Supplementary information

Theoretical study of photo-physical properties of indolylmaleimide derivatives

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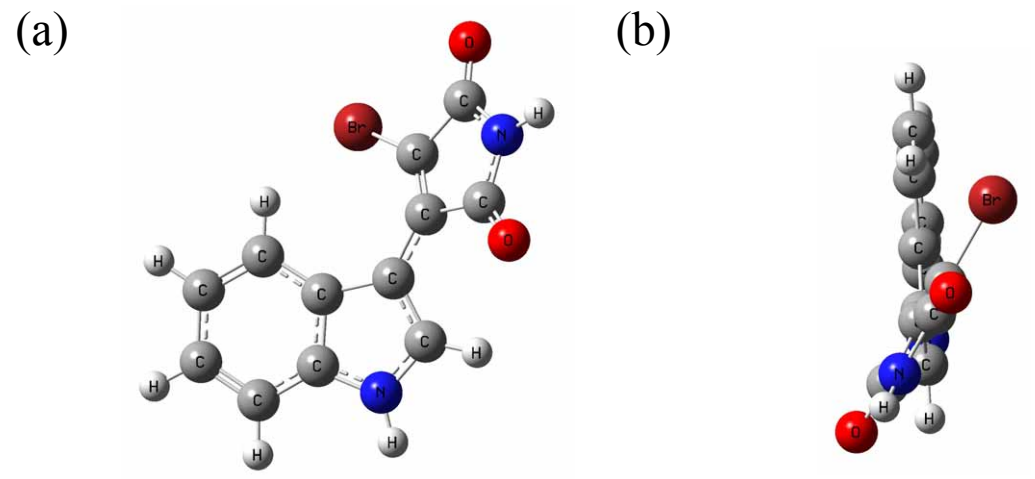


Figure S1. The x-ray measured geometry of the bromo-indolylmaleimides (**IMBr**). (a) Side view (b) Top view

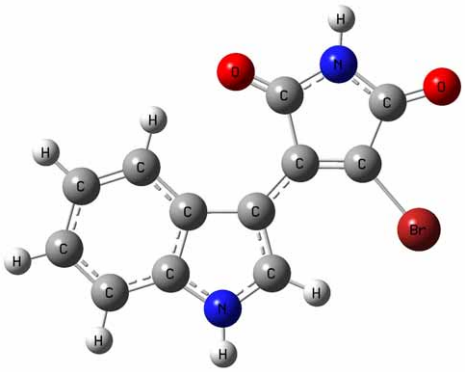
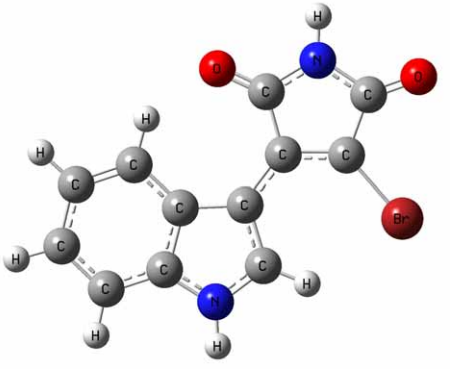
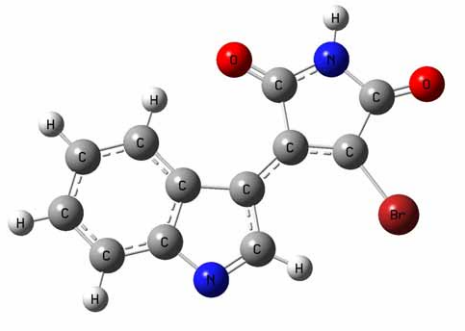
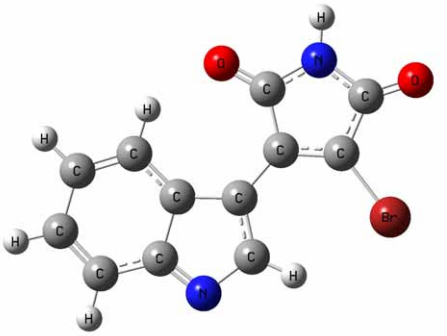
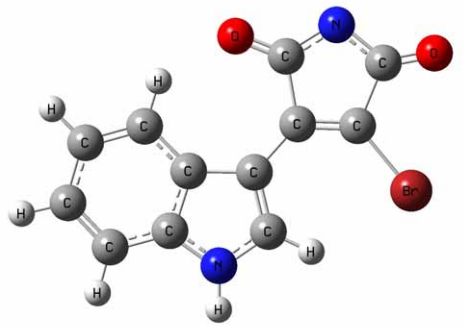
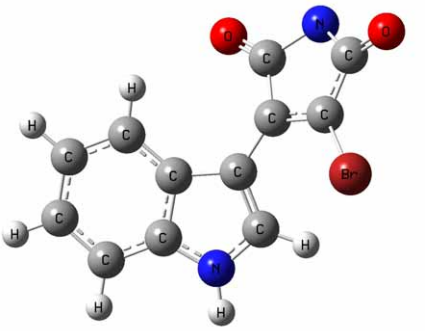
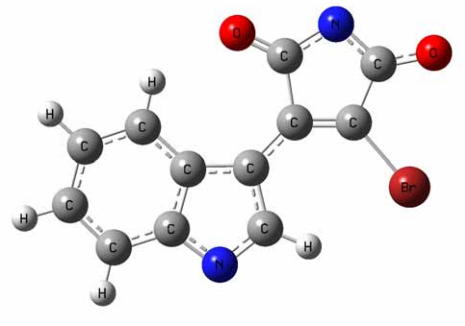
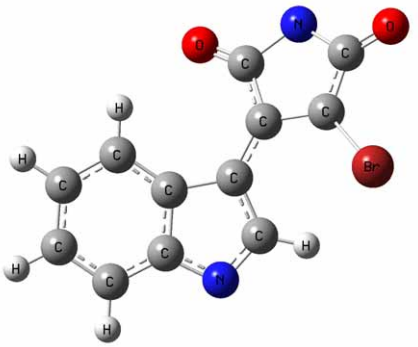
	The optimized S_0 geometry	The optimized S_1 geometry
IM-Br		
$I^{(-)}M$-Br		
$IM^{(-)}$-Br		
$I^{(-)}M^{(-)}$-Br		

