Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Can silicon substituted metal–free organic dyes achieve better efficiency compared to non-silicon organic dyes? A computational study

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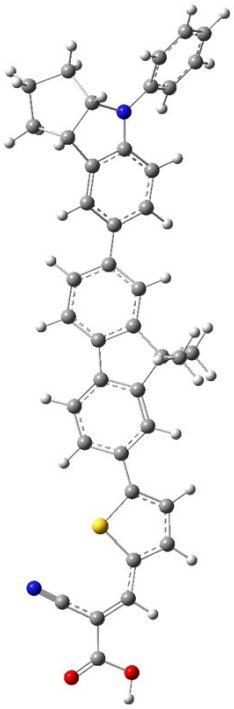
Supporting Information:



Dye **5**

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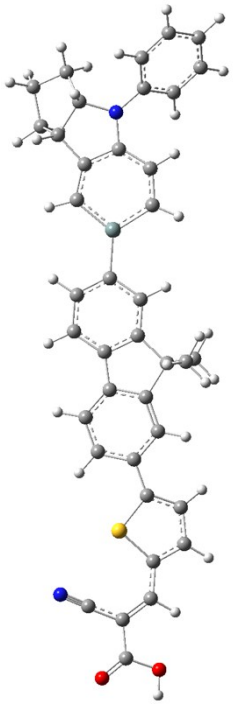

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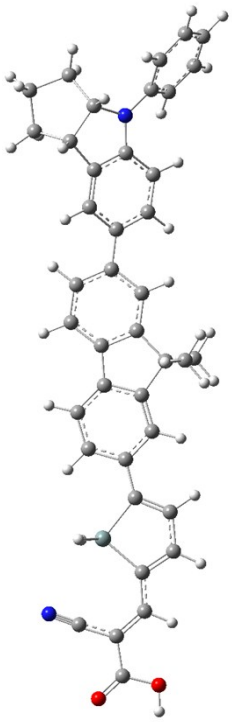

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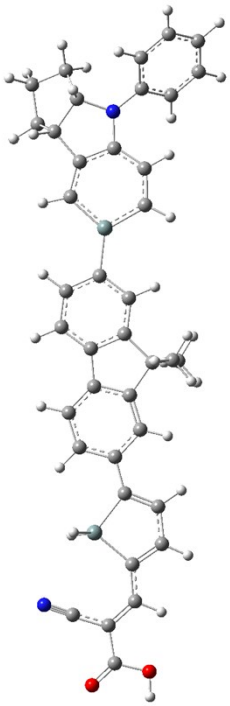

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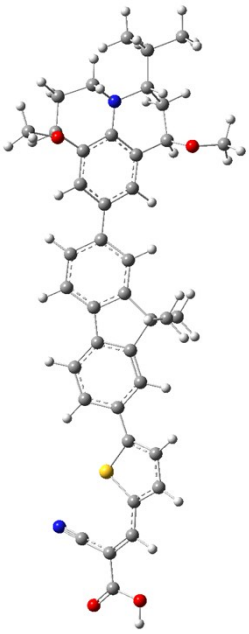

Dye **9**

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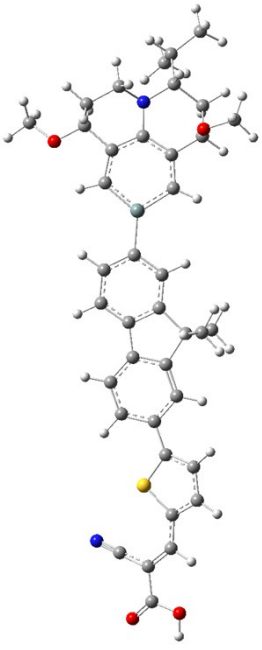

Dye **10**

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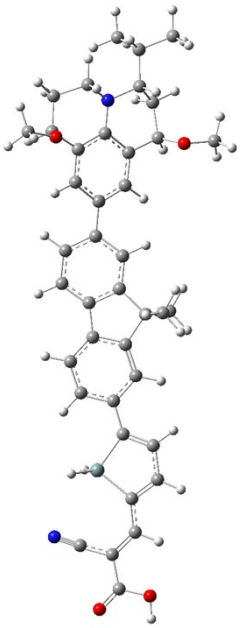
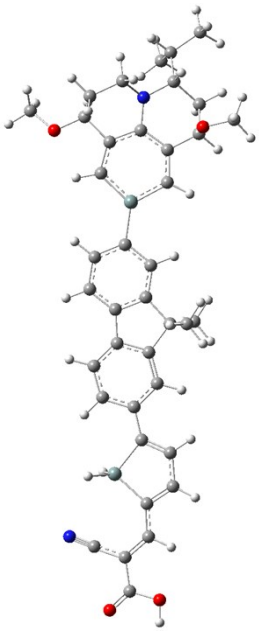


Dye **11**

E= -2249.42742 a.u.



