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Electronic Supporting Information for ***New Journal of Chemistry***:

ESIPT-based fluorescent probe for cysteine sensing with large Stokes shift over homocysteine and glutathione and its application in living cells

Peng Zhang[a], Yuzhe Xiao[a], Qian Zhang[a], Zixuan Zhang[a], Hongwei Yu[b] and Caifeng Ding[a]*

[a]*Key Laboratory of Sensor Analysis of Tumor Marker, Ministry of Education; Shandong Key Laboratory of Biochemical Analysis; Key Laboratory of Analytical Chemistry for Life Science in Universities of Shandong; College of Chemistry and Molecular Engineering. Qingdao University of Science and Technology, Qingdao 266042, PR China.*

[b]*Qingdao Municipal Center for Disease Control & Prevention, Qingdao 266033, PR China.*

*E-mail: *dingcaifeng2003@163.com*,

Contents

1. ^{1}H, ^{13}C NMR and HRMS spectra

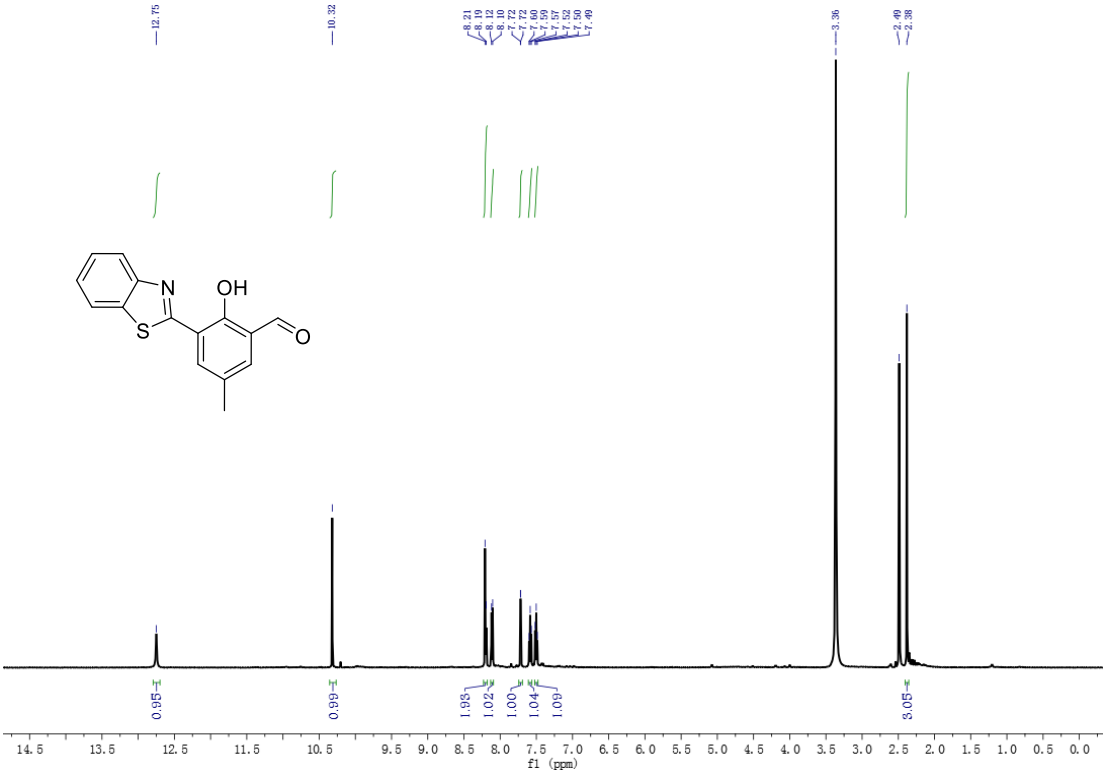


Figure S1. ^{1}H NMR spectrum (500 MHz) of HBTA in DMSO-d_6.

