Electronic Supporting Information

An alternative modular 'click-S_NAr-click' approach to develop subcellular localised fluorescent probes to image mobile Zn^{2+}

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General procedures

Unless otherwise stated, reactions were carried out using commercially available reagents, used as supplied from Sigma Aldrich, Alfa Aesar, or Tokyo Chemical Industry (TCI), in combination with solvents from Honeywell Solvents. ER-tracker red, Mito-tracker red and Lyso-tracker red were purchased from Enzo Life Sciences. The HeLa cell line used for fluorescence imaging was provided from ATCC. Anhydrous DCM and DMF were obtained from an MBRAUN MB SPS-800 solvent purification system. "H_2O" refers to deionized water.

For syntheses requiring anhydrous conditions, reactions were carried out under a nitrogen atmosphere using oven-dried glassware. Solvents were removed *in vacuo* using a Heidolph Hei-VAP Value G1 rotary evaporator with a water and dry ice bath condenser. Analytical thin layer chromatography was carried out on Merck Kiesel gel 60 aluminium-backed silica plates, with visualization using short-wave ultraviolet light (254 nm) or staining with $KMnO_4$ or phosphomolybdic acid (PMA) stain. Column chromatography was carried out using BDH (40-60 μm) silica gel.

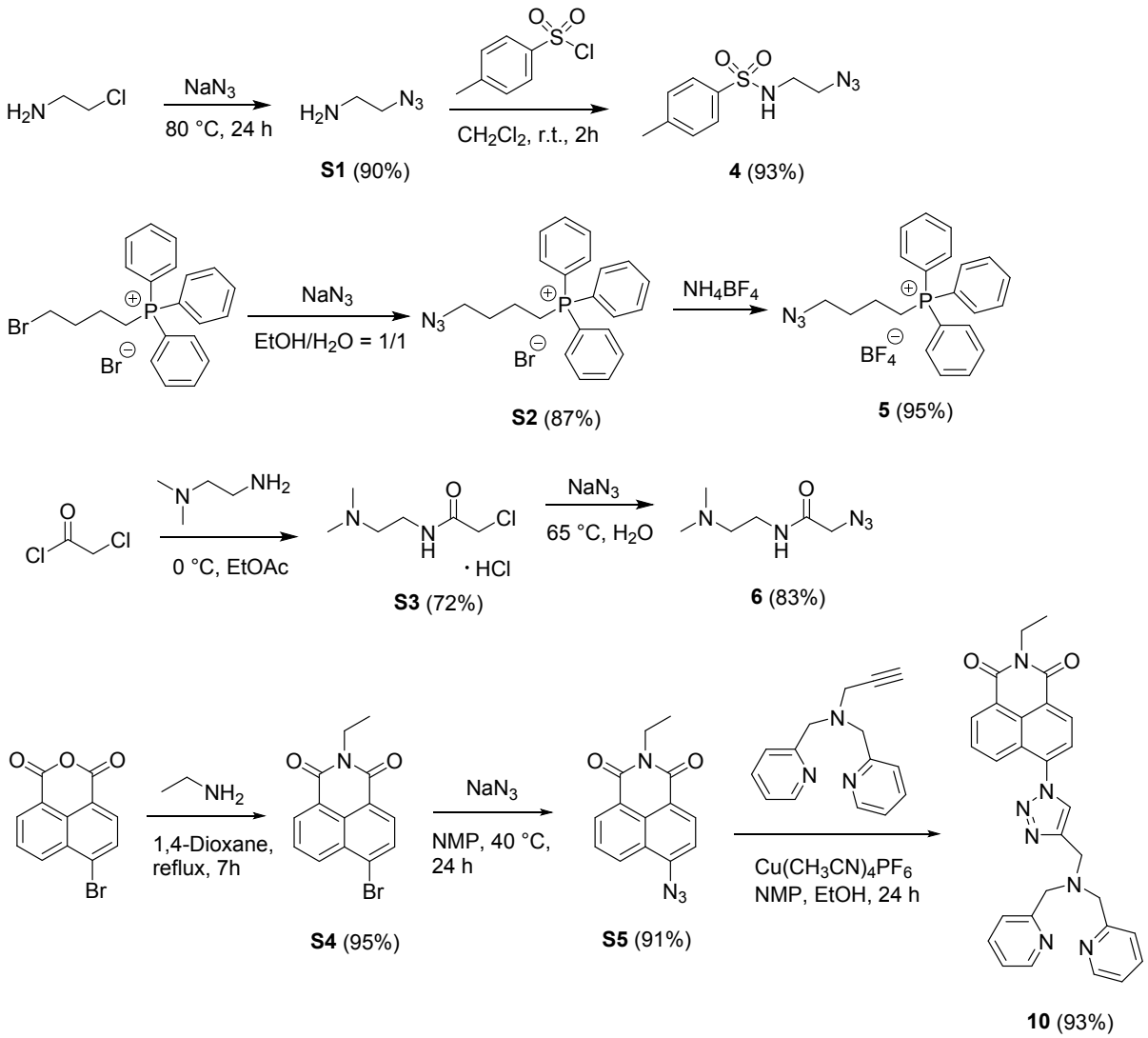
Infrared spectra were obtained on a Bruker Tensor 37 FTIR spectrometer in the range 4000-600 cm^{-1}. UV-Vis spectra were obtained on a PerkinElmer Lambda 35 UV/Vis spectrometer. Fluorescence spectra were measured on an Agilent Cary eclipse fluorescence spectrophotometer with a 1 cm path length cell. The fluorescence microscope images were obtained from a Logos CELENA S digital imaging system with 40× magnification. ^1H NMR spectra were recorded at 400 MHz on a Bruker Avance I or Bruker Avance III spectrometer. Chemical shifts are reported in δ (ppm), quoted to the nearest 0.01 ppm and referenced to the residual solvent peak used as the internal standard: $CHCl_3$ (7.26 ppm), MeOH (3.31 ppm), DMSO (2.50 ppm) and CH_3CN (1.94 ppm). Coupling constants (*J*) are measured in Hertz (Hz)

and reported to 1 d.p. Peak multiplicities for resonances are noted as standard abbreviations: s, singlet; d, doublet; dd, double doublet; dt, doublet of triplets, t, triplet; q, quartet; m, unresolved multiplet; bs, broad singlet. ^{13}C NMR spectra were recorded at 101 MHz on a Bruker Avance III spectrometer. Chemical shifts (δ) are quoted to the nearest 0.1 ppm, with reference to the given solvent $CDCl_3$ (77.2 ppm), MeOD (49.0 ppm), DMSO (39.5 ppm) and CD_3CN (118.3 ppm) as the internal standard. Electrospray ionization mass spectrometry was carried out by the EPSRC National Mass Spectrometry Service, University of Wales, Swansea on a Thermofisher LTQ Orbitrap XL. Molecular ions are reported for ^{35}Cl and ^{79}Br isotopes. Melting points were measured on a Stuart SMP3 melting point apparatus and are uncorrected.

Unless noted otherwise, the solution for all photophysical tests was a 0.01 mM HEPES buffer (pH 7.4) made up from a DMSO stock solution to dissolve probes with a 1% total DMSO concentration. $ZnCl_2$ was used as the Zn^{2+} source to simulate the chloride-rich biological environment. The medium used to incubate HeLa cells was Dulbecco's Modified Eagle Medium (DMEM), supplemented with 10% heat-deactivated fetal bovine serum (FBS). AlamarBlue™ was used to check cells' viability according to manufacturer's instructions. For co-localisation experiments, all cells were treated with probes for 1 h and then ER-tracker red, Mito-tracker red and Lyso-tracker red were added in different groups respectively for another 0.5 h incubation. For Zn^{2+} response experiments, all cells were treated with probes for 1 h, and then zinc pyrithione (100 μM) and *N*,*N*,*N*',*N*'-tetrakis(2-pyridinylmethyl)-1,2-ethanediamine (TPEN) (100 μM) were added to different groups respectively for 15 minutes incubation. All the images of cells were processed by ImageJ software and the fluorescence intensity in cells was read directly from ImageJ before processing.

Experimental procedures

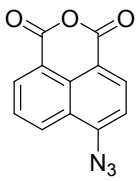
The synthetic route to different organelle targeting unit azides **4**,[1] **5**,[2,3] **6**[3,4] and non-targeting probe **10**[5] is shown below:



Scheme S1 The synthetic route towards azides **4-6** and non-targeting probe **10**.

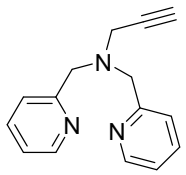
Experimental procedures

6-Azido-1*H*,3*H*-benzo[*de*]isochromene-1,3-dione (**1**)



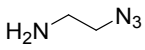
To a solution of 4-bromo-1,8-naphthalic anhydride (500 mg, 1.80 mmol) in DMF (5.0 mL), NaN_3 (175 mg, 2.69 mmol) was added and the mixture stirred at room temperature for 12 h. After the reaction was complete, water (30 mL) was added and the precipitate formed was collected by filtration, then washed with water (50 mL) and dried *in vacuo* to obtain **1** (418 mg, 97 %) as a pale-yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (dd, 1H, J = 7.3, 1.1), 8.62 (d, 1H, J = 8.0), 8.55 (dd, 1H, J = 8.5, 1.1), 7.82 (dd, 1H, J = 8.5, 7.3), 7.53 (d, 1H, J = 8.0). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7, 160.2, 145.4, 134.4, 134.1, 131.4, 130.5, 127.3, 124.5, 118.6, 115.2, 114.3. All spectroscopic data were consistent with those previously reported.[6]

N,N-bis(Pyridin-2-ylmethyl)prop-2-yn-1-amine (**2**)



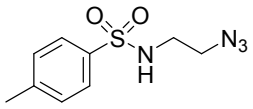
A mixture of propargylamine (1.50 g, 27.3 mmol) and potassium carbonate (22.8 g, 164 mmol) was stirred in acetonitrile (140 mL) for 5 mins. Then 2-picolyl chloride hydrochloride (9.84 g, 60.0 mmol) dissolved in acetonitrile (140 mL) was added. The resulting solution was stirred under reflux for 5 days. After the reaction was complete, the mixture was filtered and the filtrate evaporated under reduced pressure. The resulting brown oil was dissolved in distilled water (100 mL) and extracted with dichloromethane (3 × 50 mL). The organic layers were combined and dried over $MgSO_4$. The solvent was evaporated to afford **2** (6.04 g, 93%) as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56-8,53 (m, 2H), 7.69-7.61 (m, 2H), 7.54-7.48 (m, 2H), 7.19-7.12 (m, 2H), 3.92 (s, 4H), 3.42 (d, 2H, J = 2.4), 2.29 (t, 1H, J = 2.4). All spectroscopic data were consistent with those previously reported.[7]

2-Azidoethan-1-amine (**S1**)



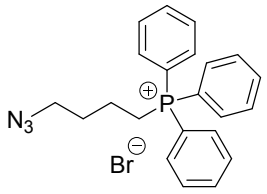
To a solution of 2-chloroethanamine hydrochloride (400 mg, 3.44 mmol) in H_2O (4.0 mL) was added NaN_3 (672 mg, 10.4 mmol) at room temperature. After stirring at 80 °C for 24 h, the reaction was quenched with aqueous KOH solution (15% w/v, 1.0 mL). The aqueous layer was extracted with diethyl ether (3 × 20 mL) and the combined organic layers were washed with brine (10 mL), dried over anhydrous $MgSO_4$, filtered and concentrated *in vacuo* to give **S1** as a colourless oil (265 mg, 90 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.36 (t, 2H, J = 5.7), 2.90-2.85 (m, 2H), 1.49-1.41 (bs, 2H). All spectroscopic data were consistent with those previously reported.[8]

N-(2-Azidoethyl)-4-methylbenzenesulfonamide **(4)**



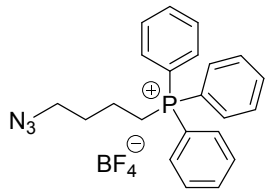
To a solution of **S1** (265 mg, 3.08 mmol) in CH_2Cl_2 (4.0 mL), 4-methylbenzenesulfonyl chloride (587 mg, 3.08 mmol) was added at room temperature and the reaction mixture was stirred for 2 h and then concentrated *in vacuo*. The residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 5:1) to give **4** as a white solid (688 mg, 93 %, M.p. 67-69 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, 2H, J = 8.3), 7.32 (d, 2H, J = 8.3), 5.06 (t, 1H, J = 5.9), 3.39 (t, 2H, J = 5.9 Hz), 3.14-3.06 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9, 136.9, 130.0, 127.2, 51.0, 42.4, 21.6. IR: (υ_{max}/cm^{-1}) 3265, 2102, 1598, 1417, 1304, 1157, 1085, 939, 811, 685. HR-ESI MS (*m/z*) [M-H]$^-$ calcd for $C_9H_{11}N_4O_2S$ 239.0603, found 239.0621.

(4-Azidobutyl)triphenylphosphonium bromide (**S2**)



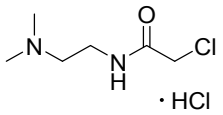
A solution of sodium azide (140 mg, 2.20 mmol) and (4-bromobutyl)triphenylphosphonium bromide (960 mg, 2.00 mmol) in EtOH/H_2O (1:1, 20 mL) was heated at reflux under N_2 overnight. The mixture was cooled to room temperature and the solvent evaporated under reduced pressure to afford a yellow oil. To the oil was added H_2O (2.0 mL) and the precipitate formed was collected by filtration, washed with water (20 mL) and dried *in vacuo* to afford **S2** (850 mg, 87%) as a white solid . ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.67 (m, 15H), 4.08-3.97 (m, 2H), 3.52-3.42 (m, 2H), 2.13-2.02 (m, 2H), 1.83-1.71 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.1 (d, J = 3.0), 133.7 (d, J = 10.0), 130.6 (d, J = 12.6), 118.2 (d, J = 86.2), 50.7, 29.2 (d, J = 16.7), 22.3 (d, J = 50.8), 19.9 (d, J = 4.0). All spectroscopic data were consistent with those previously reported.[2]

(4-Azidobutyl)triphenylphosphonium tetrafluoroborate **(5)**



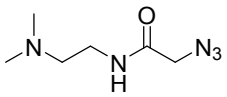
(4-Azidobutyl)triphenylphosphonium bromide **S2** (2.27 g, 5.15 mmol) was dissolved in CH_2Cl_2 (40.0 mL). This solution was thoroughly washed with a saturated aqueous solution of ammonium tetrafluoroborate (3 × 50.0 mL). The organic phase was dried over $MgSO_4$ and the solvent was removed *in vacuo* to yield **5** (2.18 g, 95%) as a white solid.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.64 (m, 15H), 3.38-3.22 (m, 4H), 1.89-1.79 (m, 2H), 1.74-1.63 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.3 (d, J = 3.0), 133.4 (d, J = 9.9), 130.6 (d, J = 12.6), 117.9 (d, J = 86.4), 50.4, 29.1 (d, J = 16.9), 21.4 (d, J = 52.0), 19.8 (d, J = 3.8). ^{31}P NMR (162 MHz, $CDCl_3$) δ 23.64. ^{19}F NMR (377 MHz, $CDCl_3$) δ -152.16 (d, J = 19.8). All spectroscopic data were consistent with those previously reported.[3]

2-Chloro-*N*-(2-(dimethylamino)ethyl)acetamide hydrochloride (**S3**)



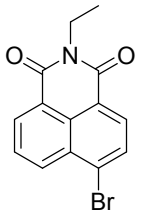
Chloroacetyl chloride (2.26 g, 20.0 mmol) in ethyl acetate (50.0 mL) was cooled to 0 ºC and a solution of *N*,*N*-dimethylethylenediamine (1.77 g, 20.0 mmol) in ethyl acetate (50.0 mL) was added dropwise. The reaction was stirred at 0 ºC for 1 h under nitrogen. The precipitate that formed was collected by filtration, washed with diethyl ether (50.0 mL) and then dried *in vacuo* to yield the product in its hydrochloride salt form **S3** (2.90 g, 72%) as a white powder. ^{1}H NMR (400 MHz, DMSO) δ 8.72-8.64 (bs, 1H), 4.13 (s, 2H), 3.50-3.44 (m, 2H), 3.15 (t, 2H, J = 6.2), 2.76 (s, 6H). All spectroscopic data were consistent with those previously reported.[4]

2-Azido-*N*-(2-(dimethylamino)ethyl)acetamide **(6)**



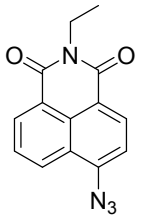
2-Chloro-*N*-(2-diethylamino-ethyl)acetamide hydrochloride **S3** (1.01 g, 5.00 mmol) was dissolved in H_2O (25.0 mL), NaN_3 (1.96 g, 30.0 mmol) was then added to the flask and the reaction mixture stirred for 48 h at 65 °C. After cooling to room temperature, the solution was adjusted to pH 10 using saturated aqueous $NaHCO_3$, and extracted with EtOAc (3 × 20.0 mL). The remaining aqueous layer was adjusted to pH 14 with aqueous NaOH (1.0 M), and extracted with EtOAc (3 × 20.0 mL). The organic extracts were combined, dried over $MgSO_4$ and the solvent was removed *in vacuo* to give **6** (0.710 g, 83%) as a pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.91-6.65 (bs, 1H), 3.91 (s, 2H), 3.34-3.26 (m, 2H), 2.41-2.34 (m, 2H), 2.19 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 57.6, 52.7, 45.2, 36.8. All spectroscopic data were consistent with those previously reported.[3]

6-Bromo-2-ethyl-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione (**S4**)



4-Bromo-1,8-naphthalic anhydride (550 mg, 2.00 mmol) and ethylamine (70% solution in water, 0.14 mL, 2.40 mmol) were refluxed in dioxane (20 mL) for 7 hours. Then the reaction mixture was cooled to room temperature and a second aliquot of ethylamine (70% solution in water, 0.10 mL, 1.60 mmol) was added and the mixture heated at reflux for another 7 hours. The solution was cooled to room temperature, poured into H_2O (100 mL) and the precipitate that formed was collected by filtration, washed with H_2O (100 mL) and dried *in vacuo* to give **S4** (0.580 g, 95%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (dd, 1H, J = 7.4, 0.8), 8.57 (dd, 1H, J = 8.4, 0.8), 8.42 (d, 1H, J = 7.9), 8.04 (d, 1H, J = 7.9), 7.84 (dd, 1H, J = 8.4, 7.4), 4.24 (q, 2H, J = 7.1), 1.34 (t, 3H, J = 7.1). All spectroscopic data were consistent with those previously reported.[5]

6-Azido-2-ethyl-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione **(S5)**



Compound **S4** (490 mg, 1.60 mmol) was dissolved in *N*-methypyrrolidionone (5.0 mL) to which sodium azide (130 mg, 1.90 mmol) was added and the mixture was stirred at 40 °C for 24 h. The reaction mixture was diluted with H_2O (30 mL) and extracted with EtOAc (3 × 20 mL). The combined organic phases were washed with brine (30 mL) and dried over $MgSO_4$, concentrated *in vacuo* to give **S5** (390 mg, 91%) as a dark brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (dd, 1H, J = 7.4, 1.0), 8.58 (d, 1H, J = 8.0), 8.43 (dd, 1H, J = 8.4, 1.0), 7.74 (dd, 1H, J = 8.4, 7.4), 7.46 (d, 1H, J = 8.0), 4.24 (q, 2H, J = 7.1), 1.33 (t, 3H, J = 7.1). All spectroscopic data were consistent with those previously reported.[5]

Photophysical properties

UV-Vis abosorption spectra

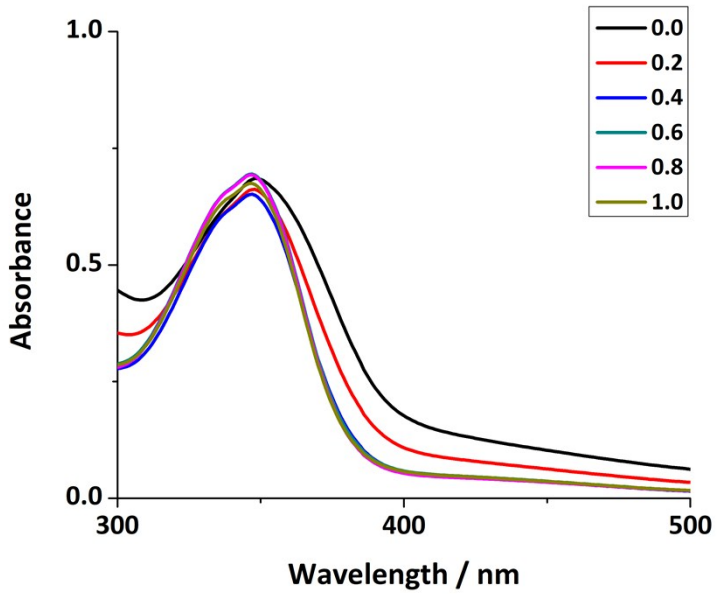


Fig. S1 The UV-Vis spectra of **7** (50 μM) and its complex with different equivalents of Zn^{2+}.

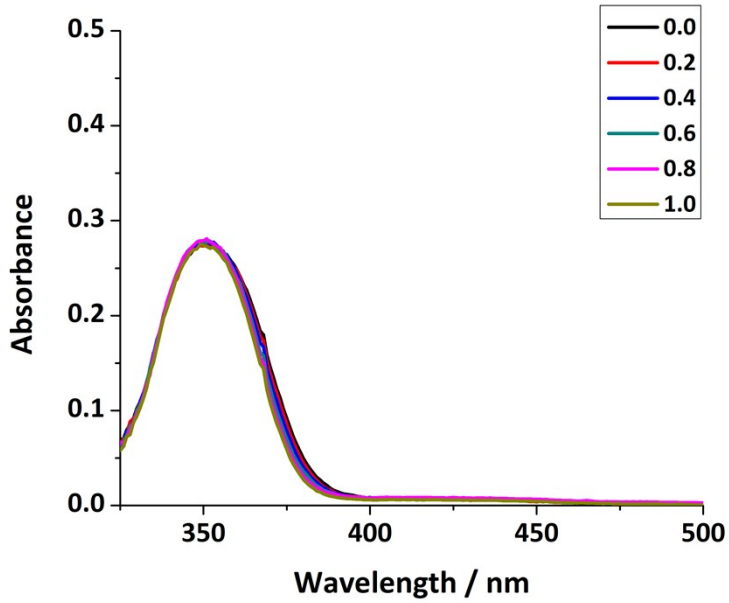


Fig. S2 The UV-Vis spectra of **8** (50 μM) and its complex with different equivalents of Zn^{2+}.

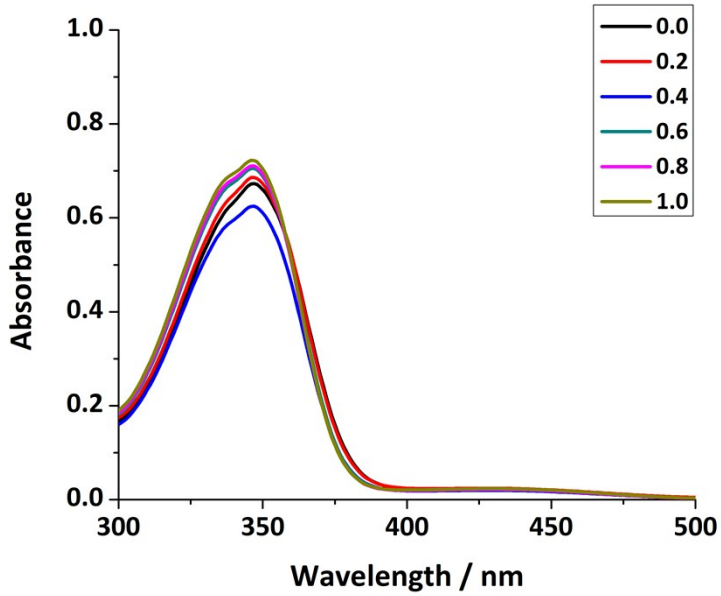


Fig. S3 The UV-Vis spectra of **9** (50 μM) and its complex with different equivalents of Zn^{2+}.

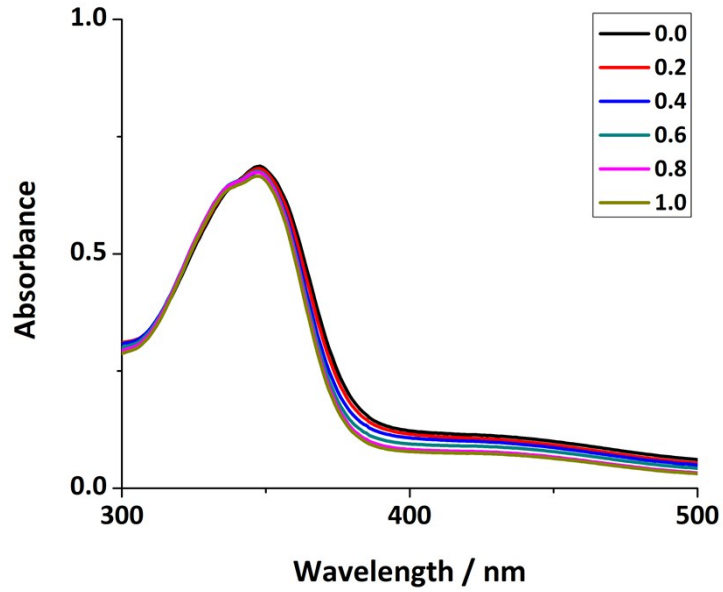


Fig. S4 The UV-Vis spectra of **10** (50 μM) and its complex with 1 equivalent of Zn^{2+}.

Fluorescence titrations

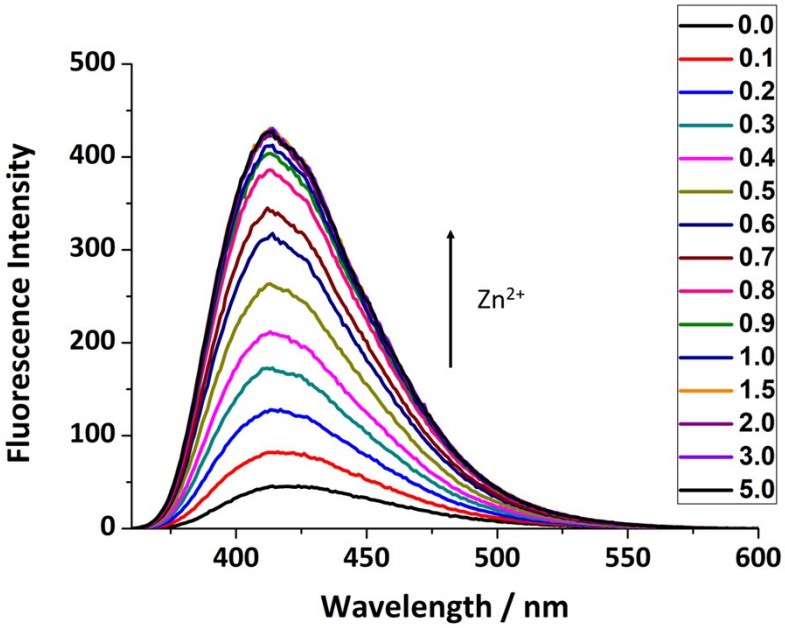


Fig. S5 The fluorescence response of **8** (50 μM) to different equivalents of Zn^{2+}. (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

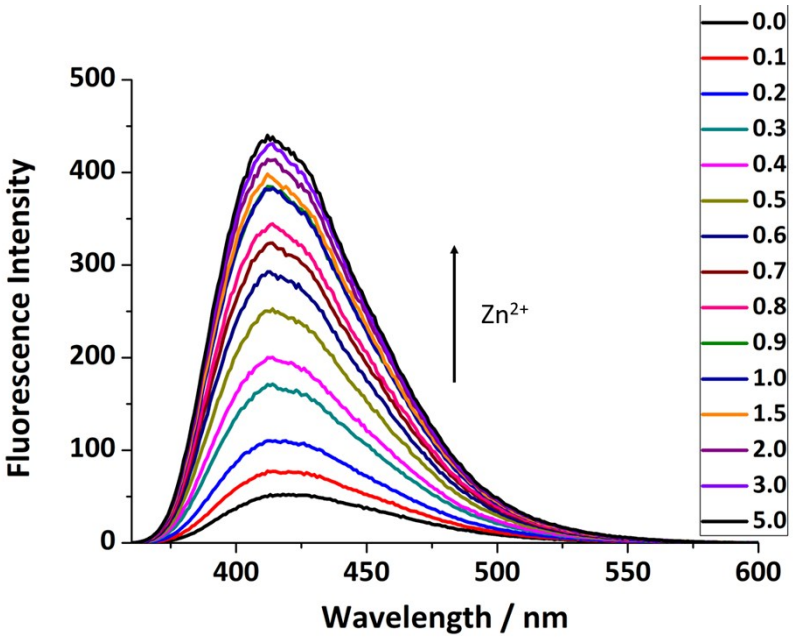


Fig. S6 The fluorescence response of **9** (50 μM) to different equivalents of Zn^{2+}. (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

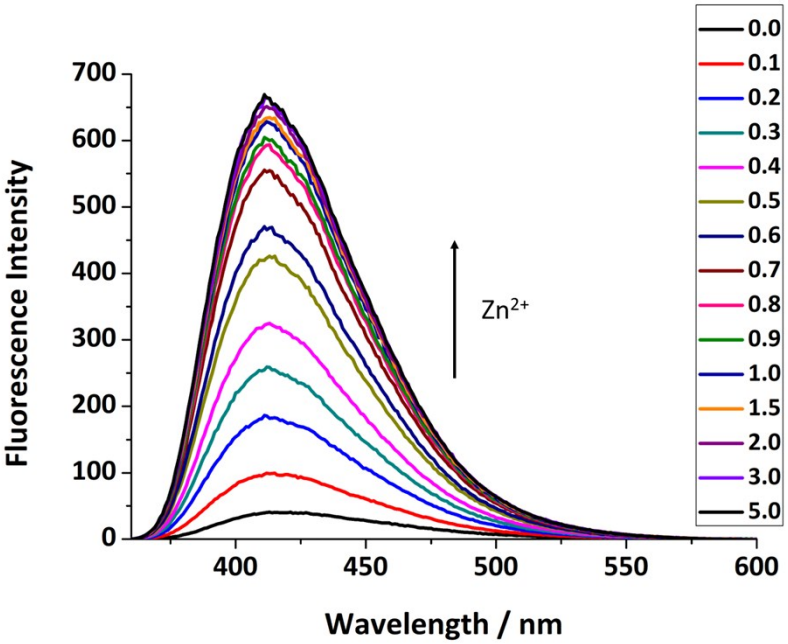


Fig. S7 The fluorescence response of **10** (50 μM) to different equivalents of Zn^{2+}. (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

Job's plot

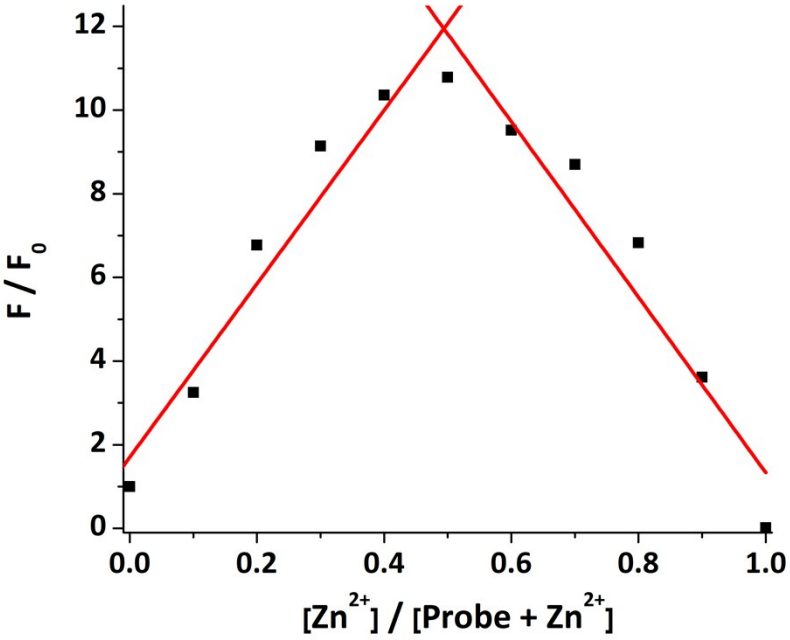


Fig. S8 The Job's plot to determine the stoichiometry of the complex formed between **7** and Zn^{2+}. The total amount of [Probe + Zn^{2+}] was 100 μM, (λ_{ex} = 346 nm, λ_{em} = 414 nm, slit width: 5/2.5 nm)

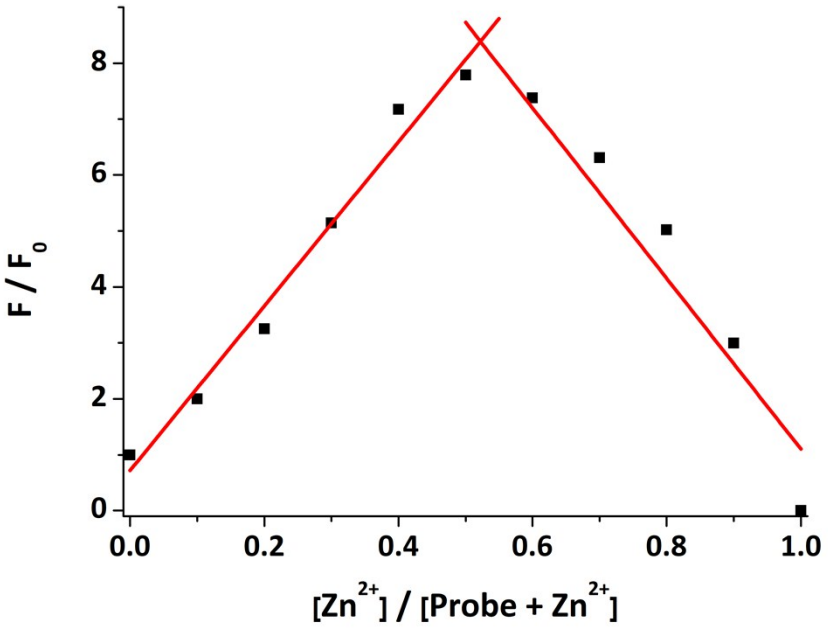


Fig. S9 The Job's plot to determine the stoichiometry of the complex formed between **8** and Zn^{2+}. The total amount of [Probe + Zn^{2+}] was 100 μM, (λ_{ex} = 346 nm, λ_{em} = 414 nm, slit width: 5/2.5 nm)

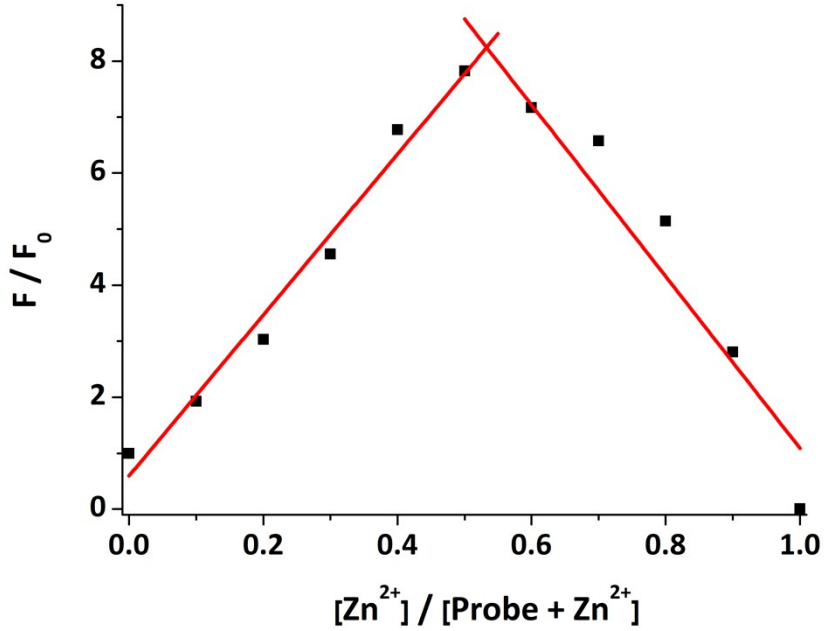


Fig. S10 The Job's plot to determine the stoichiometry of the complex formed between **9** and Zn^{2+}. The total amount of [Probe + Zn^{2+}] was 100 μM, (λ_{ex} = 346 nm, λ_{em} = 414 nm, slit width: 5/2.5 nm)

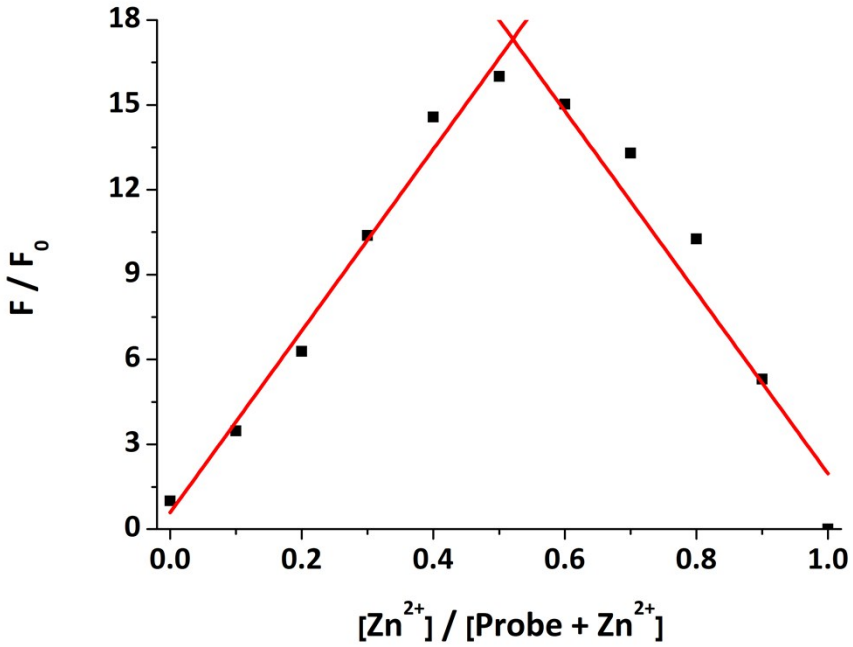


Fig. S11 The Job's plot to determine the stoichiometry of the complex formed between **10** and Zn^{2+}. The total amount of [Probe + Zn^{2+}] was 100 μM, (λ_{ex} = 346 nm, λ_{em} = 414 nm, slit width: 5/2.5 nm)

Dissociation constant measurement

A series of HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid) buffer solutions (50 mM, pH 7.2, 0.1 M KCl) containing various amounts of $ZnCl_2$ (0 ~ 9.0 mM) and 10 mM of EGTA (ethylene glycol-bis(2-aminoethylether)-*N*,*N*,*N*′,*N*′-tetraacetic acid) were prepared. The $[Zn^{2+}]_{free}$ was calculated followed the reported methods.[9–11]

The calculated $[Zn^{2+}]_{free}$ concentration of each solution is:

$[Zn^{2+}]_{total}$ (mM)	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5
$[Zn^{2+}]_{free}$ (nM)	0.00	0.14	0.29	0.46	0.66	0.87	1.11	1.39
$[Zn^{2+}]_{total}$ (mM)	4.0	4.5	5.0	6.0	7.0	8.0	9.0	
$[Zn^{2+}]_{free}$ (nM)	1.73	2.12	2.59	3.88	6.04	10.36	23.31	

To determine the apparent dissociation constants for probes **7**-**10**, the fluorescence titration curves at concentrations 1 μM, 0.1 μM and 0.01 μM were obtained and fitted to Equation S1.[11,12] (shown in Figures S12-S15)

$$\frac{F}{F_0} = 1 + \left(\frac{F_{max}}{F_0} - 1\right)\frac{[Zn^{2+}]_{free}}{K_d + [Zn^{2+}]_{free}}$$

Equation S1 Equation used to determine K_d for all probes. F is the observed fluorescence intensity, F_0 is the observed fluorescence of the probe alone. Non-linear curve fitting analysis was used to determine F_{max}/F_0 and K_d.

