

Supporting Information

DCPO based nanoparticles as near-infrared fluorescent probe for Cathepsin B

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1. Absorption spectra of DPCO and probe 1

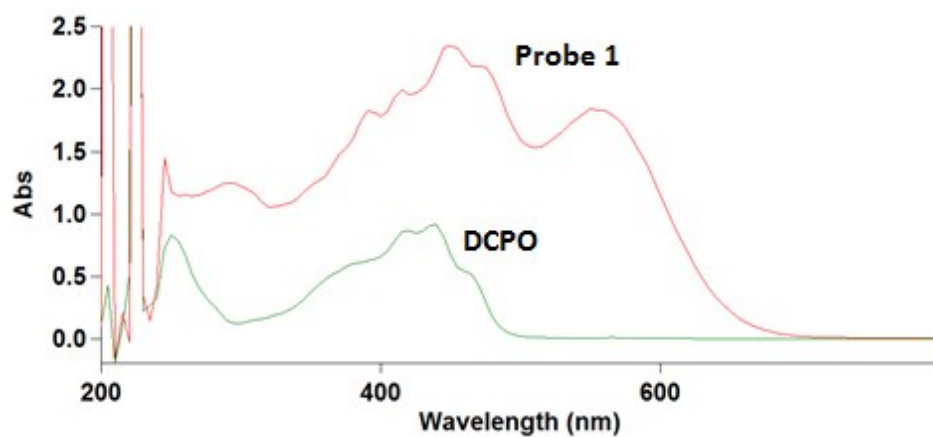


Figure S1 Absorption spectra of DPCO and probe 1 (50 μ M) in PBS buffer/DMSO (v/v=1/1, pH=7.4)

2. Emission spectra of DPCO and probe 1

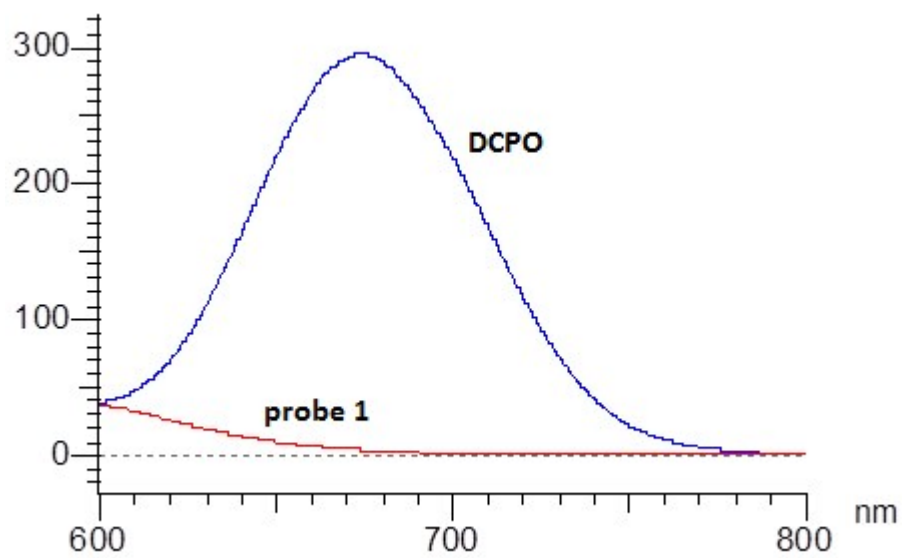


Figure S2 Emission spectra of DCPO and probe 1 (50 μ M) in PBS buffer/DMSO (v/v=1/1, pH=7.4)

