Supporting Information

Hetero Aromatic Donors as Effective Terminal Groups for DPP Based Organic Solar Cells

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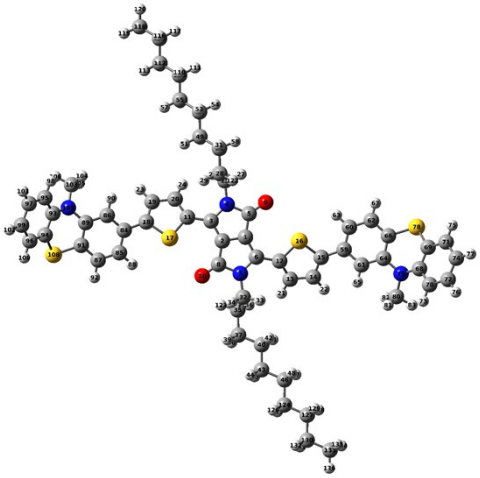
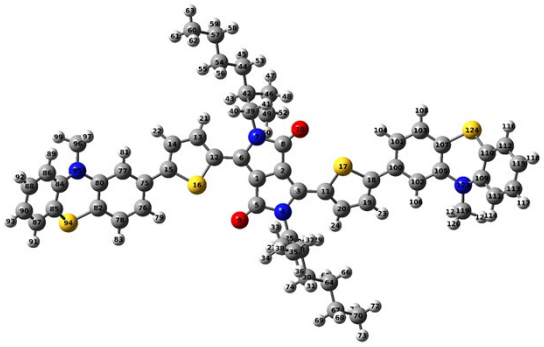
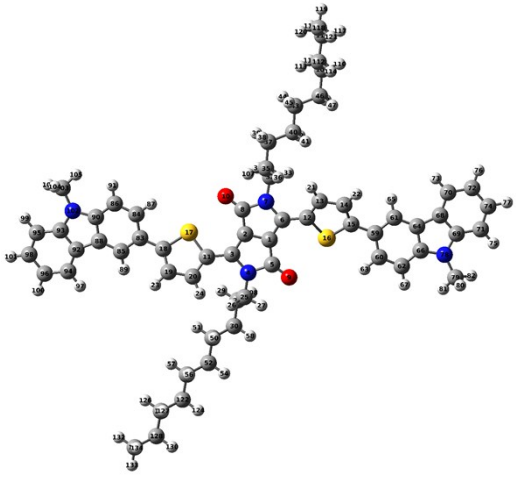
Figure S1. Structures of optimized geometries of **CSDPP5-CSDPP8** at B3LYP/6-311 G(d,p) level theory.



