35472	1.447479	-0.22093
H	-4.10902	-2.55739	0.79312
C	-6.28544	-1.05557	0.412767
C	-8.76286	-1.36327	0.203791
C	-8.16193	-2.27308	1.059944
C	6.08904	0.328917	-0.08301
C	6.048313	-0.7776	0.744214
S	7.618318	0.448333	-0.86549
C	7.226369	-1.52257	0.75653
H	5.184348	-1.01453	1.354451
C	8.211842	-1.00294	-0.06813
S	-7.54966	-0.27919	-0.46221
C	-6.7835	-2.09791	1.171716
C	-10.0984	-1.12241	-0.21195
C	9.550888	-1.36572	-0.36306
H	-6.15557	-2.69739	1.820526
C	-11.278	-1.7782	0.011457
C	-12.5807	-1.37105	-0.51743
C	-11.4668	-3.06917	0.716733
C	-13.5317	-2.46484	-0.23797
C	10.32116	-2.44398	-0.02254
C	9.889489	-3.66622	0.697958
C	11.70962	-2.64522	-0.4357
C	12.07057	-4.0379	-0.10658
C	-12.8735	-3.45211	0.498474
C	-13.5	-4.60332	0.931255
C	-14.8377	-4.77562	0.607615
H	-12.9412	-5.33695	1.503968
C	-14.8751	-2.64426	-0.56059
C	-15.5081	-3.80408	-0.1316
H	-15.3673	-5.66741	0.927094
H	-15.4338	-1.91566	-1.13326
H	-16.5537	-3.95288	-0.38187
C	11.00328	-4.6256	0.576449
C	11.04129	-5.92419	1.042647
C	13.21972	-4.78843	-0.34307
C	12.18922	-6.66609	0.805822
H	10.18609	-6.33109	1.573444
C	13.25881	-6.09857	0.117658

H	14.07213	-4.38604	-0.87489
H	12.25826	-7.69196	1.153204
H	14.14859	-6.69227	-0.06615
H	10.04008	-0.63632	-1.00394
H	-10.1735	-0.24383	-0.84729
O	8.843039	-3.8853	1.267827
O	-10.6593	-3.72052	1.342528
C	12.5741	-1.72102	-0.96454
C	-12.9171	-0.18476	-1.11811
S	1.707442	5.568018	-0.67798
C	1.715753	5.710961	1.090507
C	0.505796	5.732278	1.772005
C	2.934197	5.761158	1.756402
C	0.52299	5.799755	3.156252
H	-0.42979	5.721671	1.22363
C	2.93338	5.826827	3.140364
H	3.863495	5.771674	1.197103
C	1.732155	5.841693	3.836874
H	-0.41291	5.825963	3.704273
H	3.875442	5.874052	3.676336
H	1.738811	5.895987	4.920752
N	1.803871	3.872116	-0.91734
O	2.935391	6.107972	-1.20103
O	0.415168	5.963219	-1.17521
C	13.91452	-2.03328	-1.32523
N	15.0059	-2.2553	-1.63153
C	12.24491	-0.35238	-1.17469
N	12.00396	0.76399	-1.35113
C	-14.2274	0.096889	-1.59701
N	-15.2783	0.356917	-2.00002
C	-12.0161	0.900821	-1.30563
N	-11.3064	1.798296	-1.46792
C	0.924417	-0.68745	0.301205
H	1.522361	-1.08266	-0.5284
H	1.576676	-0.64267	1.181023
H	0.137996	-1.41044	0.511681
H	-8.73992	-3.02398	1.578914
H	7.394611	-2.41211	1.346157

Table S2: Cartesian coordinates of **PSCD1** compound.

Atom	X-axis	Y-axis	Z-axis
C	2.738168	2.229752	-0.32481
C	3.05272	3.556235	-0.67542
C	4.364993	3.970956	-0.85778

C	5.370749	3.044209	-0.65802
C	5.094621	1.717002	-0.29869
C	3.767286	1.313943	-0.14359
C	0.777478	3.405301	-0.57892
H	4.592473	4.986559	-1.15464
H	6.403083	3.361488	-0.77394
H	3.551743	0.277174	0.08731
C	1.294026	2.127031	-0.26448
C	0.451886	1.045156	0.005712
C	-0.58165	3.671137	-0.64572
C	-0.92066	1.296707	-0.04402
H	-0.98721	4.634242	-0.92405
C	-1.38367	2.588149	-0.36503
O	-2.74407	2.646307	-0.3871
C	-3.18504	1.393679	-0.08805
C	-2.1224	0.508976	0.143509
C	-2.43889	-0.81123	0.466507
C	-4.51226	1.040416	-0.01609
C	-3.76418	-1.19178	0.543044
H	-1.6689	-1.55182	0.648212
C	-4.81268	-0.28511	0.306848
H	-5.28512	1.78276	-0.18701
H	-4.00345	-2.22722	0.761957
C	-6.19263	-0.74073	0.396725
C	-8.66474	-1.07297	0.166604
C	-8.05834	-1.99033	1.01206
C	6.165435	0.751237	-0.08846
C	6.141448	-0.36286	0.730364
S	7.679436	0.881495	-0.89672
C	7.320856	-1.10398	0.716399
H	5.288024	-0.60687	1.352477
C	8.291351	-0.57481	-0.12146
S	-7.45931	0.03565	-0.47367
C	-6.68356	-1.80155	1.135652
C	-9.99885	-0.84199	-0.2545
C	9.622573	-0.93324	-0.44876
H	-6.05275	-2.4044	1.778419
C	-11.1732	-1.51476	-0.0479
C	-12.4767	-1.11463	-0.57856
C	-11.3505	-2.81348	0.641943
C	-13.4204	-2.21492	-0.30409
C	10.40775	-2.0078	-0.12656
C	10.0046	-3.21935	0.623488
C	11.78563	-2.20469	-0.57539

C	12.17443	-3.5809	-0.21277
C	-12.7552	-3.20278	0.421324
C	-13.3668	-4.36415	0.850341
C	-14.6952	-4.53294	0.528706
H	-12.8251	-5.11501	1.416071
C	-14.765	-2.3946	-0.6235
C	-15.3773	-3.55692	-0.2013
H	-15.359	-1.68363	-1.18434
C	11.13019	-4.16469	0.504214
C	11.18948	-5.44826	1.009901
C	13.33487	-4.31588	-0.44646
C	12.34069	-6.16643	0.774111
H	10.36452	-5.87721	1.569192
C	13.39414	-5.6015	0.051513
H	14.19038	-3.94426	-0.99675
H	10.0921	-0.20192	-1.10171
H	-10.0807	0.044652	-0.87775
O	8.97358	-3.44626	1.217107
O	-10.5422	-3.47019	1.260203
C	12.62309	-1.29482	-1.16789
C	-12.8226	0.067147	-1.18191
S	1.744808	5.971989	-0.59765
C	1.753573	6.107647	1.17122
C	0.544107	6.12112	1.853755
C	2.972463	6.160644	1.836105
C	0.56232	6.183925	3.238215
H	-0.39198	6.108138	1.306232
C	2.972629	6.221401	3.220245
H	3.901107	6.176852	1.275798
C	1.771932	6.228796	3.91786
H	-0.37312	6.204259	3.787252
H	3.914898	6.270953	3.755631
H	1.779345	6.27956	5.001894
N	1.853702	4.27727	-0.84344
O	2.968545	6.52213	-1.11969
O	0.449229	6.358647	-1.0926
C	13.95287	-1.61529	-1.55887
N	15.03419	-1.85334	-1.88788
C	12.275	0.060612	-1.42524
N	12.01787	1.16632	-1.64065
C	-14.1357	0.329465	-1.6629
N	-15.193	0.564337	-2.06452
C	-11.9312	1.159981	-1.3715
N	-11.2286	2.062676	-1.53496

C	1.011593	-0.30284	0.319341
H	1.603411	-0.68746	-0.51966
H	1.672302	-0.26152	1.192931
H	0.231867	-1.03231	0.532118
H	-8.62972	-2.75637	1.515756
H	7.500295	-1.99716	1.296811
F	14.47529	-6.33671	-0.15265
F	12.47335	-7.40325	1.223478
F	-15.3523	-5.61878	0.900516
F	-16.6509	-3.77039	-0.48861

Table S3: Cartesian coordinates of **PSCD2** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	2.797598	2.620105	-0.25317
C	3.102409	3.945682	-0.61595
C	4.410691	4.366928	-0.81157
C	5.423028	3.445915	-0.61995
C	5.156293	2.116852	-0.26047
C	3.832861	1.707886	-0.08925
C	0.828535	3.77929	-0.51944
H	4.629628	5.382623	-1.11444
H	6.452722	3.767578	-0.74662
H	3.62585	0.667375	0.131803
C	1.353938	2.509237	-0.1847
C	0.517629	1.429716	0.111061
C	-0.53199	4.035751	-0.59488
C	-0.85599	1.666263	0.028653
H	-0.94181	4.994589	-0.88183
C	-1.32795	2.948869	-0.31202
O	-2.6888	2.993457	-0.34642
C	-3.11977	1.737536	-0.04595
C	-2.05028	0.865594	0.201196
C	-2.35264	-0.46276	0.503215
C	-4.44305	1.367161	0.007214
C	-3.67402	-0.86022	0.560713
H	-1.57338	-1.1965	0.673684
C	-4.73061	0.036254	0.320696
H	-5.22307	2.099633	-0.17344
H	-3.9033	-1.90112	0.76384
C	-6.10587	-0.43598	0.392441
C	-8.57251	-0.7919	0.140055
C	-7.96245	-1.71202	0.980579
C	6.233901	1.154501	-0.07129
C	6.233327	0.044156	0.753493

S	7.72643	1.28595	-0.91715
C	7.415058	-0.69212	0.71555
H	5.395465	-0.19928	1.3967
C	8.362985	-0.16371	-0.1491
S	-7.37393	0.335942	-0.47967
C	-6.59108	-1.51013	1.116392
C	-9.90563	-0.56839	-0.2856
C	9.683895	-0.52117	-0.51445
H	-5.95875	-2.11286	1.757735
C	-11.076	-1.2531	-0.09089
C	-12.3807	-0.85461	-0.61935
C	-11.2437	-2.56216	0.581425
C	-13.3167	-1.96695	-0.3631
C	10.48598	-1.58789	-0.20537
C	10.11766	-2.78474	0.584504
C	11.84663	-1.78593	-0.70371
C	12.25648	-3.15334	-0.32799
C	-12.6455	-2.95958	0.350386
C	-13.2528	-4.126	0.756769
C	-14.5874	-4.31763	0.433887
H	-12.697	-4.87365	1.313274
C	-14.6546	-2.15796	-0.68701
C	-15.2783	-3.33427	-0.28723
H	-15.2378	-1.4334	-1.24092
C	11.24515	-3.72627	0.443331
C	11.33756	-4.99507	0.969077
C	13.4027	-3.892	-0.59367
C	12.4828	-5.73176	0.707395
H	10.53188	-5.40491	1.569805
C	13.50488	-5.17798	-0.07561
H	14.22312	-3.51478	-1.19065
H	10.1272	0.203131	-1.19286
H	-9.99218	0.323822	-0.90039
O	9.11044	-3.00366	1.220287
O	-10.4317	-3.21998	1.193358
C	12.65511	-0.88467	-1.34729
C	-12.7342	0.334353	-1.20388
S	1.777789	6.351923	-0.54657
C	1.784079	6.489521	1.222093
C	0.574161	6.495706	1.903942
C	3.002347	6.550456	1.887398
C	0.591429	6.559751	3.28838
H	-0.3616	6.476194	1.355999
C	3.001543	6.612137	3.271495

H	3.93091	6.572026	1.327116
C	1.800456	6.612663	3.968492
H	-0.34434	6.574673	3.837026
H	3.943222	6.667904	3.807298
H	1.807021	6.664321	5.052488
N	1.89862	4.65726	-0.7893
O	2.998364	6.909367	-1.06822
O	0.48023	6.729153	-1.04351
C	13.97157	-1.20382	-1.78244
N	15.0417	-1.43743	-2.14911
C	12.28854	0.462775	-1.62034
N	12.01529	1.561852	-1.8494
C	-14.0477	0.59696	-1.68387
N	-15.1041	0.83565	-2.08536
C	-11.8499	1.436321	-1.37258
N	-11.1529	2.346302	-1.51892
C	1.07601	0.101	0.500777
H	1.53255	-0.40947	-0.35632
H	1.850882	0.214011	1.265972
H	0.310919	-0.55705	0.911797
H	-8.52942	-2.48896	1.472351
H	7.612664	-1.58074	1.297229
Cl	-15.3706	-5.77478	0.92982
Cl	-16.9397	-3.55789	-0.70515
Cl	12.62129	-7.32694	1.355427
Cl	14.93312	-6.08508	-0.42672

Table S4: Cartesian coordinates of **PSCD3** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	2.778139	2.454216	-0.31622
C	3.087799	3.785647	-0.6548
C	4.399162	4.207703	-0.83074
C	5.407954	3.283319	-0.63901
C	5.13649	1.951491	-0.29207
C	3.810311	1.54139	-0.14131
C	0.813805	3.625208	-0.56074
H	4.623295	5.226458	-1.11898
H	6.43893	3.60646	-0.75073
H	3.597562	0.50212	0.0805
C	1.334652	2.345574	-0.25751
C	0.496753	1.258424	0.003383
C	-0.5463	3.887035	-0.62538
C	-0.87672	1.505789	-0.04533
H	-0.95552	4.850771	-0.89604
C	-1.34422	2.798456	-0.35524

O	-2.70486	2.851541	-0.37795
C	-3.14116	1.594961	-0.09108
C	-2.07511	0.711941	0.133597
C	-2.38577	-0.61266	0.444229
C	-4.46656	1.235252	-0.0245
C	-3.70923	-0.99949	0.51684
H	-1.61285	-1.35155	0.619693
C	-4.76105	-0.09481	0.286873
H	-5.24219	1.97599	-0.1898
H	-3.94349	-2.03785	0.726725
C	-6.138	-0.55725	0.370341
C	-8.60825	-0.89833	0.141066
C	-7.99337	-1.82773	0.972034
C	6.209766	0.98847	-0.09197
C	6.181033	-0.14601	0.702798
S	7.731293	1.14541	-0.87847
C	7.361149	-0.88023	0.685857
H	5.322006	-0.40746	1.309545
C	8.341539	-0.3268	-0.1297
S	-7.40845	0.226825	-0.48461
C	-6.622	-1.63432	1.094744
C	-9.9407	-0.66824	-0.26832
C	9.673619	-0.67251	-0.44411
H	-5.98648	-2.24346	1.726523
C	-11.1142	-1.35322	-0.06518
C	-12.4215	-0.94607	-0.57312
C	-11.2739	-2.6639	0.595564
C	-13.3608	-2.06122	-0.31925
C	10.45509	-1.76154	-0.14094
C	10.02895	-2.99757	0.543524
C	11.84109	-1.93907	-0.56278
C	12.22009	-3.33648	-0.25635
C	-12.6827	-3.06102	0.377342
C	-13.2801	-4.23338	0.780978
C	-14.6228	-4.42746	0.469869
H	-12.7126	-4.98219	1.324192
C	-14.702	-2.24721	-0.63481
C	-15.3248	-3.43159	-0.23976
H	-15.2864	-1.51471	-1.17748
C	11.15642	-3.94728	0.407558
C	11.1952	-5.25041	0.848638
C	13.37566	-4.06908	-0.50111
C	12.34903	-5.99112	0.608394
H	10.34473	-5.68272	1.366148

C	13.43197	-5.39467	-0.06934
H	14.2345	-3.65927	-1.01758
H	10.15548	0.076506	-1.06759
H	-10.0323	0.226912	-0.87834
O	8.986121	-3.25381	1.102501
O	-10.4619	-3.33416	1.192844
C	12.69916	-1.00593	-1.08414
C	-12.7843	0.249799	-1.13601
S	1.771042	6.200994	-0.58566
C	1.781909	6.351101	1.181251
C	0.573342	6.361232	1.865466
C	3.001613	6.421892	1.842881
C	0.593568	6.438019	3.249188
H	-0.36363	6.33616	1.319872
C	3.003666	6.496427	3.226352
H	3.92869	6.442171	1.280193
C	1.804093	6.499967	3.925951
H	-0.3409	6.456622	3.799866
H	3.946258	6.560641	3.75954
H	1.812983	6.561973	5.009352
N	1.887278	4.502052	-0.81574
O	2.992067	6.749133	-1.11528
O	0.473013	6.574887	-1.08291
C	14.03865	-1.30919	-1.4548
N	15.12814	-1.53211	-1.76633
C	12.35799	0.362057	-1.27893
N	12.10267	1.477016	-1.44152
C	-14.1038	0.520429	-1.59417
N	-15.1661	0.763518	-1.97672
C	-11.8994	1.352239	-1.29994
N	-11.1996	2.260659	-1.44088
C	1.06136	-0.08983	0.306512
H	1.652444	-0.46689	-0.53644
H	1.723259	-0.05221	1.179343
H	0.284828	-0.82353	0.516062
H	-8.55856	-2.60435	1.466282
H	7.536389	-1.78596	1.247919
C	-16.7002	-3.62943	-0.56739
N	-17.8107	-3.78265	-0.83661
C	-15.275	-5.63147	0.869153
N	-15.7821	-6.61225	1.201767
C	12.42393	-7.34635	1.046656
N	12.46234	-8.44017	1.409544
C	14.61361	-6.15352	-0.32579

N	15.57062	-6.76078	-0.53694

Table S5: Cartesian coordinates of **PSCD4** compound.

