

## Conjugated structures based on quinazolinones and their application in fluorescent labeling

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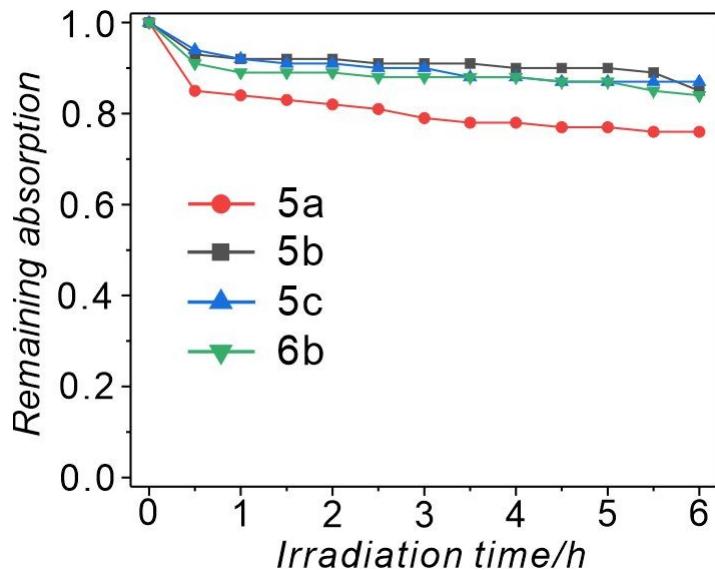
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**Fig. S1.** Photofading behaviors of probes **5a-c** and **6b** in acetonitrile.

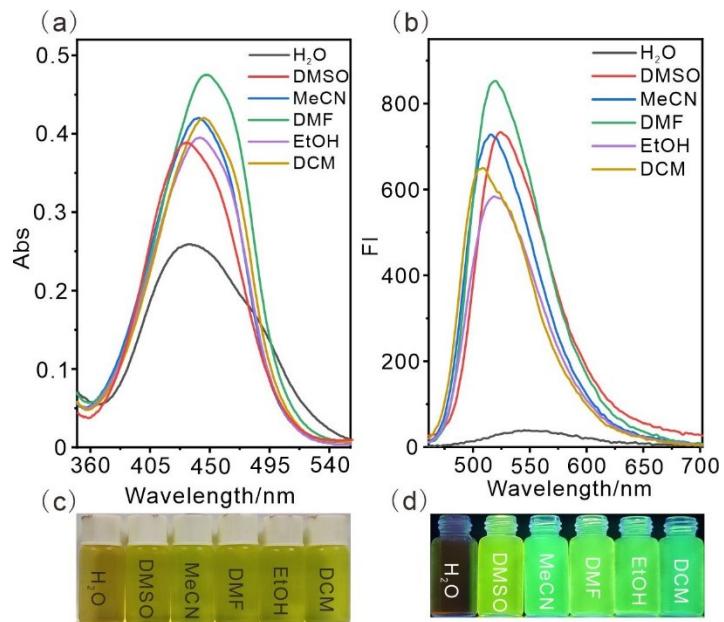
**Table S1.** Optical properties of probes **5a-c** and **6b** in organic solvents.

Probe	Solvents	$\lambda_{\text{Abs},\text{max}}^{\text{a}}$	$\lambda_{\text{Em},\text{max}}^{\text{a}}$	Stokes shift <sup>a</sup>	$\epsilon^{\text{b}}$	$\Phi^{\text{c}}$
<b>5a</b>	MeCN	451	544	93	5.23	26.6
<b>5a</b>	DMF	460	547	87	5.53	29.1
<b>5a</b>	EtOH	455	546	91	5.31	23.7
<b>5b</b>	MeCN	440	515	75	4.22	42.4
<b>5b</b>	DMF	445	518	73	4.77	58.7
<b>5b</b>	EtOH	442	516	74	3.96	39.2
<b>5c</b>	MeCN	390	508	118	2.83	1.3
<b>5c</b>	DMF	405	508	103	3.82	5.4
<b>5c</b>	EtOH	402	508	106	3.16	3.3
<b>5c</b>	Glycerol	428	530	102	2.89	36.4
<b>6b</b>	MeCN	457	497	40	4.46	51.4
<b>6b</b>	DMF	460	501	41	4.55	56.9
<b>6b</b>	EtOH	463	497	34	5.10	54.1