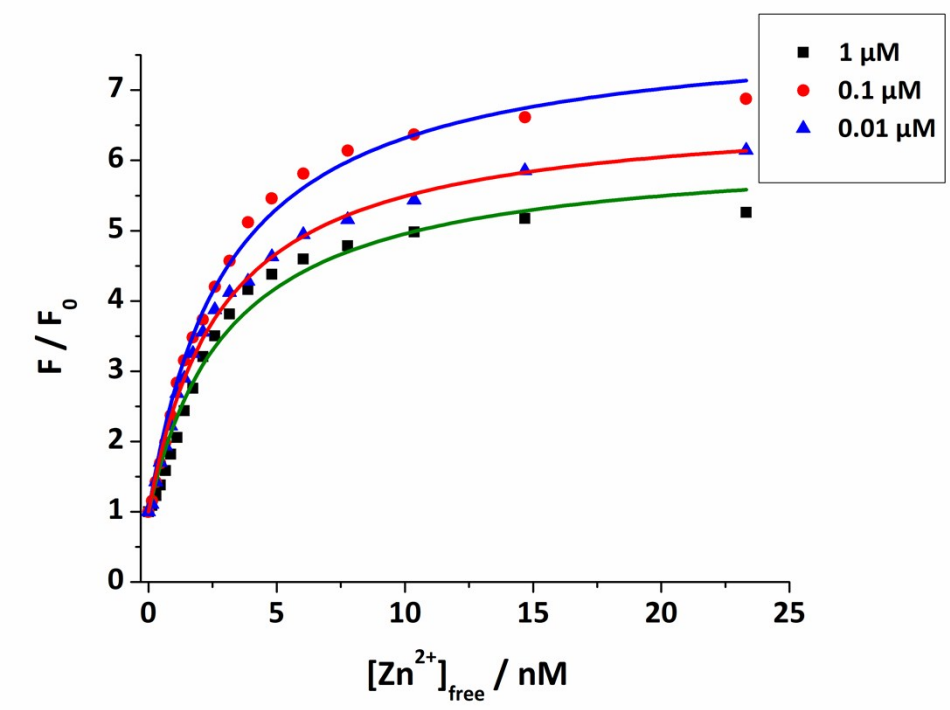


Fig. S12 The non-linear curve fitting of the fluorescence intensity of **7** at different concentrations against $[Zn^{2+}]_{free}$ applying Equation S1. (λ_{ex} = 346 nm, λ_{em} = 414 nm)

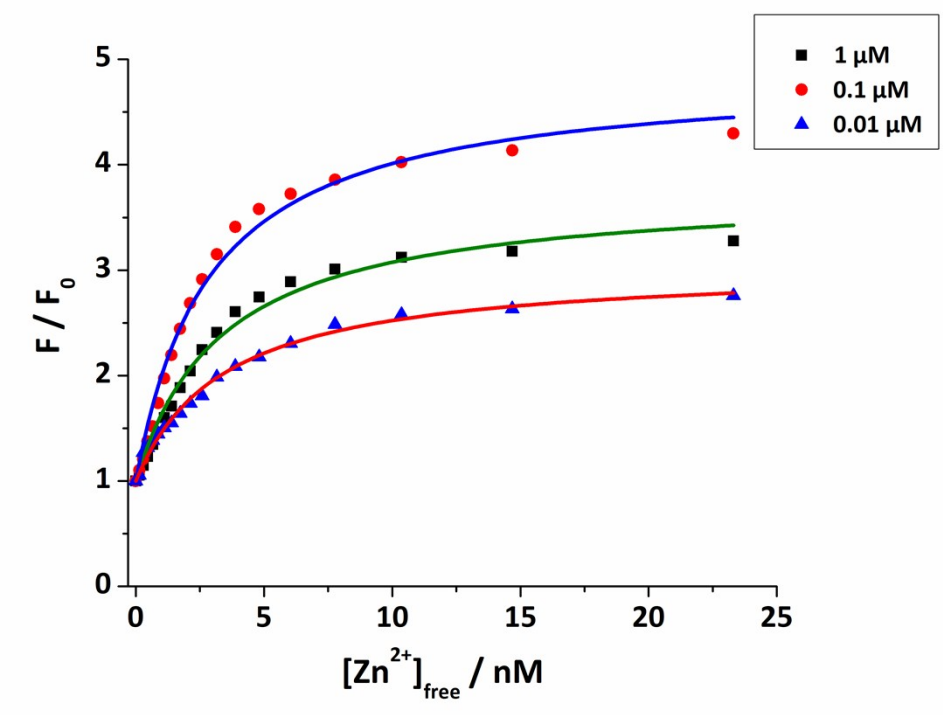


Fig. S13 The non-linear curve fitting of the fluorescence intensity of **8** at different concentrations against $[Zn^{2+}]_{free}$ applying Equation S1. (λ_{ex} = 346 nm, λ_{em} = 414 nm)

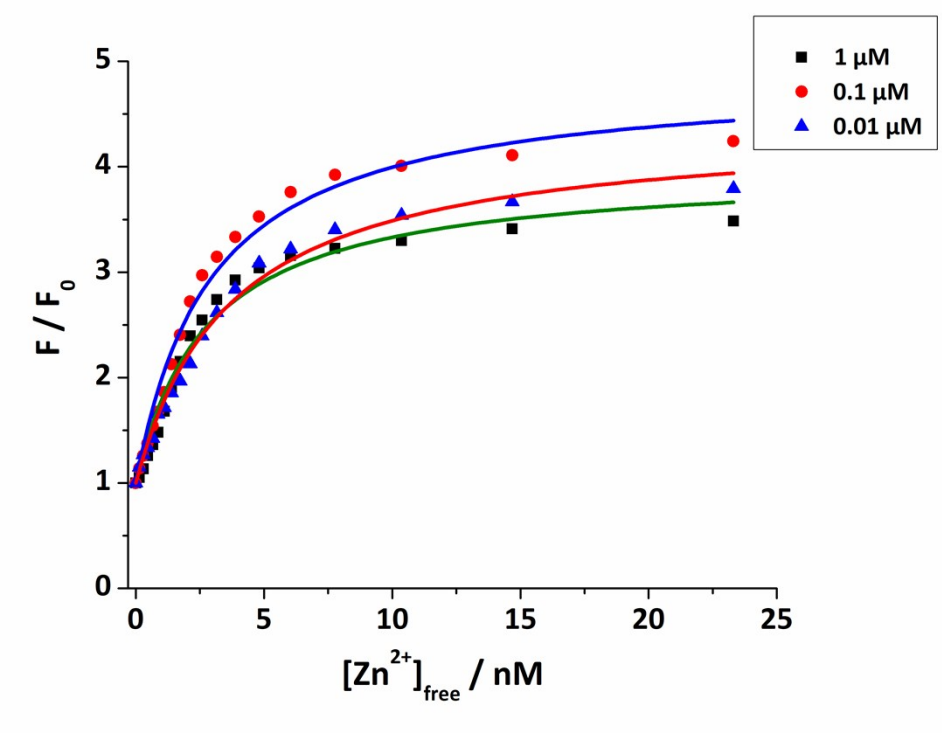


Fig. S14 The non-linear curve fitting of the fluorescence intensity of **9** at different concentrations against $[Zn^{2+}]_{free}$ applying Equation S1. (λ_{ex} = 346 nm, λ_{em} = 414 nm)

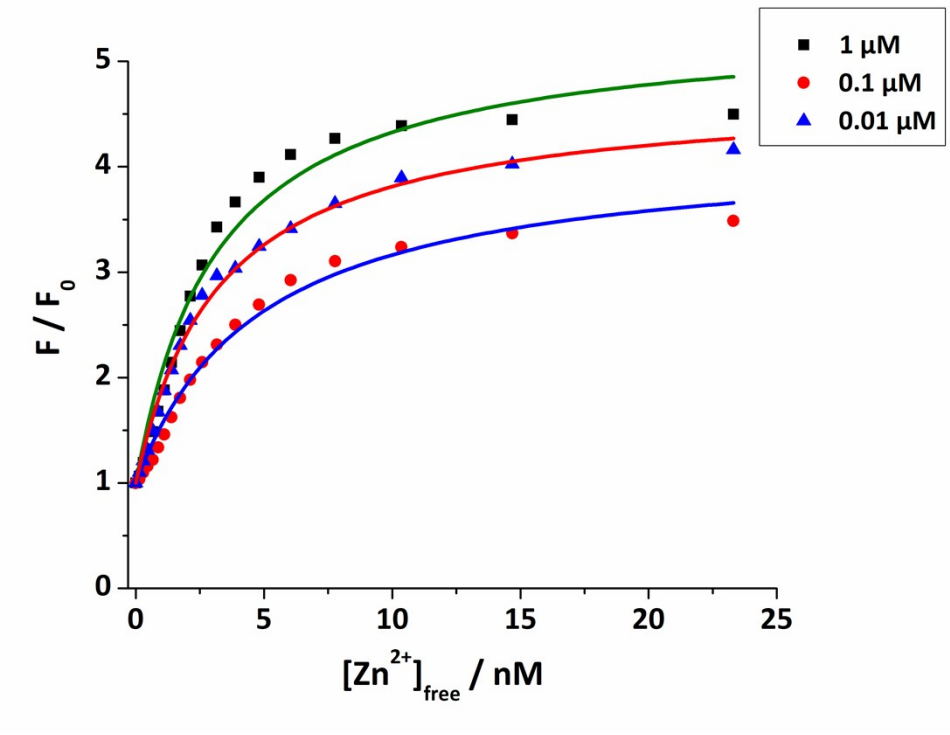


Fig. S15 The non-linear curve fitting of the fluorescence intensity of **10** at different concentrations against $[Zn^{2+}]_{free}$ applying Equation S1. (λ_{ex} = 346 nm, λ_{em} = 414 nm)

Table S1 The summary of K_d for probes **7**-**10**.

	[probe] = 1 μM		[probe] = 0.1 μM		[probe] = 0.01 μM	
	K_d	R^2	K_d	R^2	K_d	R^2
7	3.16 ± 0.34 nM	0.9789	3.05 ± 0.18 nM	0.9931	2.83 ± 0.11 nM	0.9968
8	3.38 ± 0.29 nM	0.9866	2.87 ± 0.23 nM	0.9878	3.44 ± 0.22 nM	0.9919
9	2.78 ± 0.34 nM	0.9734	2.91 ± 0.26 nM	0.9845	3.68 ± 0.26 nM	0.9911
10	3.15 ± 0.40 nM	0.9719	4.81 ± 0.47 nM	0.9850	3.24 ± 0.20 nM	0.9932

Detection limit (LOD) calculation

To determine detection limit, fluorescence spectrum of probe only was measured 20 times and the standard deviation of this blank measurement was obtained as σ. The slope K was obtained from linear fitting of the fluorescence Zn^{2+} titration data (see Fig. S16-S20). Then the detection limit was then calculated through Equation S2:

$$LOD = \frac{3\sigma}{K} \quad \text{(Equation S2)}$$

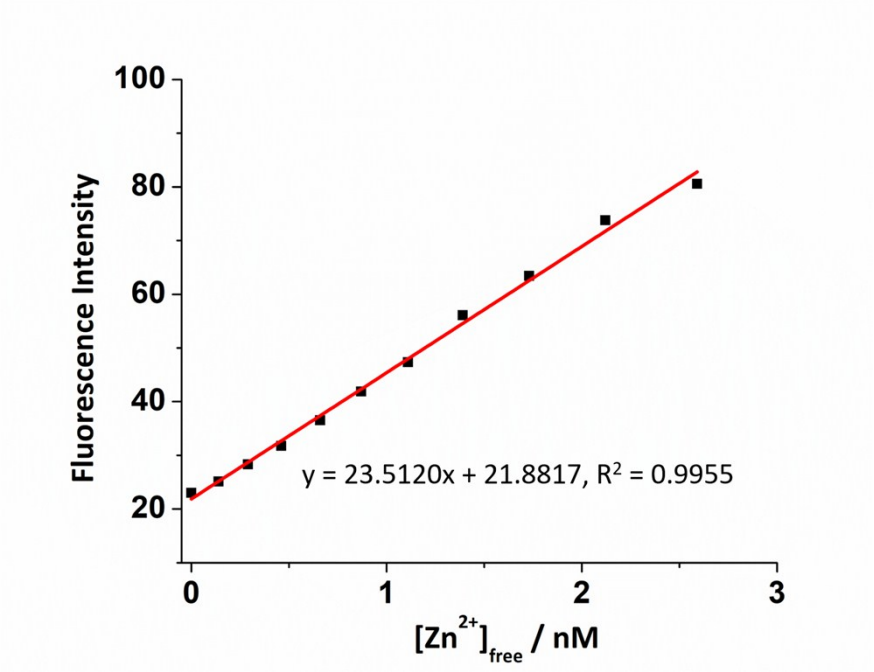


Fig. S16 Fluorescence response of **7** (1 μM) against $[Zn^{2+}]_{free}$. (λ_{ex} = 346 nm, λ_{em} = 414 nm, slit width: 5/5 nm)

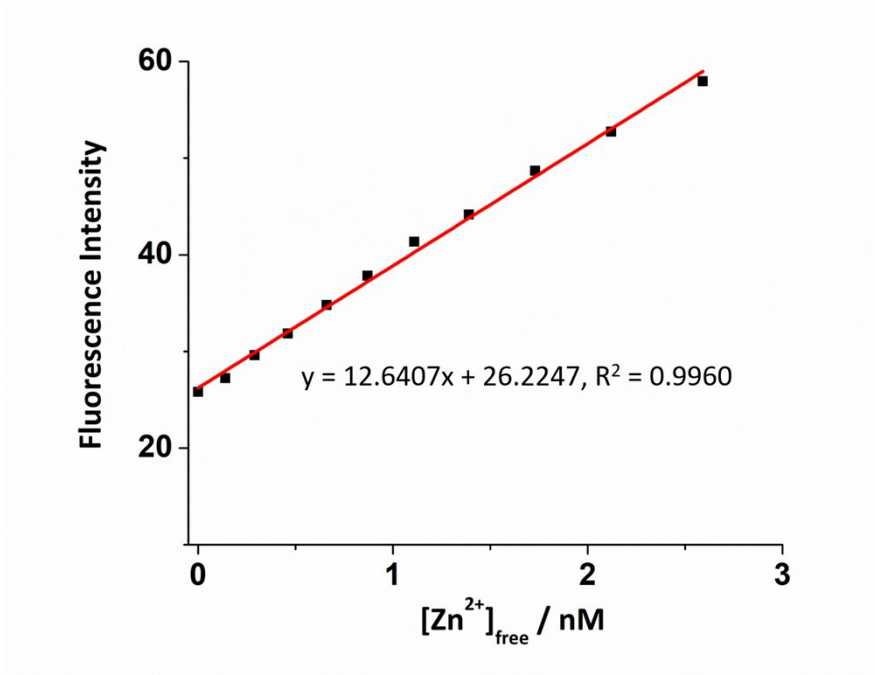


Fig. S17 Fluorescence response of **8** (1 μM) against $[Zn^{2+}]_{free}$. (λ_{ex} = 346 nm, λ_{em} = 414 nm, slit width: 5/5 nm)

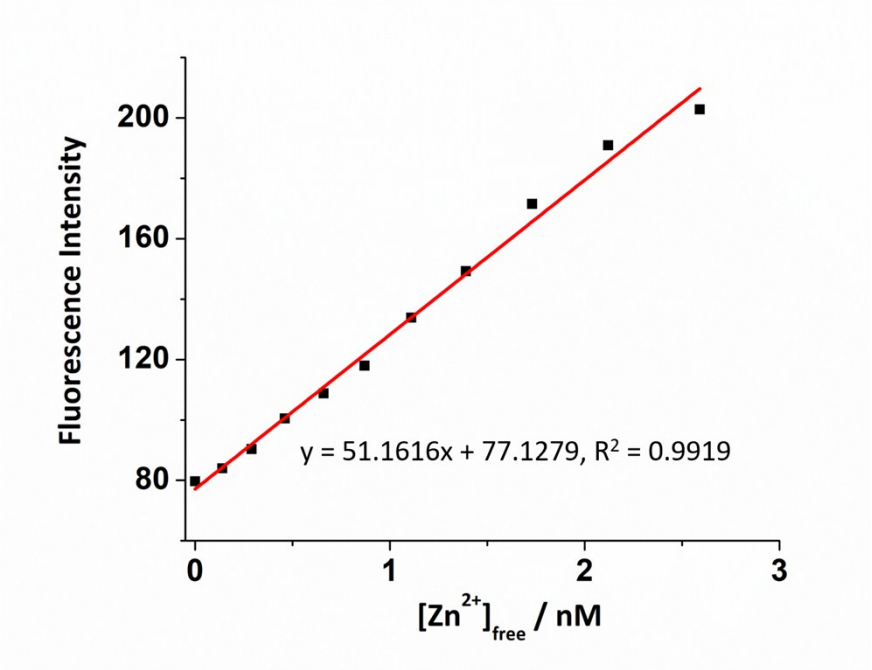


Fig. S18 Fluorescence response of **9** (1 μM) against $[Zn^{2+}]_{free}$. (λ_{ex} = 346 nm, λ_{em} = 414 nm, slit width: 5/5 nm)

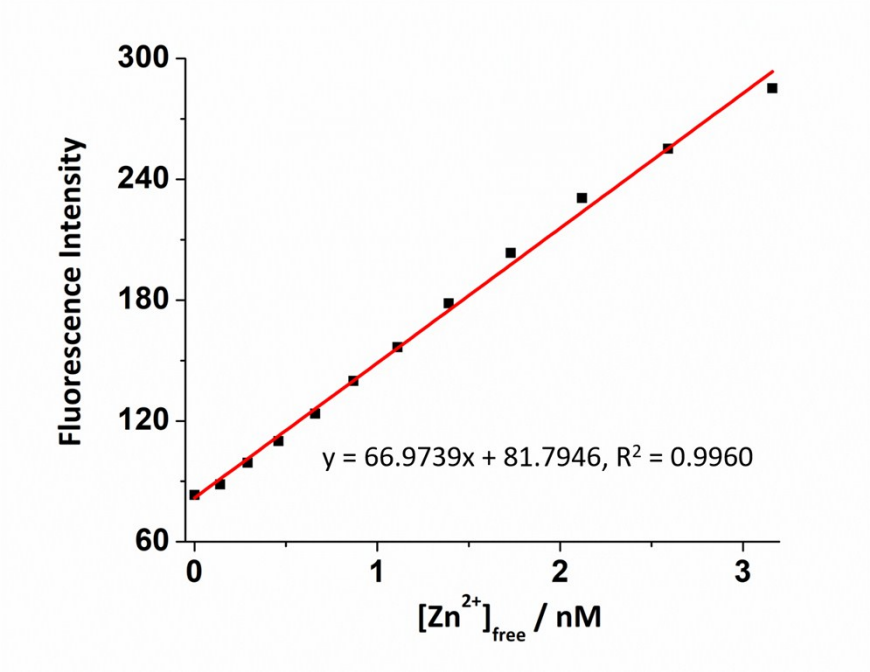


Fig. S19 Fluorescence response of **10** (1 μM) against $[Zn^{2+}]_{free}$. (λ_{ex} = 346 nm, λ_{em} = 414 nm, slit width: 5/5 nm)

Quantum yield measurements

$$\Phi_X = \Phi_{ST}\left(\frac{Grad_X}{Grad_{ST}}\right)\left(\frac{\eta_X}{\eta_{ST}}\right)^2$$

Equation S3 Equation used to calculate fluorescence quantum yield.[7] Where the subscripts *ST* and *X* denote standard and test respectively, Φ is the fluorescence quantum yield, *Grad* the gradient from the plot of integrated fluorescence intensity *vs* absorbance, and η the refractive index of the solvent.

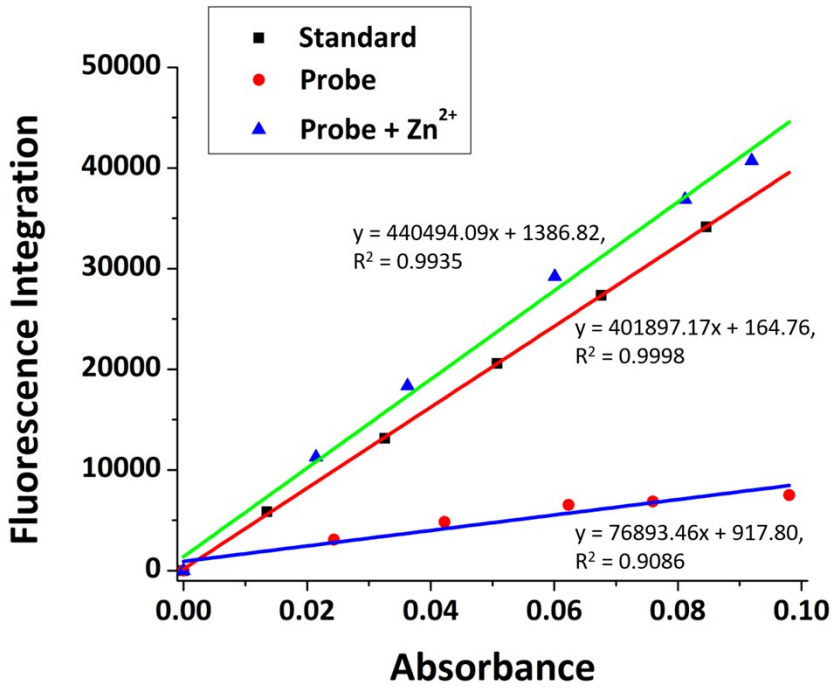


Fig. S20 Linear plots for standard sample, **7**, and **7** + Zn^{2+} to obtain quantum yields. (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

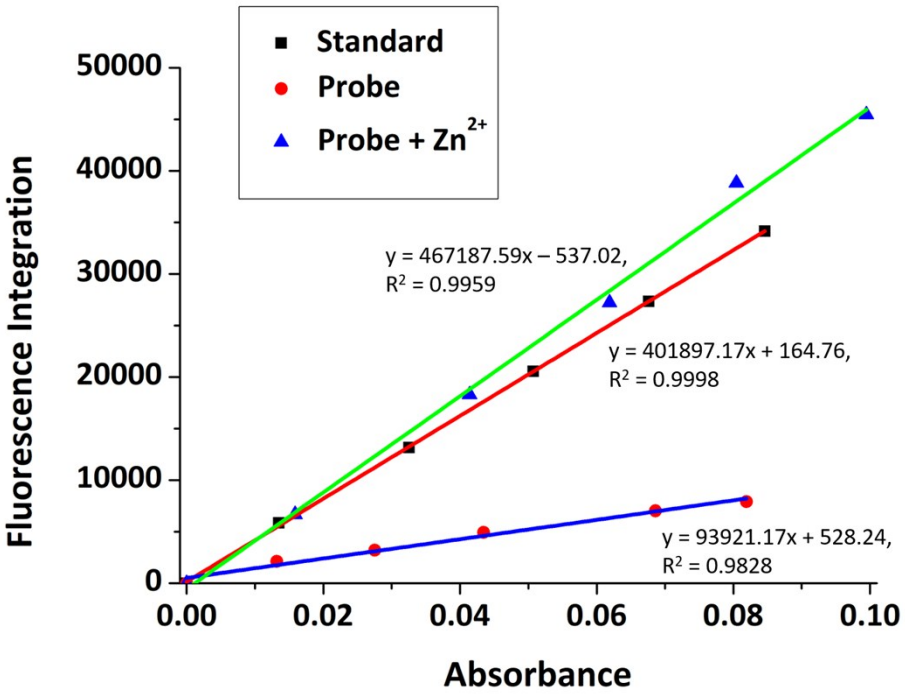


Fig. S21 Linear plots for standard sample, **8**, and **8** + Zn^{2+} to obtain quantum yields. (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

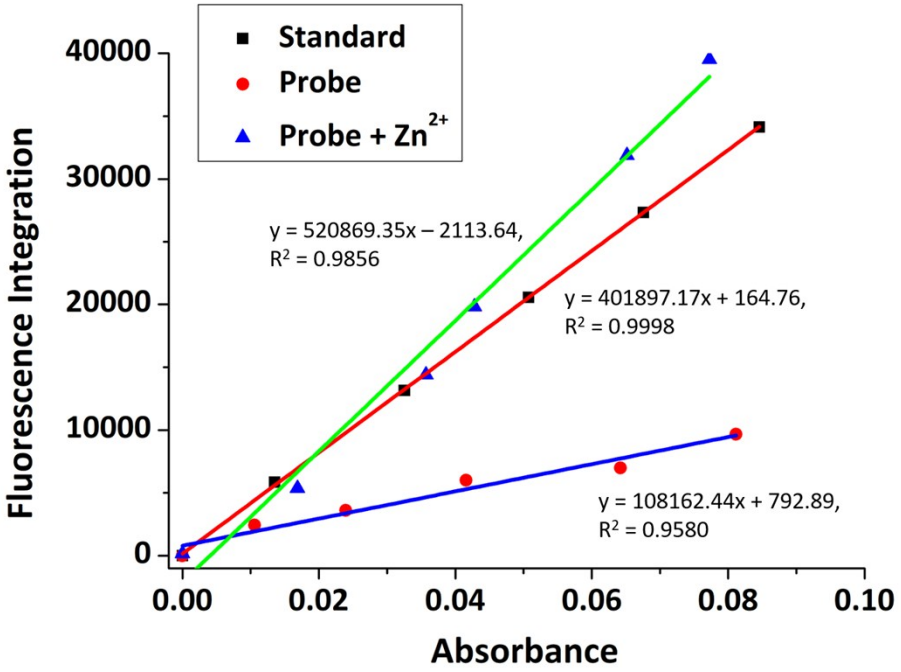


Fig. S22 Linear plots for standard sample, **9**, and **9** + Zn^{2+} to obtain quantum yields. (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

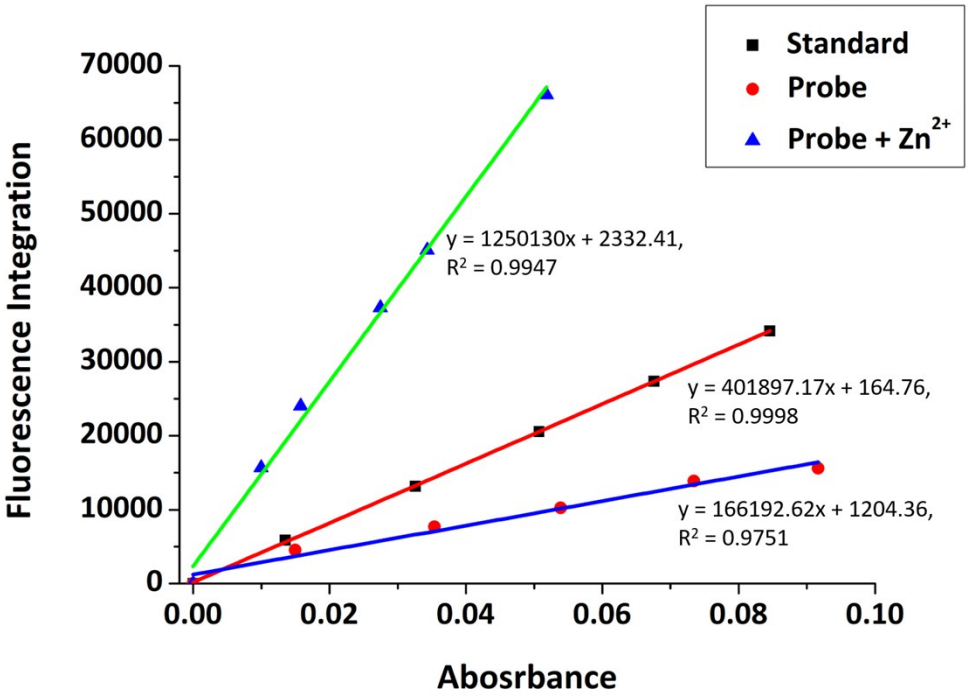


Fig. S23 Linear plots for standard sample, **10**, and **10** + Zn^{2+} to obtain quantum yields. (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

Table S2 The quantum yield of probes and their complex with 1 equivalent Zn^{2+}.

Probe	Φ_{probe}	$\Phi_{complex}$
7	0.05	0.28
8	0.06	0.30
9	0.07	0.34
10	0.11	0.81

pH profiles

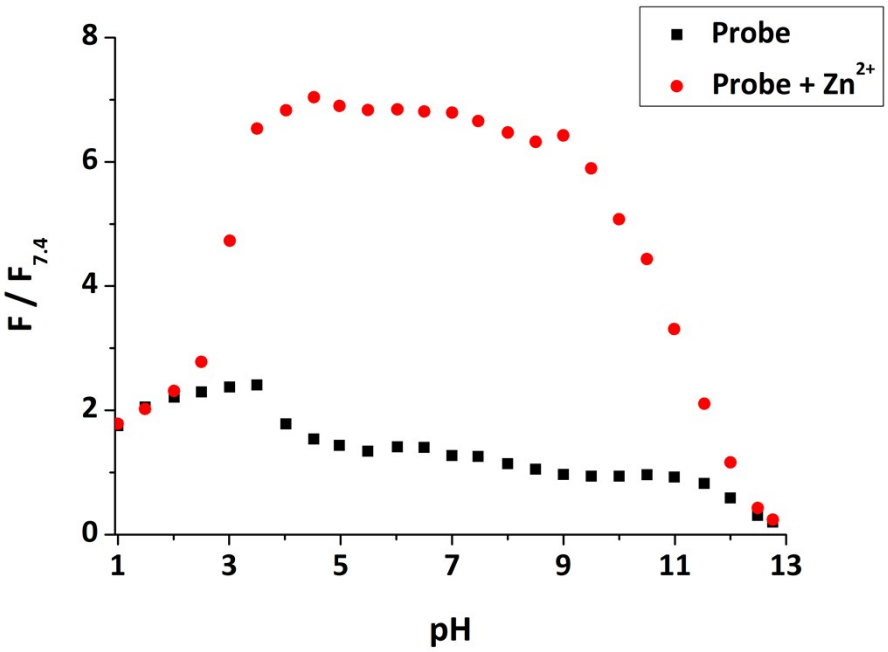


Fig. S24 The pH profile of **8** (50 μM, black dots) and its complex with 1 equivalent of Zn^{2+} (red dots). (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

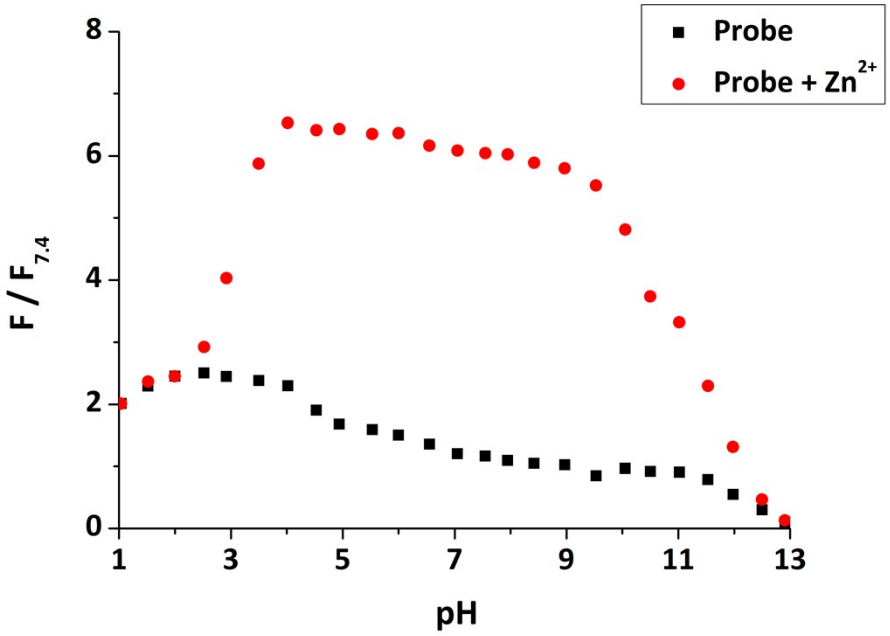


Fig. S25 The pH profile of **9** (50 μM, black dots) and its complex with 1 equivalent of Zn^{2+} (red dots). (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

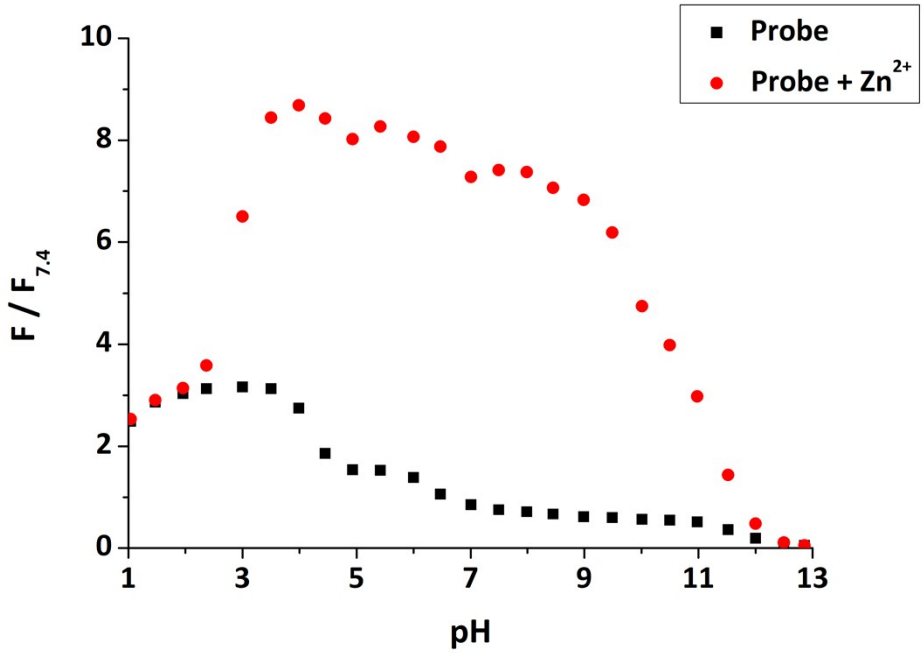


Fig. S26 The pH profile of **10** (50 μM, black dots) and its complex with 1 equivalent of Zn^{2+} (red dots). (λ_{ex} = 346 nm, slit width: 5/2.5 nm)

pK_a values

$$\frac{F - F_0}{F_{max} - F_0} = \frac{\Delta F_{1max}}{(1 + 10^{(pH - pK_{a1})})} + \frac{\Delta F_{2max}}{(1 + 10^{(pH - pK_{a2})})} + \frac{\Delta F_{3max}}{(1 + 10^{(pH - pK_{a3})})} + -$$

Equation S4 The equation used to calculate pK_a values. F_{max} is the maximum normalized emission integration ($F_{max} = 1$), F_0 is the minimum normalized emission integration obtained, and ΔF_{1max}, ΔF_{2max}, ΔF_{3max} and ΔF_{4max} are the maximum fluorescence integration changes associated with the corresponding pK_a values.

