

## Supplementary information materials for

### A pH stable fluoran-triphenylamine photosensitizer with efficient type I and type II ROS generation

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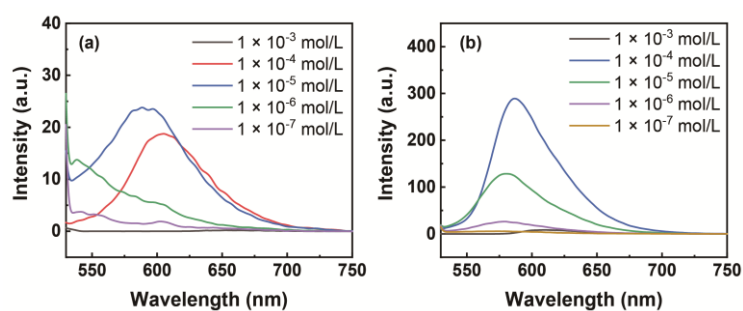
1. Photophysical properties of **FI-TPA** in different solvents

**Table S1** Photophysical properties of **FI-TPA** in different solvents

Solvents	$\lambda_{\max}$ (nm)	$\lambda_{\text{em}}$ (nm)	Stokes shift ( $\text{cm}^{-1}$ )	$\epsilon^a$ ( $\text{M}^{-1}\text{cm}^{-1}$ )
$\text{CHCl}_3$	502	575	2529	$2.46 \times 10^4$
DMF	505	592	2910	$2.70 \times 10^4$
THF	505	590	2853	$2.30 \times 10^4$
Toluene	505	600	3135	$2.30 \times 10^4$
$\text{H}_2\text{O}$	507	586	2659	$2.12 \times 10^4$

<sup>a</sup> The molar extinction coefficient was determined at the maximum absorption wavelength ( $\lambda_{\max}$ ) in DMF solution.

2. The fluorescence emission spectra of **FI-TPA** and **FI-H** at different concentrations.



**Fig. S1** The fluorescence emission spectra of (a) **FI-TPA** and (b) **FI-H** measured at different concentrations in DMF solution.

3.  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS

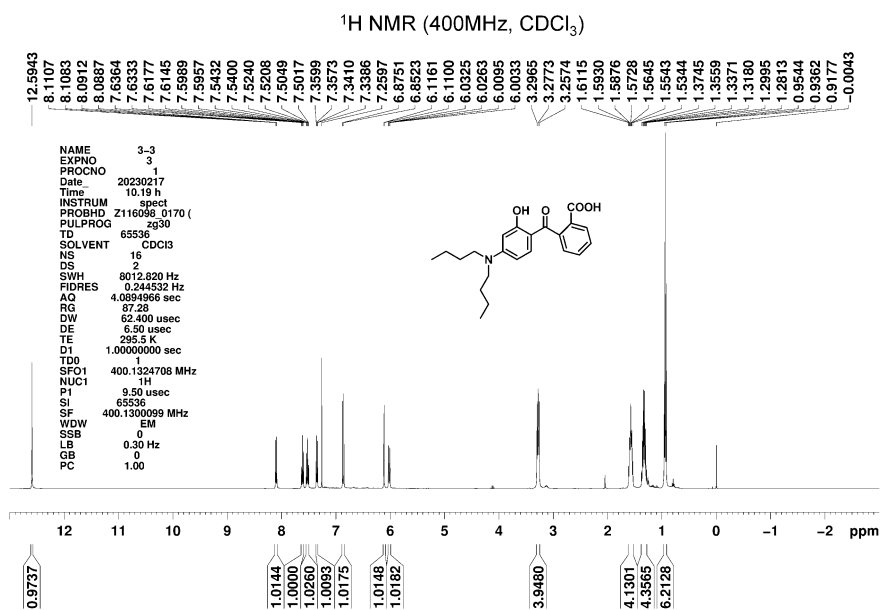


Fig. S2  $^1\text{H}$  NMR (400 MHz) spectrum of **3** ( $\text{CDCl}_3$ ).

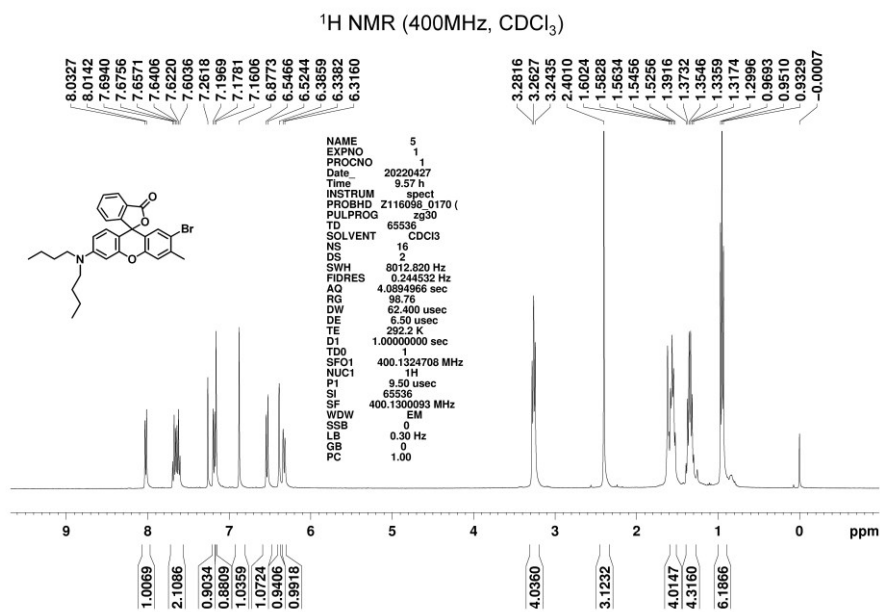


Fig. S3  $^1\text{H}$  NMR (400 MHz) spectrum of **5** ( $\text{CDCl}_3$ ).

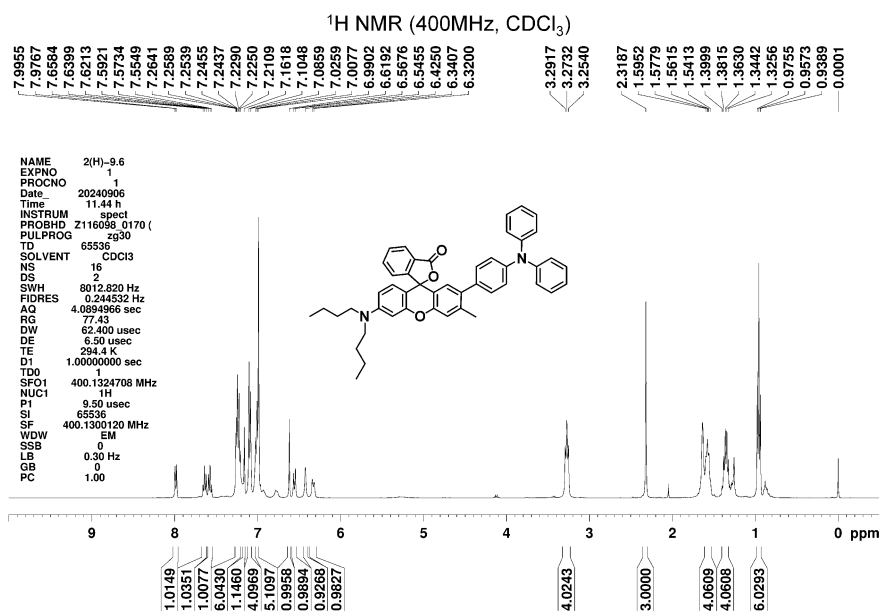


Fig. S4 <sup>1</sup>H NMR (400 MHz) spectrum of 7 (CDCl<sub>3</sub>).

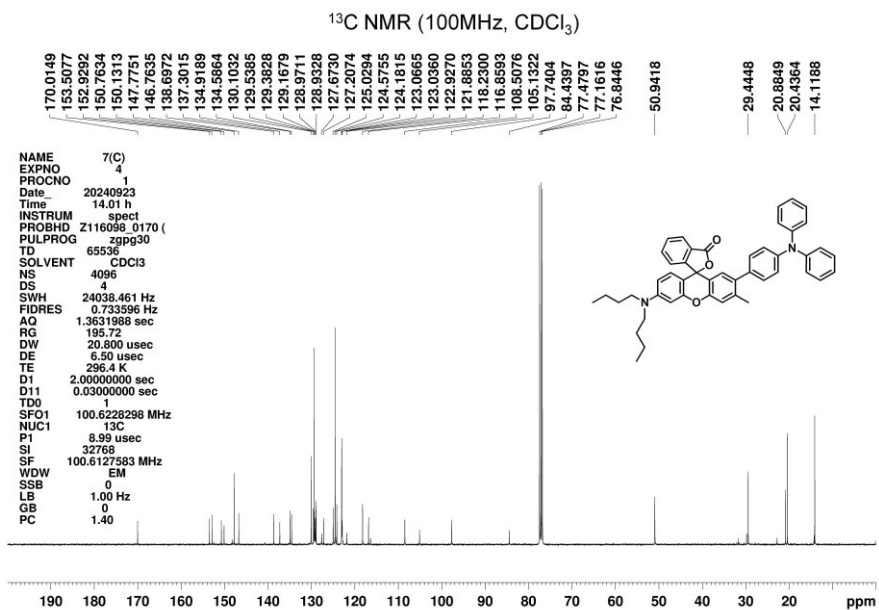
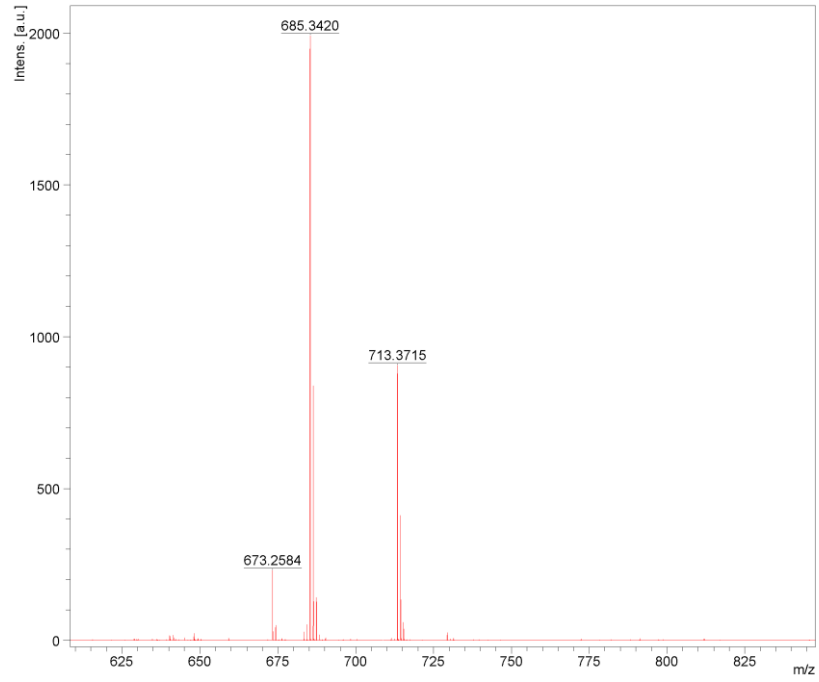


Fig. S5 <sup>13</sup>C NMR (100 MHz) spectrum of 7 (CDCl<sub>3</sub>).

