Influence of Benzothiophene Acceptor Moieties on Non-linear Optical Properties of Pyreno-Based Chromophores: First Principles DFT Framework

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

Atom	X-axis	Y-axis	Z-axis
C	-6.173517	2.889816	-0.316649
C	-4.929739	2.280545	-0.220052
C	-4.819368	0.893489	-0.090428
C	-6.007975	0.099053	-0.090051
C	-7.27005	0.744911	-0.178333
C	-7.331209	2.137578	-0.286519
C	-5.960092	-1.329768	-0.017058
C	-4.721467	-2.022753	0.039196
C	-3.534522	-1.222643	0.04566
C	-4.699175	-3.412646	0.095802
H	-3.738856	-3.917053	0.139678
C	-5.885707	-4.133915	0.101671
C	-7.103577	-3.478359	0.047711
C	-7.164031	-2.082171	-0.015163
C	-8.415657	-1.392339	-0.08362
C	-8.464344	-0.044194	-0.164256
H	-9.417799	0.47412	-0.224557
H	-9.32833	-1.982522	-0.076076
H	-6.23047	3.969122	-0.416255
H	-4.040922	2.899161	-0.254461

H	-8.30434	2.616283	-0.35587
H	-5.856847	-5.218015	0.149021
H	-8.032559	-4.042415	0.050715
C	-3.592949	0.158576	0.019129
C	-1.501261	-0.573351	0.113821
C	-0.037131	-0.59276	0.137359
C	0.617194	-1.667095	-0.472532
C	0.741853	0.387947	0.757192
C	1.997117	-1.74233	-0.488249
H	0.022335	-2.436987	-0.952827
C	2.122171	0.305871	0.741595
H	0.273401	1.216032	1.277662
C	2.781797	-0.751215	0.10965
H	2.476968	-2.569568	-1.003317
H	2.700512	1.067928	1.255616
N	-2.273256	0.572374	0.075596
N	-2.242229	-1.659272	0.094479
C	4.254628	-0.809352	0.076307
C	5.005643	0.367387	-0.04017
C	4.926851	-2.036025	0.16341
H	4.500654	1.325616	-0.136668
C	6.310547	-2.105655	0.141147
H	4.349488	-2.949191	0.277289
C	7.042194	-0.930256	0.026983
H	6.810791	-3.066974	0.221353
C	6.384062	0.304232	-0.065614
C	7.388776	1.41432	-0.195585
H	7.300666	2.146164	0.617604
H	7.258865	1.975716	-1.129837
C	8.481112	-0.695469	-0.024906
C	8.701699	0.683571	-0.156568
C	9.99056	1.181424	-0.230116
C	11.060188	0.292933	-0.170078
H	10.167311	2.248897	-0.33257
C	9.549606	-1.582021	0.034906
C	10.84044	-1.07607	-0.038268
H	12.076867	0.669965	-0.225862
H	9.37995	-2.650631	0.136906
H	11.688249	-1.752819	0.007149
C	-1.814077	1.924446	0.083261
C	-1.928149	2.670836	1.248434
C	-1.273269	2.472511	-1.069217
C	-1.495621	3.987746	1.256737

H	-2.358874	2.212706	2.134354
C	-0.837499	3.790289	-1.052024
H	-1.197799	1.864704	-1.96574
C	-0.950173	4.546771	0.106851
H	-1.582666	4.578972	2.162269
H	-0.412017	4.228269	-1.949002
H	-0.611446	5.577635	0.114733

Table S2: Cartesian coordinates of **PYFD1** compound.

Atom	X-axis	Y-axis	Z-axis
C	-12.845301	-1.289396	1.369676
C	-11.494762	-1.117557	1.096479
C	-11.014975	0.08848	0.579886
C	-11.933149	1.164869	0.364347
C	-13.31068	0.964717	0.646193
C	-13.746518	-0.268214	1.14083
C	-11.500212	2.442126	-0.114652
C	-10.131917	2.696757	-0.392125
C	-9.220376	1.612451	-0.189553
C	-9.728869	3.949847	-0.841857
H	-8.676225	4.118215	-1.046303
C	-10.661986	4.961376	-1.026455
C	-12.002004	4.734082	-0.765323
C	-12.442194	3.487192	-0.309195
C	-13.822829	3.239847	-0.028116
C	-14.235054	2.036259	0.427909
H	-15.284287	1.854706	0.645974
H	-14.532846	4.047358	-0.186365
H	-13.190271	-2.238321	1.76812
H	-10.812654	-1.934872	1.296488
H	-14.803733	-0.405527	1.351296
H	-10.337633	5.935789	-1.378471
H	-12.732826	5.525466	-0.909598
C	-9.648428	0.373315	0.250117
C	-7.45547	0.413899	-0.094346
C	-6.045126	0.025303	-0.174996
C	-5.093285	1.047921	-0.095179
C	-5.588607	-1.280791	-0.375569
C	-3.744176	0.777757	-0.206295
H	-5.436756	2.067144	0.044025
C	-4.234709	-1.545478	-0.486556
H	-6.287138	-2.105746	-0.458888
C	-3.282282	-0.527459	-0.405466

H	-3.03393	1.598392	-0.161945
H	-3.911984	-2.57324	-0.624303
N	-8.500168	-0.400592	0.301273
N	-7.873135	1.624999	-0.392003
C	-1.843139	-0.818096	-0.540475
C	-1.400178	-1.827931	-1.404112
C	-0.894806	-0.085625	0.186827
H	-2.117304	-2.390537	-1.996871
C	0.462385	-0.337064	0.068154
H	-1.233937	0.68148	0.876956
C	0.886681	-1.339804	-0.794637
H	1.177508	0.240133	0.647738
C	-0.049267	-2.082607	-1.527385
C	0.653806	-3.091311	-2.391071
H	0.438871	-2.940805	-3.456877
H	0.347471	-4.119156	-2.157771
C	2.223159	-1.81965	-1.129529
C	2.100665	-2.850837	-2.072619
C	3.231617	-3.477607	-2.564876
C	4.479697	-3.073088	-2.114817
H	3.150078	-4.282672	-3.28962
C	3.469214	-1.409703	-0.682547
C	4.615547	-2.038859	-1.176873
H	3.555336	-0.590207	0.02692
C	-8.415926	-1.760478	0.728964
C	-8.811542	-2.77337	-0.134502
C	-7.939393	-2.046098	1.998863
C	-8.727188	-4.092335	0.284133
H	-9.182658	-2.517414	-1.122837
C	-7.852459	-3.368999	2.408876
H	-7.636947	-1.232249	2.65092
C	-8.245974	-4.38992	1.553815
H	-9.034443	-4.890768	-0.383198
H	-7.477959	-3.602423	3.400075
H	-8.178501	-5.423396	1.877683
C	8.782113	-0.206132	1.502049
H	8.476822	-0.369251	2.538271
C	9.990694	0.392365	1.38339
C	10.744669	0.930715	0.247952
C	10.873169	0.442092	2.593155
C	12.13916	0.977329	0.671879
C	10.230481	1.511779	-0.878862
C	12.180476	0.755457	2.017832

O	13.39535	0.858332	2.552677
C	13.497766	1.249759	0.285922
H	5.367985	-3.580639	-2.478129
C	14.219795	1.152107	1.49304
C	15.585526	1.319598	1.593882
C	16.258537	1.589019	0.415022
H	16.09021	1.236453	2.549201
C	14.210554	1.509453	-0.889879
C	15.578787	1.678109	-0.806195
H	17.334075	1.728232	0.437627
H	13.705306	1.584128	-1.844505
H	16.143243	1.883987	-1.709418
C	8.837827	1.715313	-1.082913
N	7.72124	1.942346	-1.270102
C	11.058103	2.087564	-1.879956
N	11.697387	2.56121	-2.717089
O	10.568615	0.224883	3.740532
C	8.239367	-1.248758	-0.743982
C	5.950197	-1.639555	-0.741008
C	7.922331	-0.736482	0.495197
S	6.217679	-0.92255	0.812882
C	7.133686	-1.757552	-1.435253
H	7.190049	-2.183093	-2.430232
H	9.253878	-1.278422	-1.125584

Table S3: Cartesian coordinates of **PYFD2** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	-14.446241	-1.172886	1.430573
C	-13.095283	-1.018317	1.149324
C	-12.608502	0.169914	0.598424
C	-13.520169	1.245138	0.352203
C	-14.898249	1.062562	0.64336
C	-15.340898	-0.152341	1.175257
C	-13.080589	2.503958	-0.16803
C	-11.711674	2.741003	-0.458116
C	-10.806317	1.657657	-0.224324
C	-11.30246	3.976756	-0.94852
H	-10.24953	4.131864	-1.161732
C	-12.229775	4.988054	-1.161775
C	-13.570248	4.77752	-0.889294
C	-14.016555	3.548396	-0.392594
C	-15.397828	3.318891	-0.099649
C	-15.816334	2.132796	0.39484

H	-16.866045	1.964931	0.621392
H	-16.103159	4.125639	-0.281012
H	-14.796705	-2.107872	1.856238
H	-12.418717	-1.835165	1.369554
H	-16.398433	-0.276138	1.392409
H	-11.900515	5.948742	-1.54548
H	-14.296697	5.568508	-1.056039
C	-11.24083	0.436747	0.258175
C	-9.048737	0.449883	-0.096502
C	-7.64037	0.051874	-0.172261
C	-6.687236	1.07714	-0.191585
C	-7.183986	-1.265738	-0.274995
C	-5.339948	0.799293	-0.30418
H	-7.028856	2.104428	-0.129847
C	-5.831471	-1.538264	-0.386492
H	-7.879316	-2.096692	-0.281194
C	-4.87918	-0.5175	-0.404976
H	-4.631169	1.621595	-0.339868
H	-5.509931	-2.573927	-0.445789
N	-10.097762	-0.342436	0.331847
N	-9.46049	1.653124	-0.433585
C	-3.442463	-0.818948	-0.541618
C	-3.01407	-1.892029	-1.3328
C	-2.482746	-0.034893	0.113646
H	-3.741168	-2.496409	-1.86943
C	-1.127772	-0.297604	-0.005288
H	-2.811227	0.783479	0.747638
C	-0.717937	-1.364335	-0.795114
H	-0.40344	0.319937	0.518542
C	-1.665315	-2.158112	-1.456342
C	-0.976733	-3.232526	-2.24925
H	-1.203812	-3.163118	-3.32082
H	-1.283267	-4.238425	-1.934784
C	0.612405	-1.874915	-1.108458
C	0.474507	-2.975876	-1.967567
C	1.595609	-3.647738	-2.421705
C	2.851113	-3.219537	-2.017176
H	1.500438	-4.506073	-3.080405
C	1.865252	-1.442477	-0.706368
C	3.002257	-2.118196	-1.161432
H	1.96385	-0.572652	-0.061423
C	-10.029008	-1.690083	0.79909
C	-10.41821	-2.72313	-0.042793

C	-9.578622	-1.9431	2.085455
C	-10.352587	-4.030623	0.413583
H	-10.769634	-2.491144	-1.044081
C	-9.510818	-3.254609	2.533566
H	-9.281653	-1.113289	2.719672
C	-9.897221	-4.295924	1.699871
H	-10.654804	-4.845152	-0.236309
H	-9.15703	-3.46335	3.537801
H	-9.8444	-5.3203	2.05402
C	7.160279	-0.115773	1.367631
H	6.756633	-0.07733	2.382433
C	8.441917	0.338622	1.297282
C	9.361556	0.623246	0.199771
C	9.185017	0.478286	2.584355
C	10.705719	0.623936	0.78133
C	9.046235	1.056647	-1.058675
C	10.579459	0.59444	2.135739
O	11.732151	0.674282	2.801175
C	12.119341	0.729883	0.54053
H	3.731576	-3.760539	-2.349425
C	12.684101	0.751343	1.831769
C	14.038439	0.815732	2.086864
C	14.860262	0.861494	0.9845
H	14.443319	0.799546	3.09105
C	12.984061	0.778047	-0.556618
C	14.335512	0.850966	-0.315618
H	12.625056	0.791298	-1.578615
C	7.718866	1.367801	-1.458893
N	6.656731	1.666414	-1.79894
C	10.046712	1.356702	-2.021069
N	10.843441	1.597302	-2.821553
O	8.749866	0.455473	3.708081
C	6.634849	-1.348082	-0.793009
C	4.340503	-1.701032	-0.759737
C	6.32105	-0.713897	0.395577
S	4.60863	-0.845462	0.716488
C	5.528613	-1.904304	-1.435023
H	5.582928	-2.423355	-2.384418
H	7.649124	-1.427684	-1.168106
N	15.202483	1.055999	-1.492133
N	16.309441	0.77798	1.234398
O	16.054542	1.910036	-1.400413
O	16.73538	1.362959	2.203413

O	16.95672	0.090678	0.477288
O	14.963603	0.392286	-2.473944

Table S4: Cartesian coordinates of **PYFD3** compound.

