Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

I: Material and Methods

1.1 Materials and Physical measurements

All chemical reagents and solvents were obtained from commercial suppliers, such as Aladdin Industries (Shanghai, China), Shanghai Experimental Reagent Co., Ltd. (Shanghai, China), Beyotime Co., Ltd. (Shanghai, China). Among them, 6-methoxy-2-methylquinoline and 1.4-dioxane were purchased from Aladdin Industries (Shanghai, China). Mitochondrial red, CCK-8 and cell culture reagents were purchased from Beyotime Co., Ltd (Shanghai, China). The fluorescence spectrum was measured using a Hitachi F-7000 fluorescence spectrophotometer. The ultraviolet-visible spectrum was monitored by Hitachi U-3900 ultraviolet-visible spectrophotometer. ^{1}H NMR and ^{13}C NMR data were performed with BRUKER AVANCE III HD 600 MHz and 151 MHz NMR spectrometers (Bruker, Billerica, MA). The HR-MS measurement was performed on the AB SCIEX Tripple TOF5600 instrument. Zeiss LSM880 confocal laser scanning microscope was used to evaluate the probe's ability to respond in living cells. PerkinElmer IVIS Lumina LT III living imaging instrument was used for evaluating the imaging of **Probe** in living cells and mice.

*1.3. Synthesis of **BQ-1***

Compound A: To a round bottomed flask was added compound 1 (0.455 g, 1.7 mmol), hexamethylenetetramine (0.546 g,3.9 mmol), and trifluoroacetic acid (15 mL). The mixture was refluxed overnight. After the mixture was cooling down, the acid was neutralized with KOH solution. The precipitate was collected by filtration, and

washed with water for several times. After drying under vacuum, A was obtained. [1-2]

BQ-1: The A (0.27 g, 1.0 mmol) was added dropwise to a solution of B (0.25 g, 1.3 mmol) dissolved in ethanol, and 110 ul of piperidine was added. The mixture was heated to 90 °C, refluxed, and protected with N_2. TLC spot check. After the reaction, the solvent was removed under reduced pressure. The product was purified by column chromatography to obtain a light yellow solid product 0.15 g, 51%, (CH_2Cl_2 :CH_3OH = 20:1).

1.4. Imaging Experiments

Hela cells were cultured in humidified air containing 5% CO_2 at 37 °C in DMEM medium supplemented with 10% fetal bovine serum (additional 100 μg/mL streptomycin and 100 u/mL penicillin). The cells were washed 3 times with PBS (pH = 7.4) and then incubated with 10 μM **Probe** in pure PBS (pH = 7.4) for 20 min. After washing three times, the cells were CLSM imaged with a Zeiss LSM-880 microscope. The yellow channel was set to 570 ± 30 nm (λ_{ex} = 488 nm), and the blue channel was set to 445 ± 30 nm (λ_{ex} = 405 nm). In the mitochondrial localization experiment, we set the parameters: λ_{ex} = 488 nm, λ_{ex} = 490-550 nm. For the endogenous group, the loaded **Probe** cells were pre-incubated with Cys (150 μM) for 0.5 h.

II:

Figure S1: ^{1}H MNR (600 MHz) spectrum and ^{13}C MNR (151 MHz) spectrum of **BQ-1** in DMSO-d_6 and the HR-MS of **BQ-1** .