Atom	X-axis	Y-axis	Z-axis
C	3.122824	4.182825	-0.57069
C	4.428359	4.613291	-0.76794
C	5.445279	3.693247	-0.60163
C	5.186324	2.356732	-0.2637
C	3.865792	1.939262	-0.08701
C	0.851148	4.005242	-0.46173
H	4.641186	5.634591	-1.05551
H	6.472487	4.021717	-0.73089
H	3.663852	0.894522	0.118014
C	1.383423	2.73171	-0.15022
C	0.55324	1.644648	0.134341
C	-0.51071	4.257921	-0.52493
C	-0.82181	1.87726	0.062359
H	-0.92613	5.218933	-0.79606
C	-1.30048	3.163245	-0.25589
O	-2.66156	3.202351	-0.28495
C	-3.08573	1.939907	-0.00547
C	-2.01158	1.068444	0.224891
C	-2.30648	-0.26658	0.504644
C	-4.40653	1.561576	0.040835
C	-3.62563	-0.67192	0.556767
H	-1.52321	-0.99896	0.661562
C	-4.68643	0.223342	0.330737
H	-5.19028	2.292934	-0.12769
H	-3.84905	-1.71736	0.742213
C	-6.05852	-0.25713	0.387003
C	-8.52158	-0.61948	0.116922
C	-7.90868	-1.55732	0.940199
C	6.268686	1.39642	-0.10452
C	6.273899	0.260436	0.688941
S	7.759063	1.561965	-0.94581
C	7.457498	-0.46595	0.630788
H	5.437496	-0.00652	1.324332
C	8.405632	0.094498	-0.21842
S	-7.32463	0.527862	-0.4729
C	-6.54122	-1.35202	1.08551
C	-9.84811	-0.39397	-0.31267
C	9.72694	-0.24135	-0.58479
H	-5.90782	-1.96587	1.714907
C	-11.0234	-1.08288	-0.13496
C	-12.322	-0.67924	-0.66714

C	-11.1919	-2.38929	0.530844
C	-13.2726	-1.78019	-0.39117
C	10.53896	-1.31153	-0.29404
C	10.17025	-2.52393	0.46162
C	11.90978	-1.47869	-0.76761
C	12.34215	-2.84421	-0.39283
C	-12.6023	-2.77998	0.309625
C	-13.2136	-3.94223	0.730936
C	-14.5498	-4.1039	0.426422
H	-12.671	-4.69867	1.288393
C	-14.6215	-1.95208	-0.6942
C	-15.2336	-3.12195	-0.28471
H	-15.2146	-1.22485	-1.23573
C	11.32441	-3.44327	0.345904
C	11.42102	-4.71797	0.862296
C	13.51573	-3.55506	-0.63192
C	12.58848	-5.41404	0.623056
H	10.60948	-5.16434	1.427526
C	13.61896	-4.83064	-0.1083
H	14.35052	-3.16385	-1.20071
H	10.1699	0.503459	-1.24089
H	-9.93232	0.505909	-0.91607
O	9.151435	-2.78341	1.061182
O	-10.3864	-3.05877	1.137025
C	12.71919	-0.56325	-1.38787
C	-12.6698	0.495014	-1.28205
S	1.787462	6.587494	-0.4862
C	1.798241	6.729279	1.281445
C	0.589862	6.736676	1.965926
C	3.018248	6.795282	1.94313
C	0.61048	6.806589	3.350039
H	-0.34715	6.714491	1.420226
C	3.020663	6.862771	3.326914
H	3.945296	6.816788	1.380296
C	1.821188	6.864165	4.026797
H	-0.32383	6.823043	3.901063
H	3.963408	6.923122	3.860288
H	1.830399	6.920769	5.110494
N	1.916119	4.890305	-0.72353
O	3.00421	7.146798	-1.01394
O	0.486631	6.954529	-0.98119
C	14.0527	-0.85561	-1.78868
N	15.13762	-1.0674	-2.12297
C	12.33276	0.777493	-1.66749

N	12.04025	1.87057	-1.90017
C	-13.9788	0.752199	-1.77714
N	-15.03	0.984906	-2.1948
C	-11.7762	1.58437	-1.48225
N	-11.069	2.481983	-1.65253
C	1.118215	0.312248	0.500962
H	1.564285	-0.18743	-0.36797
H	1.902054	0.417079	1.258063
H	0.359304	-0.35172	0.913957
H	-8.47251	-2.3478	1.413638
H	7.658465	-1.37049	1.186676
N	12.65286	-6.82155	1.069222
O	13.21179	-7.59722	0.330917
O	12.09739	-7.08377	2.109245
N	14.92689	-5.50591	-0.27056
O	15.38787	-5.52731	-1.38438
O	15.43636	-5.92369	0.740804
N	-16.6295	-3.33038	-0.73412
O	-16.8626	-4.38738	-1.26886
O	-17.3909	-2.40929	-0.57414
N	-15.2424	-5.28623	0.979894
O	-14.6122	-6.31609	1.01034
O	-16.3599	-5.10684	1.40194

Table S6: Cartesian coordinates of **PSCD5** compound

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	2.924443	3.488059	-0.23485
C	3.206438	4.825853	-0.57365
C	4.508565	5.275568	-0.7498
C	5.535875	4.370919	-0.56642
C	5.292603	3.029144	-0.2371
C	3.975222	2.592327	-0.08325
C	0.93665	4.617673	-0.48563
H	4.71179	6.299365	-1.03519
H	6.559559	4.716356	-0.67838
H	3.783892	1.544673	0.115875
C	1.482894	3.350989	-0.16977
C	0.664418	2.2548	0.114288
C	-0.42783	4.853608	-0.55601
C	-0.71314	2.471224	0.038253
H	-0.85393	5.808955	-0.83065
C	-1.20548	3.750581	-0.28606
O	-2.56676	3.774682	-0.31703
C	-2.97744	2.509516	-0.03013
C	-1.89439	1.650461	0.204886

C	-2.17613	0.314614	0.494779
C	-4.29429	2.118718	0.020994
C	-3.49129	-0.10321	0.552294
H	-1.38568	-0.40894	0.656598
C	-4.56094	0.780076	0.321258
H	-5.0852	2.841538	-0.15083
H	-3.70455	-1.14922	0.746537
C	-5.92877	0.288361	0.383126
C	-8.38945	-0.09078	0.120184
C	-7.77019	-1.01828	0.950544
C	6.388052	2.08632	-0.06712
C	6.385028	0.913871	0.672295
S	7.912923	2.325526	-0.82628
C	7.585735	0.215312	0.632658
H	5.528458	0.596414	1.255256
C	8.55837	0.83746	-0.1431
S	-7.20065	1.058111	-0.48168
C	-6.4035	-0.80392	1.091408
C	-9.71773	0.124509	-0.30781
C	9.903463	0.547519	-0.4561
H	-5.76513	-1.40851	1.724767
C	-10.8898	-0.56719	-0.12012
C	-12.1896	-0.1703	-0.65302
C	-11.0537	-1.87021	0.553495
C	-13.127	-1.28647	-0.39679
C	10.70901	-0.53783	-0.20429
C	10.29716	-1.82467	0.38725
C	12.1081	-0.65478	-0.60246
C	12.5189	-2.05555	-0.3565
C	-12.4618	-2.27202	0.321629
C	-13.0725	-3.4397	0.733147
C	-14.4014	-3.63657	0.396924
H	-12.5256	-4.18288	1.306167
C	-14.4635	-1.48249	-0.7373
C	-15.0886	-2.65317	-0.33581
H	-15.0408	-0.76749	-1.31205
C	11.45812	-2.73291	0.23134
C	11.52567	-4.06331	0.592048
C	13.71029	-2.73821	-0.59309
C	12.70671	-4.74578	0.354133
H	10.67374	-4.56291	1.043975
C	13.79	-4.07794	-0.24335
H	14.58257	-2.27352	-1.03881
H	10.37391	1.345975	-1.02469

H	-9.80791	1.016877	-0.92182
O	9.245491	-2.14551	0.892444
O	-10.2473	-2.53072	1.167532
C	12.95119	0.320874	-1.06462
C	-12.5526	1.014239	-1.23721
S	1.839052	7.213739	-0.51619
C	1.842323	7.369514	1.250098
C	0.632491	7.357233	1.932115
C	3.059244	7.466416	1.913373
C	0.649012	7.439279	3.315619
H	-0.30307	7.310954	1.385374
C	3.057628	7.545322	3.296545
H	3.98636	7.503091	1.351624
C	1.856947	7.527591	3.994053
H	-0.28653	7.441022	3.864771
H	3.997854	7.629825	3.831046
H	1.862698	7.593476	5.077239
N	1.992038	5.516285	-0.73935
O	3.049694	7.785421	-1.04466
O	0.535162	7.559007	-1.0185
C	14.30563	0.072314	-1.42395
N	15.4071	-0.09628	-1.72739
C	12.57568	1.686275	-1.2092
N	12.29302	2.799777	-1.33086
C	-13.8675	1.274942	-1.7157
N	-14.9231	1.517648	-2.11638
C	-11.6702	2.118469	-1.40559
N	-10.9717	3.027273	-1.54983
C	1.24354	0.93006	0.486482
H	1.701516	0.434991	-0.37886
H	2.021023	1.045627	1.248651
H	0.490268	0.256968	0.894915
H	-8.32929	-1.80764	1.43187
H	7.781258	-0.71409	1.148923
O	13.30128	-7.20339	-0.32779
O	11.38046	-6.83409	1.235321
O	16.29562	-3.8447	-1.01689
O	15.70159	-5.63896	0.626947
O	-16.9379	-4.18689	-1.37562
O	-17.1103	-1.71491	-1.7353
O	-14.1872	-5.82823	1.82855
O	-16.4516	-4.79966	1.540323
H	-17.4761	-3.42777	1.014525
H	-16.0197	-5.6109	-0.85983

H	14.56746	-6.38133	1.756721
H	14.53509	-6.5533	-1.45676
S	-16.7939	-2.82403	-0.89215
S	-15.147	-5.15538	1.009717
S	12.69416	-6.49336	0.784658
S	15.39031	-4.84655	-0.55078
O	-17.6296	-2.64581	0.437286
O	-15.3275	-6.02759	-0.29546
O	13.64408	-6.57198	2.04485
O	15.1029	-5.81266	-1.76869

Table S7: Cartesian coordinates of **PSCD6** compound

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	2.891719	3.242204	-0.26056
C	3.187853	4.577037	-0.59669
C	4.494625	5.012976	-0.77132
C	5.512642	4.097264	-0.5872
C	5.254795	2.758255	-0.25855
C	3.932854	2.335233	-0.108
C	0.915099	4.391116	-0.51492
H	4.708504	6.035204	-1.05488
H	6.540226	4.431555	-0.69735
H	3.730516	1.289185	0.089188
C	1.448877	3.119171	-0.2002
C	0.619876	2.029511	0.077802
C	-0.44721	4.639173	-0.58896
C	-0.7552	2.258065	-0.00291
H	-0.86355	5.599374	-0.86152
C	-1.23584	3.542335	-0.32452
O	-2.59707	3.577811	-0.35851
C	-3.01928	2.31501	-0.07563
C	-1.94351	1.446864	0.158183
C	-2.23533	0.112243	0.442217
C	-4.33979	1.934531	-0.02523
C	-3.55358	-0.29504	0.498089
H	-1.45049	-0.61817	0.600593
C	-4.61666	0.597601	0.272562
H	-5.12566	2.66355	-0.19417
H	-3.77509	-1.34006	0.688069
C	-5.9874	0.11374	0.344648
C	-8.4509	-0.26533	0.10105
C	-7.82679	-1.18576	0.933101
C	6.338743	1.801831	-0.08277
C	6.323482	0.642799	0.674734
S	7.861666	2.00427	-0.85761

C	7.514317	-0.07544	0.6375
H	5.466472	0.349035	1.269551
C	8.488833	0.517941	-0.15495
S	-7.26608	0.879659	-0.51589
C	-6.45829	-0.97128	1.0637
C	-9.787	-0.05617	-0.31486
C	9.830136	0.203293	-0.47185
H	-5.81667	-1.57149	1.697965
C	-10.9483	-0.75923	-0.1151
C	-12.2619	-0.37498	-0.62845
C	-11.0922	-2.07253	0.550011
C	-13.1793	-1.50839	-0.37858
C	10.62329	-0.88434	-0.20448
C	10.20651	-2.15743	0.421058
C	12.01864	-1.02475	-0.61275
C	12.41323	-2.42559	-0.34901
C	-12.4922	-2.48953	0.323217
C	-13.0871	-3.66359	0.727393
C	-14.4215	-3.88729	0.417777
H	-12.5106	-4.39333	1.284633
C	-14.5132	-1.73028	-0.70386
C	-15.1283	-2.91707	-0.31698
H	-15.0934	-1.00882	-1.26322
C	11.35357	-3.07884	0.266472
C	11.42437	-4.39775	0.65702
C	13.5841	-3.13374	-0.59448
C	12.59346	-5.10927	0.42333
H	10.57339	-4.85986	1.14487
C	13.66975	-4.47032	-0.21947
H	14.43651	-2.68143	-1.0824
H	10.30607	0.984867	-1.05892
H	-9.89014	0.837403	-0.92566
O	9.157123	-2.45017	0.948818
O	-10.2718	-2.7254	1.155049
C	12.86785	-0.06109	-1.09025
C	-12.644	0.816861	-1.18567
S	1.844307	6.975373	-0.52265
C	1.847589	7.113008	1.245654
C	0.637492	7.10141	1.92726
C	3.064748	7.193451	1.910761
C	0.653887	7.167534	3.311595
H	-0.2982	7.066959	1.379858
C	3.063051	7.256725	3.294757
H	3.992508	7.228901	1.349944

C	1.862013	7.239765	3.99161
H	-0.28194	7.16912	3.860316
H	4.003677	7.3279	3.83054
H	1.867693	7.293128	5.075508
N	1.97997	5.280574	-0.76463
O	3.061056	7.541745	-1.04321
O	0.544387	7.340266	-1.02199
C	14.21886	-0.32711	-1.44937
N	15.3182	-0.51131	-1.7516
C	12.50706	1.306801	-1.24793
N	12.23797	2.422506	-1.38084
C	-13.9677	1.068593	-1.64364
N	-15.0319	1.302491	-2.02657
C	-11.7783	1.935945	-1.34053
N	-11.0955	2.858255	-1.47446
C	1.186463	0.699099	0.449235
H	1.642861	0.201523	-0.41552
H	1.962751	0.806662	1.21375
H	0.426168	0.032015	0.854483
H	-8.38309	-1.97172	1.422688
H	7.700303	-0.9983	1.168249
C	-16.5895	-3.06646	-0.69023
C	-15.0068	-5.2097	0.863563
C	12.60369	-6.56368	0.841785
C	14.99004	-5.15957	-0.49635
F	-16.8648	-4.28173	-1.15448
F	-17.3777	-2.83233	0.356749
F	-16.932	-2.19928	-1.64175
F	-15.0591	-6.0788	-0.14339
F	-16.2279	-5.08167	1.368792
F	-14.2475	-5.7618	1.813663
F	12.3933	-7.36634	-0.19977
F	11.63031	-6.8059	1.723231
F	13.74663	-6.91978	1.417786
F	14.82038	-6.38375	-0.98653
F	15.70884	-4.47893	-1.38868
F	15.72338	-5.24955	0.61083

Table S8: Energies of HOMO-1/LUMO+1 and HOMO-2/LUMO+2 and their differences for all the investigated chromophores (**PSCR** and **PSCD1-PSCD6**).

Compound	**HOMO-1**	**LUMO+1**	**Δ*E***	**HOMO-2**	**LUMO+2**	**Δ*E***
PSCR	-6.568	-3.339	3.229	-6.970	-2.718	4.252
PSCD1	-6.700	-3.515	3.185	-7.086	-2.919	4.167
PSCD2	-6.716	-3.565	3.151	-7.101	-2.984	4.117

PSCD3	-7.001	-4.014	2.987	-7.363	-3.645	3.718
PSCD4	-7.014	-4.069	2.945	-7.376	-3.708	3.668
PSCD5	-6,999	-4.021	2.978	-7.364	-3.670	3.694
PSCD6	-6.861	-3.778	3.083	-7.235	-3.303	3.932

Units in *eV*

Table S9: Wavelength (λ), excitation energy (E), oscillator strength (f_{os}) and nature of molecular orbital contributions of compound (**PSCR** and **PSCD1-PSCD6**).

	NO	DFT λ (*nm*)	E(*eV*)	f_{os}	MO contributions
PSCR	1	496.891	2.495	2.298	H-1→L+1 (14%), H→L (71%), H-1→L (6%), H→L+1 (5%)
	2	471.279	2.631	0.223	H-1→L (12%), H-1→L+1 (13%), H→L+1 (65%), H→L (8%)
	3	436.241	2.842	0.038	H-1→L (21%), H-1→L+1 (48%), H→L+1 (27%),
	4	434.895	2.851	0.088	H-1→L (56%), H-1→L+1 (21%), H→L (18%),
	5	404.767	3.063	0.230	H-1→L+2 (14%), H-1→L+3 (11%), H→L+2 (59%), H-5→L (3%), H-3→L+2 (3%)
	6	401.347	3.089	0.093	H-1→L+2 (10%), H-1→L+3 (26%), H→L+3 (43%), H-4→L+1 (2%), H-2→L+1 (3%), H-2→L+3 (2%)
PSCD1	1	504.452	2.458	2.219	H-1→L+1 (14%), H→L (73%), H-1→L (5%), H→L+1 (4%)
	2	478.703	2.590	0.216	H-1→L (11%), H-1→L+1 (11%), H→L+1 (68%), H→L (7%)
	3	444.244	2.791	0.057	H-1→L (14%), H-1→L+1 (57%), H→L+1 (24%),
	4	441.712	2.807	0.078	H-1→L (65%), H-1→L+1 (14%), H→L (15%), H-2→L (2%)
	5	414.026	2.995	0.269	H-1→L+2 (12%), H-1→L+3 (12%), H→L+2 (61%), H-5→L (3%), H-3→L+2 (4%)
	6	410.096	3.023	0.087	H-1→L+2 (10%), H-1→L+3 (23%), H→L+3 (43%), H-2→L+1 (6%), H-2→L+3 (2%)
PSCD2	1	511.085	2.426	2.289	H-1→L+1 (14%), H→L (75%), H-1→L (4%), H→L+1 (3%)
	2	484.067	2.561	0.249	H-1→L (10%), H-1→L+1 (12%), H→L+1 (69%), H→L (6%)
	3	449.788	2.757	0.073	H-1→L (12%), H-1→L+1 (58%), H→L+1 (24%), H→L (2%)
	4	446.002	2.780	0.074	H-1→L (69%), H-1→L+1 (12%), H→L (14%), H-2→L (2%)
	5	419.588	2.955	0.274	H-1→L+2 (12%), H-1→L+3 (11%), H→L+2 (63%), H-5→L (3%), H-3→L+2 (4%)
	6	414.940	2.988	0.096	H-1→L+2 (10%), H-1→L+3 (26%), H→L+3 (43%), H-2→L+1 (5%), H-2→L+3 (3%)
PSCD3	1	539.531	2.298	1.983	H-1→L+1 (13%), H→L (76%), H-1→L (3%), H→L+1 (3%)
	2	514.521	2.410	0.132	H-1→L (10%), H→L+1 (75%), H-1→L+1 (6%), H→L (5%)
	3	477.395	2.597	0.038	H-1→L (15%), H-1→L+1 (59%), H→L+1 (17%), H→L (2%), H→L+3 (2%)
	4	473.186	2.620	0.033	H-1→L (64%), H-1→L+1 (15%), H→L (11%), H→L+2 (3%)
	5	466.159	2.660	0.527	H-1→L+3 (20%), H→L+2 (65%), H-3→L+2 (2%), H-2→L+3 (2%), H-1→L+2 (3%)
	6	458.555	2.704	0.223	H-1→L+2 (19%), H→L+3 (60%), H-1→L (3%), H-1→L+3 (8%)
PSCD4	1	545.009	2.275	1.726	H-1→L+1 (14%), H→L (79%),
	2	523.250	2.370	0.101	H-1→L (12%), H→L+1 (78%), H-1→L+1 (5%)
	3	483.954	2.562	0.030	H-1→L (21%), H-1→L+1 (53%), H→L+1 (16%), H→L (5%),

					H→L+3 (3%)
	4	477.836	2.595	0.001	H-1→L (53%), H-1→L+1 (20%), H→L+2 (11%), H→L (8%), H→L+1 (3%)
	5	472.987	2.621	0.739	H-1→L+3 (14%), H→L+2 (59%), H-1→L (6%), H-1→L+1 (3%), H-1→L+2 (6%), H→L (3%)
	6	462.007	2.684	0.240	H-1→L+2 (12%), H-1→L+3 (14%), H→L+3 (59%), H-1→L (3%), H→L+2 (3%)
	1	541.321	2.290	1.921	H-1→L+1 (14%), H→L (76%), H-1→L (3%), H→L+1 (4%)
	2	517.723	2.395	0.103	H-1→L (11%), H→L+1 (75%), H-1→L+1 (5%), H→L (5%)
PSCD5	3	479.036	2.588	0.011	H-1→L (15%), H-1→L+1 (57%), H→L+1 (16%), H→L+3 (4%)
	4	475.108	2.610	0.001	H-1→L (56%), H-1→L+1 (12%), H→L+2 (13%), H→L (9%)
	5	471.279	2.631	0.645	H-1→L+3 (21%), H→L+2 (53%), H-1→L (6%), H-1→L+1 (7%), H-1→L+2 (2%), H→L (5%)
	6	462.852	2.679	0.257	H-1→L+2 (20%), H→L+3 (59%), H-1→L (5%), H-1→L+3 (6%), H→L+2 (2%)
	1	522.083	2.375	2.132	H-1→L+1 (14%), H→L (75%), H-1→L (3%), H→L+1 (4%)
	2	496.195	2.499	0.163	H-1→L (11%), H→L+1 (74%), H-1→L+1 (7%), H→L (6%)
PSCD6	3	461.165	2.689	0.060	H-1→L (17%), H-1→L+1 (59%), H→L+1 (18%), H→L (2%)
	4	457.608	2.709	0.082	H-1→L (64%), H-1→L+1 (16%), H→L (13%),
	5	438.231	2.829	0.333	H-1→L+3 (16%), H→L+2 (64%), H-3→L+2 (3%), H-1→L+2 (8%)
	6	433.193	2.862	0.170	H-1→L+2 (15%), H-1→L+3 (15%), H→L+3 (54%), H→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os} =oscillator strength, DFT=Density functional theory.