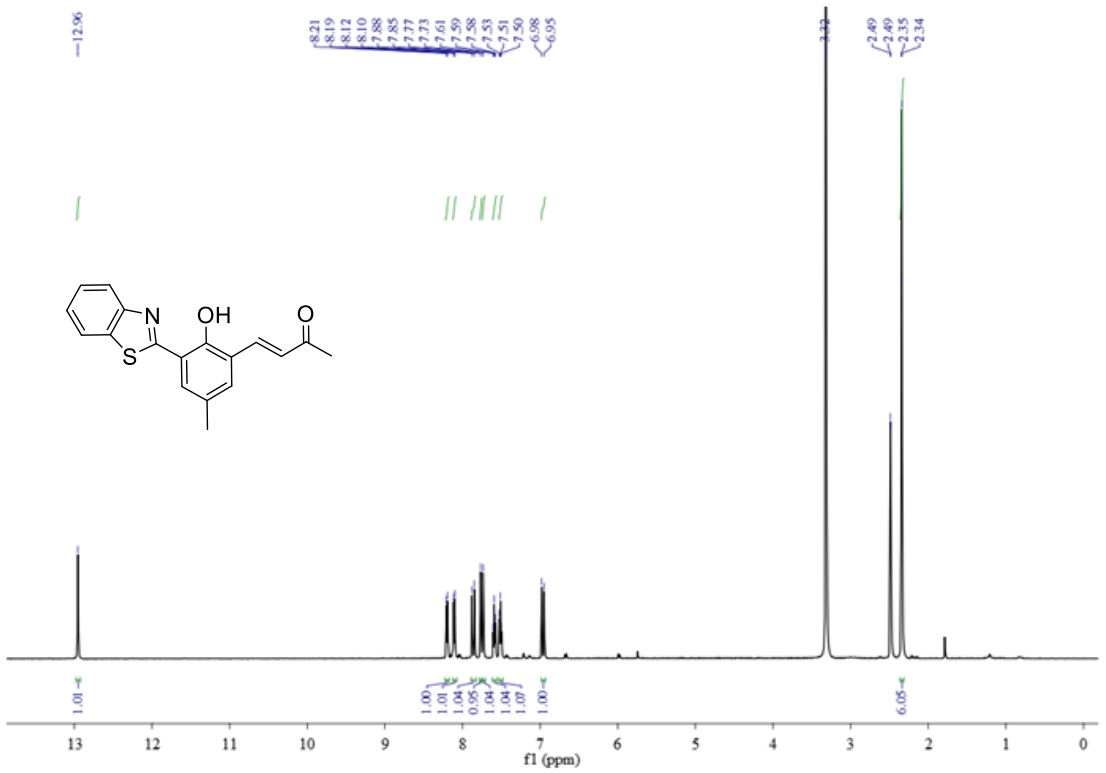


Figure S2. ^{1}H NMR spectrum (500 MHz) of HBTA-MVK in DMSO-d_6.