Figure S2. The geometry of neutral **IM-Br** and its anions. The left and right sides are the optimized S_0 and S_1 geometries, respectively.

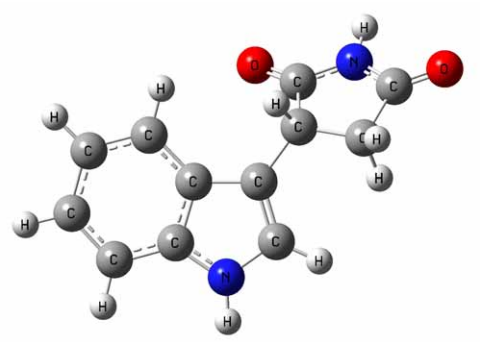
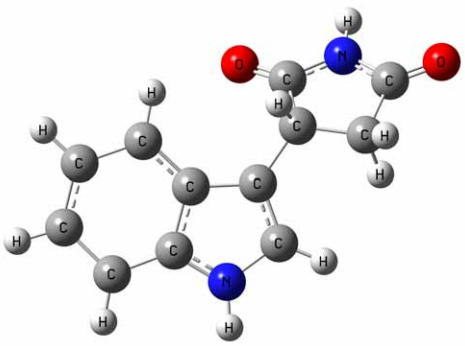
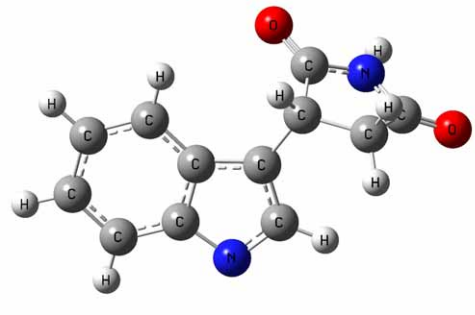
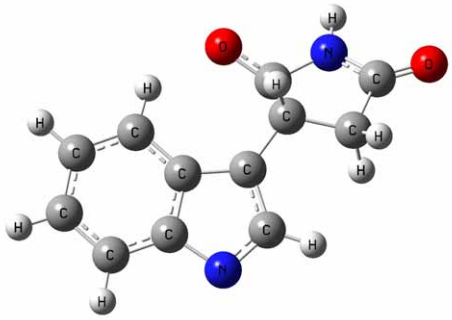
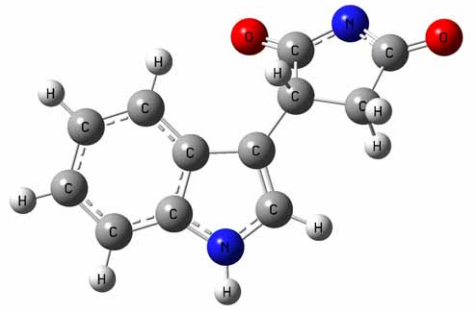
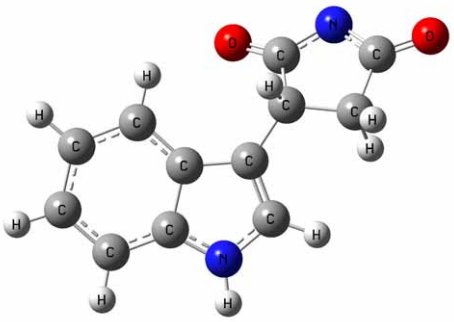
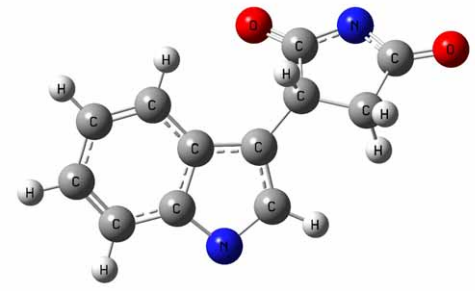
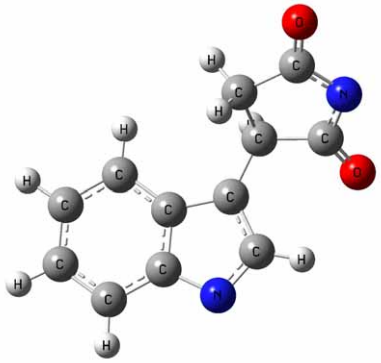
	The optimized S_0 geometry	The optimized S_1 geometry
IS		
$I^{(-)}S$		
$IS^{(-)}$		
$I^{(-)}S^{(-)}$		