Table S10: Wavelength (λ), excitation energy (E), oscillator strength (f_{os}) and nature of molecular orbital contributions of compounds (**PSCR** and **PSCD1-PSCD6**).

Compounds	**DFT λ (*nm*)**	**E(*eV*)**	f_{os}	**MO contributions**
PSCR	496.891	*2.495*	2.298	H-1→L+1 (14%), H→L (71%), H-1→L (6%), H→L+1 (5%)
PSCD1	504.452	2.458	2.219	H-1→L+1 (14%), H→L (73%), H-1→L (5%), H→L+1 (4%)
PSCD2	511.085	2.426	2.289	H-1→L+1 (14%), H→L (75%), H-1→L (4%), H→L+1 (3%)
PSCD3	539.531	2.298	1.983	H-1→L+1 (13%), H→L (76%), H-1→L (3%), H→L+1 (3%)
PSCD4	545.009	2.275	1.726	H-1→L+1 (14%), H→L (79%),
PSCD5	541.321	2.290	1.921	H-1→L+1 (14%), H→L (76%), H-1→L (3%), H→L+1 (4%)
PSCD6	522.083	2.375	2.132	H-1→L+1 (14%), H→L (75%), H-1→L (3%), H→L+1 (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os} =oscillator strength, DFT=Density functional theory.

Table S11: Percentages of π-spacer and Acceptors for HOMOs and LUMOs

Compounds	LUMO			HOMO		
	Acceptor 1	π-spacer	Acceptor 2	Acceptor 1	π-spacer	Acceptor 2
PSCR	68.5	23.1	8.5	19.3	25.5	55.2
PSCD1	69.3	22.7	8.0	18.0	24.1	57.9
PSCD2	15.5	7.0	77.5	14.0	1.3	84.7
PSCD3	75.3	18.7	6.0	16.9	20.8	62.3
PSCD4	78.6	15.9	5.4	16.5	20.4	63.1
PSCD5	76.1	18.0	5.8	16.7	20.5	62.8
PSCD6	71.6	21.2	7.1	17.4	22.1	60.5

Table S12: Open circuit voltage (V_{oc}), Band Gap (ΔE), eV_{oc}/K_BT, FF, L_D-L_A(eV) & PCE (%) of entitled compounds.

Compounds	V_{oc}	ΔE	eV_{oc}/K_BT	FF	PCE (%)	L_D-L_A(eV)
PSCR	1.72	2.02	66.409	0.958	24.17	1.053
PSCD1	1.549	1.849	59.807	0.954	21.68	1.224
PSCD2	1.502	1.802	57.992	0.953	20.99	1.271
PSCD3	1.062	1.362	41.004	0.938	14.61	1.711
PSCD4	1.015	1.315	39.18	0.935	13.92	1.758
PSCD5	1.056	1.356	40.77	0.937	14.52	1.717
PSCD6	1.293	1.593	49.93	0.947	17.96	1.48

Table S13: Dihedral angle values (θ_1 - θ_4) for the studied compound obtained by M06/ 6-311G (d,p).

Compound	θ_1		θ_2		θ_3		θ_4	
PSCR	C38-C28-S36-C41	-2.760°	S36-C27-C24-C22	-154.12°	S32-C30-C5-C4	-27.483°	-174.92°	S32-C35-C39-C45
PSCD1	C38-C28-S36-C41	-2.699°	S36-C27-C24-C22	-153.94°	C4-C5-C30-S32	-28.143°	-175.46°	S32-C35-C39-C45
PSCD2	S36-C28-C38-C27	-2.290°	S36-C27-C24-C22	-154.19°	S32-C30-C5-C4	-28.781°	-175.81°	S32-C35-C39-C45
PSCD3	C38-C28-S36-C41	-2.673°	S36-C27-C24-C22	-154.41°	C4-C5-C30-S32	-27.090°	-174.88°	S32-C35-C39-C45
PSCD4	C38-C28-S36-C41	-2.298°	S36-C27-C24-C22	-154.27°	C4-C5-C30-S32	-27.852°	-176.26°	S32-C35-C39-C45
PSCD5	C38-C28-S36-C41	-2.210°	S36-C27-C24-C22	-154.28°	C4-C5-C30-S32	-24.680°	-174.26°	S32-C35-C39-C45
PSCD6	C38-C28-S36-C41	-2.559°	S36-C27-C24-C22	-153.97°	C4-C5-C30-S32	-25.865°	-174.59°	S32-C35-C39-C45

Table S14: Bond lengths (Å) and bond angles (°) for **PSCR**

BOND LENGTH		BOND ANGLE	
DFT		DFT	
C1-C2	1.407	C1-C2-C3	121.7
C2-C3	1.388	C2-C1-C6	119.2
C3-C4	1.382	C2-C1-C8	107.5
C4-C5	1.402	C1-C2-N61	108.8
C5-C6	1.396	C2-C3-C4	117.9

C1-C6	1.39	C3-C2-N61	129.5
C1-C8	1.449	C3-C4-C5	121.9
C7-C8	1.414	C4-C5-C6	119.2
C8-C9	1.398	C4-C5-C23	121.3
C7-C10	1.386	C5-C6-C1	120
C9-C11	1.396	C6-C5-C23	119.5
C11-C12	1.409	C6-C1-C8	133.3
C10-C12	1.377	C1-C8-C7	106.9
C12-C13	1.362	C1-C8-C9	131.6
C13-C14	1.361	C7-C8-C9	121.5
C14-C15	1.402	C8-C7-C10	122.8
C11-C15	1.449	C8-C7-N61	108.8
C15-C16	1.396	C8-C9-C11	116.5
C14-C17	1.375	C8-C9-C72	120.9
C16-C18	1.381	C7-C10-C12	114.2
C17-C19	1.397	C10-C7-N61	128.3
C18-C19	1.406	C9-C11-C12	119.7
C19-C20	1.456	C9-C11-C15	135.5
C21-C22	1.386	C11-C9-C72	122.6
C5-C23	1.458	C11-C12-C10	125.2
C23-C24	1.382	C11-C12-C13	111.8
C23-S25	1.722	C12-C11-C15	104.8
C24-C26	1.394	C10-C12-C13	123
S25-C27	1.759	C12-C13-C14	106.3
C26-C27	1.386	C13-C14-C15	111.8
C21-S28	1.758	C13-C14-C17	124.1
C20-S28	1.722	C14-C15-C11	105.3
C22-C29	1.394	C14-C15-C16	117.6
C20-C29	1.382	C15-C14-C17	124.1
C21-C30	1.419	C11-C15-C16	137.1
C27-C31	1.418	C15-C16-C18	119.4
C30-C32	1.368	C14-C17-C19	117.6
C32-C33	1.464	C16-C18-C19	121.9
C32-C34	1.483	C17-C19-C18	119.3
C33-C35	1.476	C17-C19-C20	121
C31-C36	1.368	C18-C19-C20	119.7
C36-C37	1.483	C19-20-28	121.7
C36-C38	1.463	C19-C20-C29	127.6
C38-C39	1.476	C22-C21-S28	109.8
C35-C40	1.397	C21-C22-C29	113.3
C34-C40	1.474	C22-C21-C30	134.4
C40-C41	1.38	C5-C23-C24	127.4
C41-C42	1.387	C5-C23-S25	121.9

C35-C43	1.393	C24-C23-S25	110.7
C43-C44	1.389	C23-C24-C26	114.1
C42-C44	1.393	C23-S25-C27	92.1
C39-C45	1.397	C24-C26-C27	113.3
C37-C45	1.475	S25-C27-C26	109.8
C45-C46	1.38	C25-C27-31	115.8
C39-C47	1.393	C26-C27-31	134.4
C46-C48	1.387	C21-S28-C20	92.1
C47-C49	1.389	S28-C21-C30	115.7
C48-C49	1.393	S28-20-29	110.8
C37-O50	1.212	C22-C29-C20	114
C34-O51	1.212	C21-C30-32	133
C38-C52	1.372	C27-C31-C36	132.9
C33-C53	1.372	C30-C32-C33	125.1
S54-C55	1.774	C30-C32-C34	127.2
C55-C56	1.389	C33-C32-C34	107.5
C55-C57	1.389	C32-C33-C35	107.4
C56-C58	1.386	C32-C33-C53	128.1
C57-C59	1.386	C32-C34-C40	106.1
C58-C60	1.388	C32-C34-O51	129
C59-C60	1.389	C33-C35-C40	108.7
C7-N61	1.411	C33-C35-C43	132.3
C2-N61	1.41	C35-C33-C53	124.5
S54-N61	1.715	C31-C36-C37	127.3
S54-O62	1.44	C31-C36-C38	124.9
S54-O63	1.44	C37-C36-C38	107.5
C52-C64	1.423	C36-C37-C45	106
C64-N65	1.155	C36-C37-O50	129
C52-C66	1.423	C36-C38-C39	107.4
C66-N67	1.156	C36-C38-C52	127.9
C53-C68	1.423	C38-C39-C45	108.6
C68-N69	1.155	C38-C39-C47	132.3
C53-C70	1.423	C39-C38-C52	124.6
C70-N71	1.156	C35-C40-C34	110.1
C9-C72	1.493	C35-C40-C41	122.8

DFT=density functional theory

Table S15: Bond lengths (Å) and bond angles (°) for **PSCD1**

BOND LENGTH		**BOND ANGLE**	
DFT		DFT	
C1-C2	1.408	C1-C2-C3	121.7
C2-C3	1.388	C2-C1-C6	119.2
C3-C4	1.382	C2-C1-C8	107.5

C4-C5	1.402	C1-C2-N61	108.8
C5-C6	1.396	C2-C3-C4	117.9
C1-C6	1.389	C3-C2-N61	129.5
C1-C8	1.449	C3-C4-C5	121.9
C7-C8	1.414	C4-C5-C6	119.3
C8-C9	1.397	C4-C5-C23	121.3
C7-C10	1.386	C5-C6-C1	120
C9-C11	1.396	C6-C5-C23	119.4
C11-C12	1.409	C6-C1-C8	133.3
C10-C12	1.377	C1-C8-C7	106.9
C12-O13	1.362	C1-C8-C9	131.6
O13-C14	1.361	C7-C8-C9	121.5
C14-C15	1.402	C8-C7-C10	122.8
C11-C15	1.449	C8-C7-N61	108.8
C15-C16	1.396	C8-C9-C11	116.5
C14-C17	1.375	C8-C9-C72	120.9
C16-C18	1.381	C7-C10-C12	114.2
C17-C19	1.397	C10-C7-N61	128.4
C18-C19	1.406	C9-C11-C12	119.8
C19-C20	1.456	C9-C11-C15	135.5
C21-C22	1.387	C11-C9-C72	122.6
C5-C23	1.457	C11-C12-C10	125.2
C23-C24	1.383	C11-C12-O13	111.8
C23-S25	1.721	C12-C11-C15	104.8
C24-C26	1.393	C10-C12-O13	123
C25-C27	1.76	C12-O13-C14	106.3
C26-C27	1.387	O13-C14-C15	111.8
C21-S28	1.758	O13-C14-C17	124.1
C20-S28	1.722	C14-C15-C11	105.3
C22-C29	1.393	C14-C15-C16	117.6
C20-C29	1.383	C15-C14-C17	124.1
C21-C30	1.418	C11-C15-C16	137.1
C27-C31	1.417	C15-C16-C18	119.4
C30-C32	1.369	C14-C17-C19	117.6
C32-C33	1.463	C16-C18-C19	121.9
C32-C34	1.481	C17-C19-C18	119.4
C33-C35	1.475	C17-C19-C20	121
C31-C36	1.369	C18-C19-C20	119.6
C36-C37	1.481	C19-C20-S28	121.7
C36-C38	1.462	C19-C20-C29	127.6
C38-C39	1.475	C22-C21-S28	109.8
C35-C40	1.395	C21-C22-C29	113.3
C34-C40	1.474	C22-C21-C30	134.4

C40-C41	1.381	C5-C23-C24	127.3
C41-C42	1.377	C5-C23-S25	121.9
C35-C43	1.394	C24-C23-S25	110.8
C43-C44	1.38	C23-C24-C26	114.1
C42-C44	1.397	C23-S25-C27	92.1
C39-C45	1.395	C24-C26-C27	113.3
C37-C45	1.475	S25-C27-C26	109.8
C45-C46	1.381	S25-C27-C31	115.7
C39-C47	1.393	C26-C27-C31	134.5
C46-C48	1.377	C21-S28-C20	92.1
C47-C49	1.38	S28-C21-C30	115.7
C48-C49	1.397	S28-C20-C29	110.8
C37-O50	1.211	C22-C29-C20	114
C34-O51	1.211	C21-C30-C32	133
C38-C52	1.371	C27-C31-C36	133.1
C33-C53	1.371	C30-C32-C33	125.1
C54-C55	1.774	C30-C32-C34	127.1
C55-C56	1.389	C33-C32-C34	107.6
C55-C57	1.389	C32-C33-C35	107.4
C56-C58	1.386	C32-C33-C53	128.3
C57-C59	1.385	C32-C34-C40	106
C59-C60	1.389	C33-C35-C40	108.7
C7-N61	1.41	C33-C35-C43	132.1
C2-N61	1.409	C35-C33-C53	124.3
C54-N61	1.716	C31-C36-C37	127.2
C54-O62	1.44	C31-C36-C38	125
C54-O63	1.44	C37-C36-C38	107.6
C52-C64	1.423	C36-C37-C45	106
C64-C65	1.155	C36-C37-O50	129.3
C52-C66	1.423	C36-C38-C39	107.4
C66-N67	1.155	C36-C38-C52	128.2
C53-C68	1.423	C38-C39-C45	108.6
C68-N69	1.155	C38-C39-C47	132.1
C53-C70	1.423	C39-C38-C52	124.3
C70-N71	1.156	C35-C40-C34	110.2
C9-C72	1.493	C35-C40-C41	123.1
C49-F73	1.323	C40-C35-C43	119.2
C48-F74	1.323	C34-C40-C41	126.7
C42-F75	1.323	C40-C34-O51	124.7
C44-F76	1.323	C40-C41-C42	117.2

DFT=density functional theory

Table S16: Bond lengths (Å) and bond angles (°) for **PSCD2**

BOND LENGTH	**BOND ANGLE**

DFT		DFT	
C1-C2	1.408	C1-C2-C3	121.7
C2-C3	1.388	C2-C1-C6	119.2
C3-C4	1.382	C2-C1-C8	107.4
C4-C5	1.402	C1-C2-N61	108.8
C5-C6	1.396	C2-C3-C4	117.9
C1-C6	1.39	C3-C2-N61	129.4
C7-C8	1.415	C3-C4-C5	121.9
C1-C8	1.45	C4-C5-C6	119.3
C8-C9	1.397	C4-C5-C23	121.2
C7-C10	1.387	C5-C6-C1	120
C9-C11	1.396	C6-C5-C23	119.5
C11-C12	1.409	C6-C1-C8	133.3
C10-C12	1.377	C7-C8-C1	106.9
C12-O13	1.362	C7-C8-C9	121.4
O13-C14	1.361	C8-C7-C10	122.9
C14-C15	1.402	C8-C7-N61	108.8
C11-C15	1.448	C1-C8-C9	131.7
C15-C16	1.395	C8-C9-C11	116.5
C14-C17	1.375	8C-C9-C72	121.3
C16-C18	1.381	C7-C10-C12	114.2
C17-C19	1.397	C10-C7-N61	128.2
C18-C19	1.406	C9-C11-C12	119.9
C19-C20	1.456	C9-C11-C15	135.3
C21-C22	1.388	C11-C9-C72	122.3
C5-C23	1.457	C11-C12-C10	125.1
C23-C24	1.383	C11-C12-O13	111.8
C23-S25	1.721	C12-C11-C15	104.8
C24-C26	1.393	C10-C12-O13	123.1
S25-C27	1.76	C12-O13-C14	106.3
C26-C27	1.388	O13-C14-C15	111.8
C21-S28	1.759	O13-C14-C17	124.2
C20-S28	1.722	C14-C15-C11	105.3
C22-C29	1.393	C14-C15-C16	117.7
C20-C29	1.383	C15-C14-C17	124
C21-C30	1.417	C11-C15-C16	137
C27-C31	1.416	C15-C16-C18	119.4
C30-C32	1.37	C14-C17-C19	117.6
C32-C33	1.463	C16-C18-C19	121.9
C32-C34	1.481	C17-C19-C18	119.4
C33-C35	1.476	C17-C19-C20	121
C31-C36	1.37	C18-C19-C20	119.6
C36-C37	1.481	C19-C20-S28	121.7

