

Supporting Information

A highly selective and sensitive fluorescent probe for thiols based on a benzothiazole derivative

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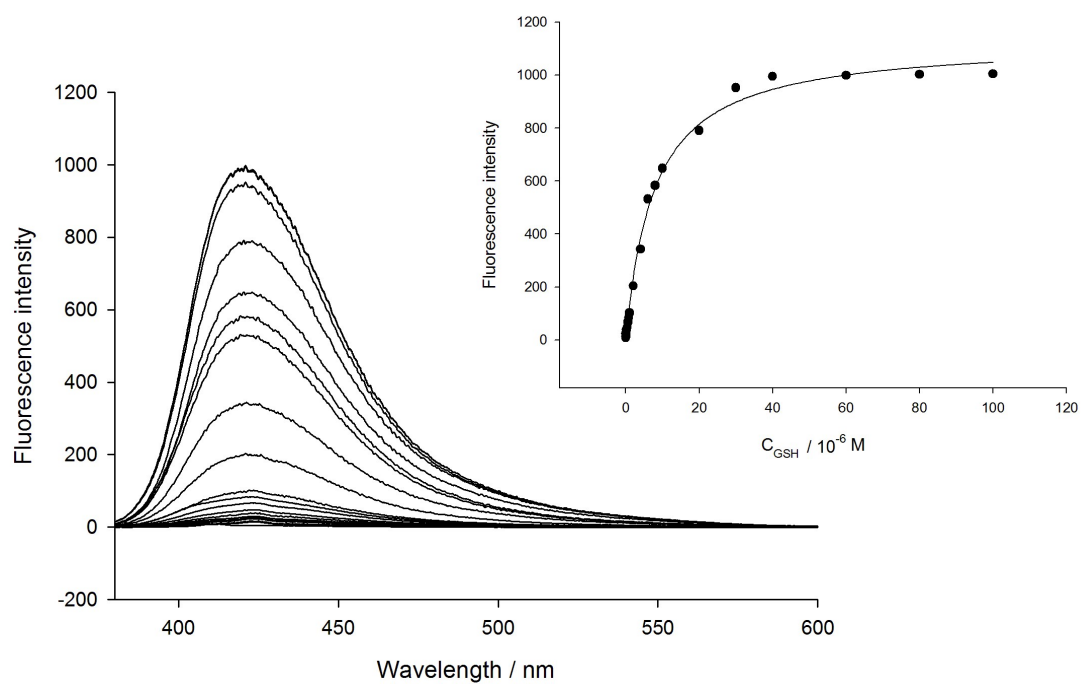


Figure S1 One-photon fluorescence spectra of probe **1** (5.0 μ M) in the presence of various concentrations of glutathione: 0, 0.02, 0.04, 0.06, 0.08, 0.1, 0.2, 0.4, 0.6, 0.8, 1, 2, 4, 6, 8, 10, 20, 30, 40, 60, 80, 100 μ M from 1 to 22 ($\lambda_{\text{ex}} = 360$ nm). Inset: fluorescence intensity at 423 nm as a function of the concentration of glutathione.

