Supporting Information

A study on optical properties for various hot drug molecules by 2020

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Molecules	Top view	Side view
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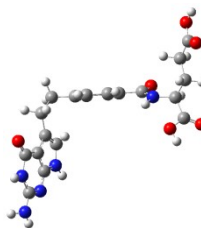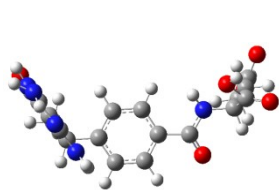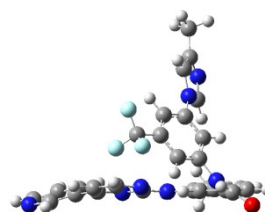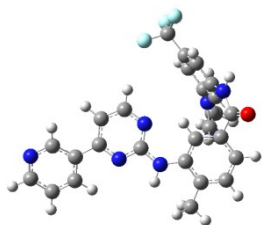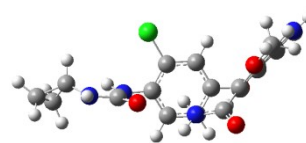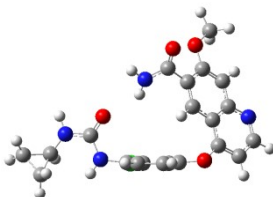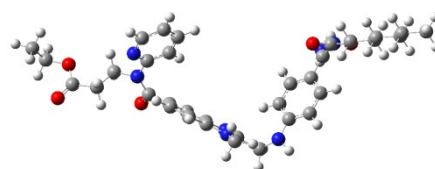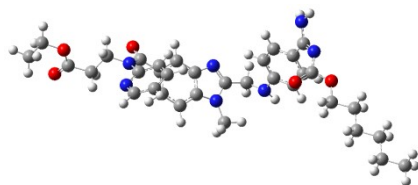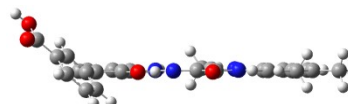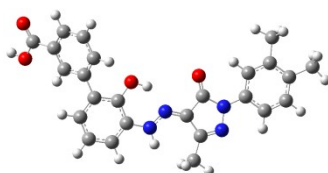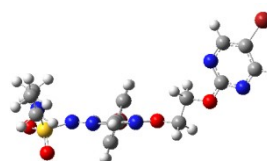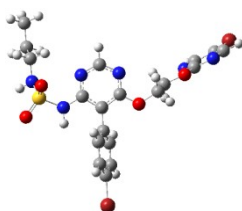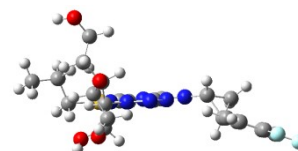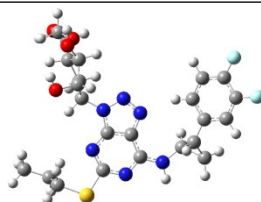