Dye **12**

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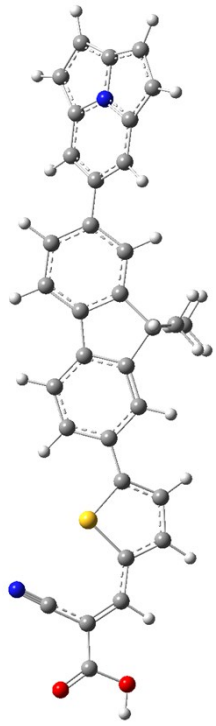

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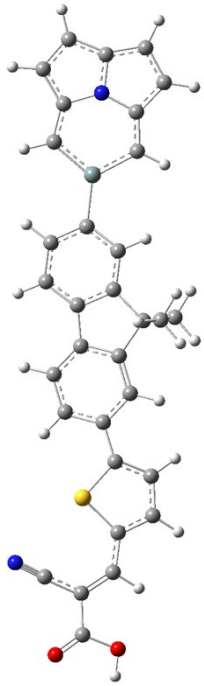

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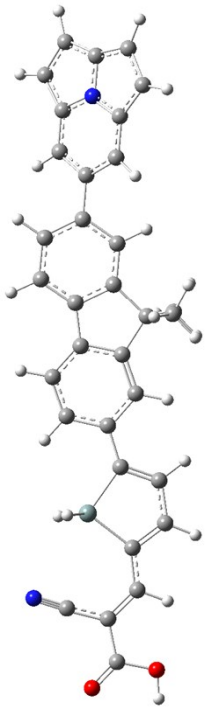
E= -2180.26975 a.u.



Dye **15**

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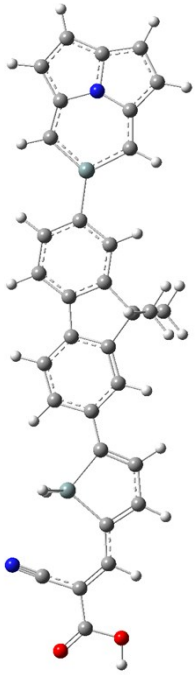

Dye **16**

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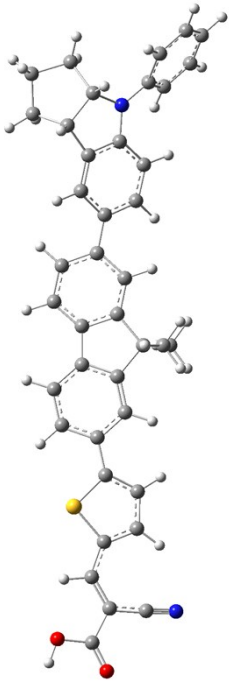
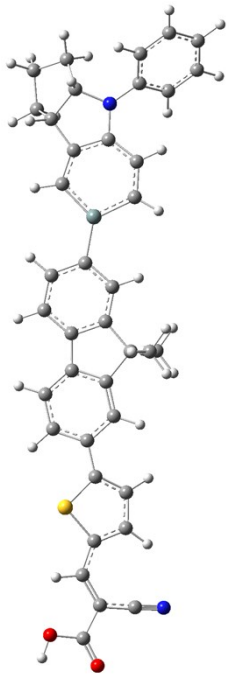
Figure S1: Most stable optimized structures of the dyes **5-16** and their corresponding electronic energies.



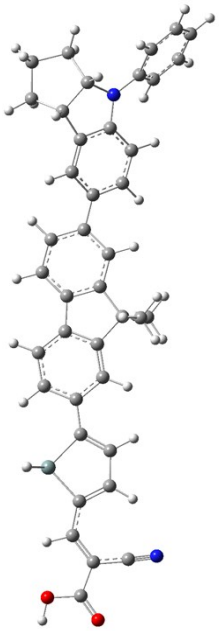
Dye **5**/

E= -2201.69793 a.u.



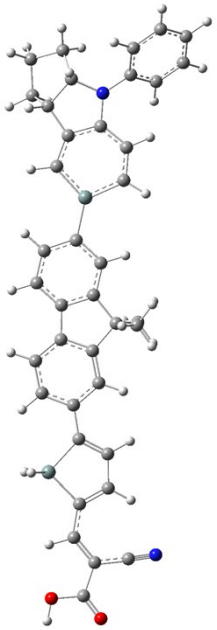
Dye **6**/

E= -2453.04751 a.u.



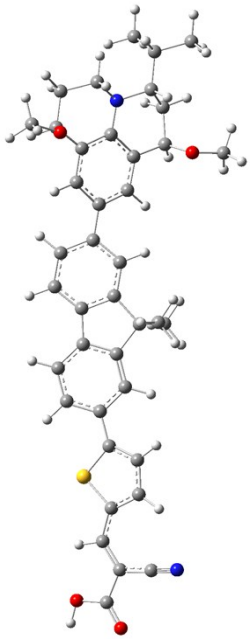
Dye **7**/

E= -2094.18241 a.u.



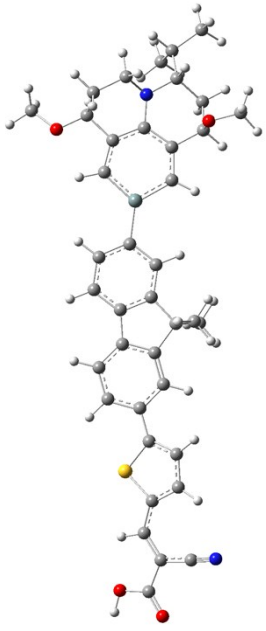
Dye **8**/

E= -2345.53198 a.u.



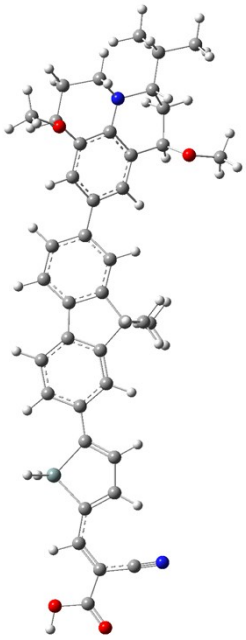
Dye **9**/

E= -2356.93709 a.u.



