Supplementary

Acceptor-Driven Synergy into Dihydropyridines-Based Compounds Uncovers Giant Static and Frequency Dependent Hyperpolarizabilities: A Quantum Exploration

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Table S1: IUPAC names of designed compounds.

Compounds	IUPAC names
CTPR	4-(9-methyl-9*H*-carbazol-3-yl)-2-oxo-6-(thiophen-2-yl)-1,2-dihydropyridine-3-carbonitrile
CTP1	(E)-2-(2-((5-(5-cyano-4-(9-methyl-9H-carbazol-3-yl)-6-oxo-1,6-dihydropyridin-2-yl)thiophen-2-yl)methylene)-6-fluoro-3-oxo-2,3-dihydro-1*H*-inden-1-ylidene)malononitrile
CTP2	(E)-2-(2-((5-(5-cyano-4-(9-methyl-9*H*-carbazol-3-yl)-6-oxo-1,6-dihydropyridin-2-yl)thiophen-2-yl)methylene)-5,6-difluoro-3-oxo-2,3-dihydro-1*H*-inden-1-ylidene)malononitrile
CTP3	(E)-2-(5,6-dichloro-2-((5-(5-cyano-4-(9-methyl-9*H*-carbazol-3-yl)-6-oxo-1,6-dihydropyridin-2-yl)thiophen-2-yl)methylene)-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile
CTP4	(E)-2-((5-(5-cyano-4-(9-methyl-9H-carbazol-3-yl)-6-oxo-1,6-dihydropyridin-2-yl)thiophen-2-yl)methylene)-1-(dicyanomethylene)-3-oxo-2,3-dihydro-1*H*-indene-5,6-dicarbonitrile
CTP5	(E)-2-(2-((5-(5-cyano-4-(9-methyl-9H-carbazol-3-yl)-6-oxo-1,6-dihydropyridin-2-yl)thiophen-2-yl)methylene)-5,6-dinitro-3-oxo-2,3-dihydro-1*H*-inden-1-ylidene)malononitrile
CTP6	(E)-2-(2-((5-(5-cyano-4-(9-methyl-9H-carbazol-3-yl)-6-oxo-1,6-dihydropyridin-2-yl)thiophen-2-yl)methylene)-3-oxo-5,6-bis(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-ylidene)malononitrile

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

Atom	x-axis	Y-axis	Z-axis
C	5.956965	-1.37582	-0.15062
C	4.76581	-0.68299	0.035932
C	3.536258	-1.17495	-0.44876
C	3.501393	-2.38452	-1.13699
C	4.684411	-3.07911	-1.32778
C	5.895499	-2.57746	-0.83861
H	6.899774	-0.99385	0.227976
H	2.561627	-2.77561	-1.51697
H	4.675761	-4.02357	-1.86214
H	6.808592	-3.14191	-1.0006
C	3.213395	0.821838	0.625236
C	2.521636	1.917902	1.134774
C	1.158699	1.980232	0.923313
C	0.464064	0.969807	0.232205
C	1.164294	-0.13477	-0.25113
C	2.536787	-0.20922	-0.06913
H	3.023935	2.703298	1.689273
H	0.605671	2.820109	1.331149
H	0.643948	-0.91954	-0.79436
N	4.554839	0.523259	0.678243
C	5.597044	1.304522	1.2983
H	6.041686	0.76657	2.142131
H	6.384508	1.536963	0.574529
H	5.183036	2.24323	1.665357
C	-0.9929	1.051345	0.04316
C	-1.63104	2.222878	-0.34865
C	-1.76708	-0.10862	0.253613
C	-3.06887	2.297204	-0.50812
C	-3.1311	-0.07566	0.11545
H	-1.28564	-1.03582	0.536506
H	-4.73783	1.157191	-0.29955
C	-0.93242	3.409268	-0.68636
N	-0.38692	4.385205	-0.98017
O	-3.70454	3.282288	-0.83559
N	-3.72602	1.093519	-0.24545
C	-3.96794	-1.23725	0.344156
C	-3.69459	-2.30791	1.156331
S	-5.50846	-1.43472	-0.44492
C	-4.71647	-3.28089	1.151099
H	-2.79754	-2.37584	1.760768

C	-5.75701	-2.94354	0.337781
H	-4.68771	-4.19319	1.733465
H	-6.66248	-3.4985	0.136303

Table S3: Cartesian coordinates of **CTP1** compound.

Atom	x-axis	Y-axis	Z-axis
C	7.59384	-4.10213	-0.37864
C	7.007018	-2.86981	-0.11365
C	5.808784	-2.46795	-0.73884
C	5.187455	-3.31749	-1.64954
C	5.766814	-4.54624	-1.91892
C	6.95561	-4.93015	-1.28875
H	8.514881	-4.40733	0.10786
H	4.264033	-3.02062	-2.13903
H	5.296372	-5.2218	-2.62595
H	7.388828	-5.89911	-1.51672
C	6.535106	-0.83149	0.689456
C	6.53004	0.381661	1.374012
C	5.500243	1.265289	1.121073
C	4.465426	0.965149	0.214524
C	4.468523	-0.26399	-0.44523
C	5.502952	-1.15851	-0.22252
H	7.301216	0.634503	2.093655
H	5.474569	2.203957	1.664672
H	3.681298	-0.50898	-1.15374
N	7.433448	-1.87047	0.742623
C	8.627125	-1.95014	1.549062
H	8.556781	-2.77109	2.270121
H	9.507535	-2.10952	0.918543
H	8.762568	-1.01854	2.097594
C	3.367476	1.912052	-0.02494
C	3.567638	3.278757	-0.16804
C	2.048568	1.408455	-0.10615
C	2.46933	4.202613	-0.3822
C	0.989971	2.249673	-0.31897
H	1.862537	0.357057	0.070104
H	0.457715	4.221497	-0.65956
C	4.854482	3.87427	-0.20112
N	5.889984	4.385394	-0.2467
O	2.56694	5.405832	-0.52935
N	1.218586	3.585858	-0.44079
C	-0.37636	1.767606	-0.39352
C	-0.78384	0.51163	-0.78391

S	-1.72477	2.76136	0.044286
C	-2.16911	0.339557	-0.71294
H	-0.09706	-0.24756	-1.13757
C	-2.83685	1.464161	-0.27615
H	-2.68099	-0.56808	-1.01129
C	-4.23967	1.693266	-0.13552
C	-5.32709	-0.58643	0.444703
C	-6.64232	1.26034	-0.26127
C	-6.64902	-1.07271	0.011991
C	-7.4384	0.02666	-0.35061
C	-5.25096	0.816829	0.068503
O	-7.00886	2.39353	-0.4621
C	-4.46235	-1.26622	1.259067
C	-4.66793	-2.61994	1.643027
N	-4.80575	-3.72086	1.96303
C	-3.35223	-0.64274	1.889998
N	-2.46406	-0.1562	2.444774
C	-7.17865	-2.35445	-0.04196
C	-8.49334	-2.47148	-0.45931
C	-9.29296	-1.3895	-0.8052
C	-8.75515	-0.11513	-0.75044
H	-6.62303	-3.25027	0.205105
H	-10.3158	-1.57044	-1.11543
H	-9.34197	0.757689	-1.01666
F	-9.02031	-3.69016	-0.53291
H	-4.58148	2.718489	-0.29558

Table S4: Cartesian coordinates of **CTP2** compound.

Atom	**x-axis**	**Y-axis**	**Z-axis**
C	8.14168	-4.10258	-0.28416
C	7.503239	-2.89479	-0.02538
C	6.292025	-2.54403	-0.65648
C	5.708432	-3.42328	-1.56426
C	6.338316	-4.62879	-1.82583
C	7.540366	-4.96057	-1.19137
H	9.075099	-4.36585	0.203118
H	4.77555	-3.16682	-2.05862
H	5.897951	-5.32612	-2.5311
H	8.014227	-5.91142	-1.41478
C	6.951151	-0.8711	0.762209
C	6.902064	0.347656	1.434494
C	5.839952	1.189777	1.174222
C	4.816677	0.842344	0.271619

C	4.866364	-0.39044	-0.37905
C	5.934039	-1.24381	-0.14926
H	7.665289	0.637112	2.148814
H	5.78003	2.132835	1.707567
H	4.090159	-0.66969	-1.08703
N	7.886048	-1.8765	0.828753
C	9.086838	-1.89771	1.628221
H	9.099944	-2.77809	2.278379
H	9.979008	-1.91458	0.993678
H	9.125663	-1.00797	2.255897
C	3.683639	1.747714	0.031284
C	3.837884	3.116588	-0.14278
C	2.383226	1.198042	-0.03773
C	2.706807	4.001494	-0.34848
C	1.293428	2.002281	-0.23511
H	2.242922	0.130638	0.072218
H	0.678524	3.966989	-0.45624
C	5.104539	3.752106	-0.19814
N	6.123234	4.293997	-0.26294
O	2.760103	5.207942	-0.49098
N	1.475729	3.343478	-0.37485
C	-0.05592	1.473006	-0.30767
C	-0.51735	0.311187	0.269674
S	-1.30937	2.2855	-1.18184
C	-1.87816	0.090347	0.040202
H	0.108215	-0.34225	0.865261
C	-2.47132	1.078022	-0.71782
H	-2.41753	-0.7788	0.39882
C	-3.80967	1.166129	-1.20769
C	-5.32441	-0.01131	0.534234
C	-6.12101	0.503973	-1.6424
C	-6.5314	-0.80785	0.263102
C	-7.02902	-0.46212	-0.99804
C	-4.95264	0.629497	-0.71866
O	-6.26091	1.041487	-2.7139
C	-4.81424	0.255406	1.776198
C	-5.3016	-0.36876	2.95703
N	-5.67498	-0.87006	3.92802
C	-3.84239	1.265913	2.007083
N	-3.08031	2.103701	2.232225
C	-7.20606	-1.74424	1.039244
C	-8.356	-2.29673	0.516072
C	-8.85138	-1.92961	-0.73744

C	-8.1908	-1.00408	-1.51417
H	-6.8732	-2.07456	2.015386
H	-8.57247	-0.72168	-2.48945
F	-9.02634	-3.20478	1.207194
F	-9.96715	-2.50046	-1.16097
H	-3.94356	1.673486	-2.16586

Table S5: Cartesian coordinates of **CTP3** compound.

Atom	x-axis	Y-axis	Z-axis
C	-9.01972	3.919421	0.739801
C	-8.36068	2.698657	0.646326
C	-7.09918	2.581021	0.027572
C	-6.4891	3.708686	-0.51434
C	-7.14157	4.927321	-0.42802
C	-8.39117	5.02727	0.193276
H	-9.9876	4.005656	1.223348
H	-5.51798	3.632538	-0.99553
H	-6.68091	5.81716	-0.84462
H	-8.8803	5.994779	0.250104
C	-7.78851	0.537463	0.798785
C	-7.7354	-0.82889	1.064424
C	-6.62856	-1.531	0.632401
C	-5.56413	-0.90358	-0.04299
C	-5.61756	0.470489	-0.27906
C	-6.72841	1.192427	0.126799
H	-8.5284	-1.33691	1.602534
H	-6.56622	-2.59146	0.853219
H	-4.80733	0.969296	-0.80484
N	-8.76498	1.455904	1.100556
C	-10.0065	1.2087	1.792763
H	-10.0126	1.689438	2.776656
H	-10.8498	1.589851	1.208948
H	-10.1437	0.136158	1.927933
C	-4.38505	-1.66845	-0.47119
C	-4.47076	-2.92805	-1.04795
C	-3.10379	-1.09998	-0.27562
C	-3.29419	-3.68364	-1.43826
C	-1.97449	-1.78341	-0.63424
H	-3.00884	-0.14844	0.23114
H	-1.27063	-3.51848	-1.51794
C	-5.70394	-3.54637	-1.37858
N	-6.69222	-4.06822	-1.67233
O	-3.29298	-4.78077	-1.96187

N	-2.09145	-3.02324	-1.1832
C	-0.64487	-1.24423	-0.41296
C	-0.29685	0.091125	-0.38187
S	0.719105	-2.2584	-0.13658
C	1.061381	0.303505	-0.14947
H	-1.01178	0.887249	-0.55113
C	1.781457	-0.87171	-0.00295
H	1.535935	1.272474	-0.09641
C	3.144095	-1.16259	0.28449
C	5.599924	-0.86821	0.664654
C	4.391625	1.041617	-0.0676
C	6.556242	0.174445	0.259363
C	5.841875	1.302983	-0.14418
C	4.25964	-0.37843	0.345491
O	3.524519	1.845963	-0.32513
C	5.932411	-2.03098	1.309236
C	7.276654	-2.40751	1.57902
N	8.355735	-2.74674	1.812228
C	4.981537	-2.95339	1.826987
N	4.241604	-3.72026	2.272996
C	7.944044	0.204908	0.234905
C	8.577698	1.366451	-0.18842
C	7.844265	2.495893	-0.57787
C	6.458155	2.463425	-0.55564
H	8.557072	-0.63951	0.521854
H	5.874971	3.327135	-0.85711
C	l10.30684500	1.383084	-0.22378
C	l8.63701900	3.941234	-1.09551
H	3.313974	-2.2223	0.458833

Table S6: Cartesian coordinates of **CTP4** compound.