C36-C38	1.463	C19-C20-C29	127.5
C38-C39	1.476	C22-C21-S28	109.8
C35-C40	1.395	2C1-C22-C29	113.3
C34-C40	1.475	C22-C21-C30	134.4
C40-C41	1.376	C5-C23-C24	127.4
C41-C42	1.386	C5-C23-S25	121.8
C35-C43	1.39	C24-C23-S25	110.8
C43-C44	1.39	C23-C24-C26	114.1
C42-C44	1.402	C23-S25-C27	92.1
C39-C45	1.395	C24-C26-C27	113.3
C37-C45	1.476	C25-C27-C26	109.8
C45-C46	1.377	S25-C27-C31	115.6
C39-C47	1.389	C26-C27-C31	134.6
C46-C48	1.387	C21-S28-C20	92.1
C47-C49	1.39	S28-C21-C30	115.7
C48-C49	1.402	S28-C20-C29	110.8
C37-O50	1.211	C22-C29-C20	114
C34-O51	1.211	C21-C30-C32	133
C38-C52	1.371	C27-C31-C36	133.2
C33-C53	1.371	C30-C32-C33	125.1
S54-C55	1.774	C30-C32-C34	127.1
C55-C56	1.389	C33-C32-C34	107.7
C55-C57	1.389	C32-C33-C35	107.3
C56-C58	1.386	C32-C33-C53	128.3
C57-C59	1.385	C32-C34-C40	105.9
C58-C60	1.388	C32-C34-O51	129.3
C59-C60	1.389	C33-C35-C40	108.7
C7-N61	1.41	C33-C35-C43	132.3
C2-N61	1.409	C35-C33-C53	124.3
S54-N61	1.716	C31-C36-C37	127.2
S54-O62	1.44	C31-C36-C38	125
S54-C63	1.44	C37-C36-C38	107.7
C52-C64	1.423	C36-C37-C45	105.9
C64-N65	1.155	C36-C37-O50	129.3
C52-C66	1.423	C36-C38-C39	107.3
C66-N67	1.155	C36-C38-C52	128.3
C53-C68	1.423	C38-C39-C45	108.7
C68-N69	1.155	C38-C39-C47	132.3
C53-C70	1.423	C39-C38-C52	124.4
C70-N71	1.156	C35-C40-C34	110.2
C9-C72	1.493	C35-C40-C41	122.8
C42-Cl73	1.727	C40-C35-C43	119
C44-Cl74	1.728	C34-C40-C41	127

C48-Cl75	1.727	C40-C34-O51	124.7
C49-Cl76	1.728	C40-C41-C42	118.2

DFT=density functional theory

Table S17: Bond lengths (Å) and bond angles (°) for **PSCD3**

BOND LENGTH		**BOND ANGLE**	
DFT		DFT	
C1-C2	1.408	C1-C2-C3	121.7
C2-C3	1.389	C2-C1-6	119.2
C3-C4	1.382	C2-C1-8	107.4
C4-C5	1.403	C1-C2-N61	108.7
C5-C6	1.396	C2-C3-C4	117.9
C1-C6	1.389	C3-C2-N61	129.5
C7-C8	1.414	C3-C4-C5	121.9
C1-C8	1.449	C4-C5-C6	119.3
C8-C9	1.397	C4-C5-C23	121.3
C7-C10	1.387	C5-C6-C1	119.9
C9-C11	1.396	C6-C5-C23	119.4
C11-C12	1.409	C6-C1-C8	133.3
C10-C12	1.376	C7-C8-C1	106.9
C12-O13	1.362	C7-C8-C9	121.5
O13-C14	1.361	C8-C7-C10	122.8
C14-C15	1.402	C8-C7-N61	108.7
C11-C15	1.449	C1-C8-C9	131.6
C15-C16	1.396	C8-C9-C11	116.5
C14-C17	1.375	C8-C9-C72	120.9
C16-C18	1.381	C7-C10-C12	114.2
C17-C19	1.397	C10-C7-N61	128.4
C18-C19	1.406	C9-C11-C12	119.8
C19-C20	1.455	C9-C11-C15	135.4
C21-C22	1.39	C11-C9-C72	122.6
C5-C23	1.456	C11-C12-C10	125.2
C23-C24	1.385	C11-C12-O13	111.8
C23-S25	1.72	C12-C11-C15	104.8
C24-C26	1.39	C10-C12-O13	123
S25-C27	1.761	C12-O13-C14	106.3
C26-C27	1.39	O13-C14-C15	111.8
C21-C28	1.76	O13-C14-C17	124.1
C20-C28	1.72	C14-C15-C11	105.3
C20-C29	1.385	C14-C15-C16	117.7
C22-C29	1.39	C15-C14-C17	124.1
C21-C30	1.413	C11-C15-C16	137
C27-C31	1.412	C15-C16-C18	119.4
C30-C32	1.374	C14-C17-C19	117.6

C32-C33	1.46	C16-C18-C19	121.9
C32-C34	1.476	C17-C19-C18	119.4
C33-C35	1.48	C17-C19-C20	121
C31-C36	1.374	C18-C19-C20	119.6
C36-C37	1.476	C19-C20-S28	121.7
C36-C38	1.46	C19-C20-C29	127.4
C38-C39	1.48	C22-C21-S28	109.8
C35-C40	1.395	C21-C22-C29	113.3
C34-C40	1.48	C22-C21-C30	134.4
C40-C41	1.376	C5-C23-C24	127.2
C41-C42	1.392	C5-C23-C25	121.9
C35-C43	1.39	C24-C23-C25	110.8
C43-C44	1.395	C23-C24-C26	114.1
C42-C44	1.41	C23-C25-C27	92.1
C39-C45	1.395	C24-C26-C27	113.3
C37-C45	1.48	C25-C27-C26	109.7
C45-C46	1.376	C25-C27-C31	115.9
C39-C47	1.39	C26-C27-C31	134.3
C46-C48	1.392	S28-C21-C30	115.8
C47-C49	1.395	S28-C20-C29	110.9
C48-C49	1.41	C20-C29-C22	114
C37-O50	1.211	C21-C30-C32	133
C34-O51	1.211	C27-C31-C36	133
C38-C52	1.371	C30-C32-C33	125
C33-C53	1.371	C30-C32-C34	127
S54-C55	1.773	C33-C32-C34	107.8
C55-C56	1.389	C32-C33-C35	107.4
C55-C57	1.389	C32-C33-C53	128.5
C56-C58	1.386	C32-C34-C40	106
C57-C59	1.385	C32-C34-O51	129.8
C58-C60	1.388	C33-C35-C40	108.5
C59-C60	1.389	C33-C35-C43	132.4
C7-N61	1.409	C35-C33-C53	124.1
C2-N61	1.407	C31-C36-C37	127
S54-N61	1.718	C31-C36-C38	124.9
S54-O62	1.439	C37-C36-C38	107.8
S54-O63	1.439	C36-C37-C45	105.9
C52-C64	1.423	C36-C37-O50	129.8
C64-N65	1.155	C36-C38-C39	107.3
C52-C66	1.423	C36-C38-C52	128.4
C66-N67	1.155	C38-C39-C45	108.5
C53-C68	1.423	C38-C39-C47	132.4
C68-N69	1.155	C39-C38-C52	124.1

C53-C70	1.423	C35-C40-C34	110.1
C70-N71	1.155	C35-C40-C41	123.1
C9- C72	1.493	C40-C35-C43	119.1
C44-C73	1.428	C34-C40-C41	126.8
C73-N74	1.153	C40-C34-O51	124.2
C42-C75	1.426	C40-C41-C42	118.2
C75-N76	1.153	C41-C42-C44	119.6
C48-C77	1.426	C41-C42-C75	119.8
C77-N78	1.153	C35-C43-C44	118.7
C49-C79	1.428	C43-C44-C42	121.3
C79-N80	1.153	C43-C44-C73	118.9

DFT=density functional theory

Table S18: Bond lengths (Å) and bond angles (°) for **PSCD4**

BOND LENGTH		**BOND ANGLE**	
DFT		DFT	
C1-C2	1.408	C1-C2-C3	121.8
C2-C3	1.389	C2-C1-C6	119.2
C3-C4	1.381	C2-C1-C8	107.4
C4-C5	1.403	C1-C2-N61	108.8
C1-C6	1.389	C2-C3-C4	117.9
C5-C6	1.396	C3-C2-N61	129.4
C7-C8	1.415	C3-C4-C5	121.9
C1-C8	1.449	C4-C5-C6	119.3
C8-C9	1.397	C4-C5-C23	121.2
C7-C10	1.387	C1-C6-C5	120
C9-C11	1.396	C6-C1-C8	133.3
C11-C12	1.409	C6C-C5-C23	119.5
C10-C12	1.376	C7-C8-C1	106.8
C12-O13	1.362	C7-C8-C9	121.4
C13-C14	1.361	C8-C7-C10	122.9
C14-C15	1.402	C8-C7-N61	108.8
C11-C15	1.448	C1-C8-C9	131.7
C15-C16	1.396	C8-C9-C11	116.4
C14-C17	1.375	C8-C9-C72	121.3
C16-C18	1.381	C7-C10-C12	114.2
C17-C19	1.398	C10-C7-N61	128.3
C18-C19	1.406	C9-C11-C12	119.9
C19-C20	1.455	C9-C11-C15	135.3
C21-C22	1.39	C11-C9-C72	122.3
C5-C23	1.456	C11-C12-C10	125.1
C23-C24	1.386	C11-C12-O13	111.8
C23-S25	1.719	C12-C11-C15	104.8

C24-C26	1.39	C10-C12-O13	123.1
S25-C27	1.761	C12-O13-C14	106.3
C26-C27	1.391	O13-C14-C15	111.8
C21-S28	1.76	O13-C14-C17	124.2
C20-S28	1.72	C14-C15-C11	105.3
C20-C29	1.386	C14-C15-C16	117.7
C22-C29	1.39	C15-C14-C17	124
C21-C30	1.412	C11-C15-C16	136.9
C27-C31	1.412	C15-C16-C18	119.4
C30-C32	1.374	C14-C17-C19	117.6
C32-C33	1.46	C16-C18-C19	121.8
C32-C34	1.476	C17-C19-C18	119.5
C33-C35	1.48	C17-C19-C20	120.9
C31-C36	1.374	C18-C19-C20	119.7
C36-C37	1.475	C19-C20-S28	121.6
C36-C38	1.46	C19-C20-C29	127.5
C38-C39	1.481	C22-C21-S28	109.8
C35-C40	1.393	C21-C22-C29	113.3
C34-C40	1.48	C22-C21-C30	134.6
C40-C41	1.379	C5-C23-C24	127.3
C41-C42	1.38	C5-C23-S25	121.8
C35-C43	1.393	C24-C23-S25	110.8
C43-C44	1.382	C23-C24-C26	114.1
C42-C44	1.392	C23-S25-C27	92.1
C39-C45	1.393	C24-C26-C27	113.3
C37-C45	1.48	S25-C27-C26	109.7
C45-C46	1.379	S25-C27-C31	115.8
C39-C47	1.393	C26-C27-C31	134.5
C46-C48	1.38	C21-S28-C20	92
C47-C49	1.383	S28-C21-C30	115.6
C48-C49	1.392	S28-C20-C29	110.9
C37-O50	1.21	C20-C29-C22	114
C34-O51	1.21	C21-C30-C32	133.2
C38-C52	1.37	C27-C31-C36	133.1
C33-C53	1.37	C30-C32-C33	125.1
S54-C55	1.773	C30-C32-C34	126.9
C55-C56	1.389	C33-C32-C34	107.9
C55-C57	1.389	C32-C33-C35	107.3
C56-C58	1.386	C32-C33-C53	128.8
C57-C59	1.385	C32-C34-C40	106
C58-C60	1.388	C32-C34-O51	129.8
C59-C60	1.389	C33-C35-C40	108.6
C7-N61	1.409	C33-C35-C43	132.3

C2-N61	1.407	C35-C33-C53	123.9
S54-N61	1.719	C31-C36-C37	126.9
S54-O62	1.439	C31-C36-C38	125.1
S54-O63	1.439	C37-C36-C38	107.9
C52-C64	1.423	C36-C37-C45	106
C64-N65	1.155	C36-C37-O50	129.8
C52-C66	1.423	C36-C38-C39	107.3
C66-N67	1.155	C36-C38-C52	128.7
C53-C68	1.423	C38-C39-C45	108.5
C68-N69	1.155	C38-C39-C47	132.3
C53-C70	1.423	C39-C38-C52	123.9
C70-N71	1.155	C35-C40-C34	110.1
C9-C72	1.493	C35-C40-C4	123
C48-N73	1.478	C40-C35-C43	119.1
N73-O74	1.208	C34-C40-C41	126.8
N73-O75	1.208	C40-C34-O51	124.3
C49-N76	1.481	C40-C41-C42	117.4
N76-O77	1.206	C41-C42-C44	120.4
N76-O78	1.207	C41-C42-N82	117.7
C44-N79	1.481	C35-C43-C44	117.9
N79-O80	1.207	C43-C44-C42	122.1
N79-O81	1.206	C43-C44-N79	116.5
C42-N82	1.478	C42-C44-N79	121.2
N82-O83	1.208	C44-C42-C82	121.7
N82-O84	1.208	C39-C45-C37	110.1

DFT=density functional theory

Table S19: Bond lengths (Å) and bond angles (°) for **PSCD5**

BOND LENGTH		**BOND ANGLE**	
DFT		DFT	
C1-C2	1.409	C1-C2-C3	121.7
C2-C3	1.389	C2-C1-C6	119.2
C3-C4	1.381	C2-C1-C8	107.4
C4-C5	1.403	C1-C2-N61	108.8
C1-C6	1.389	C2-C3-C4	117.9
C5-C6	1.396	C3-C2-N61	129.5
C7-C8	1.415	C3-C4-C5	121.9
C1-C8	1.45	C4-C5-C6	119.3
C8-C9	1.397	C4-C5-C23	121.1
C7-C10	1.387	C1-C6-C5	120
C9-C11	1.397	C6-C1-C8	133.3
C11-C12	1.409	C6-C5-C23	119.6
C10-C12	1.376	C7-C8-C1	106.8

C12-O13	1.362	C7-C8-C9	121.4
O13-C14	1.361	C8-C7-C10	122.9
C11-C15	1.448	C8-C7-N61	108.8
C14-C15	1.402	C1-C8-C9	131.8
C15-C16	1.396	C8-C9-C11	116.4
C14-C17	1.375	C8-C9-C72	121.3
C16-C18	1.381	C7-C10-C12	114.2
C17-C19	1.398	C10-C7-N61	128.3
C18-C19	1.406	C9-C11-C12	119.9
C19-C20	1.455	C9-C11-C15	135.3
C21-C22	1.39	C11-C9-C72	122.3
C5-C23	1.455	C11-C12-C10	125.1
C23-C24	1.386	C11-C12-O13	111.8
C23-S25	1.72	C12-C11-C15	104.8
C24-C26	1.39	C10-C12-O13	123.1
S25-C27	1.76	C12-O13-C14	106.3
C26-C27	1.391	O13-C14-C15	111.8
C21-S28	1.759	O13-C14-C17	124.1
C20-S28	1.72	C11-C15-C14	105.3
C20-C29	1.386	C11-C15-C16	137
C22-C29	1.391	C14-C15-C16	117.7
C21-C30	1.412	C15-C14-C17	124
C27-C31	1.411	C15-C16-C18	119.4
C30-C32	1.374	C14-C17-C19	117.6
C32-C33	1.46	C16-C18-C19	121.8
C32-C34	1.476	C17-C19-C18	119.5
C33-C35	1.48	C17-C19-C20	120.8
C31-C36	1.375	C18-C19-C20	119.7
C36-C37	1.475	C19-C20-S28	121.5
C36-C38	1.459	C19-C20-C29	127.6
C38-C39	1.48	C22-C21-S28	109.8
C35-C40	1.389	C21-C22-C29	113.3
C34-C40	1.483	C22-C21-C30	134.6
C40-C41	1.38	C5-C23-C24	127.5
C41-C42	1.385	C5-C23-S25	121.7
C35-C43	1.393	C24-C23-S25	110.8
C43-C44	1.387	C23-C24-C26	114.1
C42-C44	1.406	C23-S25-C27	92.1
C39-C45	1.389	C24-C26-C27	113.3
C37-C45	1.482	S25-C27-C26	109.8
C45-C46	1.38	S25-C27-C31	115.9
C39-C47	1.393	C26-C27-C31	134.3
C46-C48	1.385	C21-S28-C20	92

C47-C49	1.387	S28-C21-C30	115.6
C48-C49	1.406	S28-C20-C29	110.9
C37-O50	1.21	C20-C29-C22	114
C34-O51	1.21	C21-C30-C32	133.2
C38-C52	1.37	C27-C31-C36	132.8
C33-C53	1.37	C30-C32-C33	125
S54-C55	1.773	C30-C32-C34	127
C55-C56	1.389	C33-C32-C34	107.9
C55-C57	1.389	C32-C33-C35	107.2
C56-C58	1.386	C32-C33-C53	128.8
C57-C59	1.385	C32-C34-C40	105.9
C58-C60	1.388	C32-C34-O51	129.8
C59-C60	1.389	C33-C35-C40	108.7
C7-N61	1.409	C33-C35-C43	132.2
C2-N61	1.407	C35-C33-C53	123.9
S54-N61	1.719	C31-C36-C37	126.8
S54-O62	1.439	C31-C36-C38	125.1
S54-O63	1.439	C37-C36-C38	107.9
C52-C64	1.423	C36-C37-C45	105.9
C64-N65	1.155	C36-C37-O50	129.9
C52-C66	1.423	C36-C38-C39	107.3
C66-N67	1.155	C36-C38-C52	128.7
C53-C68	1.423	C38-C39-C45	108.7
C68-N69	1.155	C38-C39-C47	132.3
C53-C70	1.423	C39-C38-C52	124
C70-N71	1.155	C35-C40-C34	110.1
C9-C72	1.493	C35-C40-C41	122.8
O77-S81	1.453	C40-C35-C43	119.1
C44-S81	1.802	C34-C40-C41	127.1
O78-S81	1.429	C40-C34-O51	124.4
O80-S82	1.453	C40-C41-C42	118.2
O79-S82	1.43	C41-C42-C44	119.7
C42-S82	1.799	C41-C42-S82	115.8
O73-S83	1.453	C35-C43-C44	118.7
O74-S83	1.43	C43-C44-C42	121.4
C48-S83	1.8	C43-C44-S81	114.7
C49-S84	1.802	C42-C44-S81	123.9
O75-S84	1.428	C44-C42-S82	124.4
O76-S84	1.453	C39-C45-C37	110.1
S81-O85	1.58	C39-C45-C46	122.9
S82-O86	1.58	C45-C39-C47	119.1
S83-O87	1.58	C37-C45-C46	127
S84-O88	1.581	C45-C37-O50	124.2

DFT=density functional theory

Table S20: Bond lengths (Å) and bond angles (°) for **PSCD6**

BOND LENGTH		**BOND ANGLE**	
DFT		DFT	
C1-C2	1.408	C1-C2-C3	121.7
C2-C3	1.389	C2-C1-C6	119.2
C3-C4	1.382	C2-C1-C8	107.4
C4-C5	1.403	C1-C2-N61	108.8
C1-C6	1.389	C2-C3-C4	117.9
C5-C6	1.396	C3-C2-N61	129.5
C7-C8	1.415	C3-C4-C5	121.9
C1-C8	1.449	C4-C5-C6	119.2
C8-C9	1.397	C4-C5-C23	121.2
C7-C10	1.387	C1-C6-C5	120
C9-C11	1.396	C6-C1-C8	133.3
C11-C12	1.408	C6-C5-C23	119.5
C10-C12	1.377	C7-C8-C1	106.9
C12-O13	1.362	C7-C8-C9	121.4
O13-C14	1.361	C8-C7-C10	122.9
C14-C15	1.402	C8-C7-N61	108.8
C11-C15	1.448	C1-C8-C9	131.7
C15-C16	1.395	C8-C9-C11	116.4
C14-C17	1.375	C8-C9-C72	121.3
C16-C18	1.381	C7-C10-C12	114.2
C17-C19	1.397	C10-C7-N61	128.3
C18-C19	1.406	C9-C11-C12	119.9
C19-C20	1.455	C9-C11-C15	135.2
C21-C22	1.389	C11-C9-C72	122.3
C5-C23	1.456	C11-C12-C10	125.1
C23-C24	1.385	C11-C12-O13	111.7
C23-S25	1.721	C12-C11-C15	104.8
C24-C26	1.391	C10-C12-O13	123.2
S25-C27	1.76	C12-O13-C14	106.3
C26-C27	1.389	O13-C14-C15	111.8
C21-S28	1.759	O13-C14-C17	124.2
C20-S28	1.721	C14-C15-C11	105.3
C22-C29	1.391	C14-C15-C16	117.8
C20-C29	1.384	C15-C14-C17	124
C21-C30	1.415	C11-C15-C16	136.9
C27-C31	1.414	C15-C16-C18	119.3
C30-C32	1.372	C14-C17-C19	117.6
C32-C33	1.462	C16-C18-C19	121.9