Dye **10**/

E= -2608.28009 a.u.



Dye **11**/

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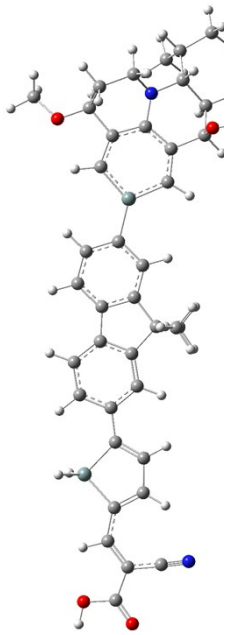
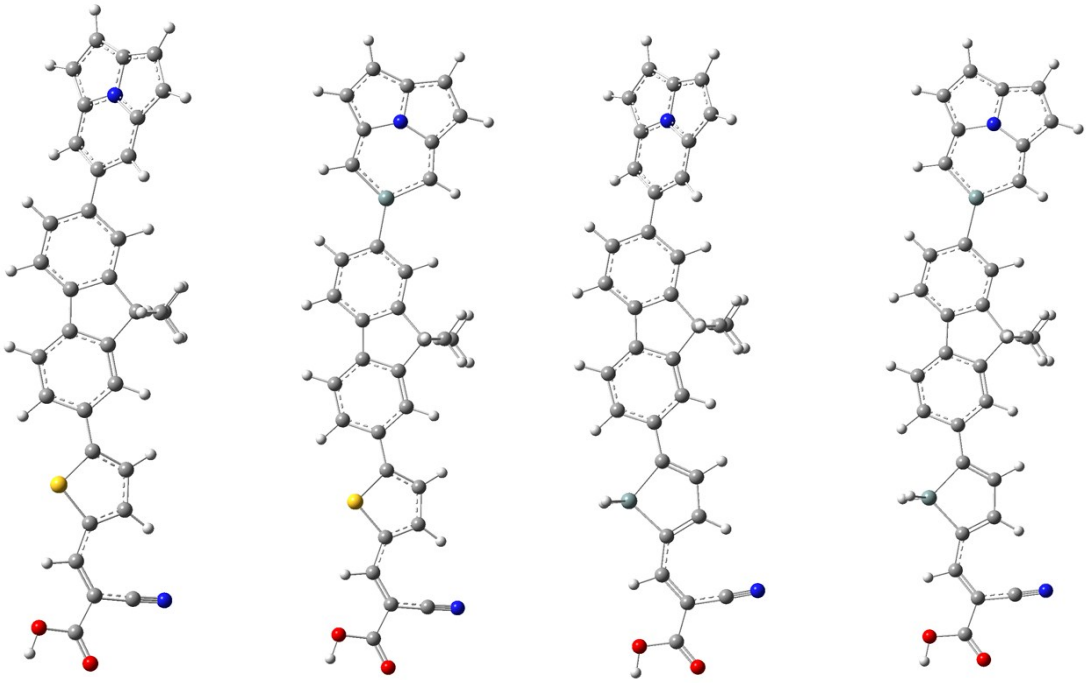


Dye **12**/

E= -2500.76452 a.u



Dye **13**$^{/}$ Dye **14**$^{/}$ Dye **15**$^{/}$ Dye **16**$^{/}$

E= -1928.90377 a.u. **E**= -2180.26937 a.u. **E**= -1821.38815 a.u. **E**= -2072.75375 a.u.

Figure S2: Optimized structures of the least stable dyes **5-16** and their corresponding electronic energies.

Table S1. Calculated maximum absorption wavelength (λ_{max}/nm) of the designed systems at M06-2X/6-31+G* level of theory.

Dyes	λ_{max} (nm)
5	428
6	481
7	488
8	527
9	423
10	455
11	485
12	503
13	413
14	431
15	473
16	481

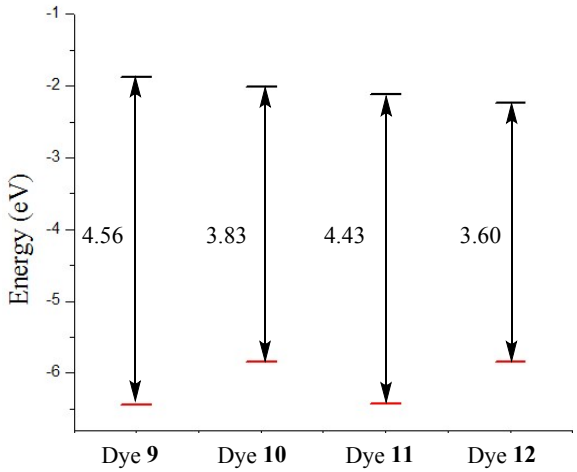


Figure S3: Calculated energy levels of HOMO and LUMO for dyes **9-12**.

