

Supporting Information

A Phenazine–based Near-infrared (NIR) Chemodosimeter for Cysteine Obtained via a Carbonyl-assisted Cycloaddition Process

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Outline

NMR and HRMS spectra	S1-S13
Plots for calculating the Detection Limited values	
UV-vis method	S14
Emission method	S15
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MTT assay for valuating the cytotoxicity	S17

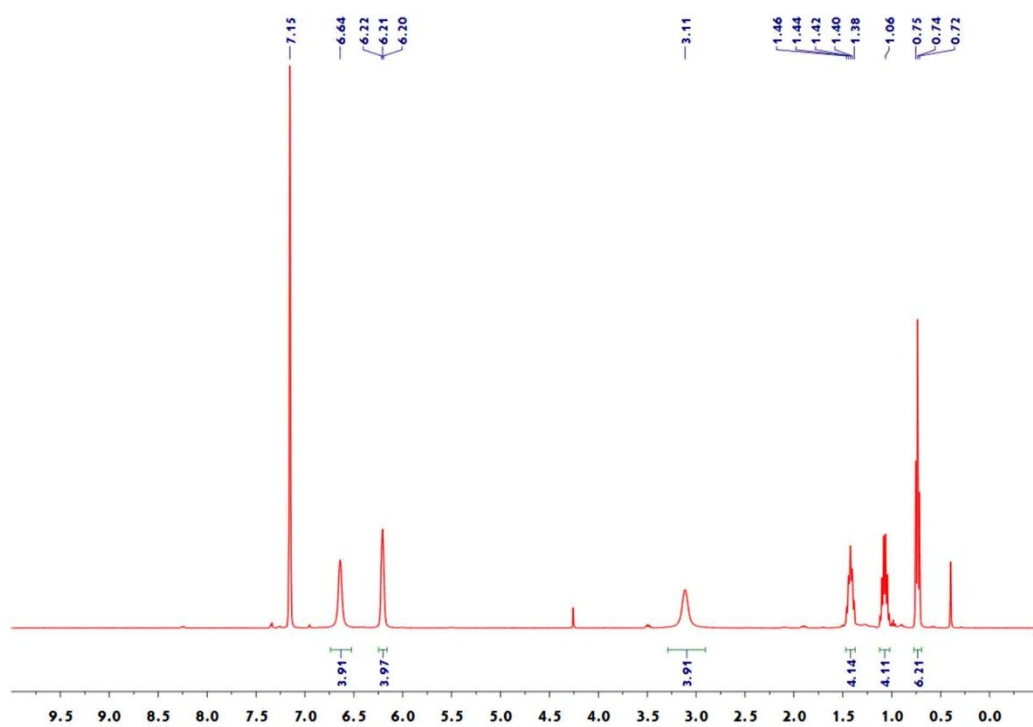


Figure S1. ¹H NMR of compound **2** in C₆D₆.

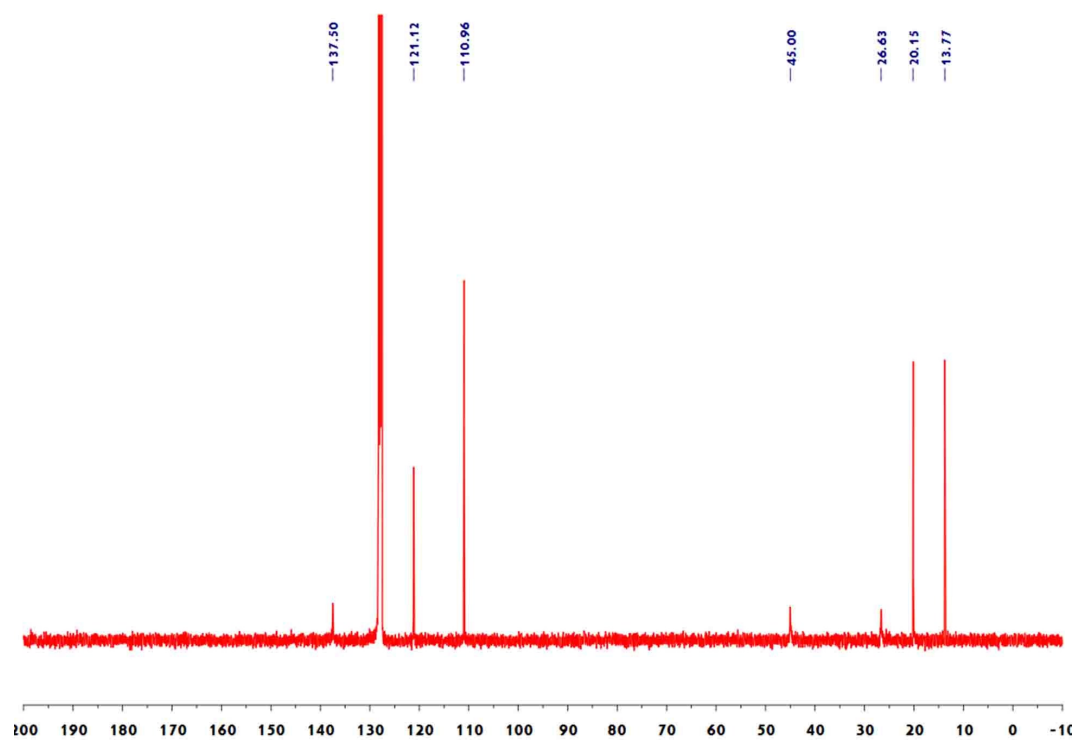


Figure S2. ¹³C NMR of compound **2** in C₆D₆.