3. HPLC of CTB assay

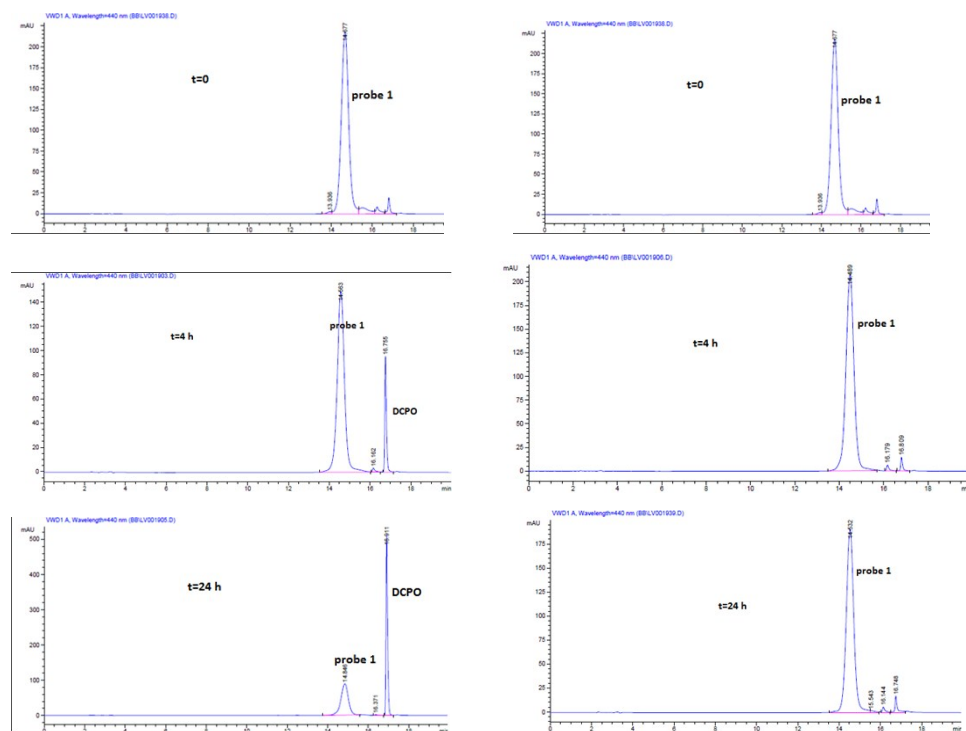


Figure S3 HPLC of CTB assay: with CTB (left) and without CTB (right). Method: From 5% ACN/95% water to 95% ACN/5% water in 20 min.

4. Stability of probe 1 in PBS

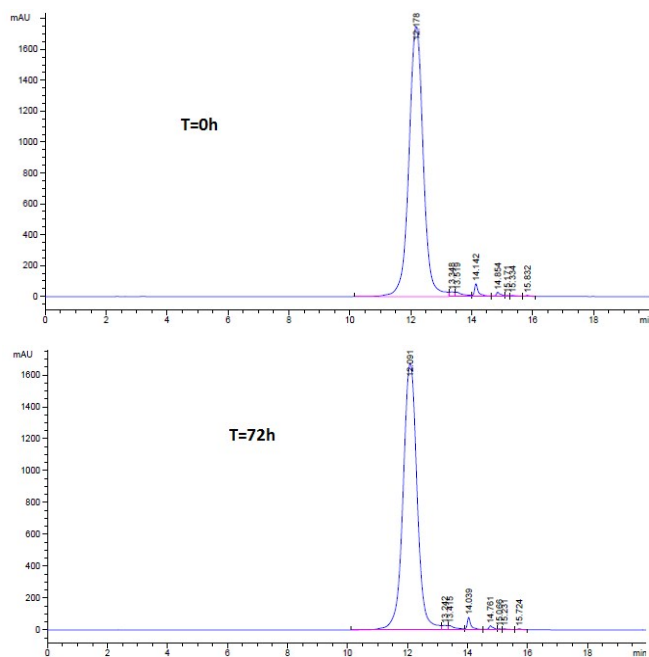


Figure S4 Stability of **probe 1** in PBS(pH=7.4, 10 mM). Method: From 10% ACN/90% water to 95% ACN/5% water in 20 min.

4. ^1H NMR and ^{13}C NMR spectra

Figure S5. ^1H NMR Spectrum of compound 3 (400 MHz, $\text{DMSO}-d_6$)

