Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Simple colorimetric and fluorescent probe with high selectivity towards cysteine over homocysteine and glutathione

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Characterization of AQDA

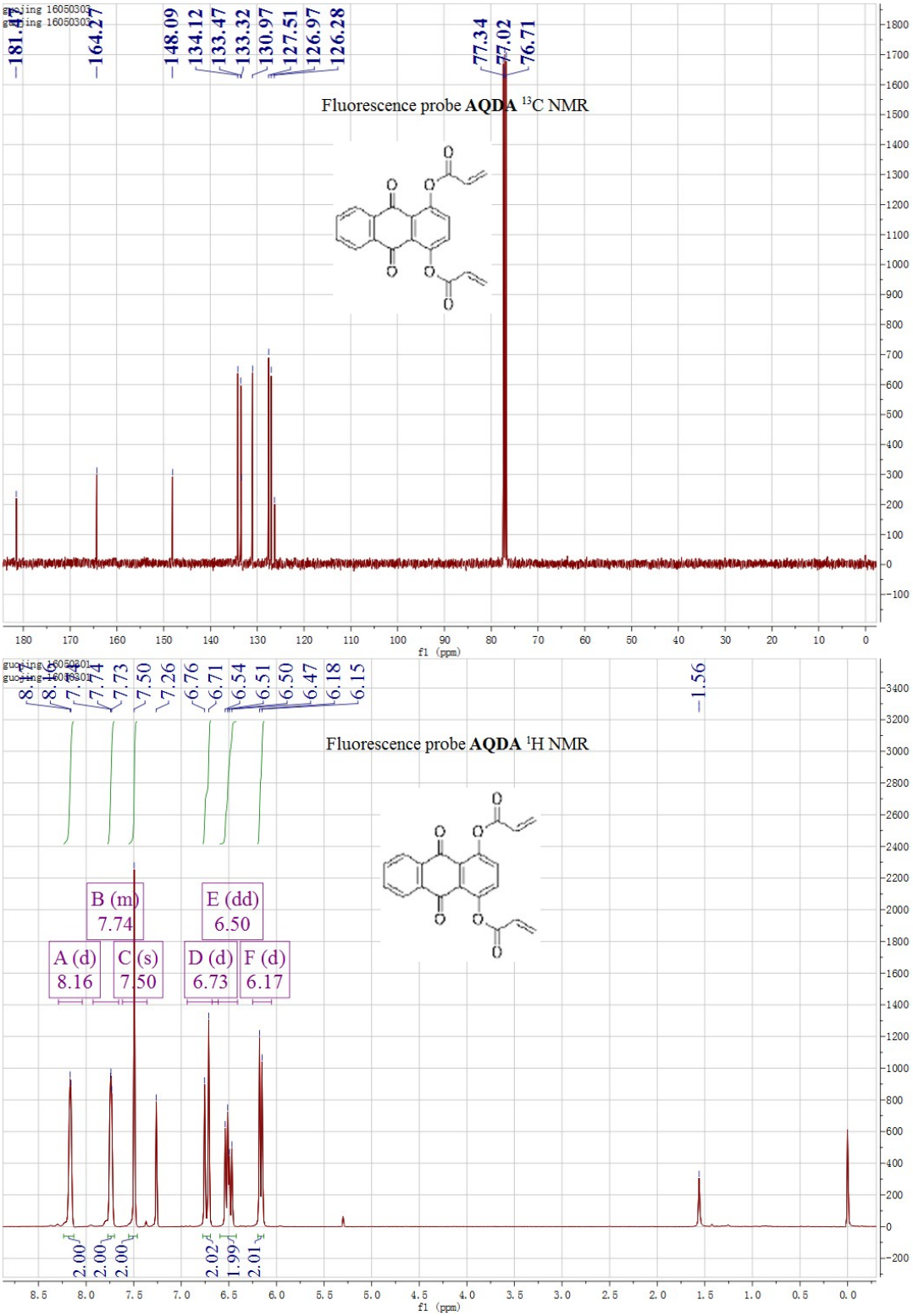

Figure S1 ^{1}H NMR spectrum of probe AQDA in $CDCl_3$; (above) ^{13}C NMR spectrum of the probe in $CDCl_3$. (bottom)