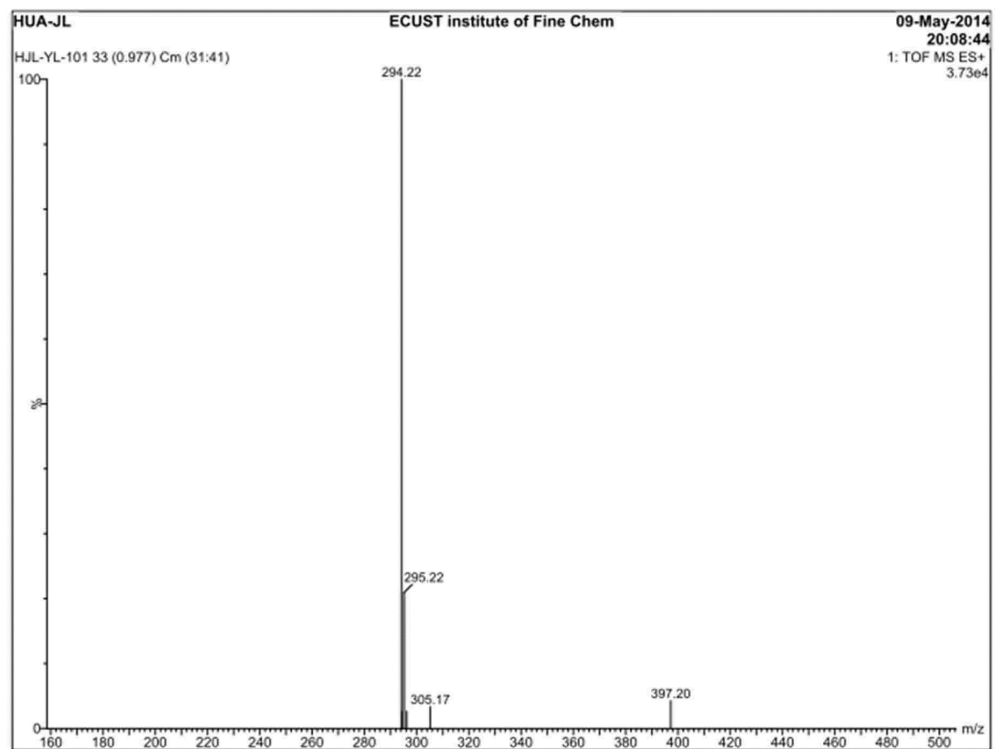


Figure S3. ESI-MS spectrum of compound **2**

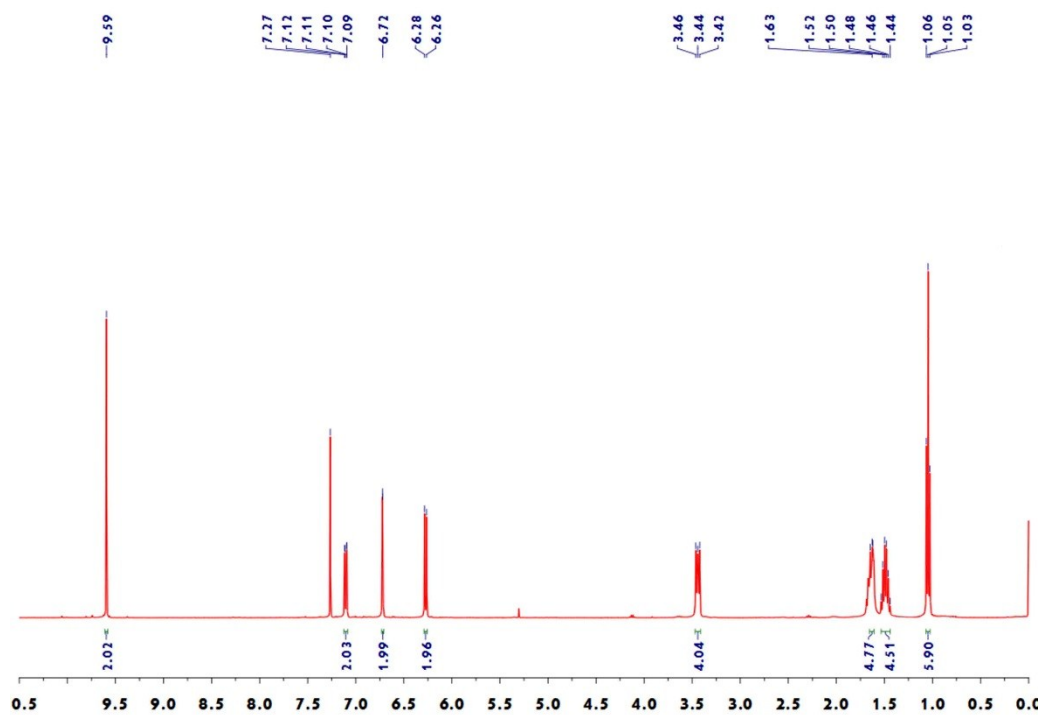