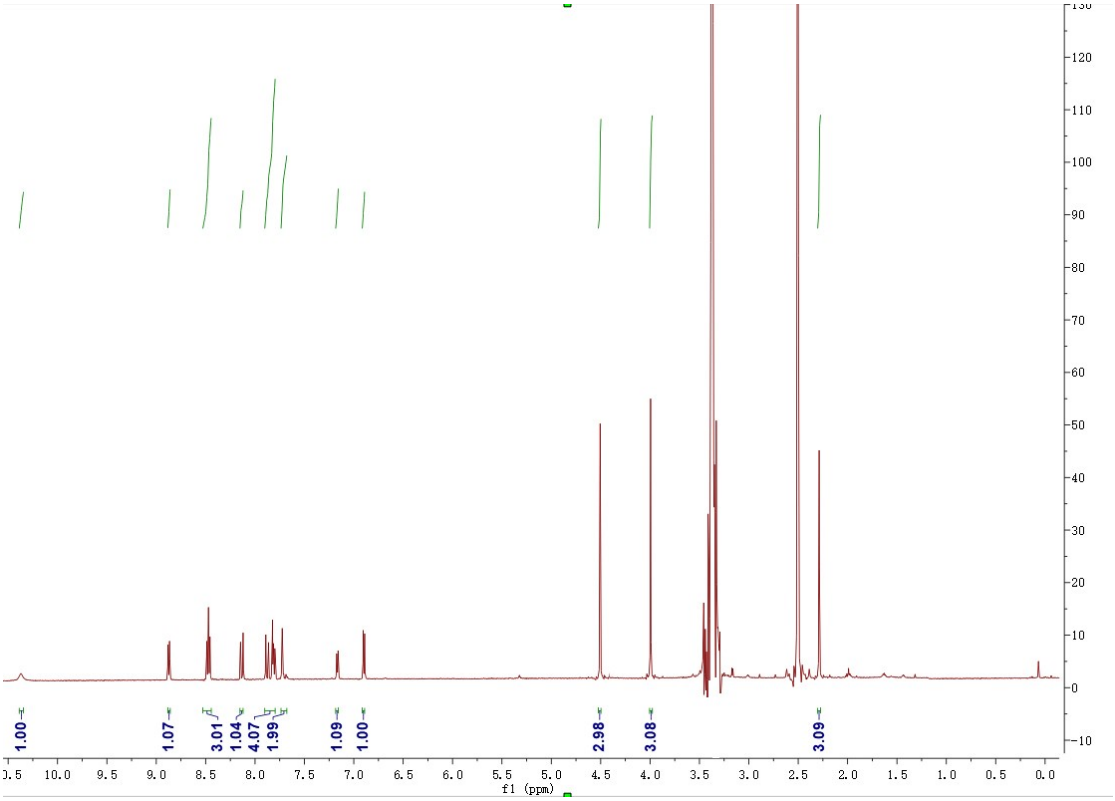


Figure S1 (a):^{1}H MNR (600 MHz) spectrum of **BQ-1** in DMSO-d_6。

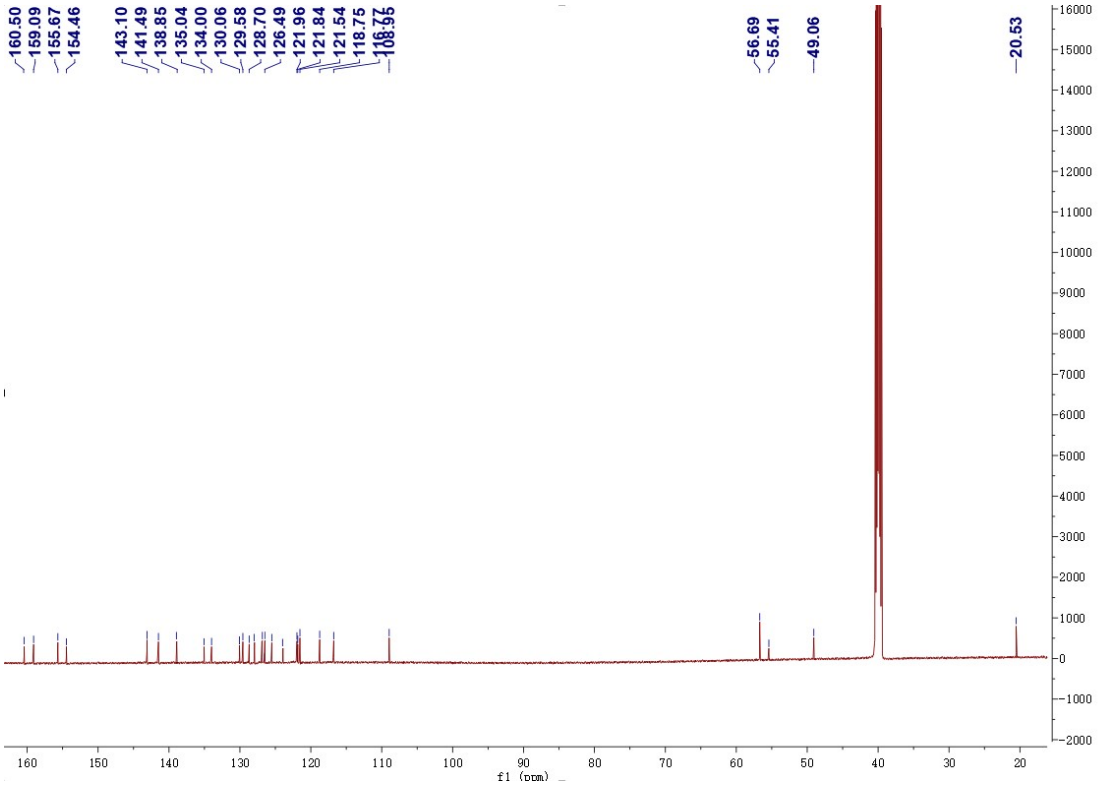


Figure S1 (b): ^{13}C MNR (151 MHz) spectrum of **BQ-1** in DMSO-d_6

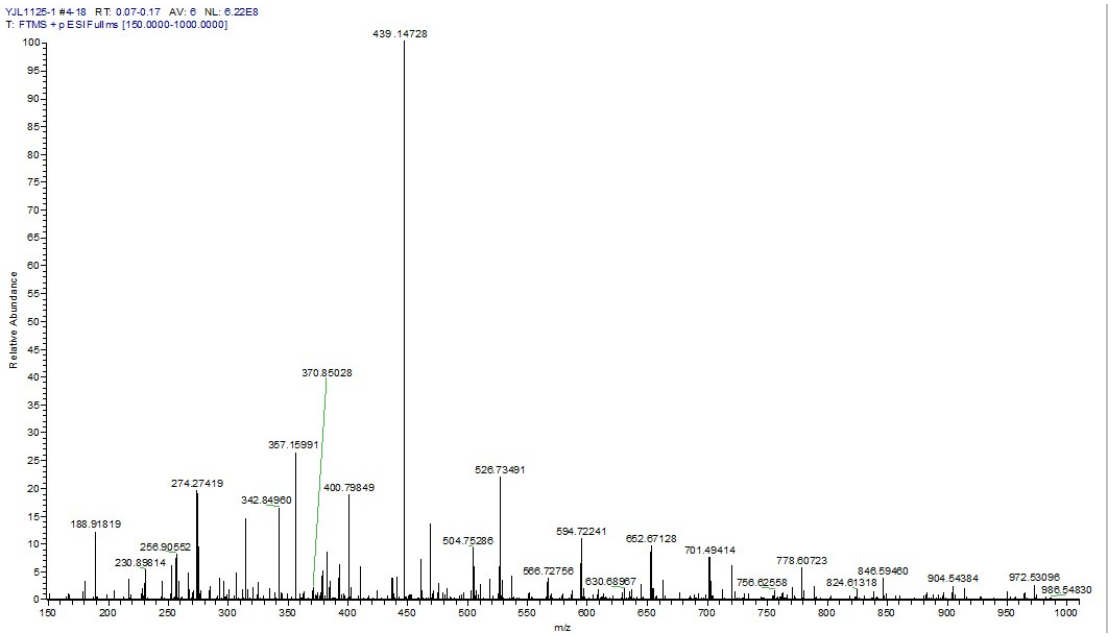


Figure S1 (c): The HR-MS of **BQ-1**

Figure S2: Fluorescence competition of **BQ-1** (10 μM) in response to various other analytes (5 mM) at 530 nm.1.H_2S, 2.L-Threonine, 3.L-Methionine, 4.L-Proline, 5.L-Aspartic acid, 6.L-Valine, 7.trans-4-Hydroxy-L-proline, 8.L-Asparagine, 9.L-Glutamic acid, 10.L-Phenylalanine, 11.L-Arginine, 12.L-Isoleucine, 13.CH_3COO^-, 14.Cl^-, 15.$H_2PO_4^-$, 16.$S_2O_3^-$, 17.H_2O_2, 18.Cys, 19.GSH, 20.Hcy, 21.NO_2^-, 22.CO_3^{2-}, 23. F^- , 24. $H_2PO_4^-$, 25.$NaHSO_3$.