Comment 1  
Comment 2



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**Instrument Info**

User BDAL@CN  
Instrument FLEX-PC  
Instrument type ultraflexTOF/TOF

Fig. S6 HRMS spectrum of 7.

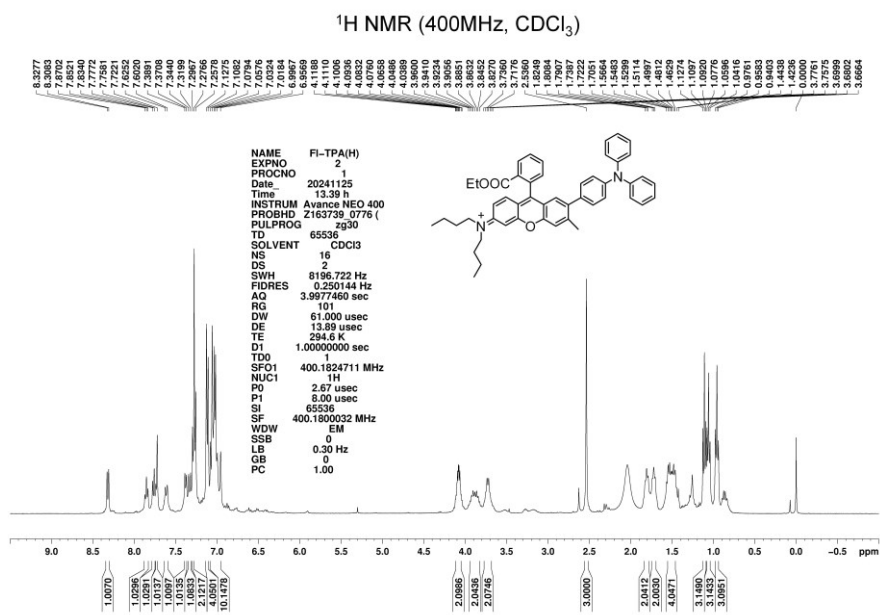


Fig. S7 <sup>1</sup>H NMR (400 MHz) spectrum of FI-TPA (CDCl<sub>3</sub>).

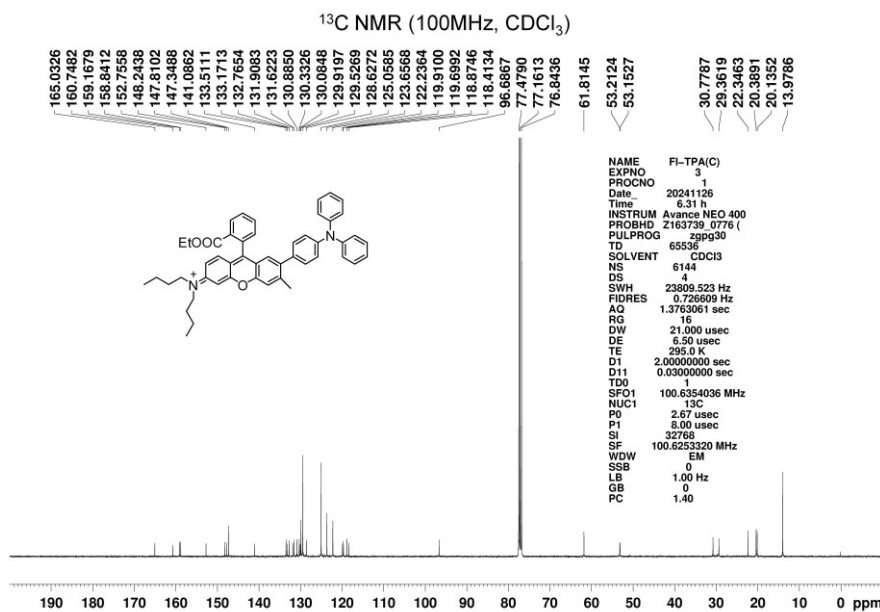
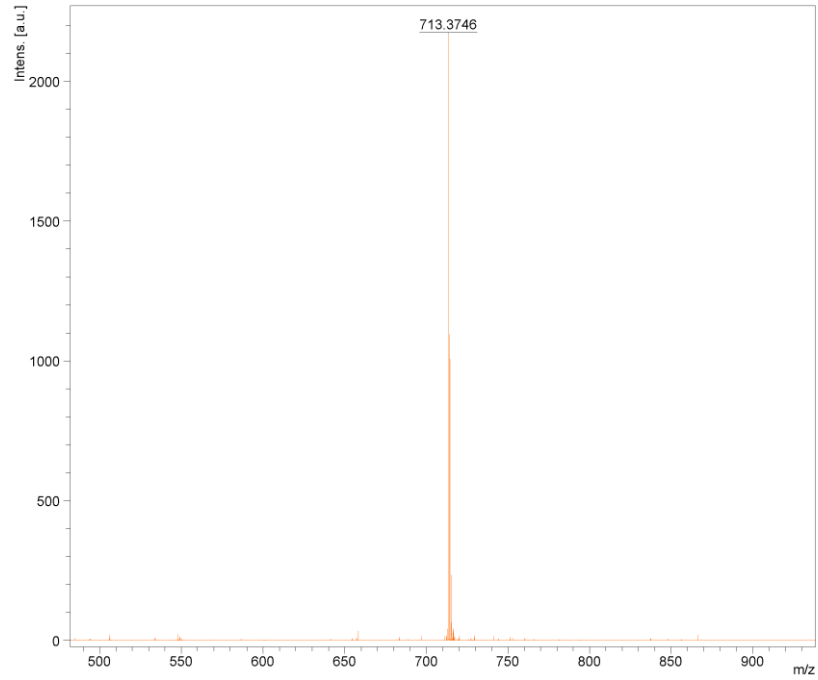


Fig. S8 <sup>13</sup>C NMR (100 MHz) spectrum of FI-TPA (CDCl<sub>3</sub>).

Comment 1  
Comment 2



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Number of shots 500  
Name of spectrum used for calibration  
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**Instrument Info**

User BDAL@CN  
Instrument FLEX-PC  
Instrument type ultraflexTOF/TOF

**Fig. S9** HRMS spectrum of FI-TPA.

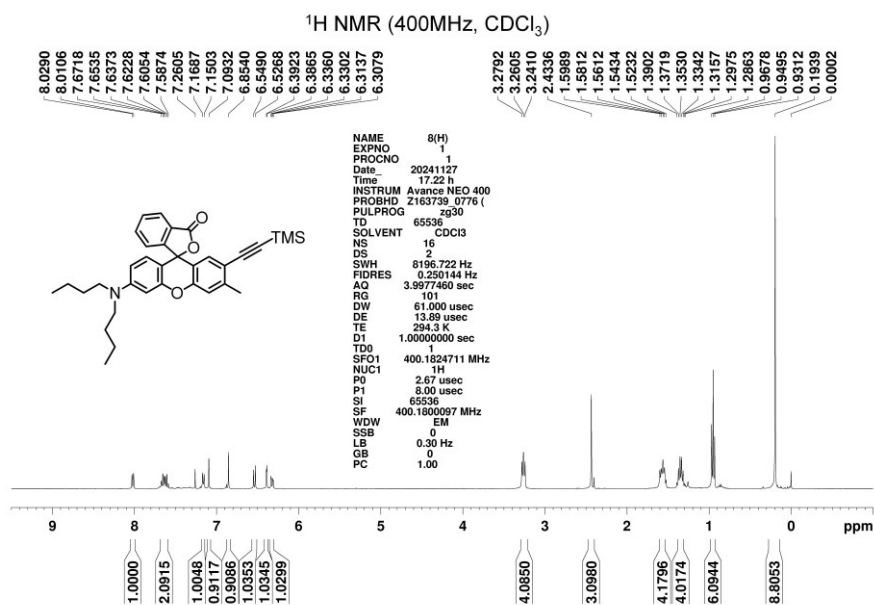


Fig. S10 <sup>1</sup>H NMR (400 MHz) spectrum of **8** (CDCl<sub>3</sub>).