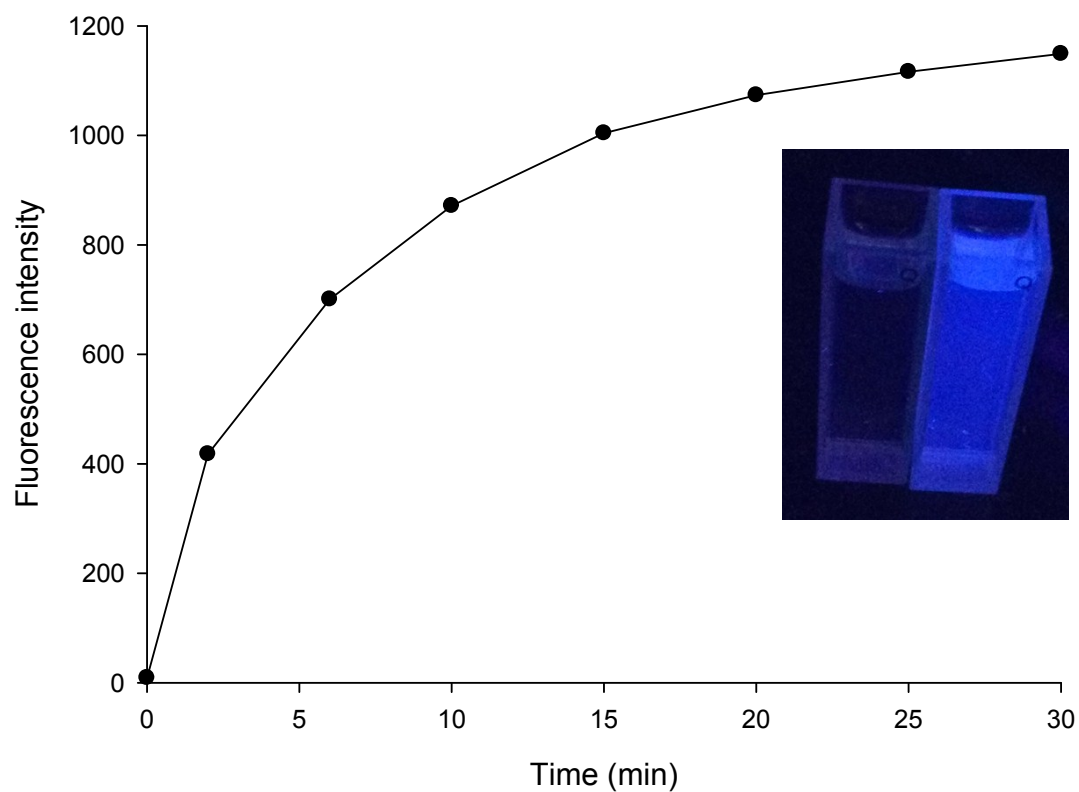


Figure S2 Time-dependent fluorescence intensity changes of probe **1** ($5.0 \mu\text{M}$) for $100 \mu\text{M}$ glutathione. Time points represent 0, 2, 6, 10, 15, 20, 25 and 30 min. The inset show the visual fluorescence color of probe **1** ($5.0 \mu\text{M}$) before (left) and after (right) incubation with with glutathione for 15 min (UV lamp, 365 nm). The fluorescence intensity is recorded at 423 nm.

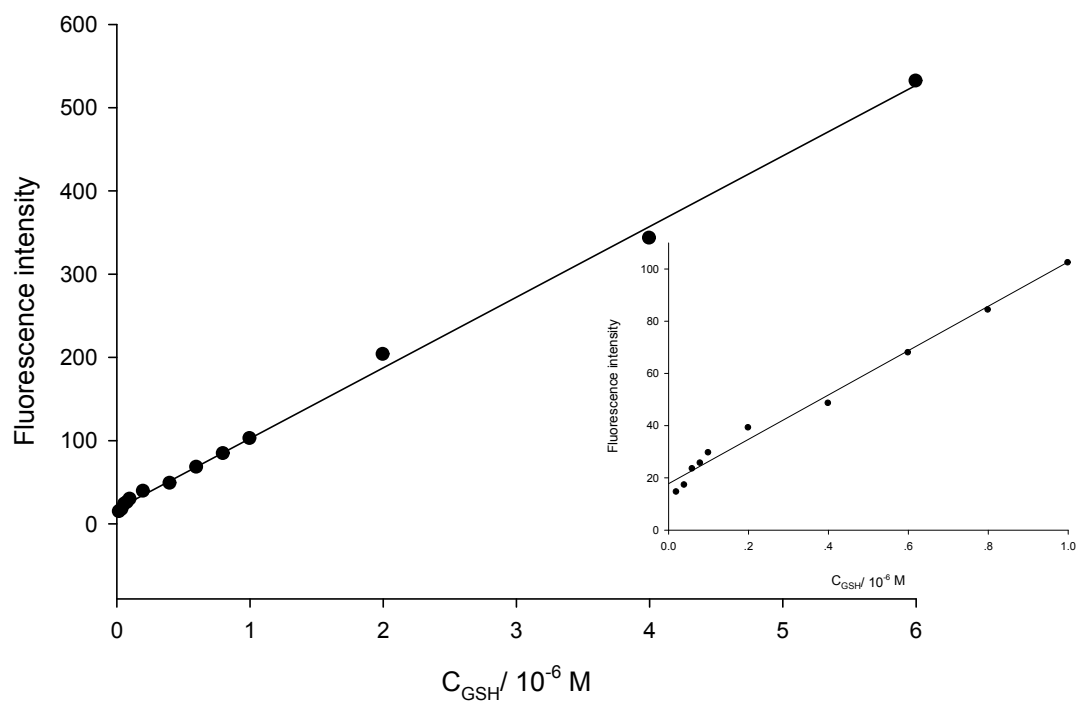


Figure S3 One-photon fluorescence titration curve of probe **1** (5.0 μM) for glutathione. Insert: the plot of fluorescence intensity of probe **1** (5.0 μM) as a function of the concentration of glutathione from 0.02 μM to 6.0 μM . The fluorescence intensity is recorded at 423 nm.