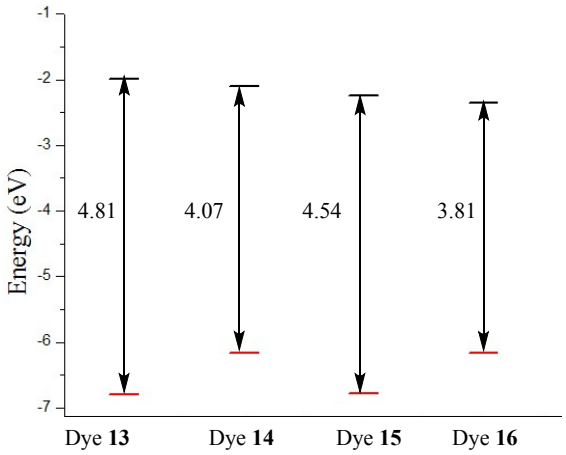
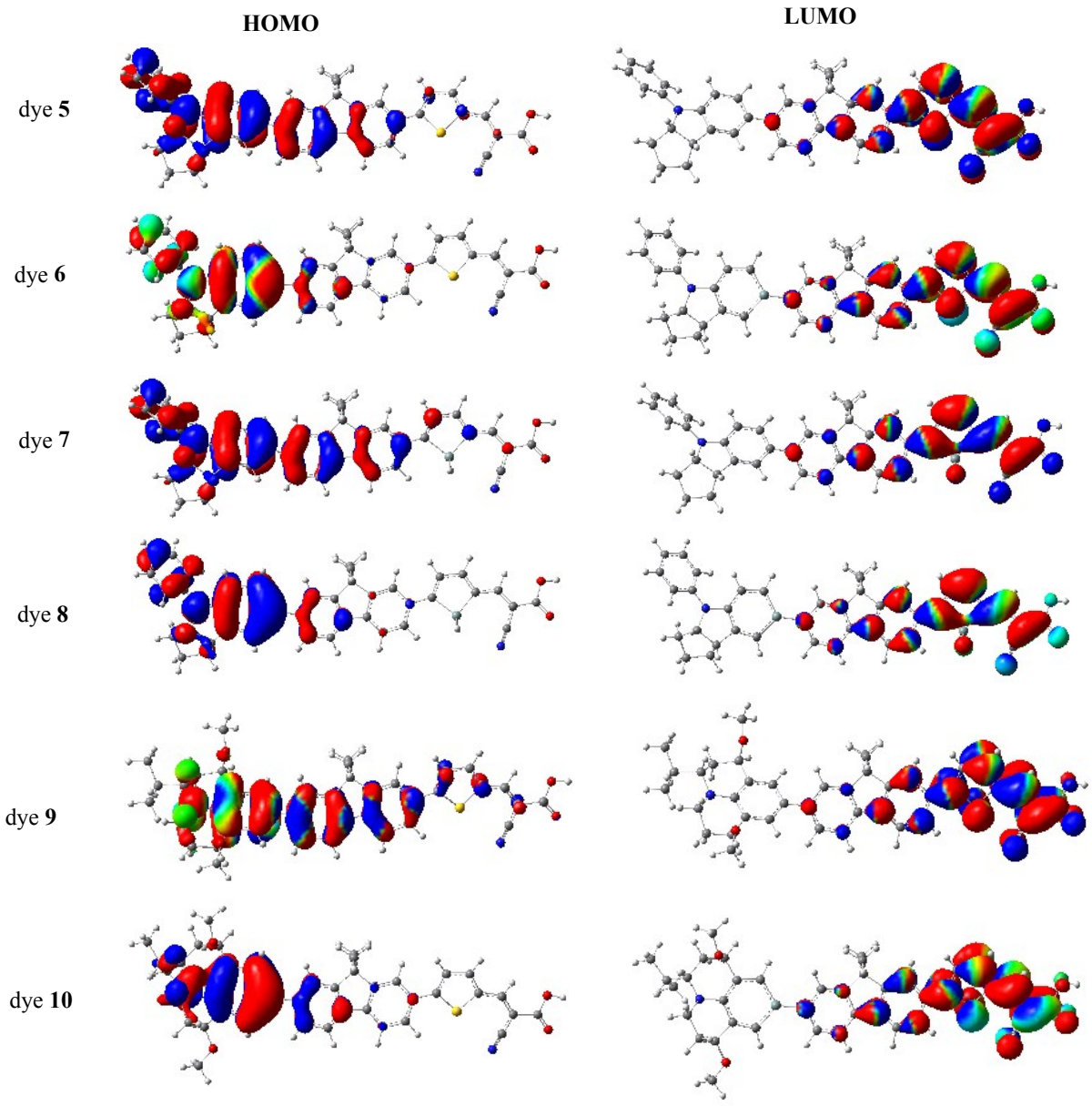


Figure S4: Calculated energy levels of HOMO and LUMO for dyes **13-16**.