Atom	x-axis	Y-axis	Z-axis
C	-7.96977	4.331511	-0.39822
C	-7.43352	3.074988	-0.13975
C	-6.24492	2.633185	-0.75599
C	-5.58062	3.467642	-1.65022
C	-6.10914	4.720599	-1.91282
C	-7.2897	5.14358	-1.29226
H	-8.88471	4.666224	0.08033
H	-4.664	3.140221	-2.13293
H	-5.60487	5.384561	-2.6074
H	-7.68294	6.130554	-1.51532
C	-7.05431	1.009521	0.642407

C	-7.10854	-0.21265	1.30859
C	-6.11406	-1.13512	1.053701
C	-5.05658	-0.86519	0.164101
C	-4.99919	0.372631	-0.47672
C	-5.99846	1.306086	-0.25304
H	-7.89892	-0.44322	2.014713
H	-6.13448	-2.0823	1.582595
H	-4.19387	0.594497	-1.17245
N	-7.90901	2.083958	0.700241
C	-9.11115	2.200455	1.489609
H	-9.03125	3.031584	2.19765
H	-9.9811	2.367797	0.846576
H	-9.27117	1.28144	2.052582
C	-3.99889	-1.85621	-0.07566
C	-4.25797	-3.2089	-0.24645
C	-2.65588	-1.41302	-0.12498
C	-3.19963	-4.17982	-0.45554
C	-1.63378	-2.29957	-0.32902
H	-2.42624	-0.37381	0.071065
H	-1.18711	-4.29093	-0.69121
C	-5.57009	-3.74396	-0.31328
N	-6.62669	-4.20595	-0.38712
O	-3.35117	-5.37401	-0.62549
N	-1.92063	-3.62222	-0.47754
C	-0.24529	-1.87866	-0.36108
C	0.224887	-0.62748	-0.70052
S	1.044556	-2.94401	0.073387
C	1.610871	-0.51688	-0.58781
H	-0.41957	0.171627	-1.04514
C	2.220836	-1.68586	-0.17399
H	2.16643	0.377887	-0.84411
C	3.601951	-1.98417	-0.01124
C	4.803678	0.230727	0.599408
C	6.021816	-1.67623	-0.11072
C	6.161485	0.652295	0.198671
C	6.8949	-0.4798	-0.16558
C	4.660431	-1.15914	0.204328
O	6.343788	-2.81746	-0.32758
C	3.970724	0.949252	1.412854
C	4.246923	2.284864	1.815079
N	4.447117	3.372453	2.146793
C	2.820297	0.378711	2.020637
N	1.899255	-0.07203	2.551036

C	6.762638	1.902553	0.161514
C	8.096832	1.98379	-0.2311
C	8.832023	0.829336	-0.57155
C	8.219557	-0.41953	-0.53928
H	6.233164	2.813707	0.409819
H	8.763593	-1.31918	-0.80596
H	3.891263	-3.02711	-0.15909
C	8.725143	3.263961	-0.28858
N	9.233998	4.297208	-0.33583
C	10.20003	0.942138	-0.95845
N	11.30606	1.032081	-1.27099

Table S7: Cartesian coordinates of **CTP5** compound.

Atom	x-axis	Y-axis	Z-axis
C	-8.39512	4.46396	-0.38872
C	-7.89185	3.193114	-0.13386
C	-6.71974	2.7189	-0.7574
C	-6.03808	3.535484	-1.65518
C	-6.53367	4.802637	-1.91415
C	-7.69846	5.257569	-1.28649
H	-9.2982	4.822953	0.094767
H	-5.13392	3.18326	-2.1439
H	-6.01561	5.452678	-2.61175
H	-8.06599	6.254919	-1.50726
C	-7.56817	1.115992	0.642071
C	-7.65602	-0.10657	1.303865
C	-6.69062	-1.05729	1.040932
C	-5.62929	-0.81501	0.148166
C	-5.53787	0.422693	-0.48875
C	-6.50861	1.384267	-0.25803
H	-8.4505	-0.31652	2.011811
H	-6.73705	-2.00597	1.565524
H	-4.72906	0.622773	-1.18706
N	-8.39031	2.215038	0.707833
C	-9.5852	2.363941	1.502656
H	-9.4856	3.204687	2.196578
H	-10.4572	2.536009	0.863496
H	-9.75593	1.457145	2.082073
C	-4.60241	-1.83626	-0.09888
C	-4.90298	-3.17872	-0.27957
C	-3.2459	-1.43441	-0.14231
C	-3.87531	-4.1804	-0.49799
C	-2.25208	-2.35146	-0.34896

H	-2.98345	-0.405	0.064369
H	-1.86655	-4.35	-0.73654
C	-6.23131	-3.67209	-0.34889
N	-7.30207	-4.09989	-0.42427
O	-4.06426	-5.36714	-0.68143
N	-2.57942	-3.66294	-0.51181
C	-0.8499	-1.97651	-0.36401
C	-0.33352	-0.74745	-0.71628
S	0.394852	-3.07426	0.118443
C	1.052626	-0.67889	-0.57637
H	-0.94589	0.064317	-1.08879
C	1.616051	-1.85855	-0.12736
H	1.641873	0.192525	-0.83804
C	2.982647	-2.19685	0.070435
C	4.245322	-0.00863	0.651777
C	5.412449	-1.97171	0.011799
C	5.626237	0.356284	0.273037
C	6.328013	-0.80683	-0.04544
C	4.064276	-1.40185	0.287527
O	5.700645	-3.12659	-0.17642
C	3.420744	0.760199	1.426516
C	3.731825	2.09836	1.793362
N	3.961238	3.189214	2.093816
C	2.239548	0.245593	2.025211
N	1.293212	-0.15982	2.547483
C	6.274793	1.58506	0.230517
C	7.610562	1.595925	-0.12075
C	8.301328	0.425879	-0.42915
C	7.663853	-0.79769	-0.39108
H	5.787183	2.5248	0.458603
H	8.192507	-1.70997	-0.64546
H	3.240754	-3.25182	-0.04615
N	8.299456	2.901194	-0.05108
O	7.735494	3.841499	-0.55746
O	9.347724	2.9291	0.548905
N	9.692292	0.457135	-0.91691
O	10.40698	-0.45907	-0.58564
O	9.995776	1.374657	-1.64451

Table S8: Cartesian coordinates of **CTP6** compound.

Atom	**x-axis**	**Y-axis**	**Z-axis**
C	-8.82457	4.56264	-0.41174
C	-8.35174	3.278865	-0.16318

C	-7.17982	2.78728	-0.77373
C	-6.46992	3.597932	-1.65496
C	-6.93658	4.876965	-1.90934
C	-8.10001	5.349986	-1.29271
H	-9.72511	4.936882	0.064759
H	-5.56603	3.232214	-2.13418
H	-6.39602	5.522543	-2.59388
H	-8.44363	6.356991	-1.50812
C	-8.07868	1.18988	0.600153
C	-8.19807	-0.03445	1.253532
C	-7.2472	-1.00154	0.997447
C	-6.16932	-0.77336	0.121069
C	-6.04545	0.466504	-0.50585
C	-7.00116	1.444894	-0.28217
H	-9.0047	-0.23276	1.95103
H	-7.31811	-1.95247	1.515247
H	-5.22251	0.655566	-1.19057
N	-8.88319	2.302352	0.659901
C	-10.0821	2.46843	1.445238
H	-9.94559	3.238443	2.211683
H	-10.9226	2.7535	0.804903
H	-10.3311	1.528833	1.937697
C	-5.15833	-1.81249	-0.11811
C	-5.4837	-3.14696	-0.31621
C	-3.7939	-1.43777	-0.13443
C	-4.47326	-4.16724	-0.52752
C	-2.81554	-2.37326	-0.33332
H	-3.51364	-0.41606	0.086854
H	-2.46408	-4.37438	-0.73506
C	-6.8207	-3.61153	-0.41155
N	-7.89899	-4.01562	-0.50805
O	-4.6826	-5.34836	-0.72554
N	-3.16723	-3.6757	-0.51543
C	-1.40534	-2.03014	-0.32296
C	-0.85288	-0.81464	-0.66409
S	-0.19465	-3.16084	0.173224
C	0.534192	-0.78373	-0.50916
H	-1.4394	0.013909	-1.04155
C	1.060391	-1.97802	-0.05712
H	1.149783	0.071937	-0.76205
C	2.417582	-2.35497	0.151552
C	3.734764	-0.20201	0.745323
C	4.853901	-2.19605	0.11149

C	5.123091	0.124102	0.362657
C	5.792202	-1.05341	0.042843
C	3.516453	-1.59176	0.381965
O	5.109321	-3.361	-0.06586
C	2.9278	0.585936	1.51925
C	3.275988	1.91284	1.893996
N	3.53292	2.995098	2.20341
C	1.729437	0.102862	2.110383
N	0.768653	-0.27666	2.625913
C	5.807075	1.329914	0.300723
C	7.14711	1.33785	-0.07017
C	7.821939	0.134717	-0.35169
C	7.126341	-1.06589	-0.30082
H	5.317369	2.270523	0.51466
H	7.615745	-2.00611	-0.52711
H	2.648151	-3.4156	0.027907
C	7.821621	2.692514	-0.08672
C	9.273719	0.064245	-0.76807
F	10.05687	0.830675	-0.01105
F	9.434106	0.440604	-2.03704
F	9.739993	-1.18105	-0.67108
F	8.671498	2.827658	-1.10187
F	6.928059	3.676002	-0.19576
F	8.496634	2.904233	1.044004

Table S9: Calculated energies (E) and energy gap (ΔE) of **HOMO-1, LUMO+1, HOMO-2** and **LUMO+2** for **CTPR** and **CTP1-CTP6**.

Compounds	HOMO-1	LUMO+1	ΔE	HOMO-2	LUMO+2	ΔE
CTPR	-6.594	-1.219	5.375	-6.603	-0.992	5.611
CTP1	-6.625	-2.855	3.770	-6.687	-2.255	4.432
CTP2	-6.633	-2.911	3.722	-6.689	-2.325	4.364
CTP3	-6.645	-2.338	4.307	-6.748	-3.011	3.737
CTP4	-6.648	-3.475	3.173	-6.782	-2.540	4.242
CTP5	-6.648	-3.619	3.029	-6.799	-2.689	4.110
CTP6	-6.639	-3.209	3.430	-6.762	-2.422	4.340

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

Table S10: Global reactivity parameters of studied compounds **CTPR** and **CTP1-CTP6**.

Compounds	IP	EA	X	η	μ	ω	σ	ΔN_{max}
CTPR	6.215	2.413	4.314	1.901	-4.314	4.894	0.263	2.269
CTP1	6.248	3.580	4.914	1.334	-4.914	9.050	0.374	3.683
CTP2	6.251	3.574	4.912	1.338	-4.912	9.014	0.373	3.671
CTP3	6.268	3.664	4.966	1.302	-4.966	9.470	0.384	3.814
CTP4	6.270	3.885	5.077	1.192	-5.077	10.809	0.419	4.257
CTP5	6.270	3.943	5.106	1.163	-5.106	11.205	0.429	4.388

CTP6	6.261	3.759	5.010	1.251	-5.010	10.032	0.399	4.004

Ionization potential (*IP*), electron affinity (*EA*), electronegativity (*X*), global hardness (η), chemical potential (μ), global electrophilicity (ω), global softness (σ) and maximum charge transfer index (ΔN_{max}); Units in *eV*

Table: S11 Wavelength, excitation energy and oscillator strength of investigated compound **CTPR**.