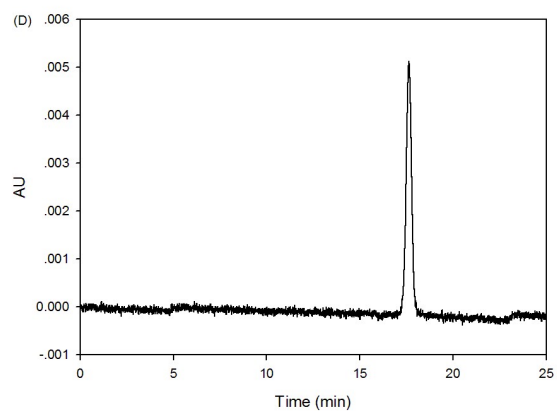
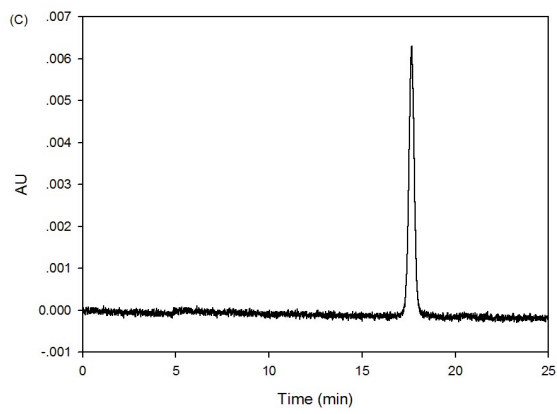
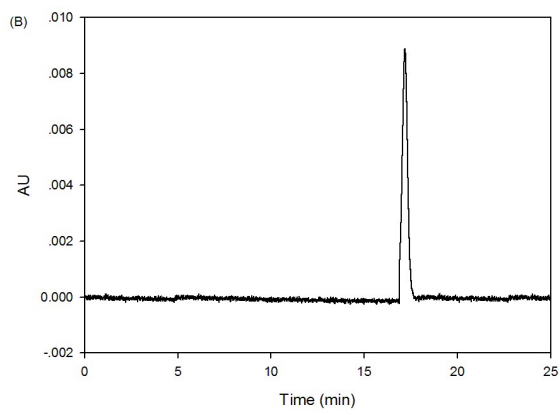
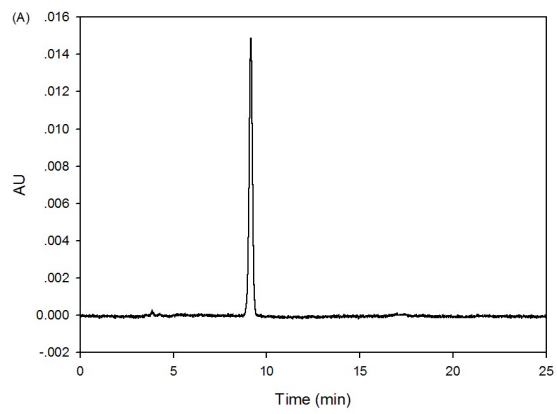


Figure S4 HPLC profiles of (A) compound **1** (5 μM), (B) compound **2** (5 μM), (C) the reaction product of compound **1** (5 μM) with cysteine (200 μM) and (D) the reaction product of compound **1** (5 μM) with glutathione (100 μM). HPLC conditions: 1.0 mL/min flow rate, Agela Technologies Venusil XBP -C18: 5 μm , 4.6 \times 250 mm column, methanol/water = 90:10 (v/v), detected at 360 nm.