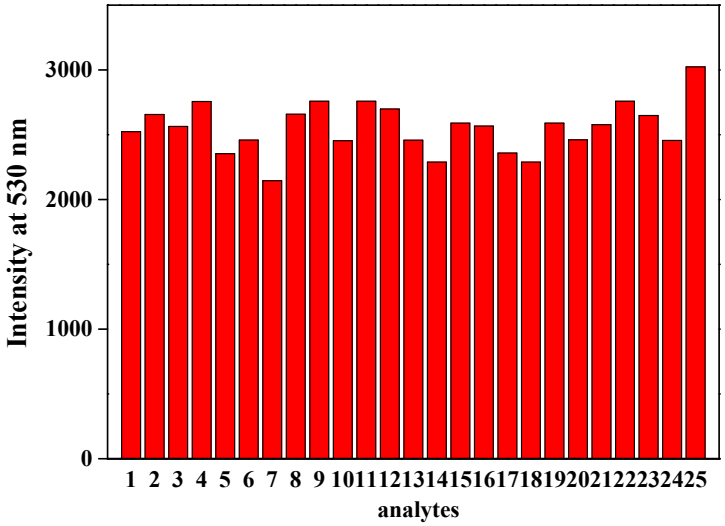


Figure S3: Fluorescence spectra of free **BQ-1** and **BQ-1** after addition of $NaHSO_3$ under different pH conditions.

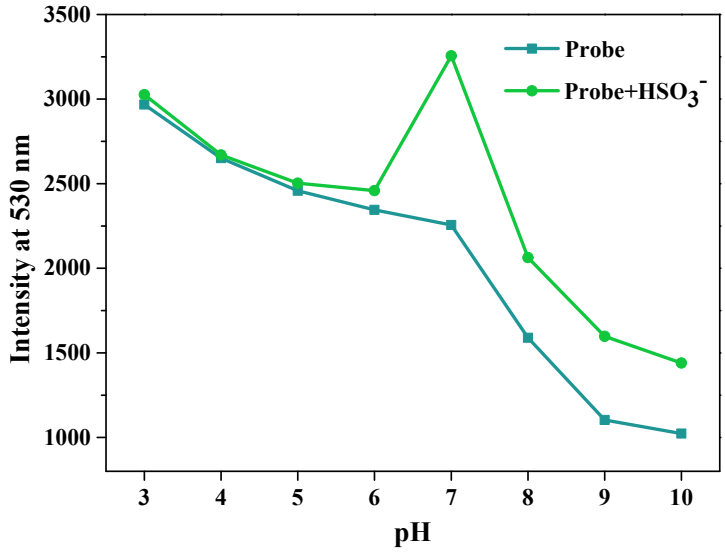


Figure S4: The ^{1}H-NMRof the reaction mechanism.