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	397.959	3.116	0.338	H→L (94%), H-2→L (3%)
2	368.069	3.369	0.538	H-2→L (52%), H-1→L (43%), H→L (3%)
3	356.830	3.475	0.020	H-2→L (42%), H-1→L (53%), H→L+1 (2%)
4	311.792	3.977	0.069	H→L+1 (88%),
5	285.935	4.336	0.041	H-2→L+1 (26%), H-1→L+1 (22%), H→L+2 (41%), H→L+3 (5%)
6	284.231	4.362	0.140	H-4→L (35%), H-3→L (48%), H-6→L (6%), H-2→L+1 (2%)

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

Table: S12 Wavelength, excitation energy and oscillator strength of investigated compound **CTP1.**

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	548.821	2.259	0.071	H→L (96%), H-2→L (2%)
2	516.407	2.401	0.728	H-2→L (88%), H-3→L (2%), H-1→L (5%), H→L (3%)
3	470.975	2.633	0.005	H-1→L (93%), H-2→L (5%)
4	417.034	2.973	0.111	H→L+1 (88%), H-2→L+1 (2%), H→L+2 (7%)
5	398.958	3.108	0.281	H-2→L+1 (80%), H-5→L (5%), H-3→L+1 (3%), H-1→L+1 (5%), H→L+1 (3%)
6	383.377	3.234	0.069	H-3→L (86%), H-4→L (6%), H-2→L (2%)

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

Table: S13 Wavelength, excitation energy and oscillator strength of investigated compound **CTP2.**

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	545.441	2.273	0.166	H→L (92%), H-2→L (6%)
2	512.141	2.421	0.668	H-2→L (90%), H-3→L (2%), H→L (6%)
3	466.667	2.657	0.005	H-1→L (98%),
4	421.729	2.940	0.127	H→L+1 (85%), H-2→L+1 (6%), H→L+2 (7%)
5	402.572	3.080	0.224	H-2→L+1 (81%), H-5→L (4%), H-5→L+1 (2%), H-3→L+1 (2%),

				H→L+1 (6%)
6	381.831	3.247	0.076	H-3→L (82%), H-4→L (9%), H-2→L (3%)

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

Table: S14 Wavelength, excitation energy and oscillator strength of investigated compound **CTP3.**

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	563.334	2.201	0.077	H→L (97%),
2	508.299	2.439	1.269	H-2→L (93%), H-1→L (2%)
3	481.979	2.572	0.008	H-1→L (95%), H-2→L (2%)
4	425.303	2.915	0.033	H→L+1 (94%), H→L+2 (3%)
5	408.542	3.035	0.104	H-2→L+1 (79%), H-5→L (2%), H-4→L (4%), H-3→L+1 (5%), H-1→L+1 (2%)
6	390.305	3.177	0.094	H-3→L (84%), H-8→L (4%), H-5→L (3%)

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

Table: S15 Wavelength, excitation energy and oscillator strength of investigated compound **CTP4.**

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	620.821	1.997	0.033	H→L (98%),
2	553.847	2.239	0.699	H-2→L (93%), H-3→L (2%)
3	523.273	2.369	0.005	H-1→L (97%),
4	501.311	2.473	0.017	H→L+1 (97%),
5	457.203	2.712	0.333	H-2→L+1 (91%), H-3→L+1 (3%), H-1→L+1 (2%)
6	435.537	2.847	0.005	H-1→L+1 (95%),

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

Table: S16 Wavelength, excitation energy and oscillator strength of investigated compound **CTP5.**

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	633.866	1.956	0.023	H→L (97%), H→L+1 (2%)
2	559.571	2.216	0.594	H-2→L (91%), H-3→L (2%)
3	532.738	2.327	0.011	H-1→L (70%), H→L+1 (26%),
4	530.936	2.335	0.007	H-1→L (26%), H→L+1 (70%),
5	474.000	2.616	0.386	H-2→L+1 (90%), H-3→L+1 (2%), H-1→L+1 (2%)
6	458.047	2.707	0.006	H-1→L+1 (94%), H-2→L+1 (2%), H-1→L (3%)

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

Table: S17 Wavelength, excitation energy and oscillator strength of investigated compound **CTP6.**

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	589.811	2.102	0.038	H→L (98%),
2	534.184	2.321	0.728	H-2→L (93%), H-3→L (2%)
3	500.966	2.475	0.005	H-1→L (97%),
4	458.064	2.707	0.033	H→L+1 (96%), H→L+2 (2%)
5	426.722	2.906	0.312	H-2→L+1 (89%), H-3→L+1 (3%)
6	402.716	3.079	0.008	H-1→L+1 (94%), H-1→L+2 (3%)

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

Table: S18 Wavelength, excitation energy and oscillator strength of investigated compound **CTPR**.

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	390.489	3.175	0.156	H→L (96%),
2	367.143	3.377	0.430	H-1→L (89%), H-2→L (8%)
3	357.612	3.467	0.036	H-2→L (87%), H-1→L (8%)
4	308.895	4.014	0.037	H→L+1 (83%), H-2→L (2%), H-2→L+2 (3%), H→L+2 (3%)
5	300.218	4.130	0.001	H-4→L (74%), H-3→L (20%), H-5→L (2%)
6	287.586	4.311	0.013	H-2→L+1 (28%), H→L+2 (53%), H-1→L+1 (7%), H→L+3 (4%)

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

Table: S19 Wavelength, excitation energy and oscillator strength of investigated compound **CTP1**.

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	593.368	2.090	0.011	H→L (99%),
2	535.523	2.315	0.504	H-2→L (65%), H-1→L (33%),
3	511.782	2.423	0.035	H-2→L (32%), H-1→L (66%),
4	433.906	2.857	0.024	H→L+1 (95%), H→L+2 (3%)
5	409.243	3.030	0.257	H-2→L+1 (65%), H-1→L+1 (24%), H-6→L (4%), H-3→L+1 (3%)
6	396.572	3.126	0.120	H-4→L (19%), H-3→L (74%),

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 **CTP2**.

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	589.811	2.102	0.012	H→L (99%),
2	537.379	2.307	0.526	H-2→L (71%), H-1→L (26%),
3	509.175	2.435	0.026	H-2→L (26%), H-1→L (72%),

4	440.207	2.817	0.020	H→L+1 (96%), H→L+2 (3%)
5	417.230	2.972	0.214	H-2→L+1 (70%), H-1→L+1 (20%), H-6→L (3%), H-3→L+1 (2%)
6	395.459	3.135	0.172	H-4→L (24%), H-3→L (68%),

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 **CTP3.**

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	594.962	2.084	0.011	H→L (99%),
2	520.133	2.384	0.480	H-2→L (25%), H-1→L (73%),
3	510.034	2.431	0.483	H-2→L (72%), H-1→L (25%),
4	439.863	2.819	0.010	H→L+1 (97%),
5	414.718	2.990	0.097	H-2→L+1 (67%), H-1→L+1 (15%), H-5→L (4%), H-5→L+1 (3%), H-3→L (2%), H-3→L+1 (4%)
6	398.036	3.115	0.183	H-3→L (75%), H-7→L (6%), H-4→L (5%), H-1→L+1 (3%)

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 **CTP4.**

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	709.251	1.748	0.006	H→L (99%),
2	600.728	2.064	0.047	H-1→L (97%), H-2→L (2%)
3	578.743	2.142	0.463	H-2→L (95%), H-1→L (2%)
4	545.273	2.274	0.008	H→L+1 (98%),
5	480.708	2.579	0.081	H-2→L+1 (21%), H-1→L+1 (76%),
6	470.385	2.636	0.146	H-2→L+1 (74%), H-1→L+1 (22%),

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 **CTP5**.

No	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	724.630	1.711	0.005	H→L (99%),
2	611.061	2.029	0.027	H-1→L (97%),
3	584.252	2.122	0.406	H-2→L (92%), H→L+1 (4%)
4	569.257	2.178	0.022	H→L+1 (95%), H-2→L (4%)
5	497.629	2.492	0.037	H-1→L+1 (92%), H-2→L+1 (6%)
6	483.124	2.566	0.217	H-2→L+1 (89%), H-1→L+1 (6%)

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 **CTP6**.

No	DFT λ (nm)	$E(eV)$	f_{os}	MO contributions
1	658.580	1.883	0.007	H→L (99%),
2	565.312	2.193	0.143	H-2→L (13%), H-1→L (85%),
3	552.761	2.243	0.387	H-2→L (84%), H-1→L (14%),
4	492.979	2.515	0.008	H→L+1 (98%),
5	444.085	2.792	0.166	H-2→L+1 (58%), H-1→L+1 (36%),
6	434.240	2.855	0.053	H-2→L+1 (35%), H-1→L+1 (61%),

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

Table S25: Percentages of Donor, π-spacer and Acceptor for LUMOs and HOMOs.

Compounds	LUMO			HOMO		
	Donor	π-spacer	Acceptor	Donor	π-spacer	Acceptor
CTPR	8.7	91.3		94.6	5.4	
CTP1	0.5	26.5	73	94.2	5.7	0.0
CTP2	0.6	25.9	73.5	94.4	5.5	0.1
CTP3	0.6	33.0	66.4	94.3	5.7	0.0
CTP4	0.3	21.6	78.1	94.3	5.7	0.0
CTP5	0.2	16.4	83.4	94.3	5.7	0.0
CTP6	0.4	25.0	74.6	94.4	5.6	0.0

Table S26: Natural bond orbital (NBO) analysis of Compound **CTPR**.

Donor(i)	Type	Acceptor(j)	Type	$E^{(2)}$ [$kcal/mol$]	$E_{(j)}$-$E_{(i)}$ [$a.u$]	$F_{(i,j)}$ [$a.u$]
C27 - C29	π	C25 - C26	π*	28.17	0.31	0.085
C11 - C16	π	C14 - C15	π*	26.07	0.29	0.079
C 1 - C 2	π	C 5 - C 6	π*	24.84	0.3	0.077
C 5 - C 6	π	C 3 - C 4	π*	23.89	0.3	0.076
C11 - C16	π	C 3 - C 4	π*	22.56	0.3	0.074
C 3 - C 4	π	C 5 - C 6	π*	21.07	0.29	0.07
C 5 - C 6	π	C 1 - C 2	π*	19.66	0.29	0.068
C 1 - C 2	π	C 3 - C 4	π*	18.36	0.31	0.068
C39 - C41	π	C36 - C37	π*	17.98	0.31	0.07
C36 - C37	π	C39 - C41	π*	15.91	0.31	0.065
C14 - C15	π	C25 - C26	π*	13.6	0.29	0.056
C25 - C26	π	C27 - C29	π*	10.86	0.3	0.052
C27 - C29	π	C36 - C37	π*	9.42	0.31	0.049
C25 - C26	π	C14 - C15	π*	4.99	0.32	0.037
C39 - C41	π	C39 - C41	π*	0.5	0.31	0.012
C26 - C32	σ	C32 - N33	σ*	8.44	1.62	0.105
C32 - N33	σ	C26 - C32	σ*	7.97	1.59	0.101
C 1 - C 6	σ	C 2 - N20	σ*	6.23	1.16	0.076
C27 - C29	σ	C29 - C36	σ*	5.98	1.24	0.077
C 2 - C 3	σ	C 1 - C 2	σ*	5.21	1.26	0.073