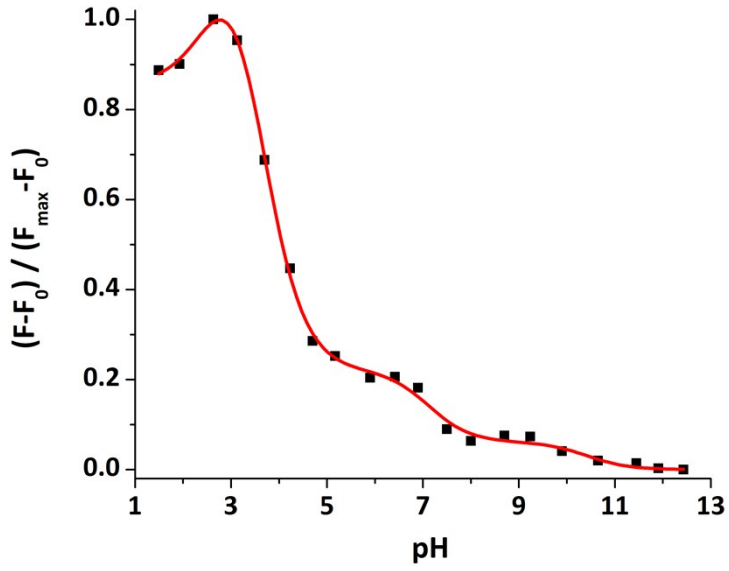


Fig. S27 Normalized integrated fluorescence emission of **7** (50 μM) *vs* pH, the nonlinear curve fitting used to determine the apparent pK_a values applying Equation S3. The determined pK_a values are: pK_{a1} = 2.65 ± 0.26, pK_{a2} = 3.62 ± 0.09, pK_{a3} = 7.13 ± 0.17, pK_{a4} = 10.42 ± 0.41, R^2 = 99.83%.

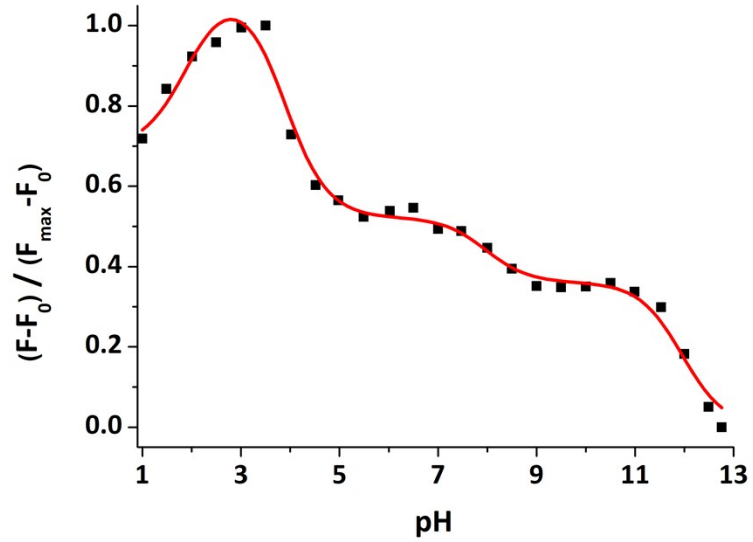


Fig. S28 Normalized integrated fluorescence emission of **8** (50 μM) *vs* pH, the nonlinear curve fitting used to determine the apparent pK_a values applying Equation S3. The determined pK_a values are: pK_{a1} = 1.91 ± 0.27, pK_{a2} = 3.88 ± 0.13, pK_{a3} = 7.97 ± 0.32, pK_{a4} = 11.95 ± 0.12, R^2 = 98.57%.

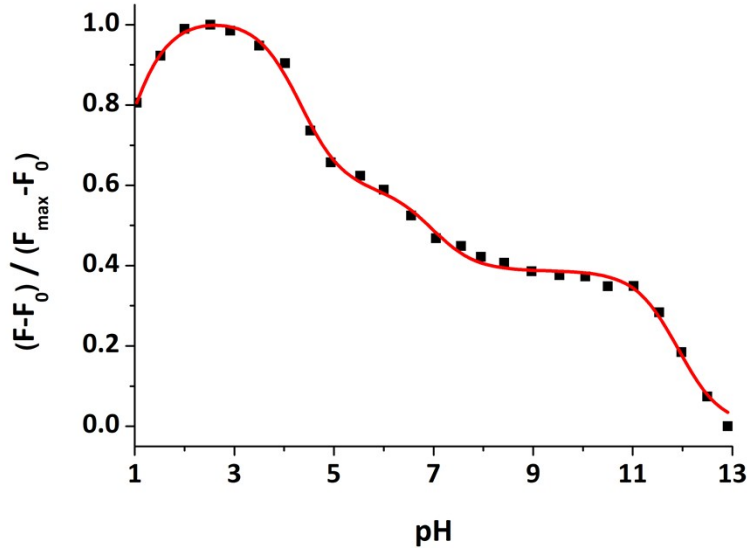


Fig. S29 Normalized integrated fluorescence emission of **9** (50 μM) *vs* pH, the nonlinear curve fitting used to determine the apparent pK_a values applying Equation S3. The determined pK_a values are: pK_{a1} = 0.70 ± 0.38, pK_{a2} = 4.33 ± 0.08, pK_{a3} = 6.99 ± 0.15, pK_{a4} = 11.91 ± 0.06, R^2 = 99.64%.

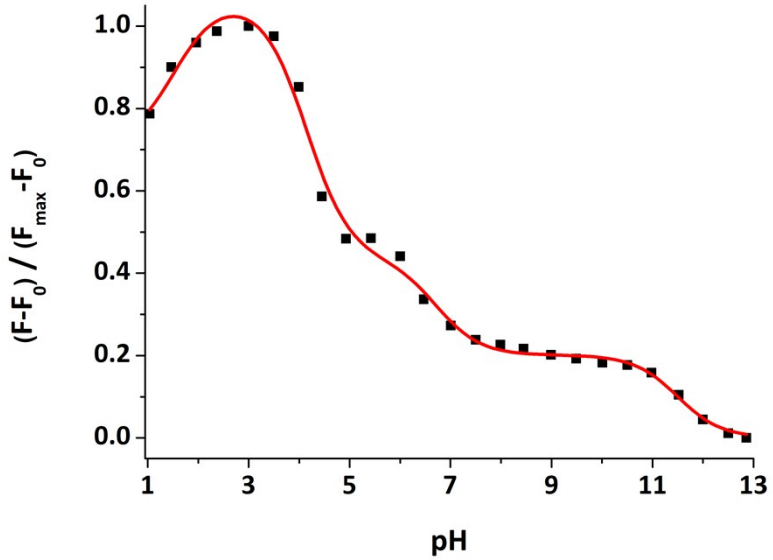


Fig. S30 Normalized integrated fluorescence emission of **10** (50 μM) *vs* pH, the nonlinear curve fitting used to determine the apparent pK_a values applying Equation S3. The determined pK_a values are: pK_{a1} = 1.53 ± 0.29, pK_{a2} = 6.73 ± 0.21, pK_{a3} = 4.14 ± 0.10, pK_{a4} = 11.50 ± 0.17, R^2 = 99.39%.

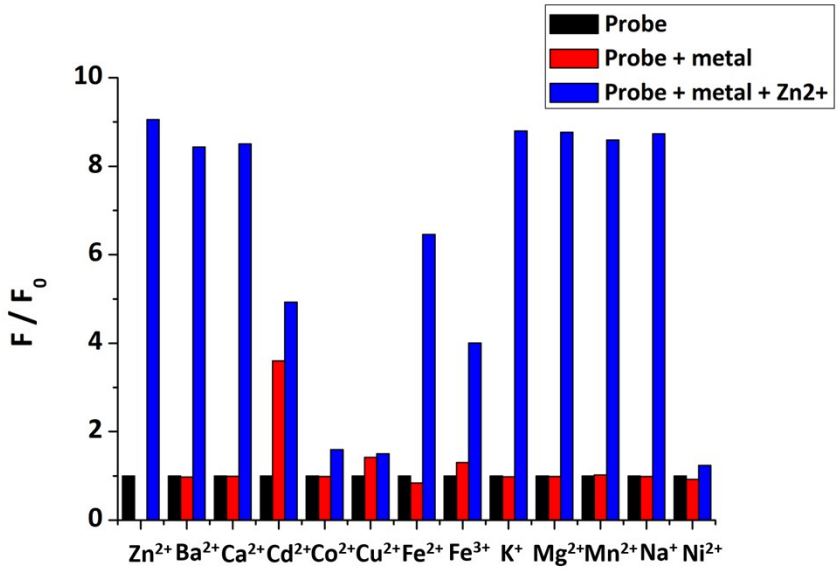


Fig. S31 Metal ion selectivity of **8**. Average normalized fluorescence intensities for **8** (50 μM) (black bars), after addition of 5 equivalents of various cations (red bars), followed by addition of 1 equivalent of $ZnCl_2$ (blue bars).

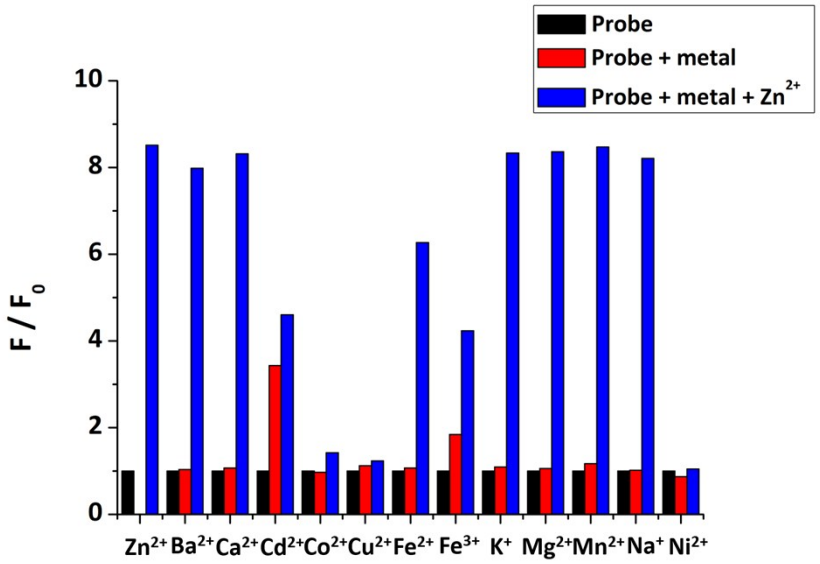


Fig. S32 Metal ion selectivity of **9**. Average normalized fluorescence intensities for **9** (50 μM) (black bars), after addition of 5 equivalents of various cations (red bars), followed by addition of 1 equivalent of $ZnCl_2$ (blue bars).

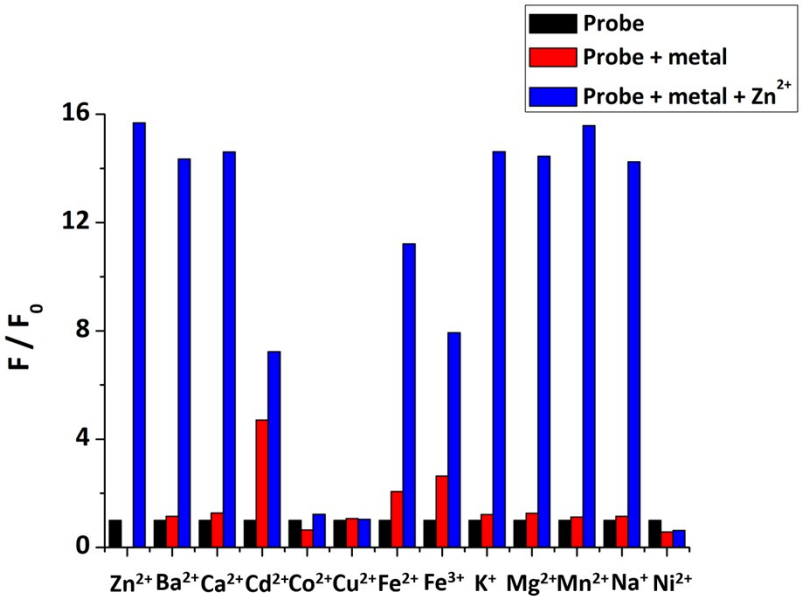


Fig. S33 Metal ion selectivity of **10**. Average normalized fluorescence intensities for **10** (50 μM) (black bars), after addition of 5 equivalents of various cations (red bars), followed by addition of 1 equivalent of $ZnCl_2$ (blue bars).

^{1}H NMR spectroscopic titration

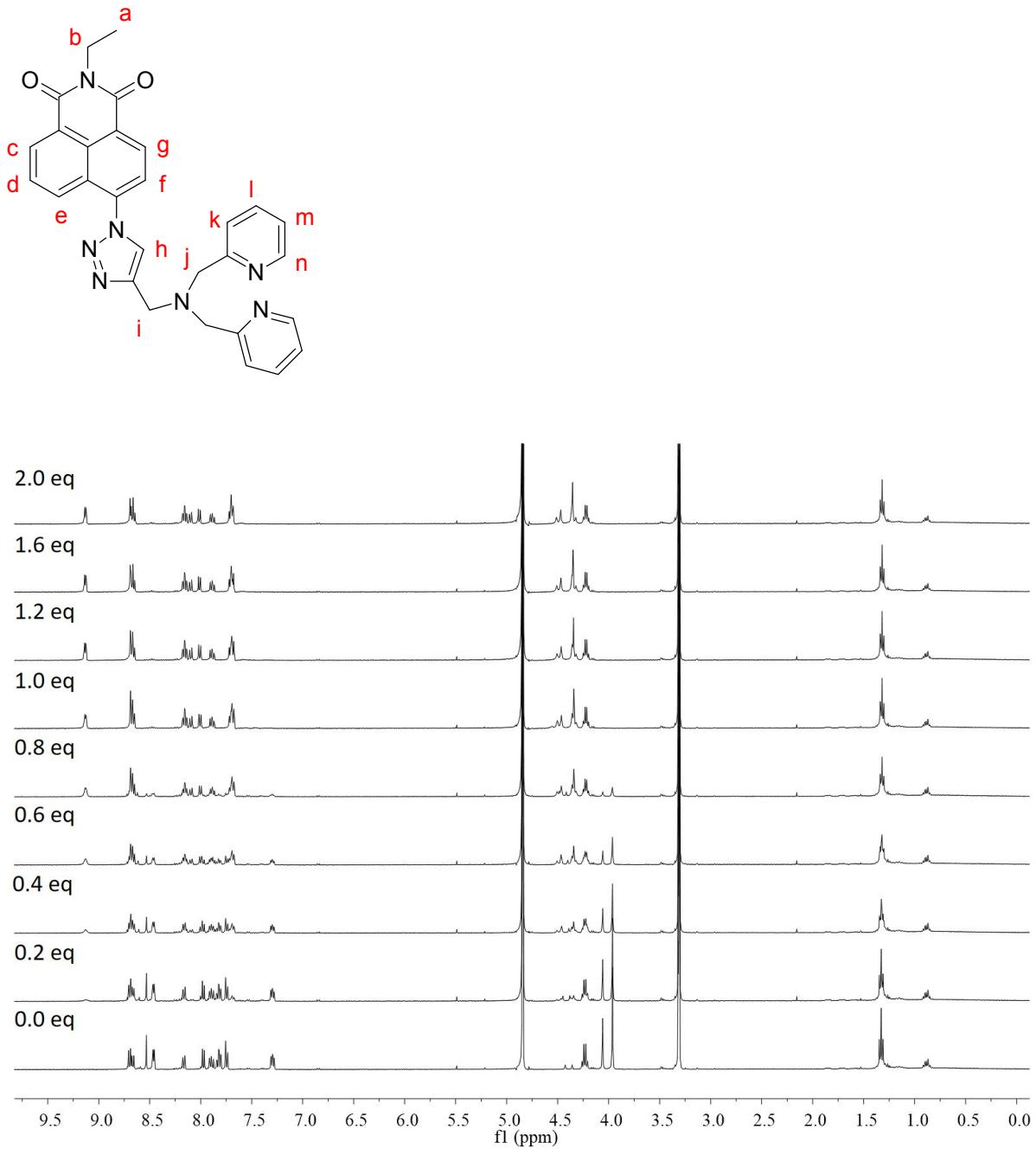


Fig. S34 ^{1}H NMR titration spectra (whole range) of probe **10** (5 mM) with different equivalents $ZnCl_2$ in CD_3OD.

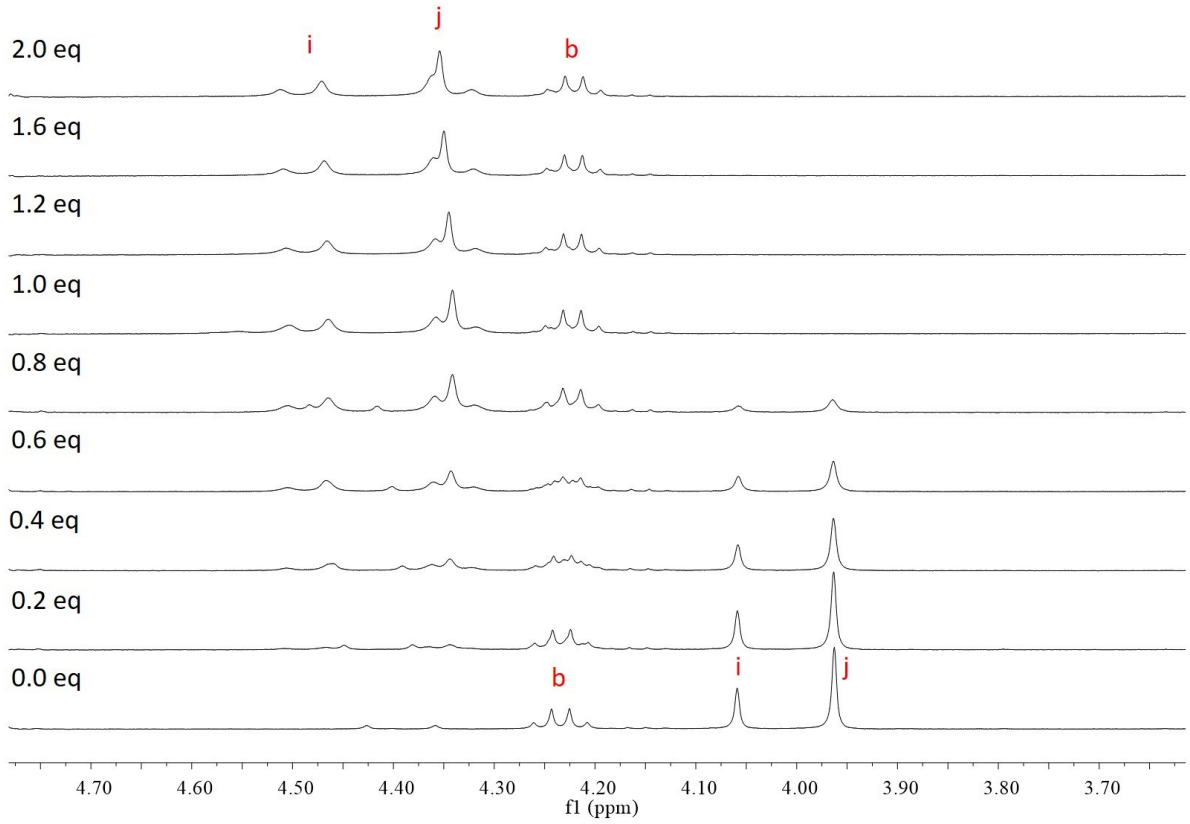
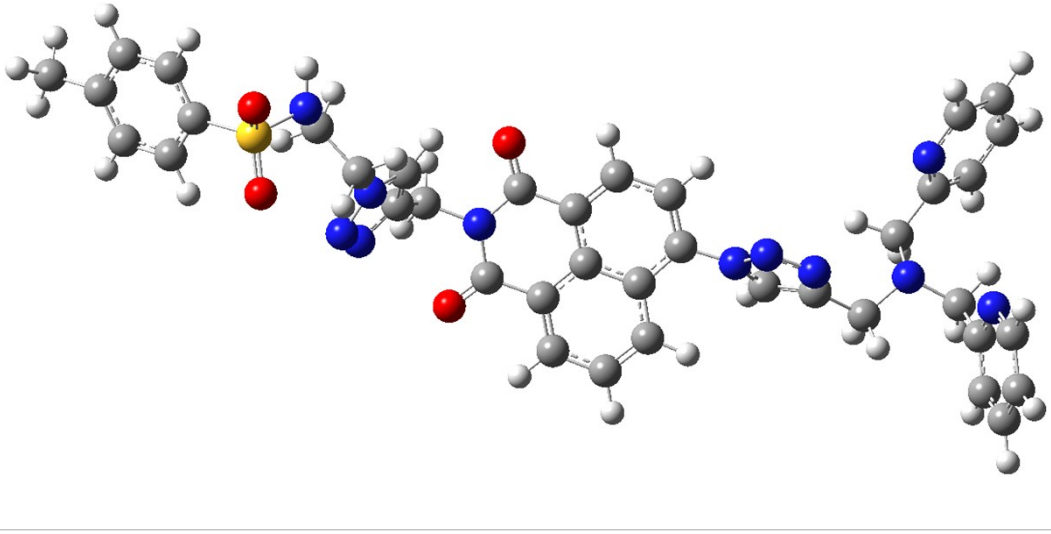


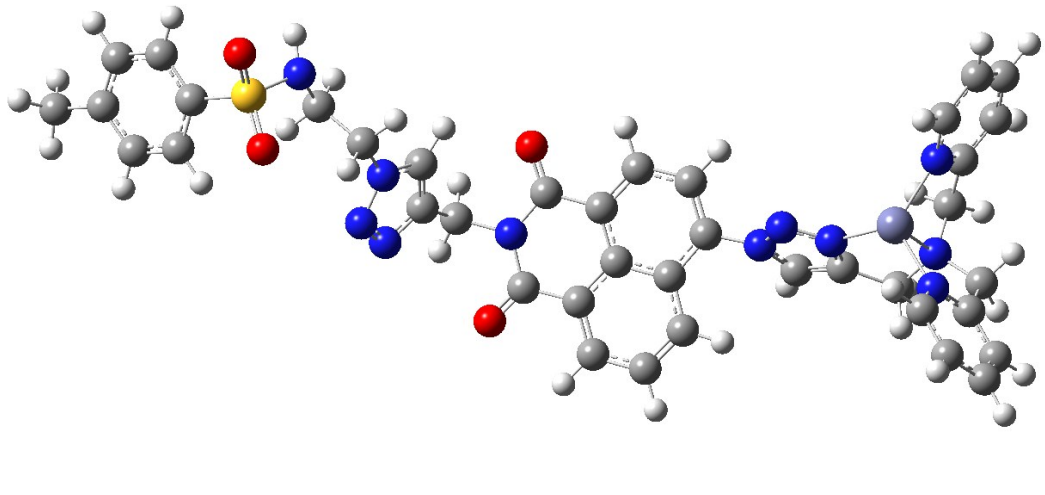
Fig. S35 ^{1}H NMR titration spectra (range 3.70 - 4.70 ppm) of probe **10** (5 mM) with different equivalents $ZnCl_2$ in CD_3OD.

Theoretical calculations

To understand the binding behaviour of the probes with Zn^{2+} and its fundamental electronic structure, DFT and TDDFT studies were performed. The structure of **7**-**10** and their complexes with Zn^{2+} were first optimized using B3LYP functional and 6-31G* basis set in Gaussian 09. Then the calculation of excited states and structures of the S_1 minima were obtained at CAMB3LYP/6-31G* level of theory. All calculations considered H_2O as solvent using a continuum model (PCM). The vertical excitations and emission energies are shown in Table S3-S6.

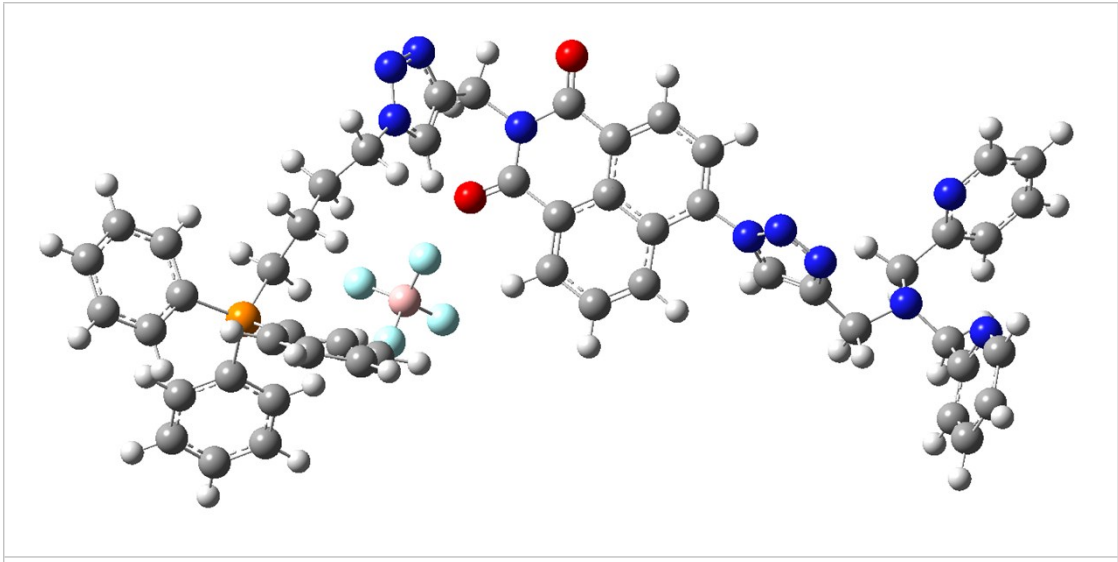


Probe **7**

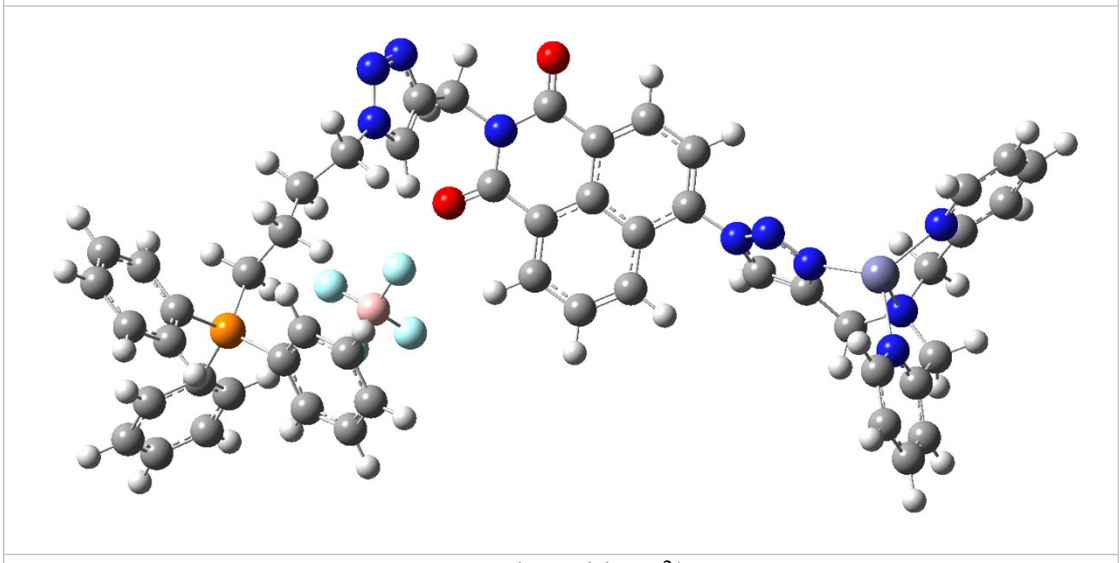


Complex with Zn^{2+}

Fig. S36 The optimized structures of **7** and its complex with Zn^{2+}.

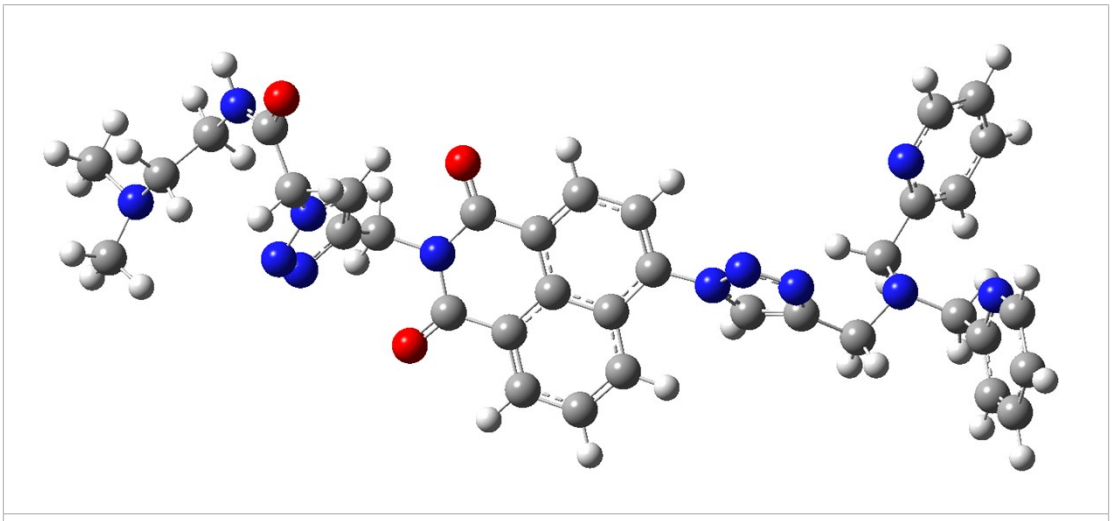


Probe **8**

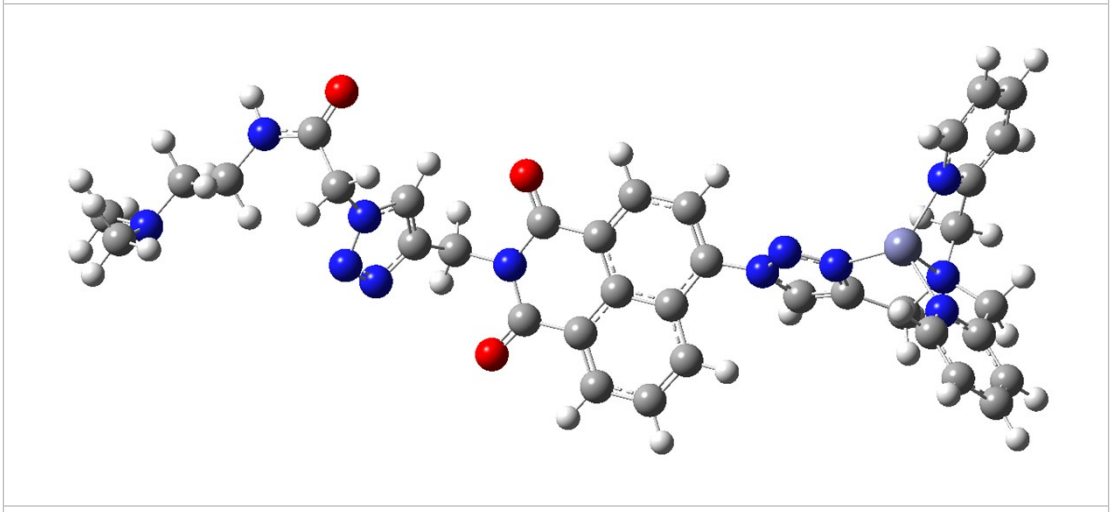


Complex with Zn^{2+}

Fig. S37 The optimized structures of **8** and its complex with Zn^{2+}.