NMR and MS data for compounds

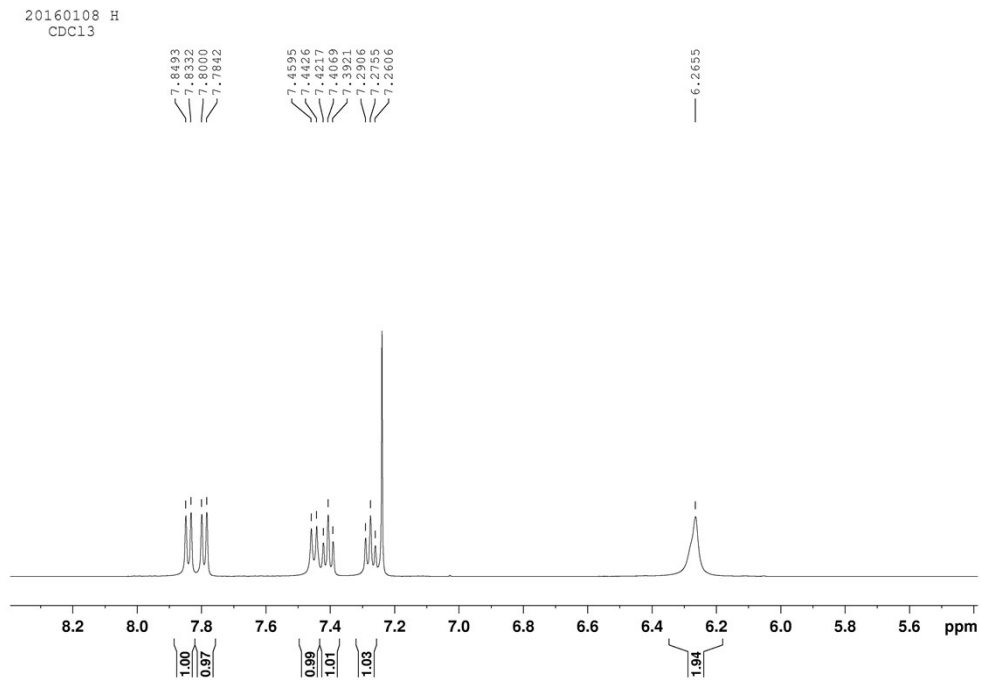
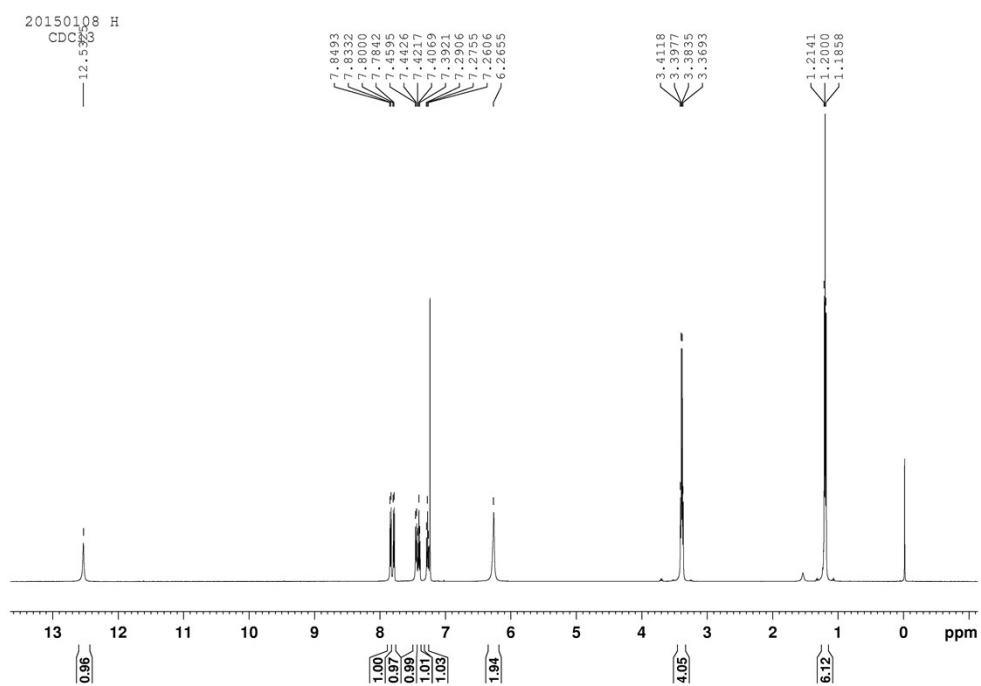


Figure S5. ¹H NMR spectrum of compound **2** in CDCl₃.