C15 - C16	σ	C11 - C16	σ^*	4.98	1.26	0.071
C27 - H30	σ	C25 - C26	σ^*	4.4	1.1	0.062
C13 - H18	σ	C14 - C15	σ^*	4.74	1.1	0.064
C14 - C25	σ	C25 - C26	σ^*	3.97	1.24	0.063
C11 - C12	σ	C12 - C13	σ^*	3.8	1.32	0.063
C36 - S38	σ	C41 - H43	σ^*	2.96	1.1	0.051
C11 - C16	σ	C15 - H19	σ^*	2.71	1.08	0.049
C25 - C27	σ	C13 - C14	σ^*	1.99	1.27	0.045
C13 - H18	σ	C12 - C13	σ^*	0.98	1.12	0.03
C41 - H43	σ	S38 - C41	σ^*	0.55	0.78	0.019
N35	LP (1)	C27 - C29	π^*	50.24	0.32	0.115
N20	LP (1)	C 1 - C 2	π^*	43.26	0.31	0.104
N20	LP (1)	C11 - C16	π^*	41.71	0.3	0.103
S38	LP (2)	C39 - C41	π^*	24.99	0.28	0.076
S38	LP (2)	C36 - C37	π^*	23.75	0.28	0.073
O34	LP (2)	C32 - N33	π^*	0.87	0.39	0.017
O34	LP (2)	C28 - N35	σ^*	29.09	0.67	0.127
O34	LP (2)	C26 - C28	σ^*	19.43	0.75	0.109
N33	LP (1)	C26 - C32	σ^*	12.23	1.06	0.102
N20	LP (1)	C21 - H22	σ^*	5.73	0.64	0.06
N20	LP (1)	C21 - H23	σ^*	4.79	0.64	0.055
O34	LP (1)	C26 - C28	σ^*	2.83	1.18	0.052
S38	LP (1)	C36 - C37	σ^*	2.51	1.24	0.05
S38	LP (1)	C39 - C41	σ^*	2.21	1.25	0.047
O34	LP (1)	C28 - N35	σ^*	1.45	1.11	0.036
O34	LP (2)	C29 - N35	σ^*	0.57	0.72	0.019

Table S27: Natural bond orbital (NBO) analysis of Compound **CTP1**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	$E^{(2)}$ **[*kcal/mol*]**	$E_{(j)}$-$E_{(i)}$ **[*a.u*]**	$F_{(i,j)}$ **[*a.u*]**
C11 - C16	π	C14 - C15	π^*	26.51	0.29	0.079
C57 - C58	π	C55 - C56	π^*	25.82	0.29	0.077
C55 - C56	π	C46 - C47	π^*	24.9	0.31	0.08
C5 - C6	π	C3 - C4	π^*	23.91	0.3	0.076
C46 - C47	π	C57 - C58	π^*	21.34	0.3	0.074
C43 - C48	π	C44 - C50	π^*	19.14	0.31	0.069
C12 - C13	π	C14 - C15	π^*	17.56	0.3	0.067
C3 - C4	π	C11 - C16	π^*	15.82	0.28	0.062
C27 - C29	π	C36 - C37	π^*	10.19	0.3	0.05
C44 - C50	π	C46 - C47	π^*	8.57	0.33	0.051
C25 - C26	π	C14 - C15	π^*	5.29	0.32	0.038

C45 - O49	π	C46 - C47	π^*	4.01	0.43	0.041
C45 - O49	π	C43 - C48	π^*	2.91	0.44	0.033
C25 - C26	π	C25 - C26	π^*	1.91	0.31	0.022
C55 - C56	π	C55 - C56	π^*	0.6	0.3	0.012
C43 - H63	σ	C44 - C48	σ^*	9.41	1.01	0.087
C26 - C32	σ	C32 - N33	σ^*	8.45	1.62	0.105
C50 - C51	σ	C51 - N52	σ^*	8.27	1.62	0.104
C32 - N33	σ	C26 - C32	σ^*	7.99	1.59	0.101
C44 - C48	σ	C43 - C48	σ^*	6.27	1.31	0.081
C50 - C51	σ	C44 - C50	σ^*	6.02	1.33	0.08
C3 - C4	σ	C3 - C16	σ^*	5.96	1.25	0.077
C37 - H40	σ	C36 - S38	σ^*	5.65	0.74	0.058
C11 - C16	σ	C11 - C12	σ^*	4.83	1.25	0.07
C15 - C16	σ	C14 - C15	σ^*	4.54	1.29	0.068
C25 - C26	σ	C14 - C25	σ^*	3.9	1.23	0.062
C28 - N35	σ	C29 - C36	σ^*	2.96	1.31	0.056
C11 - C16	σ	C11 - N20	σ^*	1.64	1.13	0.039
C39 - H42	σ	C37 - C39	σ^*	0.87	1.1	0.028
C56 - F62	σ	C55 - C56	σ^*	0.52	1.65	0.026
N35	LP (1)	C27 - C29	π^*	48.96	0.32	0.114
N20	LP (1)	C1 - C2	π^*	43.09	0.31	0.104
N20	LP (1)	C11 - C16	π^*	42.05	0.3	0.103
S38	LP (2)	C36 - C37	π^*	25.68	0.27	0.076
S 38	LP (2)	C39 - C41	π^*	23.92	0.28	0.073
F62	LP (3)	C55 - C56	π^*	21.1	0.46	0.094
O34	LP (2)	C32 - N33	π^*	0.9	0.39	0.017
O34	LP (2)	C28 - N35	σ^*	29.21	0.67	0.127
O49	LP (2)	C45 - C48	σ^*	22.84	0.71	0.115
O49	LP (2)	C45 - C47	σ^*	20.7	0.75	0.113
O34	LP (2)	C26 - C28	σ^*	19.64	0.74	0.11
N54	LP (1)	C50 - C53	σ^*	12.68	1.04	0.103
N52	LP (1)	C50 - C51	σ^*	12.59	1.04	0.102
N33	LP (1)	C26 - C32	σ^*	12.25	1.06	0.102
F62	LP (2)	C56 - C57	σ^*	6.48	1	0.072
F62	LP (2)	C55 - C56	σ^*	6.46	1	0.072
N20	LP (1)	C21 - H22	σ^*	5.54	0.64	0.059
N20	LP (1)	C21 - H23	σ^*	4.95	0.64	0.056
O34	LP (1)	C26 - C28	σ^*	2.82	1.18	0.052
O34	LP (1)	C28 - N35	σ^*	1.45	1.11	0.036
O34	LP (2)	C29 - N35	σ^*	0.57	0.72	0.019
F62	LP (2)	C46 - C55	σ^*	0.5	1.02	0.02

Table S28: Natural bond orbital (NBO) analysis of Compound **CTP2**.

Donor(*i*)	Type	Acceptor(*j*)	Type	$E^{(2)}$ [*kcal/mol*]	$E_{(j)}$-$E_{(i)}$ [*a.u*]	$F_{(i,j)}$ [*a.u*]
C11 - C16	π	C14 - C15	π^*	26.41	0.29	0.079
C1 - C2	π	C5 - C6	π^*	24.83	0.3	0.077
C55 - C56	π	C46 - C47	π^*	21.81	0.32	0.076
C46 - C47	π	C55 - C56	π^*	20.25	0.29	0.069
C1 - C2	π	C3 - C4	π^*	18.39	0.31	0.068
C39 - C41	π	C43 - C48	π^*	16.89	0.33	0.068
C36 - C37	π	C27 - C29	π^*	14.65	0.32	0.062
C25 - C26	π	C27 - C29	π^*	11.35	0.3	0.053
C27 - C29	π	C36 - C37	π^*	10.23	0.3	0.05
C43 - C48	π	C39 - C41	π^*	9.17	0.31	0.049
C44 - C50	π	C43 - C48	π^*	8.69	0.35	0.049
C25 - C26	π	C14 - C15	π^*	5.18	0.32	0.037
C45 - O49	π	C46 - C47	π^*	4.1	0.42	0.042
C25 - C26	π	C25 - C26	π^*	1.96	0.31	0.022
C51 - N52	π	C53 - N54	π^*	0.64	0.48	0.016
C43 - H63	σ	C44 - C48	σ^*	9.36	1.01	0.087
C26 - C32	σ	C32 - N33	σ^*	8.46	1.62	0.105
C51 - N52	σ	C50 - C51	σ^*	8.18	1.57	0.102
C32 - N33	σ	C26 - C32	σ^*	8	1.59	0.101
C44 - C48	σ	C43 - C48	σ^*	6.27	1.31	0.081
C50 - C53	σ	C44 - C50	σ^*	6.11	1.33	0.081
C44 - C50	σ	C50 - C53	σ^*	5.95	1.28	0.078
C15 - H19	σ	C11 - C16	σ^*	4.96	1.07	0.065
C25 - C26	σ	C32 - N33	σ^*	4.4	1.61	0.076
C4 - C5	σ	C5 - C6	σ^*	3.2	1.29	0.057
C46 - C47	σ	C45 - O49	σ^*	2.97	1.31	0.056
C27 - C29	σ	H31 - N35	σ^*	2.71	1.13	0.05
C56 - C57	σ	C55 - H59	σ^*	1.84	1.16	0.041
C37 - C39	σ	C39 - H42	σ^*	1.3	1.11	0.034
C53 - N54	σ	C44 - C50	σ^*	0.54	1.64	0.027
N35	LP (1)	C27 - C29	π^*	49.22	0.32	0.114
N20	LP (1)	C1 - C2	π^*	43.13	0.31	0.104
N20	LP (1)	C11 - C16	π^*	42.03	0.3	0.103
S38	LP (2)	C36 - C37	π^*	25.68	0.27	0.076
S38	LP (2)	C39 - C41	π^*	23.94	0.28	0.073
F61	LP (3)	C55 - C56	π^*	21.04	0.46	0.094
F62	LP (3)	C57 - C58	π^*	20.85	0.46	0.093

O34	LP (2)	C32 - N33	π^*	0.88	0.39	0.017
O34	LP (2)	C28 - N35	σ^*	29.27	0.67	0.127
O49	LP (2)	C45 - C48	σ^*	22.66	0.72	0.115
O49	LP (2)	C45 - C47	σ^*	21.14	0.75	0.114
O34	LP (2)	C26 - C28	σ^*	19.63	0.74	0.11
N54	LP (1)	C50 - C53	σ^*	12.7	1.04	0.103
F62	LP (2)	C56 - C57	σ^*	7.75	0.97	0.078
F62	LP (2)	C57 - C58	σ^*	6.38	1.01	0.072
F61	LP (2)	C55 - C56	σ^*	6.24	1.01	0.071
N20	LP (1)	C21 - H23	σ^*	5.64	0.64	0.059
N20	LP (1)	C21 - H22	σ^*	4.85	0.64	0.055
O34	LP (1)	C26 - C28	σ^*	2.83	1.18	0.052
F61	LP (1)	C55 - C56	σ^*	1.55	1.63	0.045
F62	LP (1)	C56 - C57	σ^*	1	1.59	0.036
F61	LP (1)	C56 - C57	σ^*	0.96	1.59	0.035
O34	LP (2)	C29 - N35	σ^*	0.57	0.72	0.019

Table S29: Natural bond orbital (NBO) analysis of Compound **CTP3**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	$E^{(2)}$ **[*kcal/mol*]**	$E_{(j)}$-$E_{(i)}$ **[*a.u*]**	$F_{(i,j)}$ **[*a.u*]**
C11 - C16	π	C14 - C15	π^*	26.6	0.29	0.079
C27 - C29	π	C25 - C26	π^*	25.53	0.32	0.082
C5 - C6	π	C3 - C4	π^*	23.93	0.3	0.076
C36 - C37	π	C39 - C41	π^*	20.26	0.31	0.073
C56 - C57	π	C46 - C55	π^*	19.83	0.33	0.072
C1 - C2	π	C3 - C4	π^*	18.41	0.31	0.068
C14 - C15	π	C11 - C16	π^*	17.99	0.29	0.068
C3 - C4	π	C11 - C16	π^*	15.82	0.28	0.062
C25 - C26	π	C27 - C29	π^*	11.43	0.3	0.053
C44 - C50	π	C46 - C55	π^*	9.5	0.33	0.052
C44 - C50	π	C43 - C48	π^*	8.06	0.34	0.047
C25 - C26	π	C14 - C15	π^*	5.32	0.32	0.038
C45 - O49	π	C43 - C48	π^*	3.79	0.44	0.038
C25 - C26	π	C25 - C26	π^*	1.84	0.31	0.022
C51 - N52	π	C53 - N54	π^*	0.74	0.47	0.017
C26 - C32	σ	C32 - N33	σ^*	8.46	1.62	0.105
C50 - C51	σ	C51 - N52	σ^*	8.23	1.61	0.103
C43 - H63	σ	C45 - C48	σ^*	7.35	0.97	0.076
C43 - H63	σ	C39 - C41	σ^*	6.42	1.1	0.075
C43 - C48	σ	C41 - C43	σ^*	6	1.3	0.079
C15 - C16	σ	C3 - C16	σ^*	5.99	1.25	0.077