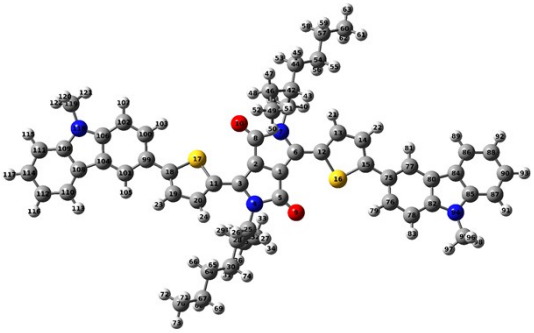
CSDPP5



CSDPP6



CSDPP7



CSDPP8

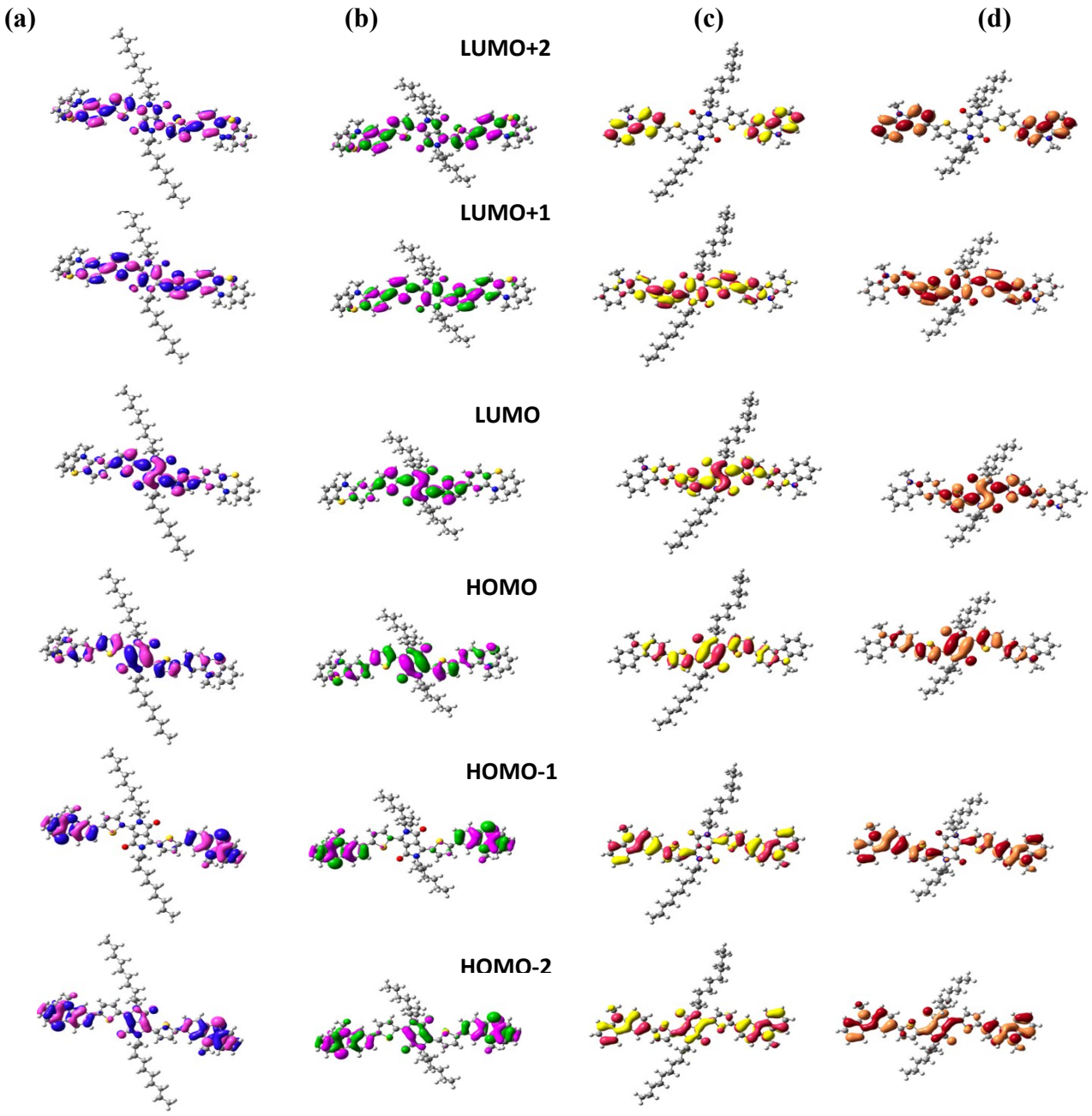


Figure S2. Molecular orbitals of (a) **CSDPP5**, (b) **CSDPP6**, (c) **CSDPP7**, and (d) **CSDPP8** in B3LYP functional, involved in transitions that contribute to the first excitation and to the next high absorbance excitation.