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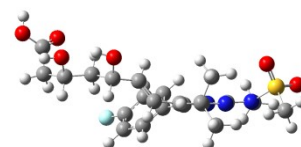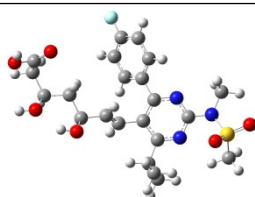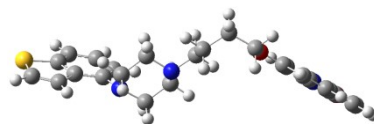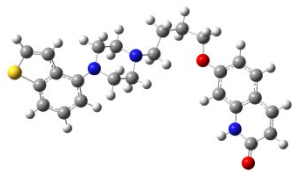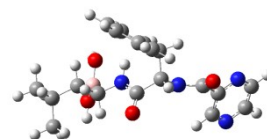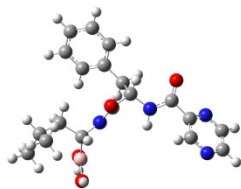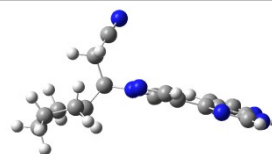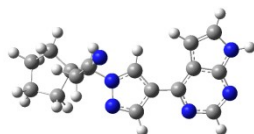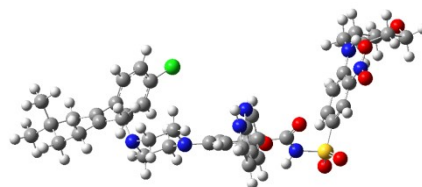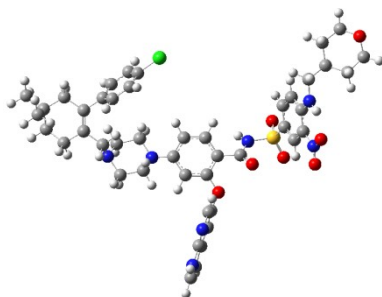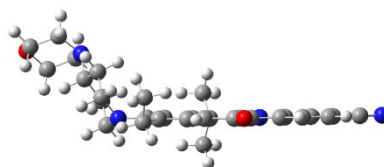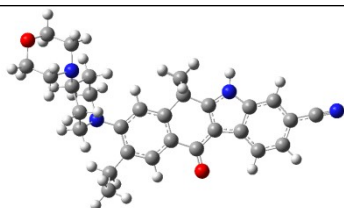
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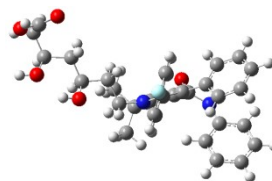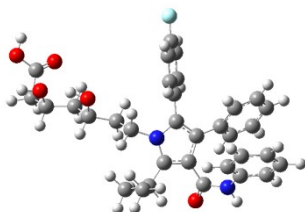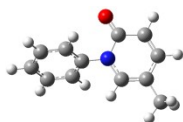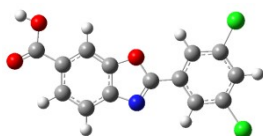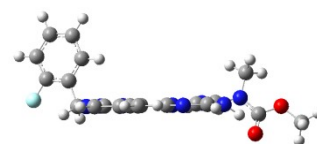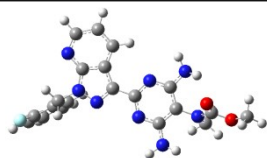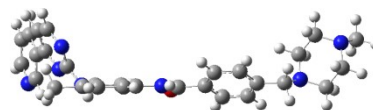