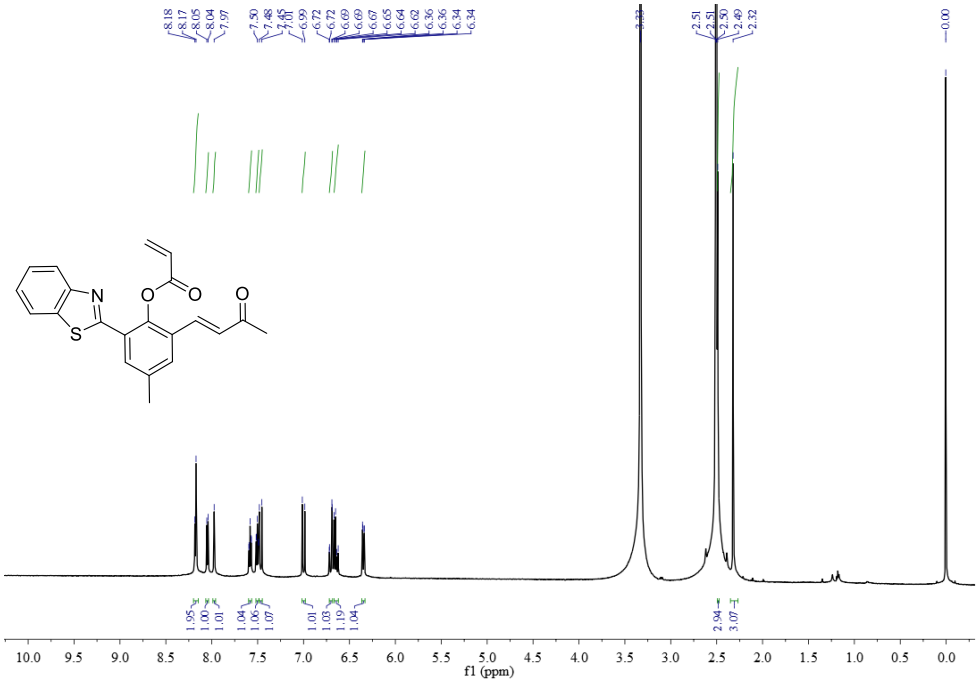


Figure S3. ^{1}H NMR spectrum (600 MHz) of ABT-MVK in DMSO-d_6.

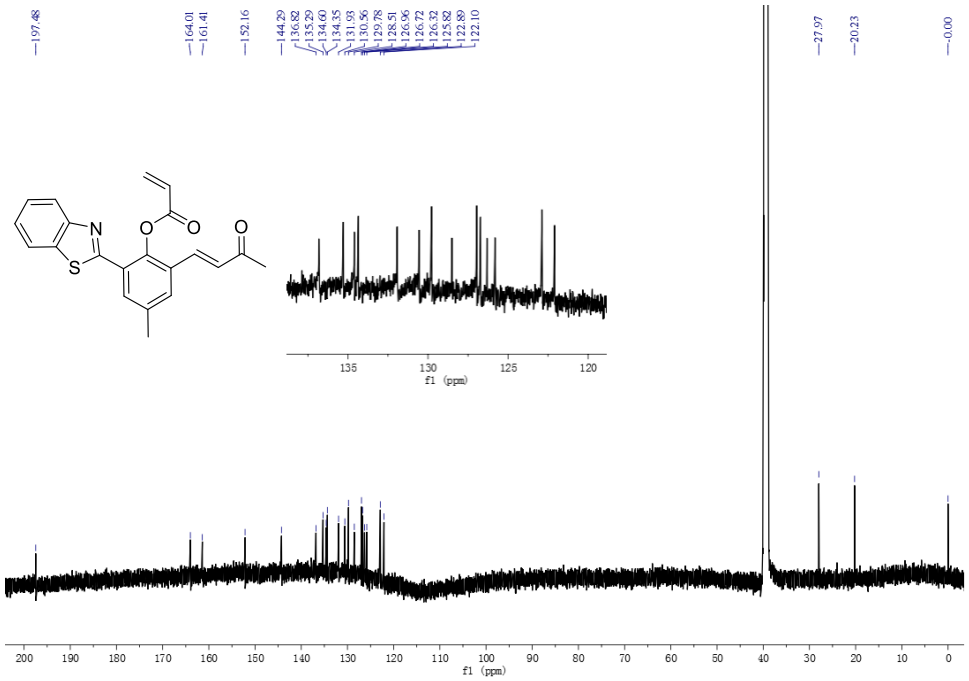
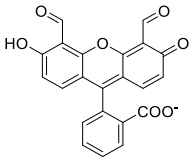
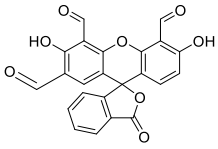
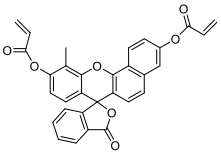
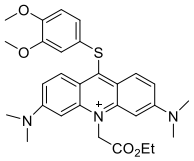
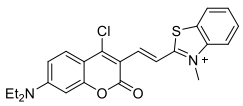
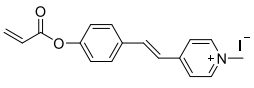
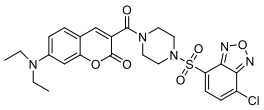
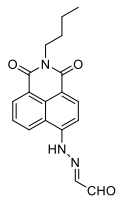
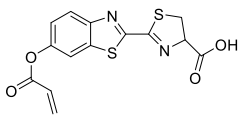
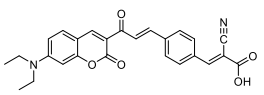
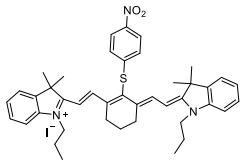
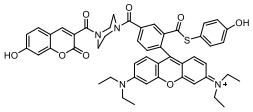
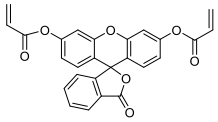
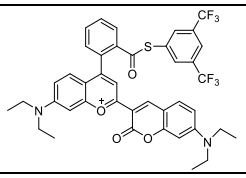
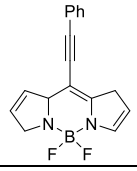
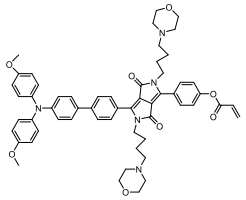
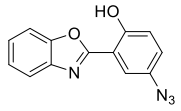
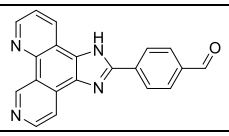
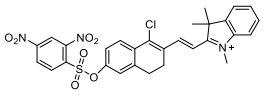
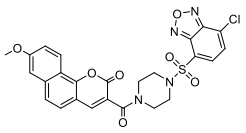
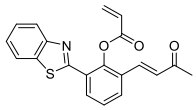