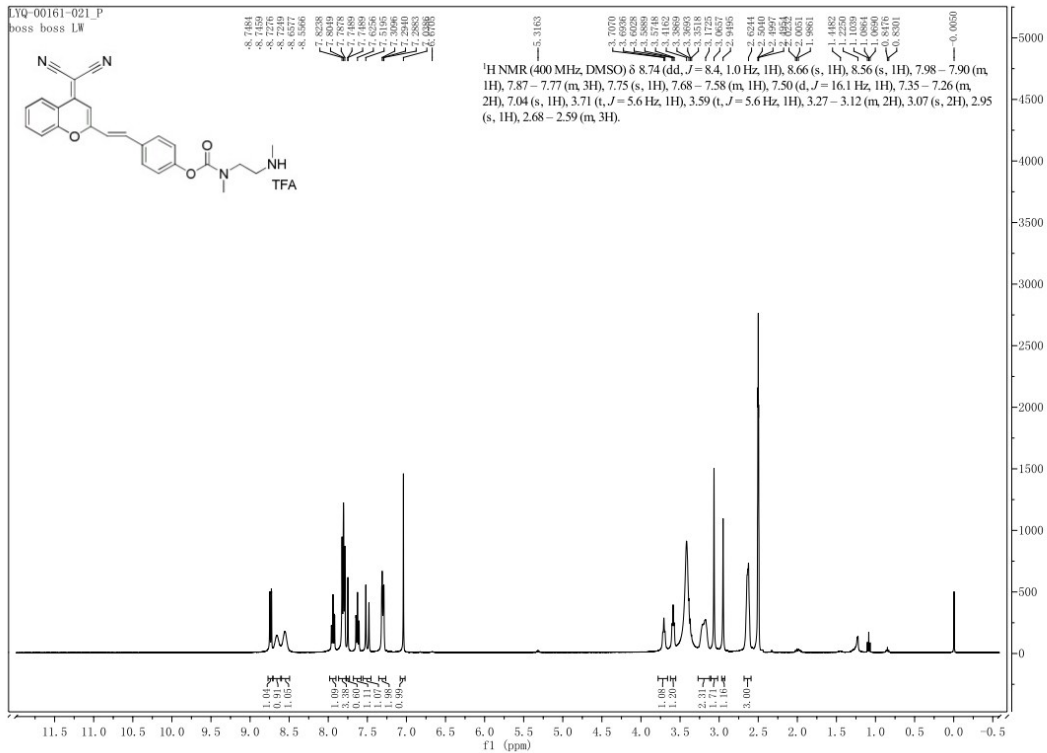


Figure S6. ¹³C NMR Spectrum of compound 3 (100 MHz, DMSO-*d*₆)

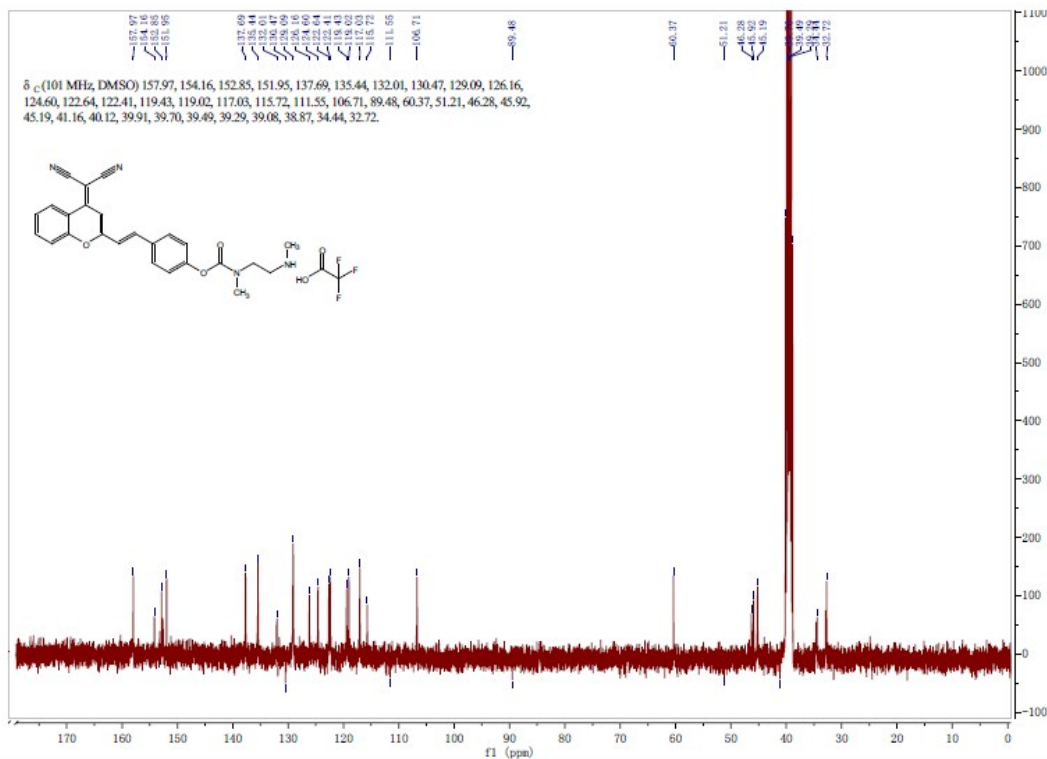


Figure S7. ¹³C NMR Spectrum of compound 5 ((400 MHz, DMSO-*d*₆)