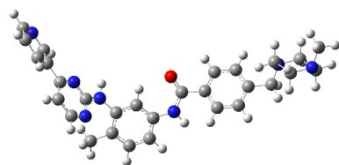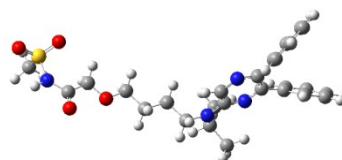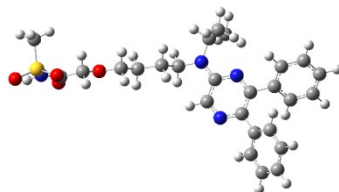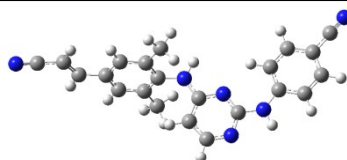
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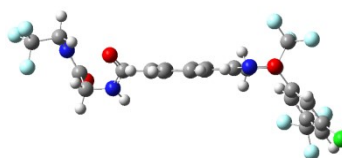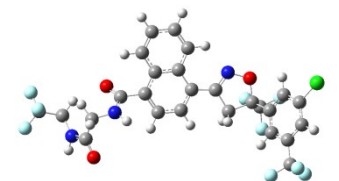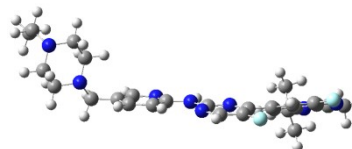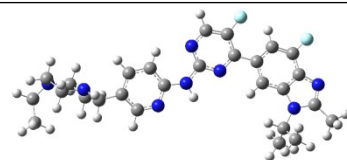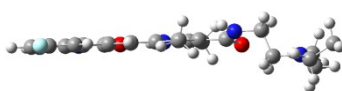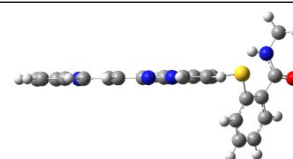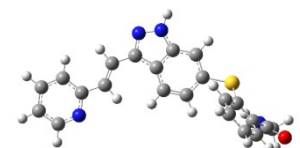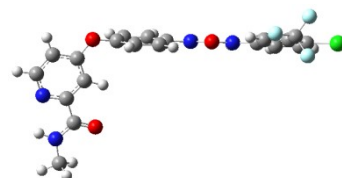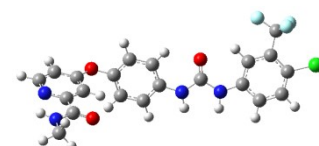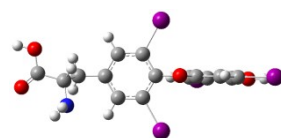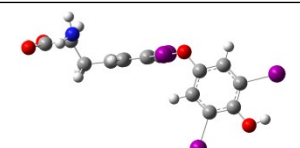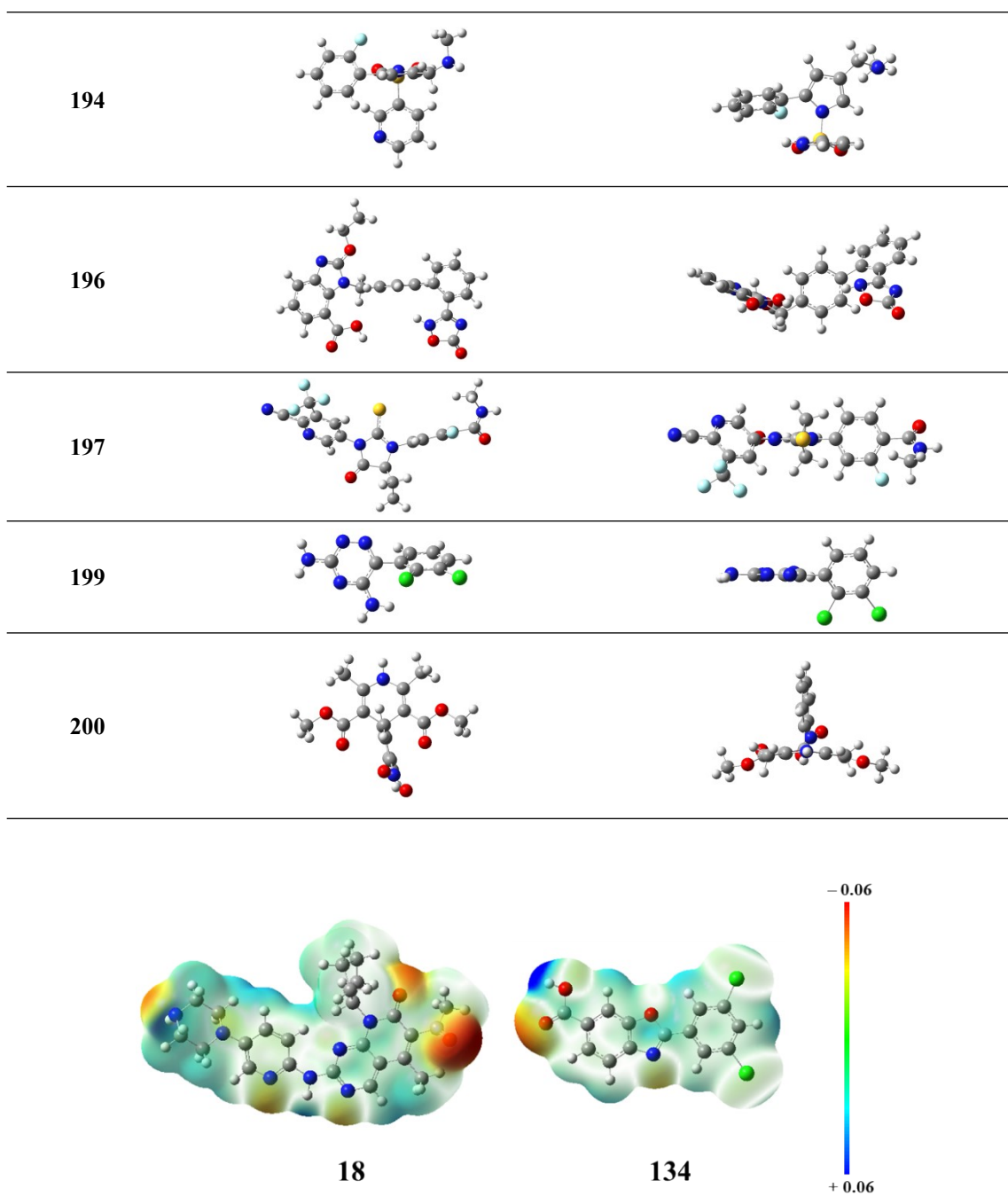
Figure S1. The electrostatic surface potential for **18** and **134** compounds based on the stable ground state geometries.