HOMO
LUMO
dye 5
dye 6
dye 7
dye 8
dye 9
dye 10

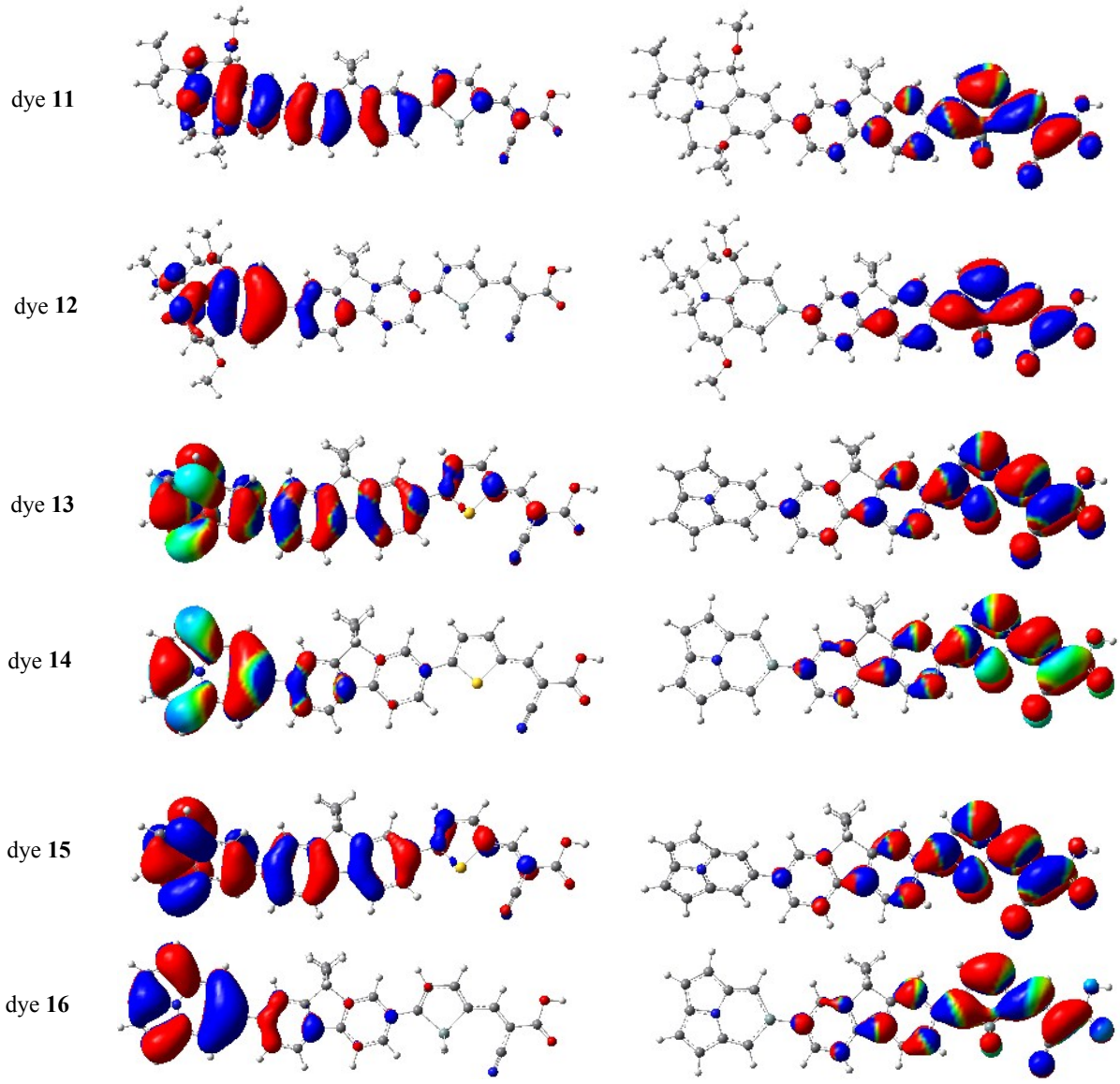
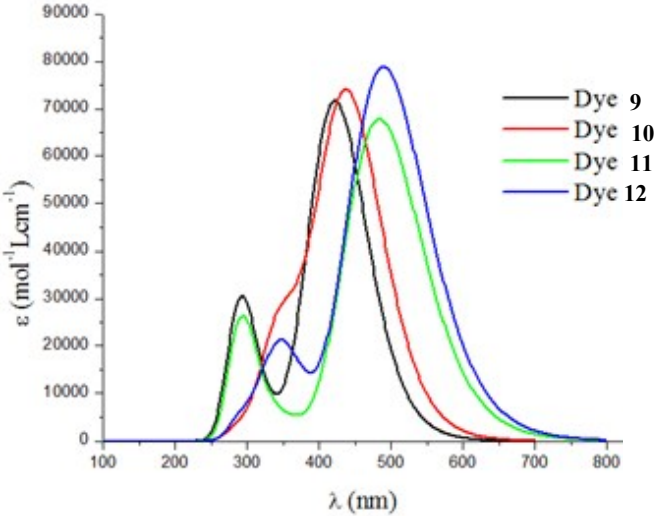


Figure S5. Illustration of frontier molecule orbitals of dyes **5**-**16**.



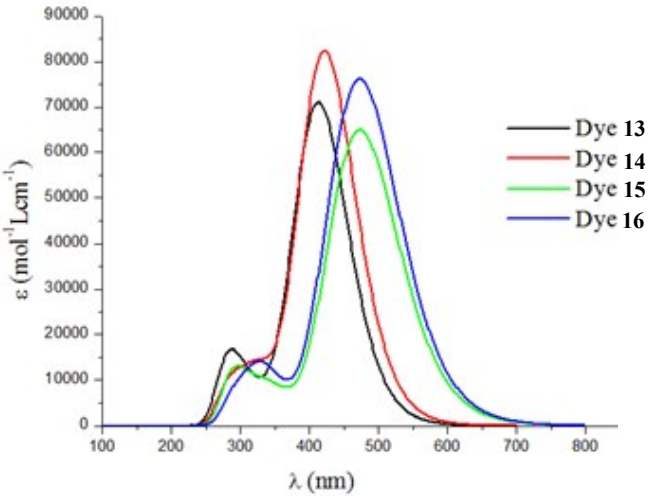
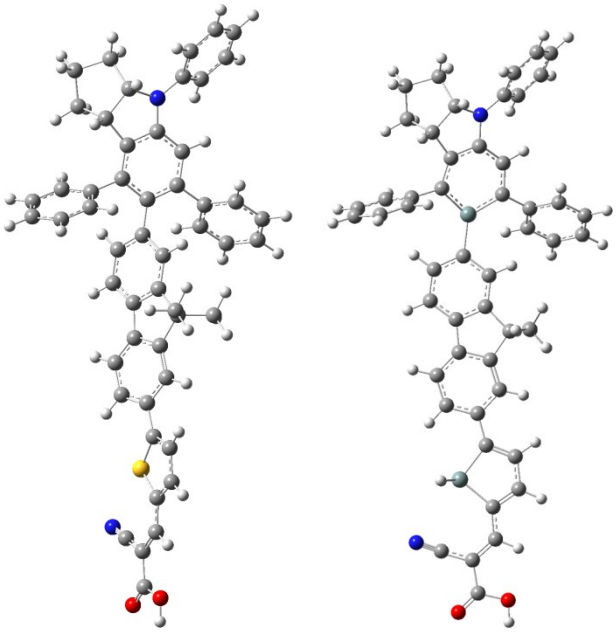