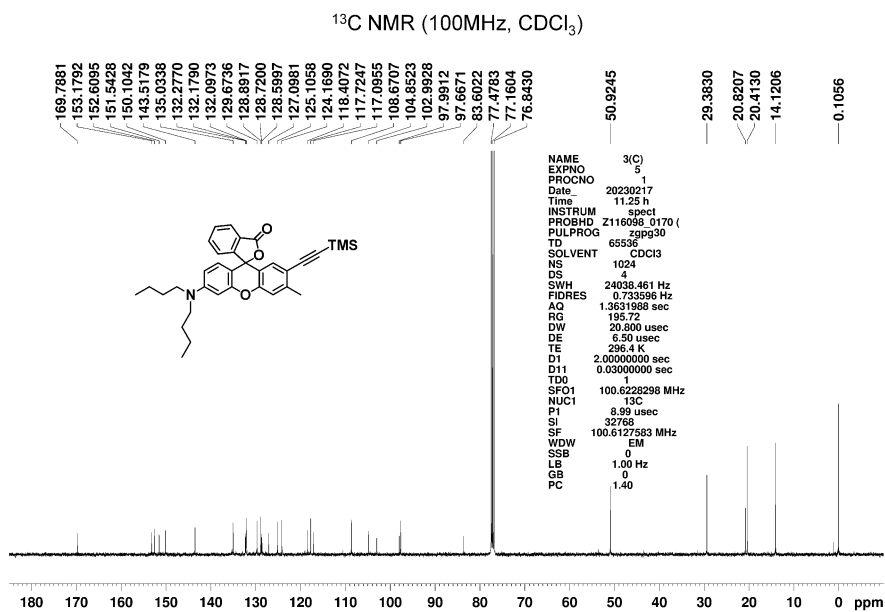
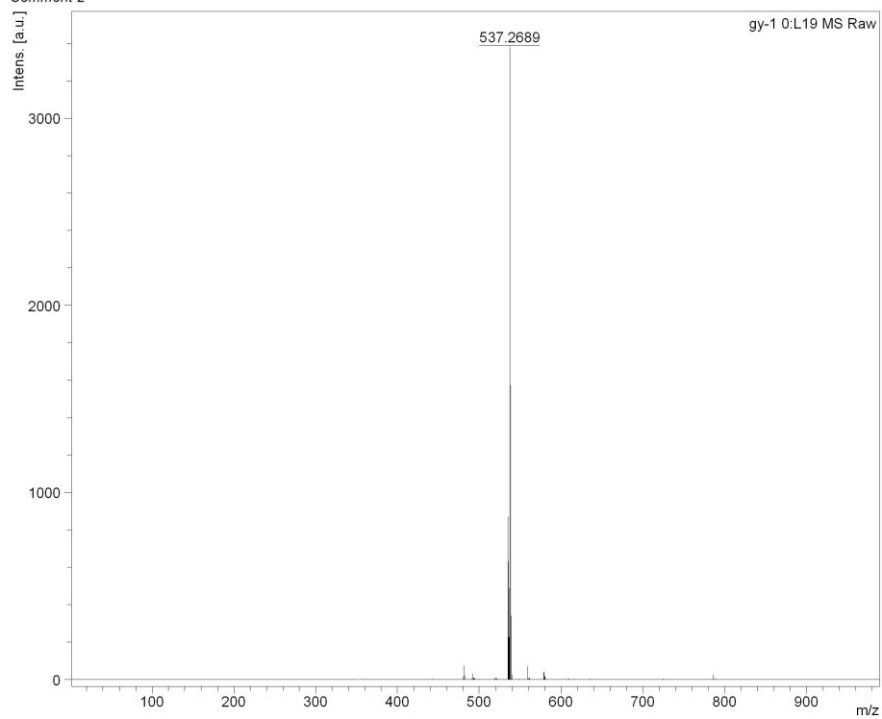


Fig. S11 <sup>13</sup>C NMR (100 MHz) spectrum of **8** (CDCl<sub>3</sub>).



Comment 1  
Comment 2



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**Instrument Info**

Bruker Daltonics flexAnalysis

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**Fig. S12** HRMS spectrum of **8**.

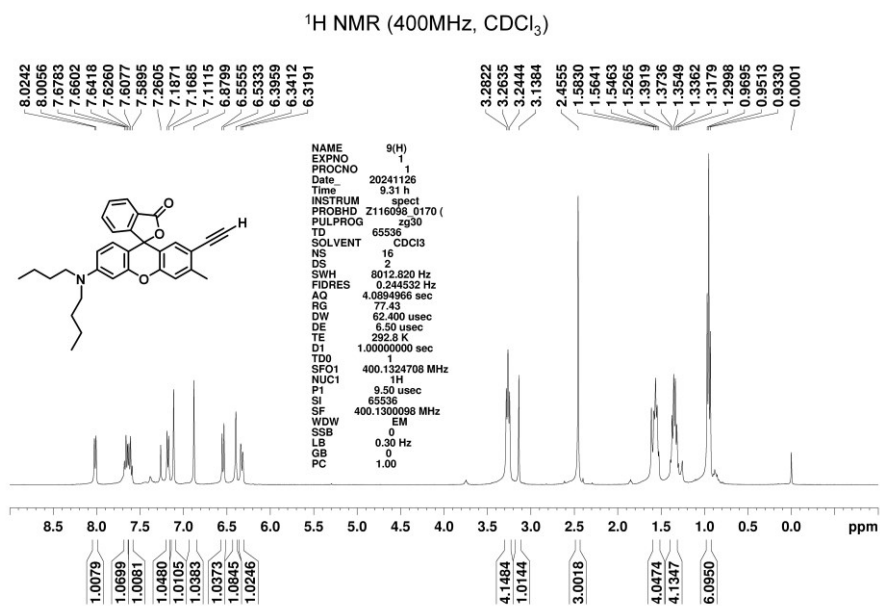


Fig. S13 <sup>1</sup>H NMR (400 MHz) spectrum of 9 (CDCl<sub>3</sub>).

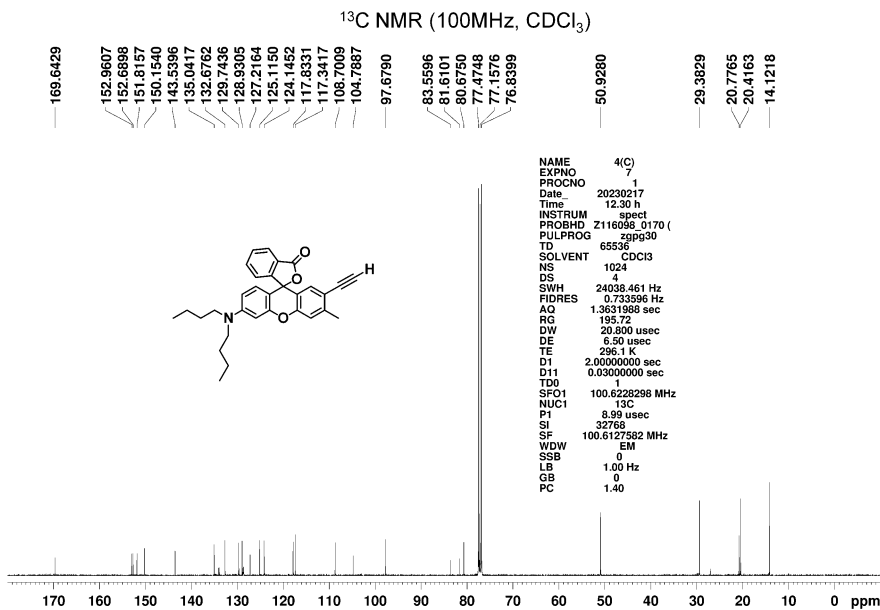
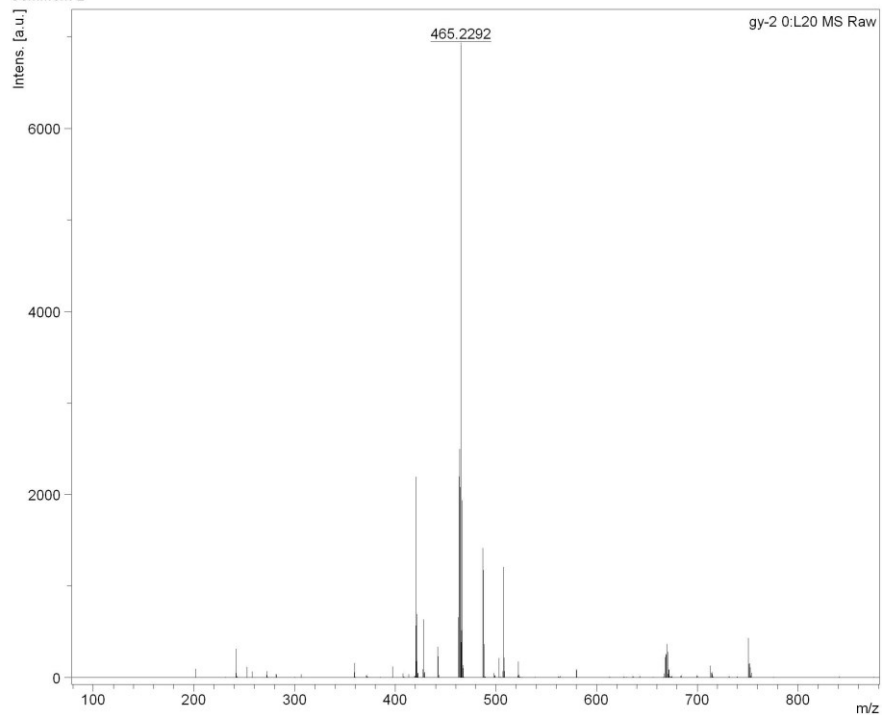


Fig. S14 <sup>13</sup>C NMR (100 MHz) spectrum of 9 (CDCl<sub>3</sub>).

Comment 1  
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Bruker Daltonics flexAnalysis

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Fig. S15 HRMS spectrum of 9.