Table S2. The calculated fluorescent spectra of all the studied 39 molecules.

Molecules	λ^{EMI}/nm	Oscillator Strength	Transition natures
3	471.6[a]	0.3880[a]	$S_1 \rightarrow S_0$ [a]
5	397.3[a]	0.5432[a]	$S_1 \rightarrow S_0$ [a]
18	690.1[a]	0.6147[a]	$S_1 \rightarrow S_0$ [a]
21	469.4[a]	0.0208[a]	$S_1 \rightarrow S_0$ [a]
	497.7[b]	0.0034[b]	$S_1 \rightarrow S_0$ [b]

24	809.4 [a]	0.0257 [a]	$S_1 \rightarrow S_0$ [a]
58	339.2 [a]	0.4459 [a]	$S_1 \rightarrow S_0$ [a]
62	654.6 [a]	0.0077 [a]	$S_1 \rightarrow S_0$ [a]
64	604.6 [a]	0.0793 [a]	$S_1 \rightarrow S_0$ [a]
67	521.5 [a]	0.0031 [a]	$S_1 \rightarrow S_0$ [a]
80	480.9 [a]	0.0249 [a]	$S_1 \rightarrow S_0$ [a]
	355.2 [b]	0.1418 [b]	$S_1 \rightarrow S_0$ [b]
87	511.6 [a]	0.0016 [a]	$S_1 \rightarrow S_0$ [a]
94	388.0 [a]	0.7767 [a]	$S_1 \rightarrow S_0$ [a]
96	769.2 [a]	0.0177 [a]	$S_1 \rightarrow S_0$ [a]
100	347.9 [a]	0.0071 [a]	$S_1 \rightarrow S_0$ [a]
104	542.8 [a]	0.4810 [a]	$S_1 \rightarrow S_0$ [a]
115	573.5 [a]	0.1361 [a]	$S_1 \rightarrow S_0$ [a]
120	483.0 [a]	0.0001 [a]	$S_1 \rightarrow S_0$ [a]
121	433.2 [a]	0.0011 [a]	$S_1 \rightarrow S_0$ [a]
126	388.3 [a]	0.5630 [a]	$S_1 \rightarrow S_0$ [a]
128	569.2 [a]	0.0057 [a]	$S_1 \rightarrow S_0$ [a]
131	456.7 [a]	0.7472 [a]	$S_1 \rightarrow S_0$ [a]
132	497.3 [a]	0.0092 [a]	$S_1 \rightarrow S_0$ [a]
133	386.4 [a]	0.2869 [a]	$S_1 \rightarrow S_0$ [a]
134	408.5 [a]	1.4772 [a]	$S_1 \rightarrow S_0$ [a]
136	428.2 [a]	0.3776 [a]	$S_1 \rightarrow S_0$ [a]
141	677.0 [a]	0.0001 [a]	$S_1 \rightarrow S_0$ [a]
149	567.0 [a]	0.2323 [a]	$S_1 \rightarrow S_0$ [a]
164	435.4 [a]	1.3784 [a]	$S_1 \rightarrow S_0$ [a]
165	454.2 [a]	0.4902 [a]	$S_1 \rightarrow S_0$ [a]
171	585.9 [a]	0.0010 [a]	$S_1 \rightarrow S_0$ [a]
180	543.9 [a]	0.6580 [a]	$S_1 \rightarrow S_0$ [a]
187	449.2 [a]	1.2937 [a]	$S_1 \rightarrow S_0$ [a]
191	512.5 [a]	0.0042 [a]	$S_1 \rightarrow S_0$ [a]
193	673.5 [a]	0.0001 [a]	$S_1 \rightarrow S_0$ [a]
194	497.7 [a]	0.0021 [a]	$S_1 \rightarrow S_0$ [a]
196	484.3 [a]	0.0012 [a]	$S_1 \rightarrow S_0$ [a]
197	514.6 [a]	0.0269 [a]	$S_1 \rightarrow S_0$ [a]
	496.7 [b]	0.0041 [b]	$S_1 \rightarrow S_0$ [b]
199	466.4 [a]	0.0162 [a]	$S_1 \rightarrow S_0$ [a]
	487.4 [b]	0.0142 [b]	$S_1 \rightarrow S_0$ [b]
200	456.5 [a]	0.0506 [a]	$S_1 \rightarrow S_0$ [a]