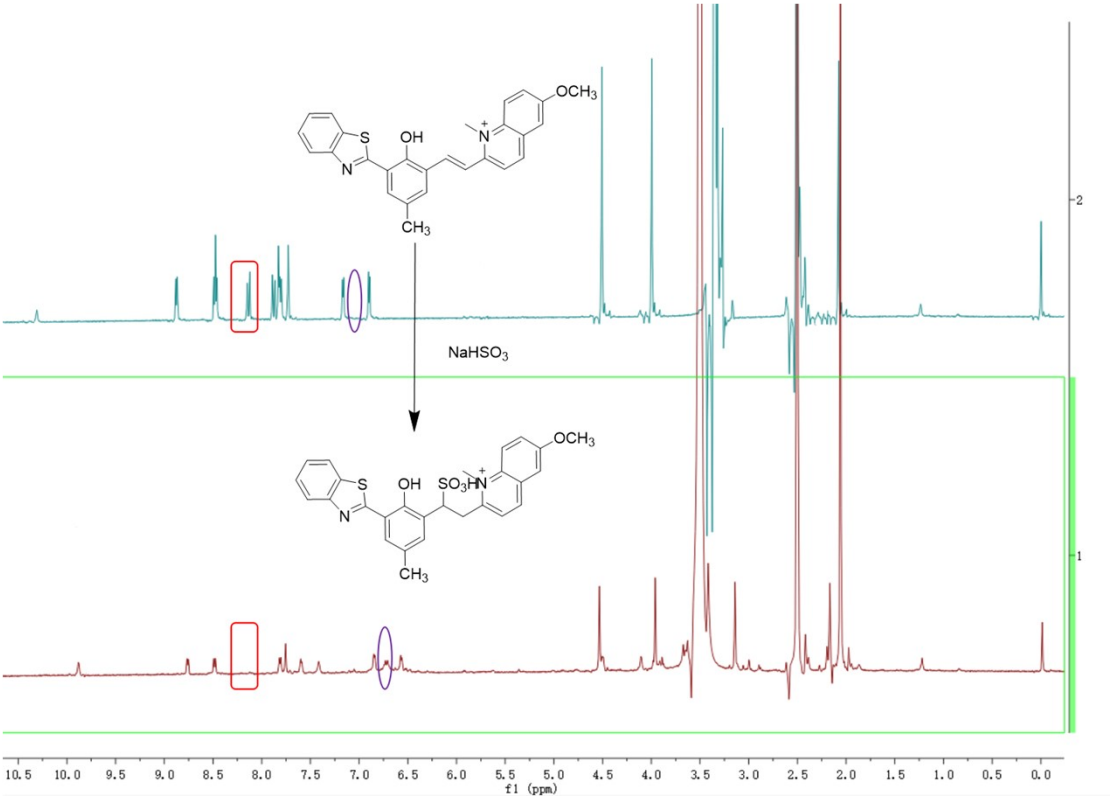


Figure S4(a} The ^{1}H-NMR of the reaction mechanism.

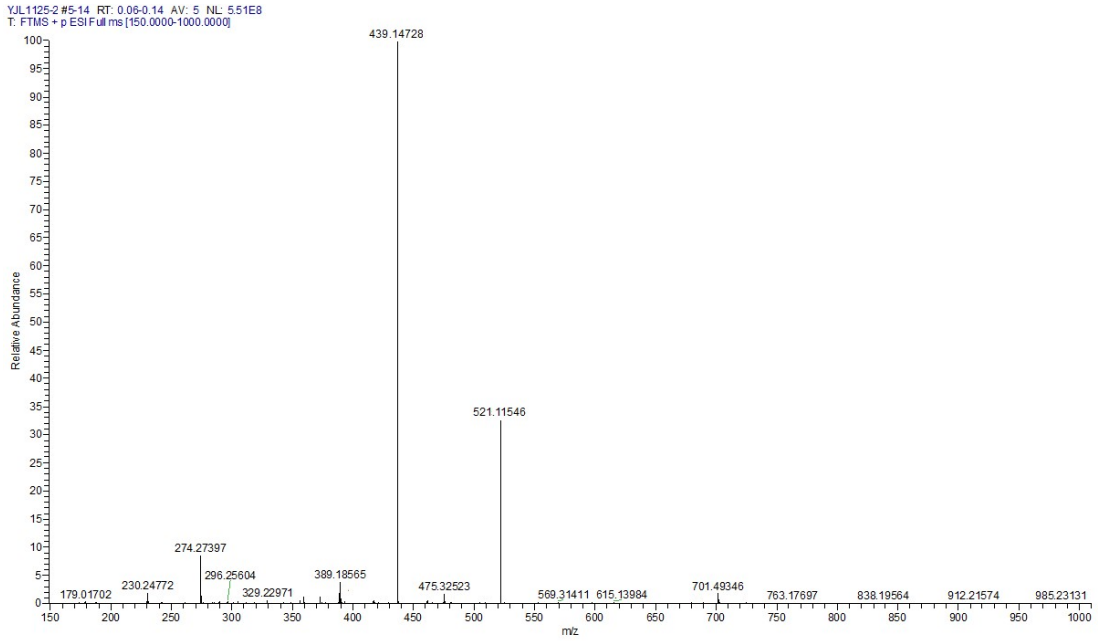


Figure S4(b) The HR-MS of the reaction mechanism.

The HR-MS spectrum of the final product: calc. for $C_{27}H_{25}N_2O_5S_2^+[M]^+$: 521.11994, found 521.11546.

Figure S5: Cell Viability Assay.

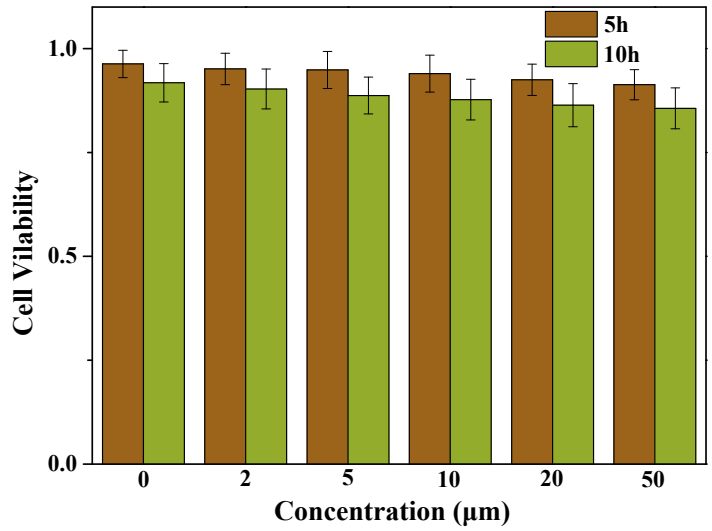


Figure S6: The fluorescence spectrum of the **BQ-1** in the presence of NAD(P)H.