Figure S4. ^1H NMR spectrum of compound **3** in CDCl_3 .

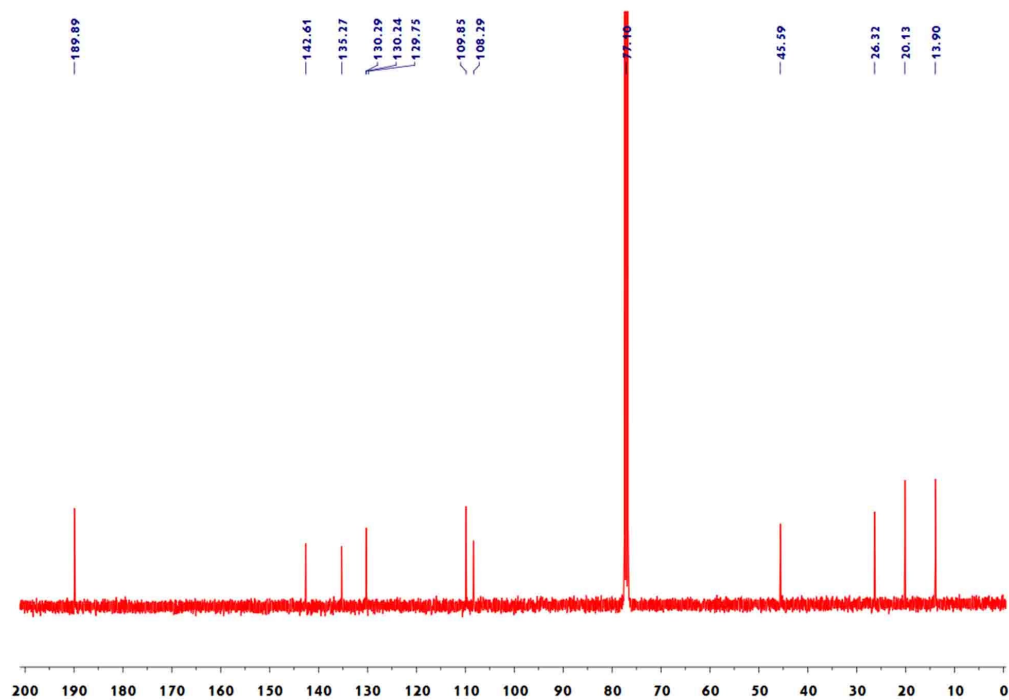


Figure S5. ^{13}C NMR spectrum of compound **3** in CDCl_3 .