C47 - C58	σ	C46 - C47	σ^*	5.76	1.3	0.077
C15 - C16	σ	C11 - C16	σ^*	4.98	1.26	0.071
C1 - H7	σ	C2 - C3	σ^*	4.69	1.08	0.064
C45 - C48	σ	C43 - C48	σ^*	3.96	1.27	0.063
C14 - C15	σ	C14 - C25	σ^*	3.82	1.2	0.06
C28 - N35	σ	C29 - C36	σ^*	2.97	1.31	0.056
C11 - C16	σ	C15 - H19	σ^*	2.73	1.08	0.049
C39 - H42	σ	C39 - C41	σ^*	1.99	1.1	0.042
C56 -Cl61	σ	C55 - C56	σ^*	0.51	1.31	0.023
N35	LP (1)	C27 - C29	π^*	48.57	0.32	0.114
N20	LP (1)	C1 - C2	π^*	43.04	0.31	0.104
N20	LP (1)	C11 - C16	π^*	42.18	0.3	0.103
S38	LP (2)	C36 - C37	π^*	27.26	0.27	0.078
S38	LP (2)	C39 - C41	π^*	21.58	0.28	0.07
Cl62	LP (3)	C56 - C57	π^*	16.44	0.31	0.071
Cl61	LP (3)	C56 - C57	π^*	16.22	0.31	0.07
O34	LP (2)	C32 - N33	π^*	0.9	0.39	0.017
O34	LP (2)	C28 - N35	σ^*	29.26	0.67	0.127
O49	LP (2)	C45 - C48	σ^*	21.01	0.73	0.112
O49	LP (2)	C45 - C47	σ^*	20.85	0.75	0.113
O34	LP (2)	C26 - C28	σ^*	19.72	0.74	0.11
N54	LP (1)	C50 - C53	σ^*	12.7	1.04	0.103
N52	LP (1)	C50 - C51	σ^*	12.67	1.04	0.103
N20	LP (1)	C21 - H22	σ^*	5.98	0.64	0.061
Cl62	LP (2)	C56 - C57	σ^*	5.64	0.86	0.062
Cl62	LP (2)	C57 - C58	σ^*	4.47	0.89	0.056
N20	LP (1)	C21 - H23	σ^*	4.4	0.64	0.052
O49	LP (1)	C45 - C48	σ^*	2.98	1.16	0.053
S38	LP (1)	C39 - C41	σ^*	2.29	1.24	0.048
Cl62	LP (1)	C56 - C57	σ^*	1.86	1.48	0.047
Cl61	LP (1)	C55 - C56	σ^*	1.74	1.5	0.046
Cl62	LP (2)	C47 - C58	σ^*	0.54	0.92	0.02

Table S30: Natural bond orbital (NBO) analysis of Compound **CTP4**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	$E^{(2)}$ **[*kcal/mol*]**	$E_{(j)}$-$E_{(i)}$ **[*a.u*]**	$F_{(i,j)}$ **[*a.u*]**
C11 - C16	π	C14 - C15	π^*	26.58	0.29	0.079
C1 - C2	π	C5 - C6	π^*	24.8	0.3	0.077
C5 - C6	π	C3 - C4	π^*	23.93	0.3	0.076
C43 - C48	π	C45 - O49	π^*	21.97	0.32	0.076
C5 - C6	π	C1 - C2	π^*	19.71	0.29	0.068

C14 - C15	π	C11 - C16	π^*	17.99	0.29	0.068
C47 - C58	π	C45 - O49	π^*	16.7	0.31	0.068
C14 - C15	π	C25 - C26	π^*	14.75	0.29	0.058
C25 - C26	π	C27 - C29	π^*	11.5	0.3	0.053
C27 - C29	π	C36 - C37	π^*	10.58	0.3	0.051
C44 - C50	π	C46 - C55	π^*	9.8	0.33	0.052
C25 - C26	π	C14 - C15	π^*	5.25	0.32	0.038
C45 - O49	π	C43 - C48	π^*	2.94	0.44	0.034
C25 - C26	π	C25 - C26	π^*	1.82	0.31	0.021
C53 - N54	π	C51 - N52	π^*	0.64	0.47	0.016
C43 - H61	σ	C44 - C48	σ^*	9.24	1.01	0.086
C57 - C64	σ	C64 - N65	σ^*	9	1.62	0.108
C56 - C62	σ	C62 - N63	σ^*	8.96	1.62	0.108
C64 - N65	σ	C57 - C64	σ^*	8.67	1.57	0.105
C43 - C48	σ	C44 - C48	σ^*	6.32	1.25	0.079
C44 - C48	σ	C43 - C48	σ^*	6.26	1.3	0.081
C15 - C16	σ	C3 - C16	σ^*	5.99	1.26	0.077
C27 - H30	σ	C29 - N35	σ^*	5.83	0.98	0.068
C43 - H61	σ	C39 - C41	σ^*	4.99	1.09	0.066
C58 - H60	σ	C56 - C57	σ^*	4.62	1.06	0.063
S38 - C41	σ	C39 - H42	σ^*	3.97	1.09	0.059
C44 - C46	σ	C50 - C53	σ^*	3.6	1.19	0.059
C28 - N35	σ	C29 - C36	σ^*	2.99	1.31	0.056
C44 - C46	σ	C44 - C48	σ^*	1.97	1.18	0.043
C43 - H61	σ	C41 - C43	σ^*	0.52	1.06	0.021
N35	LP (1)	C27 - C29	π^*	48.54	0.32	0.114
N20	LP (1)	C1 - C2	π^*	43.06	0.31	0.104
N20	LP (1)	C11 - C16	π^*	42.18	0.3	0.103
S38	LP (2)	C36 - C37	π^*	26.34	0.27	0.077
S38	LP (2)	C39 - C41	π^*	23.61	0.27	0.072
O34	LP (2)	C32 - N33	π^*	0.9	0.39	0.017
O34	LP (2)	C28 - N35	σ^*	29.25	0.67	0.127
O49	LP (2)	C45 - C48	σ^*	22.47	0.72	0.115
O49	LP (2)	C45 - C47	σ^*	21.95	0.74	0.115
O34	LP (2)	C26 - C28	σ^*	19.7	0.74	0.11
N54	LP (1)	C50 - C53	σ^*	12.72	1.04	0.103
N52	LP (1)	C50 - C51	σ^*	12.66	1.04	0.103
N33	LP (1)	C26 - C32	σ^*	12.26	1.06	0.102
N20	LP (1)	C21 - H22	σ^*	5.32	0.64	0.058
N20	LP (1)	C21 - H23	σ^*	5.16	0.64	0.057
O34	LP (1)	C26 - C28	σ^*	2.82	1.18	0.052

S38	LP (1)	C36 - C37	σ^*	2.77	1.24	0.052
O49	LP (1)	C45 - C48	σ^*	2.62	1.15	0.05
O49	LP (1)	C45 - C47	σ^*	2.55	1.16	0.049
O34	LP (1)	C28 - N35	σ^*	1.45	1.11	0.036
O34	LP (2)	C29 - N35	σ^*	0.57	0.71	0.019

Table S31: Natural bond orbital (NBO) analysis of Compound **CTP5**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	$E^{(2)}$ [*kcal/mol*]	$E_{(j)}$-$E_{(i)}$ [*a.u*]	$F_{(i,j)}$ [*a.u*]
C46 - C55	π	C56 - C57	π^*	27.52	0.28	0.078
C47 - C58	π	C56 - C57	π^*	25.81	0.27	0.075
C5 - C6	π	C3 - C4	π^*	23.93	0.3	0.076
C11 - C16	π	C3 - C4	π^*	22.51	0.3	0.074
C36 - C37	π	C39 - C41	π^*	19.76	0.31	0.072
C1 - C2	π	C3 - C4	π^*	18.42	0.31	0.068
C11 - C16	π	C12 - C13	π^*	17.98	0.29	0.067
C3 - C4	π	C11 - C16	π^*	15.82	0.28	0.062
C36 - C37	π	C27 - C29	π^*	13.99	0.32	0.06
C25 - C26	π	C27 - C29	π^*	11.5	0.3	0.053
C44 - C50	π	C46 - C55	π^*	9.93	0.33	0.052
N62 - O64	π	N62 - O64	π^*	6.5	0.4	0.054
N65 - O66	π	C56 - C57	π^*	3.04	0.48	0.038
C25 - C26	π	C25 - C26	π^*	1.8	0.31	0.021
C51 - N52	π	C53 - N54	π^*	0.63	0.48	0.016
C43 - H61	σ	C44 - C48	σ^*	9.23	1.01	0.086
C26 - C32	σ	C32 - N33	σ^*	8.46	1.62	0.105
C32 - N33	σ	C26 - C32	σ^*	8	1.59	0.101
C43 - C48	σ	C44 - C48	σ^*	6.34	1.25	0.079
C55 - C56	σ	C56 - C57	σ^*	6	1.29	0.079
C15 - C16	σ	C3 - C16	σ^*	5.98	1.26	0.077
C15 - C16	σ	C11 - C16	σ^*	4.97	1.26	0.071
C14 - C15	σ	C15 - C16	σ^*	4.51	1.3	0.069
S38 - C41	σ	C39 - H42	σ^*	3.97	1.09	0.059
C13 - C14	σ	C14 - C25	σ^*	3.85	1.19	0.06
C28 - N35	σ	C29 - C36	σ^*	2.98	1.31	0.056
C29 - C36	σ	C25 - C27	σ^*	2.18	1.28	0.047
C45 - C48	σ	C45 - O49	σ^*	1.96	1.25	0.045
C56 - N62	σ	C56 - C57	σ^*	1	1.36	0.033
C43 - H61	σ	C41 - C43	σ^*	0.52	1.06	0.021
O67	LP (3)	N65 - O66	π^*	189.12	0.17	0.16
O63	LP (3)	N62 - O64	π^*	163.13	0.18	0.155

N35	LP (1)	C27 - C29	π^*	48.34	0.32	0.113
N20	LP (1)	C1 - C2	π^*	43.07	0.31	0.104
N20	LP (1)	C11 - C16	π^*	42.19	0.3	0.103
S38	LP (2)	C36 - C37	π^*	26.4	0.27	0.077
S38	LP (2)	C39 - C41	π^*	23.54	0.27	0.072
O63	LP (2)	N62 - O64	π^*	2.26	0.2	0.022
O34	LP (2)	C32 - N33	π^*	0.9	0.39	0.017
O63	LP (2)	C56 - C57	π^*	0.86	0.31	0.016
O66	LP (2)	C56 - C57	π^*	0.58	0.31	0.013
O34	LP (2)	C28 - N35	σ^*	29.26	0.67	0.127
O49	LP (2)	C45 - C48	σ^*	22.44	0.72	0.115
O66	LP (2)	N65 - O67	σ^*	20.81	0.75	0.113
O64	LP (2)	N62 - O63	σ^*	20.51	0.76	0.113
O34	LP (2)	C26 - C28	σ^*	19.72	0.74	0.11
O64	LP (2)	C56 - N62	σ^*	16.36	0.57	0.086
O67	LP (2)	C57 - N65	σ^*	16.14	0.57	0.086
N54	LP (1)	C50 - C53	σ^*	12.72	1.04	0.103
N33	LP (1)	C26 - C32	σ^*	12.26	1.06	0.102
O67	LP (3)	N65 - O67	σ^*	8.49	0.73	0.081
N20	LP (1)	C21 - H23	σ^*	5.3	0.64	0.057
O67	LP (1)	C57 - N65	σ^*	3.98	1.08	0.06
O66	LP (1)	N65 - O67	σ^*	2.91	1.26	0.055
O63	LP (3)	N62 - O63	σ^*	1.63	0.74	0.036
O66	LP (2)	C56 - C57	σ^*	0.56	0.85	0.02