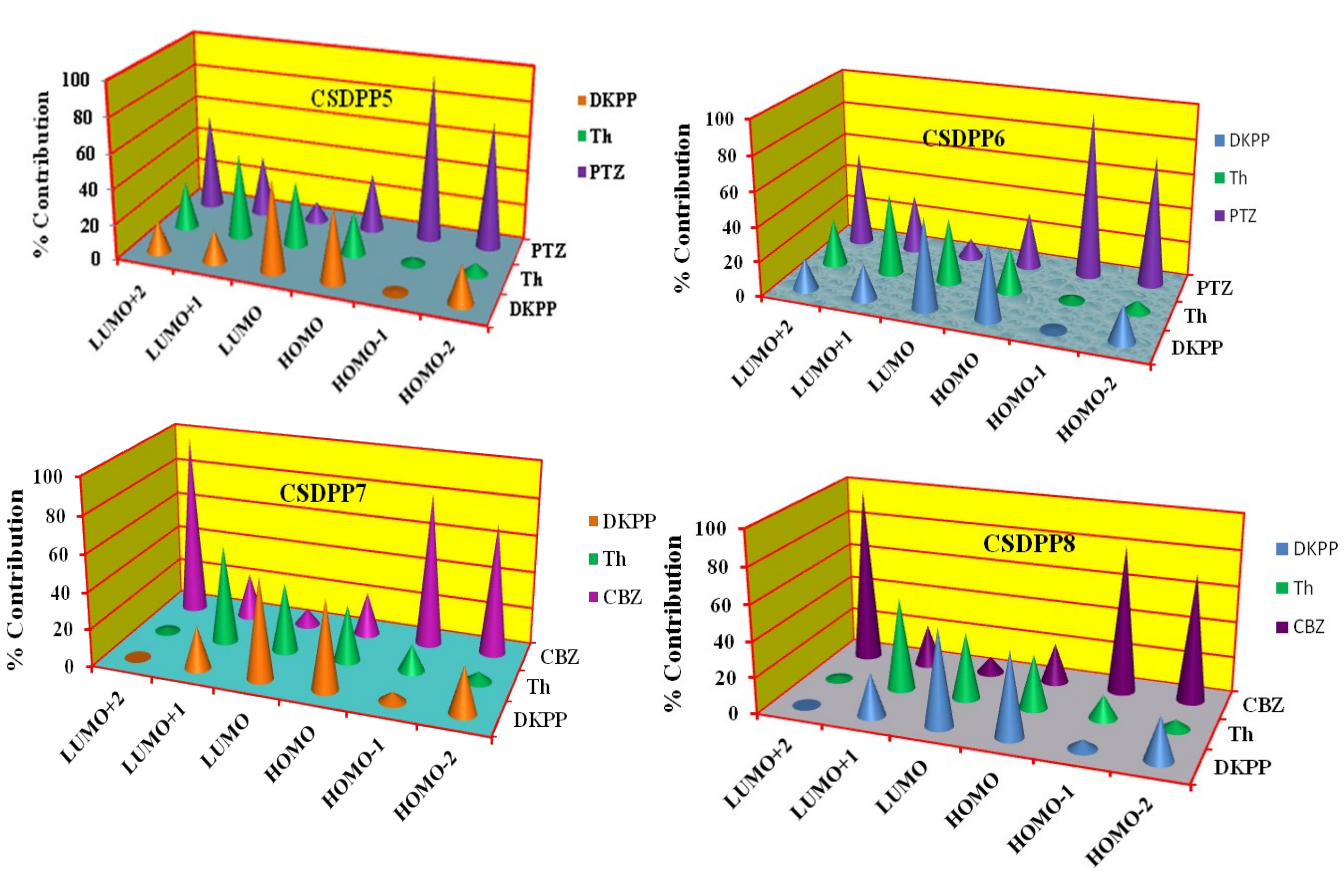


Figure S3. Percentage contributions of the orbital density of the individual groups in HOMO-2, HOMO-1, HOMO, LUMO, LUMO+1 and LUMO+2 of the **CSDPP** dyes.

Table S1. Calculated excitation energies for **CSDPP5** in THF solution.

N_ States	E (eV)	WL (nm)	f	Composition
1	2.01	615	1.2162	H → L (99%)
2	2.26	548	0.0015	H-1 → L (99%)
3	2.39	520	0.1307	H-2 → L (98%)
4	2.99	414	0.0014	H-3 → L (18%)
5	3.16	393	0.0417	H-7 → L (43%)
6	3.19	390	0.3008	H-4 → L (82%)
7	3.22	386	0.0062	H-7 → L (35%)
8	3.22	374	0.1176	H-1 → L+1 (87%)
9	3.40	365	0.0006	H-2 → L+1 (83%)
10	3.50	355	0.0097	H-12 → L (14%)

Table S2. Calculated excitation energies for **CSDPP6** in THF solution.