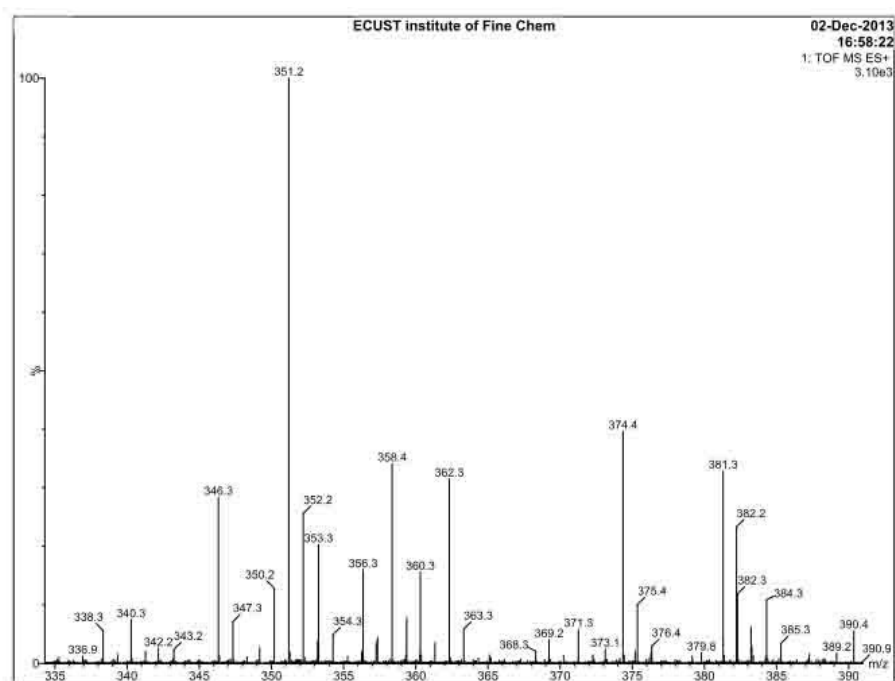


Figure S6. ESI-TOF mass spectrum of **3**

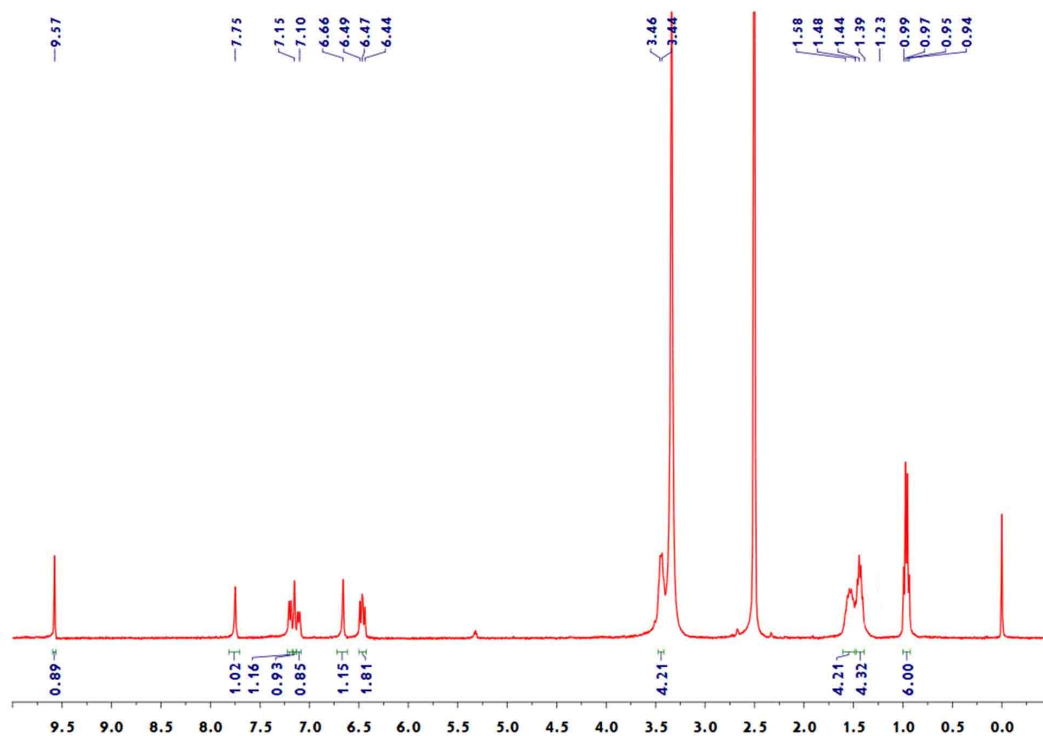


Figure S7. ¹H NMR of compound **4** in DMSO-*d*₆.