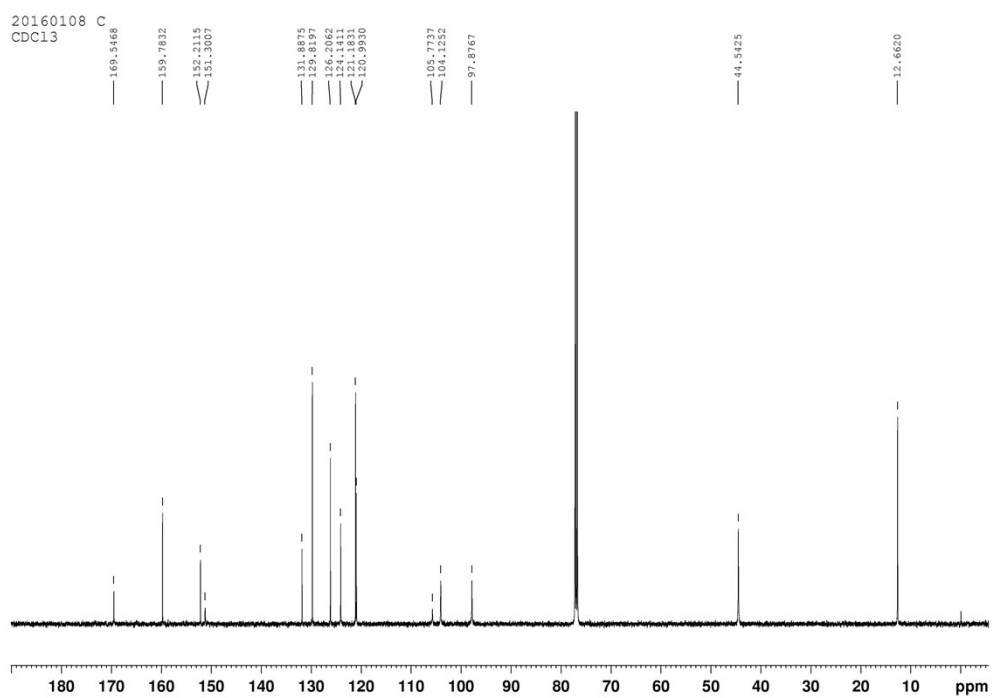


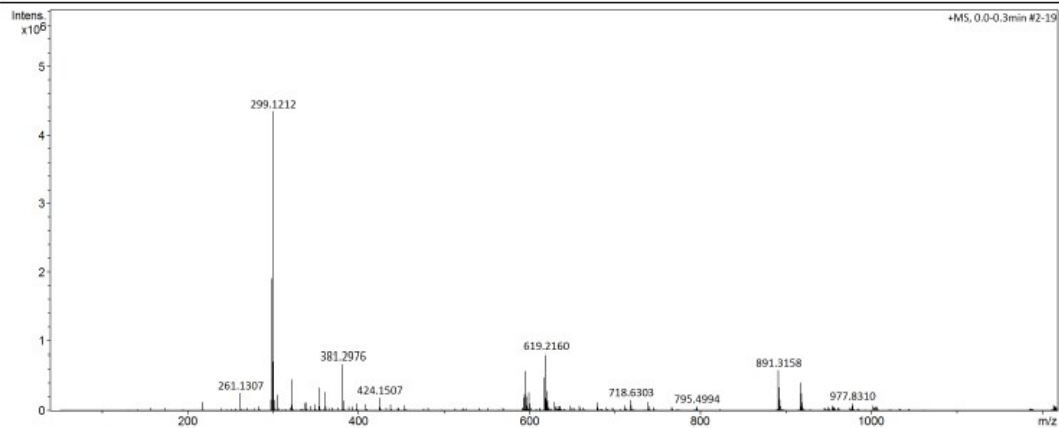
Figure S6. ¹³C NMR spectrum of compound **2** in CDCl₃.

Display Report

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Sample Name: 298
Comment:

Acquisition Date: 2016/1/14 9:52:57
Operator: BDAL@DE
Instrument: maxis HD
1820881.21303

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Scan End		Set Corona	0.1 A	Set APC Heater	0.5 jC



298.d
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Figure S7. MS spectrum of compound 2.