N_ States	E (eV)	WL (nm)	f	Composition
1	1.99	624	1.2145	H → L (99%)
2	2.24	554	0.0011	H-1 → L (99%)
3	2.36	525	0.1227	H-2 → L (98%)
4	2.97	418	0.0009	H-3 → L (17%)
5	3.13	396	0.0028	H-7 → L (51%)
6	3.15	394	0.3491	H-4 → L (88%)
7	3.19	388	0.0106	H-7 → L (26%)
8	3.30	376	0.1184	H-1 → L+1 (88%)
9	3.38	367	0.0011	H-2 → L+1 (84%)
10	3.50	355	0.0452	H-8 → L (21%)

Table S3. Calculated excitation energies for **CSDPP7** in THF solution.

N_ States	E (eV)	WL (nm)	f	Combination
1	2.05	606	1.5051	H → L (99%)
2	2.62	473	0.0027	H-1 → L (97%)
3	2.78	445	0.1448	H-2 → L (97%)
4	3.08	402	0.0015	H-3 → L (81%)
5	3.11	399	0.0603	H-4 → L (95%)
6	3.15	394	0.0036	H-7 → L (14%)
7	3.24	382	0.001	H-7 → L (33%)
8	3.43	361	0.0215	H → L+2 (78%)
9	3.44	361	0.0005	H → L+2 (13%)
10	3.55	350	0.0073	H-10 → L (17%)

Table S4. Calculated excitation energies for **CSDPP8** in THF solution.

N_States	E (eV)	WL (nm)	f	Composition
1	2.02	614.3872	1.4894	H → L (99%)
2	2.60	476.9874	0.0038	H-1 → L (97%)
3	2.77	448.2081	0.1569	H-2 → L (97%)
4	3.06	404.8832	0.001	H-3 → L (73%)
5	3.09	401.5525	0.0611	H-4 → L (96%)
6	3.11	398.1098	0.0042	H-3 → L (21%)
7	3.21	385.9043	0.0019	H-7 → L (13%)
8	3.42	362.917	0.0193	H → L+2 (89%)
9	3.43	362.2913	0.001	H → L+3 (89%)
10	3.55	349.2488	0.0182	H-10 → L (21%)

Table S5. Calculated HOMOs and LUMOs energies (eV) of the **CSDPP** molecules.

	CSDPP5	**CSDPP6**	**CSDPP7**	**CSDPP8**
L+2	-1.17	-1.18	-1.26	-1.26
L+1	-1.74	-1.77	-1.51	-1.54
L	-2.88	-2.91	-2.75	-2.77
H	-5.18	-5.16	-5.06	-5.04
H-1	-5.45	-5.45	-5.68	-5.68
H-2	-5.56	-5.56	-5.85	-5.85
H-L Gap	2.30	2.25	2.31	2.27

Table S6. Optimized geometry parameters of **CSDPP5-CSDPP8** calculated at B3LYP/6-311 G(d,p) level theory.