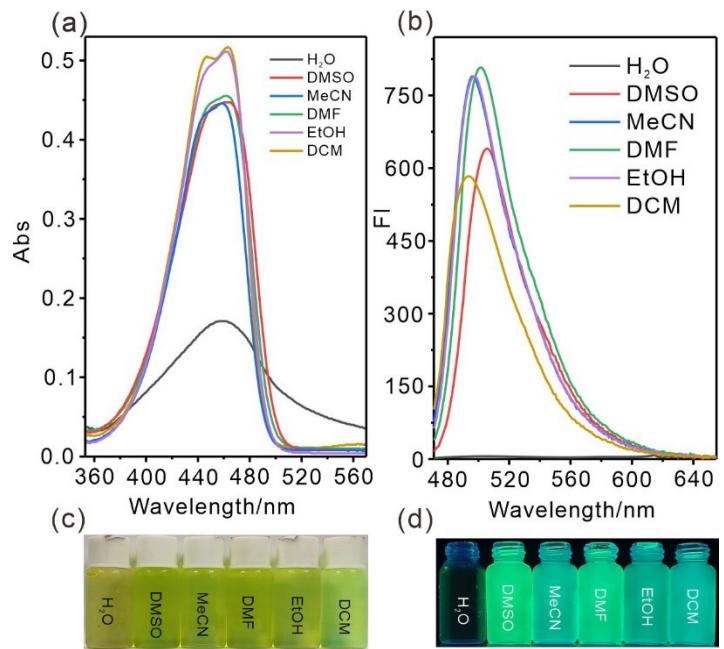
<sup>a</sup> Reported in nm.

<sup>b</sup> Reported in  $10^4 \text{ M}^{-1} \text{ cm}^{-1}$ .

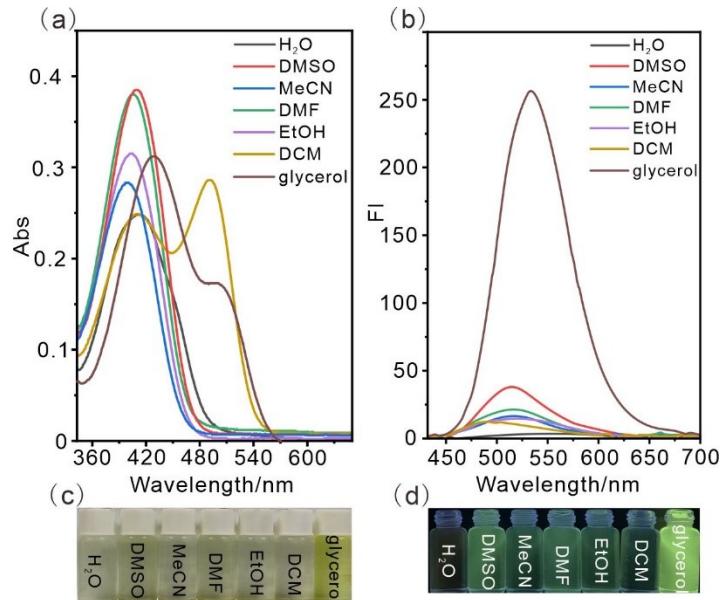
<sup>c</sup> Reported in %. Coumarin-153 ( $\Phi=0.547$  in ethanol) was used as the reference compound.



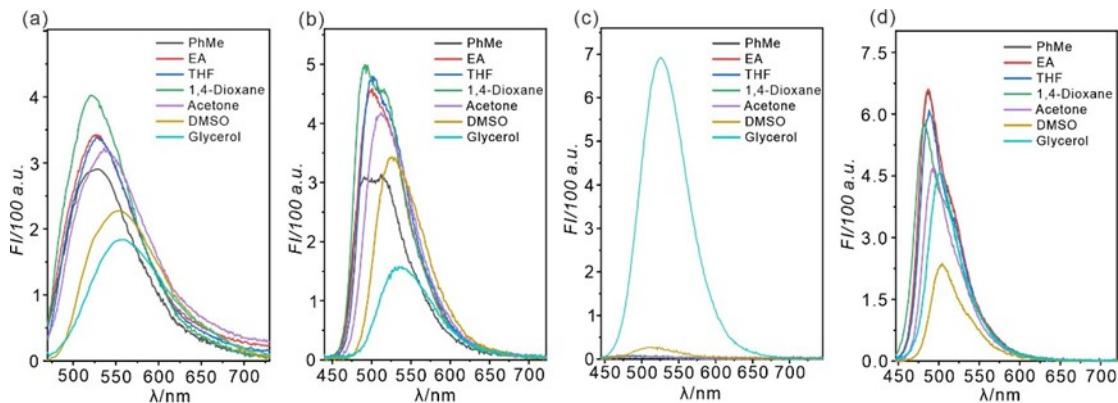
**Fig. S2.** Optical properties of probe **5b** (10  $\mu\text{M}$ ) in solvents of different polarity. (a) UV-vis absorption spectrum. (b) Fluorescence emission spectrum,  $\lambda_{\text{ex}} = 435 \text{ nm}$ , slit widths: 1.5 nm / 3 nm. (c) Photographs under daylight. (d) Photographs under a lamp at 365 nm in dark conditions.