Figure S4. ^{13}C NMR spectrum (151 MHz) of ABT-MVK in DMSO-d_6.

Table S1. Fluorescent probes for the detection of biothiols.

Probe	Analyte	Stokes shift	LOD	Spectral change	Biological application	Ref.
	Cys; Hcy	60		Off-on	Human plasma	[1]
	Hcy	32	1.88 μM	Off-on	Human plasma	[2]
	Cys	71		Off-on		[3]
	Cys; GSH	80 30	0.11 μM 5.0 nM	Off-on	HeLa Cells	[4]
	Cys; GSH	60 70	0.4 mM 0.05 μM	Off-on	COS-7 cells	[5]
	Cys	168		Ratio	HeLa Tissue slices	[6]
	Cys	130	1.4 μM	Ratio	HeLa，Zebrafish	[7]
	Cys; Hcy	85		Off-on	Tetrahymena thermophila cells	[8]
	Cys	*ca.* 210	88.0 nM	Off-on	MDA-MB-231 cells, mice	[9]
	Cys	55	122 nM	Ratio	A549/ Hela cells	[10]

	Cys	*ca.* 100	1.26 μM	Off-on	HeLa cells	[11]
	Cys; Hcy	75		Ratio	HepG2 cells	[12]
	Cys	*ca.* 42		Off-on	PC-12 cells	[13]
	Cys; Hcy	51	16 μM 18 μM	Ratio	HepG2 cells	[14]
	Cys	25	0.38 nM	Off-on	HeLa cells	[15]
	Cys	*ca.* 45	84 nM	Ratio	Hela cells	[16]
	Cys; GSH	*ca.* 160	90 nM	Off-on	Hela cells	[17]
	Cys; Hcy	*ca.* 140		Ratio	Hela cells	[18]
	Cys	40	0.19 μM	Off-on	HeLa cells	[19]
	Cys	200		Ratio	HeLa cells	[20]
	Cys	225	19 nM	Off-on	HeLa cells	this work