Figure S6: Calculated absorption spectra of dyes **9-16.**



Phenyl containing dye **5** Phenyl containing dye **8**

Figure S7. Phenyl containing dyes **5** and **8**.

Table S2. Comparison the electronic properties results of *t*-Bu containing dyes **5** and **8.**

Dyes	λ_{max} (nm)	LHE	$\Delta G_{injection}$ (eV)	ΔG_{reg} (eV)	μ_{normal} (Debye)
5	418	0.979	-1.74	-0.65	12.11
8	501	0.987	-1.81	-0.09	13.99

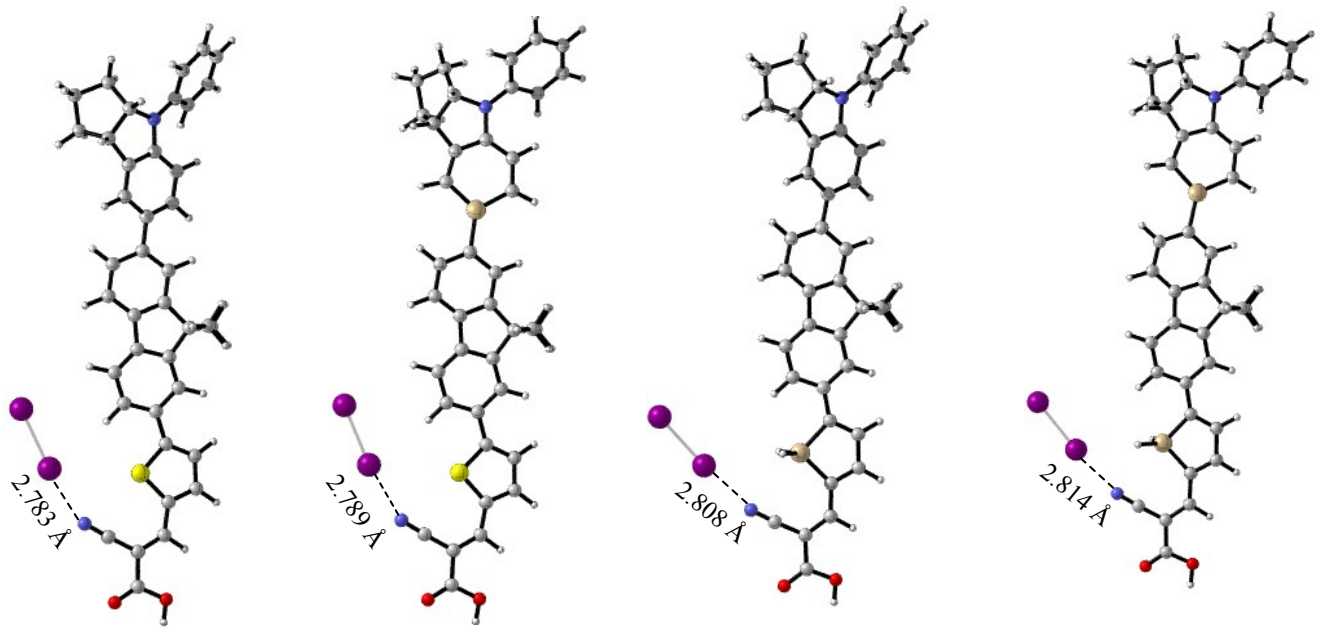
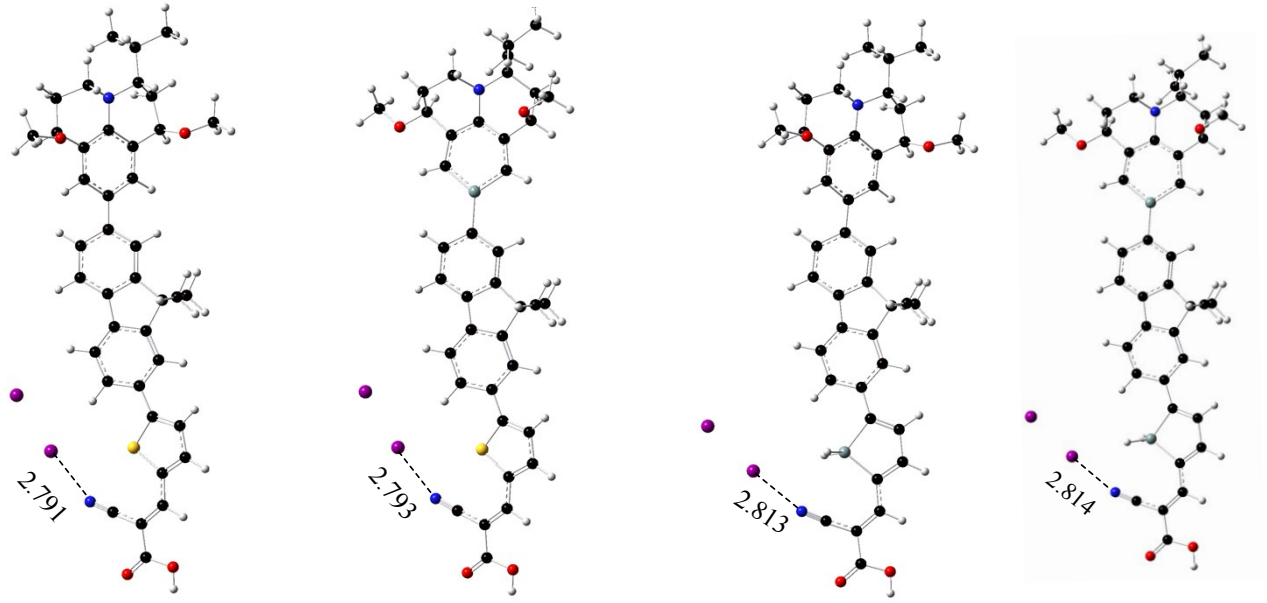
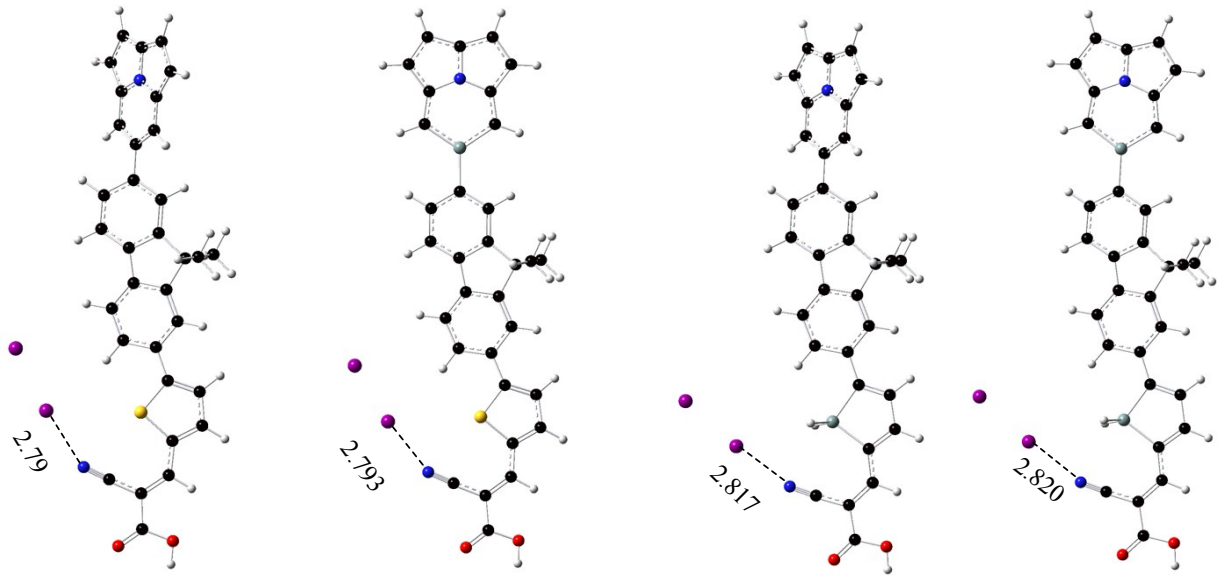