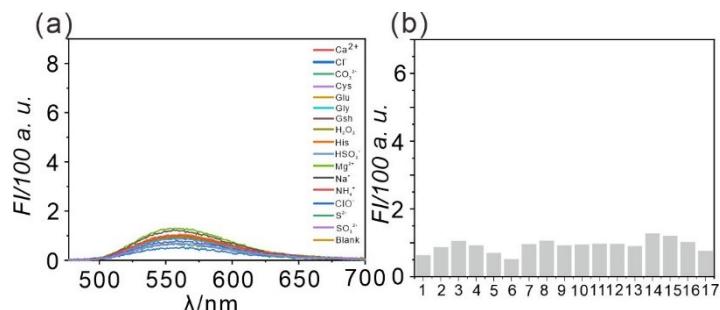
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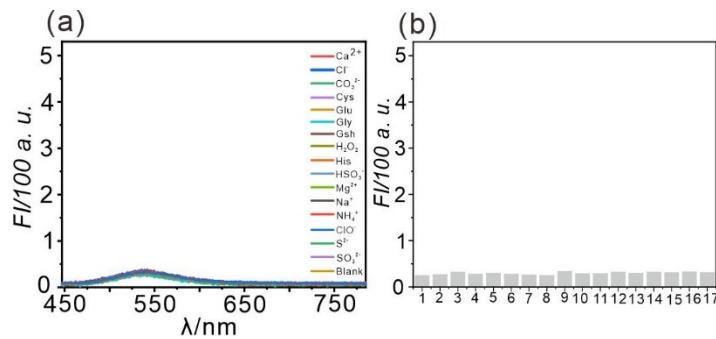
**Fig. S4.** Optical properties of probe **5c** (10  $\mu\text{M}$ ) in solvents of different polarity. (a) UV-vis absorption spectrum. (b) Fluorescence emission spectrum,  $\lambda_{\text{ex}} = 425 \text{ nm}$ , slit widths: 1.5 nm / 3 nm. (c) Photographs under daylight. (d) Photographs under a lamp at 365 nm in dark conditions.



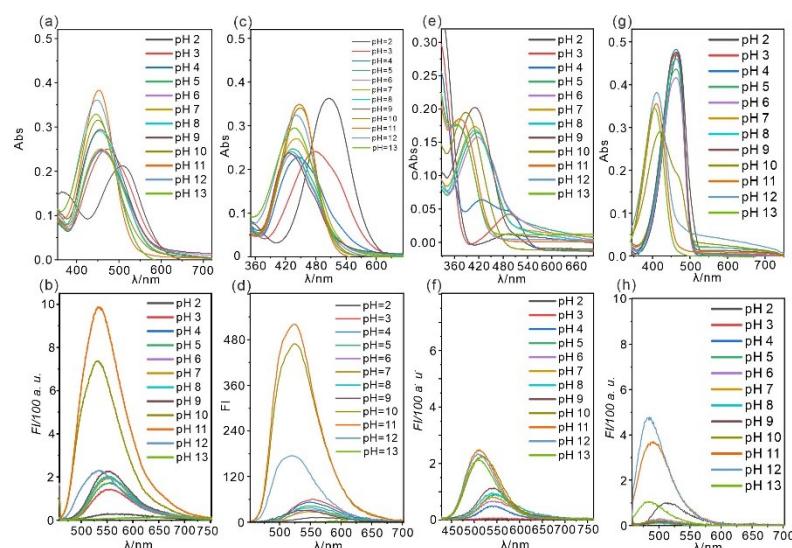
**Fig. S5.** Optical properties of probes **5a** (a), **5b** (b), **5c** (c) and **6b** (d) (10  $\mu\text{M}$ ) in solvents with different solvents.



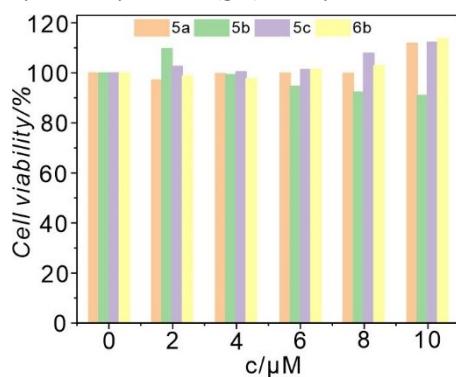
**Fig. S6.** Selectivity experiments of probe **5b**. (a) Fluorescence response of probe **5b** (10  $\mu\text{M}$ ) in the presence of 100  $\mu\text{M}$  of different biologically relevant species (excited at 435 nm, slit widths: 1.5 nm/3 nm); (b) Fluorescence histogram of probe **5b** with analyses, (1. Blank, 2.  $\text{Ca}^{2+}$ , 3.  $\text{Na}^+$ , 4.  $\text{Mg}^{2+}$ , 5.  $\text{NH}_4^+$ , 6.  $\text{ClO}^-$ , 7.  $\text{CO}_3^{2-}$ , 8.  $\text{S}^{2-}$ , 9.  $\text{SO}_3^{2-}$ , 10.  $\text{HSO}_3^-$ , 11.  $\text{Cl}^-$ , 12.  $\text{H}_2\text{O}_2$ , 13. Cys, 14. Glu, 15. Gly, 16. GSH, 17. His).