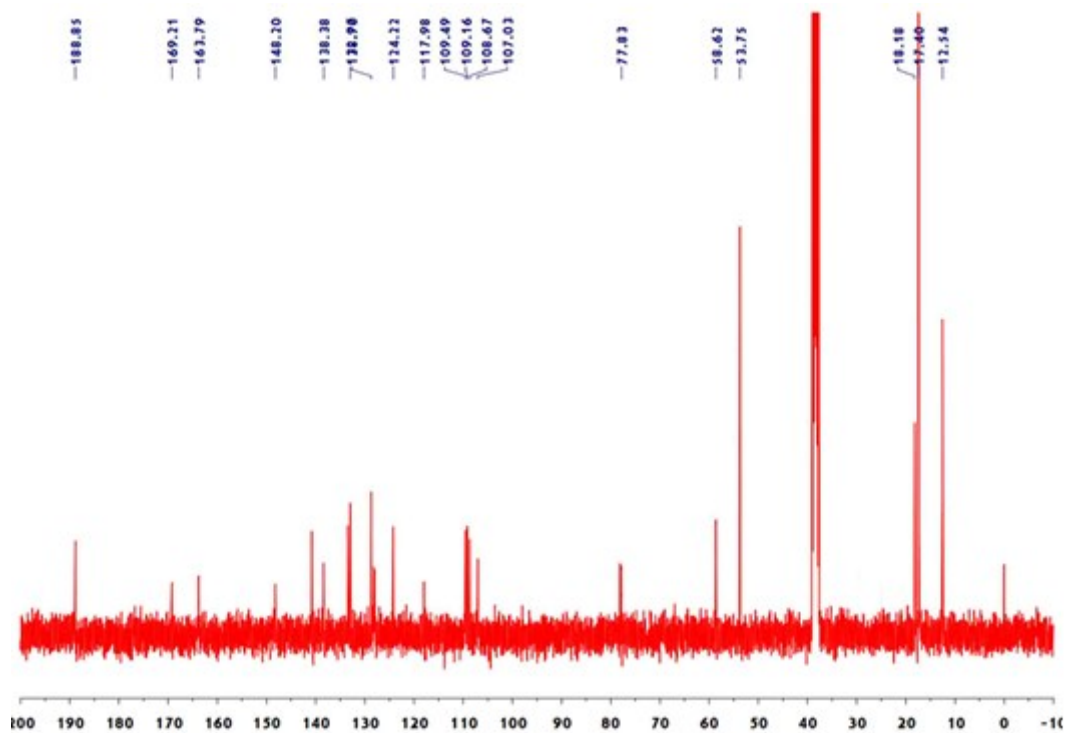


Figure S8. ¹³C NMR of compound **4** in DMSO-*d*₆.

Single Mass Analysis

Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

168 formula(e) evaluated with 11 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-30 H: 0-80 N: 0-5 O: 0-5

HJL-JL

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HJL-YL-220-2 17 (0.640) Cm (17:35)

23-Sep-2013

16:15:53

2: TOF MS ES-

1.33e+004

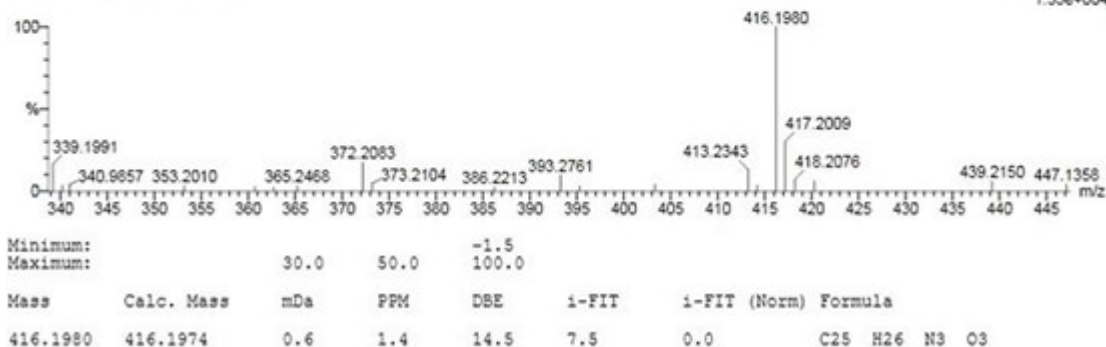


Figure S9. ESI mass spectrum of compound 4

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

PHS-H

2015-8-17 下午 02:01:09

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Date Stamp	24 Jun 2015 08:21:20	Nucleus	1H	File Name	C:\Users\qy\Desktop\print\wil-20150624\wil-20150624\1\data\111r
Frequency (MHz)	400.13	Owner	nmrsu	Number of Transients	16
Original Points Count	32768	SW(cyclical) (Hz)	8223.68	Points Count	32768
Receiver Gain	322.00	Spectrum Type	STANDARD	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.1101	Sweep Width (Hz)	8223.43	Pulse Sequence	zg30
				Temperature (degree C)	26.260

¹H NMR (400 MHz, CHLOROFORM-d) δ ppm 1.05 (q, *J*=7.03 Hz, 6 H) 1.46 - 1.54 (m, 4 H) 1.59 (br. s., 4 H) 1.67 (br. s., 4 H) 3.48 (br. s., 4 H) 6.26 (d, *J*=8.28 Hz, 1 H) 6.35 (d, *J*=8.28 Hz, 1 H) 6.82 (s, 1 H) 7.06 (d, *J*=8.28 Hz, 1 H) 7.18 (d, *J*=7.78 Hz, 1 H) 7.32 (s, 1 H) 7.92 (s, 1 H) 9.63 (s, 1 H)