Atom	Atom2	Y-axis	Z-axis
C	-15.530832	-1.130152	1.428057
C	-14.180454	-0.977484	1.143095
C	-13.691458	0.214705	0.602923
C	-14.599934	1.296137	0.372708
C	-15.977558	1.115387	0.667162
C	-16.422713	-0.103675	1.187256
C	-14.157387	2.55933	-0.134208
C	-12.788605	2.794717	-0.42644
C	-11.886589	1.70506	-0.209388
C	-12.376488	4.034935	-0.90292
H	-11.323739	4.188805	-1.11793
C	-13.300728	5.052257	-1.100295
C	-14.641024	4.843373	-0.825752
C	-15.090211	3.609953	-0.342556
C	-16.471275	3.382165	-0.047324
C	-16.892513	2.191882	0.434634
H	-17.942003	2.025378	0.663205
H	-17.174151	4.193718	-0.21636
H	-15.883047	-2.068379	1.845053
H	-13.506089	-1.799063	1.35202
H	-17.479832	-0.225925	1.40727
H	-12.96915	6.016422	-1.473135
H	-15.365045	5.639085	-0.980101
C	-12.324245	0.480094	0.259849
C	-10.133517	0.488942	-0.102386
C	-8.727387	0.085115	-0.186022
C	-7.767659	1.10426	-0.18137
C	-8.279888	-1.232944	-0.317115
C	-6.421859	0.819866	-0.29745
H	-8.102826	2.132167	-0.09727
C	-6.92922	-1.512037	-0.431994
H	-8.981283	-2.058484	-0.342882
C	-5.9699	-0.497608	-0.425986
H	-5.707251	1.637788	-0.312996
H	-6.614717	-2.548351	-0.513033
N	-11.184192	-0.304626	0.319506
N	-10.541316	1.697837	-0.423291
C	-4.535348	-0.808422	-0.564648

C	-4.115069	-1.871827	-1.373116
C	-3.569792	-0.046855	0.108171
H	-4.846041	-2.458633	-1.923753
C	-2.217298	-0.323781	-0.008323
H	-3.891686	0.764016	0.755105
C	-1.815728	-1.382349	-0.813337
H	-1.488656	0.275822	0.530173
C	-2.769124	-2.152189	-1.493846
C	-2.090051	-3.222765	-2.299813
H	-2.306309	-3.13033	-3.371936
H	-2.414705	-4.22939	-2.006694
C	-0.490363	-1.907496	-1.124401
C	-0.637821	-2.993155	-2.001331
C	0.47633	-3.676813	-2.454652
C	1.734559	-3.275396	-2.03194
H	0.373414	-4.523894	-3.126634
C	0.765602	-1.501124	-0.704851
C	1.895683	-2.18925	-1.158651
H	0.872143	-0.642782	-0.045891
C	-11.11752	-1.656806	0.773916
C	-11.515846	-2.681312	-0.074202
C	-10.659013	-1.922652	2.054738
C	-11.45151	-3.992888	0.370556
H	-11.873259	-2.43981	-1.071135
C	-10.59254	-3.23819	2.491176
H	-10.354853	-1.099434	2.694129
C	-10.98821	-4.270964	1.651281
H	-11.760861	-4.800692	-0.284382
H	-10.232459	-3.456704	3.491082
H	-10.936437	-5.298587	1.996008
C	6.071089	-0.30484	1.435938
H	5.665769	-0.279927	2.450447
C	7.360602	0.128674	1.375231
C	8.283116	0.418042	0.282035
C	8.108976	0.222872	2.665075
C	9.625026	0.39253	0.863927
C	7.977745	0.863509	-0.976222
C	9.505154	0.328497	2.217392
O	10.662923	0.389853	2.878613
C	11.036021	0.514939	0.622191
H	2.608752	-3.8269	-2.363286
C	11.60926	0.495475	1.903497
C	12.965135	0.578381	2.139743

C	13.79226	0.691076	1.0376
H	13.35129	0.578915	3.150778
C	11.890996	0.602556	-0.474626
C	13.252037	0.692449	-0.26883
H	11.494012	0.58896	-1.478888
C	6.658461	1.207567	-1.375481
N	5.603941	1.533756	-1.714068
C	8.984259	1.127774	-1.943552
N	9.78969	1.32864	-2.746771
O	7.673257	0.179303	3.787837
C	5.538407	-1.496193	-0.743746
C	3.237252	-1.8024	-0.738
C	5.225721	-0.869614	0.44904
S	3.507706	-0.96996	0.751402
C	4.427819	-2.021773	-1.403663
H	4.481841	-2.530758	-2.358481
H	6.554812	-1.592994	-1.108929
S	15.558286	0.784132	1.342542
S	14.273033	0.849811	-1.743371
O	13.30226	0.239037	-2.868354
O	14.474506	2.243221	-2.048704
O	15.362027	-0.080647	-1.630719
O	16.114581	-0.543538	1.421199
O	15.572891	1.406588	2.821994
O	16.099177	1.787946	0.468774
H	15.923976	0.758222	3.451422
H	12.86517	0.947272	-3.367426

Table S5: Cartesian coordinates of **PYFD4** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	-13.808272	-1.200321	1.417543
C	-12.455735	-1.043596	1.145172
C	-11.969421	0.139981	0.583807
C	-12.883525	1.208037	0.316538
C	-14.263128	1.023348	0.599063
C	-14.704966	-0.186691	1.142658
C	-12.445142	2.461754	-0.216925
C	-11.074976	2.700751	-0.49948
C	-10.166904	1.624677	-0.243761
C	-10.6672	3.93125	-1.00413
H	-9.613305	4.087772	-1.211514
C	-11.597089	4.935443	-1.238741
C	-12.93873	4.722987	-0.973501

C	-13.383695	3.498909	-0.463223
C	-14.76627	3.26738	-0.178012
C	-15.183661	2.086236	0.329105
H	-16.234447	1.916822	0.549434
H	-15.473577	4.068465	-0.376014
H	-14.15836	-2.131498	1.851787
H	-11.777619	-1.85496	1.380565
H	-15.763724	-0.312277	1.352733
H	-11.268963	5.892009	-1.633545
H	-13.667211	5.508379	-1.156989
C	-10.600124	0.408368	0.251341
C	-8.405507	0.425607	-0.087614
C	-6.995079	0.032293	-0.150168
C	-6.04663	1.061469	-0.187363
C	-6.531844	-1.284835	-0.225267
C	-4.697849	0.787917	-0.29121
H	-6.393201	2.088143	-0.147479
C	-5.177603	-1.553018	-0.327447
H	-7.222674	-2.119427	-0.216957
C	-4.230182	-0.528277	-0.364406
H	-3.993307	1.612962	-0.342651
H	-4.851139	-2.588158	-0.365204
N	-9.454555	-0.365049	0.343828
N	-8.819669	1.622774	-0.4432
C	-2.791473	-0.823488	-0.493405
C	-2.355007	-1.911682	-1.259092
C	-1.837528	-0.015884	0.141653
H	-3.077637	-2.534987	-1.779832
C	-0.480489	-0.268191	0.024855
H	-2.172162	0.814085	0.757014
C	-0.062621	-1.348889	-0.741419
H	0.239377	0.368555	0.531564
C	-1.004097	-2.168365	-1.379355
C	-0.307234	-3.255581	-2.147194
H	-0.540882	-3.218528	-3.218897
H	-0.600361	-4.255803	-1.803148
C	1.27194	-1.851154	-1.050079
C	1.142428	-2.97486	-1.880487
C	2.269073	-3.64366	-2.325434
C	3.521766	-3.188699	-1.941926
H	2.180555	-4.519524	-2.961578
C	2.521908	-1.391994	-0.669393
C	3.664778	-2.06283	-1.11719

H	2.613304	-0.504611	-0.047746
C	-9.385932	-1.708135	0.823952
C	-9.764285	-2.749175	-0.012935
C	-8.947227	-1.948961	2.116748
C	-9.699203	-4.052684	0.454676
H	-10.106867	-2.526198	-1.019301
C	-8.879911	-3.256582	2.576162
H	-8.658592	-1.113032	2.746748
C	-9.25532	-4.305868	1.747431
H	-9.992957	-4.873488	-0.19116
H	-8.535126	-3.456066	3.585404
H	-9.202847	-5.32707	2.110719
C	7.808204	0.096573	1.302705
H	7.3936	0.190153	2.309549
C	9.092232	0.543286	1.22636
C	10.034417	0.756991	0.131605
C	9.814776	0.750187	2.51651
C	11.368017	0.77416	0.736137
C	9.744027	1.122542	-1.1545
C	11.217547	0.825226	2.08729
O	12.358991	0.93064	2.768381
C	12.787409	0.851053	0.514434
H	4.406656	-3.726138	-2.268057
C	13.33102	0.936935	1.813549
C	14.678192	1.009554	2.091182
C	15.536874	0.98434	1.002996
H	15.046039	1.078642	3.10716
C	13.6683	0.815209	-0.567139
C	15.030126	0.883706	-0.317679
H	13.313819	0.74341	-1.58775
C	8.426588	1.427511	-1.590514
N	7.373678	1.720353	-1.962911
C	10.760337	1.3561	-2.118858
N	11.568456	1.54155	-2.922576
O	9.359974	0.796577	3.631898
C	7.289259	-1.2304	-0.805895
C	4.999982	-1.613061	-0.74132
C	6.974989	-0.551724	0.357964
S	5.266168	-0.692655	0.69536
C	6.186524	-1.826918	-1.416608
H	6.242473	-2.38283	-2.34469
H	8.301329	-1.310481	-1.186639
C	15.939685	0.849882	-1.41683

N	16.678316	0.821623	-2.301998
C	16.943751	1.055991	1.222653
N	18.081724	1.114412	1.40042

Table S6: Cartesian coordinates of **PYFD5** compound.

Atom	X-axis	Y-axis	Z-axis
C	-15.081973	-1.183057	1.446404
C	-13.731214	-1.025914	1.165586
C	-13.24702	0.16201	0.611735
C	-14.161259	1.234214	0.361789
C	-15.539058	1.049046	0.652602
C	-15.97901	-0.165447	1.187691
C	-13.724588	2.492542	-0.162056
C	-12.35614	2.732079	-0.45215
C	-11.448222	1.65174	-0.214581
C	-11.949705	3.967209	-0.946433
H	-10.897057	4.124179	-1.159662
C	-12.879418	4.975483	-1.163503
C	-14.219508	4.762507	-0.89101
C	-14.663038	3.533892	-0.390548
C	-16.043891	3.301817	-0.097691
C	-16.459677	2.116209	0.400239
H	-17.509101	1.946357	0.626644
H	-16.751179	4.106169	-0.282045
H	-15.430396	-2.117729	1.874435
H	-13.052738	-1.840466	1.388423
H	-17.036377	-0.29129	1.404494
H	-12.552376	5.935705	-1.550255
H	-14.947842	5.551117	-1.060782
C	-11.879803	0.431232	0.271505
C	-9.687712	0.448527	-0.083553
C	-8.278427	0.053855	-0.160403
C	-7.32845	1.08186	-0.189798
C	-7.818179	-1.262948	-0.256135
C	-5.980819	0.807501	-0.306108
H	-7.67297	2.108468	-0.133505
C	-6.465206	-1.531965	-0.371259
H	-8.510669	-2.096253	-0.254235
C	-5.516187	-0.508424	-0.400527
H	-5.274937	1.631857	-0.350262
H	-6.14076	-2.567019	-0.425098
N	-10.734778	-0.344931	0.347537
N	-10.102492	1.649813	-0.424011