**Fig. S7.** Selectivity experiments of probes **6b**. (a) Fluorescence response of probe **6b** (10  $\mu\text{M}$ ) in the presence of 100  $\mu\text{M}$  of different biologically relevants (excited at 440 nm, slit widths: 1.5 nm/3 nm); (b) Fluorescence histogram of probe **6b** with analyses, (1. Blank, 2.  $\text{Ca}^{2+}$ , 3.  $\text{Na}^+$ , 4.  $\text{Mg}^{2+}$ , 5.  $\text{NH}_4^+$ , 6.  $\text{ClO}^-$ , 7.  $\text{CO}_3^{2-}$ , 8.  $\text{S}^{2-}$ , 9.  $\text{SO}_3^{2-}$ , 10.  $\text{HSO}_3^-$ , 11.  $\text{Cl}^-$ , 12.  $\text{H}_2\text{O}_2$ , 13. Cys, 14. Glu, 15. Gly, 16. GSH, 17. His).

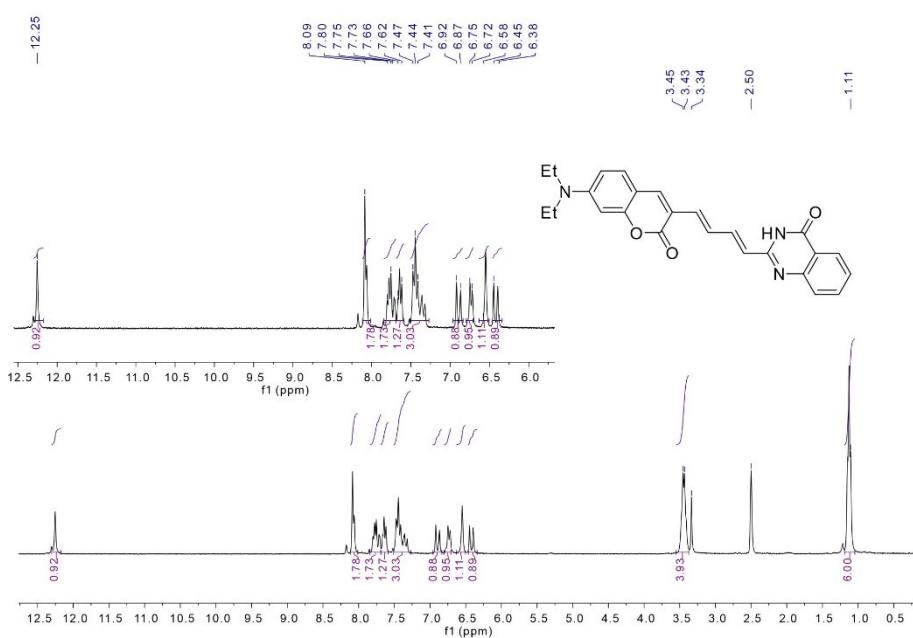


**Fig. S8.** Optical responses of probes **5a-c** and **6b** (10  $\mu\text{M}$ ) towards different pH values in PBS buffer-DMSO (9 / 1, v / v) solutions. (a-b) Absorption and emission spectra of probe **5a**; (c-d) Absorption and emission spectra of probe **5b**; (e-f) Absorption and emission spectra of probe **5c**; (g-h) Absorption and emission spectra of probe **6b**.



**Fig. S9.** Cell viabilities of HeLa cells treated by probes **5a-c** and **6b** with different concentration (0, 2, 4, 6, 8, 10  $\mu\text{M}$ ) using the CCK-8 method.

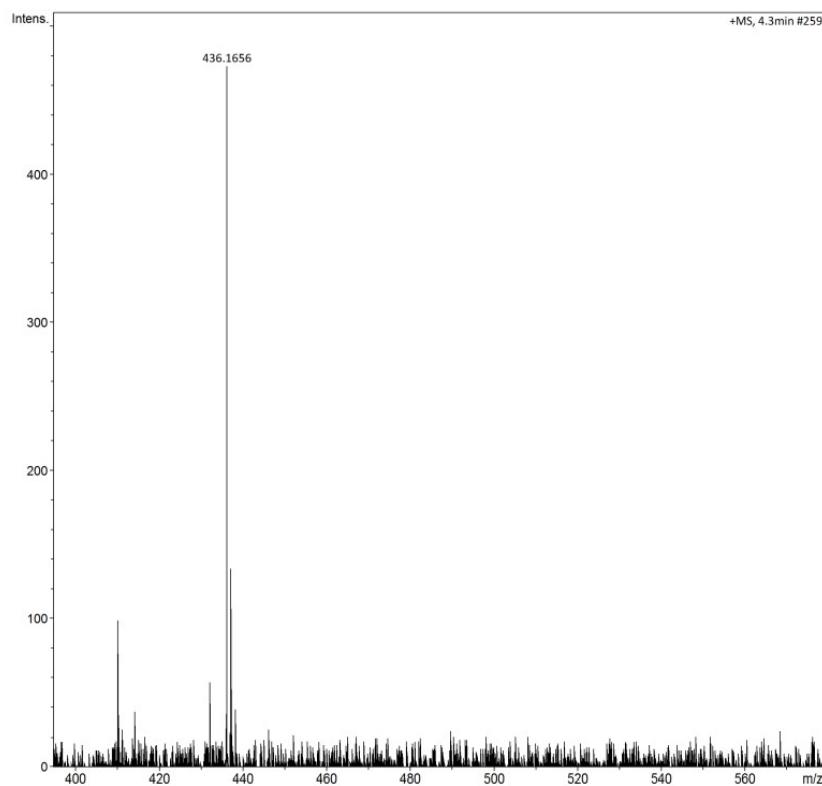
<sup>1</sup>H NMR (300Hz, DMSO-*d*<sub>6</sub>)