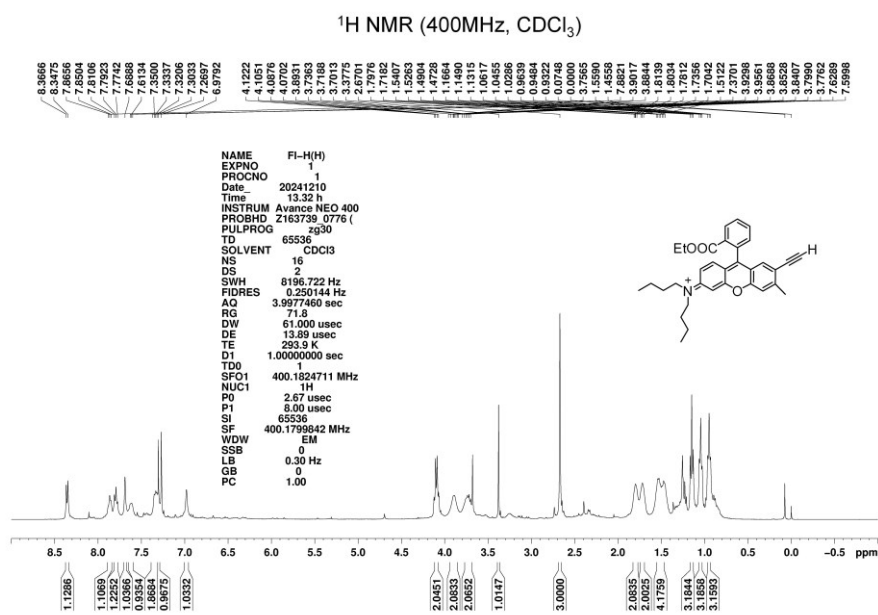


Fig. S16 <sup>1</sup>H NMR (400 MHz) spectrum of FI-H (CDCl<sub>3</sub>).

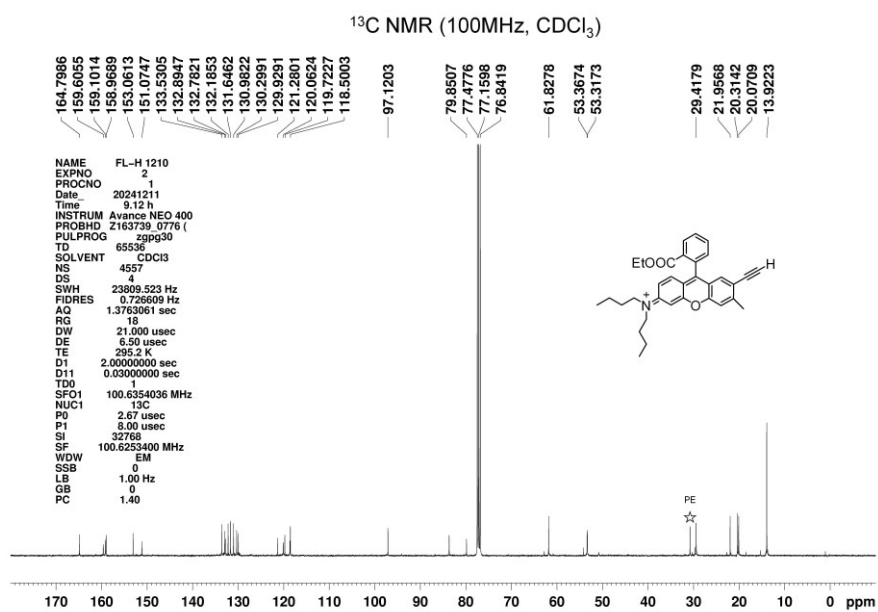


Fig. S17 <sup>13</sup>C NMR (100 MHz) spectrum of FI-H (CDCl<sub>3</sub>).

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T: FTMS + p ESI Full ms [100.0000-1500.0000]

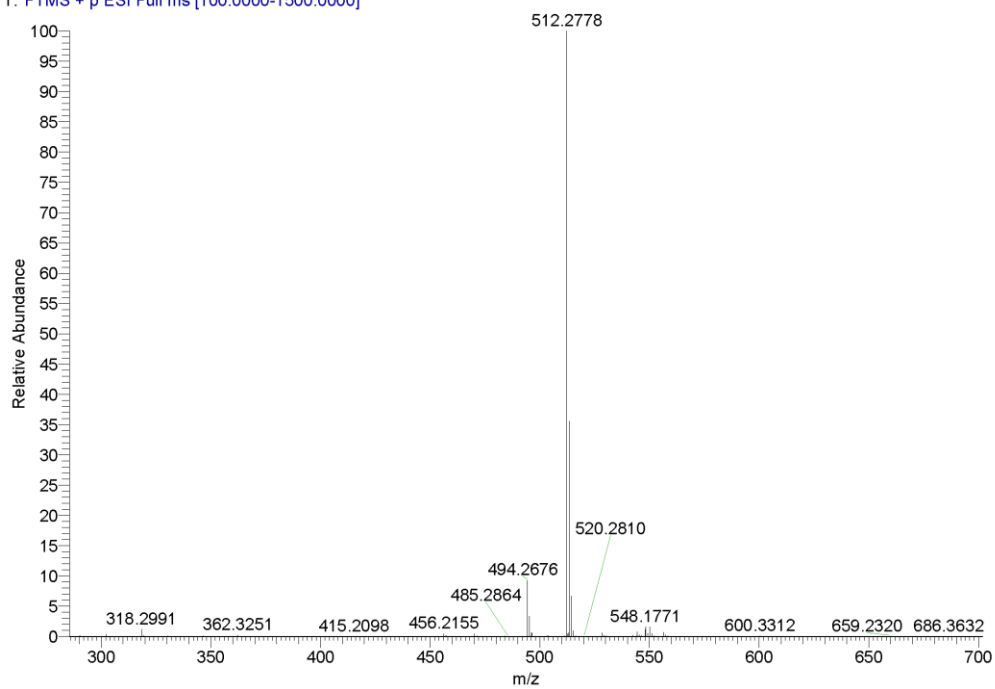
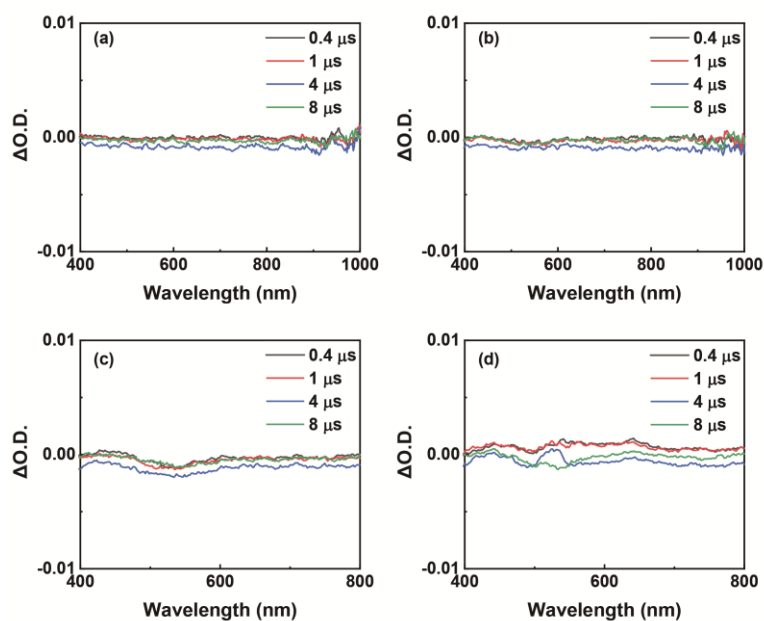
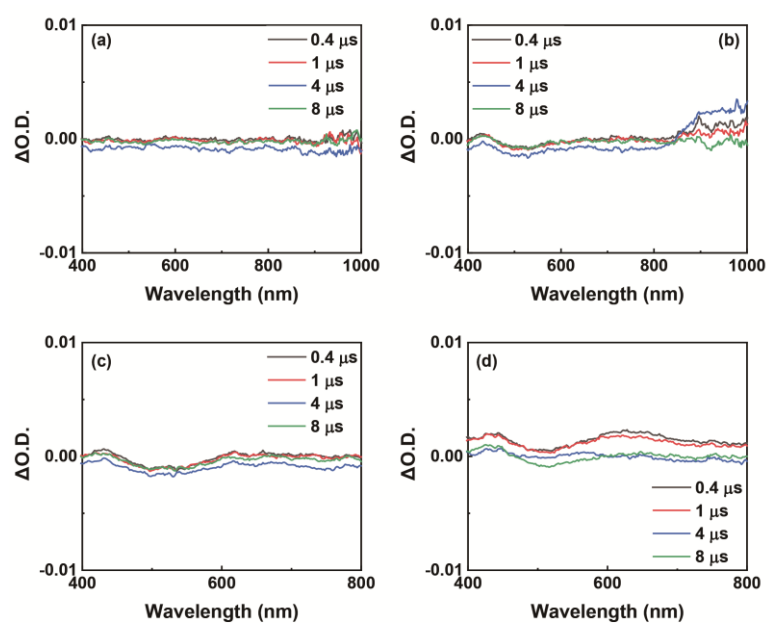


Fig. S18 HRMS spectrum of FI-H.

#### 4. Nanosecond time-resolved transient absorption spectra of compound FI-TPA



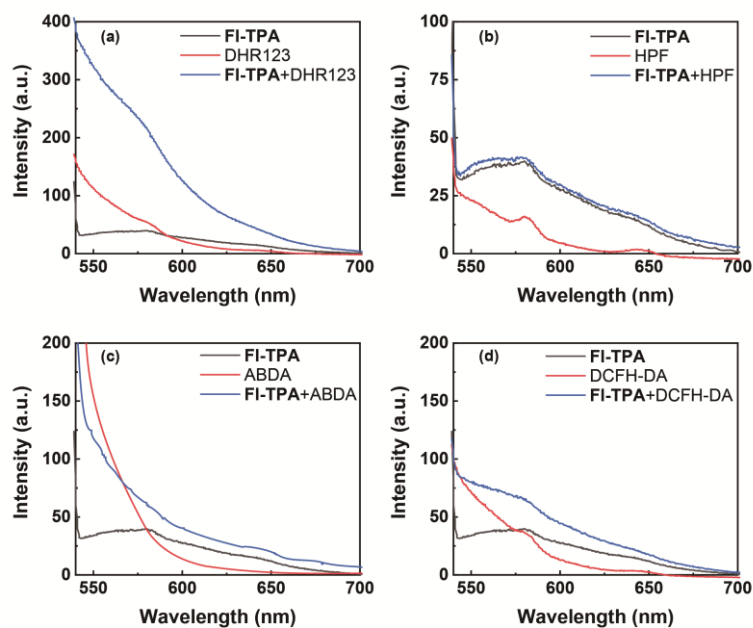
**Fig. S19** The nanosecond transient absorption spectra of FI-TPA in DMF at concentrations of  $1 \times 10^{-5}$  mol/L (a)  $5 \times 10^{-5}$  mol/L (b) were recorded in the range of 400-1000 nm, with excitation at 532 nm. (c) The nanosecond transient absorption spectra of FI-TPA in DMF at concentrations of  $1 \times 10^{-4}$  mol/L were recorded in the range of 400-800 nm, with excitation at 532 nm. (d) The nanosecond transient absorption spectra of FI-TPA in DMF at concentrations of  $1 \times 10^{-4}$  mol/L were recorded in the range of 400-800 nm, with excitation at 355 nm.