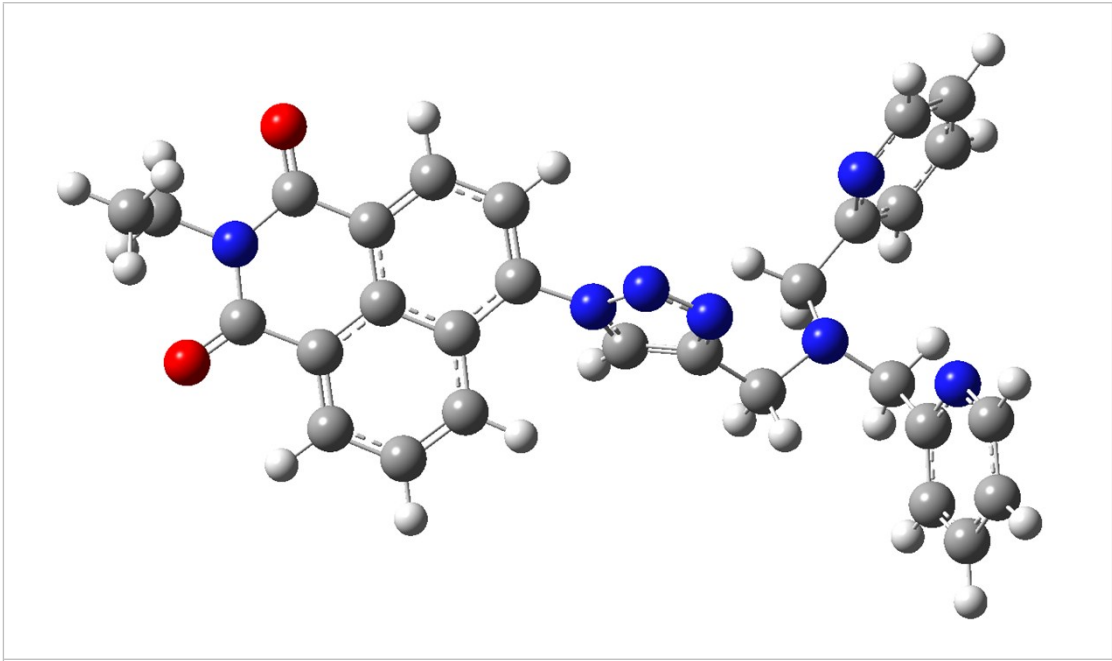


Probe **9**

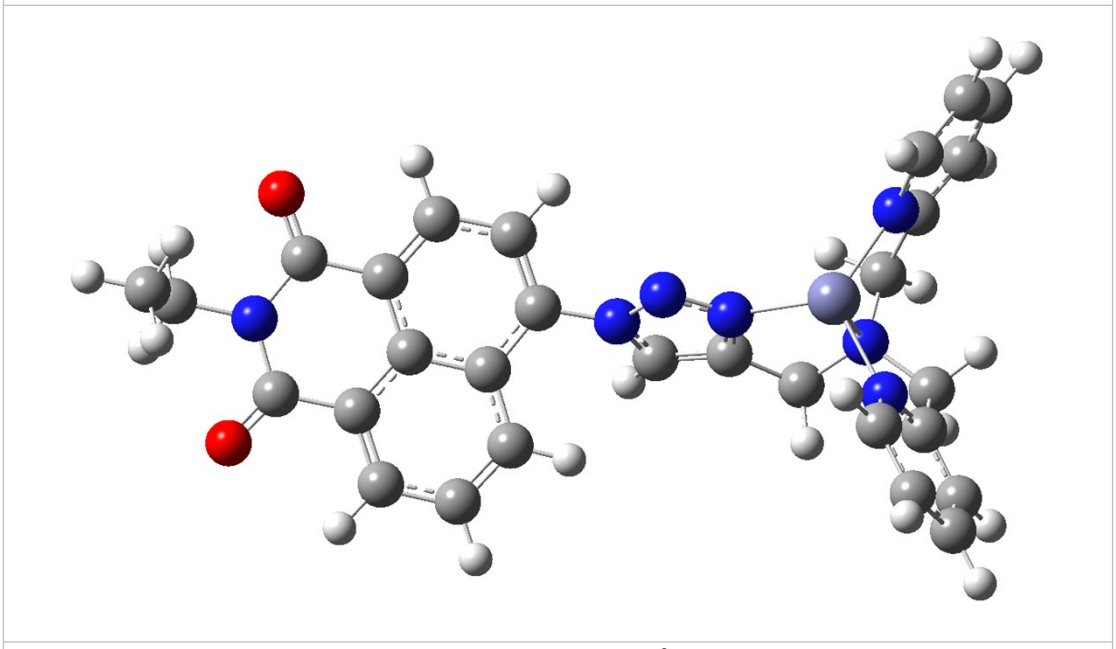


Complex with Zn^{2+}

Fig. S38 The optimized structures of **9** and its complex with Zn^{2+}.



Probe **10**



Complex with Zn^{2+}

Fig. S39 The optimized structures of **10** and its complex with Zn^{2+}.

Table S3. Comparison of the experimental data with the calculated result of vertical electronic excitation energies (eV) and the emission from S_1 to ground state of **7** and its Zn^{2+} complex.

	Electronic transition	Energy (eV)	Wavelength (nm)	Oscillator strengths (f)	Experimental data
7					
Absorption	$S_0 \rightarrow S_1$	3.90	318	0.5443	3.58 eV/346 nm
	$S_0 \rightarrow S_2$	4.26	291	0.0483	
	$S_0 \rightarrow S_3$	4.38	283	0.0002	
	$S_0 \rightarrow S_4$	4.68	265	0.0010	
	$S_0 \rightarrow S_5$	4.84	256	0.0201	
	$S_0 \rightarrow S_6$	4.93	251	0.0190	
Emission	$S_1 \rightarrow S_0$	3.14	395	0.7240	3.01 eV/412 nm
Complex of **7** with Zn^{2+}					
Absorption	$S_0 \rightarrow S_1$	3.96	313	0.5015	3.58 eV/346 nm
	$S_0 \rightarrow S_2$	4.25	291	0.0557	
	$S_0 \rightarrow S_3$	4.33	286	0.0002	
	$S_0 \rightarrow S_4$	4.62	268	0.0004	
	$S_0 \rightarrow S_5$	4.94	251	0.0329	
	$S_0 \rightarrow S_6$	5.31	234	0.0055	
Emission	$S_1 \rightarrow S_0$	3.21	386	0.6748	3.01 eV/412 nm

Table S4. Comparison of the experimental data with the calculated result of vertical electronic excitation energies (eV) and the emission from S_1 to ground state of **8** and its Zn^{2+} complex.

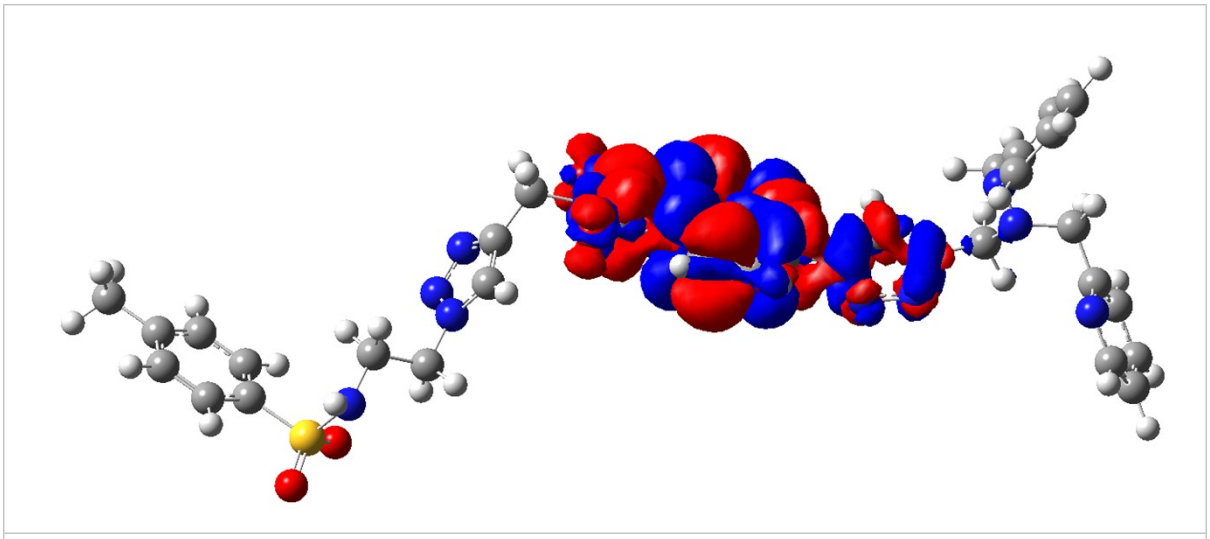
	Electronic transition	Energy (eV)	Wavelength (nm)	Oscillator strengths (f)	Experimental data
8					
Absorption	$S_0 \rightarrow S_1$	3.89	318	0.5149	3.58 eV/346 nm
	$S_0 \rightarrow S_2$	4.25	292	0.0493	
	$S_0 \rightarrow S_3$	4.38	283	0.0009	
	$S_0 \rightarrow S_4$	4.73	262	0.0034	
	$S_0 \rightarrow S_5$	4.84	256	0.0302	
	$S_0 \rightarrow S_6$	4.89	253	0.0049	
Emission	$S_1 \rightarrow S_0$	3.14	394	0.7137	3.01 eV/412 nm
Complex of **8** with Zn^{2+}					
Absorption	$S_0 \rightarrow S_1$	3.95	314	0.4796	3.58 eV/346 nm
	$S_0 \rightarrow S_2$	4.25	292	0.0530	
	$S_0 \rightarrow S_3$	4.33	286	0.0019	
	$S_0 \rightarrow S_4$	4.68	265	0.0003	
	$S_0 \rightarrow S_5$	4.84	256	0.0273	
	$S_0 \rightarrow S_6$	5.13	242	0.0178	
Emission	$S_1 \rightarrow S_0$	3.26	381	0.6351	3.01 eV/412 nm

Table S5. Comparison of the experimental data with the calculated result of vertical electronic excitation energies (eV) and the emission from S_1 to ground state of **9** and its Zn^{2+} complex.

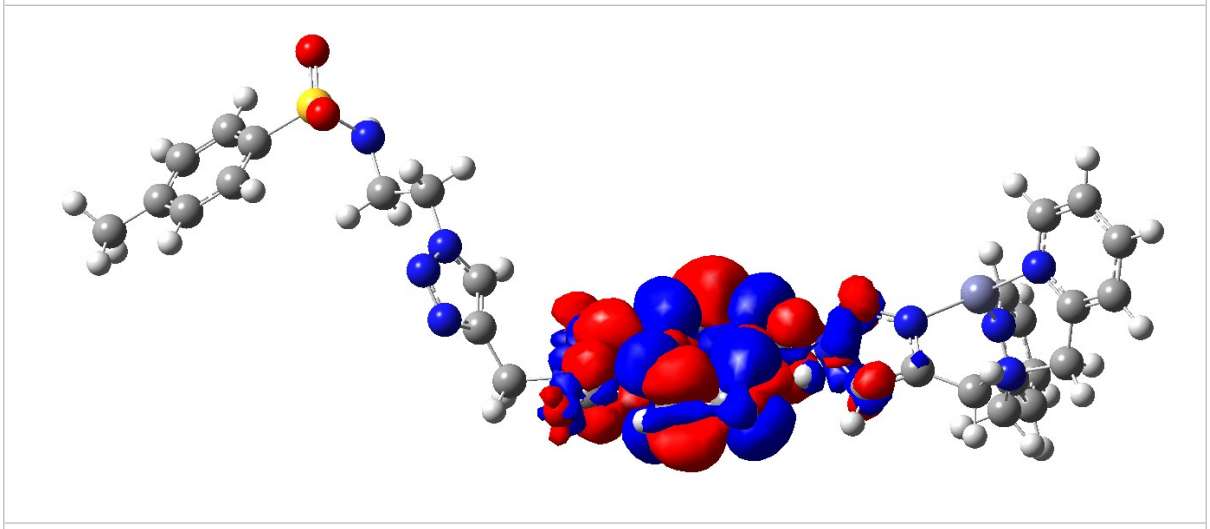
	Electronic transition	Energy (eV)	Wavelength (nm)	Oscillator strengths (f)	Experimental data
9					
Absorption	$S_0 \rightarrow S_1$	3.89	319	0.5481	3.58 eV/346 nm
	$S_0 \rightarrow S_2$	4.26	291	0.0479	
	$S_0 \rightarrow S_3$	4.39	282	0.0001	
	$S_0 \rightarrow S_4$	4.70	264	0.0022	
	$S_0 \rightarrow S_5$	4.83	257	0.0142	
	$S_0 \rightarrow S_6$	4.90	253	0.0012	
Emission	$S_1 \rightarrow S_0$	3.14	394	0.7241	3.01 eV/412 nm
Complex of **9** with Zn^{2+}					
Absorption	$S_0 \rightarrow S_1$	3.94	314	0.5169	3.58 eV/346 nm
	$S_0 \rightarrow S_2$	4.25	292	0.0543	
	$S_0 \rightarrow S_3$	4.34	286	0.0002	
	$S_0 \rightarrow S_4$	4.64	267	0.0008	
	$S_0 \rightarrow S_5$	4.95	250	0.0329	
	$S_0 \rightarrow S_6$	4.97	249	0.0015	
Emission	$S_1 \rightarrow S_0$	3.22	385	0.6710	3.01 eV/412 nm

Table S6. Comparison of the experimental data with the calculated result of vertical electronic excitation energies (eV) and the emission from S_1 to ground state of **10** and its Zn^{2+} complex.

	Electronic transition	Energy (eV)	Wavelength (nm)	Oscillator strengths (f)	Experimental data
10					
Absorption	$S_0 \rightarrow S_1$	3.92	316	0.4960	3.58 eV/346 nm
	$S_0 \rightarrow S_2$	4.27	290	0.0445	
	$S_0 \rightarrow S_3$	4.35	285	0.0004	
	$S_0 \rightarrow S_4$	4.69	264	0.0085	
	$S_0 \rightarrow S_5$	4.88	254	0.0251	
	$S_0 \rightarrow S_6$	4.96	250	0.0138	
Emission	$S_1 \rightarrow S_0$	3.15	393	0.7005	3.01 eV/412 nm
Complex of **10** with Zn^{2+}					
Absorption	$S_0 \rightarrow S_1$	3.99	311	0.4455	3.58 eV/346 nm
	$S_0 \rightarrow S_2$	4.26	291	0.0518	
	$S_0 \rightarrow S_3$	4.30	289	0.0009	
	$S_0 \rightarrow S_4$	4.65	267	0.0072	
	$S_0 \rightarrow S_5$	4.94	251	0.0369	
	$S_0 \rightarrow S_6$	5.41	229	0.0385	
Emission	$S_1 \rightarrow S_0$	3.21	386	0.6601	3.01 eV/412 nm

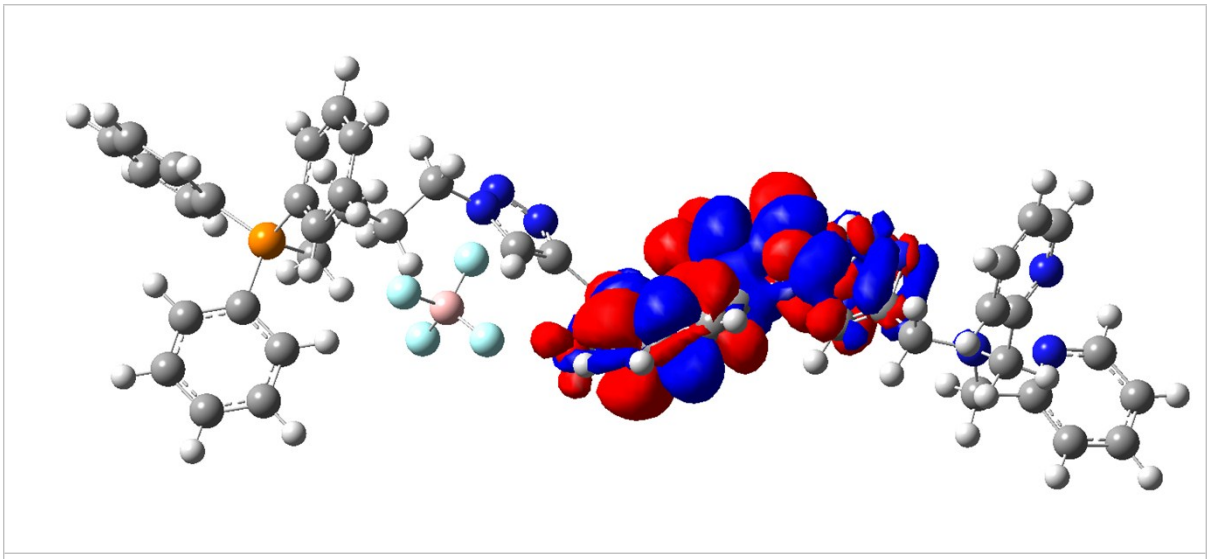


Probe **7**

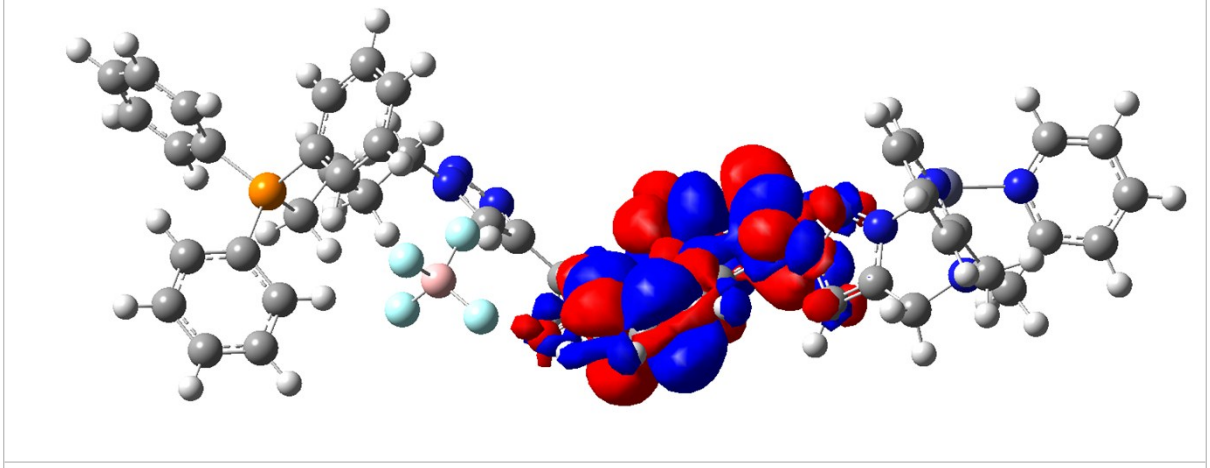


Complex with Zn^{2+}

Fig. S40. S_1-S_0 electron density map for probe **7** and its complex with Zn^{2+} (S_1 minima). Red represents positive densities and blue negative values.

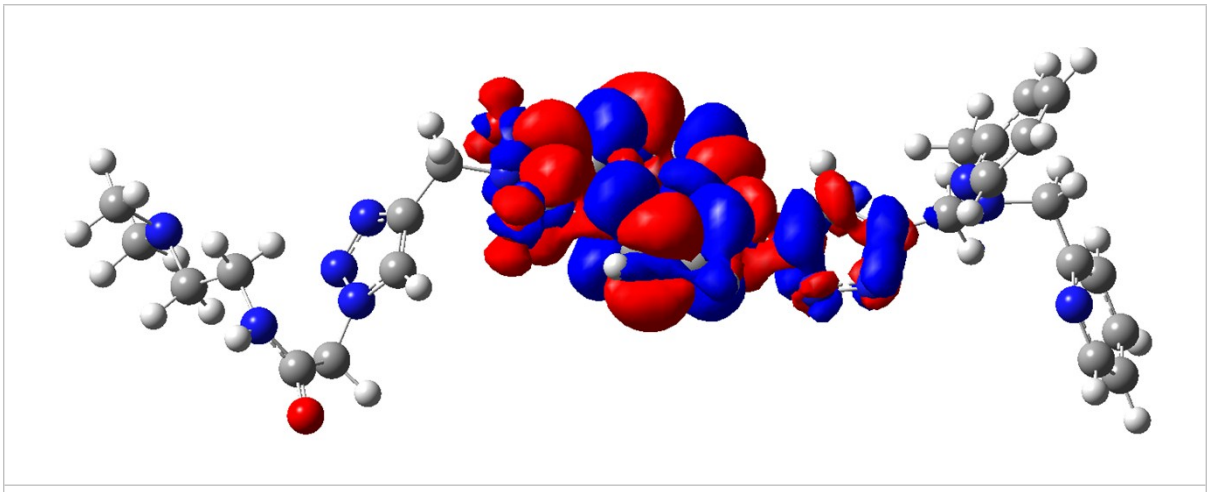


Probe **8**

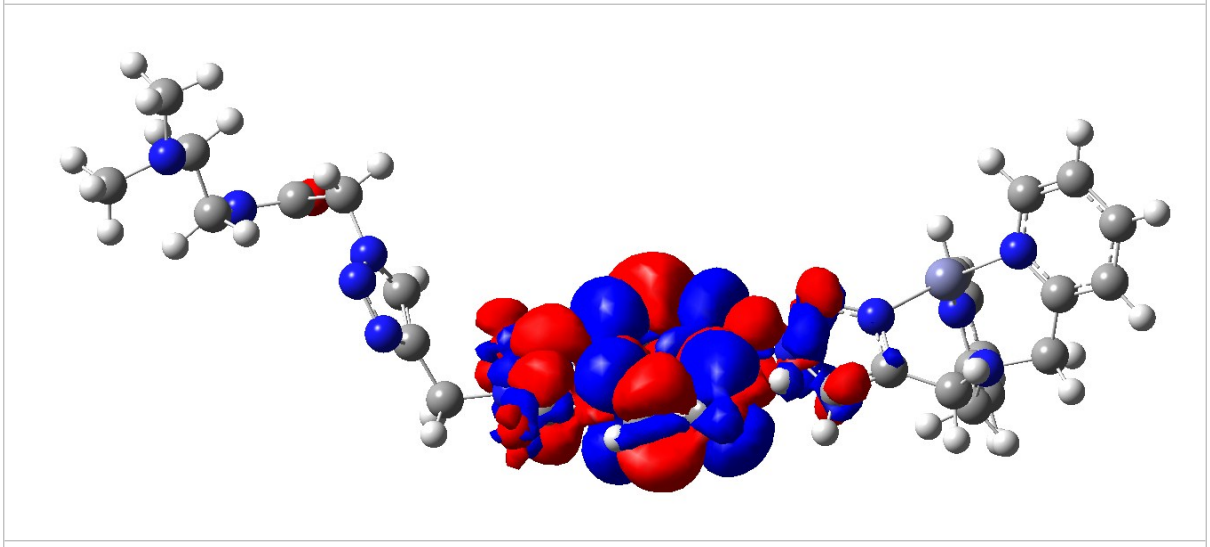


Complex with Zn^{2+}

Fig. S41. S_1-S_0 electron density map for probe **8** and its complex with Zn^{2+} (S_1 minima). Red represents positive densities and blue negative values.

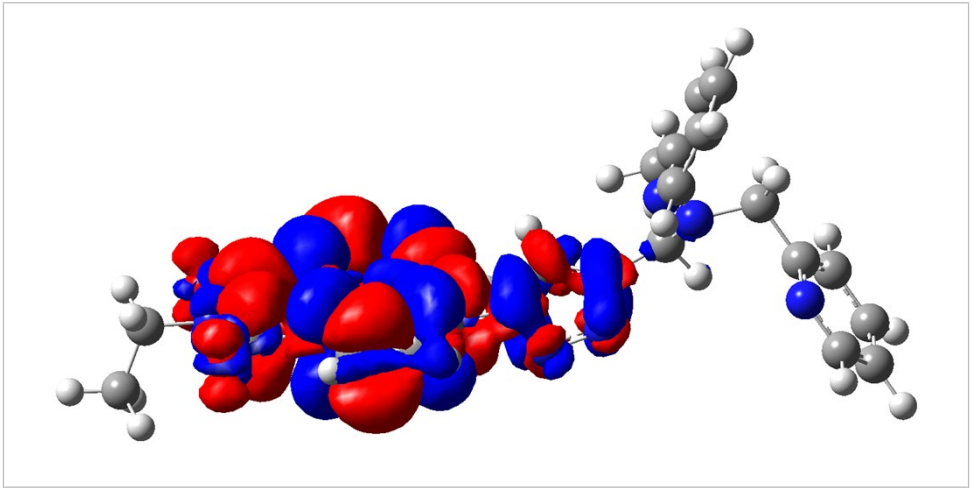


Probe **9**

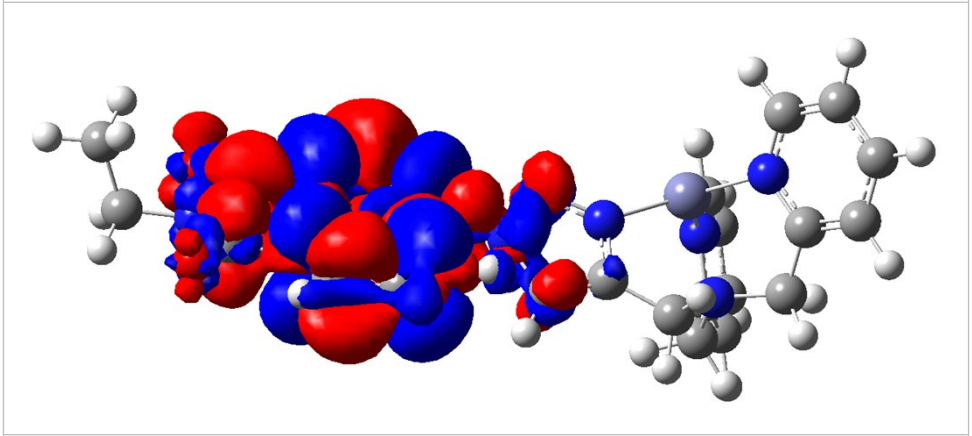


Complex with Zn^{2+}

Fig. S42. S_1-S_0 electron density map for probe **9** and its complex with Zn^{2+} (S_1 minima). Red represents positive densities and blue negative values.



Probe **1**0



Complex with Zn^{2+}

Fig. S43. S_1-S_0 electron density map for probe **10** and its complex with Zn^{2+} (S_1 minima). Red represents positive densities and blue negative values.

Biological applications

Toxicity tests for probes **7**-**10** to cells

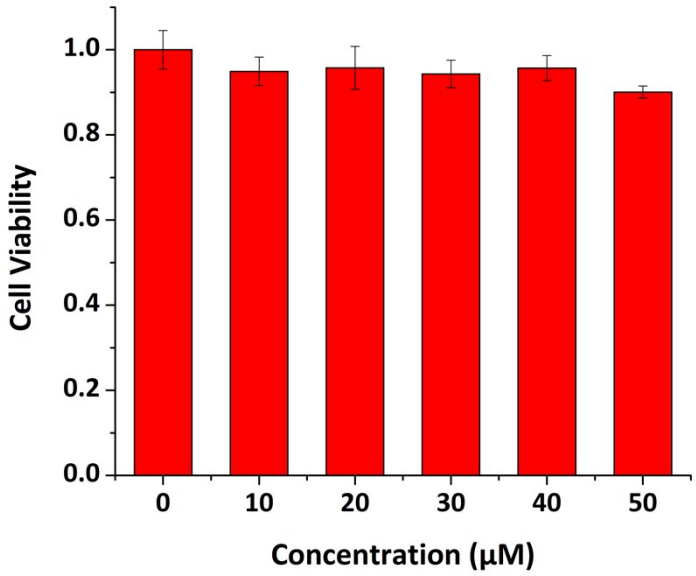


Fig. S44. The HeLa cell viability against probe **7** at different concentrations.

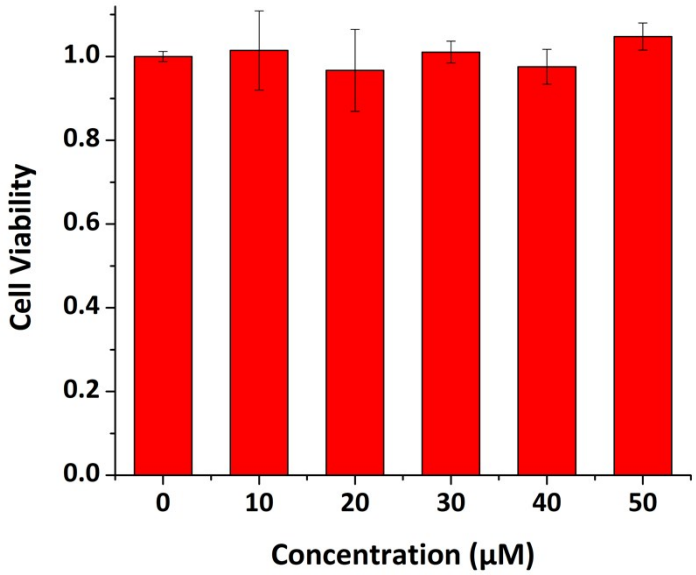


Fig. S45. The HeLa cell viability against probe **8** at different concentrations.

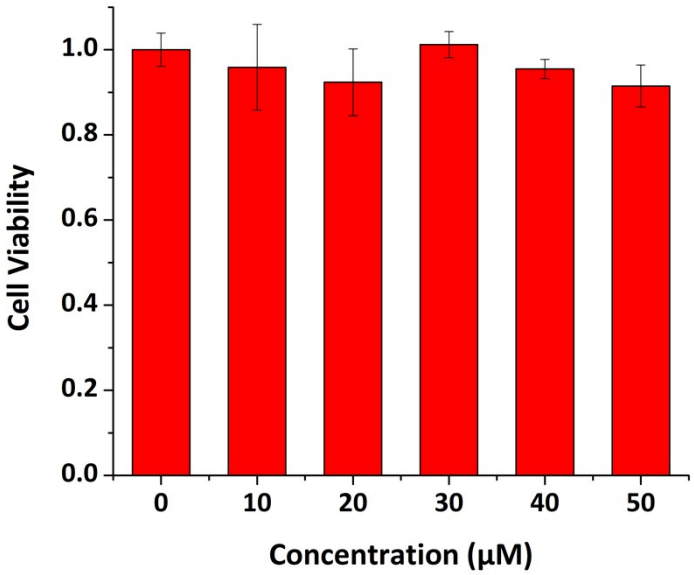


Fig. S46. The HeLa cell viability against probe **9** at different concentrations.

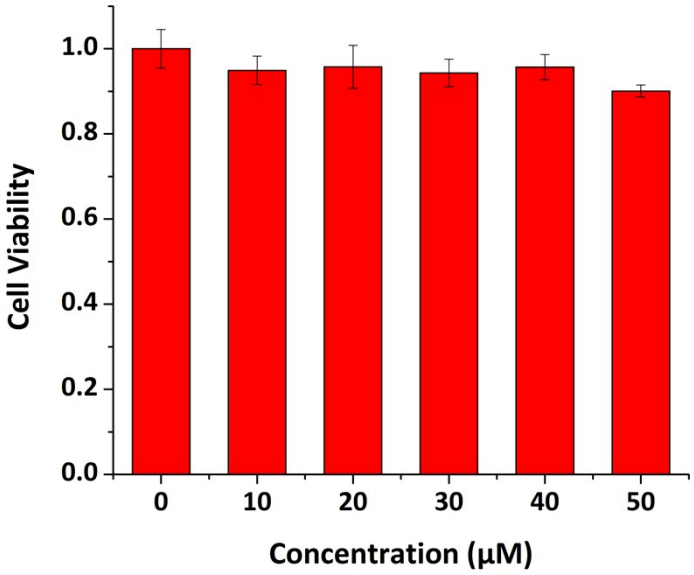


Fig. S47. The HeLa cell viability against probe **10** at different concentrations.

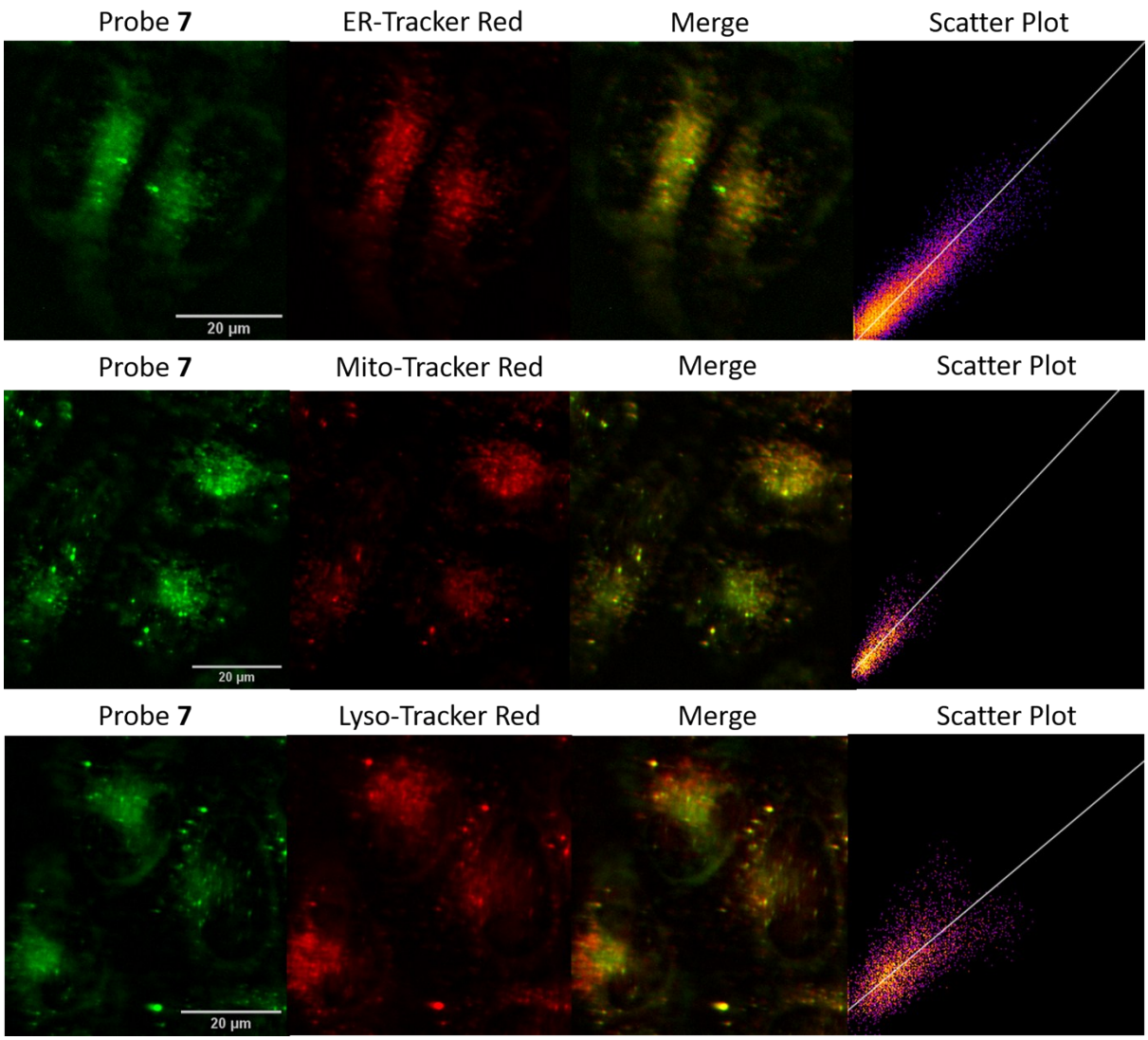


Fig. S48 The colocalization images of HeLa cells incubated with probe **7** (20 μM, GFP filter: λ_{ex} = 470/30 nm, λ_{em} = 530/50 nm) and organelle tracker red dyes (RFP filter: λ_{ex} = 530/40 nm, λ_{em} = 605/55 nm). (Scale bars = 20 μm). Pearson's correlation coefficients were 0.88, 0.73 and 0.50 compared to ER-tracker red, Mito-tracker red and Lyso-tracker red, respectively.

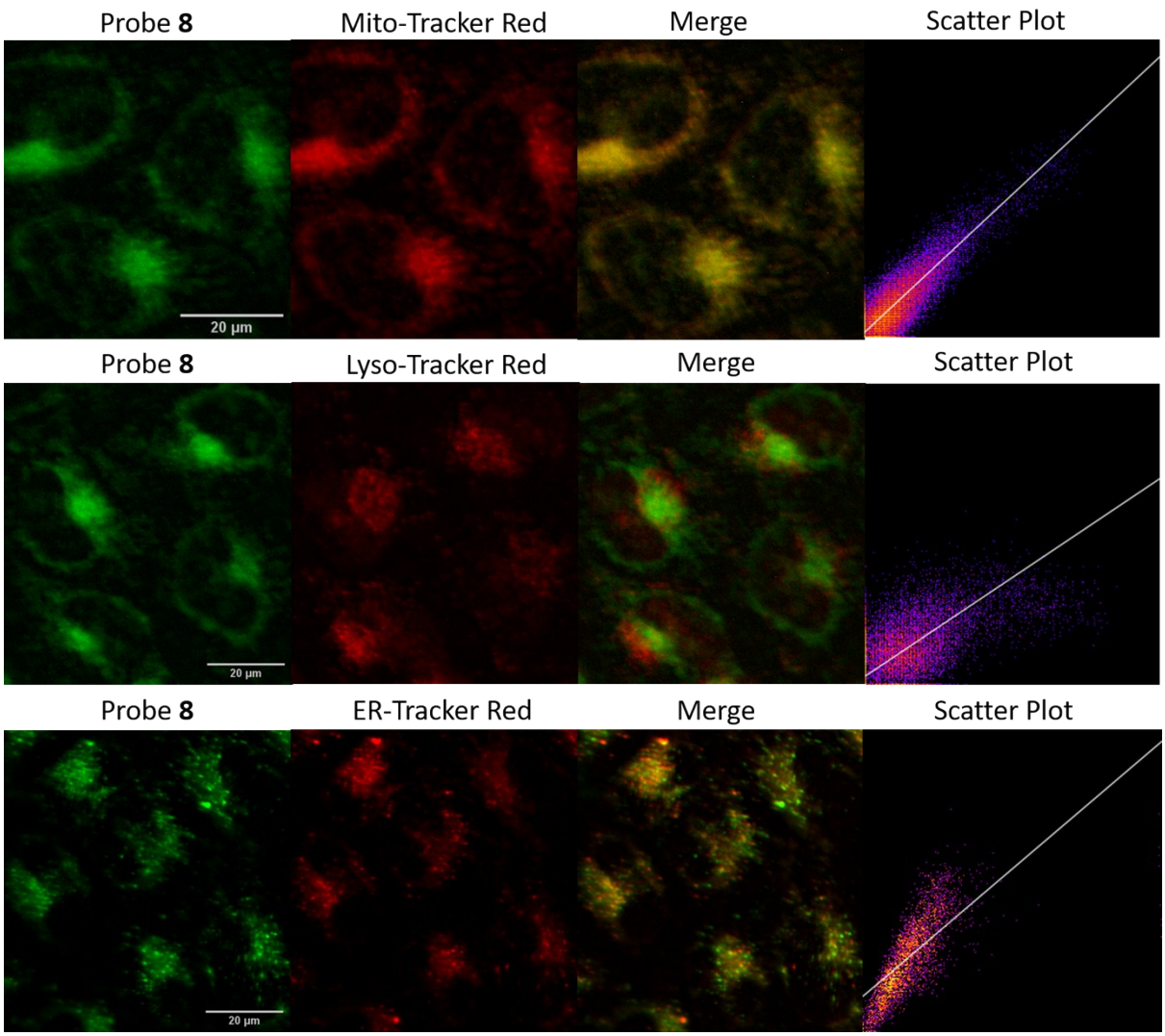


Fig. S49 The colocalization images of HeLa cells incubated with probe **8** (20 μM, GFP filter: λ_{ex} = 470/30 nm, λ_{em} = 530/50 nm) and organelle tracker red dyes (RFP filter: λ_{ex} = 530/40 nm, λ_{em} = 605/55 nm). (Scale bars = 20 μm). Pearson's correlation coefficients were 0.93, 0.41 and 0.68 compared to Mito-tracker red, Lyso-tracker red and ER-tracker red, respectively.