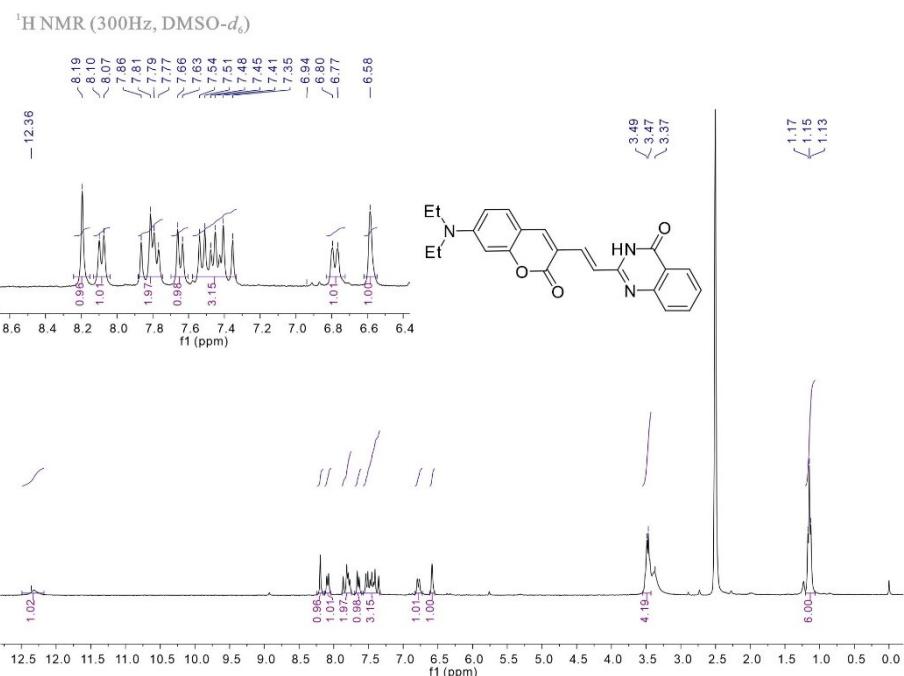
**Fig. S10.** <sup>1</sup>H NMR spectrum of probe 5a.

**Acquisition Parameter**

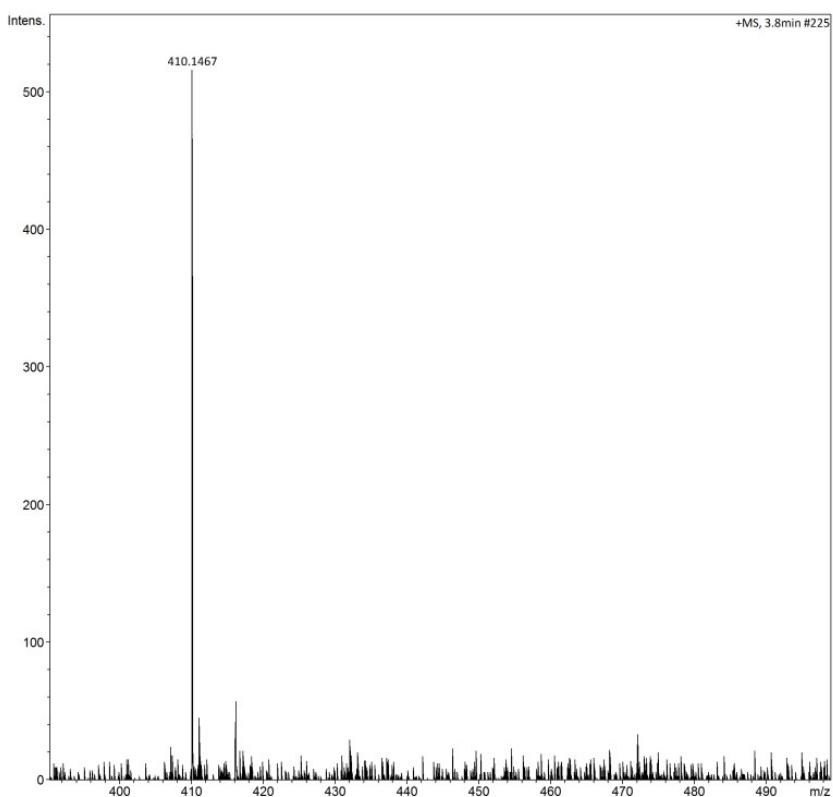
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Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Waste