C	-4.079049	-0.805633	-0.542069
C	-3.650447	-1.882327	-1.328202
C	-3.119076	-0.01349	0.103059
H	-4.377904	-2.493152	-1.856989
C	-1.763671	-0.271509	-0.021343
H	-3.447492	0.807701	0.733422
C	-1.353625	-1.341789	-0.80624
H	-1.039065	0.352303	0.494629
C	-2.301299	-2.143953	-1.456916
C	-1.612595	-3.221547	-2.24537
H	-1.845286	-3.160854	-3.316264
H	-1.914079	-4.226109	-1.921864
C	-0.022854	-1.849493	-1.122672
C	-0.160946	-2.957503	-1.972453
C	0.960547	-3.629247	-2.42575
C	2.216288	-3.194171	-2.029275
H	0.865576	-4.493223	-3.077098
C	1.23039	-1.409457	-0.729819
C	2.367894	-2.085114	-1.183626
H	1.328551	-0.534417	-0.091865
C	-10.663312	-1.691536	0.817344
C	-11.049669	-2.726785	-0.023109
C	-10.213563	-1.941392	2.104585
C	-10.981761	-4.033372	0.435491
H	-11.400715	-2.497137	-1.025059
C	-10.143475	-3.252008	2.554935
H	-9.918806	-1.109885	2.737608
C	-10.527011	-4.29552	1.722649
H	-11.281731	-4.849639	-0.213252
H	-9.790133	-3.458342	3.559826
H	-10.472415	-5.319169	2.07864
C	6.528046	-0.057047	1.32501
H	6.112549	0.003742	2.334004
C	7.816163	0.375654	1.266365
C	8.764998	0.611176	0.180565
C	8.541972	0.52389	2.5646
C	10.09602	0.583134	0.786551
C	8.482161	1.021476	-1.093739
C	9.944813	0.586166	2.139481
O	11.087778	0.64235	2.823519
C	11.517658	0.642968	0.570239
H	3.096896	-3.73559	-2.360443
C	12.059165	0.66561	1.864557

C	13.409909	0.695934	2.132576
C	14.277522	0.700367	1.055317
H	13.769414	0.712677	3.153035
C	12.40869	0.635599	-0.503556
C	13.770636	0.661672	-0.266573
H	12.044899	0.613746	-1.521359
C	7.170527	1.361883	-1.521146
N	6.12321	1.68359	-1.885515
C	9.50327	1.265586	-2.050751
N	10.313925	1.459738	-2.849923
O	8.083683	0.538972	3.67975
C	6.00248	-1.314099	-0.824062
C	3.706698	-1.661292	-0.789549
C	5.689449	-0.661862	0.353935
S	3.976044	-0.782857	0.673441
C	4.894626	-1.875732	-1.460403
H	4.94956	-2.408285	-2.402265
H	7.016699	-1.402138	-1.197286
C	14.660073	0.708022	-1.485032
C	15.750251	0.675092	1.38797
F	15.139167	1.937098	-1.694682
F	15.702717	-0.118525	-1.387686
F	13.997105	0.361013	-2.589494
F	16.463286	1.509902	0.634156
F	15.962696	1.026685	2.65809
F	16.263485	-0.548349	1.237882

Table S7: Cartesian coordinates of **PYFD6** compound.

Atom	X-axis	Y-axis	Z-axis
C	-14.033854	-1.167177	1.43015
C	-12.683001	-1.014905	1.147166
C	-12.195582	0.170934	0.591599
C	-13.10652	1.245987	0.341987
C	-14.484517	1.065735	0.634996
C	-14.92779	-0.146751	1.171885
C	-12.666291	2.502383	-0.183555
C	-11.297383	2.737183	-0.475556
C	-10.392705	1.654095	-0.238003
C	-10.887556	3.970641	-0.971242
H	-9.834655	4.124013	-1.185856
C	-11.814215	4.981814	-1.187918
C	-13.154653	4.773454	-0.913584
C	-13.601559	3.54669	-0.411591

C	-14.98278	3.319511	-0.116576
C	-15.401874	2.13578	0.383047
H	-16.451537	1.969736	0.61117
H	-15.687586	4.12612	-0.300589
H	-14.384804	-2.100278	1.859545
H	-12.00702	-1.831634	1.369699
H	-15.985245	-0.268753	1.390442
H	-11.484472	5.940674	-1.575754
H	-13.880602	5.564343	-1.082963
C	-10.827915	0.435449	0.249575
C	-8.635964	0.4454	-0.106401
C	-7.227895	0.046061	-0.180859
C	-6.274151	1.070654	-0.206351
C	-6.772151	-1.272335	-0.276168
C	-4.926999	0.791442	-0.317128
H	-6.615194	2.09848	-0.150682
C	-5.419725	-1.546218	-0.385725
H	-7.467764	-2.103033	-0.277745
C	-4.466791	-0.526168	-0.409783
H	-4.217786	1.613146	-0.357607
H	-5.098707	-2.582383	-0.438872
N	-9.685414	-0.3443	0.32578
N	-9.047016	1.647621	-0.448072
C	-3.030109	-0.829248	-0.542946
C	-2.60113	-1.907742	-1.326475
C	-2.070929	-0.041745	0.10888
H	-3.327831	-2.515016	-1.860408
C	-0.715936	-0.30647	-0.00576
H	-2.399893	0.780926	0.737046
C	-0.305478	-1.378771	-0.787688
H	0.007967	0.313687	0.51557
C	-1.252405	-2.175935	-1.445638
C	-0.56322	-3.256811	-2.229295
H	-0.787676	-3.194288	-3.301853
H	-0.872644	-4.259853	-1.908541
C	1.025011	-1.893418	-1.093966
C	0.887773	-3.000244	-1.945147
C	2.009583	-3.677367	-2.389679
C	3.264388	-3.248848	-1.982706
H	1.915559	-4.540638	-3.042167
C	2.277415	-1.459802	-0.690895
C	3.414995	-2.141085	-1.13542
H	2.375119	-0.585441	-0.051929

C	-9.618112	-1.690627	0.796994
C	-10.008013	-2.725536	-0.04225
C	-9.168616	-1.940562	2.084292
C	-9.943903	-4.031867	0.417636
H	-10.358729	-2.495827	-1.044306
C	-9.102333	-3.250932	2.535929
H	-8.871085	-1.109324	2.716371
C	-9.489362	-4.294113	1.704846
H	-10.246632	-4.847865	-0.230166
H	-8.749187	-3.457338	3.540875
H	-9.437642	-5.317567	2.061822
C	7.565096	-0.121273	1.404928
H	7.17336	-0.100552	2.424888
C	8.82939	0.365508	1.31848
C	9.731895	0.667093	0.207687
C	9.589721	0.531877	2.596128
C	11.07994	0.688996	0.77086
C	9.387294	1.094207	-1.045788
C	10.970432	0.669265	2.129056
O	12.129701	0.780102	2.777371
C	12.488349	0.824407	0.506433
H	4.145244	-3.794359	-2.306638
C	13.070887	0.86569	1.787932
C	14.424382	0.970207	2.018884
C	15.24197	1.0247	0.904913
H	14.830889	1.002549	3.021951
C	13.336796	0.868606	-0.600652
C	14.698101	0.970369	-0.391682
H	12.956409	0.83415	-1.613923
C	8.047518	1.377703	-1.425962
N	6.976049	1.656305	-1.753939
C	10.362969	1.418322	-2.02609
N	11.132144	1.679646	-2.84696
O	9.162488	0.509701	3.724137
C	7.048758	-1.373824	-0.747113
C	4.752989	-1.722985	-0.730848
C	6.727989	-0.733948	0.433478
S	5.014712	-0.859221	0.744081
C	5.943603	-1.931022	-1.395848
H	6.003578	-2.454702	-2.342538
H	8.065702	-1.454746	-1.115065
C1	15.738066	1.026635	-1.781502
C1	16.952207	1.15368	1.145641

Table S8: Cartesian coordinates of **PYFD7** compound.

Atom	X-axis	Y-axis	Z-axis
C	-13.419585	-1.238654	1.364408
C	-12.069247	-1.071091	1.087707
C	-11.585799	0.136145	0.577454
C	-12.499542	1.218386	0.373076
C	-13.877083	1.022382	0.657748
C	-14.316917	-0.211965	1.145239
C	-12.061932	2.497354	-0.097057
C	-10.693112	2.748159	-0.375705
C	-9.786086	1.657874	-0.18487
C	-10.285651	4.003093	-0.816242
H	-9.23275	4.168519	-1.021825
C	-11.214776	5.020108	-0.990685
C	-12.55519	4.79656	-0.728406
C	-12.999769	3.548054	-0.281043
C	-14.380792	3.304656	0.00161
C	-14.797234	2.099617	0.449906
H	-15.846684	1.921235	0.66953
H	-15.087587	4.11649	-0.148765
H	-13.767504	-2.188598	1.757822
H	-11.390172	-1.892722	1.280127
H	-15.374052	-0.345932	1.358235
H	-10.886932	5.995887	-1.335611
H	-13.282877	5.592221	-0.864779
C	-10.219183	0.416973	0.244868
C	-8.02739	0.449043	-0.106758
C	-6.61983	0.052234	-0.19491
C	-5.660343	1.065975	-0.097446
C	-6.17353	-1.253786	-0.417601
C	-4.313071	0.787047	-0.210879
H	-5.996322	2.085335	0.058577
C	-4.821657	-1.527248	-0.53064
H	-6.878715	-2.071425	-0.516045
C	-3.861227	-0.518524	-0.430057
H	-3.596328	1.601057	-0.151235
H	-4.507012	-2.555147	-0.684805
N	-9.075081	-0.363485	0.284906
N	-8.439245	1.665205	-0.391421
C	-2.424188	-0.820684	-0.562593
C	-1.987032	-1.825295	-1.435255
C	-1.472199	-0.107477	0.178953

H	-2.706463	-2.372915	-2.039102
C	-0.117263	-0.3737	0.066545
H	-1.806823	0.655398	0.875965
C	0.301079	-1.372347	-0.803919
H	0.600499	0.188283	0.657705
C	-0.638536	-2.095226	-1.551643
C	0.057983	-3.104712	-2.419644
H	-0.144823	-2.940013	-3.485729
H	-0.264903	-4.130486	-2.200065
C	1.633687	-1.86724	-1.132292
C	1.505067	-2.888173	-2.085792
C	2.631171	-3.527365	-2.573054
C	3.880746	-3.1449	-2.108394
H	2.544568	-4.324932	-3.305433
C	2.881379	-1.479087	-0.6709
C	4.023025	-2.120741	-1.16034
H	2.972619	-0.667177	0.046602
C	-8.996844	-1.729354	0.694364
C	-9.405635	-2.727942	-0.179632
C	-8.51121	-2.03537	1.955977
C	-9.325398	-4.053058	0.220005
H	-9.783384	-2.456337	-1.161276
C	-8.428309	-3.364397	2.346829
H	-8.197991	-1.232533	2.616553
C	-8.834929	-4.371083	1.481145
H	-9.642939	-4.840301	-0.455771
H	-8.046434	-3.613692	3.331324
H	-8.770571	-5.409342	1.789958
C	8.1906	-0.354954	1.559588
H	7.871004	-0.507502	2.593063
C	9.413255	0.219089	1.451736
C	10.184903	0.742808	0.322846
C	10.284929	0.250972	2.669167
C	11.576377	0.772931	0.761483
C	9.693989	1.324026	-0.81389
C	11.60257	0.546577	2.106161
O	12.816441	0.632054	2.651643
C	12.939693	1.033204	0.390883
H	4.764455	-3.662644	-2.468265
C	13.648275	0.919337	1.603324
C	15.016192	1.07106	1.718498
C	15.688011	1.337707	0.548872
H	15.540572	0.98239	2.661731

C	13.659122	1.291875	-0.780672
C	15.017718	1.443157	-0.677325
H	13.189388	1.390388	-1.751158
C	8.308014	1.550231	-1.037475
N	7.19812	1.795385	-1.240272
C	10.546464	1.871369	-1.809869
N	11.212598	2.317888	-2.640948
O	9.96819	0.035499	3.813238
C	7.653902	-1.390044	-0.690151
C	5.359163	-1.744576	-0.709393
C	7.332347	-0.871323	0.545926
S	5.621795	-1.031533	0.846765
C	6.548166	-1.88211	-1.391699
H	6.608505	-2.309176	-2.385727
H	8.671633	-1.435977	-1.061469
F	15.747172	1.696246	-1.760969
F	17.004327	1.499905	0.558545

Table S9: Calculated energies (*E*) and energy gap (Δ*E*) of HOMO-1, LUMO+1, HOMO-2 and LUMO+2 for **PYFR** and **PYFD1-PYFD7**.