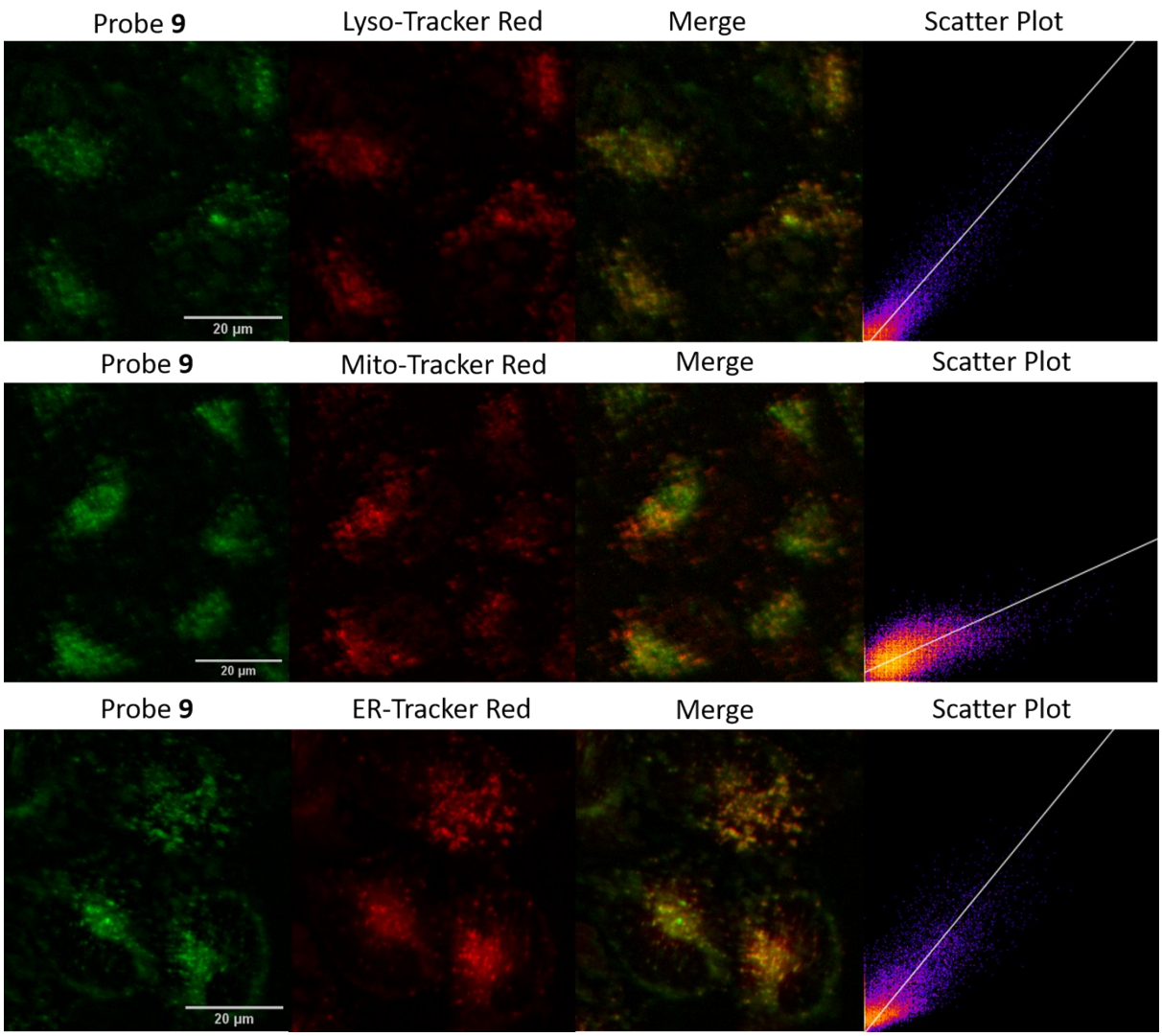


Fig. S50 The colocalization images of HeLa cells incubated with probe **9** (20 μM, GFP filter: λ_{ex} = 470/30 nm, λ_{em} = 530/50 nm) and organelle tracker red dyes (RFP filter: λ_{ex} = 530/40 nm, λ_{em} = 605/55 nm). (Scale bars = 20 μm). Pearson's correlation coefficients were 0.86, 0.47 and 0.71 compared to Lyso-tracker red, Mito-tracker red and ER-tracker red, respectively.

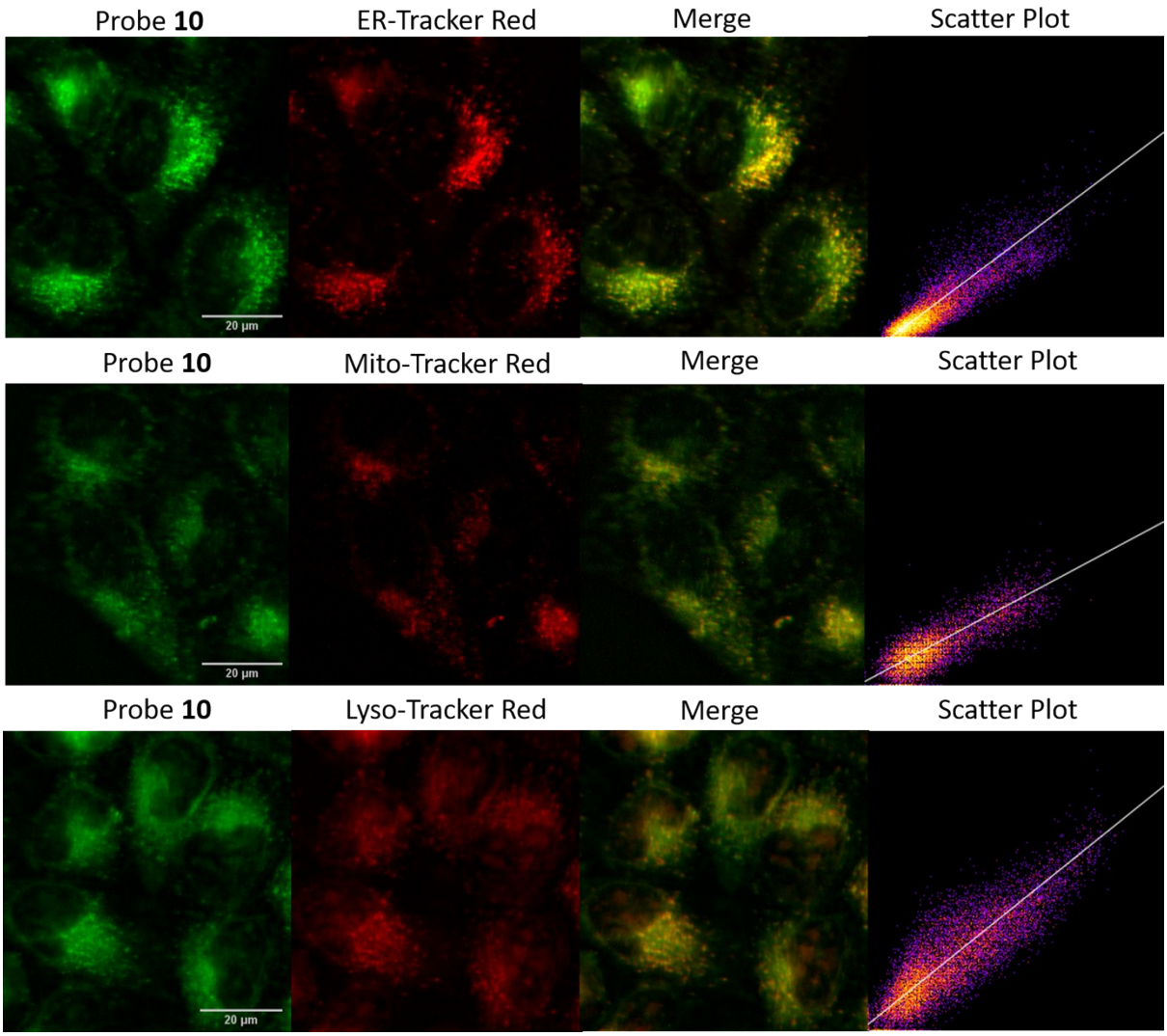


Fig. S51 The colocalization images of HeLa cells incubated with probe **10** (20 μM, GFP filter: λ_{ex} = 470/30 nm, λ_{em} = 530/50 nm) and organelle tracker red dyes (RFP filter: λ_{ex} = 530/40 nm, λ_{em} = 605/55 nm). (Scale bars = 20 μm). Pearson's correlation coefficients were 0.85, 0.78 and 0.81 compared to ER-tracker red, Mito-tracker red and Lyso-tracker red, respectively.

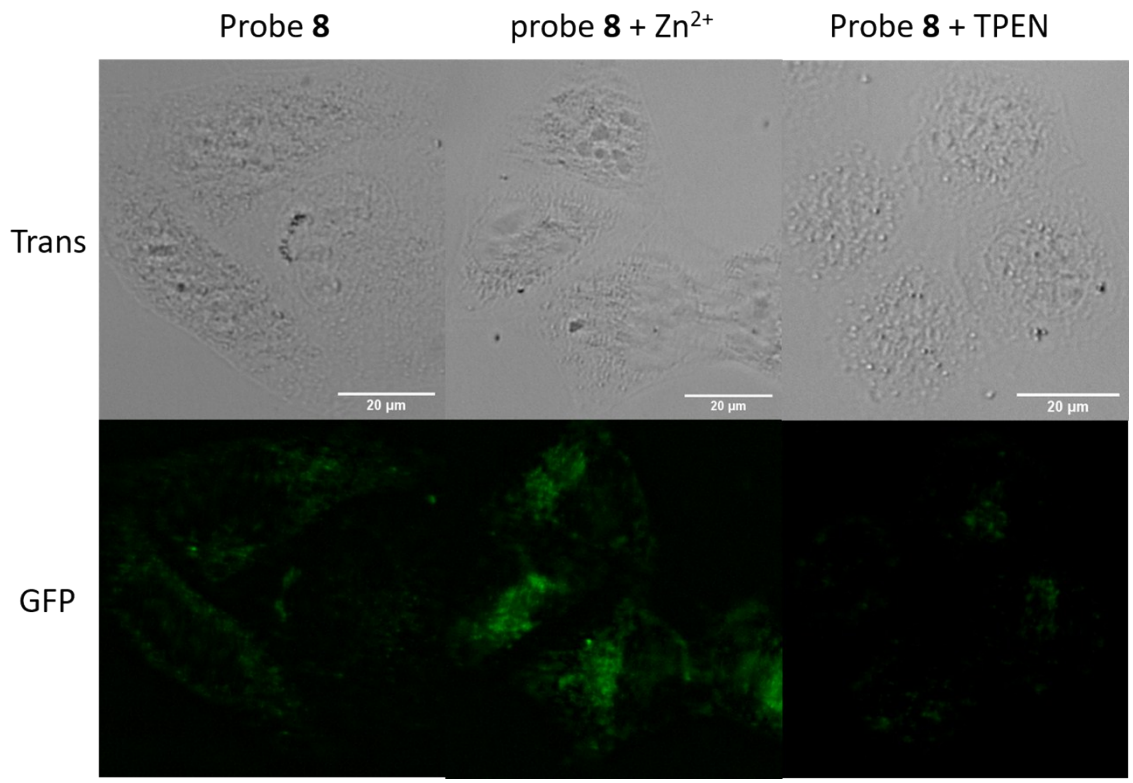


Fig. S52 Fluorescence microscopy images of HeLa cells treated with **8** (20 μM), **8** (20 μM) with zinc pyrithione (100 μM), and **8** (20 μM) with TPEN (100 μM). (Scale bars = 20 μm)

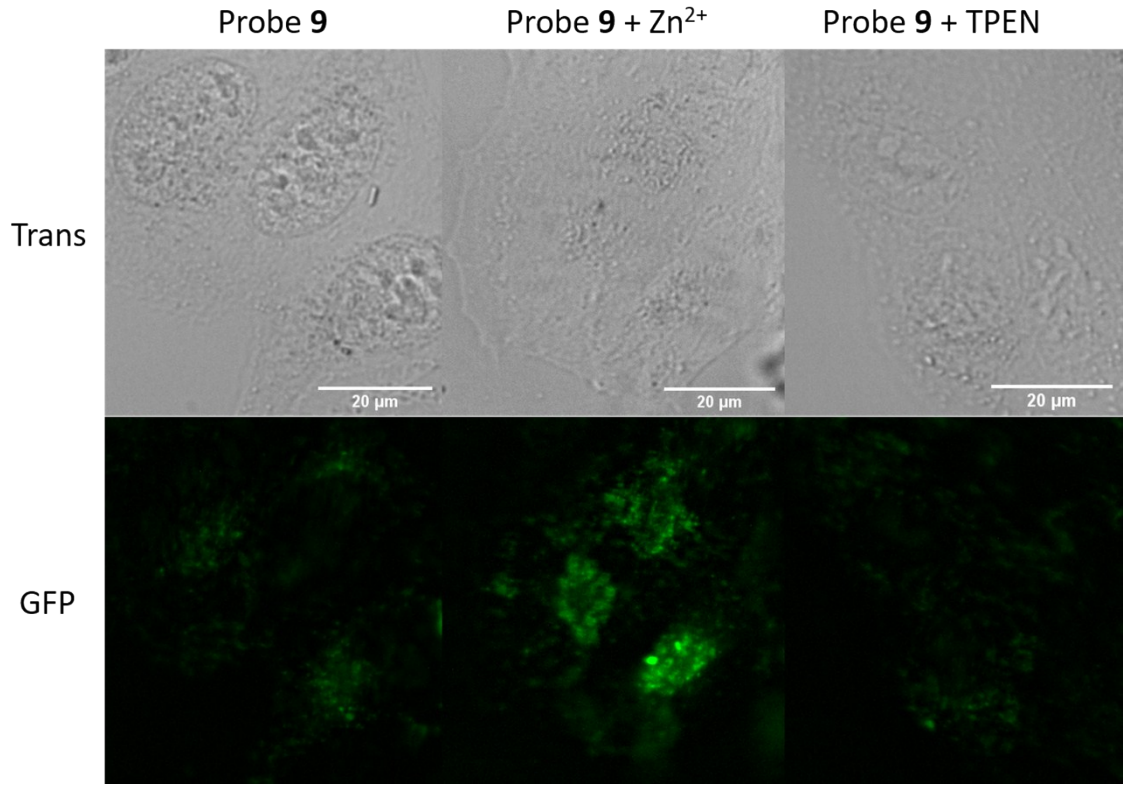


Fig. S53 Fluorescence microscopy images of HeLa cells treated with **9** (20 μM), **9** (20 μM) with zinc pyrithione (100 μM), and **9** (20 μM) with TPEN (100 μM). (Scale bars = 20 μm)

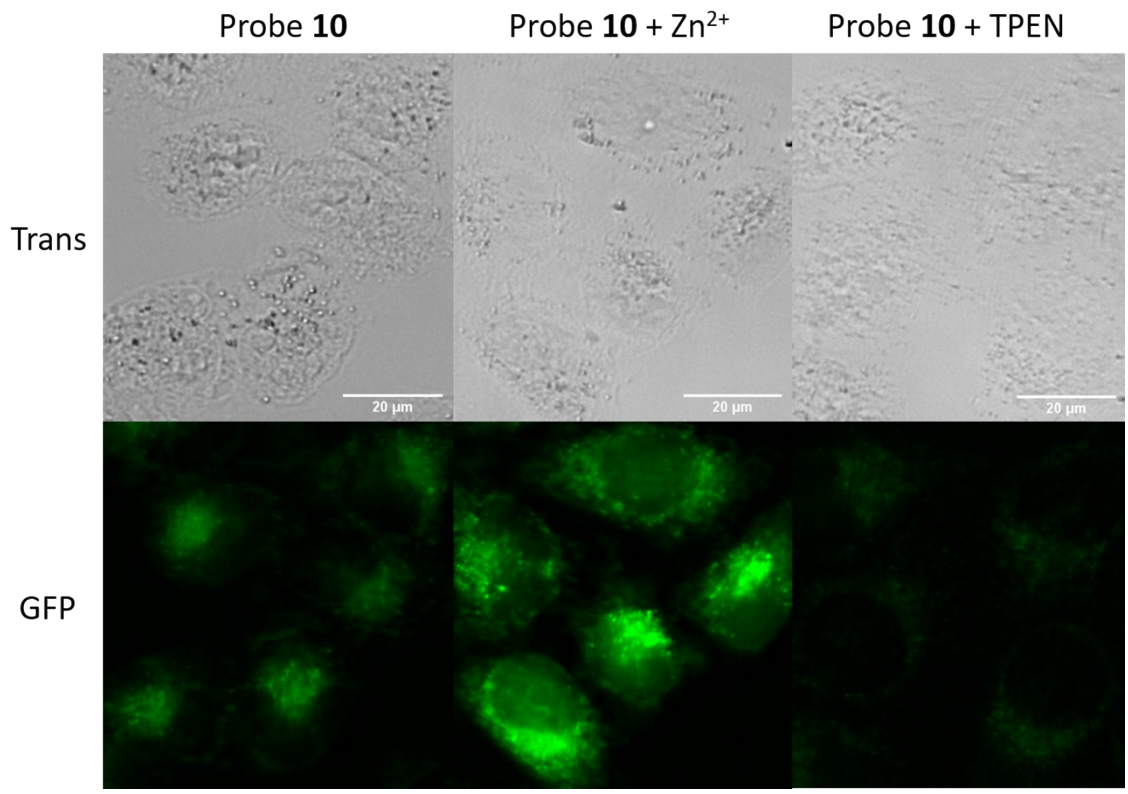


Fig. S54 Fluorescence microscopy images of HeLa cells treated with **10** (20 μM), **10** (20 μM) with zinc pyrithione (100 μM), and **10** (20 μM) with TPEN (100 μM). (Scale bars = 20 μm)

References:

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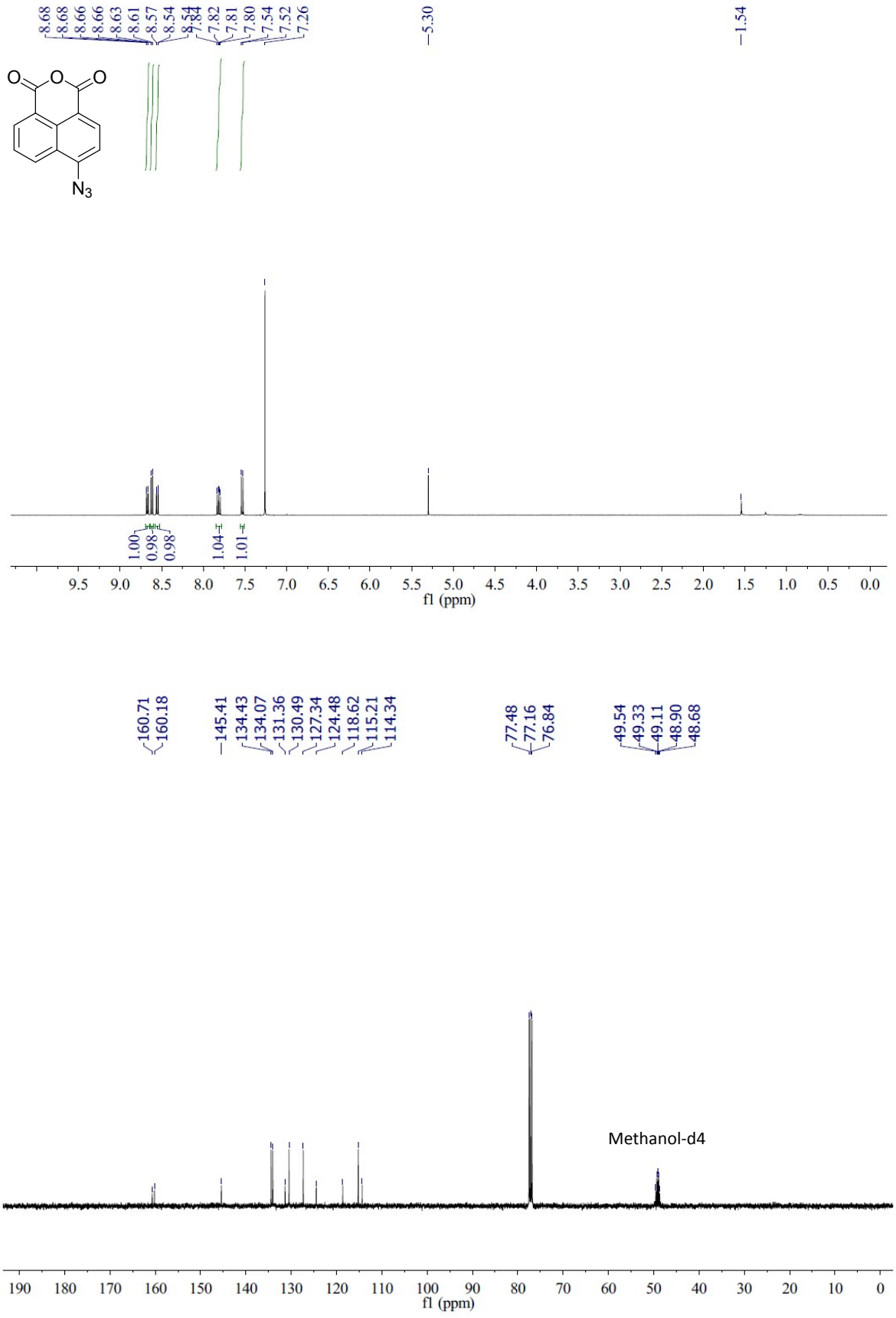
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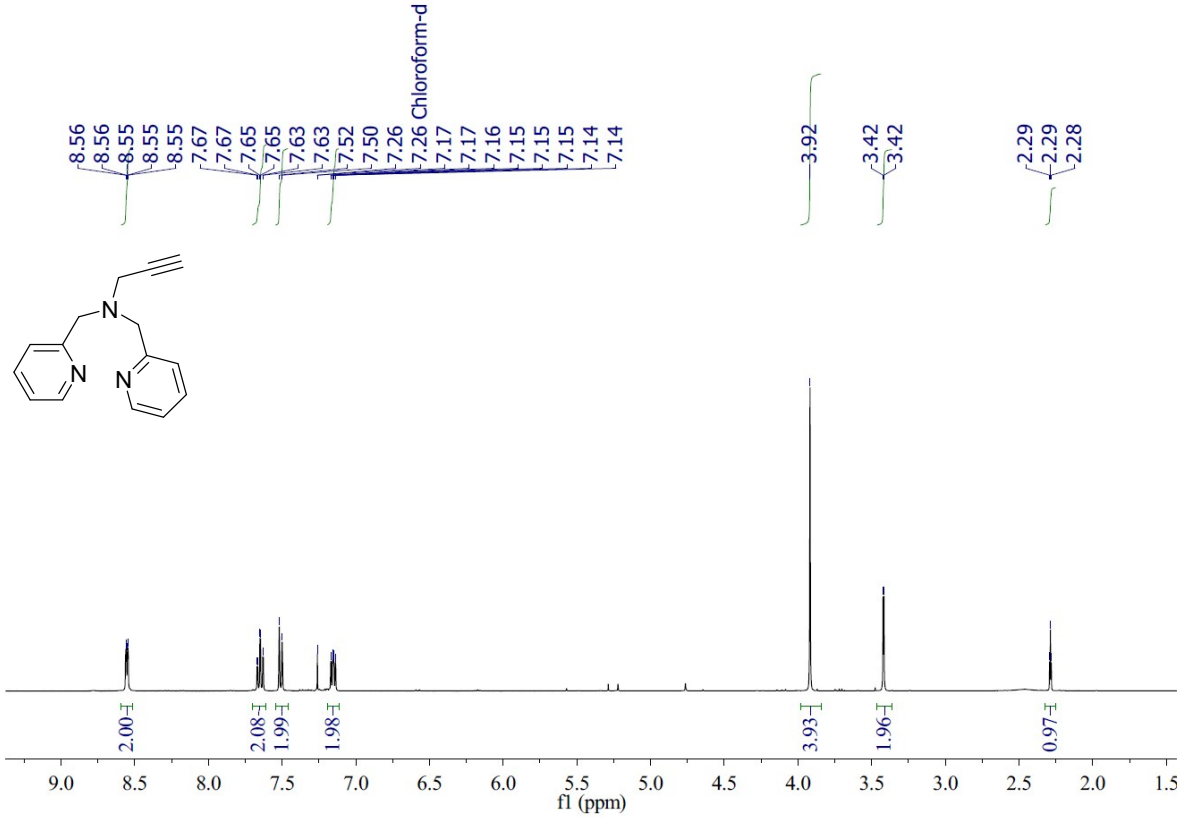
8.66
8.63
8.61
8.57
8.54
7.84
7.82
7.81
7.80
7.54
7.52
7.26
5.30
1.54
O
O
O
N3
1.00
0.98
0.98
1.04
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
160.71
160.18
145.41
134.43
134.07
131.36
130.49
127.34
124.48
118.62
115.21
114.34
77.48
77.16
76.84
49.54
49.33
49.11
48.90
48.68
Methanol-d4
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Compound **2**: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8.55
8.55
8.55
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7.63
7.63
7.52
7.50
7.26
Chloroform-d
7.17
7.17
7.16
7.15
7.15
7.15
7.14
7.14
3.92
3.42
3.42
2.29
2.29
2.28
N
N
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2.00
2.08
1.99
1.98
3.93
1.96
0.97
9.0
8.5
8.0
7.5
7.0
6.5
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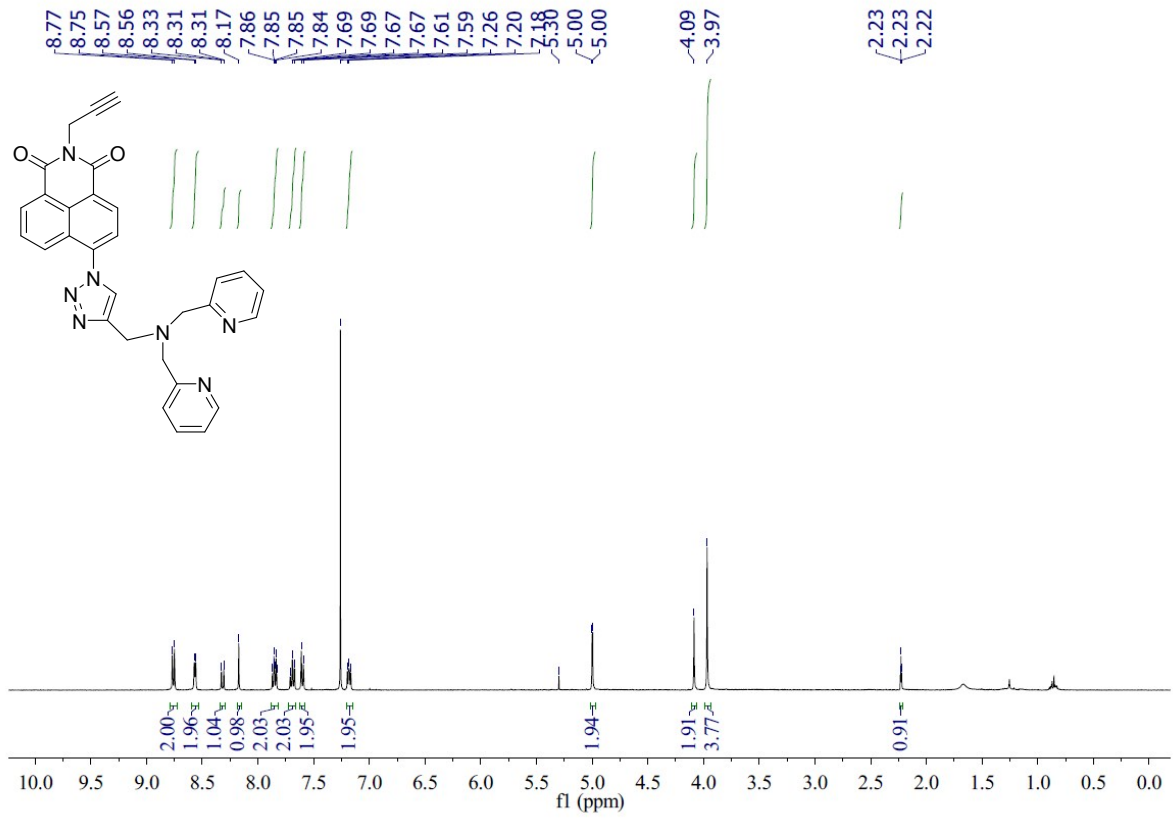
f1 (ppm)

Compound **3**: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7.85
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7.84
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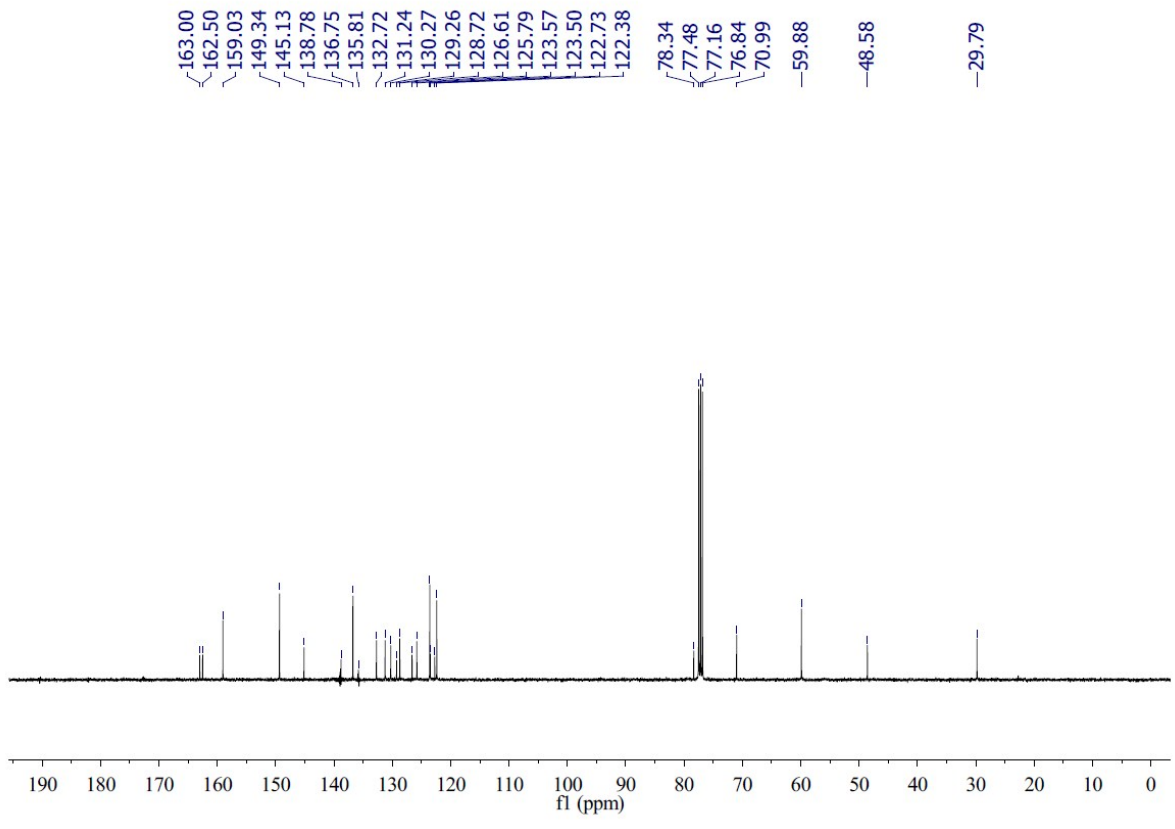
7.18
5.30
5.00
5.00
4.09
3.97
2.23
2.23
2.22
2.00
1.96
1.04
0.98
2.03
2.03
1.95
1.95
1.94
1.91
3.77
0.91
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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123.50
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122.38
78.34
77.48
77.16
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48.58
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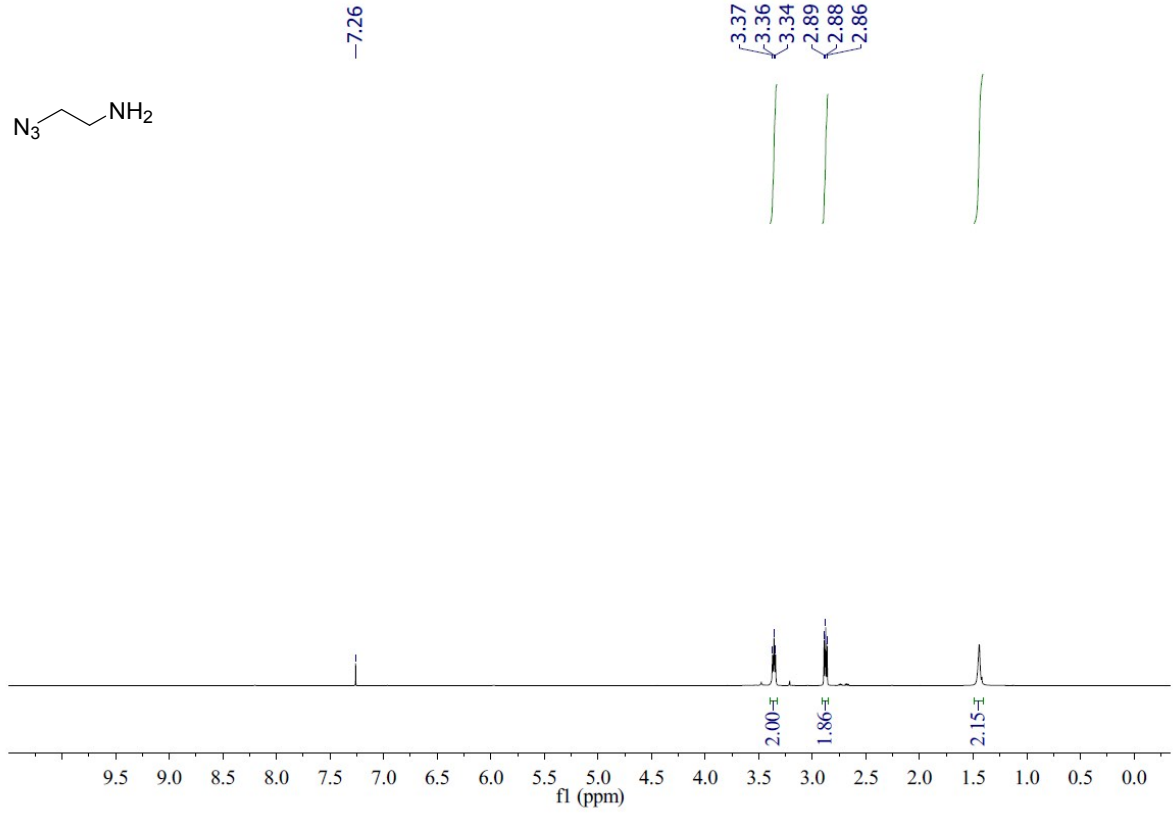
f1 (ppm)