Table S32: Natural bond orbital (NBO) analysis of Compound **CTP6**.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	$E^{(2)}$ **[*kcal/mol*]**	$E_{(j)}$-$E_{(i)}$ **[*a.u*]**	$F_{(i,j)}$ **[*a.u*]**
C11 - C16	π	C14 - C15	π^*	26.5	0.29	0.079
C1 - C2	π	C5 - C6	π^*	24.82	0.3	0.077
C43 - C48	π	C45 - O49	π^*	21.52	0.32	0.076
C5 - C6	π	C1 - C2	π^*	19.71	0.29	0.068
C11 - C16	π	C12 - C13	π^*	17.99	0.29	0.067
C3 - C4	π	C11 - C16	π^*	15.82	0.28	0.062
C14 - C15	π	C25 - C26	π^*	14.47	0.29	0.058
C25 - C26	π	C27 - C29	π^*	11.42	0.3	0.053
C27 - C29	π	C36 - C37	π^*	10.26	0.3	0.05
C43 - C48	π	C39 - C41	π^*	9.59	0.31	0.05
C25 - C26	π	C14 - C15	π^*	5.16	0.32	0.037
C45 - O49	π	C47 - C58	π^*	4.13	0.43	0.041
C45 - O49	π	C43 - C48	π^*	2.92	0.44	0.033

	C44 - C50	π	C44 - C50	π^*	1.21	0.33	0.018	
	C53 - N54	π	C51 - N52	π^*	0.63	0.47	0.015	
	C43 - H61	σ	C44 - C48	σ^*	9.3	1.01	0.087	
	C26 - C32	σ	C32 - N33	σ^*	8.46	1.62	0.105	
	C51 - N52	σ	C50 - C51	σ^*	8.22	1.57	0.102	
	C43 - C48	σ	C44 - C48	σ^*	6.3	1.25	0.079	
	C50 - C53	σ	C44 - C50	σ^*	6.03	1.33	0.08	
	C44 - C50	σ	C50 - C53	σ^*	5.88	1.28	0.077	
	C46 - C55	σ	C46 - C47	σ^*	5.5	1.3	0.076	
	C13 - H18	σ	C14 - C15	σ^*	4.74	1.09	0.064	
	C25 - C27	σ	C26 - C32	σ^*	3.99	1.24	0.063	
	C47 - C58	σ	C45 - C47	σ^*	3.43	1.19	0.058	
	C26 - C28	σ	C28 - O34	σ^*	2.9	1.3	0.055	
	C44 - C48	σ	C45 - O49	σ^*	2.71	1.3	0.053	
	C56 - C62	σ	C55 - C56	σ^*	1.94	1.26	0.044	
	C62 - F67	σ	C55 - C56	σ^*	1.05	1.64	0.037	
	C63 - F66	σ	C63 - F65	σ^*	0.5	1.34	0.024	
	N35	LP (1)	C27 - C29	π^*	48.49	0.32	0.114	
	N20	LP (1)	C1 - C2	π^*	43.09	0.31	0.104	
	N20	LP (1)	C11 - C16	π^*	42.14	0.3	0.103	
	S38	LP (2)	C36 - C37	π^*	26.15	0.27	0.077	
	S38	LP (2)	C39 - C41	π^*	23.63	0.27	0.073	
	O34	LP (2)	C32 - N33	π^*	0.9	0.39	0.017	
	F69	LP (2)	C56 - C57	π^*	0.88	0.46	0.02	
	F65	LP (2)	C56 - C57	π^*	0.78	0.46	0.019	
O34	LP (2)	C28 - N35	σ^*	29.24	0.67	0.127		
O49	LP (2)	C45 - C48	σ^*	22.61	0.72	0.115		
O49	LP (2)	C45 - C47	σ^*	21.64	0.74	0.115		
O34	LP (2)	C26 - C28	σ^*	19.7	0.74	0.11		
N54	LP (1)	C50 - C53	σ^*	12.7	1.04	0.103		
F65	LP (3)	C63 - F64	σ^*	11.86	0.71	0.083		
F67	LP (3)	C62 - F69	σ^*	10.95	0.72	0.08		
F66	LP (2)	C57 - C63	σ^*	7.01	0.81	0.068		
F67	LP (2)	C56 - C62	σ^*	6.87	0.81	0.067		
N20	LP (1)	C21 - H22	σ^*	5.74	0.64	0.06		
N20	LP (1)	C21 - H23	σ^*	4.71	0.64	0.054		
F65	LP (2)	C63 - F64	σ^*	3.99	0.72	0.048		
O34	LP (1)	C26 - C28	σ^*	2.82	1.18	0.052		
O34	LP (1)	C28 - N35	σ^*	1.45	1.11	0.036		
	F66	LP (1)	C57 - C63	σ^*	0.5	1.45	0.024	

Table S33: NBO analysis of **CTPR** and **CTP1-CTP6** by using **M06/6-311G(d,p)**.

Compounds	Donor(*i*)	Type	Acceptor(*j*)	Type	$E^{(2)}$ [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i*,*j*) [*a.u*]
CTPR	C7-C9	π	C 32-C33	π^*	16.38	0.28	0.061
	C16-C18	π	C 13-C15	π^*	23.56	0.3	0.075
	C33-C35	σ	C9-C32	σ^*	5.37	1.2	0.072
	C7-C9	σ	C5-C9	σ^*	4.6	1.27	0.068
	N1	LP (1)	C2-C4	π^*	24.86	0.29	0.079
	S34	LP (1)	C32-C33	σ^*	2.79	1.24	0.052
CTP1	C2-C4	π	C7-C9	π^*	25.45	0.3	0.078
	C32 -C33	π	C7-C9	π^*	11.56	0.32	0.056
	C37-B39	σ	C35-C37	σ^*	7.25	1.17	0.082
	C57-C64	σ	C64-N65	σ^*	8.85	1.61	0.107
	N1	LP (1)	C 2-C 4	π^*	27.58	0.29	0.083
	N63	LP (1)	C47-C62	σ^*	11.87	1.06	0.1
CTP2	C60-C61	π	C62-C65	π^*	20.3	0.29	0.071
	C13-C15	π	C 9-C11	π^*	19.4	0.3	0.07
	C3-H7	σ	C 4-S 5	σ^*	5.8	0.74	0.059
	C66-C72	σ	C72-N73	σ^*	8.86	1.61	0.107
	N28	LP (1)	C13-C15	π^*	25.54	0.29	0.08
	S5	LP (1)	C 1-C 2	σ^*	2.42	1.25	0.049
CTP3	C38-C40	π	C43-C45	π^*	24.55	0.29	0.076
	C32-C34	π	C38-C40	π^*	12.34	0.32	0.059
	C30-H33	σ	C29-S31	σ^*	5.81	0.74	0.059
	C25-C26	σ	C23-C26	σ^*	5.36	1.28	0.074
	N73	LP (1)	C53-C60	π^*	36.91	0.3	0.098
	S31	LP (1)	C29-C30	σ^*	2.48	1.25	0.05
CTP4	C50-C52	π	C45-C47	π^*	25.59	0.3	0.079
	C42-C43	π	C45-C47	π^*	10.97	0.32	0.057
	C30-H33	σ	C29-S31	σ^*	6	0.73	0.059
	C55-C67	σ	C55-C65	σ^*	5.97	1.29	0.079
	N74	LP (1)	C50-C52	π^*	32.39	0.32	0.094
	N74	LP (1)	C54-C56	σ^*	5.04	0.85	0.062
CTP5	C40-C41	π	C35-C37	π^*	14.71	0.29	0.064
	C35-C37	π	C32-C33	π^*	15.43	0.32	0.064
	N1-C22	σ	C22-C23	σ^*	1.68	1.36	0.043
	C40-S42	σ	C40-C41	σ^*	0.55	1.25	0.023
	N1	LP (1)	C2-C4	π^*	28.23	0.29	0.084
	N75	LP (1)	C61-C74	σ^*	11.87	1.06	0.1
CTP6	C40-C41	π	C35-C37	π^*	14.71	0.29	0.064
	C43-C45	π	C48-C50	π^*	26.1	0.3	0.079
	S34-C37	σ	C35-S42	σ^*	5.22	0.9	0.061

C71-C76	σ	C76-N77	σ^*	8.86	1.61	0.107
S42	LP (2)	C35-C37	π^*	25.36	0.26	0.075
N75	LP (1)	C61-C74	σ^*	11.87	1.06	0.1

Table S34: Dipole polarizability and major contributing tensor (*esu*) of the studied chromophores at diffused basis set.

Dipole Moment	**CTPR**	**CTP1**	**CTP2**	**CTP3**	**CTP4**	**CTP5**	**CTP6**
μ_x	-1.8264	-0.3612	-0.9013	0.4224	-5.5055	-5.2484	-3.2211
μ_y	-11.5239	-9.2007	-9.9746	-8.6094	-1.9319	-2.4162	-5.8020
μ_z	-4.9400	0.4820	-0.9637	-1.4843	-3.5876	-3.3901	-1.8841
$\boldsymbol{\mu_{total}}$	**12.6704**	**9.2204**	**10.0615**	**8.7466**	**6.8493**	**6.6990**	**6.8985**
Polarizability							
α_{xx}	9.303×10^{-23}	1.503×10^{-22}	1.438×10^{-22}	1.531×10^{-22}	1.605×10^{-22}	1.623×10^{-22}	1.569×10^{-22}
α_{yy}	7.711×10^{-23}	1.707×10^{-22}	1.574×10^{-22}	1.715×10^{-22}	1.876×10^{-22}	1.829×10^{-22}	1.777×10^{-22}
α_{zz}	3.963×10^{-23}	7.538×10^{-23}	7.697×10^{-23}	8.227×10^{-23}	8.222×10^{-23}	8.117×10^{-23}	7.991×10^{-23}
$\boldsymbol{\alpha_{total}}$	$\mathbf{6.992\times10^{-23}}$	$\mathbf{1.321\times10^{-22}}$	$\mathbf{1.260\times10^{-22}}$	$\mathbf{1.356\times10^{-22}}$	$\mathbf{1.434\times10^{-22}}$	$\mathbf{1.421\times10^{-22}}$	$\mathbf{1.381\times10^{-22}}$
2nd Hyper pol.							
γ_X	3.777×10^{-34}	2.226×10^{-33}	2.031×10^{-33}	2.317×10^{-33}	2.958×10^{-33}	2.909×10^{-33}	2.546×10^{-33}
γ_Y	1.002×10^{-34}	2.299×10^{-33}	2.482×10^{-33}	2.679×10^{-33}	3.021×10^{-33}	2.927×10^{-33}	2.558×10^{-33}
γ_Z	2.124×10^{-35}	1.159×10^{-33}	1.087×10^{-34}	-5.468×10^{-35}	1.647×10^{-34}	1.539×10^{-34}	1.247×10^{-34}
Average<γ>	$\mathbf{4.993\times10^{-34}}$	$\mathbf{4.641\times10^{-33}}$	$\mathbf{4.623\times10^{-33}}$	$\mathbf{4.942\times10^{-33}}$	$\mathbf{6.144\times10^{-33}}$	$\mathbf{5.991\times10^{-33}}$	$\mathbf{5.229\times10^{-33}}$
Magnitude of γ	$\mathbf{3.914\times10^{-34}}$	$\mathbf{3.202\times10^{-33}}$	$\mathbf{3.209\times10^{-33}}$	$\mathbf{3.543\times10^{-33}}$	$\mathbf{4.231\times10^{-33}}$	$\mathbf{4.130\times10^{-33}}$	$\mathbf{3.611\times10^{-33}}$

Table S35: The computed first hyperpolarizability (β_{total}) and major contributing tensors (*esu*) of studied chromophores at diffused basis set.