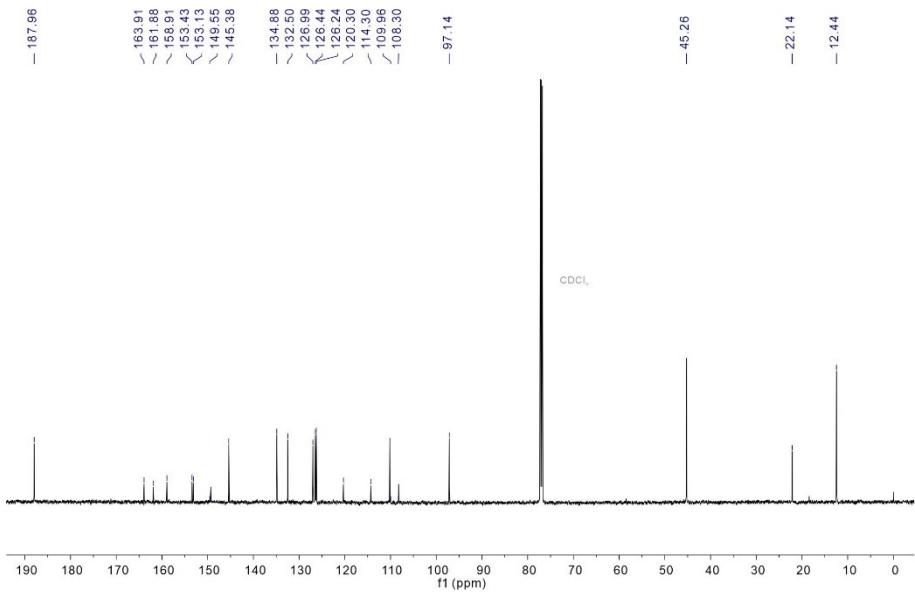
**Fig. S11** HRMS(ESI<sup>+</sup>) spectrum of probe 5a.



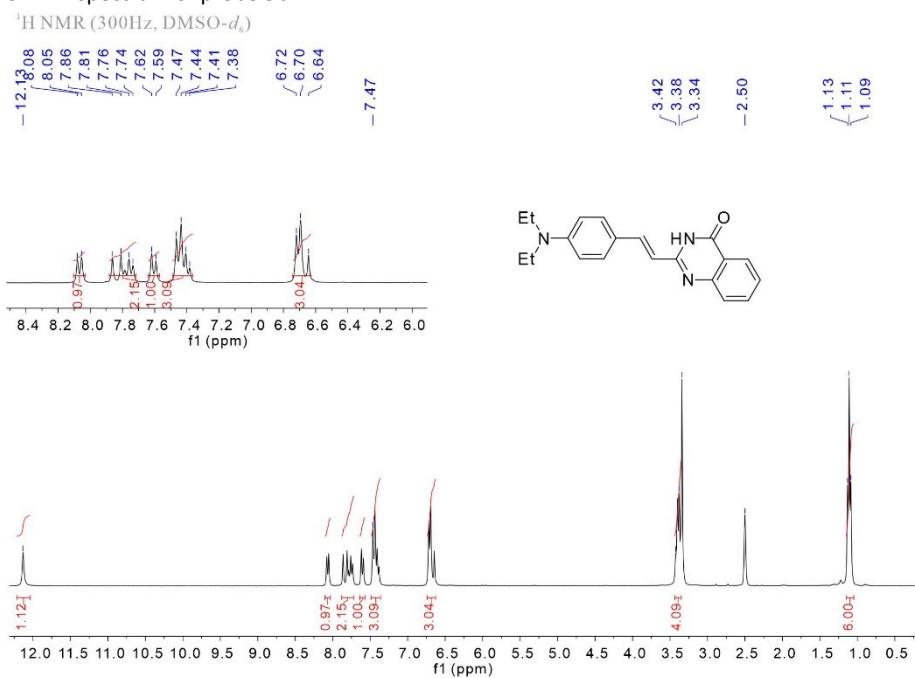
Acquisition Parameter					
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Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Waste