Figure S3. The geometry of neutral indole-succinimide (**IS**) and its anions. The left and right sides are the optimized S_0 and S_1 geometries, respectively.

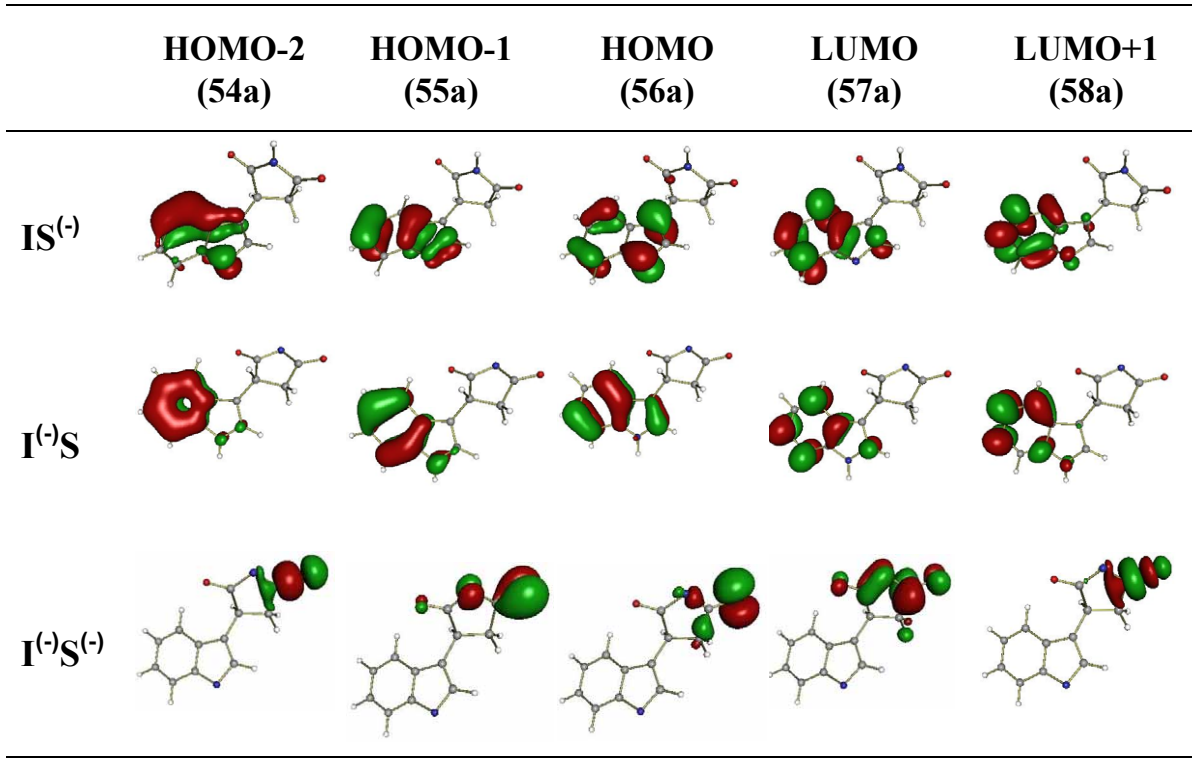


Figure S4. Natural molecular orbitals for anions of **IS**.