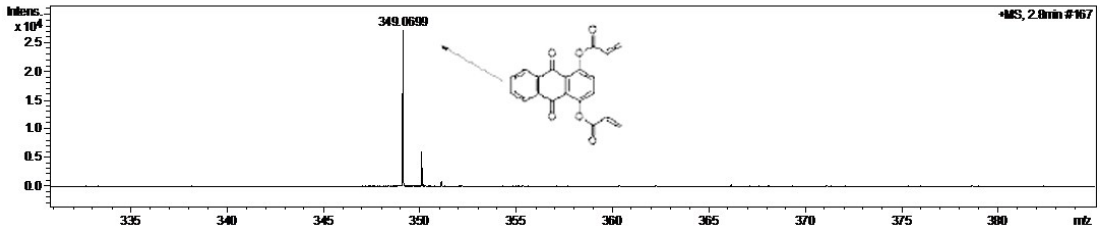

Figure S2 High-resolution mass spectra of the AQDA

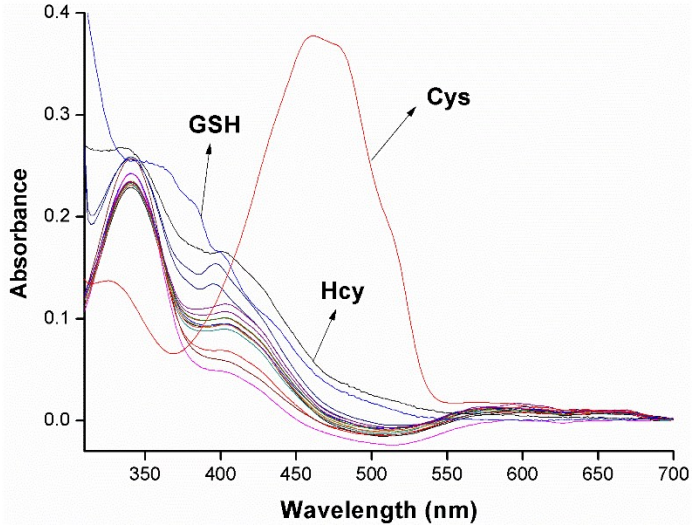

Figure S3 Absorption spectra of AQDA (50 μM) in the presence of Cys (5 equiv.), and other amino acids (50 equiv.). (including His, Ala, Asn, Asp, Gln, Arg, Glu, Met, Phe, Trp, Tyr, Lys, Ser, Hcy, GSH).