**Fig. S13** HRMS(ESI<sup>+</sup>) spectrum of probe 5b.

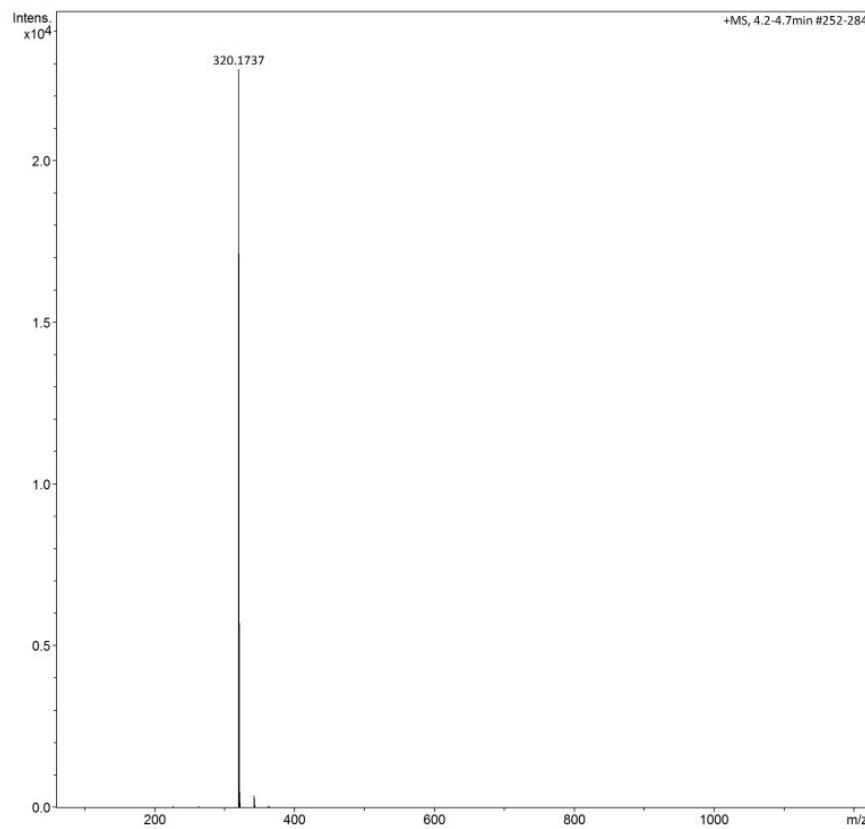


**Fig. S14.**  $^{13}\text{C}$  NMR spectrum of probe **5b**.

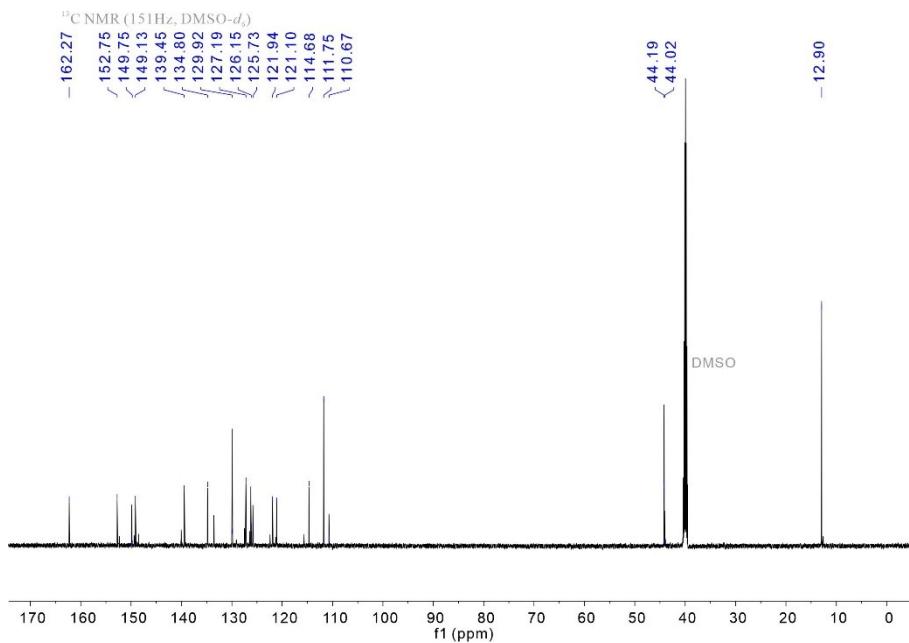


**Fig. S15.**  $^1\text{H}$  NMR spectrum of probe **5c**.

Acquisition Parameter					
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Waste