**Fig. S20** The nanosecond transient absorption spectra of FI-TPA in Tol at concentrations of  $1 \times 10^{-5}$  mol/L (a)  $5 \times 10^{-5}$  mol/L (b) were recorded in the range of 400-1000 nm, with excitation at 532 nm. (c) The nanosecond

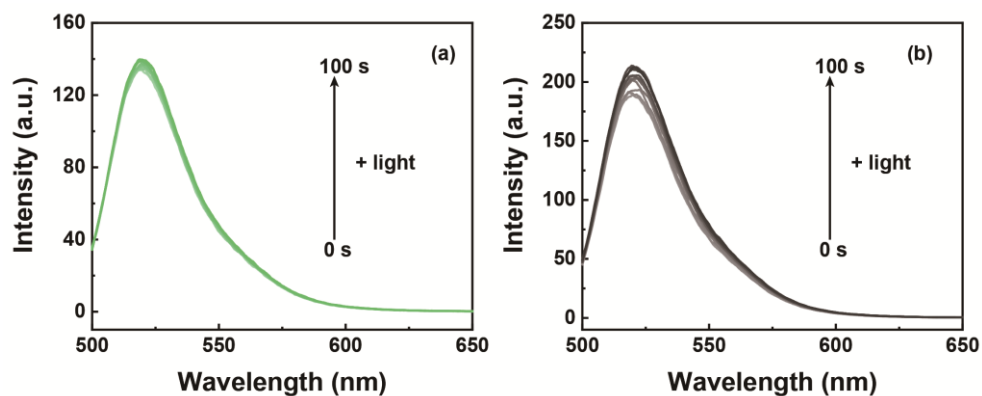
transient absorption spectra of **FI-TPA** in Tol at concentrations of  $1 \times 10^{-4}$  mol/L were recorded in the range of 400-800 nm, with excitation at 532 nm. (d) The nanosecond transient absorption spectra of **FI-TPA** in Tol at concentrations of  $1 \times 10^{-4}$  mol/L were recorded in the range of 400-800 nm, with excitation at 355 nm.

5. The effect of ROS indicators on the excited state of FI-TPA.



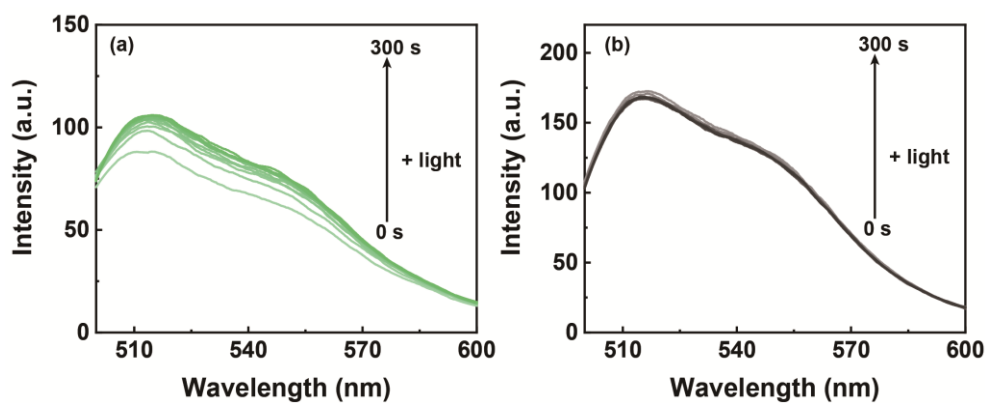
**Fig. S21** Under 530 nm excitation, the fluorescence emission spectra of (a) DHR123 (b) HPF (c) ABDA (d) DCFH-DA and FI-TPA were recorded individually and in combination in aqueous solutions at a concentration of  $1 \times 10^{-5}$  mol/L.

6. ROS generation of ICG and control group

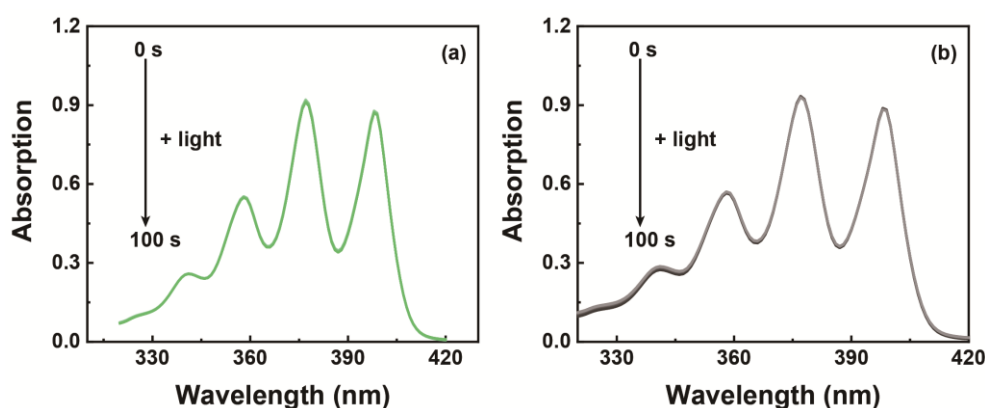


**Fig. S22** The fluorescence emission spectra of DHR123 were recorded under 100 s illumination with (a) ICG, (b) control (without test solution), at a light intensity of  $10 \text{ mW/cm}^2$ . The concentrations of PSs and DHR123 during the measurements are  $1 \times 10^{-5}$  mol/L each.

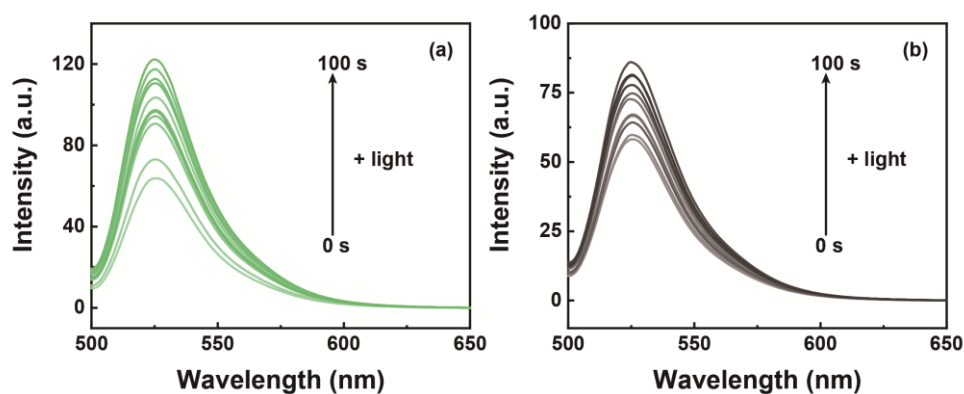




**Fig. S23** The fluorescence emission spectra of HPF were recorded under 300 s illumination with (a) ICG, (b) control (without test solution), at a light intensity of 10 mW/cm<sup>2</sup>. The concentrations of PSs and HPF during the measurements are  $1 \times 10^{-5}$  mol/L each.

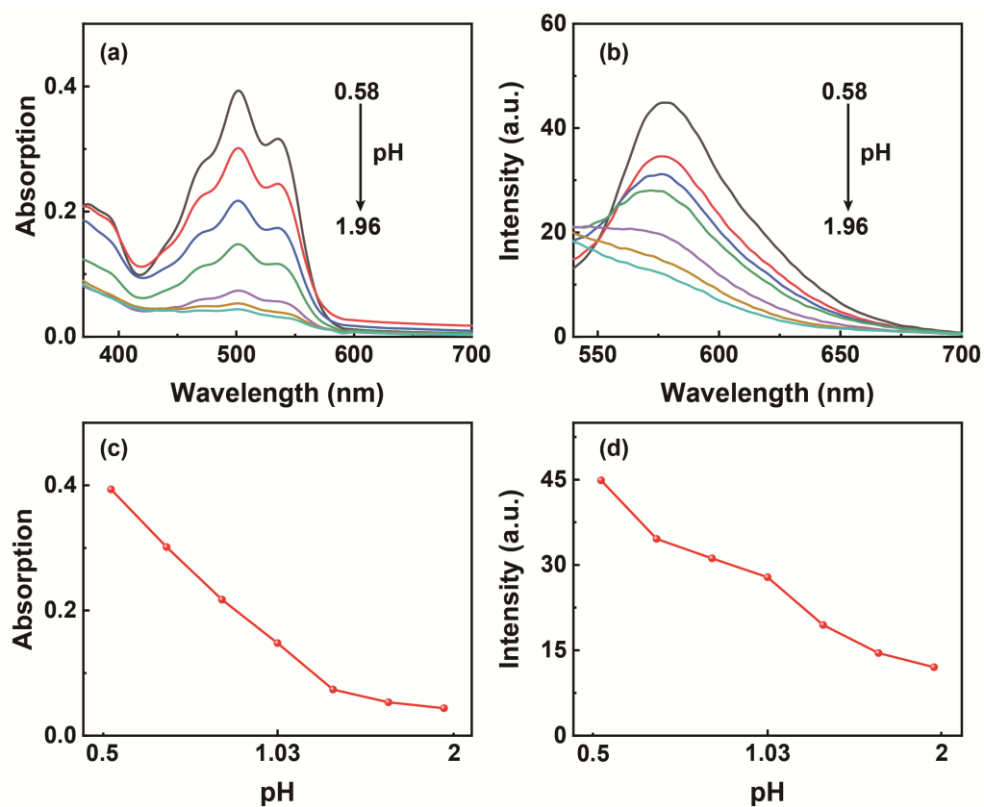


**Fig. S24** The UV-vis absorption spectra showing the changes in ABDA were recorded under 100 s illumination with (a) ICG, (b) control (without test solution), at a light intensity of 10 mW/cm<sup>2</sup>. The concentrations of PSs and ABDA during the measurements are  $1 \times 10^{-5}$  mol/L each.