Compounds	**HOMO-1**	**LUMO+1**	**Δ*E***	**HOMO-2**	**LUMO+2**	**Δ*E***
PYFR	-6.290	-1.574	4.716	-6.742	-1.016	5.726
PYFD1	-6.270	-2.849	3.421	-6.564	-1.788	4.776
PYFD2	-6.350	-3.366	2.984	-6.656	-2.873	3.783
PYFD3	-6.352	-3.232	3.120	-6.658	-1.953	4.705
PYFD4	-6.346	-3.254	3.092	-6.648	-2.233	4.415
PYFD5	-6.329	-3.101	3.228	-6.625	-1.812	4.813
PYFD6	-6.303	-2.991	3.312	-6.594	-1.803	4.791
PYFD7	-6.287	-2.920	3.367	-6.584	-1.794	4.790

Table S10: Percentage contributions of donor, acceptor and π-spacer for HOMOs and LUMOs of **PYFR** and **PYFD1-PYFD7**.

Compounds	**HOMOs**			**LUMOs**		
	Donor	**Acceptor**	**π-spacer**	**Donor**	**Acceptor**	**π-spacer**
PYFR	83.4	-	16.6	61.3	-	38.7
PYFD1	83.1	0.1	16.9	0.0	92.1	7.9
PYFD2	83.7	0.1	16.2	0.0	80.8	19.2
PYFD3	83.8	0.1	16.1	0.0	91.1	8.9
PYFD4	83.6	0.1	16.3	0.0	91.6	8.4
PYFD5	83.5	0.1	16.5	0.0	90.7	9.3
PYFD6	83.2	0.1	16.8	0.0	91.6	8.4
PYFD7	83.3	0.1	16.6	0.0	92.3	7.7

Table S11: Natural bond orbitals (NBOs) analysis of **PYFR**.

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

C9-N37	σ	C25-C26	σ*	6.74	1.28	0.083
C9-C24	σ	N36-C60	σ*	6.07	1.09	0.073
C25-N37	σ	C8-C9	σ*	5.78	1.4	0.08
C3-C24	σ	C9-C24	σ*	5.69	1.28	0.076
C42-C44	σ	C44-C46	σ*	5.41	1.29	0.075
C62-C65	σ	C60-C62	σ*	4.12	1.3	0.065
C12-C13	σ	C14-C15	σ*	3.55	1.26	0.06
C9-C24	σ	C2-C3	σ*	3.1	1.28	0.056
C38-C39	σ	C29-C33	σ*	2.18	1.27	0.047
C28-H32	σ	C28-C31	σ*	1.11	1.12	0.032
C25-N37	σ	C25-N36	σ*	1.05	1.27	0.033
C2-H20	σ	C1-C2	σ*	1	1.11	0.03
C28-H32	σ	C26-C28	σ*	0.89	1.1	0.028
C56-H59	σ	C53-C56	σ*	0.7	1.1	0.025
C56-H59	σ	C55-C56	σ*	0.68	1.11	0.025
C25-N36	σ	C60-C61	σ*	0.63	1.39	0.026
C24-N36	σ	C9-N37	σ*	0.53	1.29	0.023
C47-H48	σ	C47-C51	σ*	0.51	0.95	0.02
C47-H49	σ	C47-C51	σ*	0.51	0.94	0.02
C24-N36	σ	C25-N37	σ*	0.5	1.35	0.023
C65-C67	π	C60-C62	π*	23.98	0.29	0.075
C65-C67	π	C60-C62	π*	23.98	0.29	0.075
C61-C63	π	C60-C62	π*	23.3	0.29	0.074
C42-C44	π	C38-C40	π*	23.28	0.29	0.074
C50-C51	π	C42-C44	π*	20.78	0.29	0.07
C8-C10	π	C9-C24	π*	19.76	0.29	0.068
C8-C10	π	C7-C14	π*	19.3	0.3	0.069
C2-C3	π	C9-C24	π*	18.81	0.3	0.068
C9-C24	π	C8-C10	π*	18.15	0.32	0.069
C9-C24	π	C25-N37	π*	16.11	0.29	0.062
C15-C16	π	C7-C14	π*	14.65	0.31	0.065
C4-C5	π	C15-C16	π*	14.22	0.3	0.063
C42-C44	π	C50-C51	π*	13.85	0.3	0.058
C60-C62	π	C28-C31	π*	0.60	0.32	0.012
N36	LP(1)	C25-N37	π*	51.64	0.3	0.111
N36	LP(1)	C9-C24	π*	34.74	0.32	0.095
N36	LP(1)	C60-C62	π*	1.64	0.3	0.02
N37	LP(1)	C25-N36	σ*	10.08	0.81	0.081
N37	LP(1)	C9-C24	σ*	6.93	0.96	0.074
N37	LP(1)	N36-C60	σ*	0.67	0.77	0.02

Table S12: Natural bond orbitals (NBOs) analysis of **PYFD1**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C69-H70	σ	C71-C72	σ*	9.4	1	0.086
C75-C91	σ	C91-N92	σ*	8.5	1.61	0.105
C91-N92	σ	C75-C91	σ*	8.34	1.57	0.103
C75-C89	σ	C89-N90	σ*	8.21	1.62	0.103
C89-N90	σ	C75-C89	σ*	8.11	1.57	0.101

C71-C73	σ	C76-O77	σ*	7.08	1.02	0.076
C9-N37	σ	C25-C26	σ*	6.59	1.28	0.082
C69-C71	σ	C71-C72	σ*	5.95	1.23	0.077
C5-C6	σ	C4-C5	σ*	4.77	1.27	0.07
C44-C50	σ	C42-C44	σ*	4.37	1.25	0.066
C94-C98	σ	C95-C98	σ*	3.84	1.28	0.063
C74-C78	σ	C73-C76	σ*	3.67	1.14	0.058
C78-C84	σ	O77-C80	σ*	2.56	1.04	0.046
C58-C60	σ	C60-H64	σ*	1.38	1.14	0.036
C82-H86	σ	C81-H83	σ*	0.74	0.93	0.023
C71-C72	σ	C76-O77	σ*	0.61	1.06	0.023
O77-C80	σ	C76-O77	σ*	0.53	1.3	0.024
C78-C84	σ	C74-C76	σ*	0.51	1.27	0.023
C78-C84	σ	C74-C76	σ*	0.51	1.27	0.023
C47-H49	σ	C47-C51	σ*	0.5	0.95	0.02
C81-C82	π	C78-C80	π*	25.5	0.28	0.078
C38-C39	π	C44-C46	π*	24.63	0.3	0.078
C63-C65	π	C58-C60	π*	24.09	0.29	0.075
C25-N37	π	C9-C24	π*	23.87	0.36	0.088
C7-C14	π	C3-C4	π*	22.89	0.28	0.072
C59-C61	π	C63-C65	π*	21.54	0.3	0.072
C1-C2	π	C5-C6	π*	20.9	0.3	0.072
C8-C10	π	C7-C14	π*	19.38	0.29	0.069
C74-C76	π	C78-C80	π*	14.4	0.32	0.063
C72-C75	π	C69-C71	π*	8.02	0.35	0.047
C73-O93	π	C74-C76	π*	4.64	0.43	0.043
C74-C76	π	C74-C76	π*	0.67	0.32	0.013
C91-N92	π	C89-N90	π*	0.65	0.48	0.016
C89-N90	π	C91-N92	π*	0.64	0.47	0.016
N36	LP(1)	C25-N37	π*	51.69	0.3	0.111
O77	LP(2)	C78-C80	π*	25.53	0.38	0.092
N36	LP(1)	C58-C60	π*	1.47	0.3	0.019
N90	LP(1)	C75-C89	σ*	12.69	1.04	0.103
N37	LP(1)	C25-N36	σ*	9.91	0.81	0.08
N37	LP(1)	N36-C58	σ*	0.68	0.77	0.021

Table S13: Natural bond orbitals (NBOs) analysis of **PYFD2**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C69-H70	σ	C71-C72	σ*	9.39	1	0.087
C75-C89	σ	C89-N90	σ*	8.59	1.62	0.106
C89-N90	σ	C75-C89	σ*	8.4	1.57	0.103
C78-C80	σ	C72-C74	σ*	7.86	1.18	0.086
C71-C73	σ	C76-O77	σ*	6.99	1.01	0.075
C69-C71	σ	C71-C72	σ*	6.14	1.24	0.078
C72-C75	σ	C75-C87	σ*	5.95	1.28	0.078
O77-C80	σ	C73-C76	σ*	5.38	1.39	0.078
C50-C55	σ	C44-C50	σ*	4.93	1.24	0.07
C29-H34	σ	C26-C27	σ*	4.4	1.09	0.062

C29-C33	σ	C27-C29	σ*	3.98	1.31	0.065
C60-H64	σ	C63-C65	σ*	3.64	1.11	0.057
C24-N36	σ	N36-C58	σ*	2.82	1.19	0.052
C25-C26	σ	C25-N36	σ*	1.76	1.11	0.04
C94-S95	σ	C92-C94	σ*	0.66	1.24	0.026
C84-C85	σ	C85-N99	σ*	0.63	1.02	0.023
N99-O101	σ	N99-O104	σ*	0.56	1.56	0.027
C47-H49	σ	C46-C47	σ*	0.51	0.94	0.02
C47-H49	σ	C47-C51	σ*	0.5	0.95	0.02
C81-C82	σ	C82-N100	σ*	0.5	1.02	0.021
C38-C39	π	C44-C46	π*	24.73	0.3	0.078
C31-C33	π	C26-C28	π*	24.48	0.29	0.076
C63-C65	π	C58-C60	π*	24.12	0.29	0.075
C55-C56	π	C52-C53	π*	20.16	0.3	0.07
C74-C76	π	C78-C80	π*	16.04	0.3	0.065
C72-C75	π	C74-C76	π*	9.36	0.32	0.05
N100-O102	π	N100-O102	π*	7.01	0.36	0.053
N99-O101	π	N99-O101	π*	6.59	0.4	0.054
C73-O91	π	C74-C76	π*	4.79	0.42	0.043
C72-C75	π	C72-C75	π*	1.51	0.33	0.02
C74-C76	π	C74-C76	π*	0.89	0.32	0.015
C87-N88	π	C89-N90	π*	0.61	0.47	0.015
C89-N90	π	C87-N88	π*	0.6	0.48	0.015
N36	LP(1)	C25-N37	π*	51.77	0.3	0.111
O103	LP(2)	C81-C82	π*	0.64	0.32	0.014
O91	LP(2)	C73-C76	σ*	24.22	0.73	0.12
O102	LP(2)	N100-O103	σ*	20.72	0.75	0.112
O102	LP(2)	C82-C85	σ*	0.56	0.84	0.02

Table S14: Natural bond orbitals (NBOs) analysis of **PYFD3**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C69-H70	σ	C71-C72	σ*	9.33	1	0.086
C75-C89	σ	C89-N90	σ*	8.63	1.61	0.106
C89-N90	σ	C75-C89	σ*	8.35	1.57	0.103
C78-C80	σ	C72-C74	σ*	7.81	1.19	0.086
C74-C76	σ	C78-C84	σ*	7.03	1.3	0.085
C9-N37	σ	C25-C26	σ*	6.56	1.28	0.082
C81-C82	σ	C82-C85	σ*	6.19	1.28	0.079
C71-C72	σ	C74-C78	σ*	6.07	1.19	0.076
C74-C78	σ	C78-C84	σ*	5.74	1.27	0.076
C42-C44	σ	C44-C46	σ*	5.5	1.29	0.075
C55-C56	σ	C56-C93	σ*	4.08	1.21	0.063
C44-C46	σ	C44-C50	σ*	3.18	1.2	0.055
C29-C33	σ	C38-C39	σ*	2.06	1.28	0.046
S99-O105	σ	C82-S99	σ*	1.01	0.92	0.028
C28-H32	σ	C31-H35	σ*	0.82	0.94	0.025
C65-H68	σ	C61-C65	σ*	0.71	1.11	0.025
C25-N36	σ	C58-C59	σ*	0.63	1.39	0.026