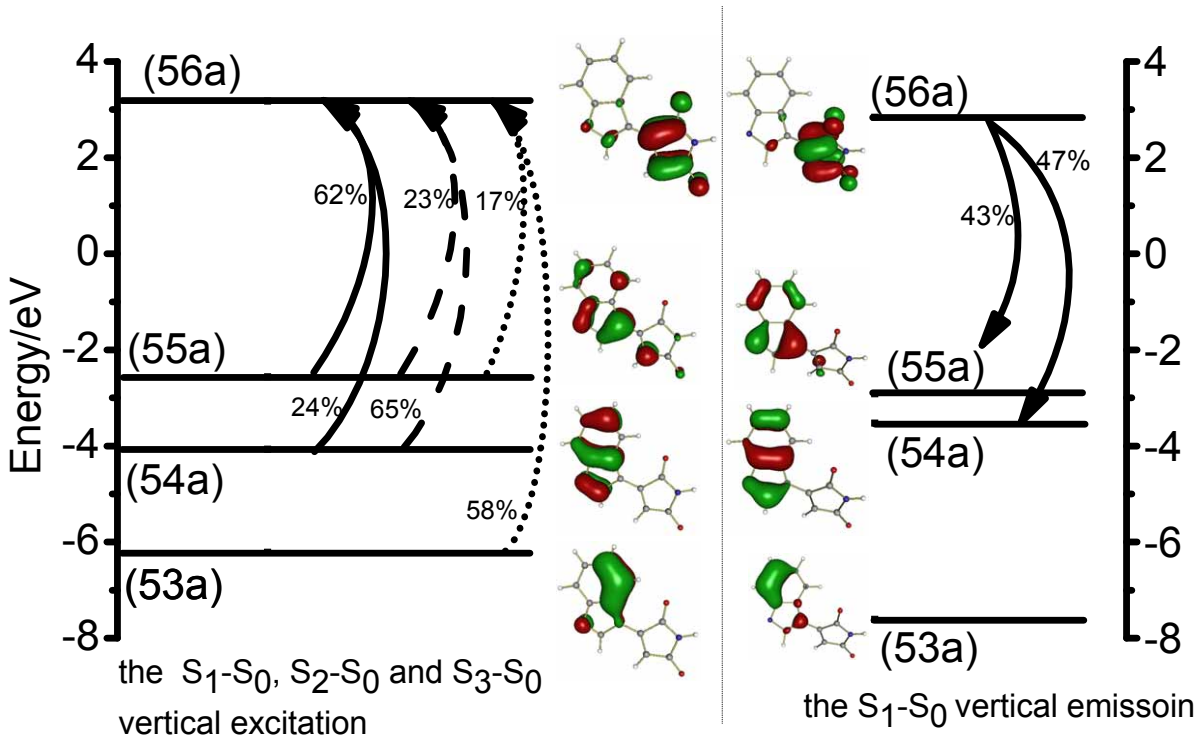


Figure S5. Natural molecular obitals of $\mathbf{I^{(-)}M}$. The left side is for $S_1 \leftarrow S_0$ (solid line) , $S_2 \leftarrow S_0$ (dash line) and $S_3 \leftarrow S_0$ (short dot line) vertical excitations at the optimized S_0 geometry, and the right side is $S_1 \rightarrow S_0$ vertical emission at the optimized S_1 geometry.