**Fig. S25** The fluorescence emission spectra of DCFH-DA were recorded under 100 s illumination with (a) ICG, (b) control (without test solution), at a light intensity of 10 mW/cm<sup>2</sup>. The concentrations of PSs and DCFH-DA during the measurements are  $1 \times 10^{-5}$  mol/L each.

7. Compound **5** in its acid-induced ring-opened form pH stability



**Fig. S26** (a) The UV-vis absorption spectra and (b) fluorescence emission spectra of compound **5** in its acid-induced ring-opened form at different pH values ( $\lambda_{\text{ex}} = 500$  nm). (c) Changes in the UV-vis absorption intensity at 502 nm and (d) changes in the fluorescence emission intensity at 577 nm for compound **5** in its acid-induced ring-opened form at different pH values.

## 8. Theoretical calculation

The optimized structure of  $S_0$  state of **FI-TPA**

C	3.42392300	-1.11254300	0.85726800
C	4.78740600	-0.92132000	1.02900400
C	5.64407700	-0.86048800	-0.07655700
C	5.08561600	-0.98907800	-1.35490300
C	3.72069800	-1.17335100	-1.51672500
N	7.03535100	-0.67384700	0.09234100
C	7.76536600	0.13722700	-0.81935800
C	7.71746300	-1.30206800	1.17013500
C	9.00140200	-0.29100500	-1.31538200
C	9.71966100	0.50830200	-2.19695400
C	9.21298000	1.73796700	-2.60984800
C	7.97960400	2.16421600	-2.12306500
C	7.26311000	1.37704600	-1.22940800
C	8.65848500	-0.59121900	1.92284200
C	9.33453700	-1.20997300	2.96787900
C	9.07445500	-2.53970800	3.28961400
C	8.13353900	-3.24827400	2.54634200
C	7.46504600	-2.64058200	1.49025000
C	-4.12084700	1.07581200	0.85335600
C	-5.44348700	0.83595400	0.67691500
C	-5.91257300	-0.30240500	-0.07695200
C	-4.93026200	-1.17706400	-0.60341600
C	-3.59590400	-0.91726600	-0.41346400
C	-3.11678300	0.21343800	0.31595200
O	-2.72469300	-1.79936200	-0.95607900
N	-7.22818300	-0.52220400	-0.27136600
C	-1.75021200	0.41787700	0.45396600
C	-0.85276300	-0.53937500	-0.10690800
C	-1.38507700	-1.63474900	-0.80892500
C	-0.56717100	-2.60154400	-1.37506500
C	0.81378000	-2.50943800	-1.27210200
C	1.38836500	-1.40435300	-0.57644300
C	0.55170300	-0.46026600	-0.00970800
C	-0.85957700	2.79748600	0.75145600
C	-1.22338200	1.54502400	1.27875800
C	-0.37154700	3.78733000	1.61031000
C	-0.23918600	3.54917700	2.97047700
C	-0.59821600	2.31143700	3.49081900
C	-1.08697200	1.31876300	2.64907000
C	1.65724300	-3.60126200	-1.87211500
C	-7.64619200	-1.73478800	-1.01530900
C	-9.12354600	-1.82868600	-1.38281600
C	-9.39702500	-3.10656600	-2.18479400
C	-10.86804900	-3.25090000	-2.57595400
C	-8.24964800	0.30942700	0.38531900
C	-8.56909200	-0.13107700	1.81775500
C	-9.65003400	0.74213100	2.45917900
C	-9.98447400	0.31703800	3.88967900
C	2.85967000	-1.24407100	-0.41632300
C	-0.99743300	3.06225900	-0.71102400
O	-1.39314700	2.23876300	-1.51200600
O	-0.63821000	4.30418000	-1.04878800
C	-0.28818100	6.09085100	-2.60449400
C	-0.73654600	4.65509400	-2.45824000

H	2.78607900	-1.15986800	1.73218700
H	5.19119900	-0.82058900	2.02802200
H	5.72448800	-0.94139700	-2.22708700
H	3.32258300	-1.25559000	-2.52060400
H	9.39743700	-1.25066100	-1.00805600
H	10.67496300	0.16051500	-2.57217200
H	9.77206800	2.35632600	-3.30126200
H	7.57652900	3.12250900	-2.42898600
H	6.31131800	1.72208900	-0.84556400
H	8.85894200	0.44614400	1.68630100
H	10.05953600	-0.64401500	3.54095400
H	9.59853300	-3.01777600	4.10802200
H	7.92686600	-4.28624100	2.77932900
H	6.74512900	-3.20308200	0.90927500
H	-3.81162200	1.94295700	1.42070300
H	-6.14937700	1.52032600	1.11869900
H	-5.19048800	-2.06534900	-1.15511500
H	-1.02802000	-3.43762000	-1.88559500
H	0.98544400	0.37819600	0.51838500
H	-0.09618600	4.74803500	1.19960100
H	0.14147500	4.32669700	3.62048400
H	-0.50072300	2.11359800	4.55099700
H	-1.36608100	0.35573400	3.05818000
H	1.05837800	-4.49352600	-2.05257800
H	2.08363900	-3.29050400	-2.82955500
H	2.49180200	-3.86231300	-1.22028800
H	-7.06837100	-1.76433500	-1.94104100
H	-7.36330000	-2.61618600	-0.42937000
H	-9.74932800	-1.83438100	-0.48659100
H	-9.41912200	-0.96180700	-1.98118200
H	-8.77656700	-3.10853600	-3.08699000
H	-9.08817300	-3.97655500	-1.59587400
H	-11.03485700	-4.16749000	-3.14597700
H	-11.51000300	-3.28650700	-1.69163900
H	-11.19689400	-2.41004900	-3.19258100
H	-7.92689200	1.34894100	0.36453700
H	-9.14845100	0.27088400	-0.22331500
H	-8.89528700	-1.17604900	1.80917100
H	-7.65742800	-0.09562200	2.42266200
H	-9.32008600	1.78663900	2.45596000
H	-10.55639100	0.70473500	1.84535000
H	-10.75769500	0.95701300	4.32063000
H	-10.34917900	-0.71329600	3.91968900
H	-9.10384200	0.37713500	4.53497400
H	-0.35093200	6.38107600	-3.65514700
H	-0.92429100	6.76272100	-2.02576900
H	0.74524000	6.21565900	-2.27675200
H	-0.10668700	3.96863000	-3.02459900
H	-1.77084700	4.51388900	-2.77282200

The optimized structure of S<sub>1</sub> state of **FI-TPA**

C	3.91007700	-2.05560800	0.64863800
C	5.26093400	-1.79720800	0.74125700
C	5.82055300	-0.72003200	0.02869900
C	4.98859900	0.08329600	-0.77328900
C	3.64066000	-0.19366100	-0.85777400
N	7.18944000	-0.44870600	0.11861900
C	7.65561500	0.88711200	0.08891700
C	8.12096700	-1.50751000	0.24088100
C	8.80413600	1.20790100	-0.64865700
C	9.25334300	2.51713200	-0.67574900
C	8.57524100	3.50835600	0.03326200
C	7.43803900	3.18598700	0.77186300
C	6.97181200	1.88219000	0.80222000
C	9.20272000	-1.38501100	1.12423000
C	10.10945600	-2.42494800	1.24015500
C	9.95411600	-3.58181000	0.47717300
C	8.88187300	-3.69849200	-0.40573600
C	7.96238700	-2.66989200	-0.52709600
C	-3.98126300	1.13675700	0.55912900
C	-5.31676800	0.81477000	0.46742500
C	-5.74496500	-0.47508700	0.05697700
C	-4.72605100	-1.41906600	-0.20553600
C	-3.39469800	-1.07272200	-0.10808300
C	-2.94885700	0.21673100	0.26128700
O	-2.50041600	-2.08150300	-0.37836800
N	-7.08022200	-0.79010000	-0.09590200
C	-1.55528800	0.48978900	0.34175600
C	-0.64934400	-0.57180600	0.05223400
C	-1.15221900	-1.84281500	-0.30048700
C	-0.32091400	-2.90497300	-0.60298100
C	1.07001000	-2.78068600	-0.56688900
C	1.60618400	-1.51861600	-0.22888800
C	0.75594100	-0.45174200	0.05145900
C	-1.17712300	2.98640600	-0.01975400
C	-1.05791300	1.82229000	0.76710900
C	-0.74905100	4.21990100	0.48319500
C	-0.17817400	4.31624600	1.74416500
C	-0.04591700	3.17242900	2.52430500
C	-0.48747200	1.94731500	2.03924500
C	1.91891800	-3.97388100	-0.92960600
C	-7.43814700	-2.17354600	-0.44511800
C	-8.88149500	-2.38624200	-0.89790100
C	-9.09288200	-3.81375100	-1.41354800
C	-10.53540500	-4.08008100	-1.84547200
C	-8.10428600	0.05988200	0.51756400
C	-8.28405200	-0.15035500	2.02609700
C	-9.35987500	0.76368500	2.61690800
C	-9.55837800	0.56138000	4.11990100
C	3.06784100	-1.26647900	-0.15316000
C	-1.69153300	2.92452700	-1.42231700
O	-1.51447000	1.99799500	-2.18493700
O	-2.35545800	4.04073200	-1.76212500
C	-3.52691500	5.45962500	-3.29459100
C	-2.83602500	4.12481700	-3.13171200
H	3.49003800	-2.86062900	1.23615600
H	5.88386400	-2.39095300	1.39562200