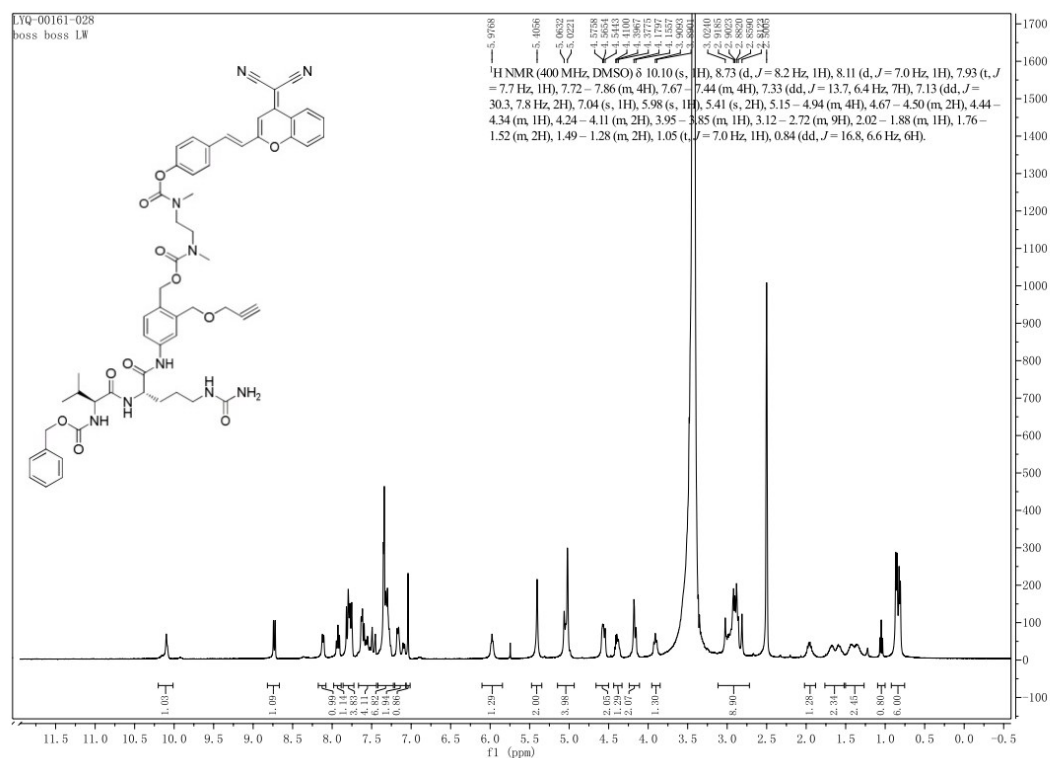


Figure S8. ^{13}C NMR Spectrum of compound compound 5 ((400 MHz, DMSO- d_6)