Hyper pol	**CTPR**	**CTP1**	**CTP2**	**CTP3**
$\boldsymbol{\beta_{xxx}}$	-9.291×10^{-29}	-2.853×10^{-28}	-2.346×10^{-28}	-2.904×10^{-28}
$\boldsymbol{\beta_{xxy}}$	-3.451×10^{-29}	1.687×10^{-28}	1.489×10^{-28}	1.979×10^{-28}
$\boldsymbol{\beta_{xyy}}$	1.793×10^{-29}	-1.825×10^{-28}	-1.817×10^{-28}	-2.075×10^{-28}
$\boldsymbol{\beta_{yyy}}$	-1.851×10^{-30}	2.548×10^{-28}	2.691×10^{-28}	2.236×10^{-28}
$\boldsymbol{\beta_{xxz}}$	-8.571×10^{-30}	9.975×10^{-30}	1.013×10^{-29}	1.150×10^{-29}
$\boldsymbol{\beta_{yyz}}$	-2.221×10^{-30}	3.795×10^{-29}	2.843×10^{-29}	4.965×10^{-29}
$\boldsymbol{\beta_{xzz}}$	1.793×10^{-30}	2.506×10^{-30}	6.147×10^{-30}	4.747×10^{-30}
$\boldsymbol{\beta_{yzz}}$	1.571×10^{-30}	-3.756×10^{-30}	-5.277×10^{-30}	-7.268×10^{-30}
$\boldsymbol{\beta_{zzz}}$	2.350×10^{-31}	9.787×10^{-31}	4.936×10^{-30}	6.439×10^{-30}
$\boldsymbol{\beta_{total}}$	$\mathbf{8.172\times10^{-29}}$	$\mathbf{6.287\times10^{-28}}$	$\mathbf{5.836\times10^{-28}}$	$\mathbf{6.478\times10^{-28}}$

Hyper pol	**CTP4**	**CTP5**	**CTP6**
$\boldsymbol{\beta_{xxx}}$	-3.755×10^{-28}	-3.710×10^{-28}	-3.354×10^{-28}
$\boldsymbol{\beta_{xxy}}$	2.520×10^{-28}	2.459×10^{-28}	2.145×10^{-28}
$\boldsymbol{\beta_{xyy}}$	-2.815×10^{-28}	-2.737×10^{-28}	-2.377×10^{-28}
$\boldsymbol{\beta_{yyy}}$	3.866×10^{-28}	3.725×10^{-28}	3.291×10^{-28}
$\boldsymbol{\beta_{xxz}}$	1.723×10^{-31}	4.728×10^{-30}	3.257×10^{-30}
$\boldsymbol{\beta_{yyz}}$	3.657×10^{-29}	4.118×10^{-29}	3.623×10^{-29}
$\boldsymbol{\beta_{xzz}}$	-8.886×10^{-30}	-5.352×10^{-30}	-5.679×10^{-30}
$\boldsymbol{\beta_{yzz}}$	6.869×10^{-30}	4.114×10^{-30}	4.214×10^{-30}
$\boldsymbol{\beta_{zzz}}$	-8.585×10^{-30}	-3.460×10^{-30}	-4.991×10^{-30}

β_{total}	**9.279×10^{-28}**	**9.012×10^{-28}**	**7.977×10^{-28}**

Table S36: Dynamic first and second order hyperpolarizability (β), and (γ) values of studied chromophores in *esu* at diffused basis set.

Parameters	**Frequency (ω)[a]**	**CTPR**	**CTP1**	**CTP2**	**CTP3**
$\beta(-\omega;\omega,0)$	0.085645	4.908×10^{-28}	8.098×10^{-27}	1.214×10^{-26}	3.729×10^{-26}
$\beta(-2\omega;\omega,\omega)$	0.085645	6.446×10^{-28}	1.013×10^{-27}	3.580×10^{-27}	5.314×10^{-27}
$\gamma(-\omega,\omega,0,0)$	0.085645	4.996×10^{-33}	-2.923×10^{-31}	-6.221×10^{-31}	-1.802×10^{-30}
$\gamma(-2\omega,\omega,\omega,0)$	0.085645	-2.635×10^{-32}	-2.297×10^{-32}	1.257×10^{-30}	-2.775×10^{-31}

Parameters	**Frequency (ω)[a]**	**CTP4**	**CTP5**	**CTP6**
$\beta(-\omega;\omega,0)$	0.085645	5.714×10^{-25}	4.484×10^{-25}	2.300×10^{-26}
$\beta(-2\omega;\omega,\omega)$	0.085645	2.735×10^{-27}	1.718×10^{-25}	1.820×10^{-27}
$\gamma(-\omega,\omega,0,0)$	0.085645	5.057×10^{-29}	6.156×10^{-30}	1.626×10^{-30}
$\gamma(-2\omega,\omega,\omega,0)$	0.085645	4.522×10^{-31}	-6.597×10^{-30}	-3.950×10^{-31}

Table S37: Hole-electron analysis indices for $S_0\rightarrow S_1$ excitation (with highest f_{osc}) of compounds **CTPR** and its derivatives

Compound	**Excitation**	**E (*eV*)**	**H_{ct}**	**$S_{r\ (a.u)}$**	***H* (Å)**	**HDI**	**EDI**
CTPR	$S_0\rightarrow S_1$	3.115	2.310	0.35395	*3.109*	8.41	7.16
CTP1	$S_0\rightarrow S_1$	2.259	2.486	0.1691	3.04	8.31	6.08
CTP2	$S_0\rightarrow S_1$	2.273	2.771	0.2186	3.613	8.04	6.21
CTP 3	$S_0\rightarrow S_1$	2.201	2.609	0.1256	3.554	8.29	5.86
CTP 4	$S_0\rightarrow S_1$	1.997	2.334	0.1007	3.391	8.37	6.13
CTP 5	$S_0\rightarrow S_1$	1.956	2.395	0.0978	3.449	8.51	6.07
CTP 6	$S_0\rightarrow S_1$	2.102	2.256	0.1070	3.335	8.41	6.21

Equations S1-S8 are used to calculate global reactivity descriptors.

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

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

$$X = -\frac{(E_{HOMO} + E_{LUMO})}{2} \quad (3)$$

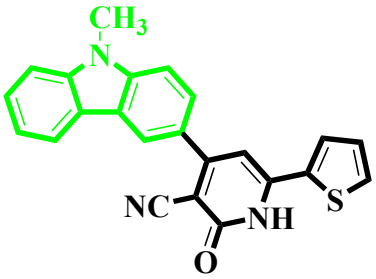
$$\eta = -\frac{E_{LUMO} - E_{HOMO}}{2} \quad (4)$$

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

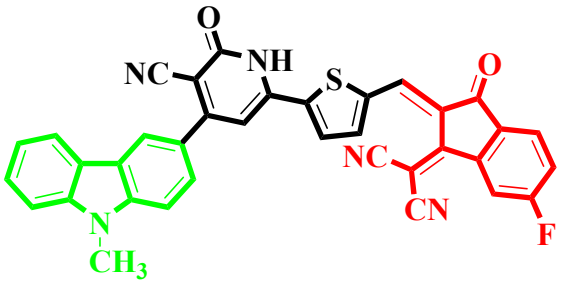
$$\sigma = \frac{1}{2\eta} \quad (6)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (7)$$

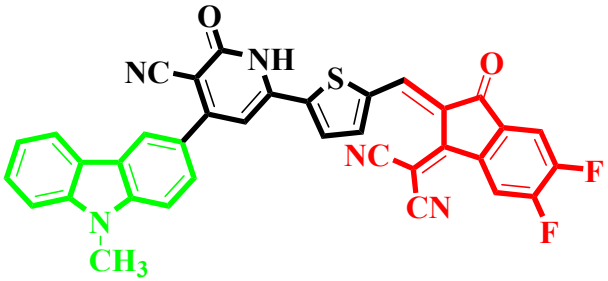
$$\Delta Nmax = -\frac{\mu}{\eta} \quad (8)$$