H	5.41532800	0.88818100	-1.35539900
H	3.01789600	0.41092900	-1.50391900
H	9.31411000	0.43976300	-1.21385700
H	10.12879300	2.76911400	-1.26001200
H	8.93402100	4.52938100	0.01144800
H	6.92094300	3.95097900	1.33634600
H	6.10593900	1.62200300	1.39565500
H	9.30713500	-0.49455600	1.72903200
H	10.93452400	-2.33865700	1.93521500
H	10.66863900	-4.38971100	0.56933100
H	8.76976400	-4.58868300	-1.01094300
H	7.14412900	-2.74446900	-1.23036700
H	-3.71424700	2.13466100	0.88156300
H	-6.03713300	1.57733600	0.71955400
H	-4.94835800	-2.43919700	-0.47602000
H	-0.77515300	-3.84716800	-0.88594100
H	1.18806600	0.50852100	0.29921400
H	-0.85173100	5.10320700	-0.13242600
H	0.15953100	5.27630700	2.11418500
H	0.39074600	3.23328500	3.51394100
H	-0.40490100	1.06394200	2.66090700
H	1.35414800	-4.66242600	-1.55943000
H	2.82150000	-3.68545000	-1.47005700
H	2.23544500	-4.53396700	-0.04440800
H	-6.79207700	-2.47909700	-1.26981300
H	-7.21963800	-2.84921100	0.39416000
H	-9.57960100	-2.20447200	-0.07606000
H	-9.12838500	-1.67398300	-1.69212300
H	-8.41893500	-3.99786800	-2.25693300
H	-8.80892400	-4.52674700	-0.63190700
H	-10.65611700	-5.10235900	-2.21122200
H	-11.22922800	-3.94033800	-1.01190200
H	-10.83879700	-3.40128500	-2.64735700
H	-7.86921600	1.10368400	0.30984100
H	-9.04671100	-0.12856500	0.00741000
H	-8.54796600	-1.19652100	2.21577100
H	-7.33046700	0.02705900	2.53397700
H	-9.09284900	1.80831400	2.42171600
H	-10.30857900	0.58898000	2.09724900
H	-10.33089800	1.22738400	4.51159700
H	-9.85984000	-0.46595900	4.34258700
H	-8.63479700	0.76249500	4.66985400
H	-3.90107600	5.54964200	-4.31640900
H	-4.37355100	5.54995100	-2.61176500
H	-2.83732700	6.28507100	-3.10929800
H	-1.98190400	4.02129800	-3.80190800
H	-3.51439200	3.28960200	-3.30867000

The optimized structure of T<sub>1</sub> state of **FI-TPA**

C	-3.58084400	-0.51296100	-0.99994100
C	-4.92907600	-0.25219300	-1.06360100
C	-5.79876100	-0.77873500	-0.08421200
C	-5.26033100	-1.57864900	0.94616800
C	-3.91318600	-1.85551800	0.97538700
N	-7.16220800	-0.51064000	-0.13249400
C	-7.92126100	-0.40259200	1.06404800
C	-7.82176900	-0.33901000	-1.37924200
C	-9.18034600	-1.01002500	1.14505100
C	-9.91751600	-0.89972600	2.31335700
C	-9.41493400	-0.18117100	3.39726700
C	-8.16547800	0.42973100	3.31011300
C	-7.41438300	0.32230300	2.14994500
C	-8.75148100	0.69635900	-1.53674800
C	-9.39407900	0.85752100	-2.75393100
C	-9.12536300	-0.01008700	-3.81170800
C	-8.20645300	-1.04503100	-3.64879300
C	-7.55157600	-1.21432300	-2.43882000
C	3.98643100	1.20204700	-0.52334500
C	5.32586700	0.89823000	-0.41560200
C	5.76682500	-0.39802300	-0.04236400
C	4.75724000	-1.36704800	0.16667700
C	3.42397000	-1.03618100	0.05307900
C	2.96462300	0.25561900	-0.28055400
O	2.53823700	-2.07010500	0.27395500
N	7.10321500	-0.69983900	0.12548900
C	1.56560100	0.51028700	-0.38064100
C	0.67135100	-0.57963700	-0.15663800
C	1.19430900	-1.85314200	0.17169600
C	0.37504400	-2.94408300	0.40298800
C	-1.01542300	-2.84541600	0.35851400
C	-1.57928200	-1.57804000	0.05739100
C	-0.72953100	-0.49281000	-0.20669700
C	1.10629000	2.97497700	0.08732000
C	1.05577400	1.85205800	-0.76398300
C	0.66819800	4.22194400	-0.37155600
C	0.15643100	4.37044000	-1.65283800
C	0.09435700	3.26721000	-2.49721500
C	0.54564000	2.02920300	-2.05492700
C	-1.82202000	-4.10271800	0.57343700
C	7.47677600	-2.08835500	0.43668000
C	8.91330400	-2.29306500	0.91433300
C	9.13703900	-3.73399300	1.38564900
C	10.57397200	-3.99183900	1.84073400
C	8.12657600	0.18802600	-0.43252000
C	8.34415900	0.03295700	-1.94308800
C	9.41751700	0.98408200	-2.47708000
C	9.65313700	0.83653200	-3.98111300
C	-3.02909000	-1.33214200	0.00908300
C	1.56300600	2.85056200	1.50554800
O	1.40000400	1.87076100	2.20191300
O	2.15814500	3.97188300	1.94139600
C	3.20951500	5.33689000	3.60452500
C	2.57787600	3.99040200	3.33341100
H	-2.93218200	-0.08871700	-1.75489900
H	-5.32031500	0.38354000	-1.84536300

H	-5.91310500	-1.99980900	1.69772100
H	-3.53097900	-2.47133400	1.77633500
H	-9.56014000	-1.57936400	0.30732000
H	-10.88379800	-1.38285800	2.38202300
H	-9.99729800	-0.09492300	4.30591700
H	-7.78007800	1.00260800	4.14384300
H	-6.45533300	0.81640800	2.06953100
H	-8.94589600	1.37663500	-0.71846400
H	-10.10072400	1.66766600	-2.88106800
H	-9.63354000	0.11810800	-4.75909400
H	-8.00877500	-1.73074900	-4.46275100
H	-6.85696300	-2.03208900	-2.30032000
H	3.70885300	2.20711400	-0.81433400
H	6.03821600	1.68107100	-0.62572900
H	4.99006000	-2.39249200	0.40710100
H	0.84357300	-3.89831600	0.61254300
H	-1.17005900	0.47211300	-0.41637500
H	0.71673300	5.07382600	0.29299100
H	-0.19016900	5.33986300	-1.98870700
H	-0.29574800	3.36968200	-3.50274200
H	0.51711500	1.17828300	-2.72490900
H	-1.22766400	-4.97668600	0.30439400
H	-2.11421000	-4.22590800	1.62067400
H	-2.73309500	-4.11743400	-0.02492700
H	6.81793300	-2.43229700	1.23574600
H	7.28842500	-2.73830700	-0.42988900
H	9.62598300	-2.07199700	0.11499200
H	9.13066100	-1.60480100	1.73777300
H	8.44788000	-3.95772400	2.20685600
H	8.88237500	-4.42405100	0.57394000
H	10.70359700	-5.02403400	2.17413500
H	11.28356400	-3.81250600	1.02829800
H	10.84818100	-3.33626400	2.67190300
H	7.86856700	1.21990600	-0.19450600
H	9.06010200	-0.00317200	0.09277600
H	8.63004100	-1.00168500	-2.16174400
H	7.39944900	0.21231500	-2.46651900
H	9.12847200	2.01690300	-2.25284000
H	10.35701900	0.80684800	-1.94184800
H	10.42271000	1.52819400	-4.33201200
H	9.97716300	-0.17748200	-4.23142400
H	8.73882600	1.04118900	-4.54504900
H	3.53610000	5.37866600	4.64558300
H	4.08039100	5.49816400	2.96674300
H	2.49737700	6.14686100	3.43710600
H	1.70105000	3.81610100	3.95812700
H	3.27965900	3.17079000	3.49060600



The optimized structure of S<sub>0</sub> state of **FI-H**

C	-0.68280800	-1.25787600	-0.42836000
C	-2.01596300	-1.23143500	-0.18768000
C	-2.70278600	-0.00369700	0.13859900
C	-1.92547100	1.18179100	0.17526400
C	-0.57766400	1.13382100	-0.07128100
C	0.11800900	-0.07492800	-0.38386000
O	0.09135700	2.31035600	-0.00942000
N	-4.02409900	0.01313200	0.39546100
C	1.48590900	-0.04630300	-0.60903900
C	2.16258700	1.21232600	-0.56225900
C	1.42272400	2.36872800	-0.25515400
C	2.01492000	3.62451700	-0.18854900
C	3.36943000	3.77530800	-0.42879600
C	4.14298300	2.61901100	-0.74684800
C	3.53848200	1.37386100	-0.80850700
C	2.90743200	-2.11405500	-0.11586100
C	2.22416200	-1.27755100	-1.01728600
C	3.57584500	-3.24265600	-0.60008000
C	3.57598200	-3.54461400	-1.95407500
C	2.90122800	-2.71765600	-2.84416700
C	2.23017600	-1.59334100	-2.37658600
C	4.01176800	5.12830900	-0.35945200
C	-4.68127400	1.31332500	0.67588600
C	-6.12871700	1.25191000	1.15275100
C	-6.65900700	2.66139000	1.44096700
C	-8.10994500	2.65512300	1.92315000
C	-4.85151700	-1.19426100	0.23466300
C	-5.31237900	-1.43071200	-1.20743800
C	-6.18133900	-2.68431200	-1.33361000
C	-6.65404900	-2.93596200	-2.76611800
C	5.54261100	2.73793100	-1.00444300
C	6.72088800	2.84037000	-1.22166700
C	2.90983200	-1.79708400	1.34264800
O	2.35916700	-0.82577300	1.82226400
O	3.58278000	-2.69488500	2.06725300
C	4.44624500	-3.59257500	4.11281200
C	3.64217700	-2.46712700	3.50414100
H	-0.20624000	-2.19917900	-0.66513600
H	-2.56380300	-2.15761100	-0.24777800
H	-2.35989600	2.14509400	0.38591200
H	1.39631700	4.47913100	0.05306900
H	4.13629500	0.50688800	-1.05244700
H	4.09614100	-3.88294900	0.09761200