**Fig. S16.** HRMS( $\text{ESI}^+$ ) spectrum of probe **5c**.



**Fig. S17**  $^{13}\text{C}$  NMR spectrum of probe **5c**.

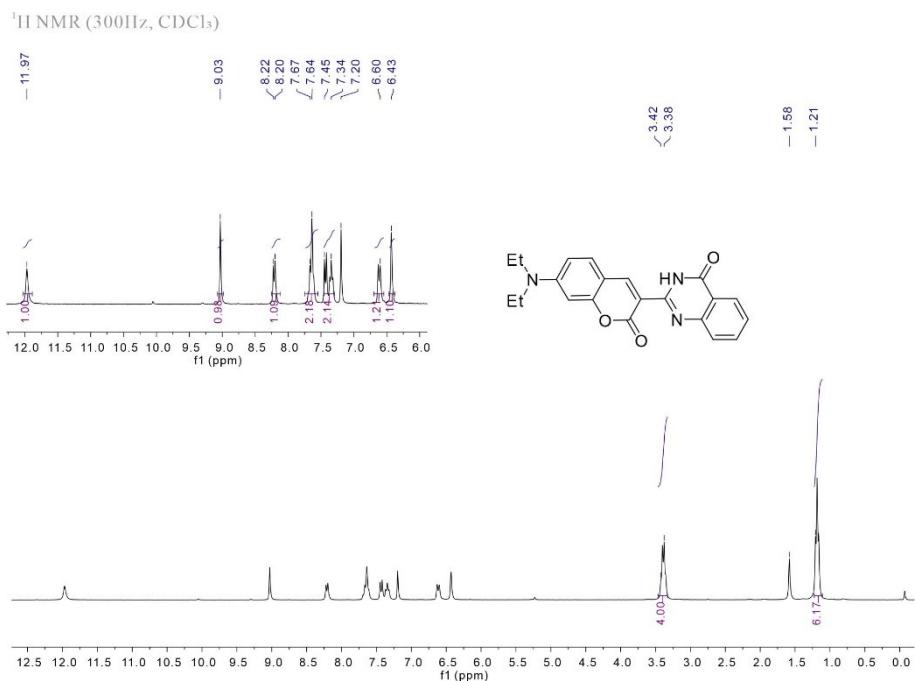


Fig. S18. <sup>1</sup>H NMR spectrum of probe 6b.

Acquisition Parameter					
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Scan End	1500 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Waste

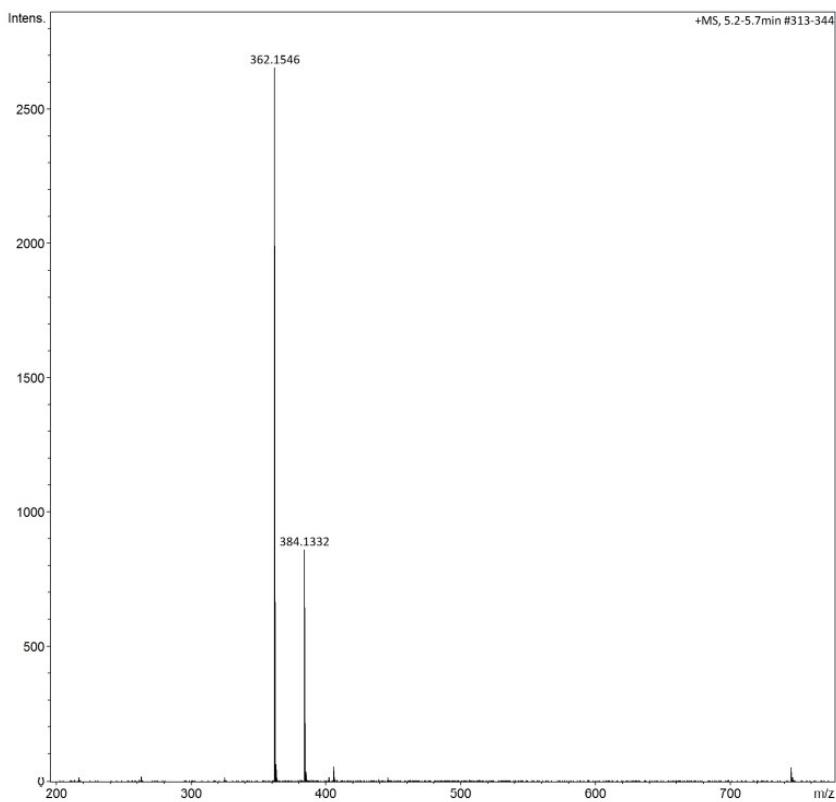
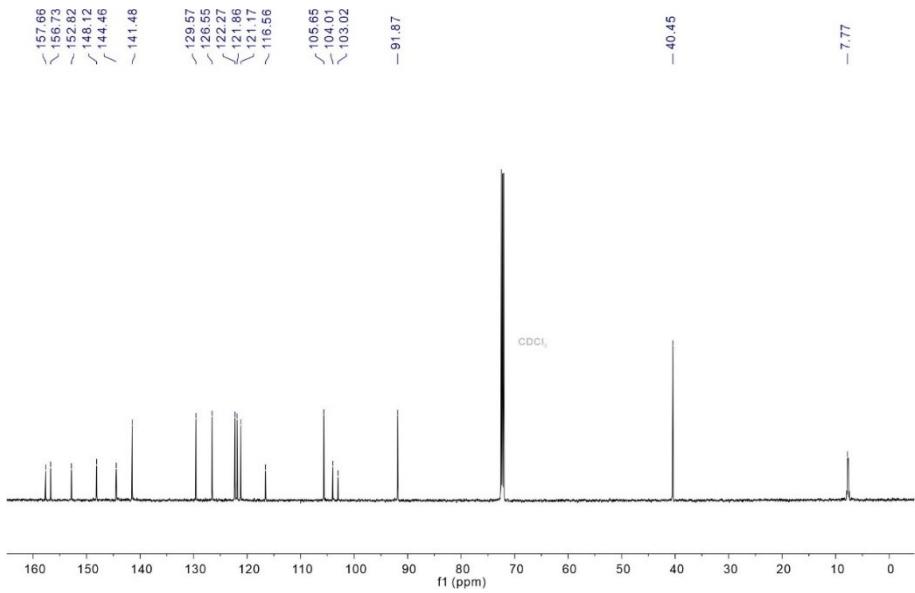


Fig. S19 HRMS(ESI<sup>+</sup>) spectrum of probe 6b.



**Fig. S20**  $^{13}\text{C}$  NMR spectrum of probe **6b**.