C32-C34	1.479	C17-C19-C18	119.4
C33-C35	1.479	C17-C19-C20	121
C31-C36	1.372	C18-C19-C20	119.5
C36-C37	1.478	C19-C20-S28	121.8
C36-C38	1.461	C19-C20-C29	127.4
C38-C39	1.479	C22-C21-S28	109.8
C35-C40	1.388	C21-C22-C29	113.3
C34-C40	1.478	C22-C21-C30	134.3
C40-C41	1.377	C5-C23-C24	127.4
C41-C42	1.388	C5-C23-S25	121.8
C35-C43	1.391	C24-C23-S25	110.8
C43-C44	1.392	C23-C24-C26	114.1
C42-C44	1.407	C23-S25-C27	92.1
C39-C45	1.389	C24-C26-C27	113.3
C37-C45	1.479	S25-C27-C26	109.8
C45-C46	1.377	S25-C27-C31	115.9
C39-C47	1.39	C26-C27-C31	134.3
C46-C48	1.388	C21-S28-C20	92
C47-C49	1.391	S28-C21-C30	115.9
C48-C49	1.407	S28-C20-C29	110.8
C37-O50	1.211	C22-C29-C20	114
C34-O51	1.21	C21-C30-C32	132.9
C38-C52	1.37	C27-C31-C36	132.9
C33-C53	1.37	C30-C32-C33	125.1
S54-C55	1.774	C30-C32-C34	127.1
C55-C56	1.389	C33-C32-C34	107.7
C55-C57	1.389	C32-C33-C35	107.3
C56-C58	1.386	C32-C33-C53	128.5
C57-C59	1.385	C32-C34-C40	105.9
C58-C60	1.388	C32-C34-O51	129.6
C59-C60	1.389	C33-C35-C40	108.7
C7-N61	1.41	C33-C35-C43	132.6
C2-N61	1.408	C35-C33-C53	124.2
S54-N61	1.717	C31-C36-C37	127
S54-O62	1.44	C31-C36-C38	125
S54-O63	1.44	C37-C36-C38	107.7
C52-C64	1.423	C36-C37-C45	105.9
C64-N65	1.155	C36-C37-O50	129.6
C52-C66	1.423	C36-C38-C39	107.2
C66-N67	1.155	C36-C38-C52	128.4
C53-C68	1.423	C38-C39-C45	108.7
C68-N69	1.155	C38-C39-C47	132.5
C53-C70	1.423	C39-C38-C52	124.3

C70-N71	1.155	C35-C40-C34	110.3
C9-C72	1.493	C35-C40-C41	122.5
C44-C73	1.516	C40-C35-C43	118.7
C42-C74	1.513	C34-C40-C41	127.2
C48-C75	1.513	C40-C34-O51	124.5
C49-C76	1.515	C40-C41-C42	119.2
C73-F77	1.33	C41-C42-C44	119.2
C73-F78	1.331	C41-C42-C74	116.5
C73-F79	1.332	C35-C43-C44	119.7
C74-F80	1.331	C43-C44-C42	120.7
C74-F81	1.328	C43-C44-C73	116.2
C74-F82	1.336	C42-C44-C73	123
C75-F83	1.332	C44-C42-C74	124.2
C75-F84	1.335	C39-C45-C37	110.2
C75-F85	1.328	C39-C45-C46	122.5
C76-F86	1.33	C45-C39-C47	118.8
C76-F87	1.333	C37-C45-C46	127.3
C76-F88	1.331	C45-C37-O50	124.5

DFT=density functional theory

Table S21: IUPAC names of the reference and designed chromophores.

Abbreviation	IUPAC Name
PSCR	2,2'-((2Z,2'Z)-((5,5'-(12-methyl-7-(phenylsulfonyl)-7H-benzofuro[2,3-b]carbazole-3,10-diyl)bis(thiophene-5,2-diyl))bis(methanylylidene))bis(3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile
PSCD1	2,2'-((2Z,2'Z)-((5,5'-(12-methyl-7-(phenylsulfonyl)-7H-benzofuro[2,3-b]carbazole-3,10-diyl)bis(thiophene-5,2-diyl))bis(methanylylidene))bis(5,6-difluoro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile
PSCD2	2,2'-((2Z,2'Z)-((5,5'-(12-methyl-7-(phenylsulfonyl)-7H-benzofuro[2,3-b]carbazole-3,10-diyl)bis(thiophene-5,2-diyl))bis(methanylylidene))bis(5,6-dichloro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile
PSCD3	(2Z,2'Z)-2,2'-((5,5'-(12-methyl-7-(phenylsulfonyl)-7H-benzofuro[2,3-b]carbazole-3,10-diyl)bis(thiophene-5,2-diyl))bis(methanylylidene))bis(1-(dicyanomethylene)-3-oxo-2,3-dihydro-1H-indene-5,6-dicarbonitrile)
PSCD4	2,2'-((2Z,2'Z)-((5,5'-(12-methyl-7-(phenylsulfonyl)-7H-benzofuro[2,3-b]carbazole-3,10-diyl)bis(thiophene-5,2-diyl))bis(methanylylidene))bis(5,6-dinitro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile
PSCD5	(2Z,2'Z)-2,2'-((5,5'-(12-methyl-7-(phenylsulfonyl)-7H-benzofuro[2,3-b]carbazole-3,10-diyl)bis(thiophene-5,2-diyl))bis(methanylylidene))bis(1-(dicyanomethylene)-3-oxo-2,3-dihydro-1H-indene-5,6-disulfonic acid)
PSCD6	2,2'-((2Z,2'Z)-((5,5'-(12-methyl-7-(phenylsulfonyl)-7H-benzofuro[2,3-b]carbazole-3,10-diyl)bis(thiophene-5,2-diyl))bis(methanylylidene))bis(3-oxo-5,6-bis(trifluoromethyl)-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile

Table S22: Equations for calculating global reactivity descriptors (GRDs) of **PSCR** and **PSCD1-PSD6**

$$IP = -E_{HOMO} \quad (1)$$

$$EA = -E_{LUMO} \quad (2)$$

$$X = \frac{[IP + EA]}{2} \quad (3)$$

$$\eta = \frac{[IP - EA]}{2} \quad (4)$$

$$\mu = \frac{E_{HOMO} + E_{LUMO}}{2} \quad (5)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (6)$$

$$\sigma = \frac{1}{2\eta} \quad (7)$$

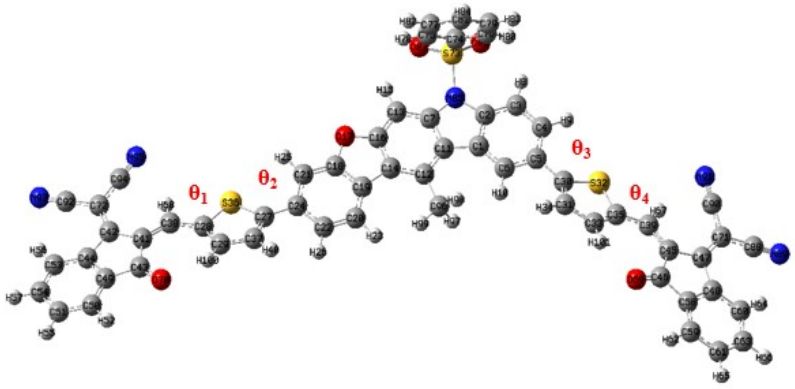
Table S23: Reorganization Energy (*eV*) of entitled Compounds.

Compounds	λ_e **(*eV*)[a]**	λ_h **(*eV*)[b]**
PSCR	0.00032553	0.00023206
PSCD1	0.00034201	-0.00027591
PSCD2	0.00034764	-0.00007466
PSCD3	0.00038431	-0.00029709
PSCD4	0.00011124	-0.00585749
PSCD5	0.00011465	0.00019163

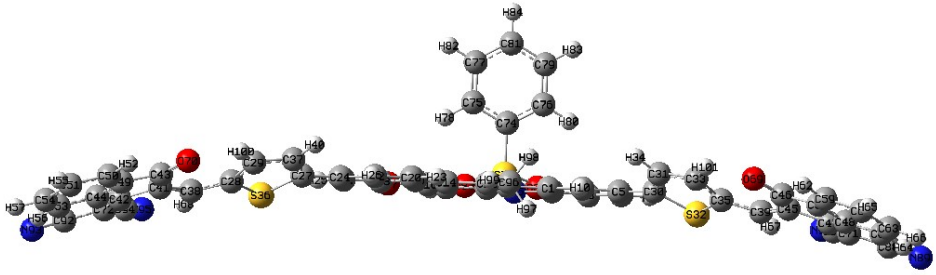
[a] reorganization energy of electron [b] reorganization energy of hole.

Table S24. Hole-electron analysis indices for $S_0 \rightarrow S_1$ excitation (with highest f_{osc}) of compounds **PSCR** to **PSCD6.**

Compound	Excitation	E (*eV*)	*D* (Å)	E_{Coul} (*eV*)	S_r	*H* (Å)	*t* (Å)	HDI	EDI
PSCR	$S_0 \rightarrow S_1$	2.495	2.709	2.2262	0.5765	8.611	-4.506	4.01	4.68
PSCD1	$S_0 \rightarrow S_1$	2.458	2.844	2.1833	0.5577	8.595	-4.199	4.02	4.70
PSCD2	$S_0 \rightarrow S_1$	2.426	2.955	2.1636	0.5547	8.578	-4.046	4.07	4.67
PSCD3	$S_0 \rightarrow S_1$	2.298	3.148	2.0180	0.4947	8.890	-3.442	4.01	4.42
PSCD4	$S_0 \rightarrow S_1$	2.275	4.317	1.8473	0.4540	9.007	-2.889	3.96	4.29
PSCD5	$S_0 \rightarrow S_1$	2.290	2.932	2.0085	0.4867	8.966	-3.341	4.02	4.40
PSCD6	$S_0 \rightarrow S_1$	2.375	2.754	2.1089	0.5283	8.780	-3.779	3.99	4.54