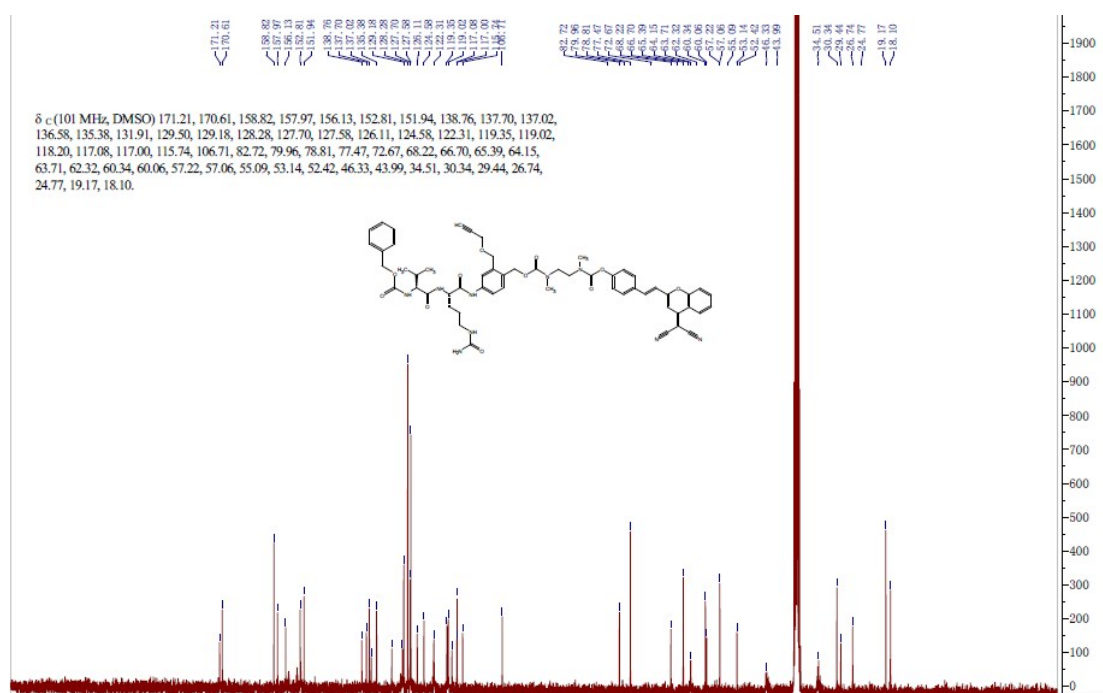


Figure S9. ^1H NMR Spectrum of probe 1 ((400 MHz, DMSO- d_6)

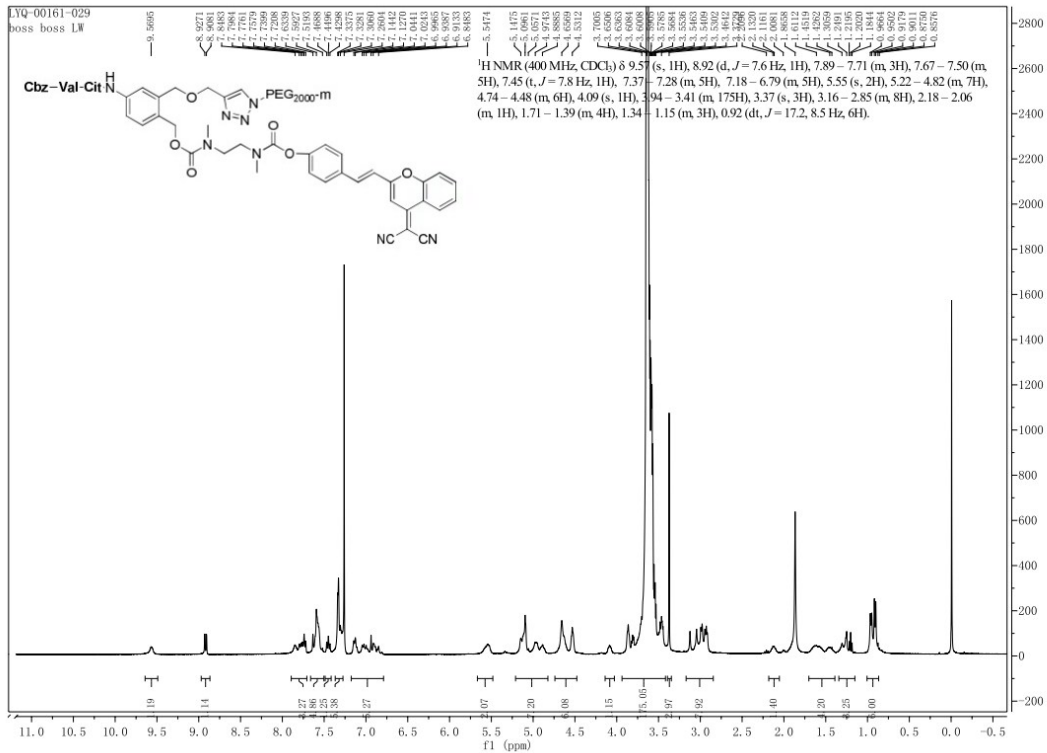


Figure S10. HR-MS of compound 5

Elemental Composition Report

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Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

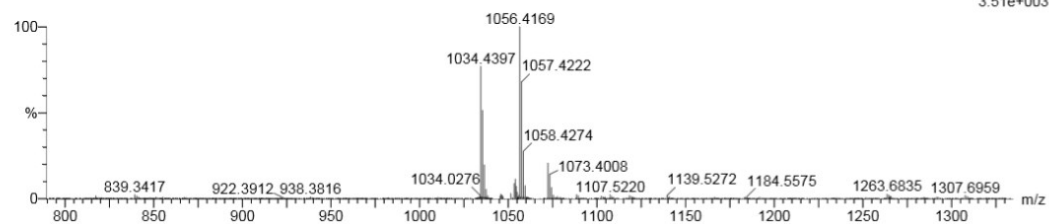
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 56-56 H: 53-62 N: 9-9 O: 11-11 Na: 0-1 I: 0-1

LYQ-00161-028-1C 14 (0.796)

1: TOF MS ES+



Minimum:

Maximum: 500.0 1000.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1034.4397	1034.4412	-1.5	-1.5	31.5	35.4	0.0	C56 H60 N9 O11