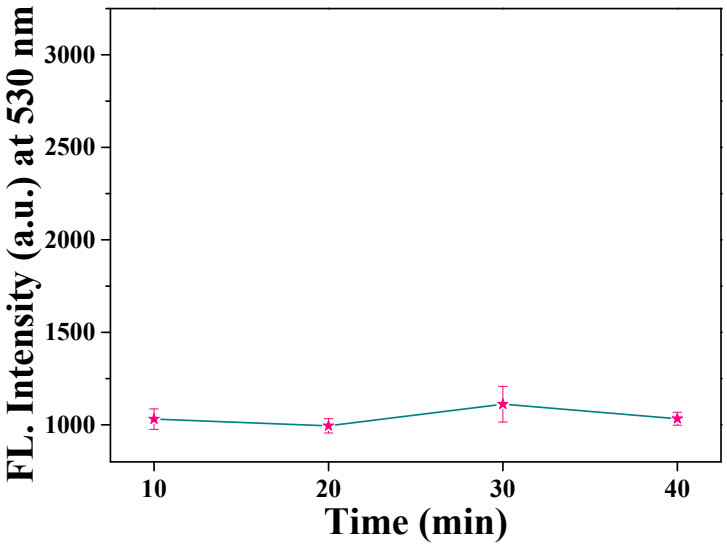
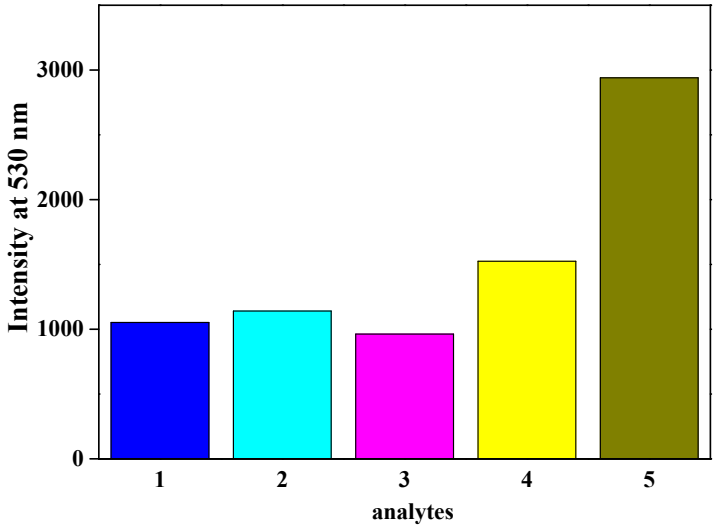


Figure S6 In the presence of NAD(P)H, the fluorescence emission spectrum of the BQ-1 (10 μM) in 40 minutes. MeOH:PBS=1:1 (pH=7.4), slit width: 10 nm/10 nm.

Figure S7: Selective experiments with **BQ-1** (10 μM) and other analytes(5 mM).



In the existence of other ananlytes (5 mM), the fluorescence intensity of the **BQ-1** (10 μM) in MeOH:PBS=1:1 (pH=7.4), slit width: 10 nm/10 nm. 1.$S_2O_3^{2-}$, 2.Na_2S_2, 3.O_2^-, 4.HOCl, 5.$NaHSO_3$.

Reference

[1]D. Dahal, L. McDonald, X. Bi, C. Abeywickrama, F. Gombedza, M. Konopka, S. Paruchuri and Y. Pang, An NIR-emitting lysosome-targeting probe with large Stokes shift via coupling cyanine and excited-state intramolecular proton transfer, Chem. Commun., 53 (2017) 3697-3700.

[2]X. He, Y. Wu, W. Jin, X. Wang, C. Wu, Y. Shang, Highly efficient AgNO3-catalyzed approach to 2-(benzo[d]azol-2-yl) phenols from salicylaldehydes with 2-aminothiophenol, 2-aminophenol and benzene-1,2-diamine, Appl Organometal Chem., 32 (2018) 4284-4295.