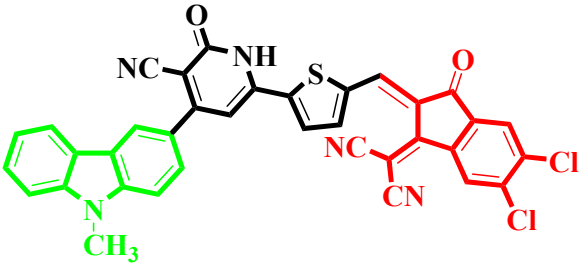
CTPR



CTP1



CTP2



CTP3

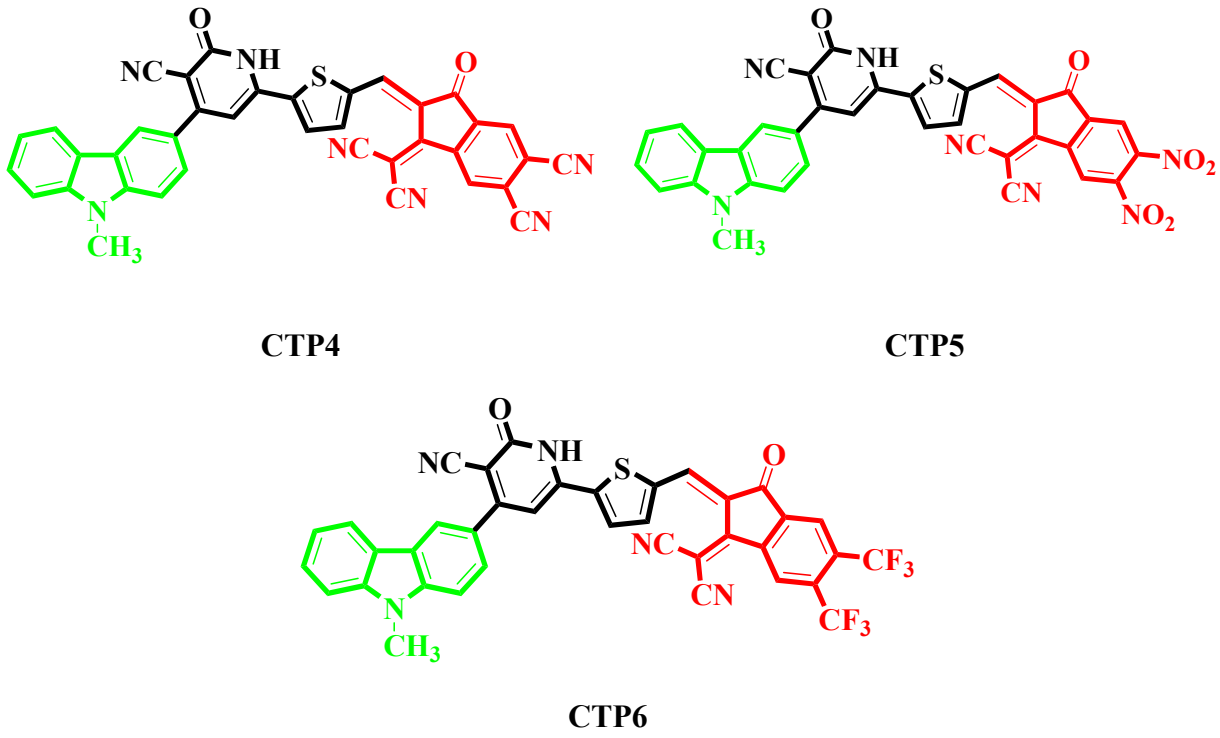
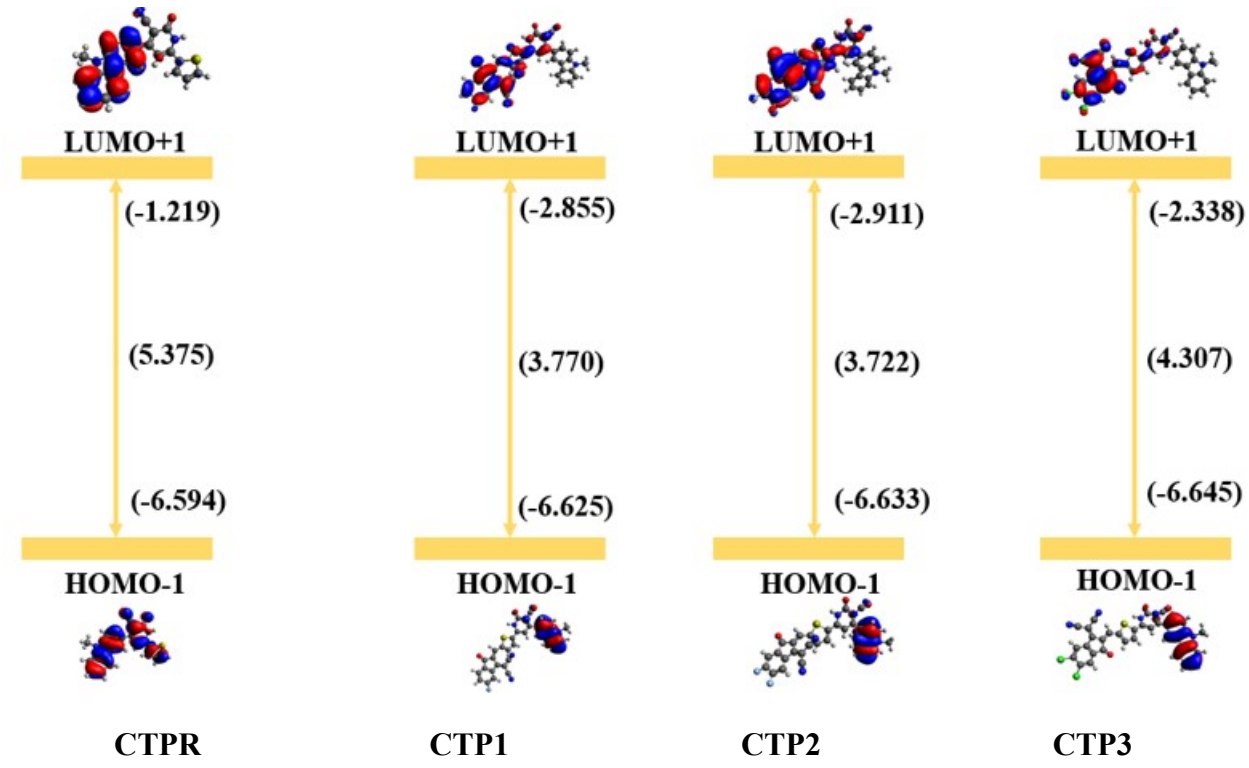
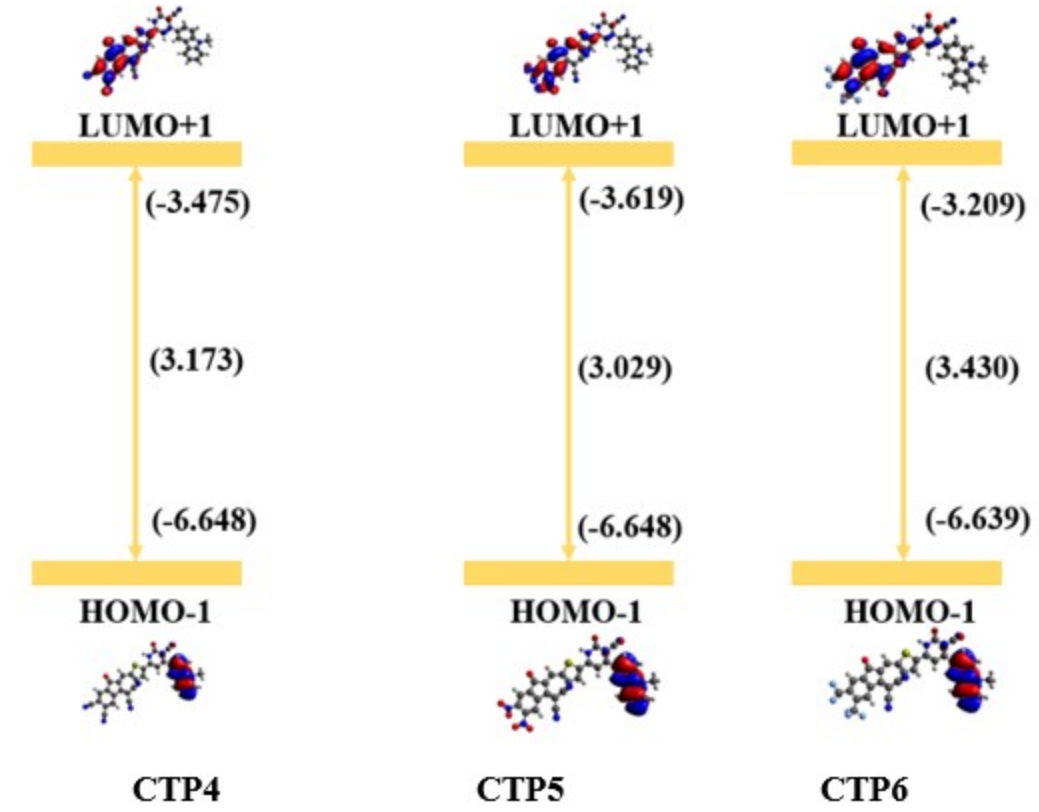
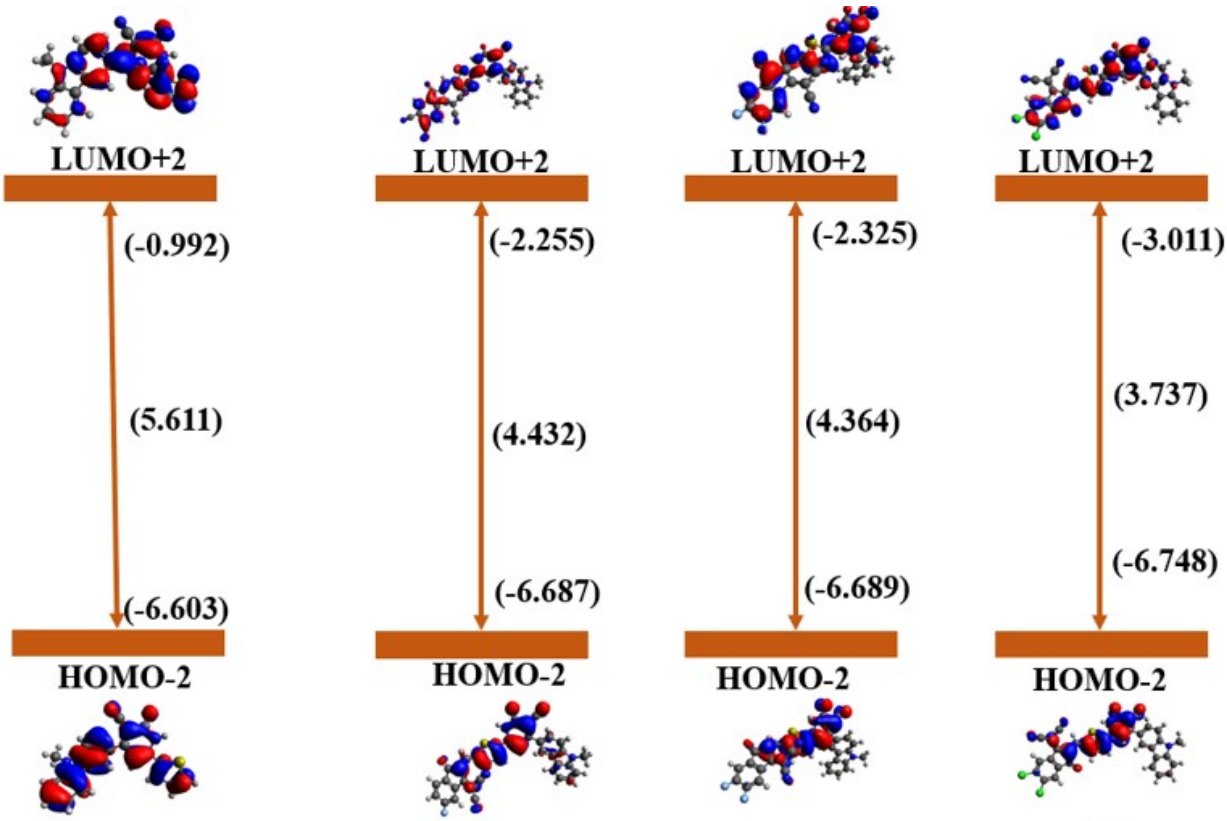


Figure S1: Chemical structures of **CTPR** and **(CTP1-CTP6)**.





CTP4 CTP5 CTP6



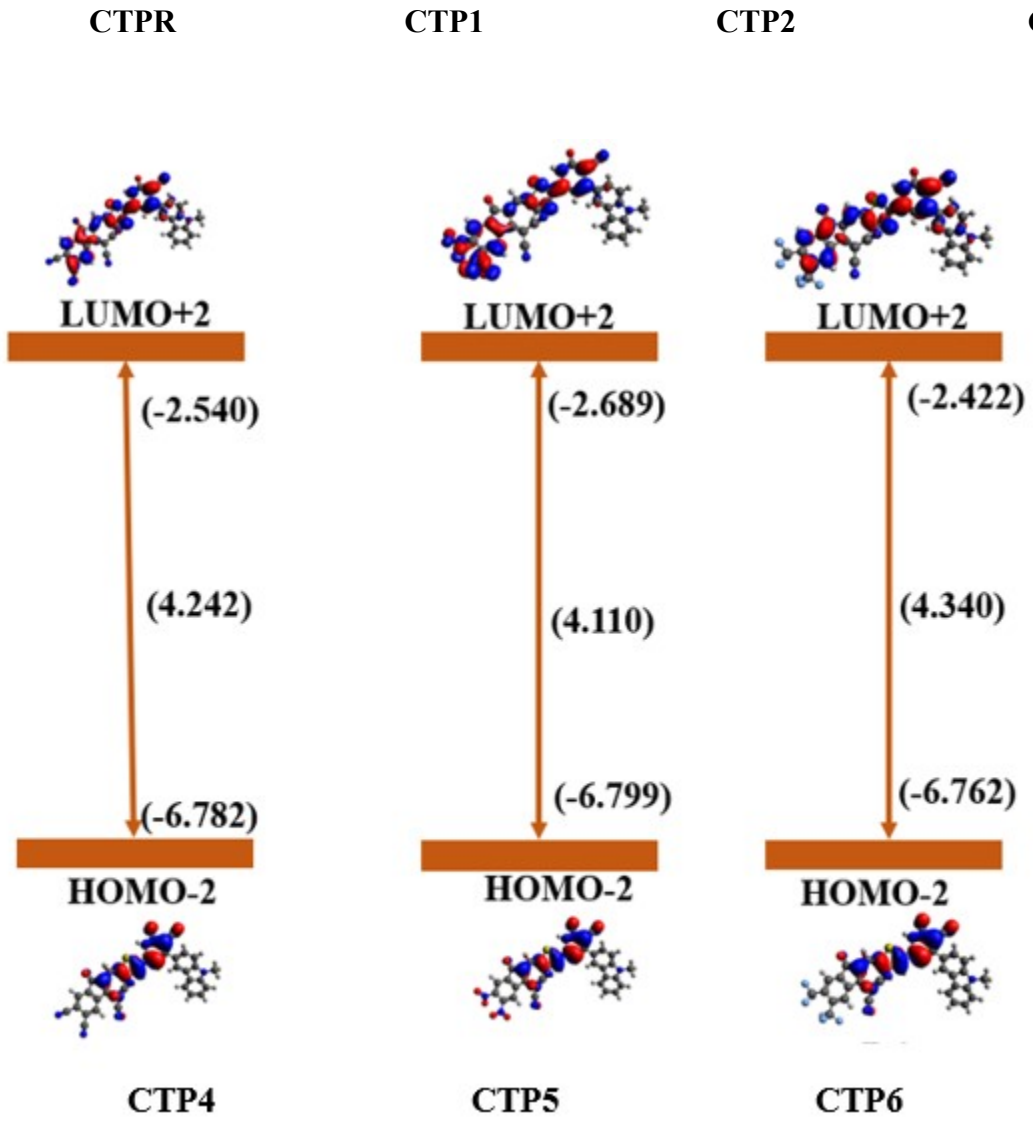


Figure S2: FMO pictograms of **CTPR** and **(CTP1-CTP6)** for HOMO-1, LUMO+1, HOMO-2, LUMO+2 and their energy gaps in *eV***.**