C47-H48	σ	C47-C51	σ*	0.51	0.95	0.02
C47-H49	σ	C47-C51	σ*	0.51	0.95	0.02
O77-C80	σ	C76-O77	σ*	0.51	1.31	0.023
C38-C39	π	C44-C46	π*	24.75	0.3	0.078
C31-C33	π	C26-C28	π*	24.5	0.29	0.076
C63-C65	π	C58-C60	π*	24.12	0.29	0.075
C50-C51	π	C55-C56	π*	24.02	0.28	0.074
C25-N37	π	C9-C24	π*	23.88	0.36	0.088
C8-C10	π	C9-C24	π*	19.84	0.29	0.068
C15-C16	π	C13-C14	π*	16.57	0.31	0.068
C92-C94	π	C93-C96	π*	15.78	0.31	0.063
C93-C96	π	C55-C56	π*	11.6	0.32	0.056
C73-O91	π	C74-C76	π*	4.76	0.42	0.043
C87-N88	π	C89-N90	π*	0.62	0.47	0.015
C89-N90	π	C87-N88	π*	0.59	0.48	0.015
N36	LP(1)	C25-N37	π*	51.75	0.3	0.111
N36	LP(1)	C9-C24	π*	34.53	0.32	0.095
O106	LP(2)	C81-C82	π*	0.75	0.32	0.014
O91	LP(2)	C71-C73	σ*	21.68	0.71	0.113
O105	LP(2)	C82-C85	σ*	0.53	0.9	0.02
C69-H70	σ	C71-C72	σ*	9.33	1	0.086

Table S15: Natural bond orbitals (NBOs) analysis of **PYFD4**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C69-H70	σ	C71-C72	σ*	9.44	1	0.087
C82-C101	σ	C101-N102	σ*	8.97	1.62	0.108
C85-C99	σ	C99-N100	σ*	8.84	1.62	0.107
C101-N102	σ	C82-C101	σ*	8.66	1.57	0.105
C75-C89	σ	C89-N90	σ*	8.58	1.62	0.106
C69-C71	σ	C71-C72	σ*	6.15	1.24	0.078
C9-C24	σ	N36-C58	σ*	6.05	1.09	0.073
C72-C75	σ	C75-C87	σ*	5.93	1.28	0.078
C69-C71	σ	C69-C94	σ*	5.71	1.31	0.077
C81-C82	σ	O77-C80	σ*	5.64	1.07	0.069
C92-H98	σ	C94-S95	σ*	5.52	0.75	0.057
C74-C78	σ	C78-C84	σ*	5.42	1.26	0.074
C84-C85	σ	C74-C78	σ*	5.29	1.23	0.072
C50-C51	σ	C50-C55	σ*	5.17	1.28	0.073
C39-H41	σ	C44-C46	σ*	4.94	1.1	0.066
C71-C73	σ	C73-O91	σ*	2.1	1.25	0.046
C71-C72	σ	C71-C73	σ*	1.02	1.12	0.03
C47-H48	σ	C47-C51	σ*	0.51	0.95	0.02
C47-H49	σ	C46-C47	σ*	0.51	0.94	0.02
C47-H49	σ	C47-C51	σ*	0.5	0.95	0.02
C38-C39	π	C44-C46	π*	24.72	0.3	0.078
C31-C33	π	C26-C28	π*	24.47	0.29	0.076
C63-C65	π	C58-C60	π*	24.12	0.29	0.075
C25-N37	π	C9-C24	π*	23.91	0.36	0.088

C74-C76	π	C72-C75	π*	22.49	0.32	0.076
C26-C28	π	C31-C33	π*	21.43	0.3	0.072
C55-C56	π	C52-C53	π*	20.15	0.3	0.07
C81-C82	π	C84-C85	π*	19.37	0.31	0.069
C84-C85	π	C78-C80	π*	18.54	0.29	0.067
C25-N37	π	C26-C28	π*	8.11	0.36	0.051
C87-N88	π	C89-N90	π*	0.61	0.47	0.015
C89-N90	π	C87-N88	π*	0.61	0.48	0.015
N36	LP(1)	C25-N37	π*	51.79	0.3	0.111
O77	LP(2)	C78-C80	π*	27.82	0.38	0.095
N36	LP(1)	C58-C60	π*	1.19	0.3	0.017
O91	LP(2)	C73-C76	σ*	24.11	0.73	0.12
N100	LP(1)	C85-C99	σ*	12.32	1.05	0.101
N37	LP(1)	N36-C58	σ*	0.68	0.77	0.021
C69-H70	σ	C71-C72	σ*	9.44	1	0.087

Table S16: Natural bond orbitals (NBOs) analysis of **PYFD5**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C69-H70	σ	C71-C72	σ*	9.48	1	0.087
C75-C89	σ	C89-N90	σ*	8.57	1.62	0.106
C89-N90	σ	C75-C89	σ*	8.39	1.57	0.103
C75-C87	σ	C87-N88	σ*	8.29	1.62	0.104
C78-C80	σ	C72-C74	σ*	7.96	1.18	0.087
C9-N37	σ	C25-C26	σ*	6.54	1.28	0.082
C71-C72	σ	C69-C71	σ*	6.11	1.3	0.08
C84-C85	σ	C82-C85	σ*	5.99	1.27	0.078
C81-C82	σ	O77-C80	σ*	5.56	1.07	0.069
C8-C10	σ	C7-C8	σ*	5.25	1.27	0.073
C40-C42	σ	C44-C50	σ*	5.00	1.23	0.07
C15-H18	σ	C5-C16	σ*	4.91	1.06	0.064
C55-H57	σ	C50-C51	σ*	4.84	1.1	0.065
C7-C14	σ	C7-C8	σ*	4.45	1.25	0.067
C44-C50	σ	C39-C46	σ*	3.92	1.27	0.063
C85-C99	σ	C81-C82	σ*	2.64	1.27	0.052
C25-N37	σ	C26-C28	σ*	1.89	1.42	0.046
C47-H49	σ	C46-C47	σ*	0.51	0.94	0.02
C69-H70	σ	C94-S95	σ*	0.51	0.73	0.017
C47-H49	σ	C47-C51	σ*	0.5	0.95	0.02
C38-C39	π	C44-C46	π*	24.7	0.3	0.078
C31-C33	π	C26-C28	π*	24.48	0.29	0.076
C63-C65	π	C58-C60	π*	24.12	0.29	0.075
C25-N37	π	C9-C24	π*	23.92	0.36	0.088
C52-C53	π	C50-C51	π*	22.96	0.31	0.076
C84-C85	π	C81-C82	π*	21.62	0.3	0.073
C78-C80	π	C81-C82	π*	20.77	0.3	0.072
C31-C33	π	C27-C29	π*	19.59	0.3	0.07
C26-C28	π	C25-N37	π*	18.94	0.28	0.065
C72-C75	π	C72-C75	π*	1.55	0.33	0.02

C87-N88	π	C89-N90	π*	0.61	0.47	0.015
C89-N90	π	C87-N88	π*	0.61	0.48	0.015
O77	LP(2)	C74-C76	π*	34.67	0.39	0.104
S95	LP(2)	C92-C94	π*	22.72	0.27	0.07
F101	LP(2)	C84-C85	π*	0.91	0.48	0.02
O91	LP(2)	C73-C76	σ*	23.86	0.73	0.119
O91	LP(2)	C71-C73	σ*	21.73	0.71	0.113
F104	LP(1)	C82-C100	σ*	0.5	1.46	0.024
C69-H70	σ	C71-C72	σ*	9.48	1	0.087

Table S17: Natural bond orbitals (NBOs) analysis of **PYFD6**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C69-H70	σ	C71-C72	σ*	9.5	1	0.087
C75-C89	σ	C89-N90	σ*	8.55	1.61	0.105
C89-N90	σ	C75-C89	σ*	8.37	1.57	0.103
C75-C87	σ	C87-N88	σ*	8.27	1.62	0.104
C87-N88	σ	C75-C87	σ*	8.19	1.57	0.102
C71-C73	σ	C76-O77	σ*	7.07	1.02	0.076
C74-C76	σ	C78-C84	σ*	6.79	1.29	0.084
C71-C72	σ	C69-C71	σ*	6.11	1.3	0.08
C78-C84	σ	C74-C78	σ*	5.82	1.23	0.075
C69-C71	σ	C69-C94	σ*	5.66	1.3	0.077
C92-C96	σ	C56-C93	σ*	5.19	1.21	0.071
C52-C53	σ	C47-C51	σ*	5.05	1.15	0.068
C40-C42	σ	C44-C50	σ*	5.00	1.23	0.07
C15-H18	σ	C7-C14	σ*	4.68	1.09	0.064
C10-H11	σ	C12-C13	σ*	3.82	1.11	0.058
C7-C8	σ	C4-C5	σ*	2.67	1.25	0.052
C44-C50	σ	C55-C56	σ*	1.85	1.22	0.043
C47-H49	σ	C46-C47	σ*	0.51	0.94	0.02
C47-H49	σ	C47-C51	σ*	0.51	0.95	0.02
C81-H83	σ	C82-Cl100	σ*	0.50	0.68	0.017
C38-C39	π	C44-C46	π*	24.67	0.3	0.078
C63-C65	π	C58-C60	π*	24.12	0.29	0.075
C25-N37	π	C9-C24	π*	23.91	0.36	0.088
C44-C46	π	C38-C39	π*	22.56	0.29	0.073
C59-C61	π	C63-C65	π*	21.58	0.3	0.072
C55-C56	π	C52-C53	π*	20.19	0.3	0.07
C69-C71	π	C72-C75	π*	19.48	0.3	0.07
C3-C4	π	C9-C24	π*	18.03	0.29	0.065
C15-C16	π	C5-C6	π*	16.52	0.31	0.068
C7-C14	π	C15-C16	π*	14.43	0.3	0.063
C74-C76	π	C74-C76	π*	0.72	0.32	0.014
C87-N88	π	C89-N90	π*	0.62	0.47	0.015
C89-N90	π	C87-N88	π*	0.62	0.48	0.015
N36	LP(1)	C25-N37	π*	51.78	0.3	0.111
S95	LP(2)	C93-C96	π*	27.18	0.28	0.078
N36	LP(1)	C58-C60	π*	1.20	0.3	0.017

O91	LP(2)	C73-C76	σ*	23.55	0.73	0.119
N88	LP(1)	C75-C87	σ*	12.7	1.04	0.103
Cl100	LP(2)	C80-C81	σ*	0.56	0.91	0.02

Table S18: Natural bond orbitals (NBOs) analysis of **PYFD7**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C69-H70	σ	C71-C72	σ*	9.35	1	0.086
C75-C89	σ	C89-N90	σ*	8.52	1.61	0.105
C89-N90	σ	C75-C89	σ*	8.34	1.57	0.103
C75-C87	σ	C87-N88	σ*	8.23	1.62	0.104
C71-C73	σ	C76-O77	σ*	7.14	1.02	0.076
C74-C76	σ	C78-C84	σ*	6.72	1.29	0.083
C96-H97	σ	C93-S95	σ*	5.65	0.75	0.058
C25-N36	σ	C3-C24	σ*	4.87	1.35	0.073
C44-C50	σ	C42-C44	σ*	4.37	1.25	0.066
C80-C81	σ	C82-F100	σ*	4.1	1.05	0.059
C94-S95	σ	C56-C93	σ*	3.99	1.18	0.061
C74-C76	σ	C74-C78	σ*	3.65	1.23	0.06
C5-C16	σ	C3-C4	σ*	3.29	1.23	0.057
C25-N36	σ	N36-C58	σ*	2.92	1.2	0.053
C10-C12	σ	C13-H23	σ*	2.58	1.13	0.048
C8-C9	σ	C10-C12	σ*	1.95	1.28	0.045
C4-C5	σ	C16-H17	σ*	1.78	1.1	0.04
C47-H49	σ	C46-C47	σ*	0.51	0.94	0.02
C78-C84	σ	C74-C76	σ*	0.51	1.28	0.023
C47-H49	σ	C47-C51	σ*	0.50	0.95	0.02
C38-C39	π	C44-C46	π*	24.65	0.3	0.078
C63-C65	π	C58-C60	π*	24.08	0.29	0.075
C25-N37	π	C9-C24	π*	23.84	0.36	0.088
C5-C6	π	C1-C2	π*	23.75	0.29	0.075
C69-C71	π	C73-O91	π*	22.06	0.31	0.074
C52-C53	π	C55-C56	π*	21.8	0.3	0.073
C74-C76	π	C73-O91	π*	20.89	0.33	0.075
C81-C82	π	C84-C85	π*	19.17	0.32	0.07
C84-C85	π	C78-C80	π*	18.62	0.3	0.07
C5-C6	π	C15-C16	π*	17.24	0.31	0.069
C89-N90	π	C87-N88	π*	0.64	0.48	0.016
C74-C76	π	C74-C76	π*	0.63	0.32	0.013
C81-C82	π	C81-C82	π*	0.55	0.31	0.012
C93-C96	π	C55-C56	π*	11.42	0.32	0.056
N36	LP(1)	C25-N37	π*	51.69	0.3	0.111
N36	LP(1)	C9-C24	π*	34.5	0.32	0.094
N36	LP(1)	C58-C60	π*	1.53	0.3	0.019
O91	LP(2)	C73-C76	σ*	23.46	0.74	0.119
N88	LP(1)	C75-C87	σ*	12.7	1.04	0.103
N37	LP(1)	N36-C58	σ*	0.68	0.77	0.021