CSDPP5		**CSDPP6**		**CSDPP7**		**CSDPP8**	
			Bond lengths (°A)				
C_6-C_{12}	1.44	C_6-C_{12}	1.44	C_6-C_{12}	1.44	C_6-C_{12}	1.44
C_{15}-C_{59}	1.46	C_{15}-C_{75}	1.46	C_{15}-C_{59}	1.46	C_{15}-C_{75}	1.46
C_3-C_{11}	1.44	C_3-C_{11}	1.44	C_3-C_{11}	1.44	C_3-C_{11}	1.44
C_{18}-C_{84}	1.46	C_{18}-C_{100}	1.46	C_{18}-C_{83}	1.46	C_{18}-C_{99}	1.46
			Dihedral angles (°)				
S_{17}-C_{11}-C_3-C_2	18.97	N_7-C_6-C_{12}-C_{13}	11.54	C_2-C_3-C_{11}-S_{17}	19.10	N_4-C_3-C_{11}-C_{20}	18.16
S_{17}-C_{11}-C_3-N_4	-163.37	N7-C6-C12-S16	-167.87	C_2-C_3-C_{11}-C_{20}	-159.74	C_2-C_3-C_{11}-C_{20}	-159.35
C_{20}-C_{11}-C_3-C_2	-159.91	S_{16}-C_{12}-C_6-C_1	11.57	S_{17}-C_{11}-C_3-N_4	-162.96	S_{17}-C_{11}-C_3-C_2	18.96
C_{20}-C_{11}-C_3-N_4	17.74	C_{13}-C_{12}-C_6-C_1	-169.01	S_{17}-C_{11}-C_3-C_2	19.11	S_{17}-C_{11}-C_3-N_4	-163.51
S_{17}-C_{18}-C_{84}-C_{85}	-27.27	S_{16}-C_{15}-C_{75}-C_{76}	-26.77	S_{17}-C_{18}-C_{83}-C_{84}	-28.28	S_{17}-C_{18}-C_{99}-C_{100}	-28.09
S_{17}-C_{18}-C_{84}-C_{86}	152.15	S_{16}-C_{15}-C_{75}-C_{77}	153.67	S_{17}-C_{18}-C_{83}-C_{35}	152.08	S_{17}-C_{18}-C_{99}-C_{101}	152.28
C_{85}-C_{84}-C_{18}-C_{19}	152.06	C_{14}-C_{15}-C_{75}-C_{77}	-28.09	C_{19}-C_{18}-C_{83}-C_{85}	-28.16	C_{19}-C_{18}-C_{99}-C_{101}	-27.91
C_1-C_6-C_{12}-C_{13}	-157.19	C_{14}-C_{15}-C_{75}-C_{76}	152.47	C_{19}-C_{18}-C_{83}-C_{84}	151.47	C_{19}-C_{18}-C_{99}-C_{100}	151.71
C_6-C_{12}-C_{13}-N_7	-9.91	C_2-C_3-C_{11}-S_{17}	19.39	N_7-C_6-C_{12}-C_{13}	20.72	S_{16}-C_{15}-C_{75}-C_{78}	-28.07
N_7-S_{16}-C_6-C_{12}-C_1	-39.97	C_2-C_3-C_{11}-C_{20}	-158.78	N_7-C_6-C_{12}-S_{16}	-160.57	S_{16}-C_{15}-C_{75}-C_{77}	152.11
S_{16}-C_6-C_{12}-C_1	-21.78	C_{20}-C_{11}-C_3-N_4	18.28	S_{16}-C_{12}-C_6-C_1	20.90	C_{77}-C_{75}-C_{15}-C_{14}	-28.00
C_6-C_{12}-C_1-C_{13}	-38.98	S_{17}-C_{11}-C_3-N_4	-163.54	C_1-C_6-C_{12}-C_{13}	157.80	C_{14}-C_{15}-C_{75}-C_{76}	151.82
S_{16}-C_{15}-C_{59}-C_{60}	-28.63	S_{17}-C_{18}-C_{100}-C_{101}	-27.14	S_{16}-C_{15}-C_{59}-C_{60}	-29.48	C_1-C_6-C_{12}-S_{16}	11.29
C_{61}-S_{16}-C_{15}-C_{59}	-24.65	S_{17}-C_{18}-C_{100}-C_{102}	152.49	S_{16}-C_{15}-C_{59}-C_{61}	151.09	C_1-C_6-C_{12}-C_{13}	-169.49
C_{14}-C_{15}-C_{59}-C_{61}	-29.87	C_{19}-C_{18}-C_{100}-C_{102}	-28.33	C_{14}-C_{15}-C_{59}-C_{61}	-29.33	N_7-C_6-C_{12}-C_{13}	11.46
C_{60}-C_{59}-C_{15}-C_{14}	150.70	C_{19}-C_{18}-C_{100}-C_{101}	152.03	C_{14}-C_{15}-C_{59}-C_{60}	150.09	N_7-C_6-C_{12}-S_{16}	-167.75