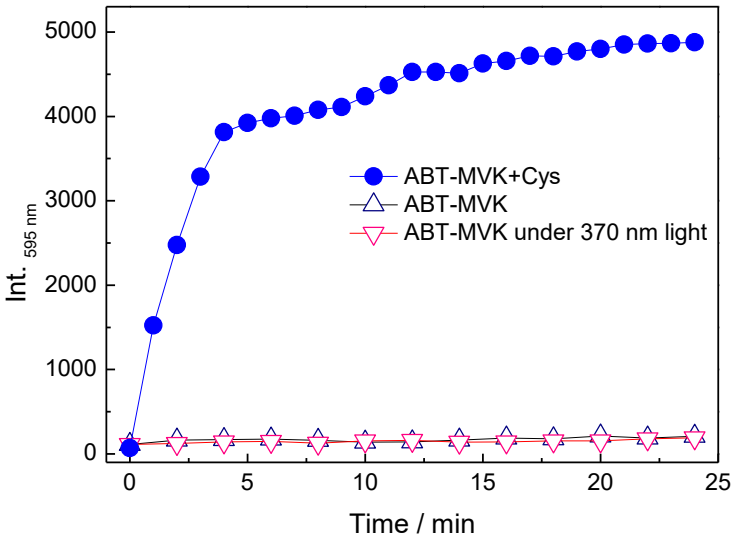


Figure S5. The stability of ABT-MVK (10 μM) in PBS buffer with (black triangles) or without (red triangles) 370 nm light irritation.

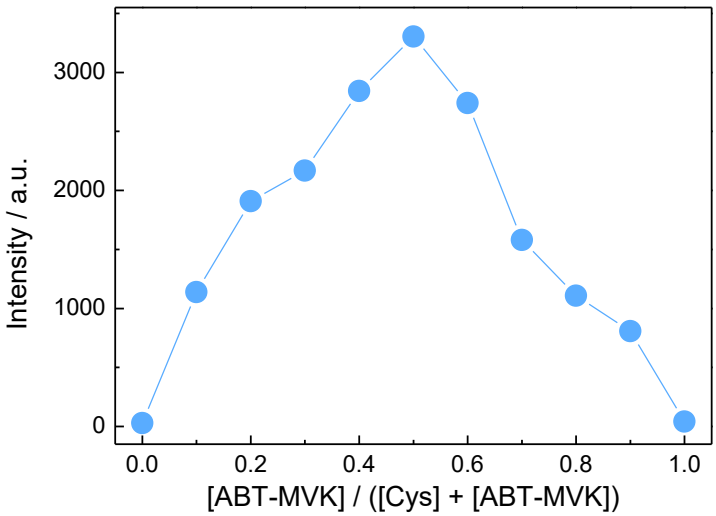


Figure S6. Job plot of Cys binding to ABT-MVK in 10 mM PBS buffer, measured by fluorescence spectra.

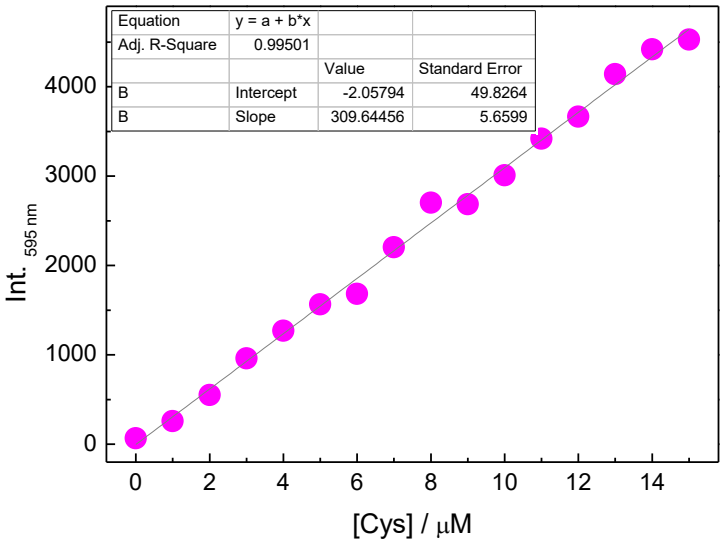


Figure S7. The limit of detection for Cys by fluorescence of ABT-MVK at 10 μM. The limit of detection was calculated to be 19 nM.