Table S19: Wavelength, excitation energy and oscillator strength of investigated compound **PYFR**

NO	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	371.032	3.342	0.886	H→L (90%), H→L+4 (3%)
2	351.708	3.525	0.201	H→L+1 (75%), H-2→L (5%), H→L+2 (3%), H→L+4 (5%)
3	333.578	3.717	0.142	H-2→L+1 (14%), H→L+1 (13%), H→L+2 (29%), H→L+4 (13%), H-2→L (7%), H-1→L (6%), H→L+3 (3%), H→L+5 (5%), H→L+6 (4%)
4	323.626	3.831	0.127	H→L+2 (49%), H→L+3 (35%), H-2→L (2%), H-2→L+1 (2%), H-1→L (4%), H→L+4 (2%)
5	317.363	3.907	0.094	H→L+2 (13%), H→L+3 (53%), H→L+4 (18%), H-1→L (9%)

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 **PYFD1**

NO	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	553.649	2.239	0.013	H→L (97%)
2	501.554	2.472	0.005	H→L+1 (96%)
3	497.869	2.490	0.210	H-3→L (14%), H-2→L (25%), H-1→L (51%), H→L+1 (2%)
4	442.122	2.804	0.749	H-2→L+1 (18%), H-1→L+1 (56%), H-5→L (3%), H-3→L+1 (8%), H-1→L (7%)
5	421.328	2.943	0.197	H-3→L (22%), H-2→L (27%), H-1→L (36%), H-4→L (4%), H-3→L+1 (2%), H-2→L+1 (3%), H-1→L+1 (2%)
6	391.093	3.170	0.130	H-3→L+1 (23%), H-2→L+1 (26%), H-1→L+1 (36%), H-5→L (3%), H-4→L+1 (5%)

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 **PYFD2**

NO	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	685.981	1.807	0.008	H→L (99%)
2	663.053	1.870	0.002	H→L+1 (99%)
3	525.892	2.358	0.201	H-3→L (24%), H-3→L+1 (11%), H-1→L (40%), H-2→L (8%), H-2→L+1 (2%), H-1→L+1 (7%)
4	500.118	2.479	0.338	H-3→L+1 (15%), H-1→L (27%), H-1→L+1 (42%), H-2→L+1 (6%), H→L+2 (3%)
5	484.863	2.557	0.012	H→L+2 (97%)
6	468.041	2.649	0.253	H-3→L (35%), H-1→L (26%), H-1→L+1 (22%), H-4→L (9%), H-2→L (5%)

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 **PYFD3** at M06/6-311G(d,p) in gaseous phase.

NO	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	697.363	1.778	0.005	H→L (99%)
2	635.263	1.952	0.006	H→L+1 (99%)

3	533.105	2.326	0.216	H-3→L (34%), H-2→L (10%), H-1→L (48%), H-4→L (3%)
4	489.418	2.533	0.203	H-3→L (10%), H-3→L+1 (12%), H-1→L (20%), H-1→L+1 (43%), H-4→L (5%), H-2→L+1 (6%)
5	470.850	2.633	0.465	H-3→L (25%), H-1→L (29%), H-1→L+1 (25%), H-4→L (6%), H-3→L+1 (6%), H-2→L (4%), H-2→L+1 (3%)
6	443.656	2.795	0.013	H-2→L (84%), H-4→L (4%), H-3→L (9%)

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 **PYFD4** at M06/6-311G(d,p) in gaseous phase.

NO	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	671.419	1.847	0.007	H→L (97%), H→L+1 (2%)
2	640.150	1.937	0.005	H→L+1 (97%), H→L (2%)
3	522.897	2.371	0.183	H-3→L (35%), H-2→L (10%), H-1→L (44%), H-4→L (3%), H-3→L+1 (3%)
4	489.998	2.530	0.439	H-3→L+1 (15%), H-1→L (12%), H-1→L+1 (58%), H-2→L+1 (8%)
5	463.336	2.676	0.294	H-3→L (33%), H-1→L (40%), H-1→L+1 (10%), H-4→L (9%), H-2→L (4%)
6	443.895	2.793	0.495	H-3→L+1 (48%), H-2→L+1 (10%), H-1→L+1 (27%), H-4→L+1 (9%)

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 **PYFD5** at M06/6-311G(d,p) in gaseous phase.

NO	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	629.777	1.969	0.007	H→L (98%)
2	583.235	2.126	0.007	H→L+1 (98%)
3	512.310	2.420	0.213	H-3→L (35%), H-2→L (12%), H-1→L (44%), H-4→L (2%), H-3→L+1 (2%)
4	469.282	2.642	0.495	H-3→L+1 (15%), H-1→L (16%), H-1→L+1 (51%), H-3→L (3%), H-2→L+1 (8%)
5	447.693	2.769	0.412	H-3→L (33%), H-1→L (35%), H-1→L+1 (10%), H-4→L (6%), H-3→L+1 (5%), H-2→L (6%), H-2→L+1 (2%)
6	423.154	2.930	0.318	H-3→L+1 (44%), H-1→L+1 (34%), H-4→L+1 (8%), H-2→L+1 (8%)

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 **PYFD6** at M06/6-311G(d,p) in gaseous phase.

NO	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	591.923	2.095	0.009	H→L (98%)

2	540.943	2.292	0.011	H→L+1 (98%)
3	506.968	2.446	0.203	H-3→L (28%), H-2→L (18%), H-1→L (46%),
4	455.942	2.719	0.742	H-3→L+1 (14%), H-2→L+1 (12%), H-1→L (13%), H-1→L+1 (52%),
5	435.185	2.849	0.348	H-3→L (31%), H-2→L (12%), H-1→L (37%), H-4→L (5%), H-3→L+1 (5%), H-2→L+1 (3%), H-1→L+1 (5%)
6	407.588	3.042	0.207	H-3→L+1 (36%), H-2→L+1 (13%), H-1→L+1 (38%), H-4→L+1 (6%), H-1→L (2%)

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

Table S26: Wavelength, excitation energy and oscillator strength of investigated compound **PYFD7** at M06/6-311G(d,p) in gaseous phase.

NO	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	589.082	2.105	0.008	H→L (98%)
2	529.191	2.343	0.012	H→L+1 (99%)
3	510.076	2.431	0.186	H-3→L (27%), H-2→L (18%), H-1→L (48%),
4	451.722	2.745	0.586	H-3→L+1 (13%), H-2→L+1 (11%), H-1→L (12%), H-1→L+1 (52%), H-5→L (2%), H-3→L (4%)
5	436.149	2.843	0.311	H-3→L (29%), H-2→L (12%), H-1→L (36%), H-4→L (5%), H-3→L+1 (6%), H-2→L+1 (3%), H-1→L+1 (7%)
6	403.253	3.075	0.176	H-3→L+1 (36%), H-2→L+1 (14%), H-1→L+1 (35%), H-5→L (2%), H-4→L+1 (6%)

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

Table S27: Wavelength, excitation energy and oscillator strength of investigated compound **PYFR** at M06/6-311G(d,p) in chloroform solvent.

No	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	372.347	3.330	1.124	H→L (86%), H→L+1 (4%), H→L+2 (3%)
2	354.981	3.493	0.411	H→L+1 (79%), H-2→L (3%), H-2→L+2 (3%), H→L (6%), H→L+2 (6%)
3	333.443	3.718	0.283	H-2→L (14%), H-2→L+1 (11%), H-1→L (12%), H→L+2 (44%), H-1→L+1 (2%), H→L+1 (6%), H→L+5 (4%)
4	314.274	3.945	0.387	H-1→L (62%), H-1→L+1 (15%), H→L (2%), H→L+1 (4%), H→L+2 (8%)
5	300.197	4.130	0.022	H→L+3 (78%), H-2→L (2%), H→L+4 (6%), H→L+5 (5%)
6	297.160	4.172	0.031	H-1→L+1 (47%), H-3→L (9%), H-3→L+1 (4%), H-2→L (4%), H-1→L (7%), H→L+2 (6%), H→L+4 (8%), H→L+5 (5%)

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

Table S28: Wavelength, excitation energy and oscillator strength of investigated compound **PYFD1** at M06/6-311G(d,p) in chloroform solvent.

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

1	528.807	2.345	0.142	H-2→L (10%), H-1→L (35%), H→L (53%),
2	506.906	2.446	0.082	H-2→L (19%), H-1→L (32%), H→L (46%),
3	470.136	2.637	0.250	H-1→L+1 (16%), H→L+1 (80%),
4	447.483	2.771	0.718	H-2→L+1 (20%), H-1→L+1 (54%), H→L+1 (19%), H-5→L (3%)
5	418.089	2.966	0.061	H-2→L (60%), H-1→L (29%), H-4→L (3%), H-3→L (2%), H-2→L+1 (3%)
6	385.044	3.220	0.048	H-2→L+1 (55%), H-1→L+1 (27%), H-5→L (8%), H-4→L+1 (3%), H-3→L+1 (2%)

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

Table S29: Wavelength, excitation energy and oscillator strength of investigated compound **PYFD2** at M06/6-311G(d,p) in chloroform solvent.

No	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	583.592	2.125	0.059	H→L (89%), H-1→L (3%), H→L+1 (6%)
2	568.970	2.179	0.001	H→L+1 (89%), H-1→L+1 (3%), H→L (7%)
3	532.327	2.329	0.248	H-2→L (11%), H-2→L+1 (22%), H-1→L (22%), H-1→L+1 (33%), H-3→L+1 (2%), H→L+1 (4%)
4	500.542	2.477	0.778	H-2→L+1 (10%), H-1→L (48%), H-1→L+1 (22%), H-2→L (9%), H-1→L+2 (3%)
5	461.680	2.686	0.007	H→L+2 (95%), H-2→L (3%)
6	448.487	2.765	0.154	H-2→L (48%), H-1→L (20%), H-4→L (3%), H-3→L (6%), H-2→L+1 (6%), H-1→L+1 (9%), H→L+2 (3%)

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

Table S30: Wavelength, excitation energy and oscillator strength of investigated compound **PYFD3** at M06/6-311G(d,p) in chloroform solvent.

No	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	582.195	2.130	0.043	H→L (92%), H-1→L (6%)
2	540.896	2.292	0.044	H→L+1 (95%), H-1→L+1 (3%)
3	536.125	2.313	0.237	H-2→L (32%), H-1→L (54%), H-3→L (3%), H→L (7%)
4	484.011	2.562	0.888	H-2→L+1 (22%), H-1→L+1 (67%), H→L+1 (3%)
5	448.860	2.762	0.108	H-2→L (47%), H-1→L (35%), H-4→L (3%), H-3→L (7%), H-2→L+1 (5%)
6	422.131	2.937	0.124	H-2→L+1 (54%), H-1→L+1 (27%), H-4→L+1 (4%), H-3→L+1 (7%), H-1→L (3%)

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

Table S31: Wavelength, excitation energy and oscillator strength of investigated compound **PYFD4** at M06/6-311G(d,p) in chloroform solvent.

No	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	572.147	2.167	0.050	H→L (90%), H-1→L (6%), H→L+1 (2%)
2	545.825	2.272	0.041	H→L+1 (94%), H-1→L+1 (3%), H→L (2%)
3	529.666	2.341	0.210	H-2→L (32%), H-1→L (54%), H-3→L (3%), H→L (7%)

4	487.417	2.544	0.968	H-2→L+1 (22%), H-1→L+1 (68%), H→L+1 (3%)
5	443.133	2.798	0.111	H-2→L (47%), H-1→L (33%), H-4→L (3%), H-3→L (6%), H-2→L+1 (7%)
6	424.429	2.921	0.117	H-2→L+1 (54%), H-1→L+1 (26%), H-4→L+1 (3%), H-3→L+1 (6%), H-2→L (3%), H-1→L (5%)

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

Table S32: Wavelength, excitation energy and oscillator strength of investigated compound **PYFD5** at M06/6-311G(d,p) in chloroform solvent.