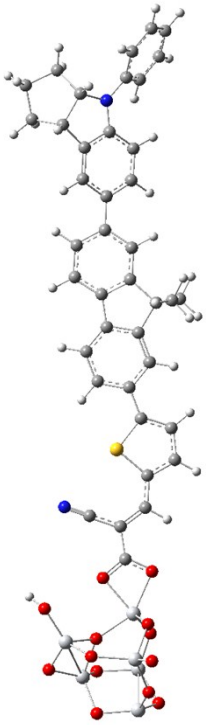
Figure S8. Optimized molecular structure of dye...I_2 complexes at M06-2X/6-31G* (LANL2DZ basis set for I atom) level of theory.



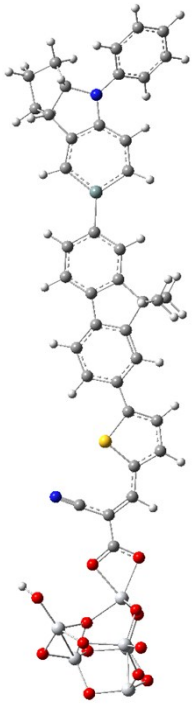


Dye **13** Dye **14** Dye **15** Dye **16**

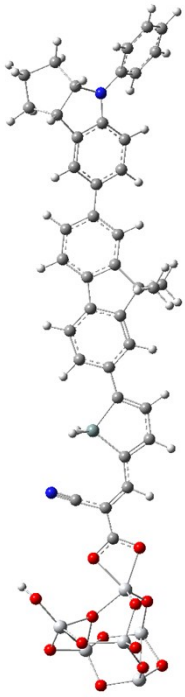
Figure S9: Optimized molecular structure of dye...I_2 complexes at M06-2X/6-31G* (LANL2DZ basis set for I atom) level of theory.