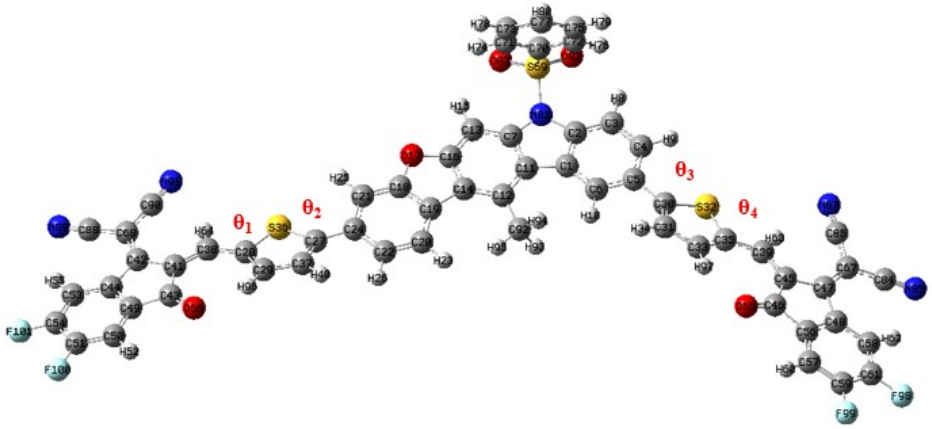


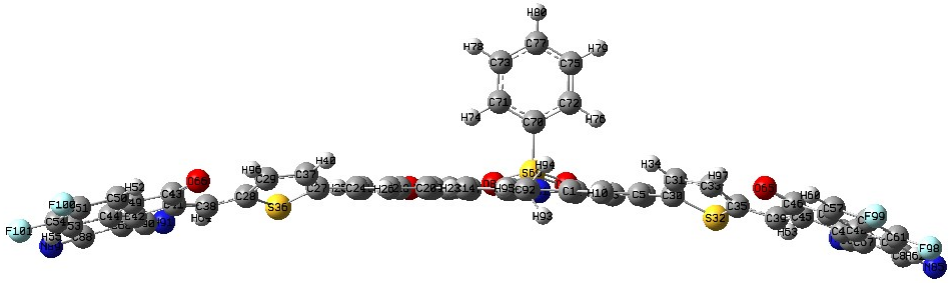
Front View



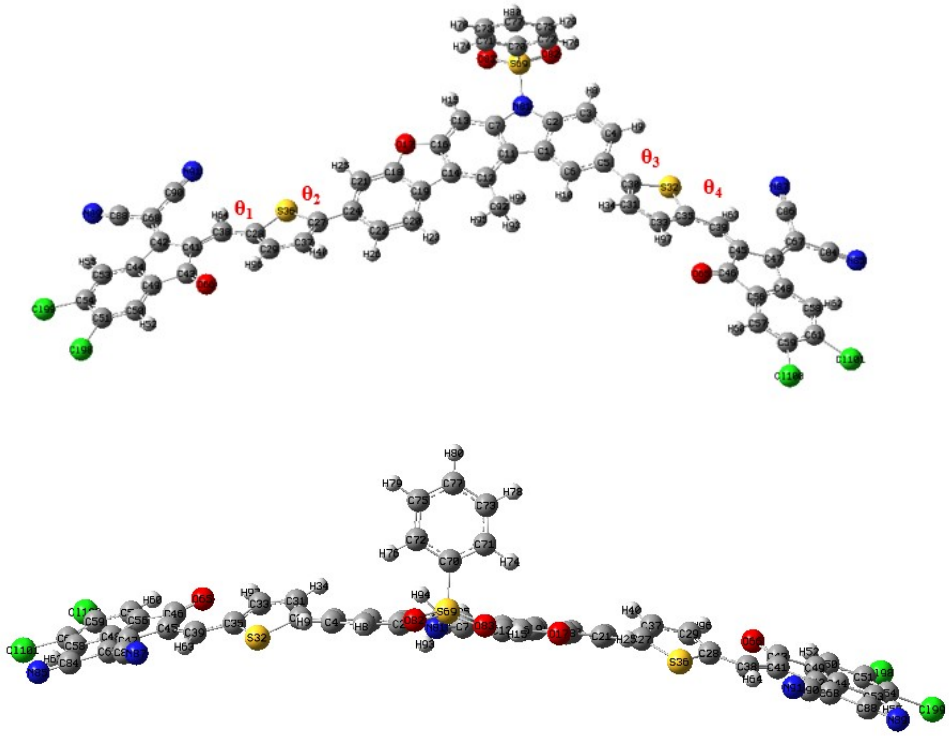
Side View

PSCR

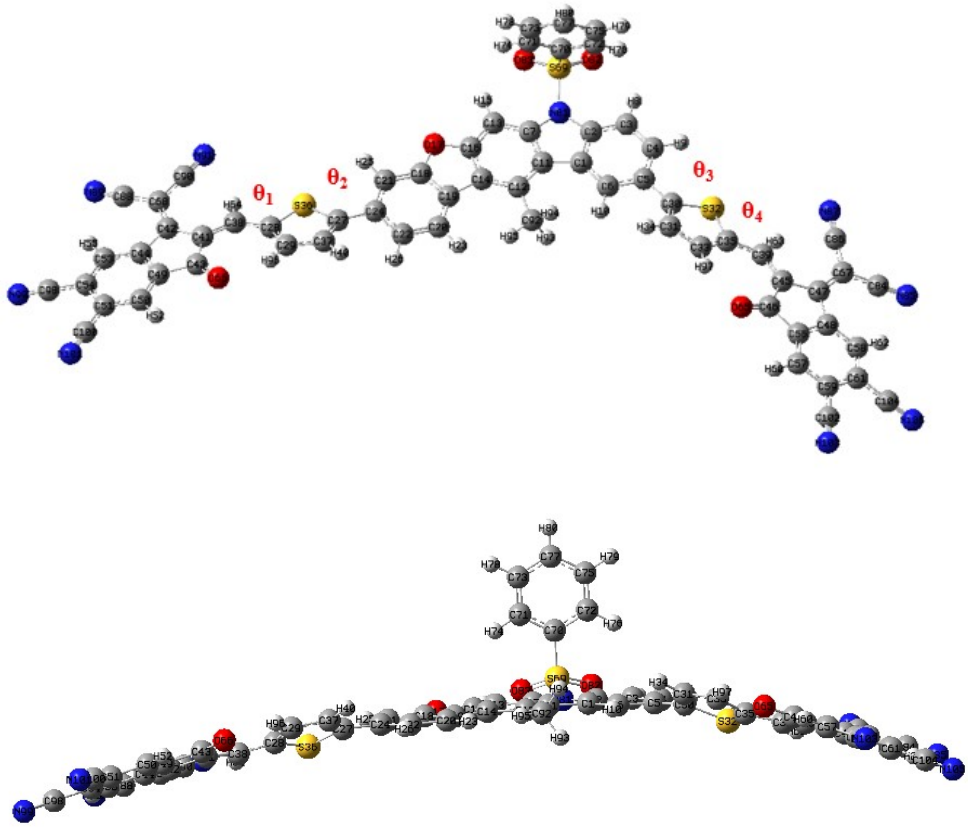




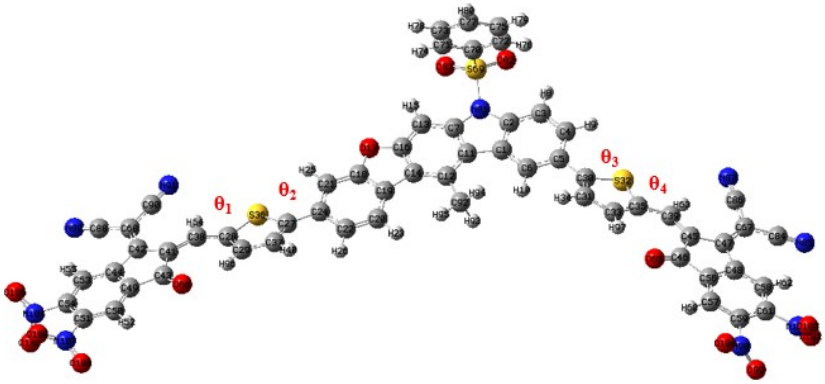
PSCD1

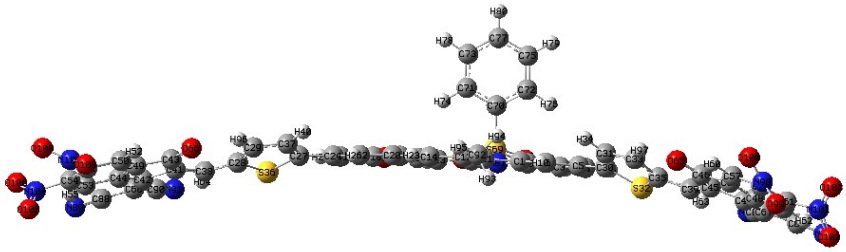


PSCD2

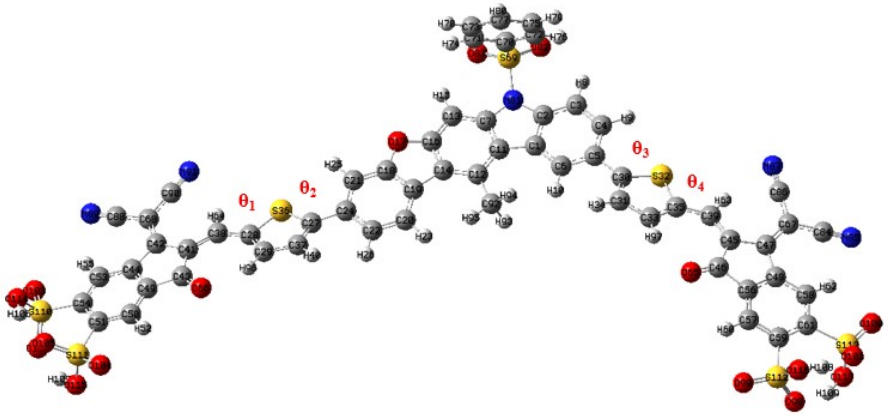


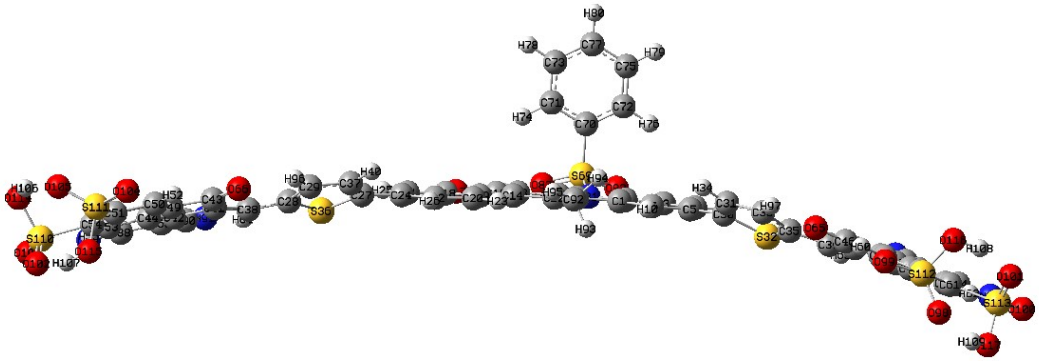
PSCD3



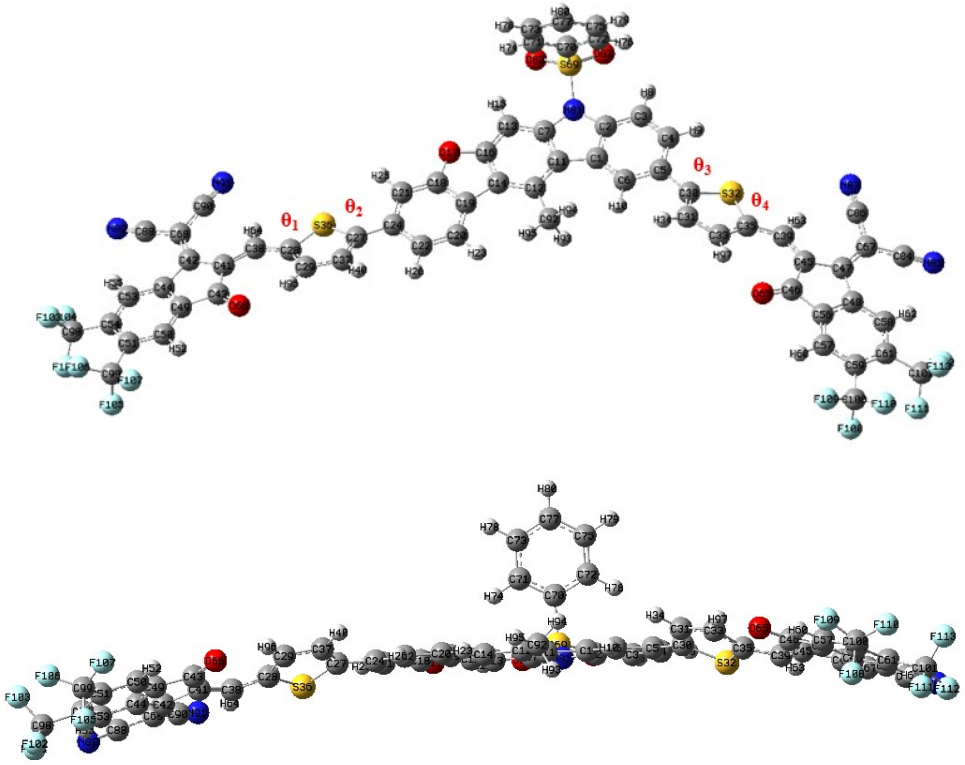


PSCD4



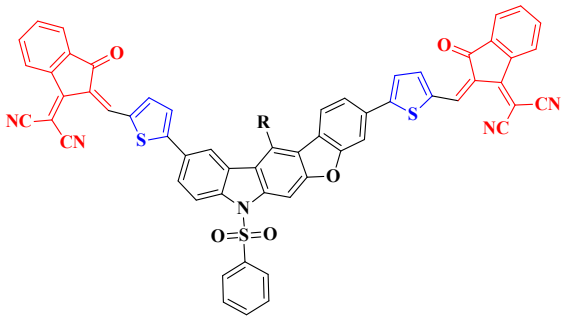


PSCD5

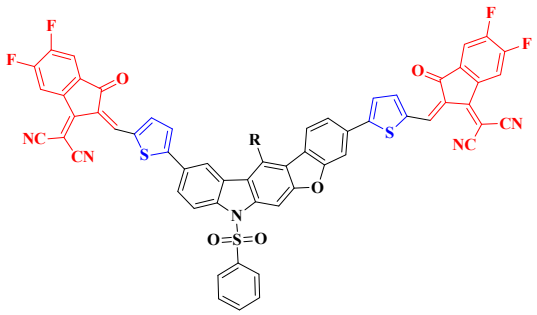


PSCD6

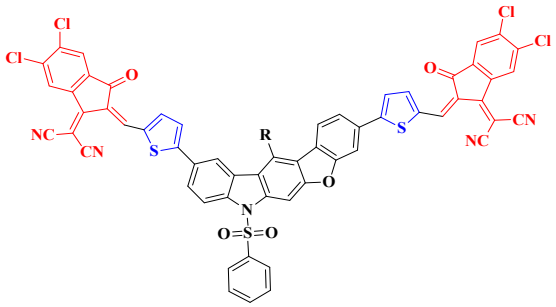
Figure S1: The geometric optimization and dihedral angle (**θ)** of the entitled chromophores (**PSCR** and **PSCD1-PSD6**).



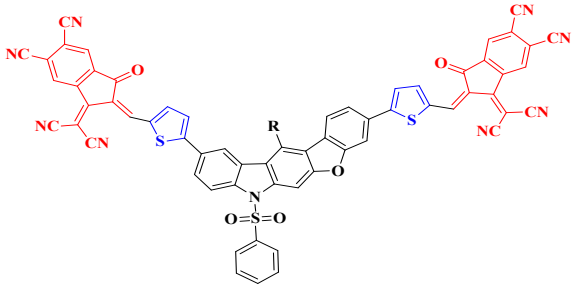
PSCR



PSCD1



PSCD2



PSCD3

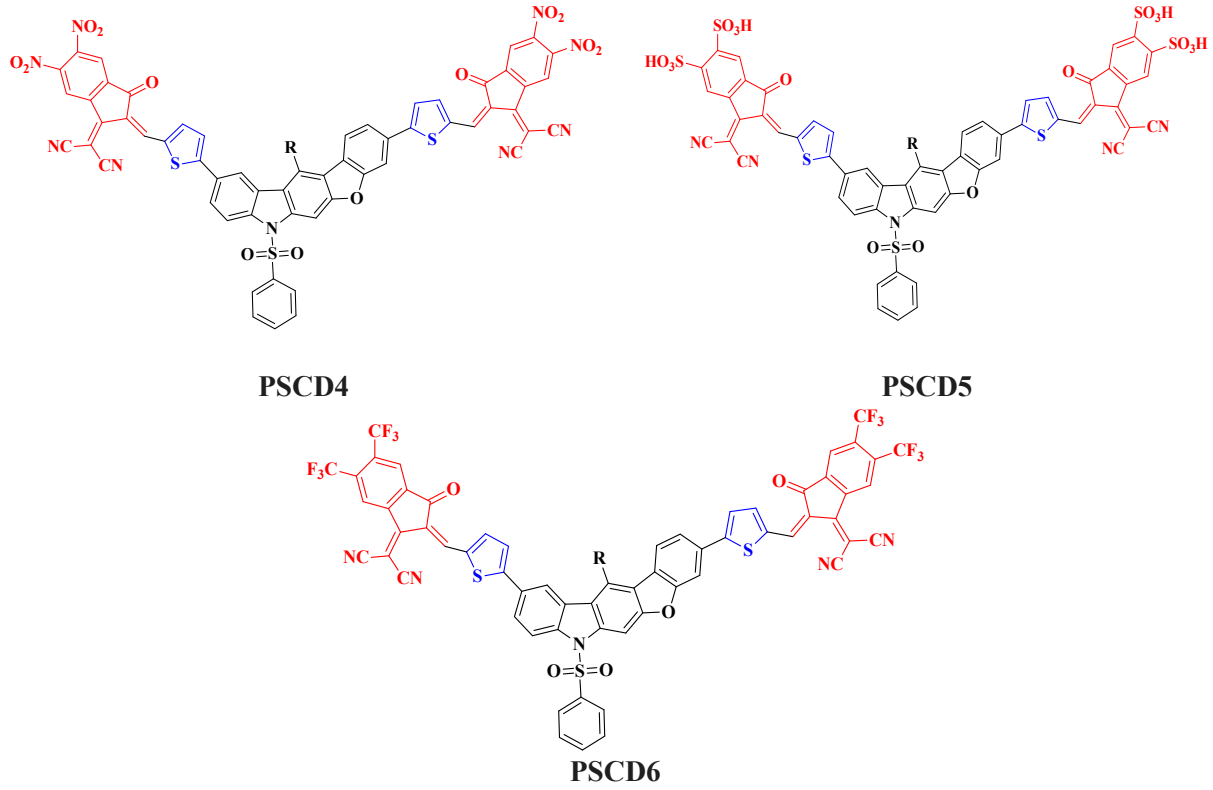
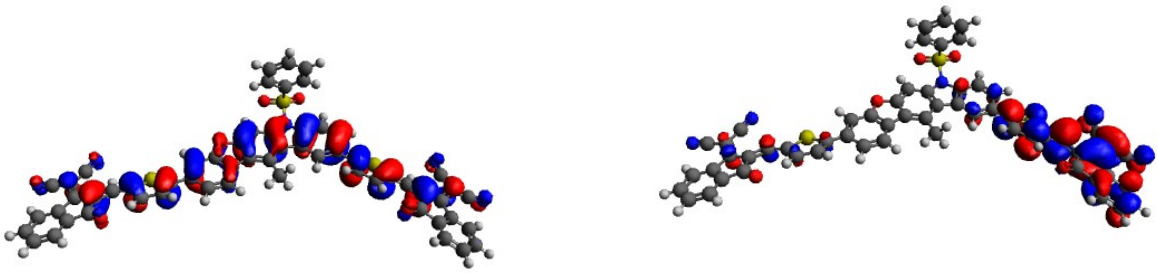
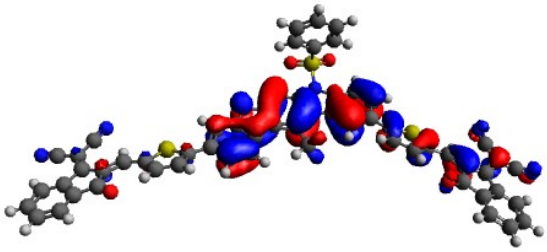
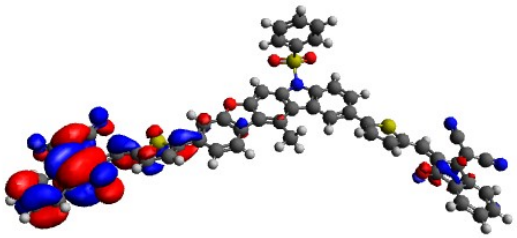


Figure S2: Chemical structures of the studied compounds **PSCR** and **PSCD1-PSD6.**



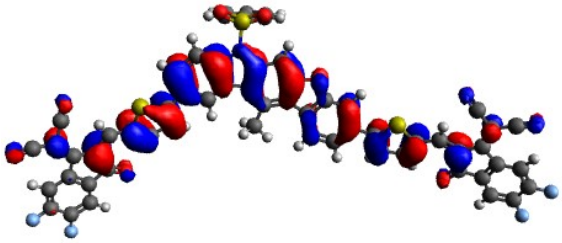


HOMO-2

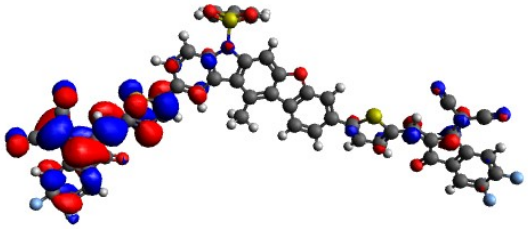


LUMO+2

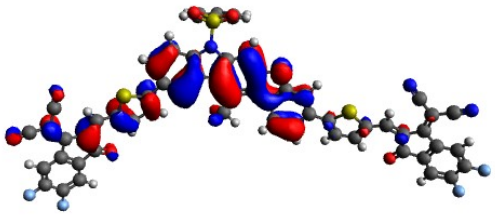
PSCR



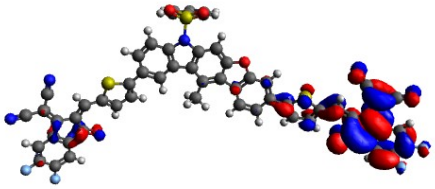
HOMO-1



LUMO+1

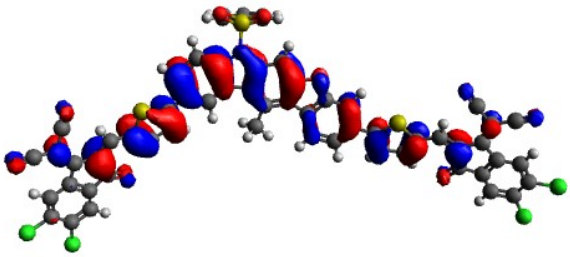


HOMO-2

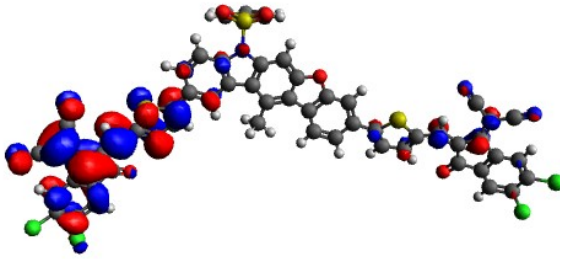


LUMO+2

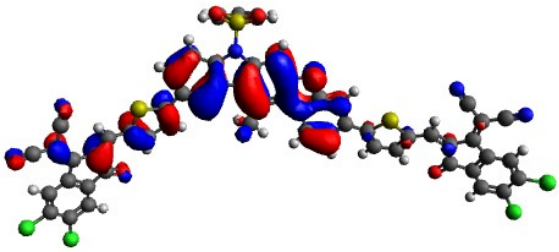
PSCD1



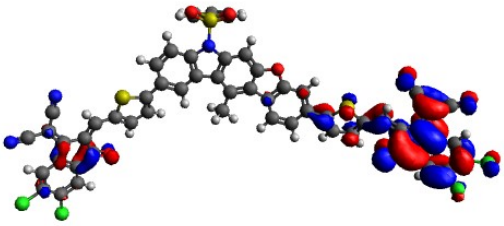
HOMO-1



LUMO+1

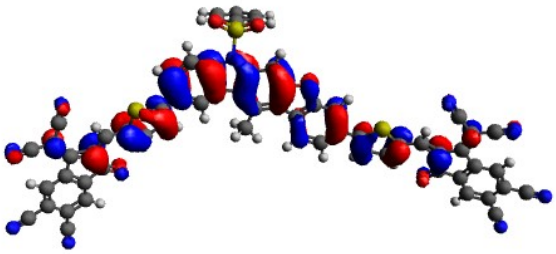


HOMO-2

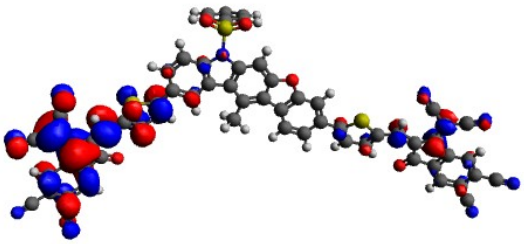


LUMO+2

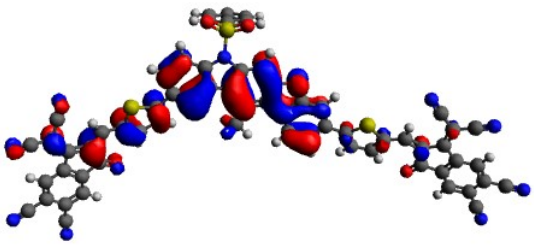
PSCD2

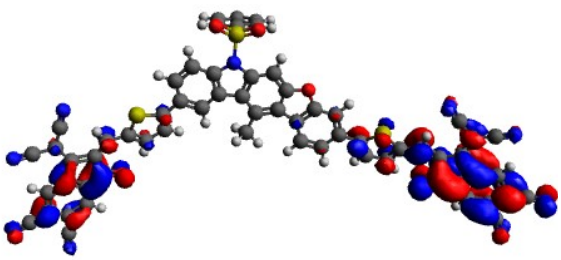


HOMO-1



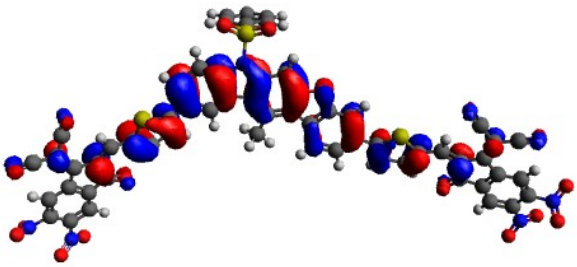
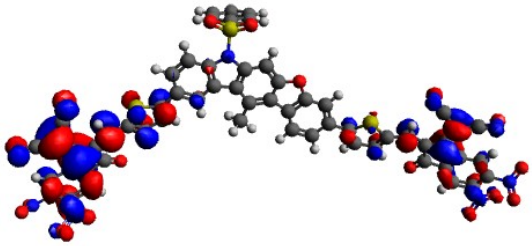
LUMO+1