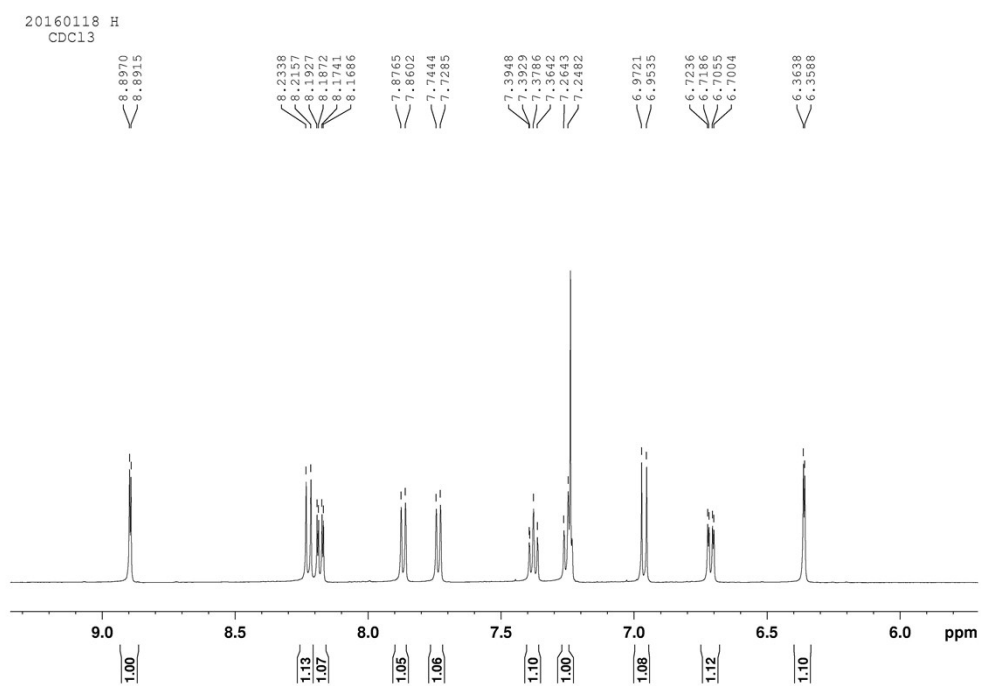
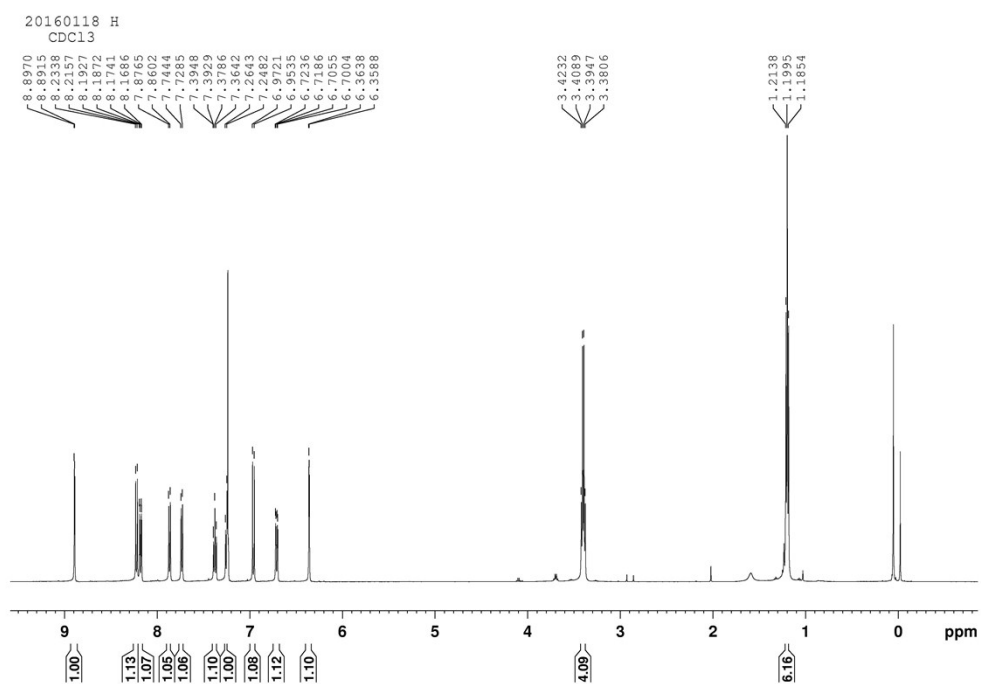


Figure S8. ¹H NMR spectrum of compound **1** in CDCl₃.