No	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	557.408	2.224	0.063	H→L (88%), H-1→L (9%)
2	523.118	2.370	0.184	H-2→L (31%), H-1→L (52%), H→L (10%),
3	514.287	2.411	0.097	H→L+1 (93%), H-1→L+1 (5%)
4	470.243	2.637	0.926	H-2→L+1 (22%), H-1→L+1 (66%), H→L+1 (5%)
5	434.971	2.850	0.100	H-2→L (52%), H-1→L (33%), H-4→L (3%), H-3→L (5%), H-2→L+1 (5%)
6	408.084	3.038	0.099	H-2→L+1 (57%), H-1→L+1 (27%), H-4→L+1 (3%), H-3→L+1 (5%), H-1→L (3%)

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

Table S33: Wavelength, excitation energy and oscillator strength of investigated compound **PYFD6** at M06/6-311G(d,p) in chloroform solvent.

No	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	544.818	2.276	0.090	H-1→L (17%), H→L (77%), H-2→L (4%)
2	518.893	2.389	0.141	H-2→L (27%), H-1→L (47%), H→L (22%),
3	494.178	2.509	0.149	H→L+1 (90%), H-1→L+1 (8%)
4	461.577	2.686	0.968	H-2→L+1 (22%), H-1→L+1 (62%), H-5→L (2%), H→L+1 (9%)
5	427.856	2.898	0.081	H-2→L (56%), H-1→L (31%), H-4→L (3%), H-3→L (3%), H-2→L+1 (4%)
6	397.998	3.115	0.089	H-2→L+1 (58%), H-1→L+1 (27%), H-5→L (2%), H-4→L+1 (3%), H-3→L+1 (4%)

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

Table S34: Wavelength, excitation energy and oscillator strength of investigated compound **PYFD7** at M06/6-311G(d,p) in chloroform solvent.

No	DFT λ (*nm*)	*E (eV)*	f_{os}	MO contributions
1	541.345	2.290	0.104	H-1→L (24%), H→L (67%), H-2→L (7%)
2	517.463	2.396	0.115	H-2→L (24%), H-1→L (41%), H→L (32%),
3	481.174	2.577	0.174	H-1→L+1 (11%), H→L+1 (86%),
4	453.922	2.731	0.782	H-2→L+1 (21%), H-1→L+1 (59%), H→L+1 (13%), H-5→L (3%)
5	426.664	2.906	0.061	H-2→L (58%), H-1→L (31%), H-4→L (3%), H-3→L (3%), H-2→L+1 (3%)

6	391.327	3.168	0.069	H-2→L+1 (58%), H-1→L+1 (27%), H-5→L (4%), H-4→L+1 (3%), H-3→L+1 (3%)

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

Table S35: Dipole polarizability and major contributing tensors (*D*) of the studied compounds (**PYFR** and **PYFD1-PYFD7**).

System	μ_x	μ_y	μ_z	μ_{total}
PYFR	-1.961	5.801	0.217	6.127
PYFD1	1.418	-9.884	0.732	10.013
PYFD2	-10.834	-10.973	4.495	16.062
PYFD3	-12.854	-10.894	5.677	17.780
PYFD4	-11.423	-10.697	5.028	16.438
PYFD5	7.040	10.473	3.533	13.105
PYFD6	-3.404	-10.368	2.892	11.290
PYFD7	1.908	10.480	2.011	10.841

Table S36: Average linear polarizability $\langle\alpha\rangle$ and major contributing tensor (*esu*) of the studied compounds (**PYFR** and **PYFD1-PYFD7**).

System	$\alpha_{xx}\times10^{-22}$	$\alpha_{yy}\times10^{-22}$	$\alpha_{zz}\times10^{-22}$	$\langle\alpha\rangle\times10^{-22}$
PYFR	1.589	1.187	4.380	1.072
PYFD1	2.723	1.420	1.108	1.750
PYFD2	2.961	1.445	1.176	1.861
PYFD3	2.998	1.482	1.217	1.899
PYFD4	3.019	1.426	1.170	1.872
PYFD5	2.874	1.429	1.152	1.819
PYFD6	2.925	1.417	1.160	1.834
PYFD7	2.732	1.417	1.160	1.752

Table S37: The computed first hyper-polarizability (β_{tot}) and major contributing tensors (*esu*) of (**PYFR** and **PYFD1-PYFD7**).

First Hyper-polarizability	PYFR	PYFD1	PYFD2	PYFD3	PYFD4	PYFD5	PYFD6	PYFD7
$\beta_{xxx}\times10^{-28}$	0.272	-1.437	-4.049	-3.328	-3.501	2.733	-1.749	1.568
$\beta_{xxy}\times10^{-29}$	0.096	-4.215	-9.629	-8.181	-9.345	7.201	-5.706	4.412
$\beta_{xyy}\times10^{-29}$	-1.101	-2.438	-3.593	-3.049	-3.738	2.892	-2.815	2.422
$\beta_{yyy}\times10^{-29}$	-0.243	-1.567	-1.616	-1.404	-1.704	1.408	-1.496	1.501
$\beta_{xxz}\times10^{-29}$	0.105	-4.968	-8.041	-7.396	-6.976	-6.020	-5.533	-5.652
$\beta_{yyz}\times10^{-30}$	-0.412	-5.263	-5.869	-5.131	-6.054	-5.139	-4.941	-5.185
$\beta_{xzz}\times10^{-29}$	0.0166	-1.552	-2.808	-2.596	-2.408	2.092	-1.672	1.786
$\beta_{yzz}\times10^{-30}$	-0.682	-3.784	-6.896	-5.611	-6.401	5.306	-4.544	4.201
$\beta_{zzz}\times10^{-30}$	0.0143	-7.662	-11.94	-13.80	-10.97	-11.55	-9.762	-9.078
$\beta_{tot}\times10^{-28}$	0.1650	2.036	4.937	4.128	4.365	3.445	2.431	2.204

Table S38: Second hyper-polarizability (γ_{tot}) and major contributing tensor (*esu*) of the studied compounds (**PYFR** and **PYFD1-PYFD7**).

System	$\gamma_x\times10^{-33}$	$\gamma_y\times10^{-34}$	$\gamma_z\times10^{-34}$	$\gamma_{tot}\times10^{-33}$
PYFR	1.025	0.4847	0.03492	1.077

PYFD1	2.574	2.278	1.185	2.921
PYFD2	4.180	2.735	1.772	4.631
PYFD3	3.609	2.432	1.647	4.017
PYFD4	3.841	2.717	1.572	4.269
PYFD5	3.157	2.294	1.429	3.529
PYFD6	3.095	2.383	1.338	3.467
PYFD7	2.664	2.264	1.279	3.018

Table S39: Frequency dependent First hyperpolarizability (*esu*) of studied comp. **PYFR** and **PYFD1-PYFD7**.

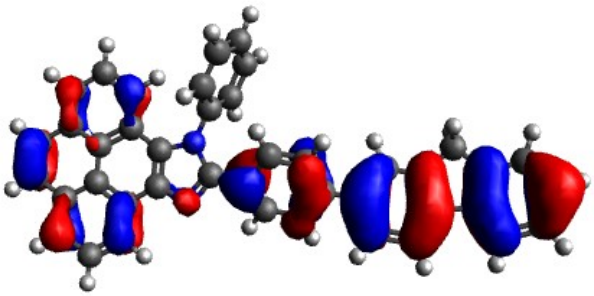
Parameters	**Frequency ω**	**PYFR ×10^{-29}**	**PYFD1 ×10^{-28}**	**PYFD2 ×10^{-28}**	**PYFD3 ×10^{-28}**	**PYFD4 ×10^{-28}**	**PYFD5 ×10^{-28}**	**PYFD6 ×10^{-28}**	**PYFD7 ×10^{-28}**
β (−ω;ω,0,)	0.000	1.650	2.036	4.937	4.128	4.365	3.445	2.431	2.204
β (-2, ω;ω,ω)	0.000	1.650	2.036	4.937	4.128	4.365	3.445	2.431	2.204
β (−ω;ω,0)	1907.21nm	1.823	2.118	5.048	4.234	4.453	3.502	2.544	2.282
β (−2ω;ω,ω)	1907.21nm	2.388	2.849	6.904	5.769	6.021	4.682	3.503	3.101

Table S40: Frequency dependent Second hyperpolarizability (*esu*) of studied comp. **PYFR** and **PYFD1-PYFD7**.

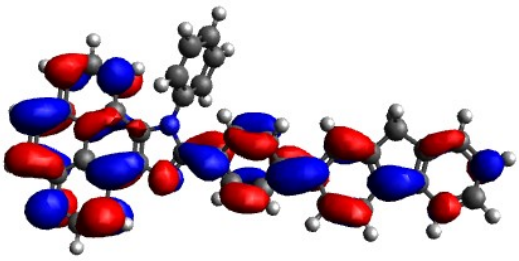
Parameters	**Frequency ω**	**PYFR ×10^{-33}**	**PYFD1 ×10^{-33}**	**PYFD2 ×10^{-33}**	**PYFD3 ×10^{-33}**	**PYFD4 ×10^{-33}**	**PYFD5 ×10^{-33}**	**PYFD6 ×10^{-33}**	**PYFD7 ×10^{-33}**
γ(−ω,ω,0,0)	0.000	1.077	2.921	4.632	4.017	4.269	3.529	3.467	3.018
	1907.21*nm*	1.008	2.929	4.883	4.185	4.430	3.618	3.516	3.041
γ(−2ω,ω,ω,0)	0.000	1.077	2.921	4.632	4.017	4.269	3.529	3.467	3.018
	1907.21*nm*	1.139	3.779	7.539	6.114	6.430	4.998	4.686	3.992

Table S41: Calculated energies (E_{HOMO} , E_{LUMO}) and energy gap (ΔE) of the entitled compounds in eV at DFT approach.

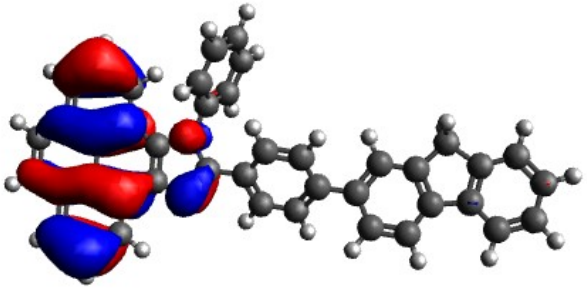
Compounds	E_{HOMO}	E_{LUMO}	ΔE (eV)
PYFR	-5.735	-1.723	4.012
PYFD1	-5.729	-3.125	2.604
PYFD2	-5.739	-3.399	2.340
PYFD3	-5.740	-3.391	2.349
PYFD4	-5.738	-3.350	2.388
PYFD5	-5.735	-3.285	2.450
PYFD6	-5.731	-3.220	2.511
PYFD7	-5.733	-3.198	2.535