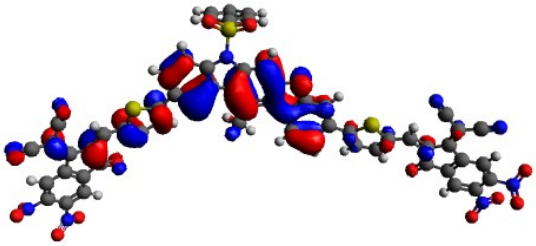
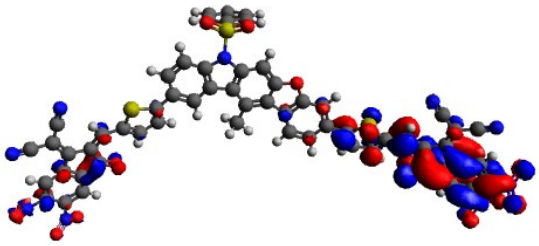


HOMO-2 **LUMO+2**

PSCD3

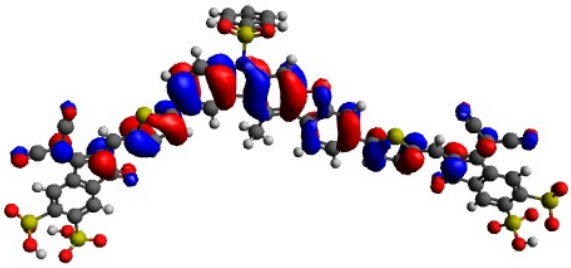
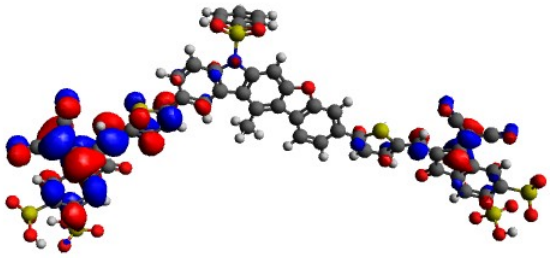



HOMO-1 **LUMO+1**

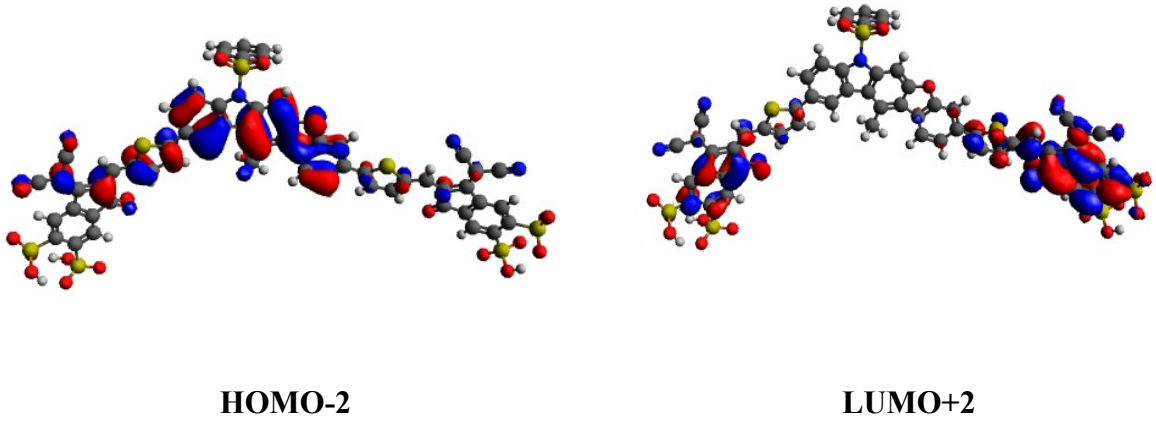



HOMO-2 **LUMO+2**

PSCD4

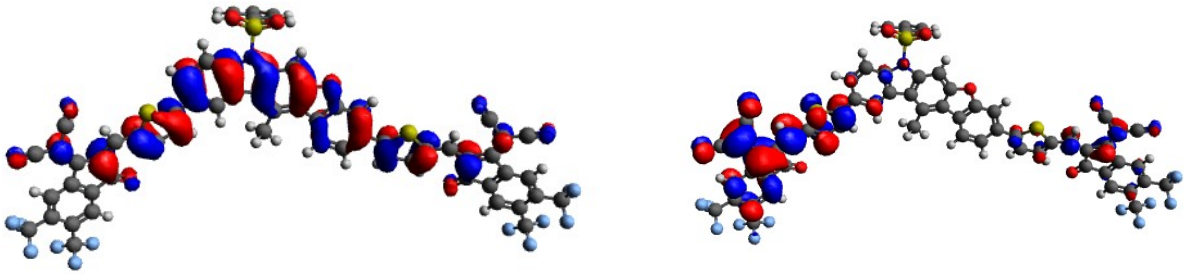



HOMO-1 **LUMO+1**

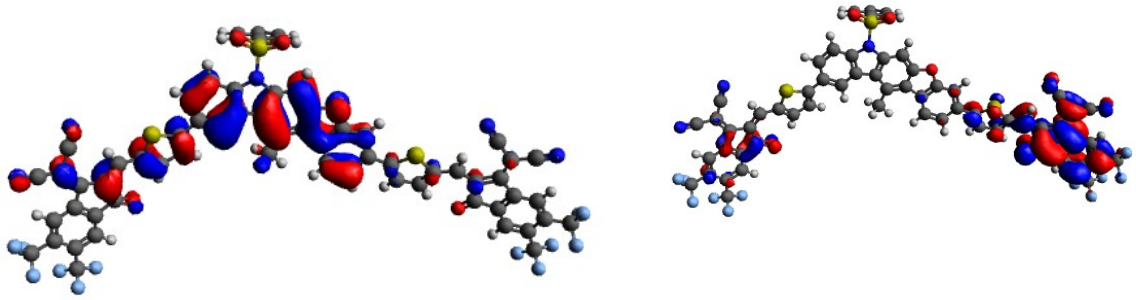


HOMO-2 **LUMO+2**

PSCD5



HOMO-1 **LUMO+1**



HOMO-2 **LUMO+2**

PSCD6

Figure S3: HOMO-1/LUMO+1 and HOMO-2/LUMO+2 of the entitled compounds (**PSCR** and **PSCD1-PSD6**).

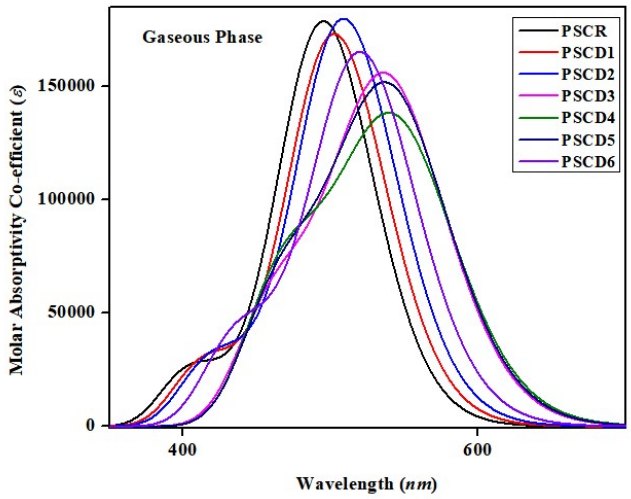
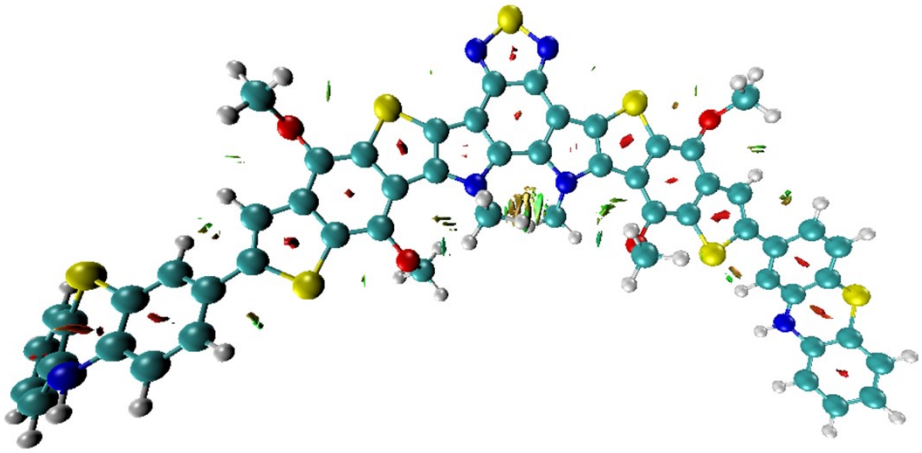
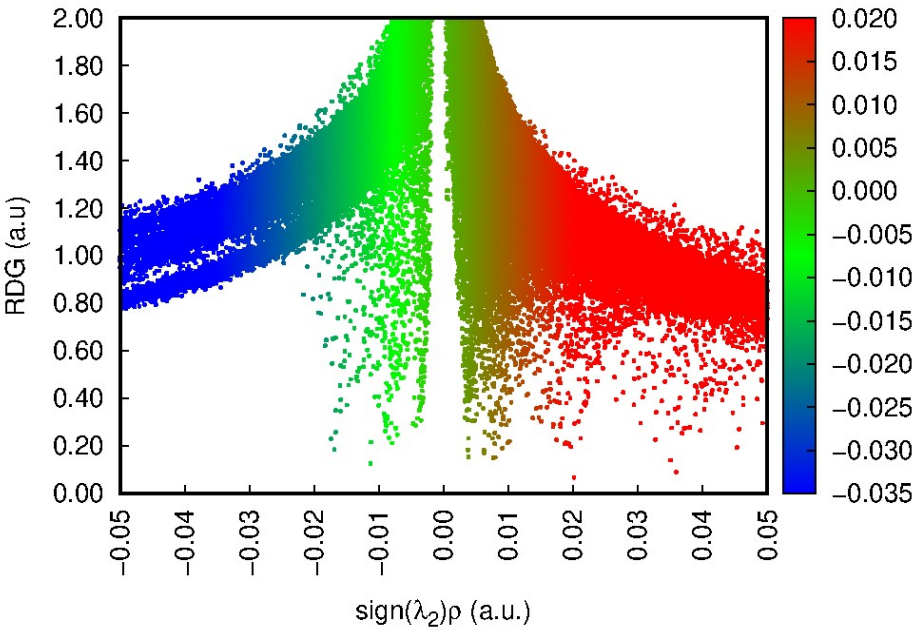
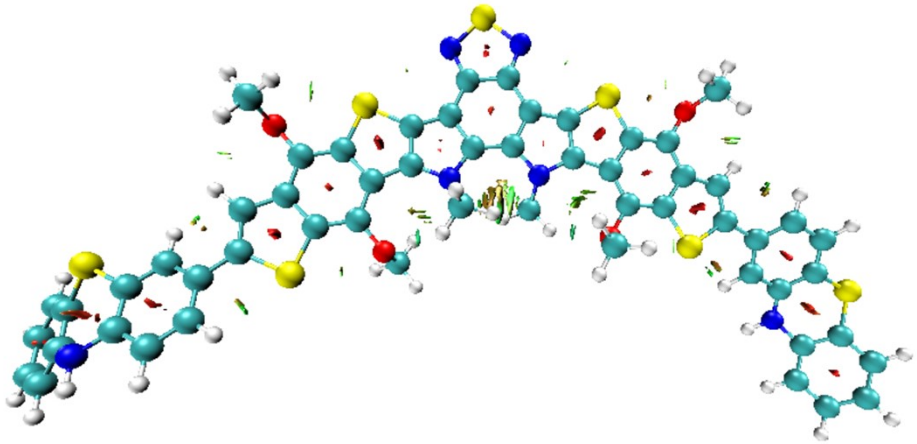


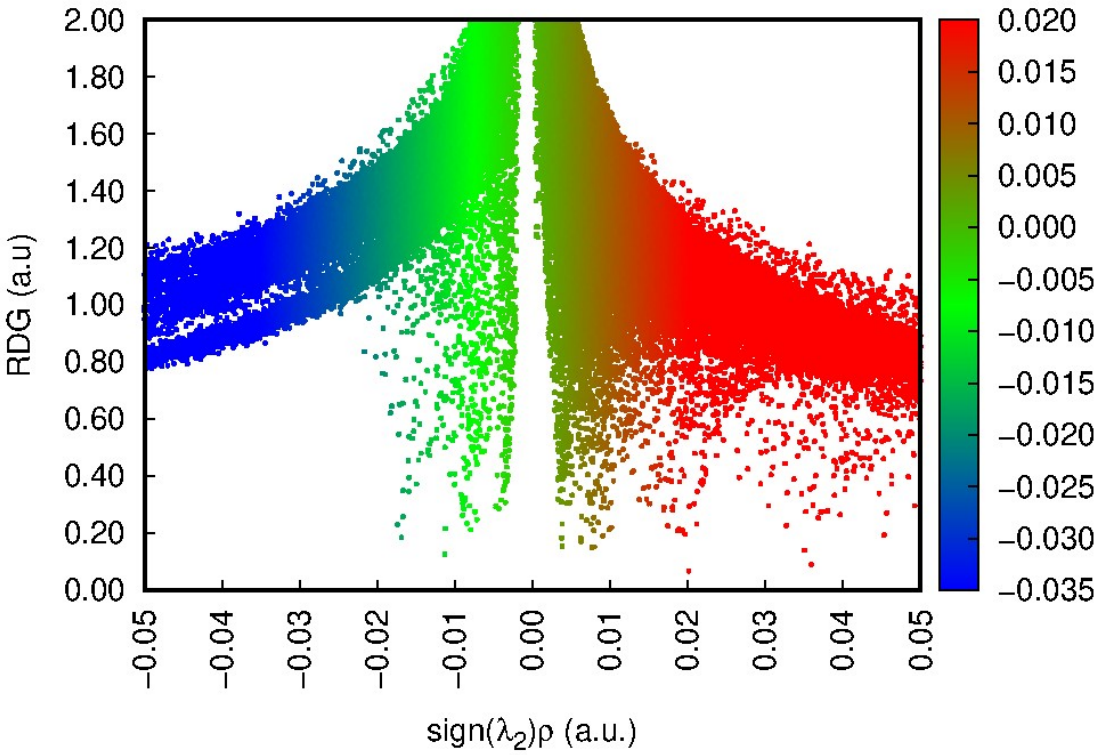
Figure S4: The simulated absorption spectra of the studied compounds (**PSCR** and **PSCD1-PSCD6**).



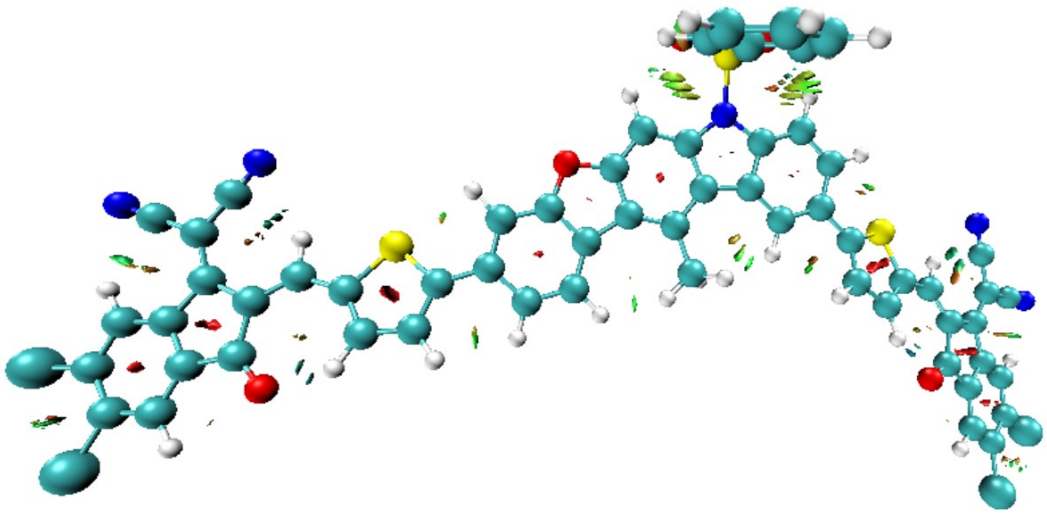

2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
RDG (a.u)
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ2)ρ (a.u.)
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

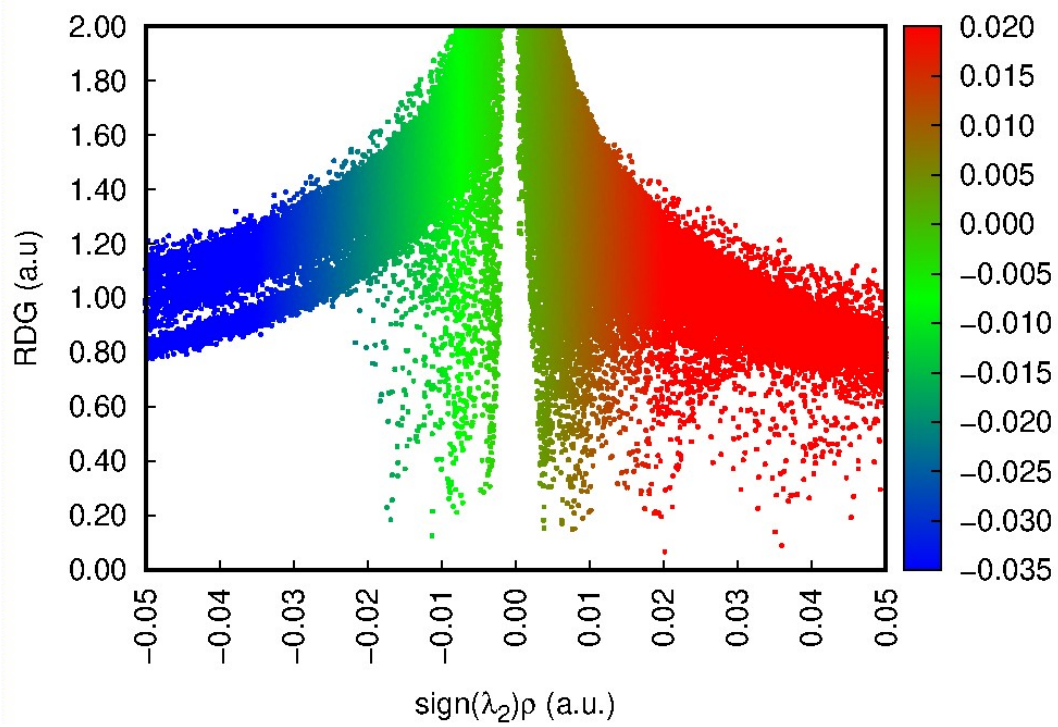
PSCR



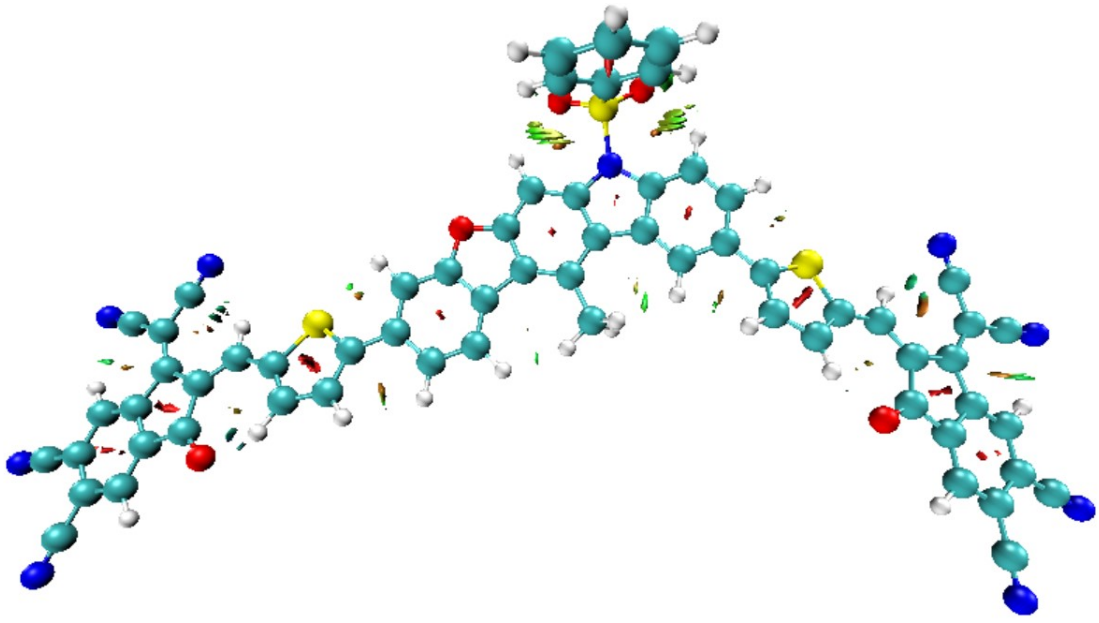

RDG (a.u)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ2)ρ (a.u.)
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