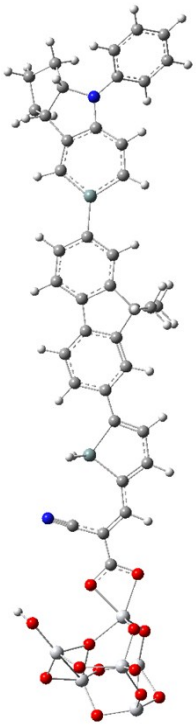
Dye **5**@TiO_2



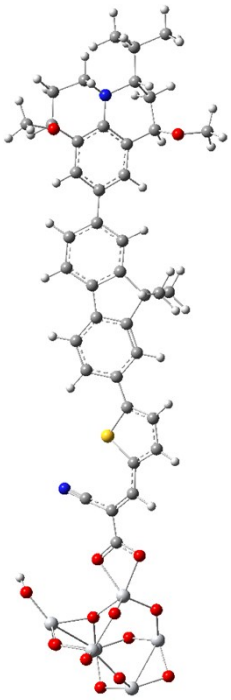
Dye **6**@TiO_2



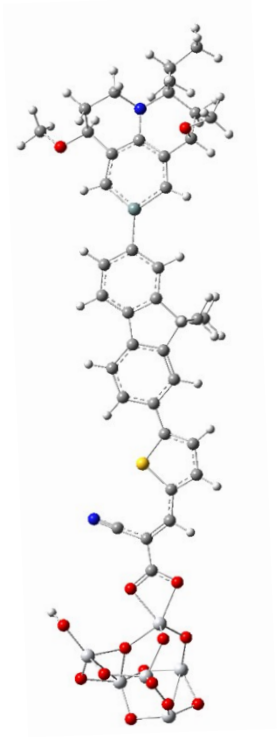
Dye **7**@TiO_2



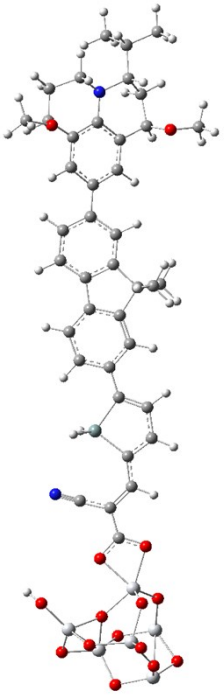
Dye **8**@TiO_2



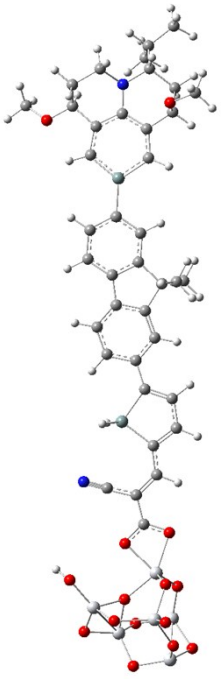
Dye **9**@TiO_2



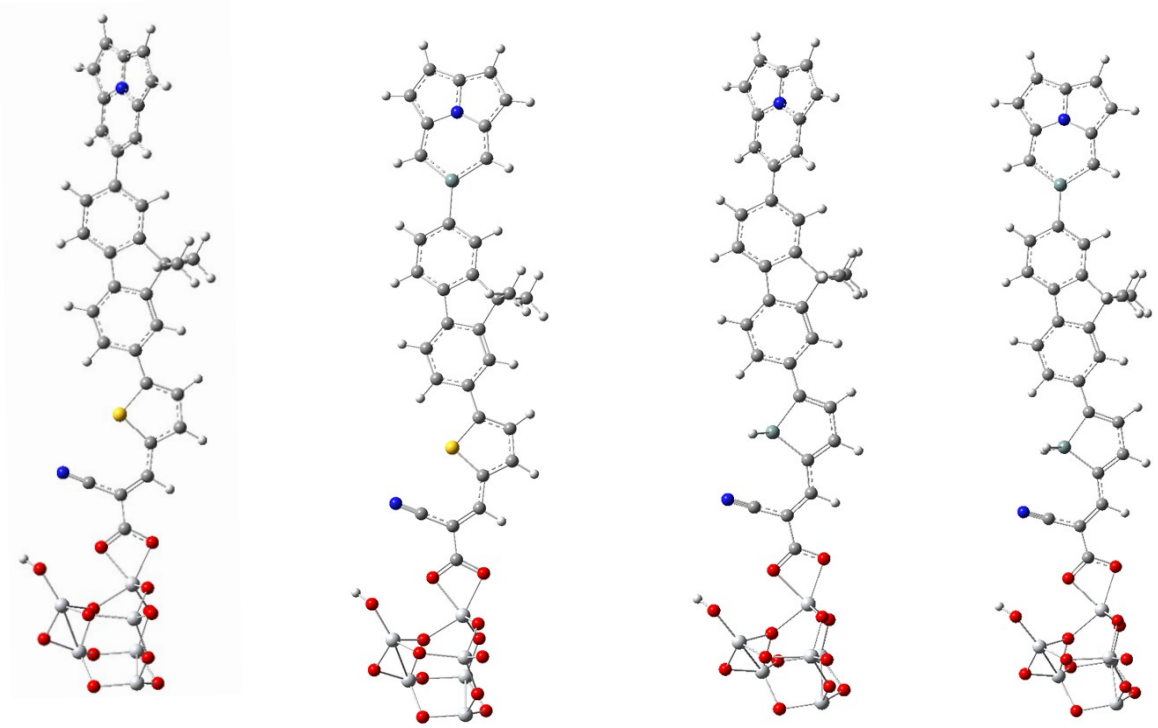
Dye **10**@TiO_2



Dye **11**@TiO_2



Dye **12**@TiO_2



Dye **13**@TiO_2 Dye **14**@TiO_2 Dye **15**@TiO_2 Dye **16**@TiO_2

Figure S10: Optimized structures of the dyes **5-16@**TiO_2.