H	4.09956500	-4.42205900	-2.31166100
H	2.89298600	-2.94343300	-3.90318900
H	1.70531100	-0.95160100	-3.07315500
H	3.28398100	5.89801800	-0.10757600
H	4.80723800	5.14045900	0.39004200
H	4.47598100	5.38537900	-1.31500500
H	-4.09487500	1.81515600	1.44776300
H	-4.62397700	1.93067700	-0.22708800
H	-6.76802000	0.78163500	0.40107900
H	-6.20031600	0.65100100	2.06408600
H	-6.02511900	3.14053800	2.19429400
H	-6.57714500	3.27125000	0.53521300
H	-8.46239800	3.66974700	2.12105400
H	-8.77265000	2.21165200	1.17513100
H	-8.21671300	2.07889300	2.84616800
H	-4.29915600	-2.05417300	0.60946800
H	-5.71311300	-1.09328600	0.88810400
H	-5.87204100	-0.55643300	-1.55497700
H	-4.43823800	-1.51940200	-1.86038700
H	-5.61694000	-3.55277100	-0.97708700
H	-7.04998400	-2.59040400	-0.67318100
H	-7.27060100	-3.83566800	-2.82533900
H	-7.25004300	-2.09794400	-3.13757200
H	-5.80609900	-3.06740700	-3.44376900
H	7.76448000	2.92929900	-1.41385600
H	4.50655700	-3.44666000	5.19312600
H	3.97590900	-4.55911500	3.92427700
H	5.46164700	-3.61152700	3.71337900
H	4.10289700	-1.49397400	3.67549300
H	2.62150400	-2.43817300	3.88635000

The optimized structure of S<sub>1</sub> state of **FI-H**

C	0.92661100	-1.18593700	0.89829800
C	2.28794300	-1.21279300	0.70087500
C	2.96005000	-0.09878000	0.13416700
C	2.16959800	1.02681500	-0.22655700
C	0.79496600	1.01421000	-0.00654900
C	0.12180900	-0.06951200	0.56448900
O	0.15027900	2.14437600	-0.39797900
N	4.30994500	-0.07573300	-0.06095300
C	-1.30662500	0.00973400	0.74334600
C	-1.95328000	1.19583200	0.34363800
C	-1.18996400	2.25682500	-0.23813600
C	-1.76139900	3.44812100	-0.66120600
C	-3.12292800	3.67116600	-0.52911300
C	-3.91561300	2.63632400	0.06141000
C	-3.33598000	1.44302900	0.48111500
C	-2.85963100	-2.01210500	0.70600200
C	-2.04439400	-1.09629700	1.40191100
C	-3.55901100	-2.99471100	1.41425500
C	-3.44832300	-3.09388800	2.79369800
C	-2.63773900	-2.19996200	3.48422600
C	-1.94646600	-1.21255800	2.79192600
C	-3.74251800	4.95674300	-0.98475700
C	4.99751200	1.03549900	-0.72026200
C	5.42803100	2.14613700	0.25456000
C	6.18924100	3.26394200	-0.46151000
C	6.62609600	4.37802800	0.49123400
C	5.16053900	-1.17577000	0.38682600
C	5.30086300	-2.29526200	-0.66262100
C	6.21534900	-3.41919200	-0.17034500
C	6.37516600	-4.53648300	-1.20273800
C	-5.31486500	2.82463800	0.22779300
C	-6.50031000	2.98488000	0.36883300
C	-2.93796100	-1.97911100	-0.78585900
O	-2.10751100	-1.46050000	-1.50406000
O	-4.02601700	-2.60440800	-1.25298400
C	-5.44839400	-3.42618300	-2.99540600
C	-4.16941000	-2.67726900	-2.69901600
H	0.44785300	-2.05918400	1.32103700
H	2.83074900	-2.10541100	0.96705600
H	2.59617600	1.91630500	-0.66215800
H	-1.11714400	4.20253900	-1.09481100
H	-3.96381700	0.68645100	0.92996500
H	-4.18097200	-3.69156900	0.87024800
H	-3.99001400	-3.86604800	3.32532500
H	-2.54579300	-2.26441800	4.56150700
H	-1.32915600	-0.50803400	3.33581200
H	-2.99095000	5.62750600	-1.39887200
H	-4.50412700	4.77613900	-1.74878400
H	-4.24395500	5.46636700	-0.15716600
H	5.88022800	0.61646700	-1.20592000
H	4.36862200	1.43999200	-1.51232000
H	4.54161300	2.55366300	0.74995700
H	6.05543800	1.71138300	1.03818700
H	7.06832100	2.84190400	-0.95940400
H	5.55826100	3.68399600	-1.25174900
H	7.16687700	5.16122400	-0.04469000

H	5.76416300	4.84100500	0.97893300
H	7.28497600	3.99225600	1.27360500
H	6.14379600	-0.75464800	0.60120400
H	4.77107800	-1.57538700	1.32321900
H	4.31158600	-2.69515200	-0.90133700
H	5.70106300	-1.86622000	-1.58598100
H	7.19823500	-3.00476900	0.07662700
H	5.81198200	-3.83403600	0.75921300
H	7.03113800	-5.32501400	-0.82712200
H	5.41085700	-4.99100600	-1.44480800
H	6.80770800	-4.15623200	-2.13192000
H	-7.54868200	3.12563700	0.49378700
H	-5.58232200	-3.49489800	-4.07682300
H	-5.41456700	-4.43898700	-2.59026100
H	-6.31316800	-2.90885700	-2.57635500
H	-4.19010800	-1.66032400	-3.09162300
H	-3.29334600	-3.18492300	-3.10387300

The optimized structure of T<sub>1</sub> state of **FI-H**

C	-0.70718500	-1.13148200	-0.86046400
C	-2.07558200	-1.05996600	-0.74037700
C	-2.70115300	0.16041700	-0.39546100
C	-1.88277400	1.30029000	-0.19187300
C	-0.51408400	1.20098200	-0.33430600
C	0.12782500	-0.00664400	-0.67044200
O	0.18348300	2.35935800	-0.13791400
N	-4.07473900	0.25708200	-0.27334500
C	1.55916000	-0.03006900	-0.79999900
C	2.26000800	1.18236700	-0.58584400
C	1.54550200	2.36226900	-0.24954200
C	2.17716000	3.57217000	-0.01926100
C	3.55934200	3.68734300	-0.11012200
C	4.30659200	2.52316000	-0.44701300
C	3.66302900	1.31259600	-0.67507500
C	2.74482500	-2.24867400	-0.33225300
C	2.26496000	-1.26920000	-1.22579000
C	3.40789200	-3.37519400	-0.83260600
C	3.59391800	-3.54819300	-2.19631700
C	3.12676800	-2.58346600	-3.08124600
C	2.47383900	-1.45657600	-2.59504300
C	4.23911600	5.00130500	0.14054400
C	-4.70066600	1.23164700	0.62249000
C	-5.07273600	0.59696100	1.97817400
C	-5.70313700	1.63110800	2.91435000
C	-6.08107400	1.03059400	4.26933000
C	-4.93986400	-0.77197700	-0.87639500
C	-6.28465100	-0.25147700	-1.39105000
C	-7.02142700	-1.34975300	-2.16566600
C	-8.38119500	-0.88247900	-2.68559600
C	5.72853000	2.58966900	-0.55193500
C	6.92725800	2.64698000	-0.64020800
C	2.54441000	-2.10145300	1.14126300
O	1.77877800	-1.31255700	1.65714100
O	3.30612400	-2.94874700	1.84718200
C	4.09611400	-3.94576500	3.87534300
C	3.16404200	-2.90755700	3.29366000
H	-0.25172100	-2.08272600	-1.09896100
H	-2.65738100	-1.96053900	-0.86166900
H	-2.29531700	2.27468500	0.01901000
H	1.56967600	4.43216300	0.23359000
H	4.25400900	0.44341900	-0.92811900
H	3.77317200	-4.12004700	-0.14014600
H	4.10280900	-4.43011600	-2.56467000
H	3.26966900	-2.70365400	-4.14820300
H	2.11591800	-0.70345800	-3.28649500
H	3.51414600	5.77554800	0.38882600
H	4.95524200	4.92215800	0.96294300
H	4.80355300	5.32562600	-0.73794000
H	-4.01815900	2.05729200	0.79119300
H	-5.58807100	1.62668900	0.13242900
H	-5.76901200	-0.23078300	1.82055800
H	-4.16941900	0.17945900	2.43164400
H	-5.00414700	2.46029000	3.06265500
H	-6.59330700	2.05536300	2.43915900
H	-6.52767100	1.78659100	4.91874500

H	-6.80431800	0.21919900	4.15387700
H	-5.20349100	0.62657500	4.78059200
H	-4.39008400	-1.20946000	-1.70545800
H	-5.10282100	-1.55994900	-0.13200200
H	-6.91527700	0.08258800	-0.56438300
H	-6.11527000	0.60968800	-2.04413400
H	-6.40146700	-1.68015200	-3.00507600
H	-7.15628400	-2.22179400	-1.51740700
H	-8.88353200	-1.68046000	-3.23634500
H	-9.03558000	-0.58010800	-1.86385500
H	-8.27371900	-0.02804200	-3.35896800
H	7.98802200	2.69626500	-0.71839200
H	4.01098800	-3.93603200	4.96382400
H	3.84085600	-4.94619600	3.52162700
H	5.13392800	-3.73438800	3.61198500
H	3.41035200	-1.90091700	3.63281900
H	2.12122200	-3.10837500	3.54127900