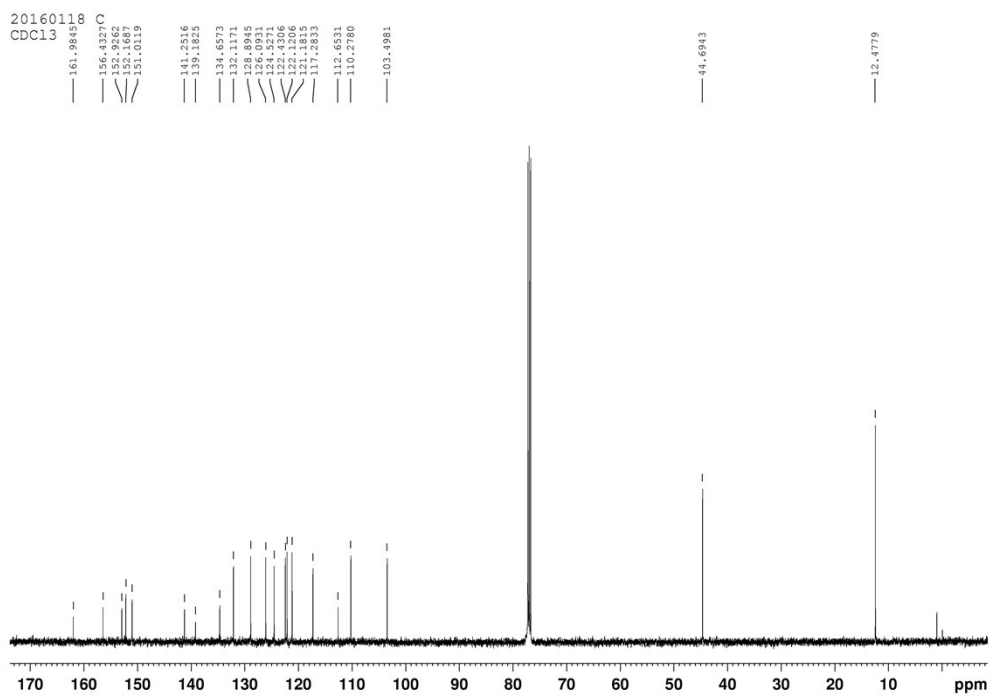
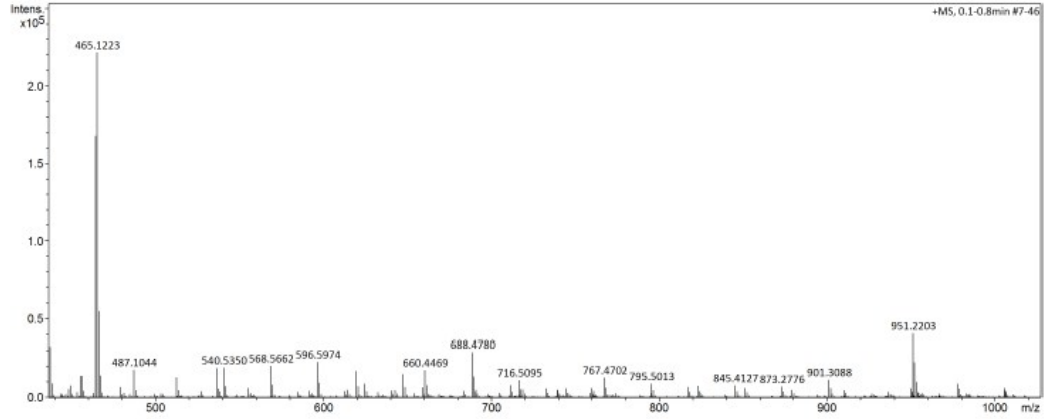


Figure S9. ^{13}C NMR spectrum of compound **1** in CDCl_3 .

Display Report

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Comment			

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MQJ.d
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Figure S10. MS spectrum of compound 1.