a: the results were from the level of TD-DFT//B3LYP/6-31+G(d)/SMD(H_2O). b: the results were from the level of TD-DFT//M06-2X/6-31+G(d)/SMD(H_2O).

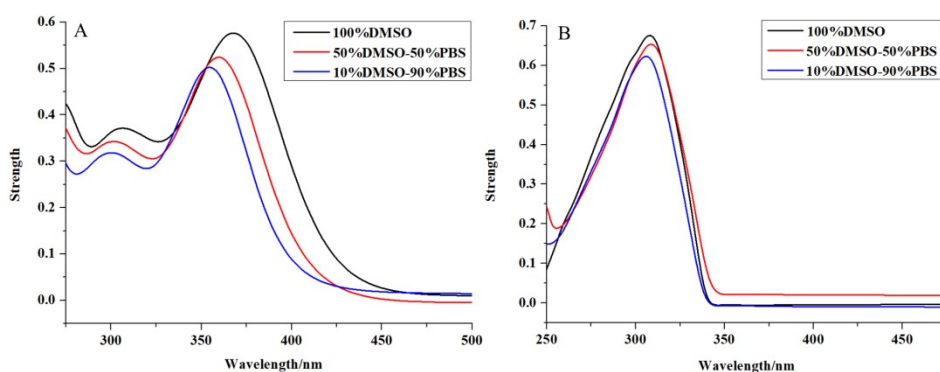Figure S2. The UV-vis spectra of (A) molecule **18** and (B) **134** with the concentration of 100 μM in different solvent (100%DMSO, 50%DMSO and 10%DMSO).

Table S3. Calculated ground state transient dipole moment (μ_{00}) of **18** and **134** compounds with DMSO and H_2O solvent model.

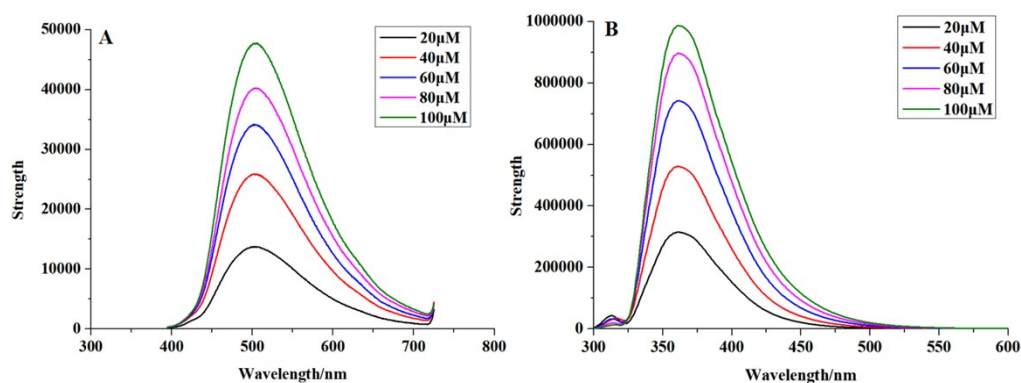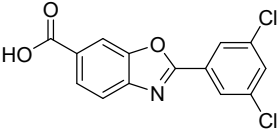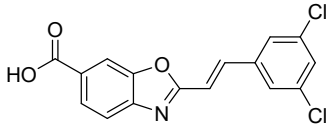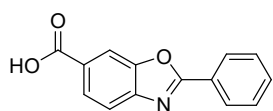| Molecules	μ_{00}/Debye	
	DMSO	H_2O
18	5.7895	7.0117
134	2.2178	2.6613