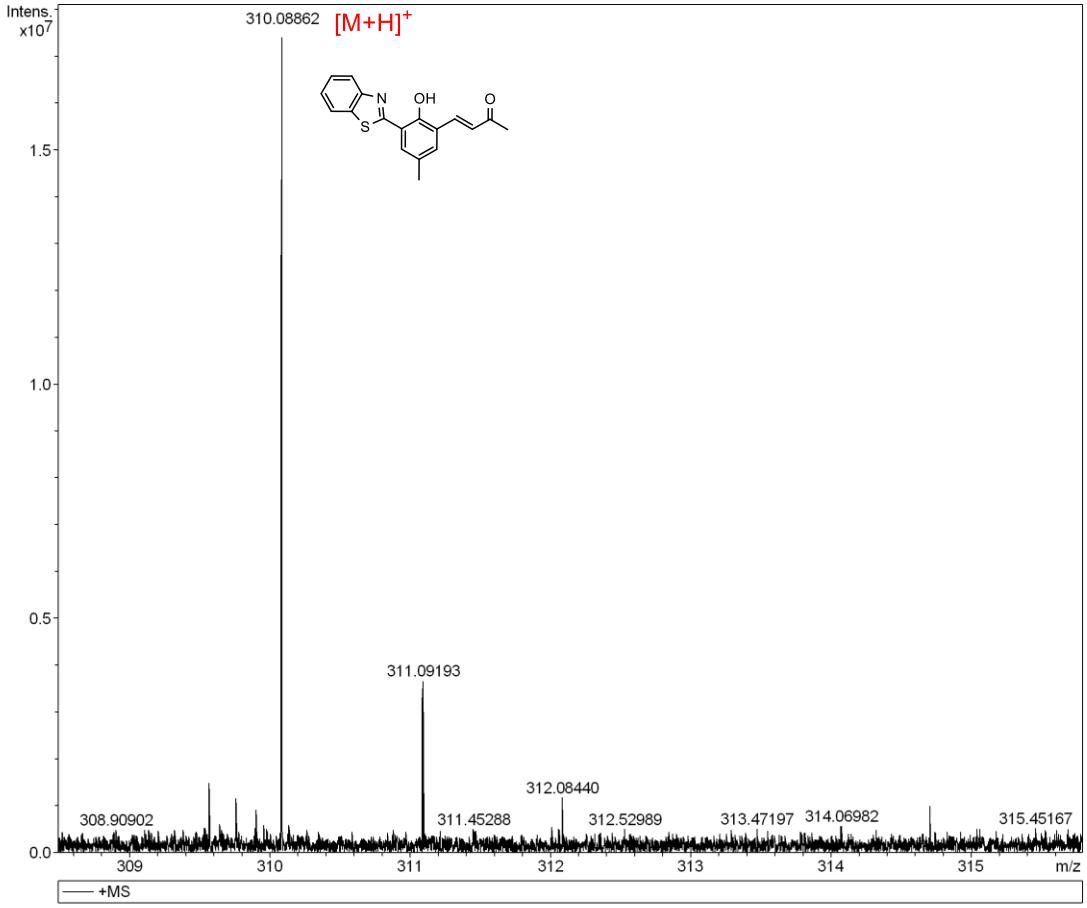


Figure S8. HRMS spectra of ABT-MVK before (a) and after (b) treated with Cys in 10 mM PBS buffer. [ABT-MVK] = [Cys] = 10 μM.