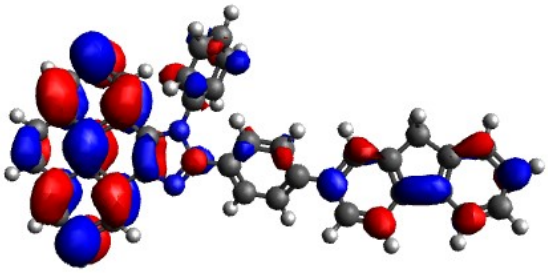
HOMO -1



LUMO +1

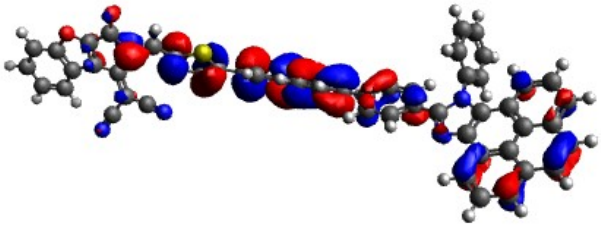


HOMO -2

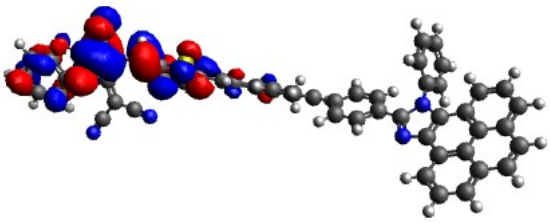


LUMO +2

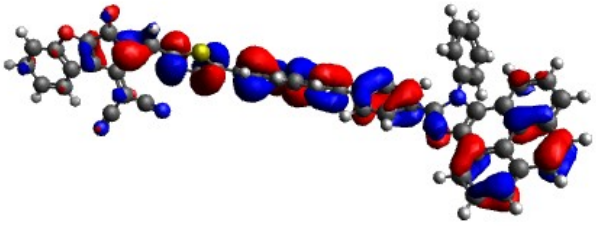
PYFR



HOMO -1



LUMO +1



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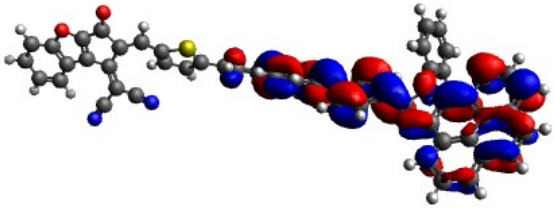
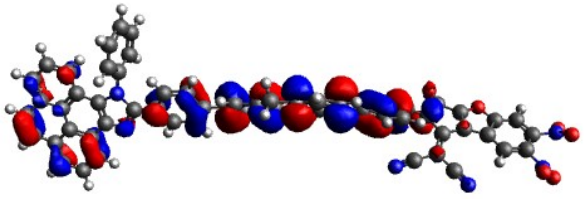
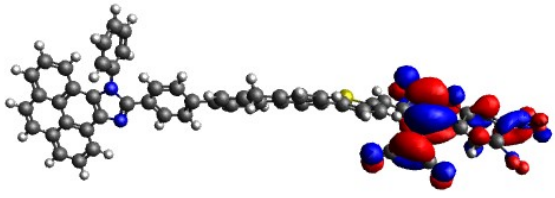


LUMO +2

PYFD1





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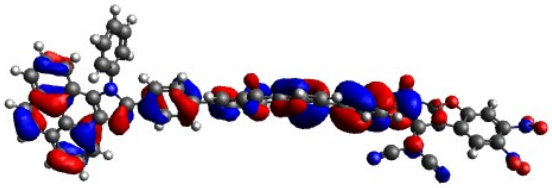
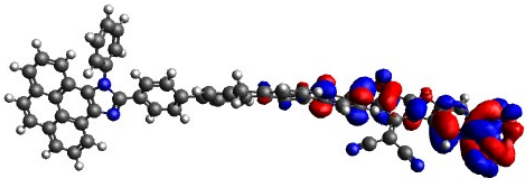


LUMO +1



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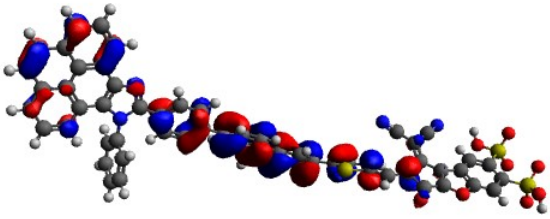
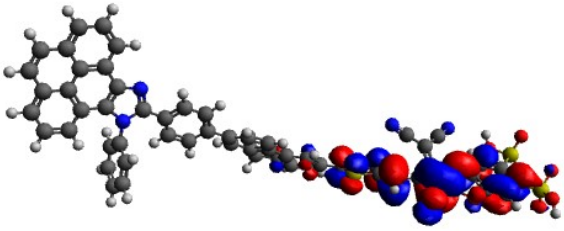


LUMO +2



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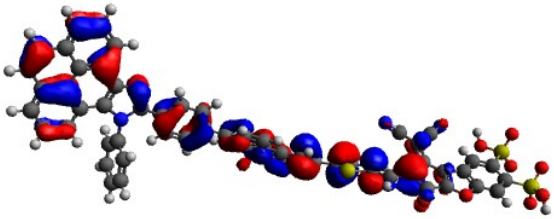
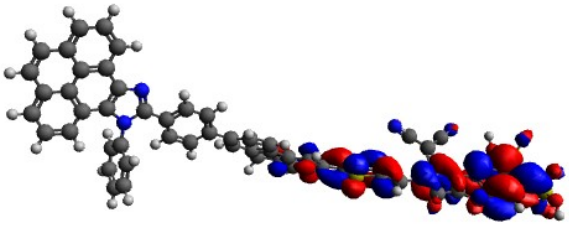


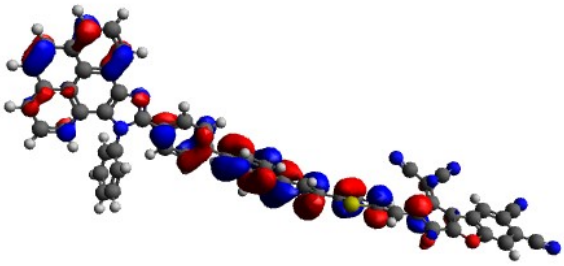
LUMO +1

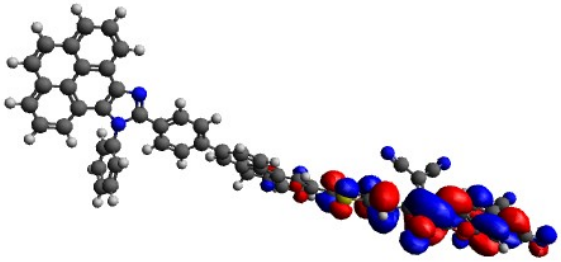


HOMO -2

LUMO +2

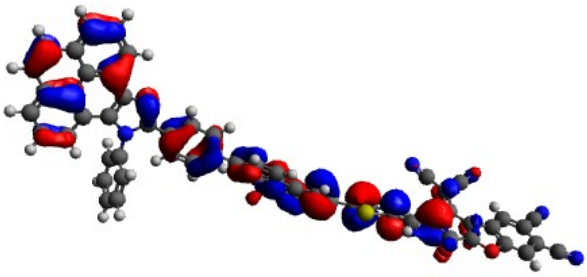
PYFD3

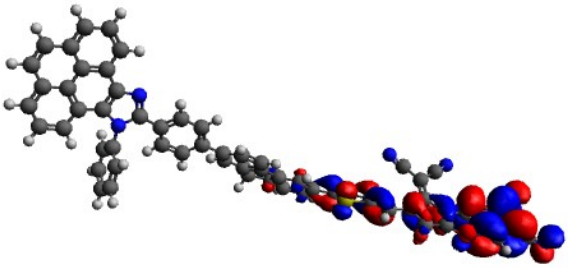




HOMO-1

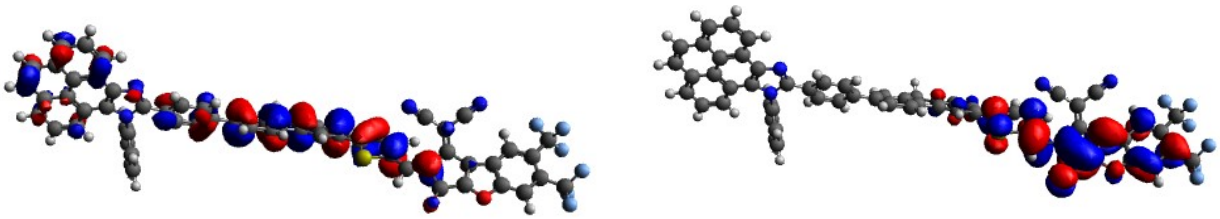
LUMO+1



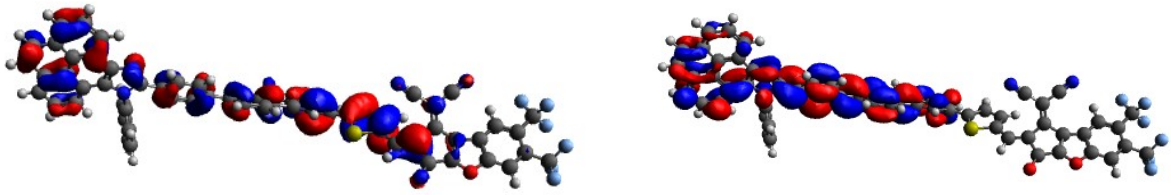


HOMO-2 LUMO+2

PYFD4

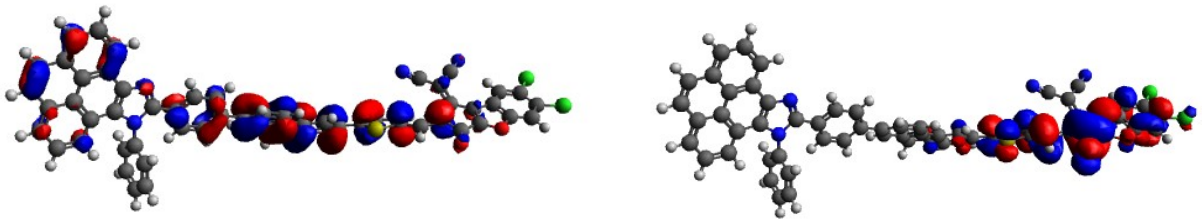


HOMO-1 LUMO+1

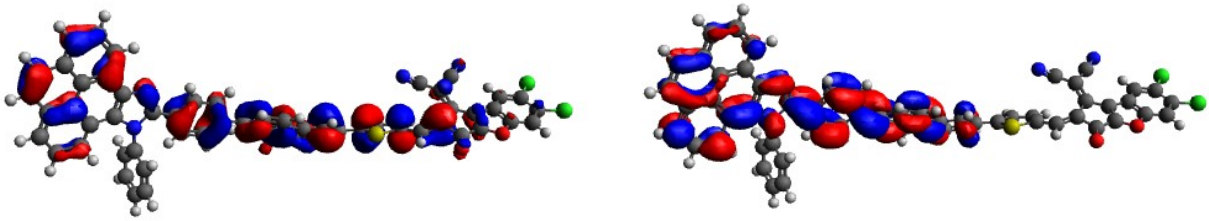


HOMO-2 LUMO+2

PYFD5

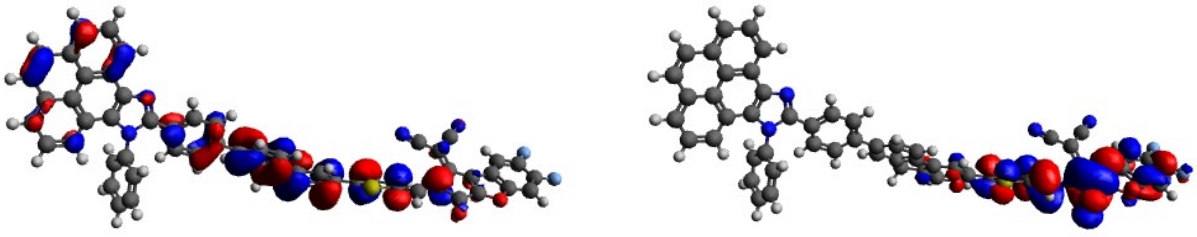


HOMO-1 LUMO+1

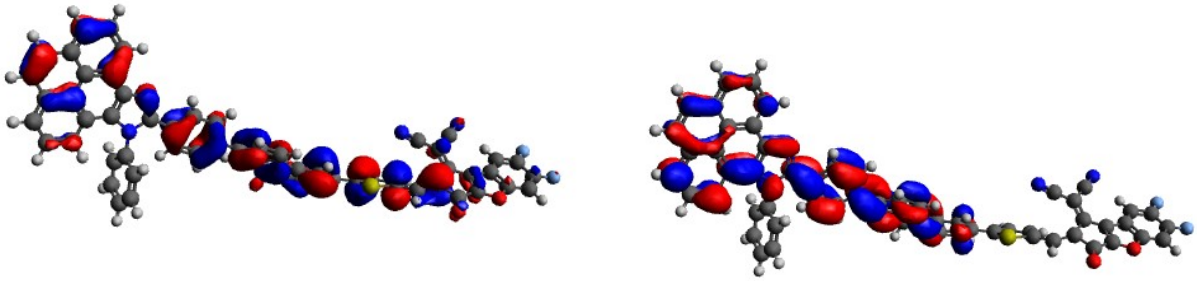


HOMO-2 LUMO+2

PYFD6



HOMO-1 LUMO+1



HOMO-2 **LUMO+2**

PYFD7

Figure S1: HOMO-1/LUMO+1 and HOMO-2/LUMO+2 of **PYFR** and **PYFD1-PYFD7** compounds.