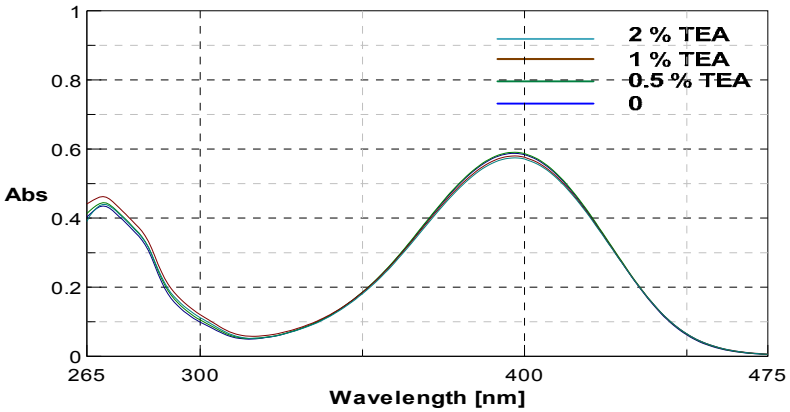


Figure S6. Absorption spectra of **IM** (0.05 mM) in 0, 0.5 1 or 2 % triethylamine (TEA)-CH_3CN solution

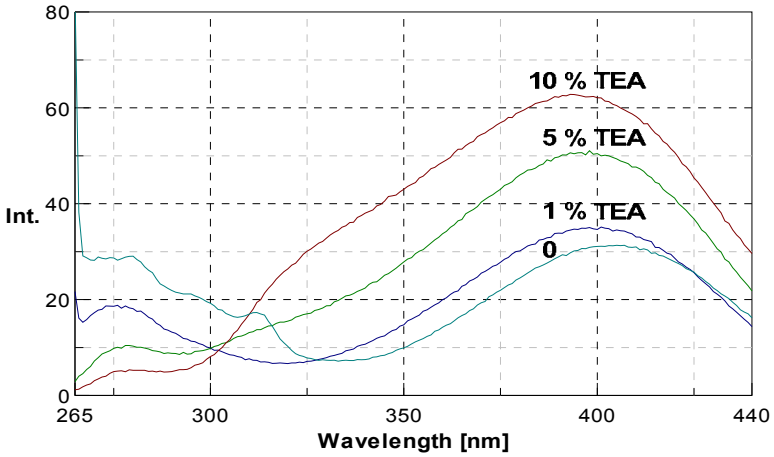


Figure S7. The fluorescence excitation spectra of **IM** (10 µM) in 0, 1, 5 or 10 % triethylamine (TEA)- CH_3CN solution

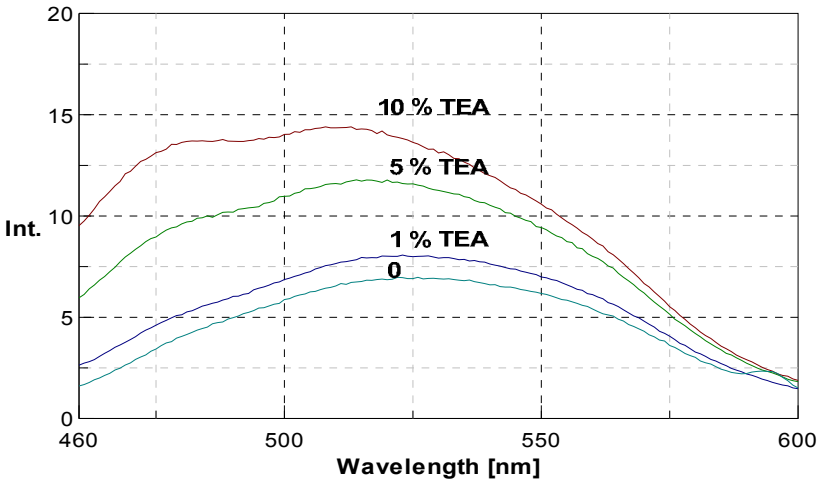


Figure S8. The fluorescence emission spectra of **IM** (10 µM) in 0, 1, 5 or 10 % triethylamine (TEA)-CH_3CN solution.

Table S1. The excitation energy of **$I^{(-)}$M-Br**, **IS** and **$I^{(-)}$M**.

Molecule	Excitation energy (cm^{-1})		
	Theoretical result		Experiment data
	Vdz(Basis set)	Pople(Basis set)	
$I^{(-)}$M-Br	23873, 31207	21958, 29189	24054
IS	37974, 47370	37389, 46317	35780, 45583
$I^{(-)}$M	22935, 29409, 39598	24553, 25129, 35518	25209, 36973

Table S2. The emission energy of **$I^{(-)}$M-Br**, **IS** and **$I^{(-)}$M**.

Molecule	Emission energy(cm^{-1})		
	Theoretical result		Experimental data
	Vdz(Basis set)	Pople(Basis set)	
$I^{(-)}$M-Br	15556	14863	17731
IS	33363	36491	30159
$I^{(-)}$M	18512	16509	19497