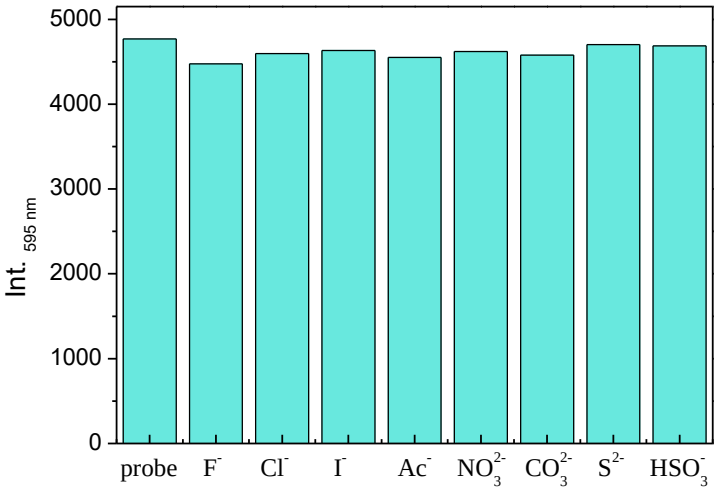


Figure S9. Fluorescence intensity of ABT-MVK at 595 nm in 10 mM PBS buffer pH 8.0 in the presence of 20 μM Cys upon addition of 50 μM of competition anions, such as F^-, Cl^-, I^-, Ac^-, NO_3^-, CO_3^{2-}, S^{2-}, and HSO_3^-. [ABT-MVK] = 10 μM, λ_{ex} = 370 nm.

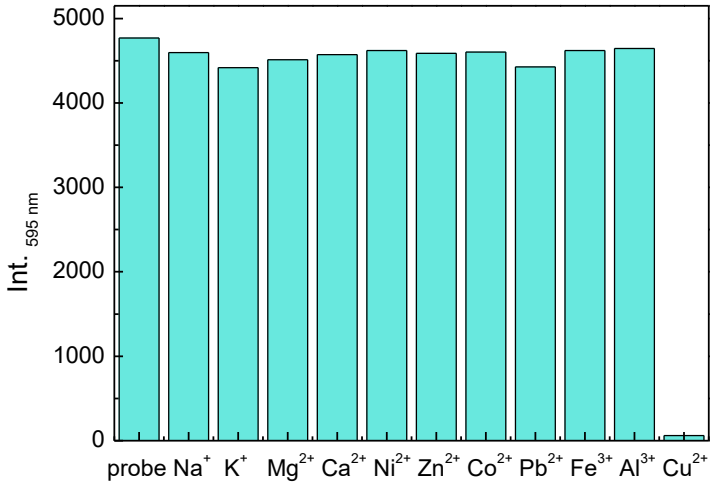


Figure S10. Fluorescence intensity of ABT-MVK at 595 nm in 10 mM PBS buffer pH 8.0 in the presence of 20 μM Cys upon addition of 50 μM of competition cations, such as Na^+, K^+, Mg^{2+}, Ca^{2+}, Ni^{2+}, Zn^{2+}, Co^{2+}, Pb^{2+}, Fe^{3+}, Al^{3+} and Cu^{2+}. [ABT-MVK] = 10 μM, λ_{ex} = 370 nm.