Figure S3. The emission spectra of compound **18** (A) and **134** (B) with different concentration in 10%DMSO-90%PBS solvent.

Table S4. The calculated energies of HOMO, LUMO and HOMO-LUMO gap for molecules **134**, **134-E** and **134-RETCl**.

Molecules	HOMO/eV	LUMO/eV	HOMO-LUMO gap /eV
134	-6.97	-2.65	4.32
134-E	-6.64	-2.90	3.74

134-RETCl	-6.63	-2.29	4.34
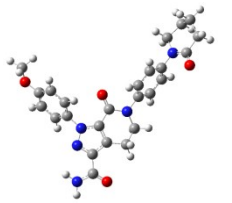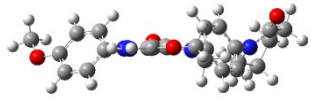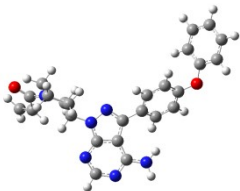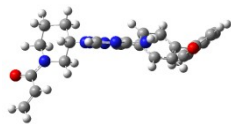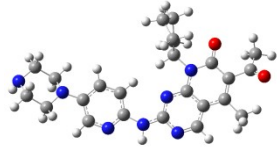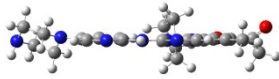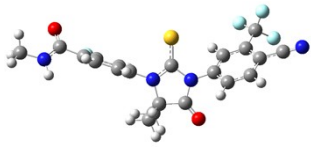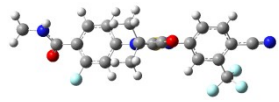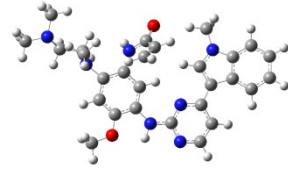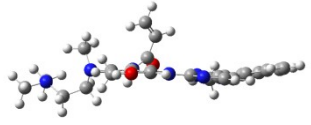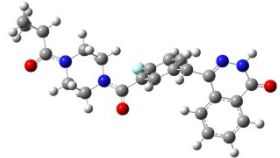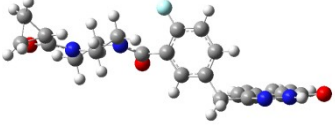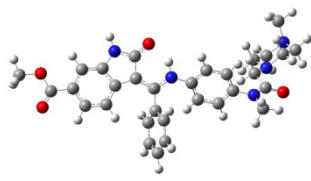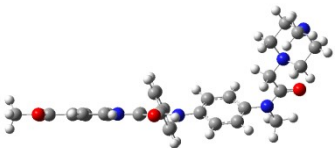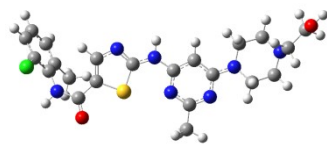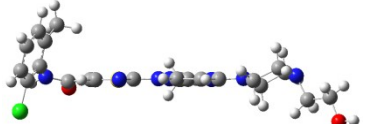
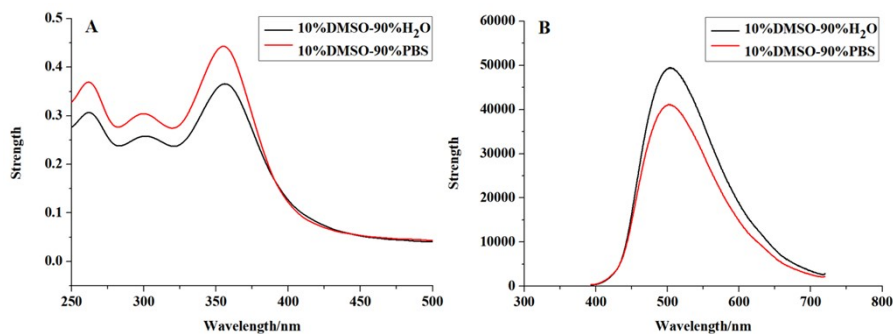Figure S4. The UV-vis (A) and emission spectra (by excited at 370 nm, B) of compound **18** using 10%DMSO-90%H$_2$O and 10%DMSO-90%PBS solvent from experiments.
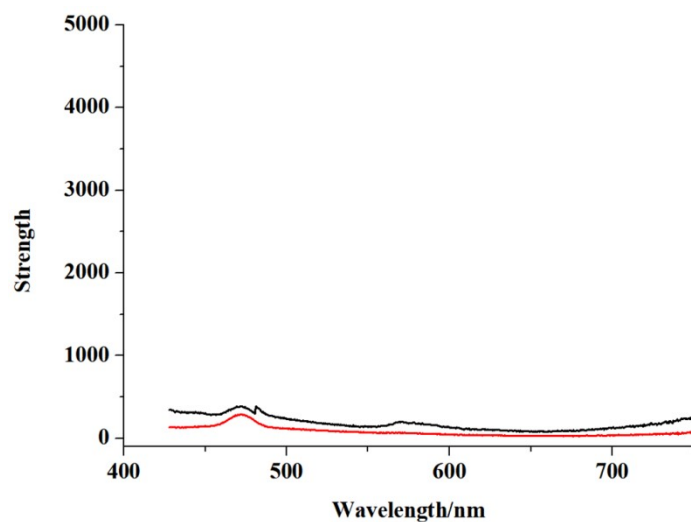