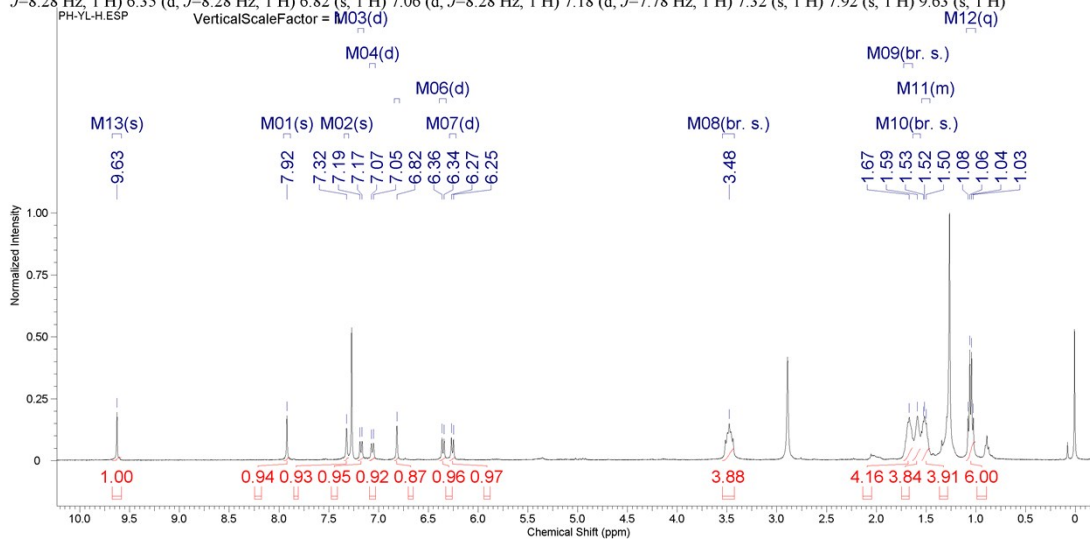
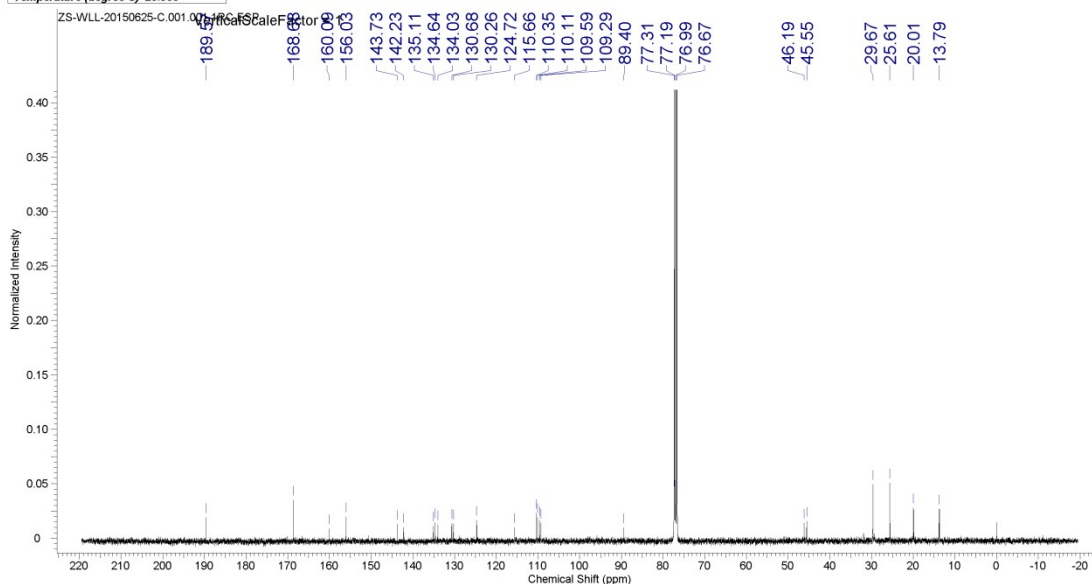


Fig S10. ¹H NMR spectrum of PHS in CDCl₃.

PHS-C

2015-8-17 下午 01:59:30

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Date Stamp	25 Jun 2015 13:22:08	File Name	H:\zs-wll-20150625-cl\1\data\1\1\1	Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	2000	Origin	spect
Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	1150.00
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10060.8047	Original Points Count	32768
Temperature (degree C)	28.960	Spectrum Type	STANDARD	SW(cyclical) (Hz)	24038.46
				Sweep Width (Hz)	24037.73

Fig S11. ^{13}C NMR spectrum of PHS in CDCl_3 .

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 30.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

249 formula(e) evaluated with 18 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-34 H: 0-60 N: 0-4 O: 0-12

JL-HUA

ECUST Institute of Fine Chem

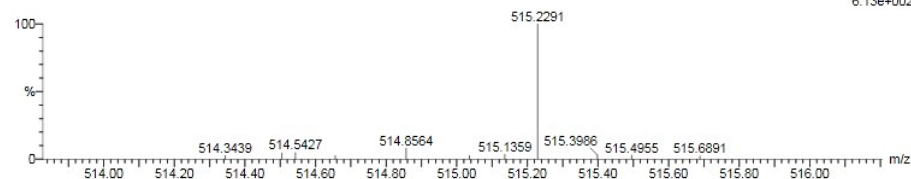
21-Sep-2013

16:41:22

1: TOF MS ES+

6.13e+002

HJL-YL-322 7 (0.298) Cm (5:10)



Minimum:

Maximum:

30.0 50.0 -1.5 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
515.2291	515.2294	-0.3	-0.6	16.5	36.4	0.0	C29 H31 N4 O5