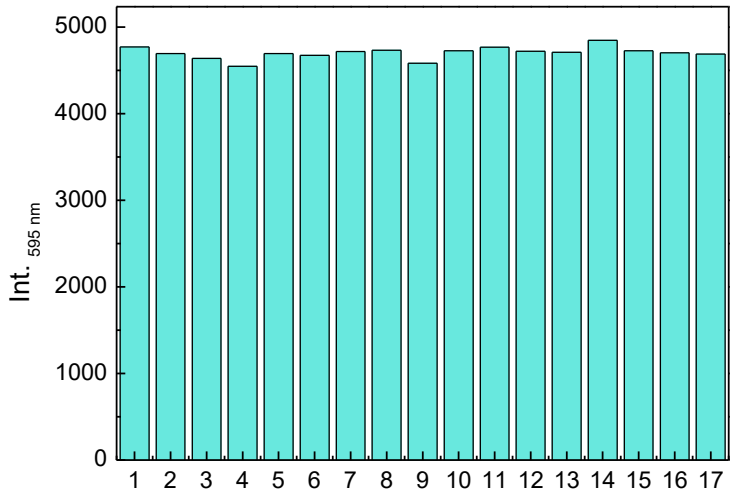


Figure S11. Fluorescence intensity of ABT-MVK at 595 nm in 10 mM PBS buffer pH 8.0 in the presence of 20 μM Cys upon addition of 50 μM competition amino acids, 1-17: Free, Ala, Asp, Gln, Glu, Gly, His, Ile, Leu, Lys, Met, Pro, Ser, Thr, Val, Hcy and GSH. [ABT-MVK] = 10 μM, λ_{ex} = 370 nm.

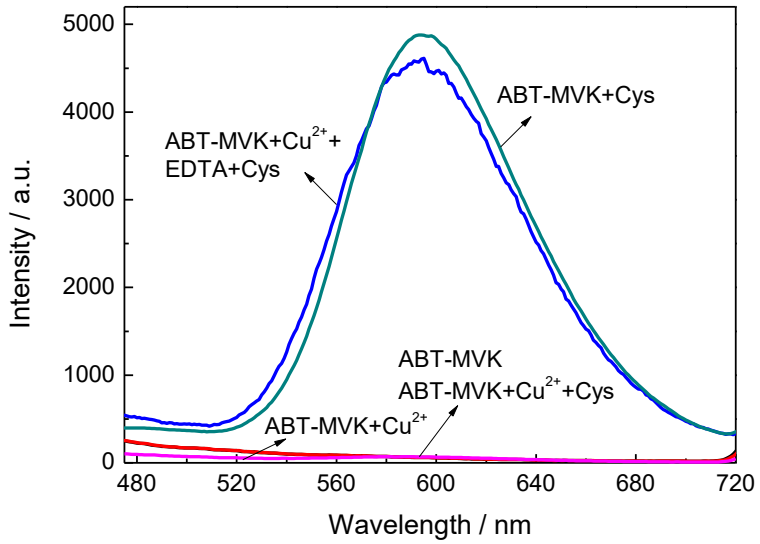


Figure S12. Fluorescence spectra of ABT-MVK, ABT-MVK+Cys, ABT-MVK+Cu^{2+}, ABT-MVK+Cu^{2+}+Cys and ABT-MVK+Cu^{2+}+EDTA+Cys in 10 mM PBS buffer. [ABT-MVK] = 10 μM, λ_{ex} = 370 nm.

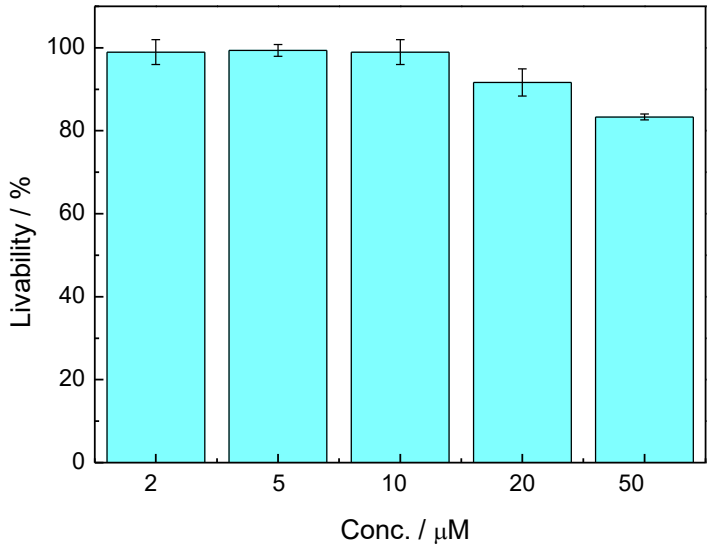


Figure S13. Cytotoxicity of ABT-MVK against HeLa cells as determined by CCK-8 assay: HeLa cells were treated with ABT-MVK (2-50 μM) for 2 hours.

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