Figure S5. The emission spectra of compound **134** by excitation at 405 nm (black) and 488 nm (red) wavelength in 10%DMSO-90%PBS solvent.
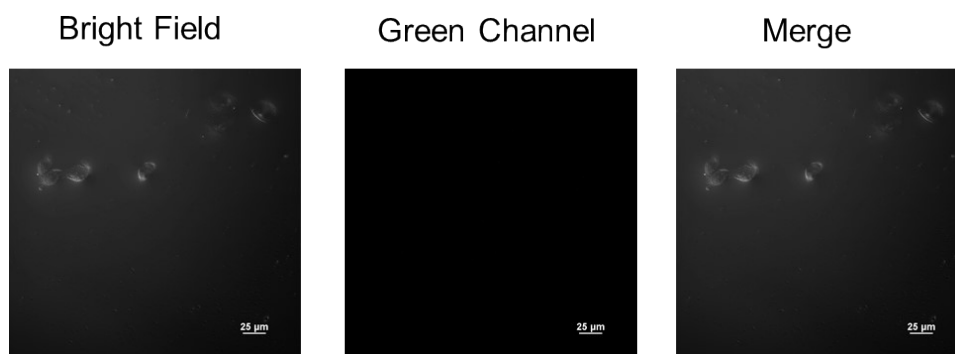

Figure S6. Confocal microscopy colocalization images of compound **134** with 10 μM in HeLa cells.

Table S5. Calculated TPA properties including the maximum TPA cross-section (δ^{TPA}_{max}), corresponding TPA wavelength (λ^{TPA}_{max}), and transition nature of **18** and **134** in gas (a) and water (b) by B3LYP functional.

Molecules	λ^{TPA}_{max}/nm	δ^{TPA}_{max}/GM	Transition nature
18	815.7[a]	319[a]	$S_0 \rightarrow S_1$[a]
	879.4[b]	989[b]	$S_0 \rightarrow S_1$[b]
134	618.4[a]	3[a]	$S_0 \rightarrow S_1$[a]
	661.2[b]	4[b]	$S_0 \rightarrow S_1$[b]