Fig S12. HRMS spectrum of PHS

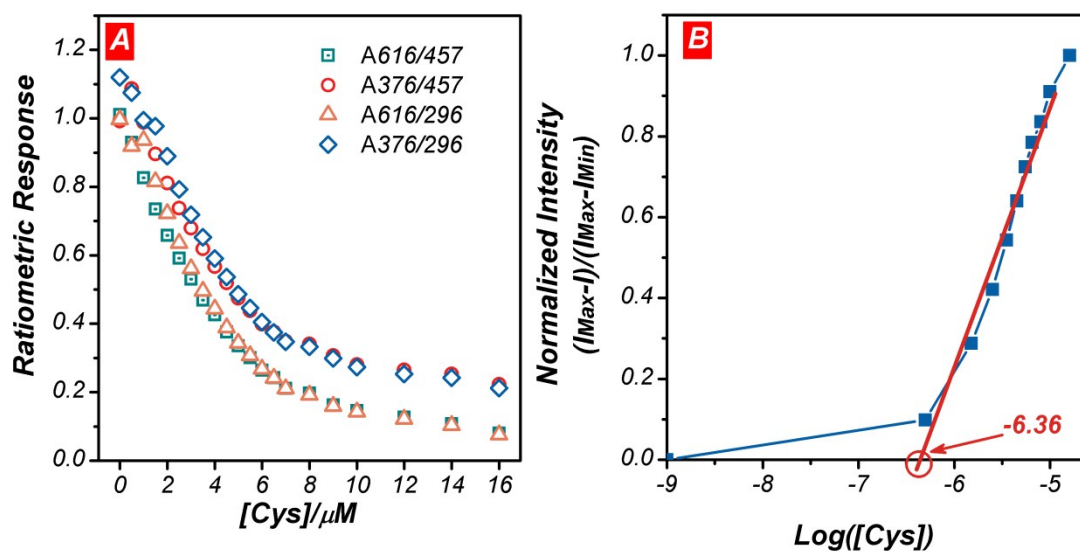


Fig S13. (a) Ratiometric plots of **PHS** with absorbance at 296 nm, 376 nm, 457 nm and 616 nm. (b) Detection limit of **PHS** by UV-vis spectra (Data were collected at 616 nm). The intensity was normalized between the minimum absorbance, found at 16 μM Cys, and the maximum absorbance, found at zero Cys (shown on the graph as 1 nM) .

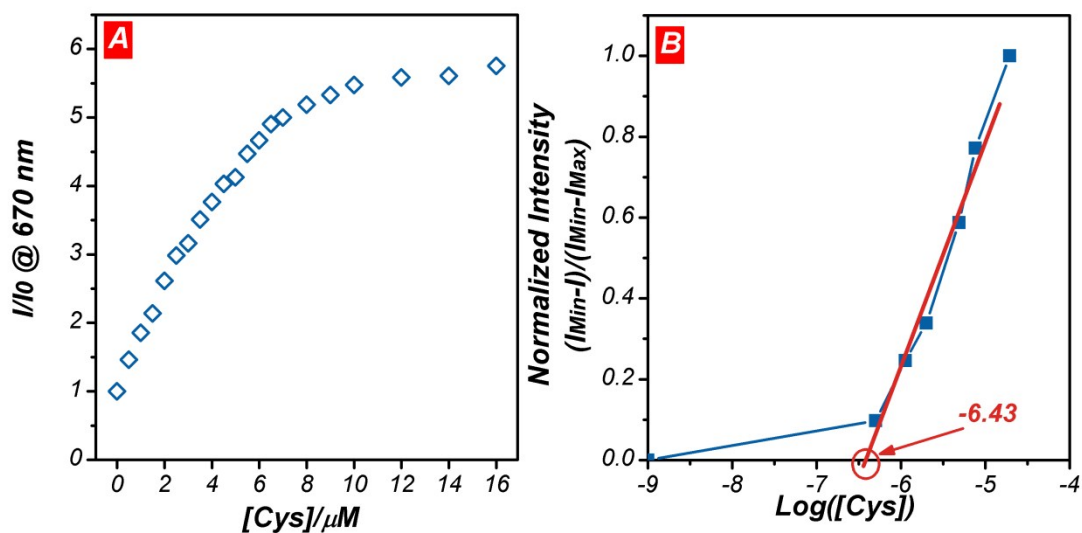


Fig S14. (a) Intensity enhancement plots of **PHS** at 670 nm. (b) Detection limit of **PHS** by emission spectra (Data were collected at 670 nm). The intensity was normalized between the minimum emission intensity, found at zero cys (shown on the graph as 1 nM), and the maximum absorbance, found at 16 μM Cys.