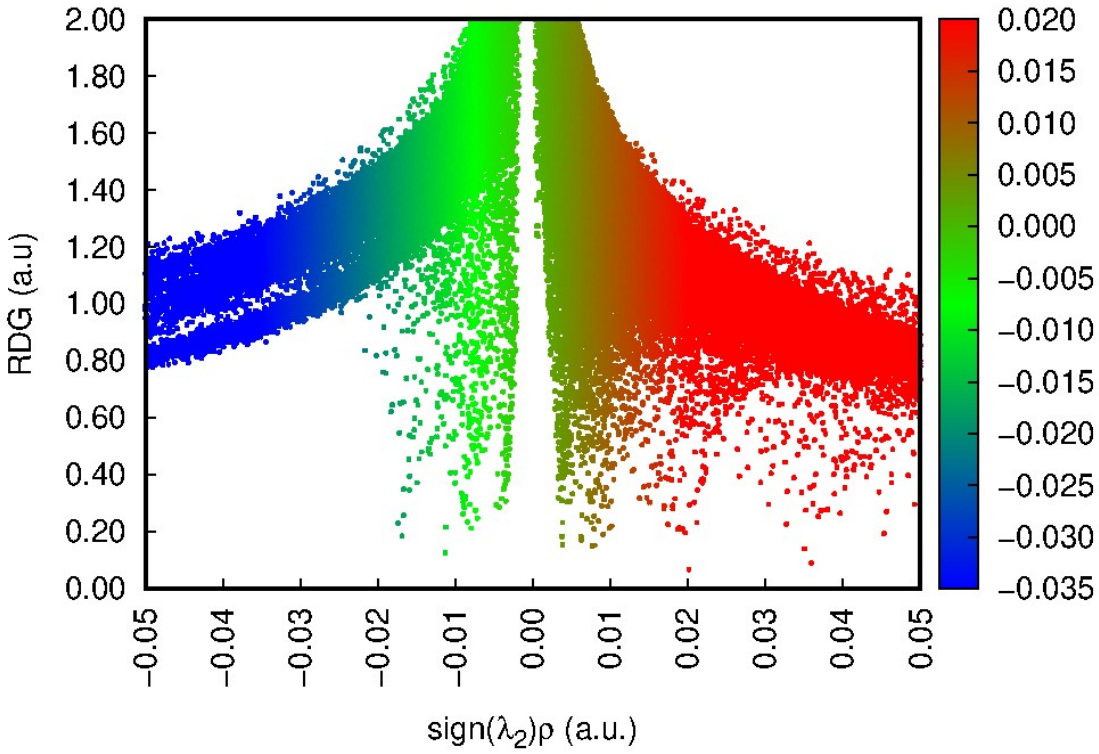
PSCD1



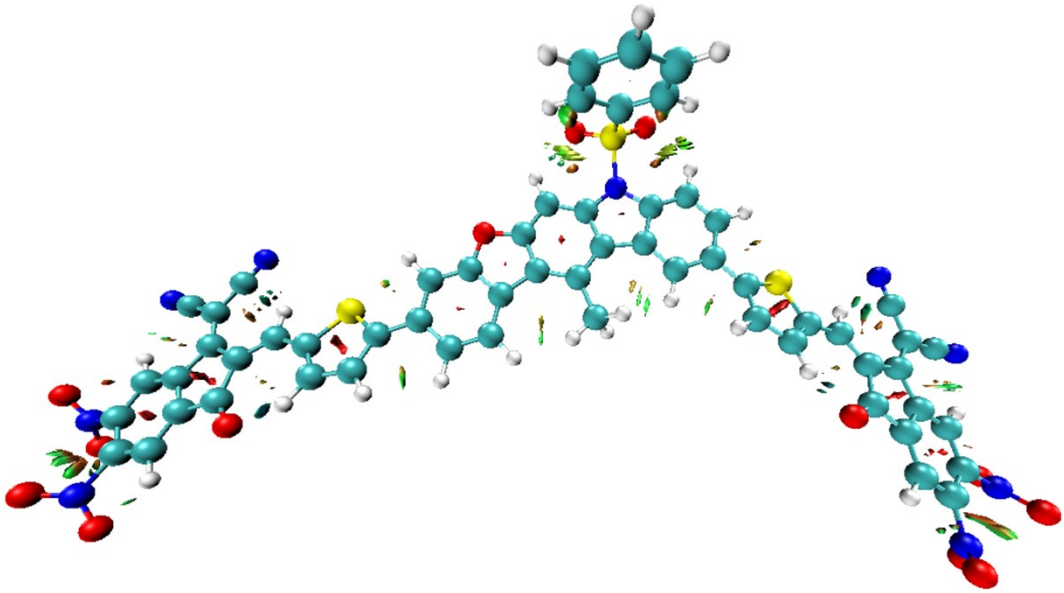

RDG (a.u)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ2)ρ (a.u.)
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

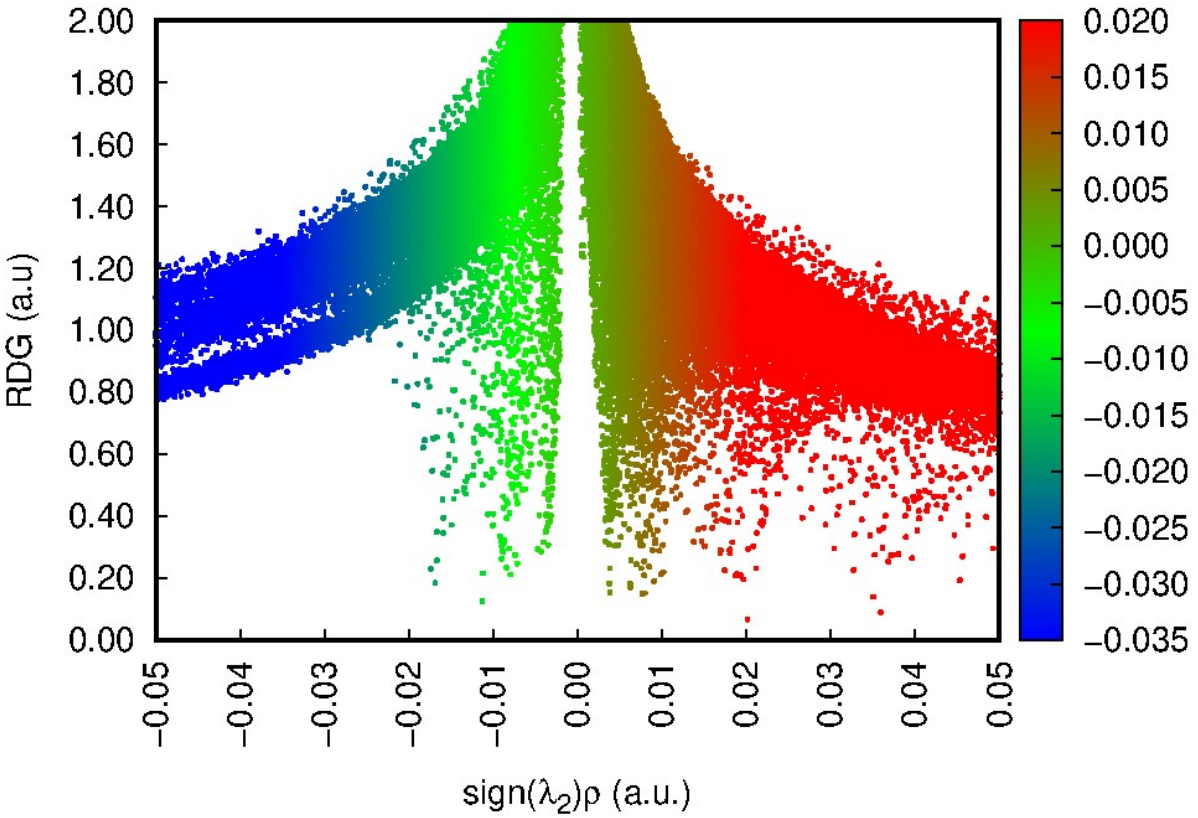
PSCD2



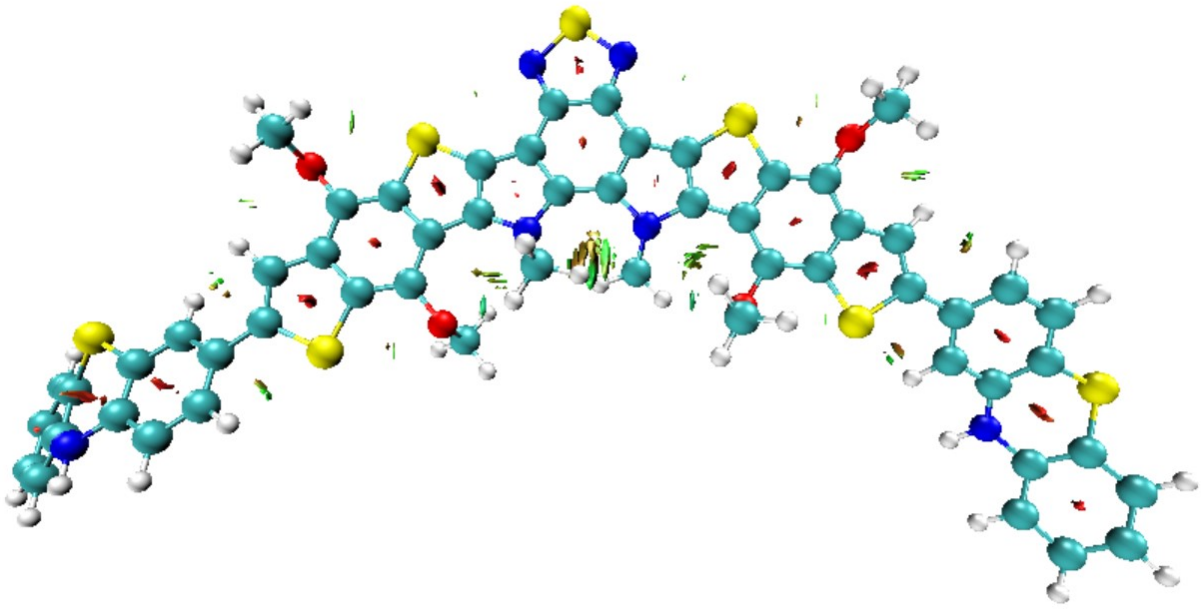

RDG (a.u)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ2)ρ (a.u.)
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

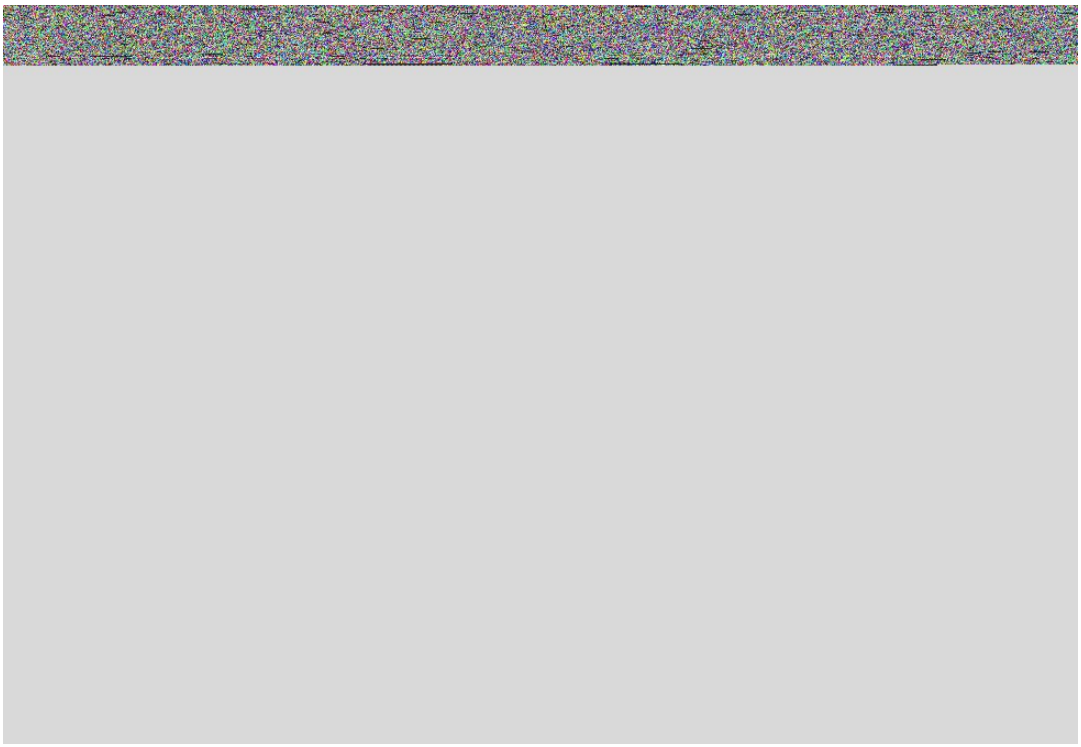
PSCD3



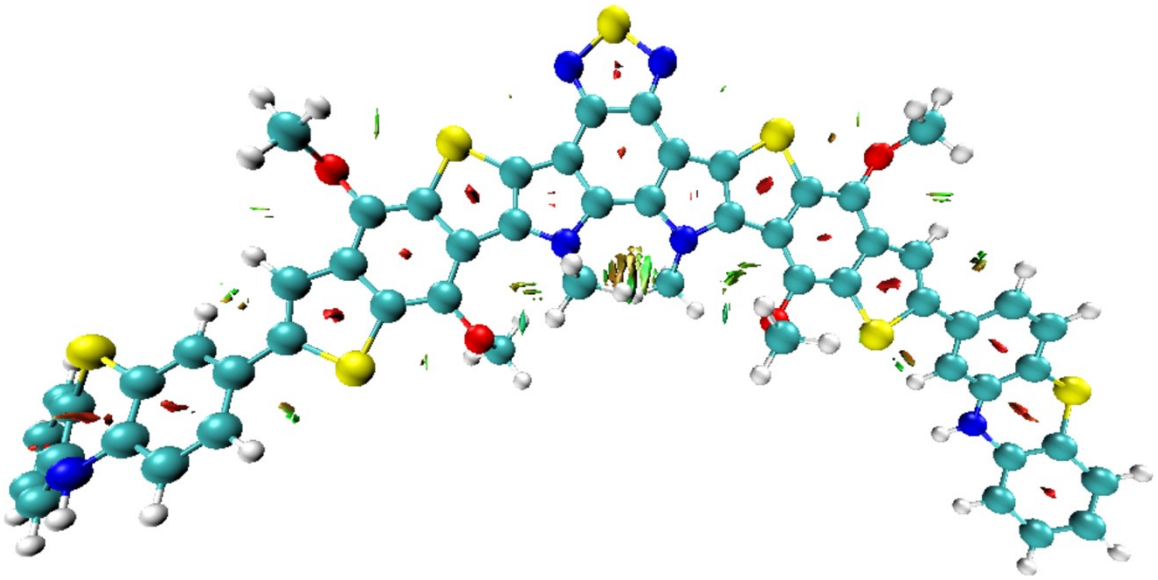

RDG (a.u)
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ2)ρ (a.u.)
0.020
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
−0.025
−0.030
−0.035

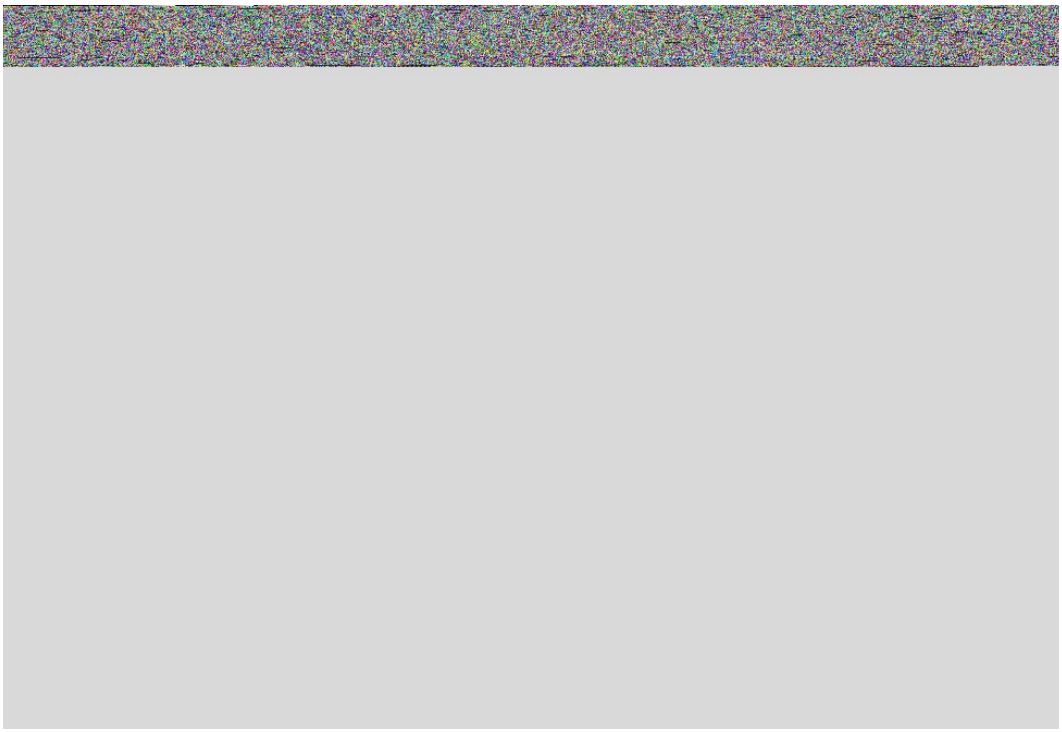
PSCD4





PSCD5





PSCD6

Figure S5: NCI isosurface and index plot of **PSCR** and **PSCD1**-**PSCD6** in chloroform with M06/6-311G(d,p) level at cutoff = 0.5.