Compound **S1**: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NH2
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1.86
2.15
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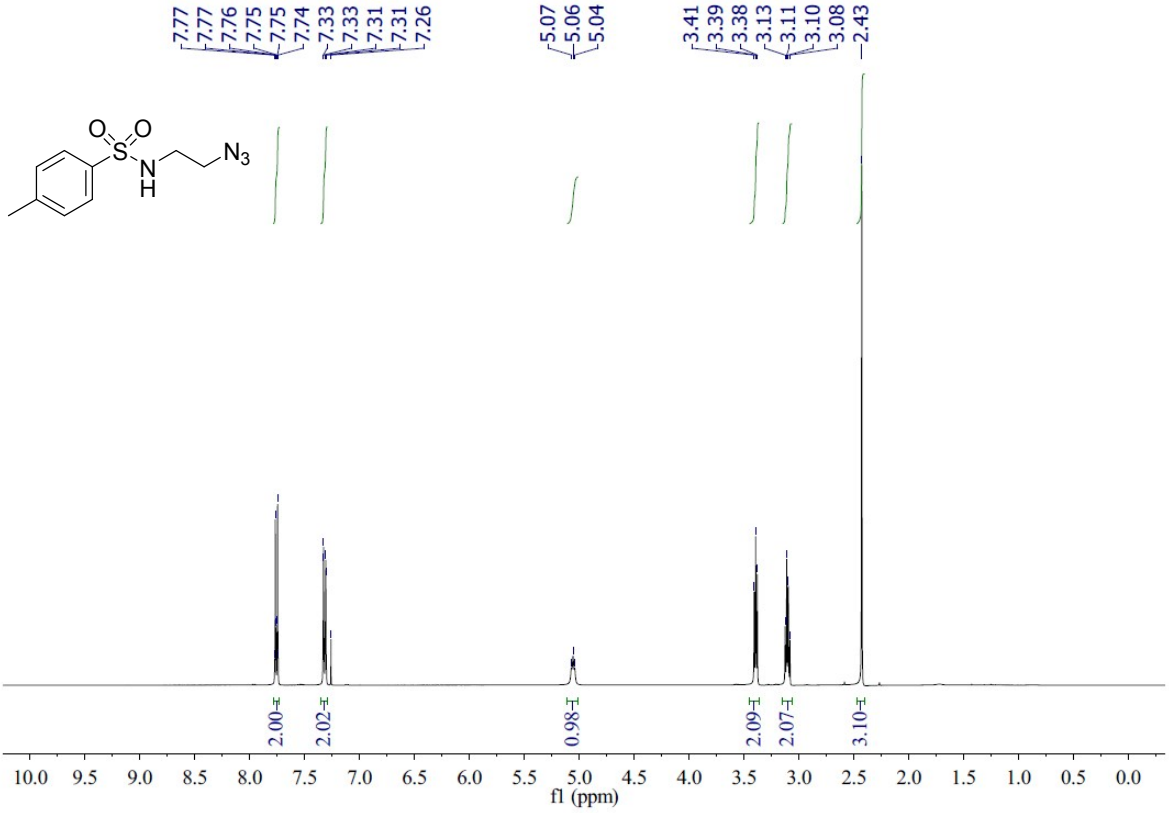
f1 (ppm)

Compound **4**: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5.07
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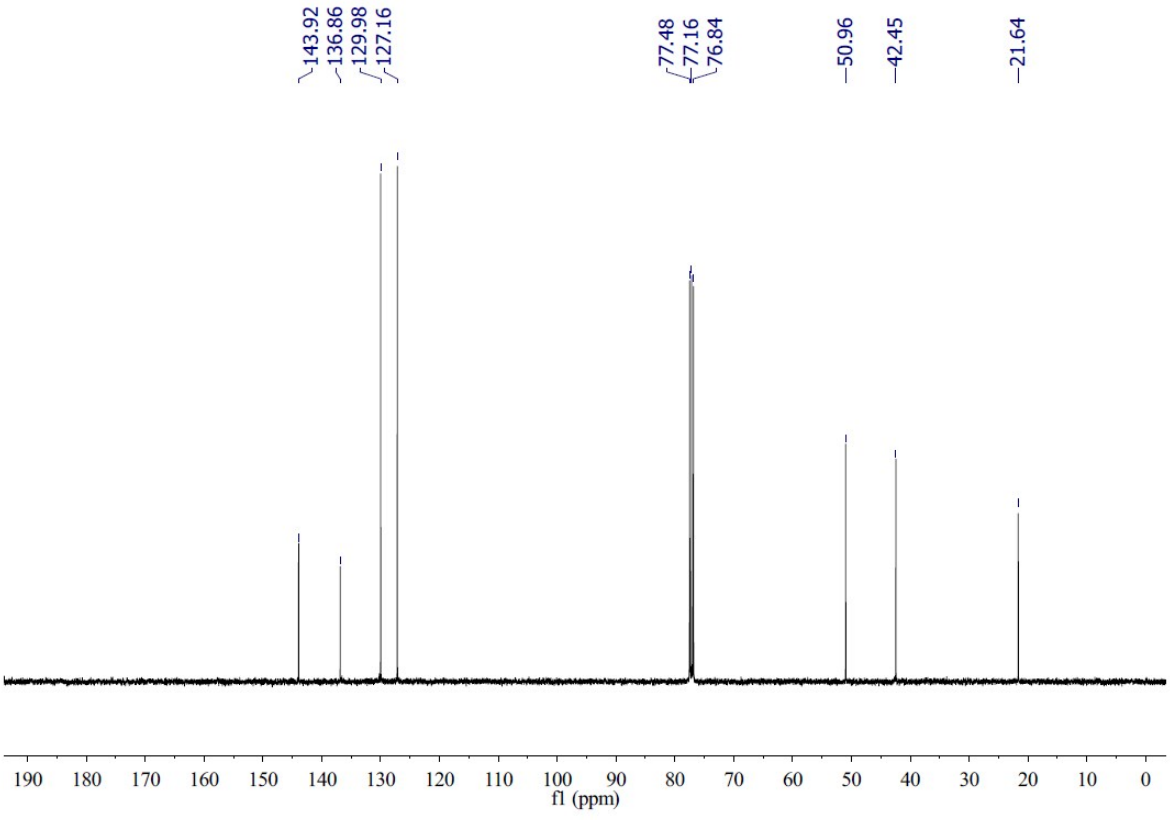
3.39
3.38
3.13
3.11
3.10
3.08
2.43
O
O
S
N
H
N3
2.00
2.02
0.98
2.09
2.07
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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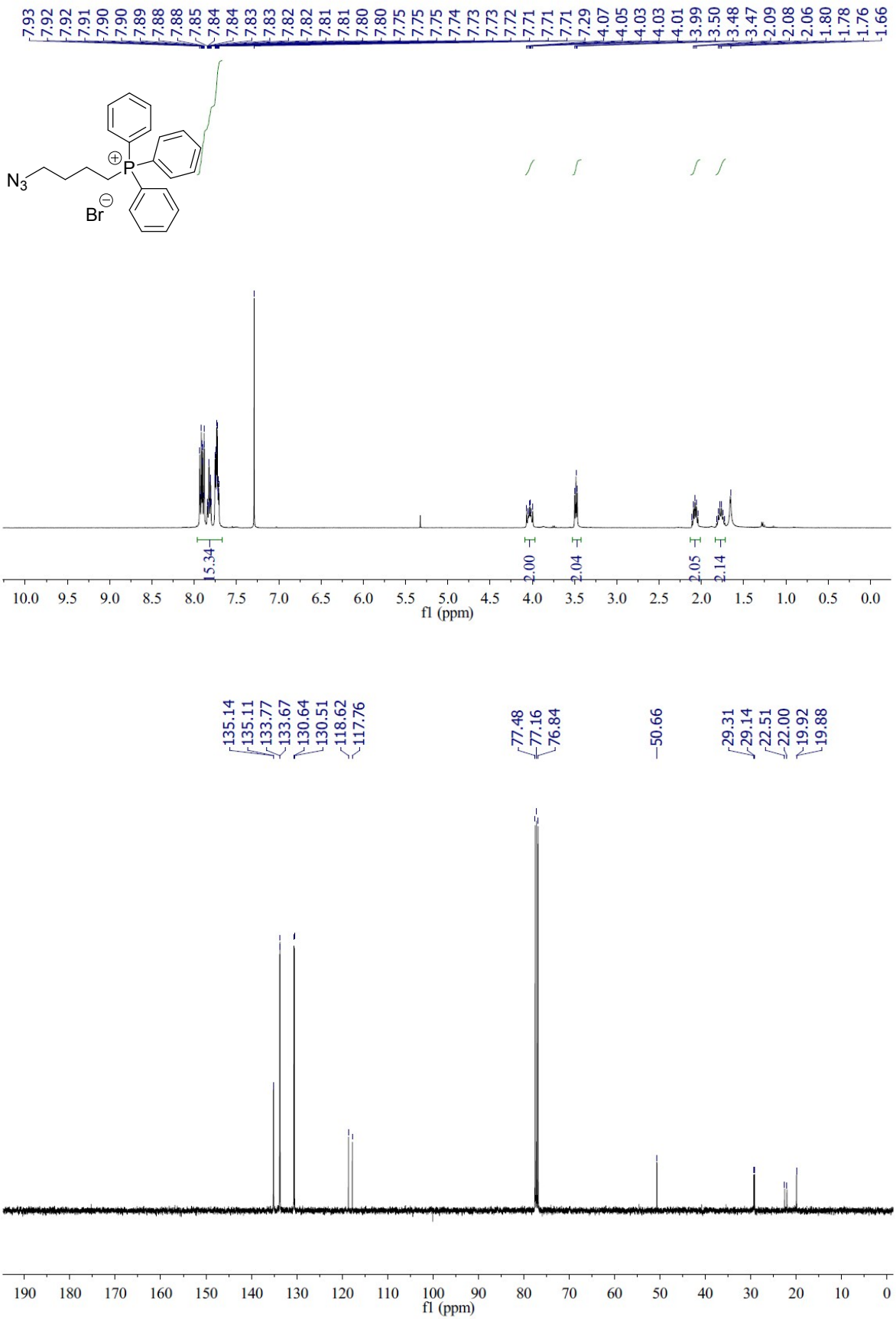
f1 (ppm)

Compound **S2**: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N3
P
Br
15.34
2.00
2.04
2.05
2.14
fl (ppm)
135.14 135.11 133.77 133.67 130.64 130.51 118.62 117.76
77.48 77.16 76.84
50.66
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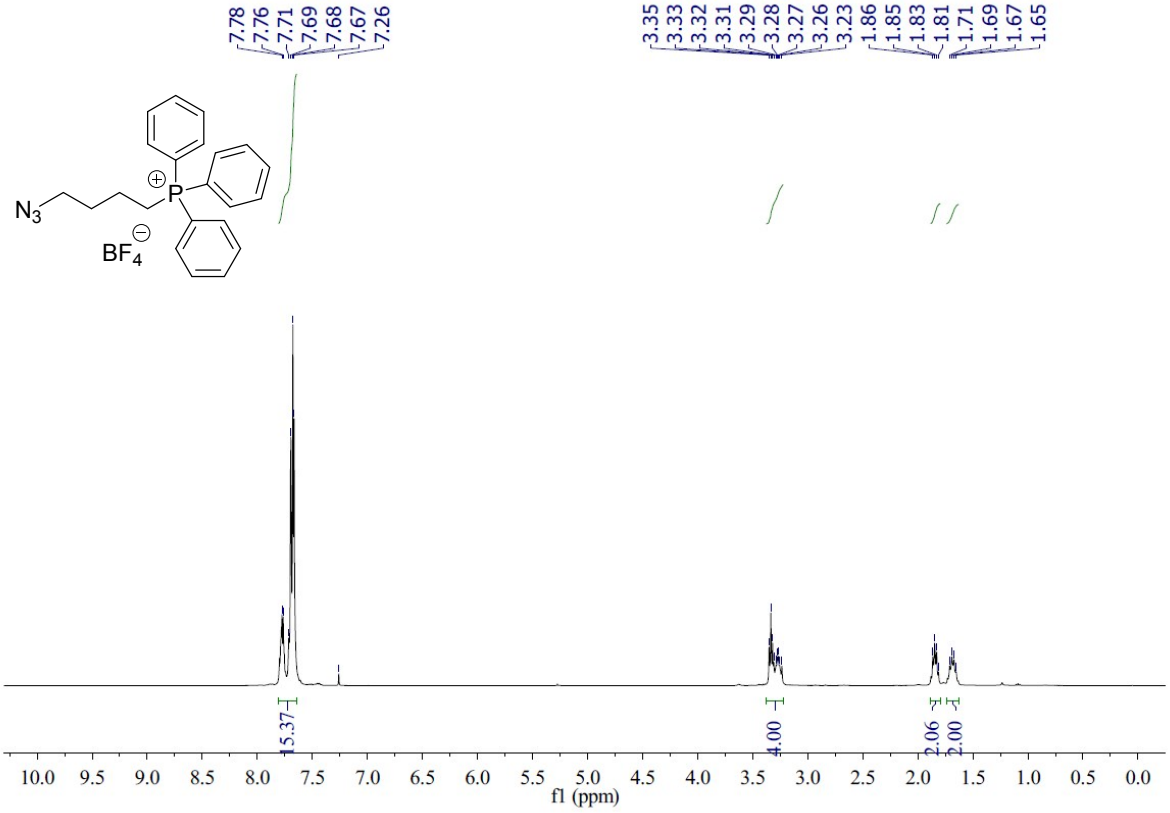
fl (ppm)

Compound **5**: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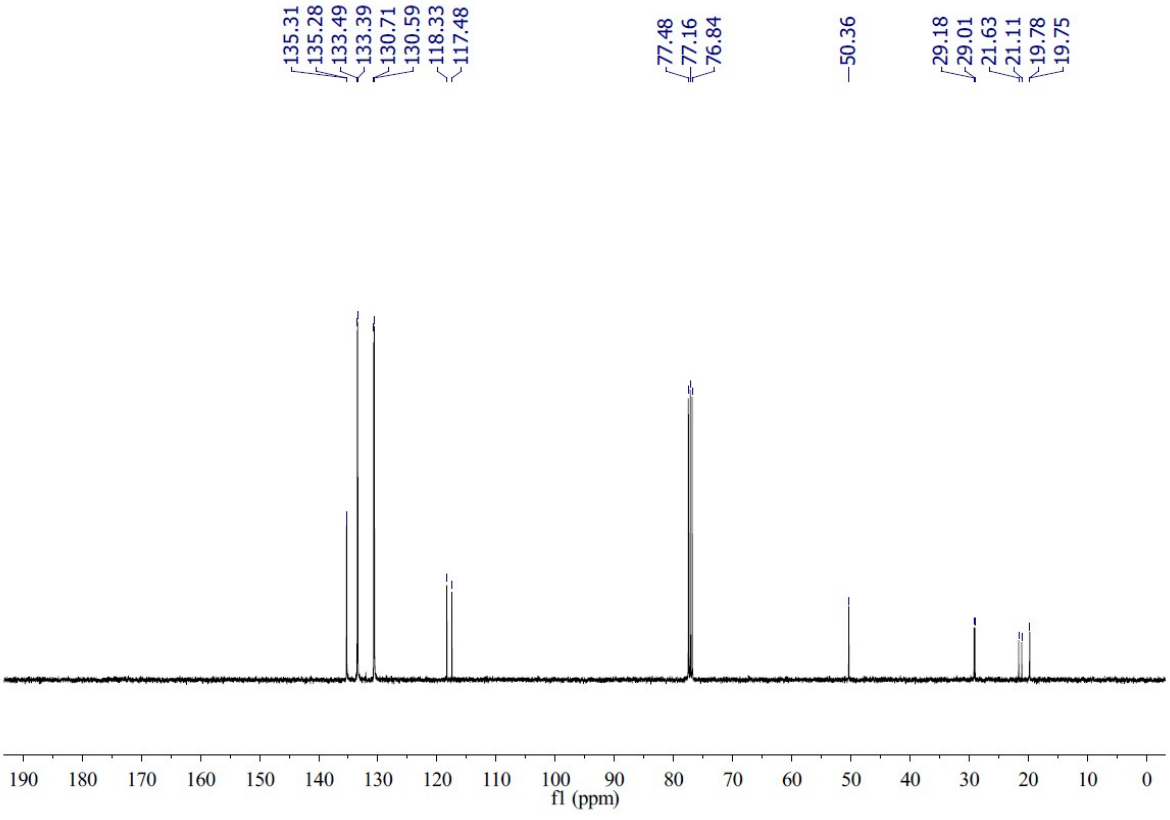
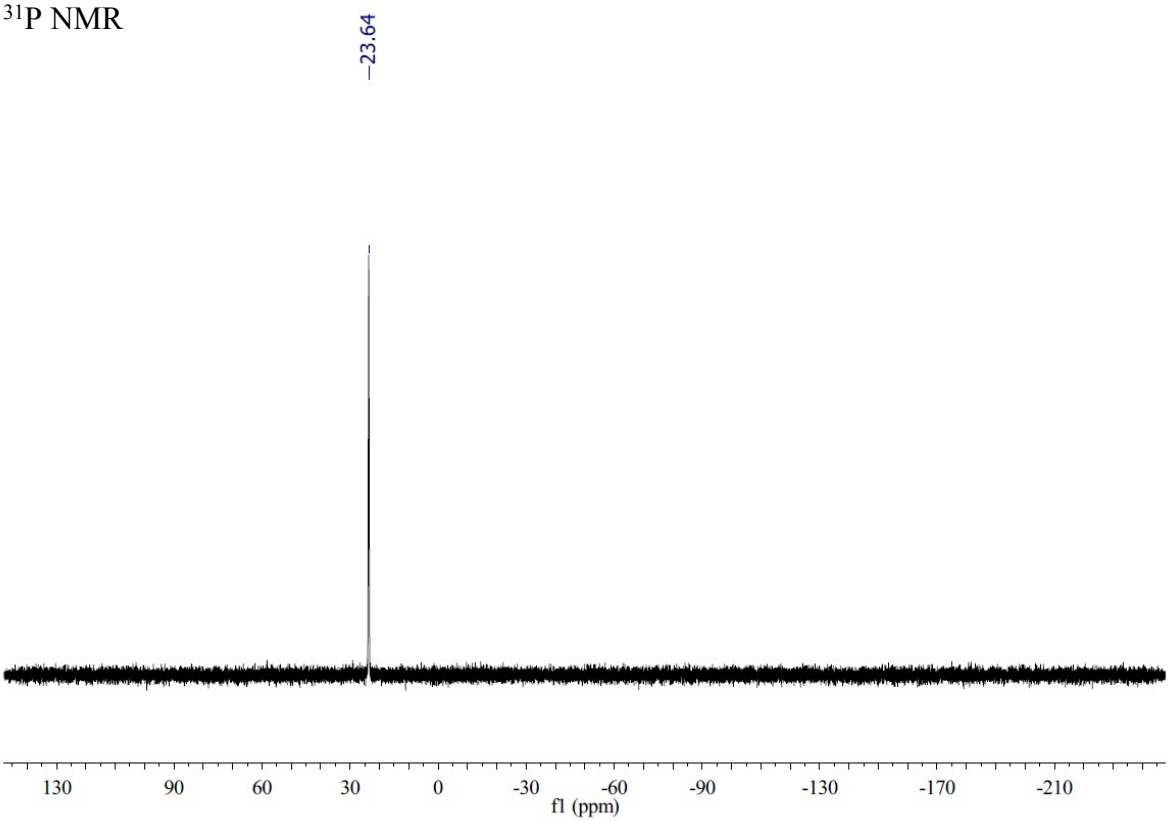
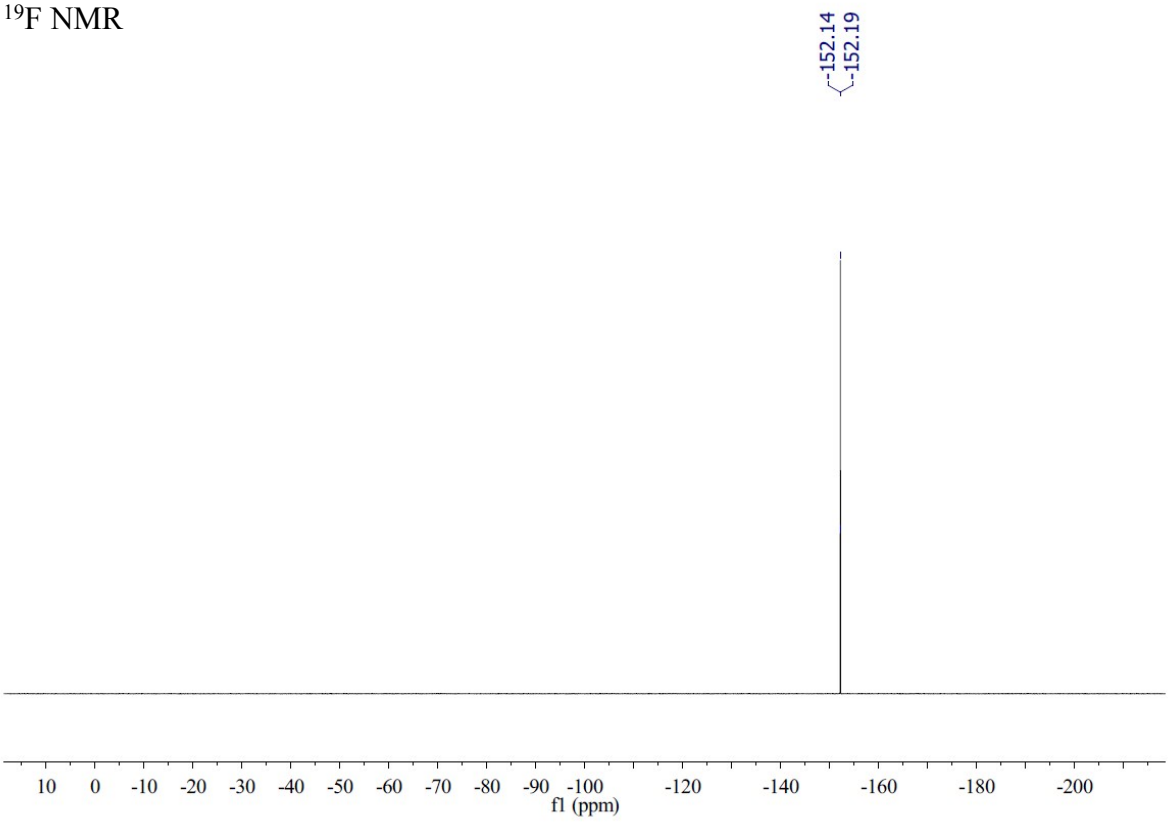
3.35
3.33
3.32
3.31
3.29
3.28
3.27
3.26
3.23
1.86
1.85
1.83
1.81
1.71
1.69
1.67
1.65
N3
P
BF4
15.37
4.00
2.06
2.00
fl (ppm)


135.31
135.28
133.49
133.39
130.71
130.59
118.33
117.48
77.48
77.16
76.84
50.36
29.18
29.01
21.63
21.11
19.78
19.75
fl (ppm)

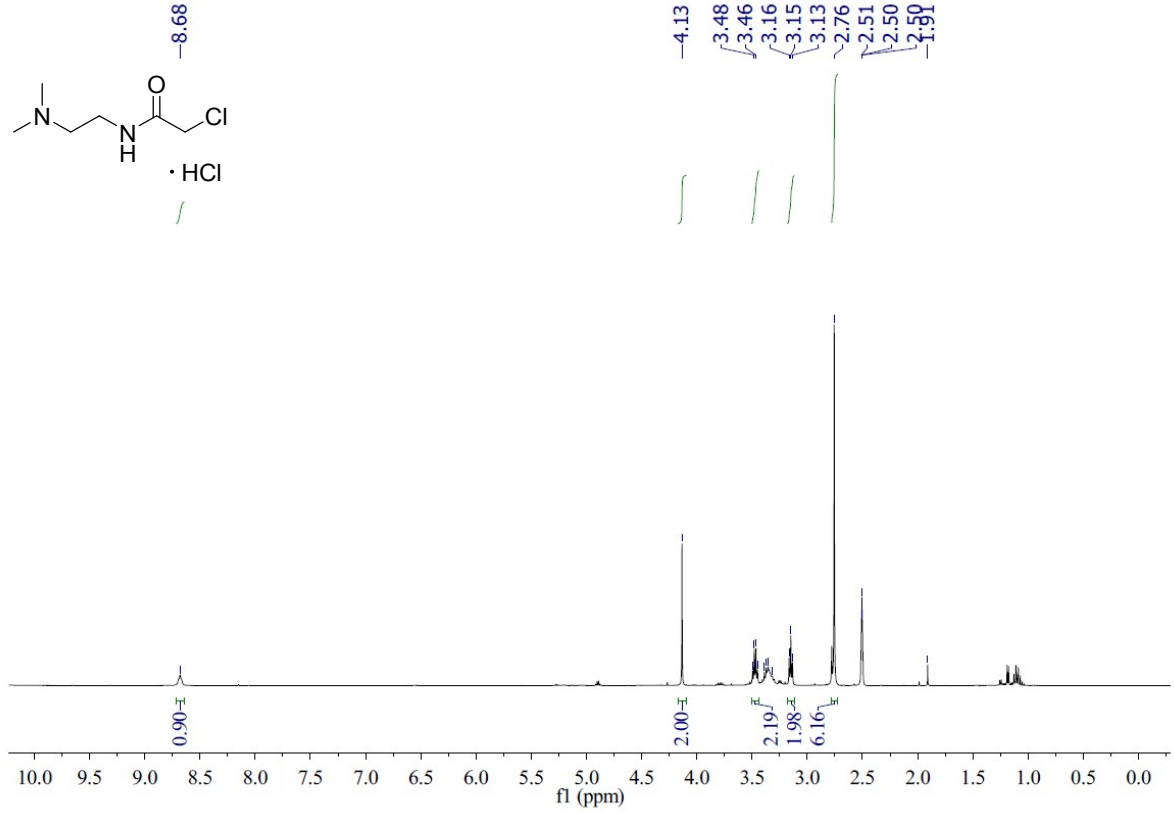
^{31}P NMR



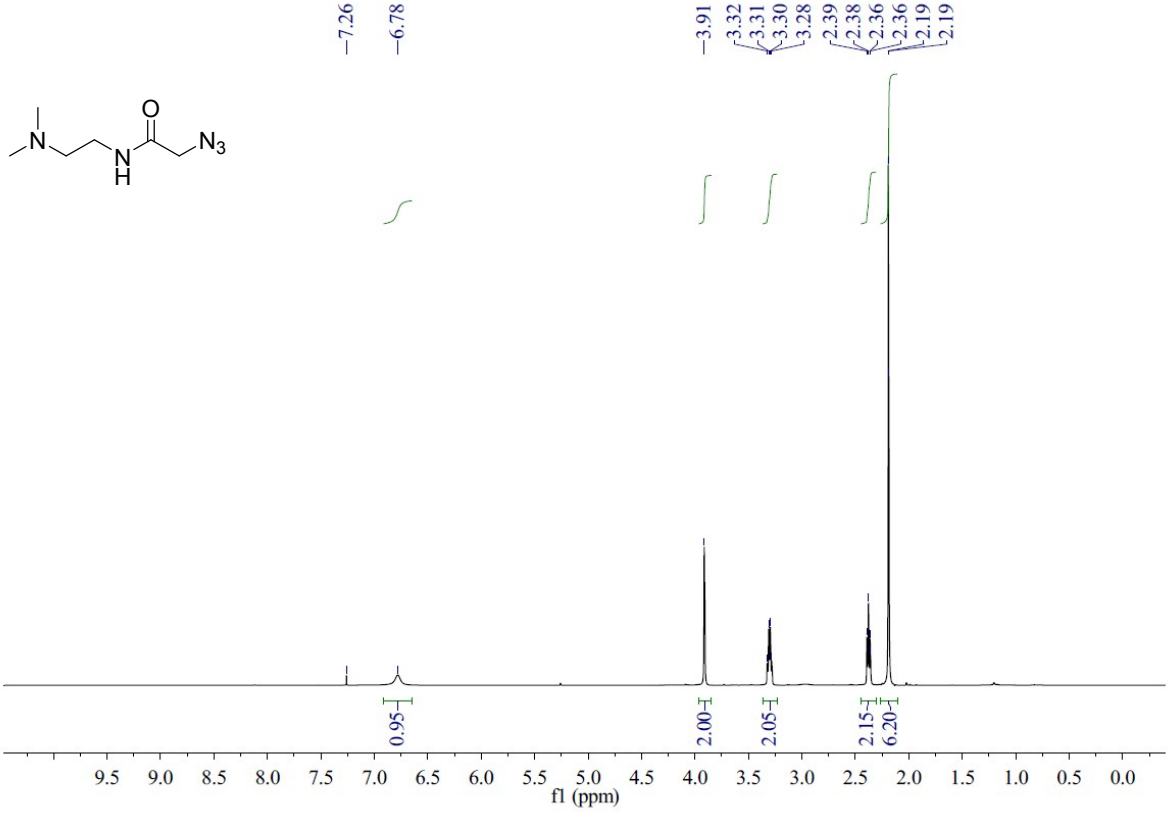
^{19}F NMR

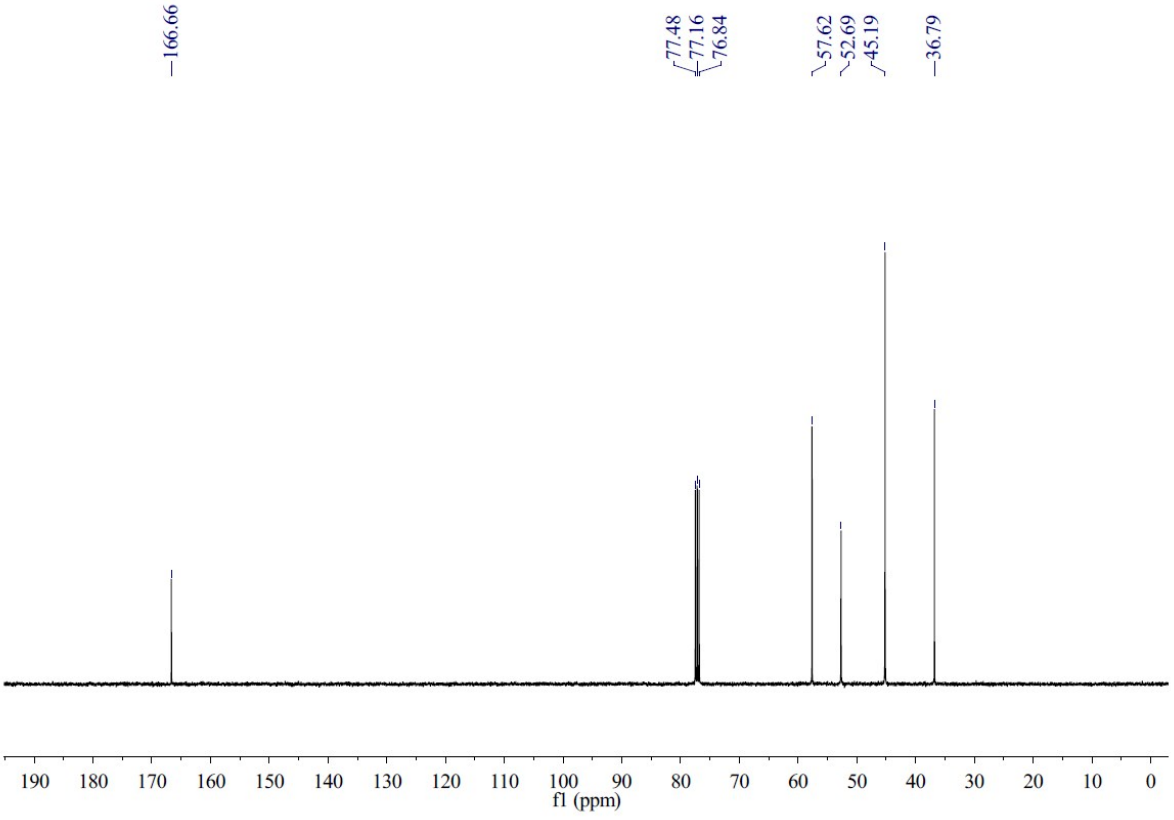


Compound **S3**:

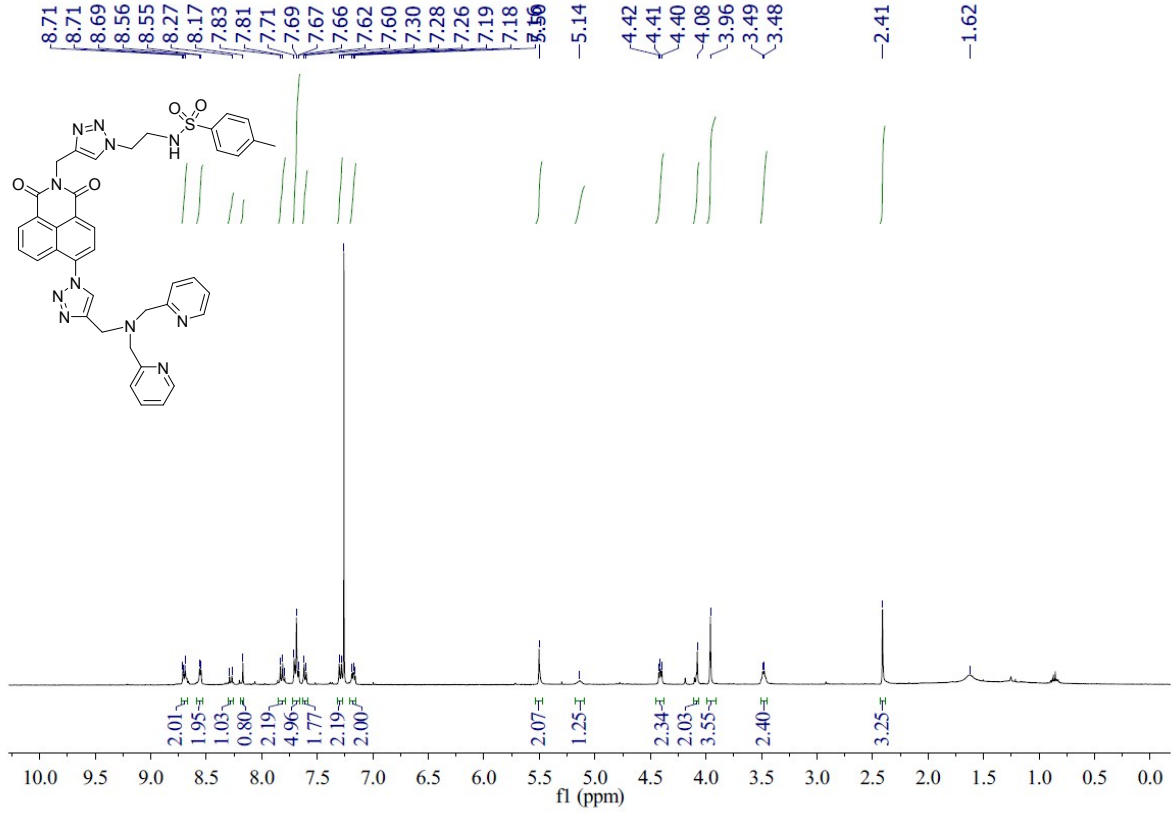

8.68
4.13
3.48
3.46
3.16
3.15
3.13
2.76
2.51
2.50
1.91
O
N
N
H
Cl
· HCl
0.90
2.00
2.19
1.98
6.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