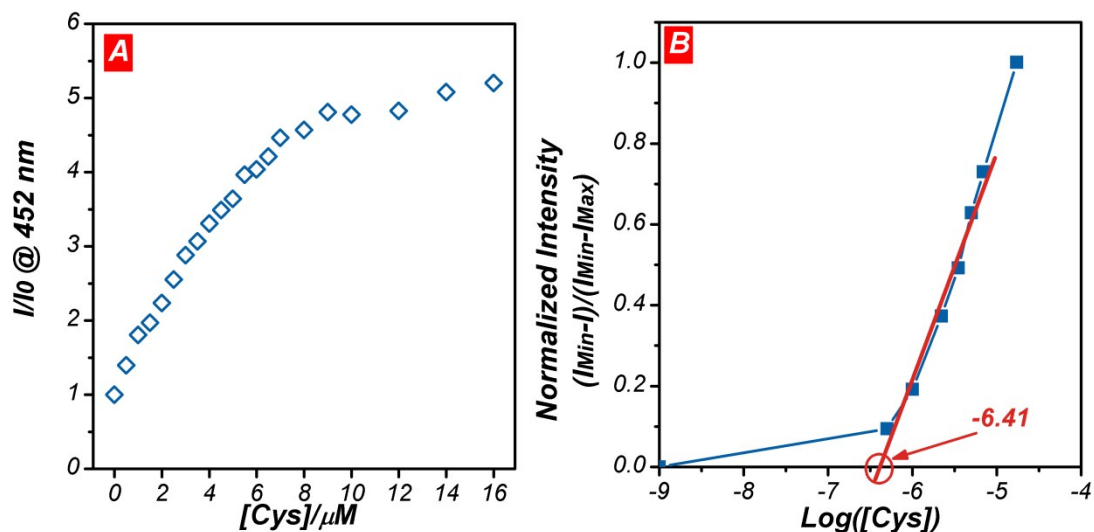


Fig S15. (a) Excitation intensity enhancement plots of **PHS** at 452 nm. (b) Detection limited of **PHS** by emission spectra (Data were collected at 452 nm). The intensity was normalized between the minimum emission intensity, found at zero Cys (shown on the graph as 1 nM), and the maximum absorbance, found at 16 μM Cys.

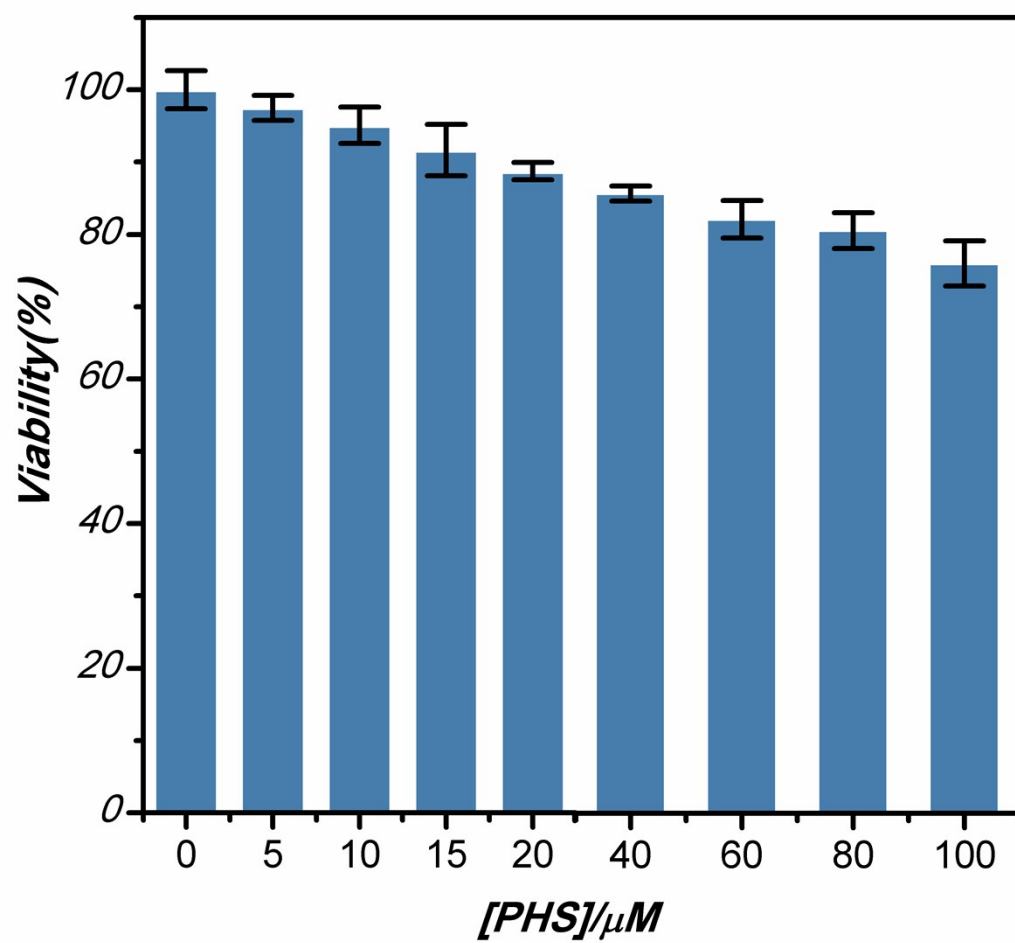


Fig S16.MTT assay of **PHS** with 0~ 100 μM Cys.