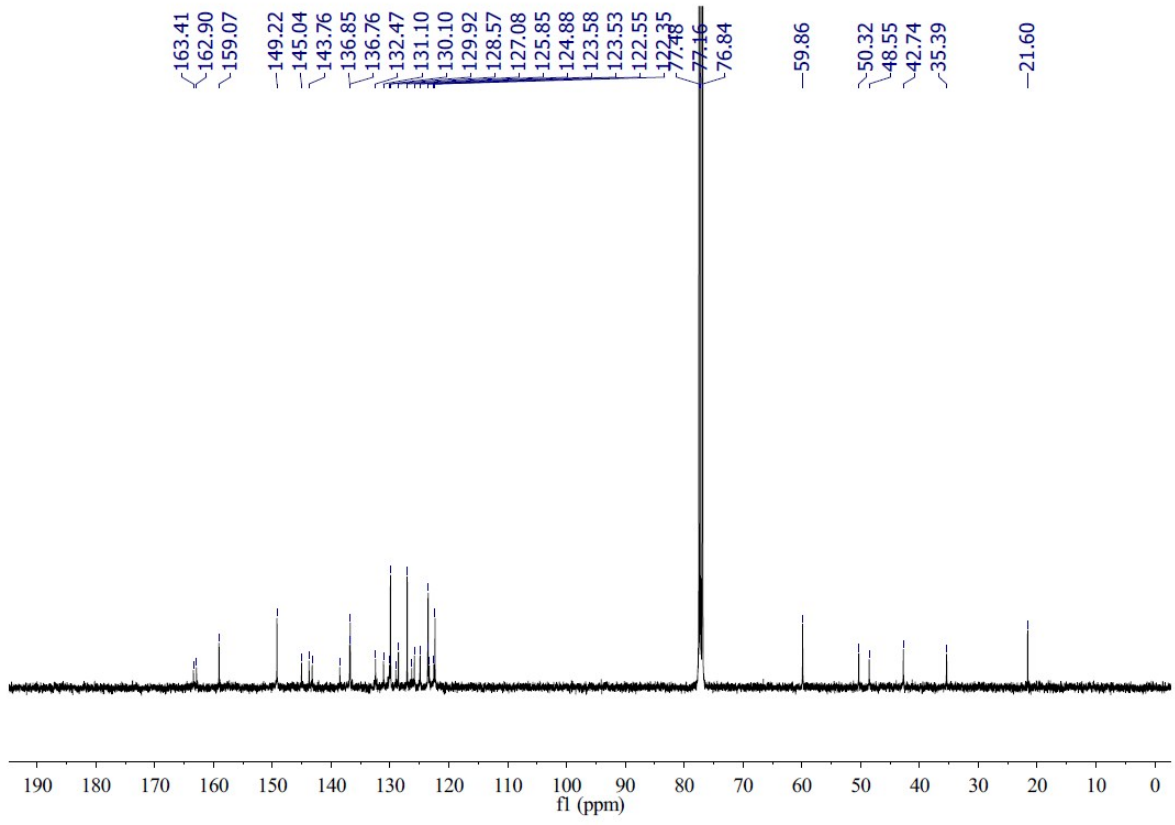
Compound **6**:


7.26
6.78
3.91
3.32
3.31
3.30
3.28
2.39
2.38
2.36
2.36
2.19
2.19
O
N
N
H
N3
0.95
2.00
2.05
2.15
6.20
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

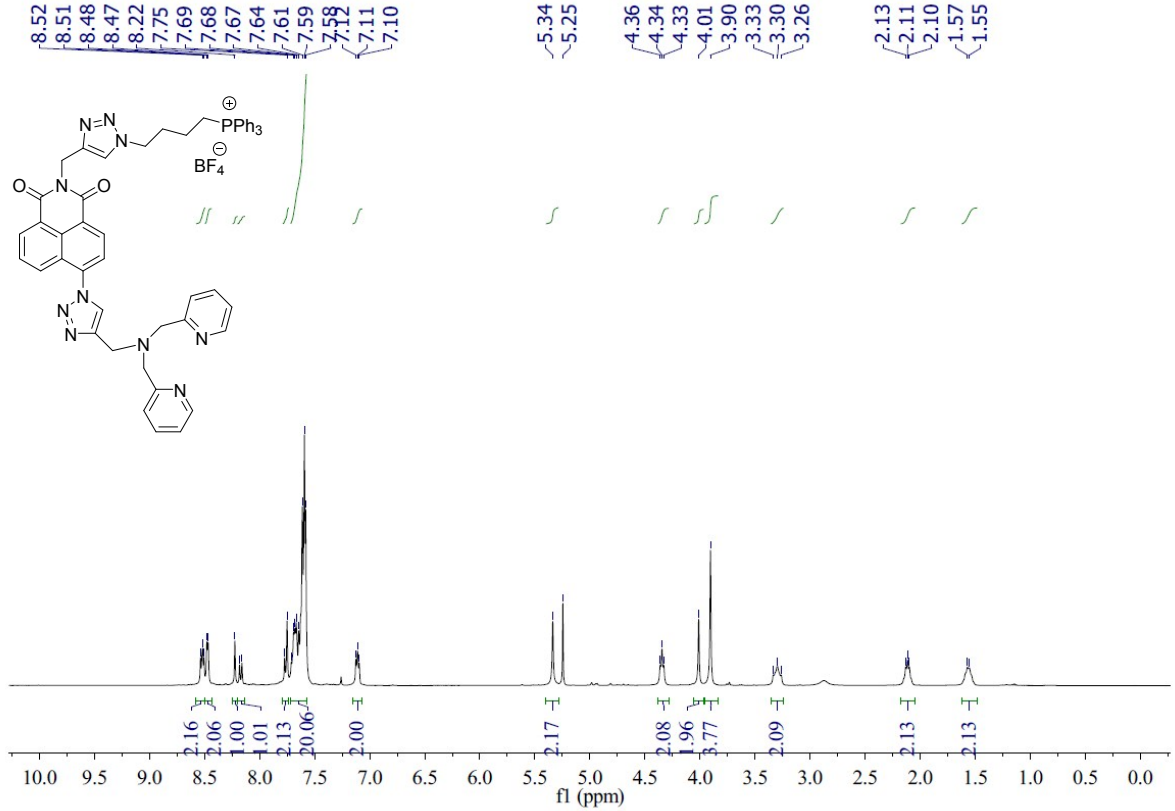

166.66
77.48
77.16
76.84
57.62
52.69
45.19
36.79
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

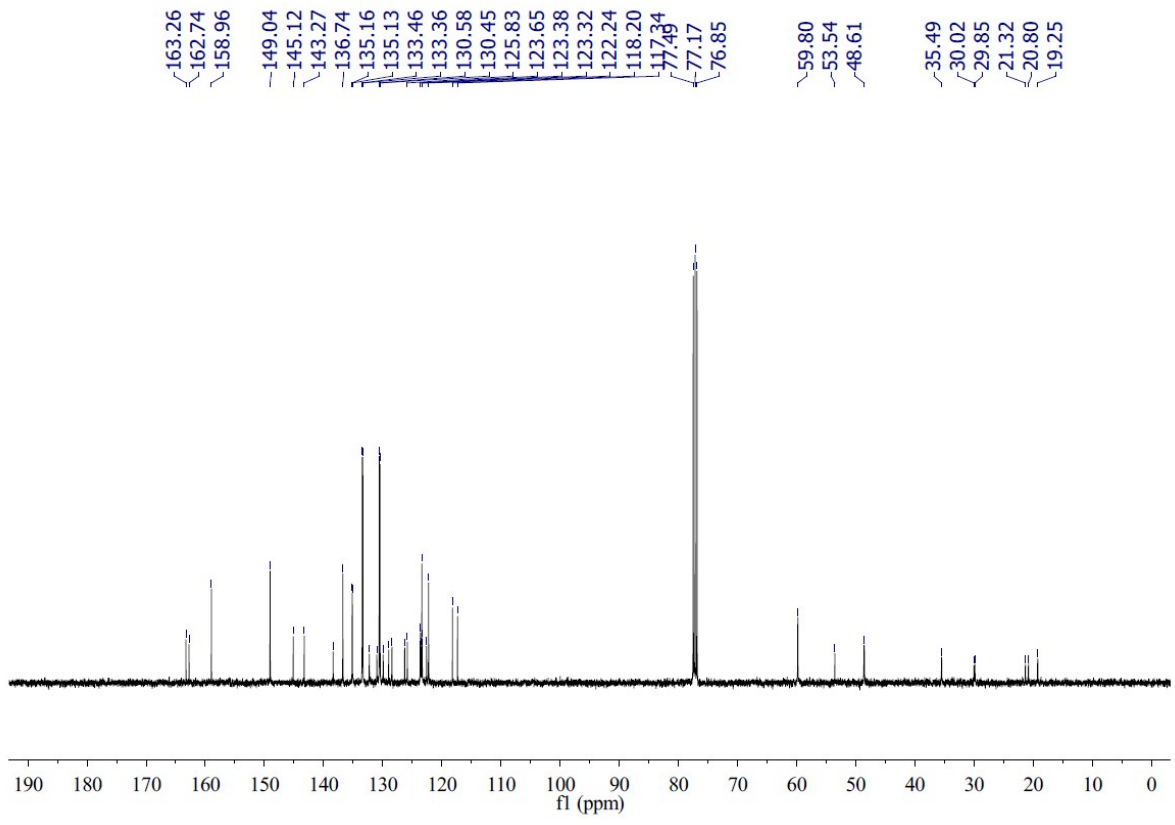
Compound **7**:


8.71
8.71
8.69
8.56
8.55
8.27
8.17
7.83
7.81
7.71
7.69
7.67
7.66
7.62
7.60
7.30
7.28
7.26
7.19
7.18
5.14
4.42
4.41
4.40
4.08
3.96
3.49
3.48
2.41
1.62
2.01
1.95
1.03
0.80
2.19
4.96
1.77
2.19
2.00
2.07
1.25
2.34
2.03
3.55
2.40
3.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

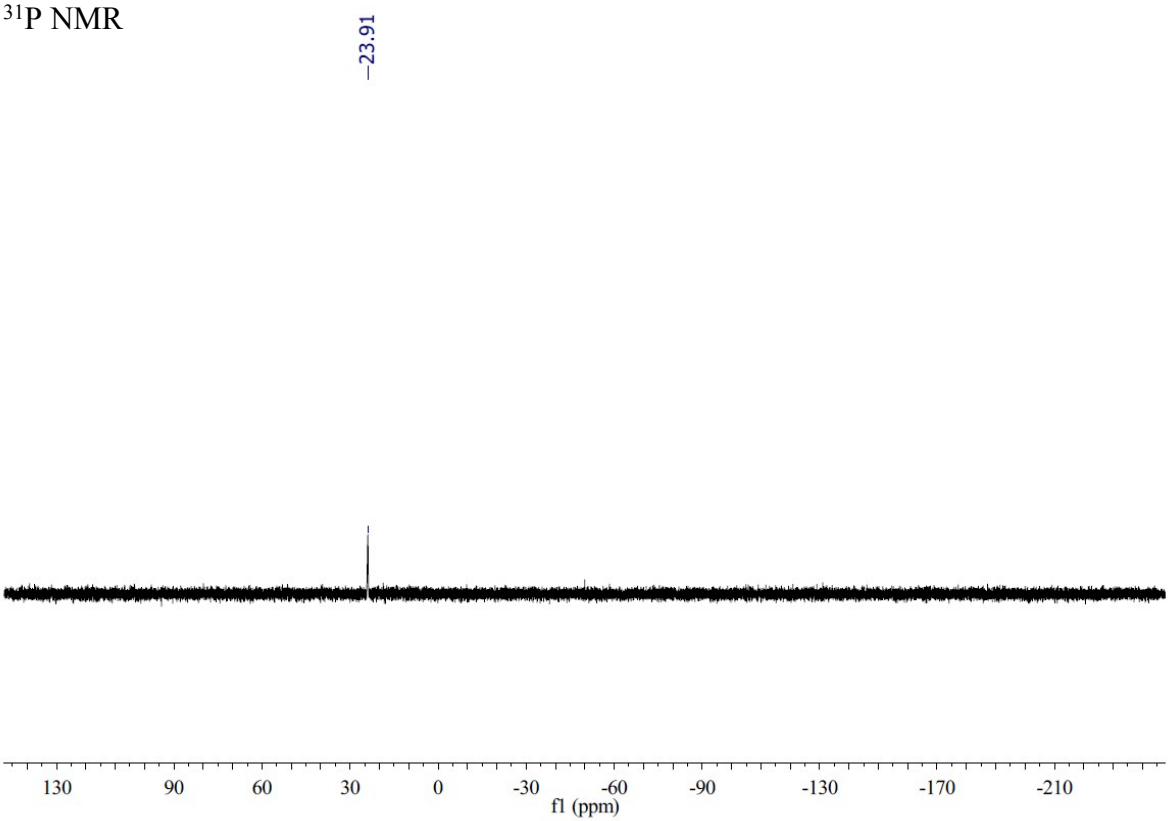

163.41
162.90
159.07
149.22
145.04
143.76
136.85
136.76
132.47
131.10
130.10
129.92
128.57
127.08
125.85
124.88
123.58
123.53
122.55
122.35
77.48
77.16
76.84
59.86
50.32
48.55
42.74
35.39
21.60
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Compound **8**:

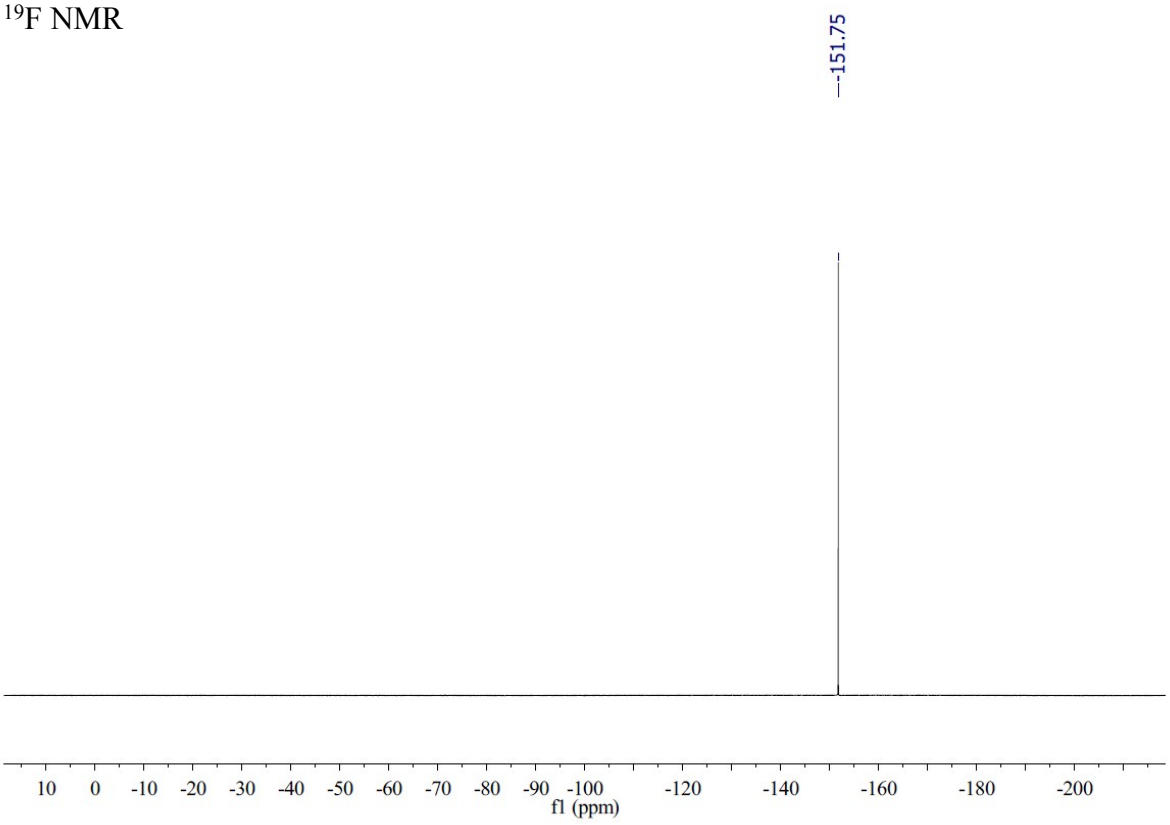

8.52
8.51
8.48
8.47
8.22
7.75
7.69
7.68
7.67
7.64
7.61
7.59
7.58
7.12
7.11
7.10
5.34
5.25
4.36
4.34
4.33
4.01
3.90
3.33
3.30
3.26
2.13
2.11
2.10
1.57
1.55
PPh3
BF4
2.16
2.06
1.00
1.01
2.13
20.06
2.00
2.17
2.08
1.96
3.77
2.09
2.13
2.13
fl (ppm)


163.26
162.74
158.96
149.04
145.12
143.27
136.74
135.16
135.13
133.46
133.36
130.58
130.45
125.83
123.65
123.38
123.32
122.24
118.20
117.34
77.49
77.17
76.85
59.80
53.54
48.61
35.49
30.02
29.85
21.32
20.80
19.25
fl (ppm)

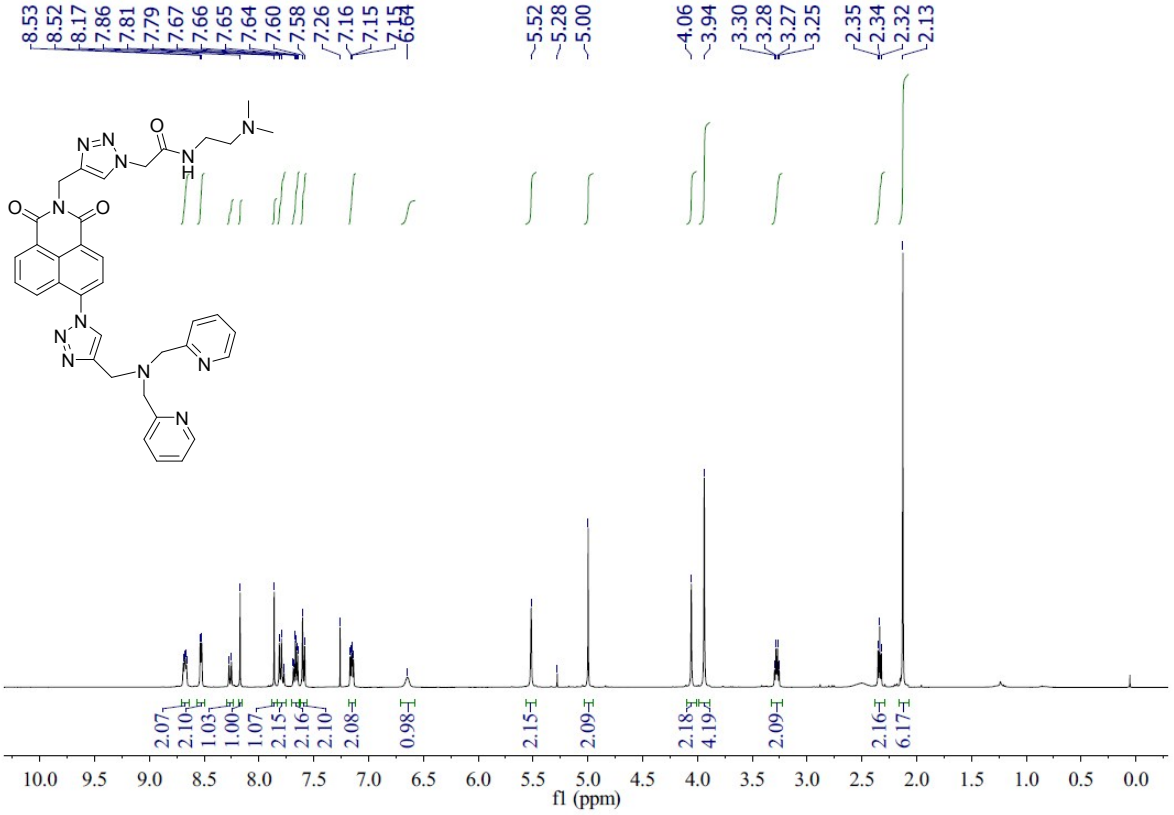
^{31}P NMR

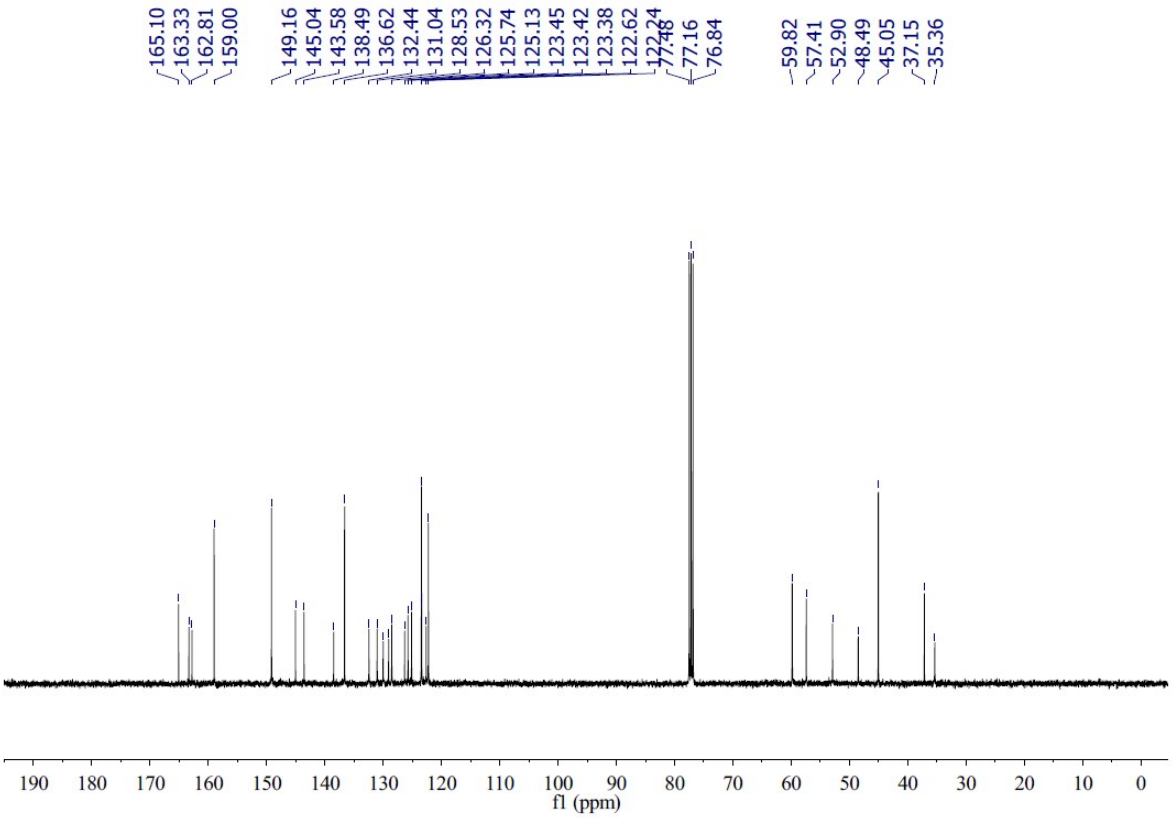


^{19}F NMR

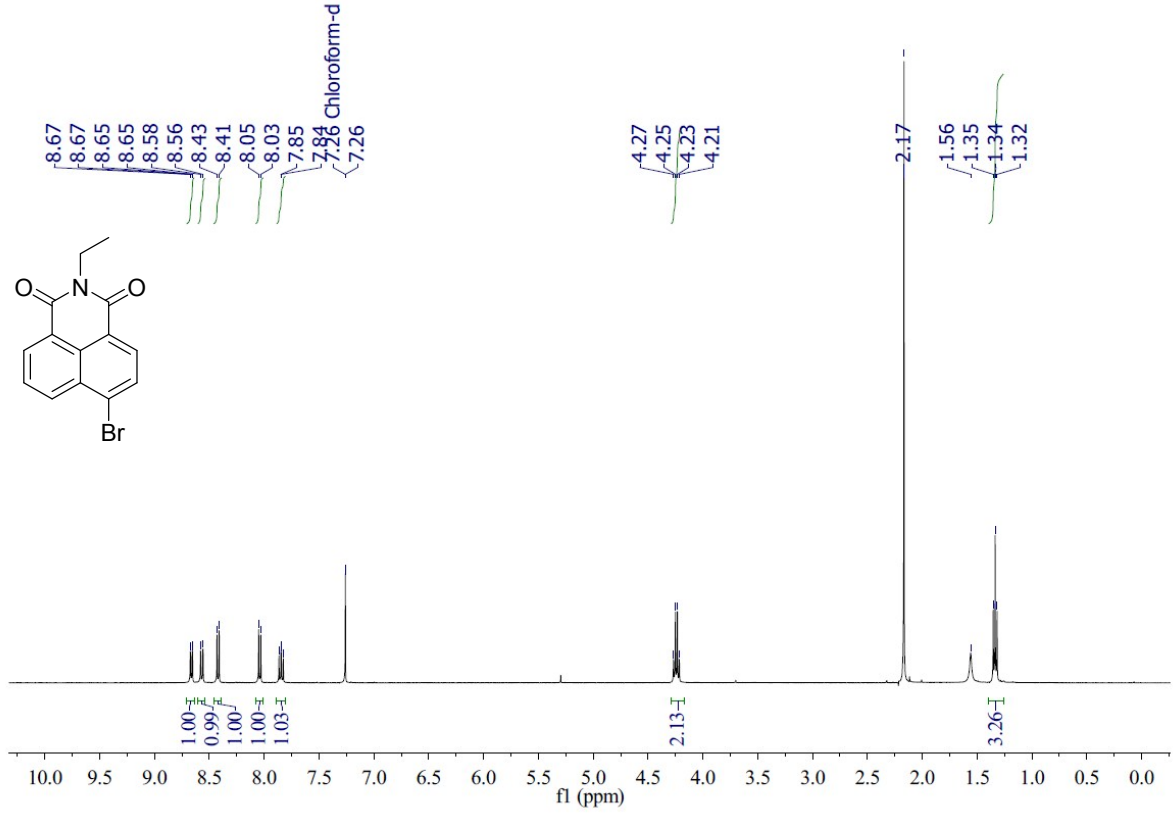


Compound **9**:

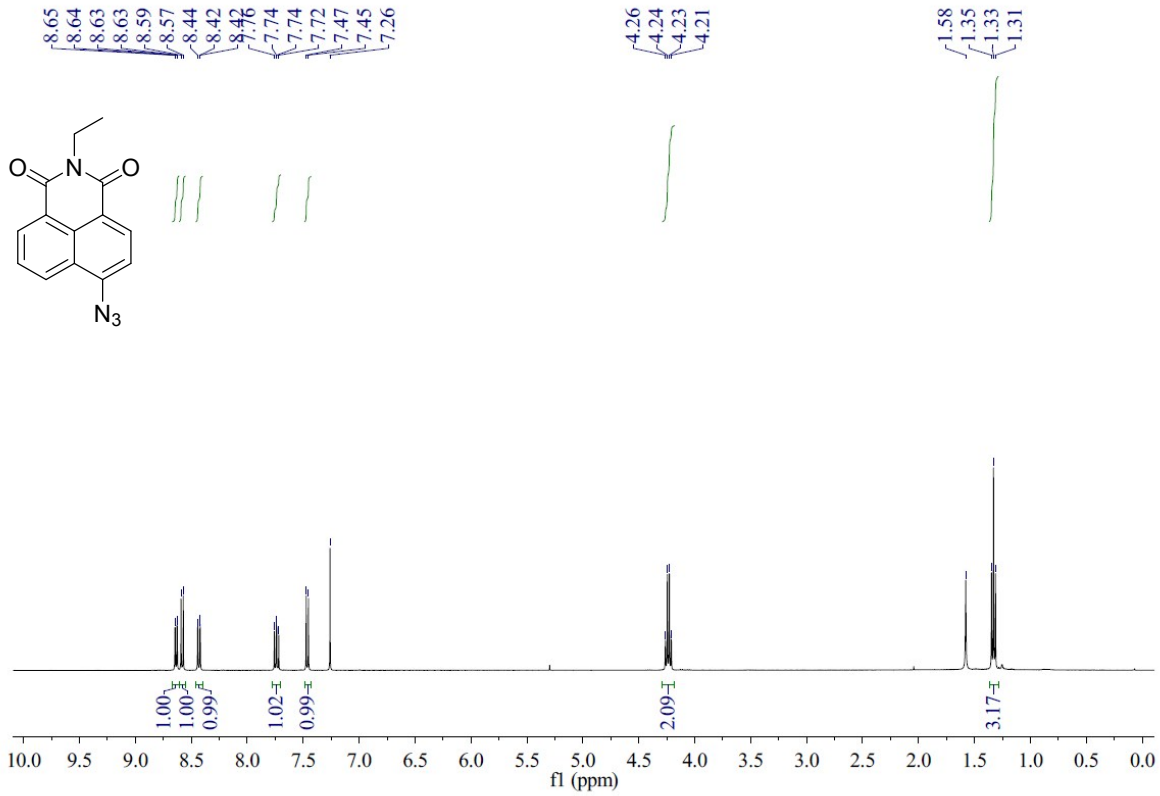

8.53
8.52
8.17
7.86
7.81
7.79
7.67
7.66
7.65
7.64
7.60
7.58
7.26
7.16
7.15
6.84
5.52
5.28
5.00
4.06
3.94
3.30
3.28
3.27
3.25
2.35
2.34
2.32
2.13
2.07
2.10
1.03
1.00
1.07
2.15
2.16
2.10
2.08
0.98
2.15
2.09
2.18
4.19
2.09
2.16
6.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


165.10
163.33
162.81
159.00
149.16
145.04
143.58
138.49
136.62
132.44
131.04
128.53
126.32
125.74
125.13
123.45
123.42
123.38
122.62
122.24
77.48
77.16
76.84
59.82
57.41
52.90
48.49
45.05
37.15
35.36
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

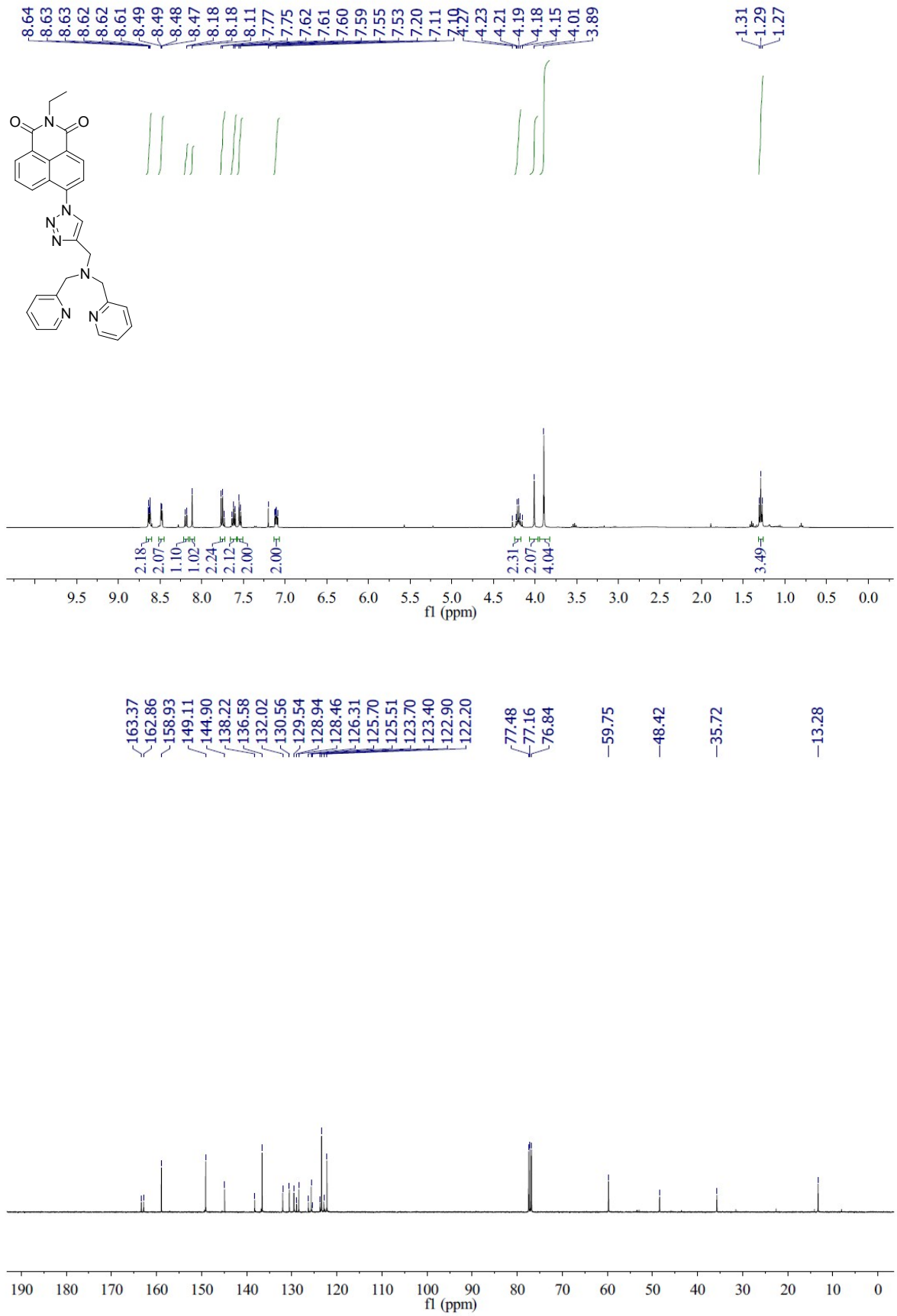
Compound **S4**:


8.67
8.67
8.65
8.65
8.58
8.56
8.43
8.41
8.05
8.03
7.85
7.84
7.26
7.26
Chloroform-d
4.27
4.25
4.23
4.21
2.17
1.56
1.35
1.34
1.32
O
N
O
Br
1.00
0.99
1.00
1.00
1.03
2.13
3.26
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

Compound **S5**:


8.65
8.64
8.63
8.63
8.59
8.57
8.44
8.42
7.74
7.74
7.72
7.47
7.45
7.26
4.26
4.24
4.23
4.21
1.58
1.35
1.33
1.31
O
N
O
N3
1.00
1.00
0.99
1.02
0.99
2.09
3.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

Compound **10**:


8.64
8.63
8.63
8.62
8.62
8.61
8.49
8.49
8.48
8.47
8.18
8.18
8.11
7.77
7.75
7.62
7.61
7.60
7.59
7.55
7.53
7.20
7.11
7.10
4.27
4.23
4.21
4.19
4.18
4.15
4.01
3.89
1.31
1.29
1.27
2.18
2.07
1.10
1.02
2.24
2.12
2.00
2.00
2.31
2.07
4.04
3.49
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
163.37
162.86
158.93
149.11
144.90
138.22
136.58
132.02
130.56
129.54
128.94
128.46
126.31
125.70
125.51
123.70
123.40
122.90
122.20
77.48
77.16
76.84
59.75
48.42
35.72
13.28
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Cartesian coordinates of probe **7**:

H	-3.57544400	2.92763100	0.63801900
C	-2.74657700	0.46234700	-0.32288800
C	-2.02949800	1.69653600	-0.26476500
C	-2.56537200	2.90902200	0.24552800
C	-2.14400100	-0.70285400	-0.75823000
C	-0.67493500	1.69061700	-0.72502900
C	-0.07961000	0.48692500	-1.18091200
C	-0.80397500	-0.69149200	-1.18115500
C	0.07778300	2.89303600	-0.70103900
C	-0.48615100	4.06121800	-0.21870900
C	-1.80861200	4.06304700	0.26480800
H	-2.23332500	4.97941800	0.66152600
H	0.10903000	4.96765600	-0.20892000
H	-2.71849400	-1.62144200	-0.78288000
H	-0.33183000	-1.60396400	-1.52716000
C	1.47852000	2.91298400	-1.18462100
O	2.15957100	3.93209200	-1.19527300
C	1.32585500	0.47549600	-1.64783100
O	1.88959300	-0.54772100	-2.02716500
N	2.00735500	1.69675700	-1.64463300
C	3.40044800	1.69113200	-2.14331200
H	3.62067800	2.70439000	-2.47406900
H	3.42817100	1.01362600	-2.99683900
N	-4.10617700	0.39550500	0.09574500
C	-7.69373700	1.00865600	0.35731600
H	-7.98536000	1.27418200	1.37879900
H	-7.79877800	1.92627200	-0.25021200
N	-8.59527700	-0.06102800	-0.09335600
C	-8.43337700	-0.33096900	-1.52984100
H	-8.84418200	0.48860800	-2.14785900
H	-7.35861500	-0.37951700	-1.73276700
C	-9.99372400	0.24521300	0.24179000
H	-10.61897000	-0.50000100	-0.26031200
H	-10.29899400	1.23592000	-0.14294500
C	-9.04921100	-1.64923000	-1.95965800
C	-10.65347400	-2.92675800	-3.22815300
C	-8.99033100	-3.94573900	-1.84304200
C	-10.07101200	-4.08434900	-2.71739200
H	-11.49574400	-2.98185100	-3.91203000
H	-8.50685900	-4.82919800	-1.42838100
H	-10.43681500	-5.07028500	-2.98644100
C	-10.27916800	0.16756100	1.72989000
C	-10.93257900	1.17939100	3.81882900
C	-10.43548700	-1.15130600	3.60760300
C	-10.81856900	-0.07554800	4.41242100
H	-11.22784500	2.04704500	4.40203600
H	-10.34123200	-2.14779300	4.03689100
H	-11.02169500	-0.22460100	5.46823700
N	-8.48133100	-2.76648100	-1.46732100
N	-10.17144300	-1.04780500	2.29966600
C	-10.65798200	1.30216200	2.45601700
H	-10.73553800	2.26438800	1.95841100
C	-10.13423000	-1.69000200	-2.84236100

H	-10.56242100	-0.76586800	-3.21932700
N	-4.49744600	-0.54568300	1.00348700
N	-5.78155100	-0.41582200	1.16746800
C	-6.25132300	0.59529900	0.37097700
C	-5.18204200	1.11928300	-0.32130700
H	-5.10830800	1.89901000	-1.06331000
C	4.69120300	0.03768200	-0.58529300
H	4.27058100	-0.93834200	-0.76823100
C	4.40637500	1.28442500	-1.10783000
N	5.23691700	2.19142200	-0.51365500
N	6.01290500	1.57237900	0.33881800
N	5.68315400	0.26119100	0.30891600
C	6.42836900	-0.69705700	1.11913800
H	6.80042000	-0.16097100	1.99264700
H	5.74377700	-1.48108000	1.44950900
C	7.60005500	-1.30262800	0.32980600
H	8.24129200	-0.50058700	-0.05557300
H	7.22484700	-1.85896800	-0.53258400
N	8.34694400	-2.25152900	1.17071300
H	8.54227700	-3.14686400	0.72993700
S	9.68237300	-1.71435700	2.03455600
O	10.18007700	-2.89822300	2.74731400
O	9.23654400	-0.52388100	2.77254300
C	10.93733400	-1.19271800	0.87037000
C	11.76549000	-2.15324800	0.27699600
C	11.06348900	0.16014400	0.54928500
C	12.72218500	-1.74411900	-0.64557700
H	11.67069500	-3.20083200	0.54330100
C	12.02960600	0.54996000	-0.37952400
H	10.42962200	0.89685000	1.03019900
C	12.86971200	-0.38936200	-0.99080100
H	13.36991700	-2.48696700	-1.10371500
H	12.13174000	1.60283300	-0.62748900
C	13.91892600	0.03349500	-1.98963200
H	14.92656000	-0.18835900	-1.61752700
H	13.80141900	-0.50607900	-2.93662000
H	13.86458500	1.10546900	-2.19873000

Cartesian coordinates of the Zn^{2+} complex of **7**:

H	-3.21900100	3.09952200	0.92613000
C	-2.34943900	1.12217400	-0.82262100
C	-1.62265500	2.20617800	-0.25059100
C	-2.17701700	3.16879500	0.63450500
C	-1.75129000	0.17816200	-1.63133900
C	-0.23502700	2.29981200	-0.58476500
C	0.36490800	1.32957800	-1.42690300
C	-0.38103000	0.28063900	-1.93072900
C	0.54157500	3.36129500	-0.05424600
C	-0.03520700	4.29167300	0.79176800
C	-1.39644800	4.18765200	1.14056600
H	-1.83243100	4.91456100	1.81783000
H	0.57714900	5.09457100	1.18705200
H	-2.34365000	-0.63042500	-2.04386800
H	0.09614700	-0.45377800	-2.56910300

C	1.97935700	3.48557300	-0.39626200
O	2.68225600	4.39244100	0.03239300
C	1.80520100	1.42410400	-1.77182700
O	2.36636000	0.59656600	-2.48350800
N	2.51457200	2.50899000	-1.25203100
C	3.94348600	2.61773300	-1.62503800
H	4.22083500	3.66268000	-1.50043500
H	4.01765700	2.34300800	-2.67739400
N	-3.75249100	0.97787700	-0.55592100
C	-7.37277500	1.52288700	-0.46983000
H	-7.62043500	2.04799000	0.45818800
H	-7.62182400	2.19470900	-1.29854700
N	-8.16853900	0.26920500	-0.51361600
C	-8.33077400	-0.25585500	-1.88608000
H	-9.18858400	0.19765500	-2.39575100
H	-7.43724100	0.02385100	-2.45570900
C	-9.44167900	0.35907800	0.23207800
H	-10.10546900	-0.42624700	-0.14710500
H	-9.94953200	1.31475600	0.05918400
C	-8.44278400	-1.77024200	-1.90379400
C	-9.11957800	-3.83309000	-2.93440200
C	-7.81339200	-3.79588900	-0.93012900
C	-8.45337600	-4.52555600	-1.92274700
H	-9.63920300	-4.37073400	-3.72093700
H	-7.29091800	-4.28200800	-0.11390600
H	-8.43430000	-5.60885100	-1.89454600
C	-9.23658000	0.12392600	1.71847400
C	-9.89257600	0.36827500	4.01743000
C	-8.04303300	-1.00710700	3.37559300
C	-8.85721600	-0.49483100	4.37695100
H	-10.54235400	0.79551400	4.77436700
H	-7.21628900	-1.67209200	3.59911500
H	-8.67508200	-0.76222600	5.41141600
N	-7.80838600	-2.44867600	-0.92294300
N	-8.23077900	-0.70421700	2.07646300
C	-10.08178500	0.68394700	2.67285500
H	-10.87554300	1.35484000	2.36249900
C	-9.11740000	-2.43937100	-2.92200200
H	-9.62921000	-1.87197000	-3.69186300
N	-4.20855500	-0.15645000	-0.00726700
N	-5.50902400	-0.02614600	0.04551000
C	-5.91022100	1.17327400	-0.46644200
C	-4.77140500	1.83102500	-0.86597200
H	-4.60970800	2.78419100	-1.34367800
C	5.06720500	0.40143000	-0.81711500
H	4.64995800	-0.38683900	-1.42314000
C	4.84864900	1.76520700	-0.78657900
N	5.63719900	2.29765800	0.19336500
N	6.32467100	1.34029500	0.76185600
N	5.97937700	0.18047200	0.15839600
C	6.62644300	-1.06844000	0.54768800
H	6.88937100	-0.98320400	1.60229900
H	5.90850000	-1.88217200	0.42654600
C	7.88383500	-1.33330000	-0.29532700
H	8.57567300	-0.48613500	-0.21151100

H	7.61388900	-1.42742300	-1.35000200
N	8.51065500	-2.60320400	0.10534900
H	8.78819900	-3.19962300	-0.67023200
S	9.69419300	-2.60211700	1.29714200
O	10.10078100	-4.00678600	1.43394800
O	9.12335200	-1.87012600	2.43702900
C	11.09854900	-1.66724000	0.70127500
C	12.03893000	-2.29227500	-0.12659200
C	11.22923600	-0.32059400	1.04639400
C	13.11378100	-1.55257200	-0.60778400
H	11.93695800	-3.34286900	-0.37788200
C	12.31447300	0.40430100	0.55199400
H	10.50535200	0.14748300	1.70419700
C	13.26929600	-0.19447000	-0.27981900
H	13.84835600	-2.03687400	-1.24583900
H	12.41976500	1.45119300	0.82279500
C	14.44705500	0.58807600	-0.80670200
H	15.39043800	0.18542900	-0.41816000
H	14.50087100	0.53117100	-1.90009600
H	14.38734600	1.64223600	-0.52205900
Zn	-7.02804700	-1.28063900	0.54437500

Cartesian coordinates of probe **8**:

H	-3.62656400	1.00095200	-1.11988500
C	-4.34883500	-1.29675400	0.25340800
C	-3.16607000	-1.02972300	-0.49950400
C	-2.90543100	0.19353600	-1.17359300
C	-4.49800700	-2.46546100	0.97616500
C	-2.16898300	-2.05369400	-0.53629900
C	-2.33799100	-3.24573300	0.21317800
C	-3.48102200	-3.43501900	0.96944900
C	-0.99003500	-1.85080200	-1.29798000
C	-0.76632600	-0.64833900	-1.94637700
C	-1.72757300	0.37902200	-1.86897800
H	-1.53523700	1.32880800	-2.35744500
H	0.16960300	-0.49568900	-2.47074200
H	-5.40878100	-2.62796600	1.54059600
H	-3.59003100	-4.34662700	1.54597800
C	0.02607900	-2.92028100	-1.38900400
O	1.02002100	-2.83501900	-2.10413500
C	-1.27689700	-4.28112600	0.23311900
O	-1.35090400	-5.28831000	0.92897400
N	-0.16603100	-4.05751500	-0.59143900
C	0.92560900	-5.05159800	-0.58001400
H	1.25500300	-5.17888800	-1.61317900
H	0.51477200	-5.99208900	-0.21802500
N	-5.40583300	-0.34615400	0.29204700
C	-8.10699400	1.86854000	-0.75001100
H	-8.05140700	2.86306700	-0.29613000
H	-7.89619900	1.99622200	-1.82752600
N	-9.45743300	1.34237100	-0.50728300
C	-9.69948700	0.10328400	-1.25874700
H	-9.82189100	0.29788600	-2.34013200
H	-8.81630700	-0.53250500	-1.14229000

C	-10.48482900	2.35376300	-0.79247400
H	-11.45813700	1.85496700	-0.75262900
H	-10.37520600	2.77244600	-1.80998000
C	-10.89686700	-0.65702200	-0.72704800
C	-13.14596800	-1.49673100	-0.94265900
C	-11.80658900	-1.85929900	1.00778300
C	-13.01598400	-2.04384800	0.33204600
H	-14.06634700	-1.61286300	-1.50784600
H	-11.66872500	-2.27785200	2.00369100
H	-13.82409900	-2.60095300	0.79549600
C	-10.48808900	3.47044400	0.23122700
C	-10.12494800	5.76638600	0.86970700
C	-10.88461300	4.09637200	2.40700400
C	-10.52060400	5.42308900	2.16062700
H	-9.83265000	6.78440400	0.62838600
H	-11.20431900	3.79454400	3.40333000
H	-10.55089900	6.15784100	2.95900900
N	-10.76529400	-1.18628100	0.50405400
N	-10.87417500	3.13429900	1.47665700
C	-10.10880400	4.77282800	-0.11060500
H	-9.80397500	4.99927100	-1.12809000
C	-12.06781200	-0.79166400	-1.48032500
H	-12.12984500	-0.34733100	-2.46927900
N	-5.93627300	0.04949200	1.48551100
N	-6.91734600	0.86280000	1.22143000
C	-7.04806500	1.00620000	-0.13498900
C	-6.08392500	0.23120900	-0.73855700
H	-5.84913100	0.03397400	-1.77266500
C	2.67318400	-3.38633200	0.39780700
H	2.51191200	-2.43439700	-0.08144100
C	2.06422100	-4.62182700	0.29940700
N	2.68424900	-5.47449600	1.16521000
N	3.64541700	-4.82957200	1.78826100
N	3.63530400	-3.56063000	1.33109000
C	4.58965800	-2.55534400	1.79561600
H	5.12469900	-2.99325600	2.64089200
H	4.01300800	-1.69637100	2.15180700
C	5.53217900	-2.12059800	0.66865400
H	6.19094500	-2.95285800	0.39310800
H	4.93198700	-1.86792800	-0.20813000
C	6.35546500	-0.88820200	1.06584100
H	5.69730800	-0.15387300	1.54206700
H	7.12030300	-1.15412400	1.80440500
C	6.97510400	-0.25279900	-0.18933000
H	7.59286400	-0.96468500	-0.74919600
H	6.17856200	0.05898200	-0.87209500
C	8.13439300	2.07053500	-1.52834700
C	6.94436100	2.51850500	-2.13114400
C	9.36037600	2.24101400	-2.18938400
C	6.99504900	3.14971600	-3.37242300
H	5.97732700	2.35775700	-1.66722300
C	9.39715900	2.87570400	-3.43192700
H	10.28294600	1.87663900	-1.75360900
C	8.21896800	3.33557300	-4.02120600
H	6.07394700	3.49164300	-3.83452800

H	10.34941100	3.00455100	-3.93721400
H	8.25164100	3.82911900	-4.98803400
C	7.24532800	2.28665400	1.32965200
C	7.98716200	2.83712100	2.38641100
C	5.86653900	2.54798400	1.23203200
C	7.35903100	3.65906600	3.32268100
H	9.04365200	2.62480400	2.49673400
C	5.25087400	3.36934300	2.17528300
H	5.26088600	2.10774300	0.44815000
C	5.99397400	3.93000000	3.21699300
H	7.94022400	4.08091700	4.13687800
H	4.18561400	3.56402900	2.09590200
H	5.50834700	4.56841800	3.94912000
C	9.67971100	0.73724600	0.63060600
C	10.68181900	1.71381500	0.78685700
C	9.96882400	-0.60741900	0.91077200
C	11.95227900	1.34385700	1.22271300
H	10.47872600	2.75626900	0.56174000
C	11.24390600	-0.96729900	1.34814300
H	9.21725000	-1.37912300	0.79116200
C	12.23341800	0.00432300	1.50536600
H	12.72059800	2.10169100	1.33833800
H	11.46045500	-2.00891400	1.56326800
H	13.22449700	-0.28096300	1.84499000
P	8.02644300	1.22073100	0.07823600
F	4.27358700	-0.54608300	-1.99138400
F	3.99961300	1.53334600	-1.05924500
F	2.22766200	0.50881200	-2.10466800
F	3.00420900	-0.30325400	-0.08946200
B	3.36328300	0.28861800	-1.31833000

Cartesian coordinates of the Zn^{2+} complex of **8**:

H	-3.32238500	-0.37613800	2.06234400
C	-4.04381100	1.84609100	0.55156800
C	-2.80986200	1.55494300	1.20259000
C	-2.55130100	0.37851000	1.95570100
C	-4.21488300	2.96725700	-0.23441900
C	-1.75608100	2.50895000	1.04158400
C	-1.94149100	3.65192000	0.22250300
C	-3.15093700	3.86947100	-0.41024200
C	-0.50874200	2.28392000	1.67775900
C	-0.28729400	1.12567600	2.40247700
C	-1.31483600	0.16956800	2.53154900
H	-1.12839000	-0.74405700	3.08636500
H	0.69296000	0.94639100	2.83160800
H	-5.17097100	3.14816500	-0.71180800
H	-3.27331100	4.74398700	-1.03866100
C	0.57787000	3.28127900	1.55336300
O	1.63982900	3.18269800	2.15890400
C	-0.82813800	4.61020500	-0.00291300
O	-0.93614900	5.57489800	-0.75052500
N	0.36553900	4.35958300	0.68342300
C	1.49775200	5.28785800	0.48272800

H	1.94045400	5.46568600	1.46481900
H	1.08866100	6.22101100	0.10011600
N	-5.15619300	0.94769500	0.67333700
C	-7.94185100	-1.03394700	1.99027900
H	-7.57232500	-2.04037700	2.21061500
H	-8.24603800	-0.58527100	2.94230600
N	-9.08367400	-1.15950600	1.04681800
C	-9.98967900	0.00797600	1.08913300
H	-10.76326300	-0.10686000	1.85705500
H	-9.39013700	0.88121400	1.36994600
C	-9.78649400	-2.45596100	1.15044000
H	-10.77644400	-2.33342100	0.69634900
H	-9.94800500	-2.75171000	2.19333900
C	-10.62217100	0.29451000	-0.26228300
C	-12.33576300	1.27775500	-1.63117800
C	-10.40470500	0.23820100	-2.58656700
C	-11.60401500	0.91419300	-2.76237800
H	-13.28310800	1.79767000	-1.73094600
H	-9.80099700	-0.08089200	-3.42874800
H	-11.95587100	1.13982700	-3.76238800
C	-9.04904100	-3.54847500	0.39460200
C	-8.48182600	-5.85067500	0.00365400
C	-7.74048500	-4.10638000	-1.45668500
C	-7.78162900	-5.45709400	-1.13677600
H	-8.52679300	-6.89658900	0.28963100
H	-7.20183500	-3.74296700	-2.32465400
H	-7.26942800	-6.17692700	-1.76460600
N	-9.92588400	-0.06262000	-1.36331300
N	-8.36054400	-3.17494900	-0.70731500
C	-9.11952100	-4.88425800	0.78035500
H	-9.66740300	-5.15835400	1.67541900
C	-11.84088100	0.96069500	-0.36753400
H	-12.38826300	1.22692300	0.53023600
N	-5.72955700	0.46331700	-0.43702500
N	-6.74460200	-0.25269000	-0.02886400
C	-6.84827800	-0.23967700	1.33094300
C	-5.82007000	0.54561400	1.79621000
H	-5.53169200	0.85656200	2.78760800
C	3.13202200	3.52125100	-0.53785200
H	3.03865000	2.61579500	0.04151500
C	2.52169400	4.75920400	-0.48163200
N	3.02930400	5.52976400	-1.48723900
N	3.92016700	4.83326800	-2.15505200
N	3.98125300	3.61188700	-1.58615000
C	4.87886500	2.56749400	-2.08213700
H	5.32061800	2.94965300	-3.00465500
H	4.26335400	1.69670900	-2.32876700
C	5.93856200	2.18837000	-1.03800600
H	6.69312200	2.98129900	-0.97061900
H	5.45569100	2.10949100	-0.06075000
C	6.59678000	0.83663600	-1.35350500
H	5.80868000	0.10352200	-1.55668100
H	7.22139100	0.90854800	-2.25171500
C	7.41345100	0.36269800	-0.14107600
H	8.21898200	1.06456600	0.10307500

H	6.76063800	0.31785700	0.73551100
C	8.73880500	-1.74657800	1.40362700
C	7.84293400	-1.62910600	2.48314100
C	10.05126200	-2.19197000	1.62347700
C	8.27032100	-1.96091300	3.76832100
H	6.81942300	-1.30279400	2.32474300
C	10.46600900	-2.51735800	2.91512000
H	10.74846000	-2.28165800	0.79747400
C	9.57846000	-2.40125300	3.98626300
H	7.57846100	-1.87265400	4.60049000
H	11.48320100	-2.85859700	3.08115900
H	9.90504300	-2.65335700	4.99092100
C	7.02681100	-2.52955800	-0.91752000
C	6.68544400	-2.49931300	-2.28218000
C	6.45809100	-3.49922200	-0.07898100
C	5.78087100	-3.42790100	-2.79356100
H	7.13034400	-1.76755800	-2.94894200
C	5.55694100	-4.42733500	-0.60115500
H	6.71563800	-3.53728600	0.97292800
C	5.21641500	-4.39192900	-1.95411900
H	5.52271400	-3.40029300	-3.84765700
H	5.12427300	-5.17845000	0.05253200
H	4.51537300	-5.11724200	-2.35650600
C	9.62049800	-1.23058800	-1.38920500
C	10.05287600	-2.40204900	-2.03557200
C	10.32823100	-0.03147600	-1.57583600
C	11.17778800	-2.36851400	-2.85836100
H	9.51475100	-3.33487300	-1.90310900
C	11.44895600	-0.00676100	-2.40540800
H	10.01871900	0.88365800	-1.08307400
C	11.87412500	-1.17232700	-3.04594000
H	11.50573400	-3.27657100	-3.35470900
H	11.98695300	0.92488000	-2.55010900
H	12.74700100	-1.14863400	-3.69152100
P	8.19239200	-1.29459900	-0.26915700
F	4.95720300	0.99495100	2.04914400
F	4.80487900	-1.17412000	1.33330400
F	3.04718800	-0.22225100	2.47992200
F	3.52474200	0.45980500	0.33220400
B	4.07259200	0.01507000	1.55612100
Zn	-8.27686700	-1.17235000	-0.99484800

Cartesian coordinates of probe **9**:

H	-1.99859700	2.93562000	-0.55545800
C	-1.35398400	0.29201100	-0.02723100
C	-0.53365500	1.33112500	-0.56234300
C	-0.98086200	2.65753800	-0.80331300
C	-0.83942700	-0.95596700	0.26975900
C	0.83166200	1.00943100	-0.84109900
C	1.33653500	-0.28174100	-0.54450000
C	0.51363400	-1.23990400	0.01997300
C	1.68419100	1.99953800	-1.39343300
C	1.20712200	3.27518200	-1.63873000

C	-0.12694000	3.60502600	-1.33063100
H	-0.48337800	4.61506500	-1.50413900
H	1.87879700	4.01576200	-2.05876600
H	-1.49387200	-1.71589800	0.68024000
H	0.91900000	-2.21933100	0.24742100
C	3.09715300	1.68403700	-1.70823800
O	3.86791800	2.50625200	-2.19007300
C	2.75139300	-0.61395200	-0.82315000
O	3.24570000	-1.70344600	-0.54365500
N	3.52841500	0.37652300	-1.43302900
C	4.93347300	0.03166900	-1.73546300
H	5.26732800	0.69969800	-2.52698600
H	4.94049700	-0.99618300	-2.09848300
N	-2.73375600	0.52326400	0.22759400
C	-6.25919800	1.30589300	-0.26558400
H	-6.67025300	1.95999200	0.50970500
H	-6.23242800	1.89428200	-1.20097100
N	-7.14024200	0.13430200	-0.37536600
C	-6.78677700	-0.69662000	-1.53511500
H	-7.05382000	-0.20280700	-2.48769800
H	-5.69991800	-0.82517700	-1.53011100
C	-8.55399100	0.53652200	-0.41351500
H	-9.14298100	-0.35088700	-0.66428000
H	-8.74355300	1.28722900	-1.20296500
C	-7.42076600	-2.07039100	-1.46754000
C	-8.97853900	-3.73022900	-2.26044600
C	-7.51247500	-4.10708200	-0.40621800
C	-8.51690400	-4.57834000	-1.25609400
H	-9.75759100	-4.05074700	-2.94625900
H	-7.12395400	-4.74562800	0.38580100
H	-8.91741700	-5.57930600	-1.13028100
C	-9.03674800	1.05601300	0.92498500
C	-9.80414300	2.83229700	2.36260900
C	-9.53938800	0.57580400	3.11592700
C	-9.89049000	1.89968700	3.39397700
H	-10.06664900	3.87316200	2.52891700
H	-9.60101100	-0.18053500	3.89702000
H	-10.22230100	2.18220600	4.38810600
N	-6.96845800	-2.88767200	-0.49789000
N	-9.12225200	0.15028800	1.91761000
C	-9.37011400	2.40233100	1.10751700
H	-9.28685800	3.09862700	0.27829400
C	-8.42041100	-2.45537700	-2.36723600
H	-8.75464400	-1.76313800	-3.13436300
N	-3.27810900	0.19024100	1.43419000
N	-4.55296000	0.44209600	1.36553400
C	-4.86232100	0.93259200	0.12407500
C	-3.70116800	0.98439700	-0.61315200
H	-3.49807200	1.27596500	-1.63155200
C	5.90802700	-0.57882300	0.60274600
H	5.36650900	-1.45165800	0.92969100
C	5.83166300	0.18318900	-0.54630600
N	6.74989000	1.19141100	-0.45121500
N	7.38611000	1.08835500	0.68560100
N	6.88179500	0.01243500	1.33473800

C	7.42060200	-0.38794900	2.62300600
H	8.13341200	0.38651500	2.91806500
H	6.61711600	-0.40940700	3.36120200
C	8.10699300	-1.76264100	2.70197600
O	8.01946800	-2.37365900	3.76753900
N	8.79469600	-2.26542700	1.64447700
H	9.23291400	-3.15036100	1.87415900
C	9.22561800	-1.64164900	0.38910200
H	9.61974000	-2.45492000	-0.22417300
H	8.37626800	-1.22507100	-0.15356200
C	10.28827600	-0.55091900	0.58906300
H	9.85221500	0.24303600	1.20098700
H	11.14529900	-0.96391100	1.15406700
C	11.19041000	1.39515600	-0.52820000
H	11.43174700	1.81569400	-1.51071900
H	10.41698500	2.01966500	-0.06955900
H	12.10168300	1.45225900	0.09801500
C	11.66048500	-0.79831700	-1.39681800
H	12.61972300	-0.89152700	-0.85136900
H	11.26317800	-1.80550300	-1.55487800
H	11.86879100	-0.36473200	-2.38080600
N	10.68884200	0.03298100	-0.69038200

Cartesian coordinates of the Zn^{2+} complex of **9**:

H	1.88135600	-3.04419000	-0.20466800
C	1.18320300	-0.43485500	-0.87255700
C	0.37188000	-1.60653700	-0.82790300
C	0.84320000	-2.90134800	-0.48224900
C	0.65927100	0.81417500	-1.13539000
C	-1.01552400	-1.44244500	-1.13506800
C	-1.53777400	-0.15563000	-1.42073600
C	-0.71468300	0.95486500	-1.40071300
C	-1.86925600	-2.57507800	-1.13744700
C	-1.37132000	-3.82531800	-0.81719700
C	-0.01332500	-3.98287900	-0.47728400
H	0.36104100	-4.96457600	-0.20665300
H	-2.04258500	-4.67683300	-0.82439300
H	1.31310400	1.67825700	-1.15854600
H	-1.13301700	1.93134700	-1.61565700
C	-3.30267500	-2.43575500	-1.49049500
O	-4.06789200	-3.39134100	-1.52913800
C	-2.97540700	0.01386300	-1.74787800
O	-3.47347700	1.11133100	-1.97875400
N	-3.75702400	-1.14321700	-1.79769800
C	-5.17054800	-0.98282500	-2.20493800
H	-5.49304700	-1.94273800	-2.60389600
H	-5.18728500	-0.23406100	-2.99707000
N	2.59736800	-0.53603700	-0.65547200
C	6.12449300	-1.43162200	-1.04371400
H	6.33009700	-2.29197400	-0.39909700
H	6.26118900	-1.76344600	-2.07884400
N	7.07365500	-0.34976800	-0.67697700
C	7.26723100	0.63763000	-1.76098500
H	8.05565100	0.32675200	-2.45598500

H	6.33568400	0.68525700	-2.33632000
C	8.34326100	-0.85981100	-0.11580100
H	9.09262300	-0.06599200	-0.21219700
H	8.71859200	-1.72183100	-0.67906900
C	7.55299600	2.02676700	-1.21762300
C	8.43313700	4.25180300	-1.44211700
C	7.18511000	3.58054800	0.48527500
C	7.87702700	4.56817900	-0.20222500
H	8.98992500	4.99574600	-2.00268800
H	6.74384300	3.76652300	1.45798700
H	7.98190600	5.55593200	0.23140900
C	8.20322900	-1.20301400	1.35767600
C	8.87581900	-2.38884400	3.33644500
C	7.18783900	-0.69438400	3.39767100
C	7.95703100	-1.63597700	4.06816500
H	9.48729800	-3.13993800	3.82598500
H	6.45143900	-0.08851500	3.91362900
H	7.83033900	-1.77676100	5.13531700
N	7.02671600	2.33906200	-0.01355900
N	7.31038000	-0.48415400	2.07288800
C	8.99726200	-2.17247200	1.96462600
H	9.69950800	-2.74459500	1.36810100
C	8.27249600	2.96509700	-1.95340900
H	8.69640800	2.68766800	-2.91242600
N	3.19709800	0.24056900	0.25828800
N	4.47500800	-0.02500300	0.16526500
C	4.71865800	-0.95899100	-0.80034900
C	3.50199200	-1.29013100	-1.34447100
H	3.21959300	-1.95402000	-2.14569200
C	-6.26579500	0.63887800	-0.47403900
H	-5.80085100	1.60127000	-0.61502300
C	-6.08641300	-0.58678700	-1.08578500
N	-6.94945600	-1.47733500	-0.51302100
N	-7.64651400	-0.87000100	0.41131900
N	-7.23447800	0.41840900	0.44497100
C	-7.85646000	1.36937900	1.36191900
H	-8.51185900	0.79226400	2.01392100
H	-7.08210500	1.84529900	1.96530200
C	-8.57525300	2.48823400	0.58645400
O	-7.97272400	3.53328200	0.33722200
N	-9.84240700	2.25988900	0.16750600
H	-10.24754900	3.03986300	-0.33902800
C	-10.69667300	1.09212300	0.38282000
H	-11.25190900	0.92869200	-0.54510700
H	-10.07958500	0.20532700	0.53935600
C	-11.65441600	1.28347800	1.57033600
H	-11.05192600	1.42372800	2.47521700
H	-12.23439700	2.21648200	1.42810000
C	-13.07118300	0.10049600	3.12566800
H	-13.66543000	-0.80922100	3.26340500
H	-12.25950700	0.09395700	3.86055900
H	-13.72395300	0.96822100	3.34058400
C	-13.59029300	0.04185300	0.78347300
H	-14.27745000	0.90887000	0.82746700
H	-13.18115200	-0.01506900	-0.22922100

H	-14.17761200	-0.86610200	0.95552300
N	-12.51754800	0.12014100	1.77347300
Zn	6.17353200	0.77994500	0.96284200

Cartesian coordinates of probe **10**:

H	-1.51485600	-2.37496100	-0.73607300
C	-1.86683700	0.13156800	0.39614500
C	-2.83961700	-0.74928400	-0.16755700
C	-2.53842800	-2.01832900	-0.73017200
C	-2.23228900	1.32099400	0.99723000
C	-4.20585100	-0.32682700	-0.13028800
C	-4.55878800	0.90545400	0.47562900
C	-3.58345500	1.70569500	1.04237500
C	-5.21211600	-1.15966200	-0.68332000
C	-4.87860800	-2.38148600	-1.24074200
C	-3.53778900	-2.81250400	-1.25496900
H	-3.29051300	-3.78115800	-1.67709100
H	-5.66502600	-3.00291700	-1.65483300
H	-1.46598500	1.96048100	1.41972900
H	-3.87070800	2.64193300	1.50734500
C	-6.63292700	-0.73635400	-0.65988000
O	-7.53329600	-1.43054000	-1.12218600
C	-5.97420900	1.34658400	0.51636900
O	-6.31796500	2.39962300	1.04502100
N	-6.92052400	0.50813500	-0.08366300
C	-8.33261400	0.94291500	-0.06167000
C	-9.06918100	0.47267200	1.19244200
H	-8.79874400	0.53833800	-0.95978600
H	-8.32683100	2.03109600	-0.12238400
H	-10.10763000	0.82005900	1.16201200
H	-9.07505300	-0.61986200	1.25556600
H	-8.59921500	0.87523300	2.09503600
N	-0.48404300	-0.21036000	0.37452800
C	2.85541600	-1.07649500	-0.81094500
H	3.20310400	-2.02265500	-0.38261500
H	2.65385900	-1.27007500	-1.88073800
N	3.92542300	-0.08828700	-0.61745400
C	3.64090100	1.16406600	-1.33311700
H	3.75003900	1.04390100	-2.42668800
H	2.59373100	1.41897200	-1.14077400
C	5.23281800	-0.63946300	-1.00290800
H	5.95182000	0.18598100	-0.98428600
H	5.22076300	-1.03420100	-2.03578400
C	4.49657400	2.32391600	-0.85985600
C	5.02497400	3.77107800	0.84788300
C	6.16750700	4.02068300	-1.23909900
C	5.96921700	4.44774500	0.07182000
H	4.83991500	4.08105800	1.87544400
H	6.88982000	4.51452800	-1.88293100
H	6.52491200	5.28251000	0.48730200
C	5.73160000	-1.71479900	-0.05576600
C	6.46296500	-2.25008200	2.05826400
C	6.40577100	-3.98271100	0.40979500
C	6.68276100	-3.58653400	1.71613600

H	6.67339100	-1.90368600	3.06917200
H	6.56058000	-5.01071500	0.09451700
H	7.06109100	-4.28726900	2.45373600
N	0.24416000	-0.19903200	1.52822200
N	1.47218700	-0.49502400	1.21451300
C	1.57040600	-0.69301800	-0.13755800
C	0.31904200	-0.50985300	-0.68351900
H	-0.04373700	-0.54238200	-1.69900300
C	5.41932300	2.94122800	-1.71149900
H	5.54670000	2.57949500	-2.72757500
C	5.92196200	-3.03158800	-0.48963800
H	5.69346600	-3.30358200	-1.51596500
N	6.00252600	-1.32753600	1.20507200
N	4.29941700	2.73689700	0.40656400

Cartesian coordinates of the Zn^{2+} complex of **10**:

H	1.64843000	-2.18069900	0.80323800
C	2.08754300	0.52763300	0.36274400
C	3.02978800	-0.53747800	0.45248500
C	2.68820700	-1.89632400	0.68560900
C	2.46391700	1.82388200	0.08146500
C	4.40630500	-0.19800000	0.26578100
C	4.78229900	1.13999600	-0.01389900
C	3.82351700	2.13076100	-0.11206300
C	5.39353000	-1.21293000	0.34334000
C	5.02688000	-2.52444500	0.58592500
C	3.66917800	-2.86417800	0.75159700
H	3.39380900	-3.89891400	0.92719800
H	5.79799500	-3.28506300	0.63834400
H	1.71156000	2.60204200	0.02018400
H	4.12977800	3.14726100	-0.33023100
C	6.82701400	-0.88136100	0.15292500
O	7.70899800	-1.73194700	0.20296000
C	6.21209700	1.49312200	-0.21509600
O	6.56952800	2.63655600	-0.47745900
N	7.14699800	0.46152000	-0.08941000
C	8.57294800	0.80235700	-0.28118200
C	9.00762500	0.68833600	-1.74210100
H	9.14514900	0.12134000	0.34834200
H	8.70383800	1.82047900	0.08471600
H	10.06839100	0.94633900	-1.83167300
H	8.87071700	-0.33263800	-2.11129200
H	8.43405100	1.37223000	-2.37525700
N	0.68867000	0.25607800	0.54356100
C	-2.52771200	-0.71126600	2.00071500
H	-2.58890600	-1.80192900	1.93429900
H	-2.50534100	-0.45580200	3.06588700
N	-3.71969100	-0.14239400	1.32116100
C	-4.07871900	1.20281100	1.81740500
H	-4.71907800	1.15076400	2.70570100
H	-3.15147500	1.70207800	2.12077700
C	-4.86452800	-1.07742700	1.27962200
H	-5.76940000	-0.48695500	1.09598900
H	-5.00826900	-1.58992400	2.23761700

C	-4.73604200	2.04982000	0.74086900
C	-4.88666400	2.57376600	-1.52946200
C	-6.12630600	3.88237600	0.04376900
C	-5.75434900	3.62751700	-1.27661200
H	-4.57285300	2.32338200	-2.53661800
H	-6.81037200	4.69165000	0.27794500
H	-6.13210000	4.22557500	-2.09776200
C	-4.71759500	-2.08396400	0.15111300
C	-3.95173800	-2.49119200	-2.01663200
C	-5.17926000	-4.20341800	-0.88275800
C	-4.50384200	-3.76536300	-2.02218700
H	-3.40758200	-2.10158800	-2.86980000
H	-5.61580200	-5.19636000	-0.84852900
H	-4.39860600	-4.39656400	-2.89699000
N	-0.16359400	0.46322800	-0.46919100
N	-1.34673500	0.15320800	-0.00366100
C	-1.28052700	-0.24909100	1.29745200
C	0.04312700	-0.17759400	1.66362300
H	0.55639900	-0.37938400	2.59026800
C	-5.61473800	3.08121800	1.06298600
H	-5.88882000	3.25172600	2.09852000
C	-5.28341400	-3.35430500	0.21824500
H	-5.79866500	-3.66810600	1.11957500
N	-4.05809600	-1.67171800	-0.95344100
N	-4.38888700	1.80417700	-0.54180800
Zn	-3.22009800	0.17139800	-0.79396700