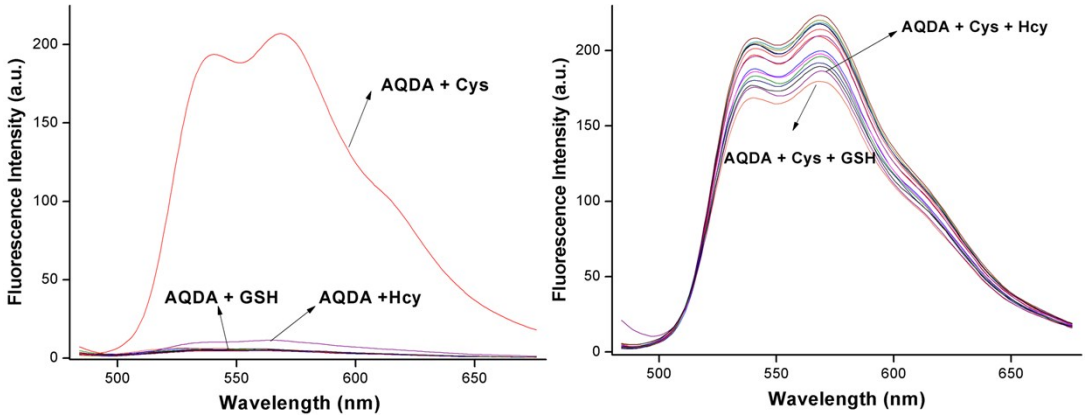

Figure S4 (left) Fluorescence spectra of AQDA (10 μM) in the presence of Cys (5 equiv.), Hcy (50 equiv.), GSH (500 equiv.) and other amino acids (50 equiv.). (including His, Ala, Asn, Asp, Gln, Arg, Glu, Met, Phe, Trp, Tyr, Lys and Ser) (right) Fluorescence spectra of the sensor (10 μM) towards Cys (5 equiv.) in addition of other amino acids (50 equiv.) (His, Ala, Asn, Asp, Gln, Arg, Glu, Met, Phe, Trp, Tyr, Lys, Ser, Hcy and GSH)

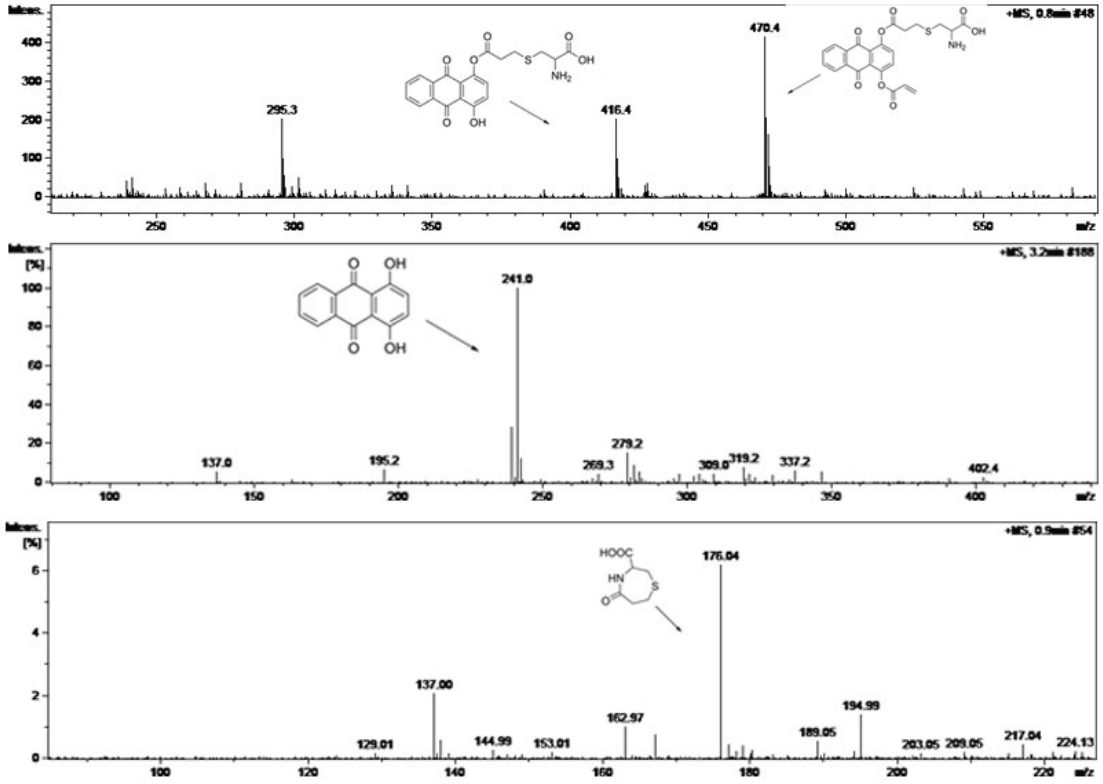

Figure S5 Mass spectra of the conjugate addition adducts, hydrolyzation intermediates of AQDA with the addition of Cys (above). Mass spectra of the end product of AQDA treated with Cys (middle). Mass spectra of the lactam ring (bottom).

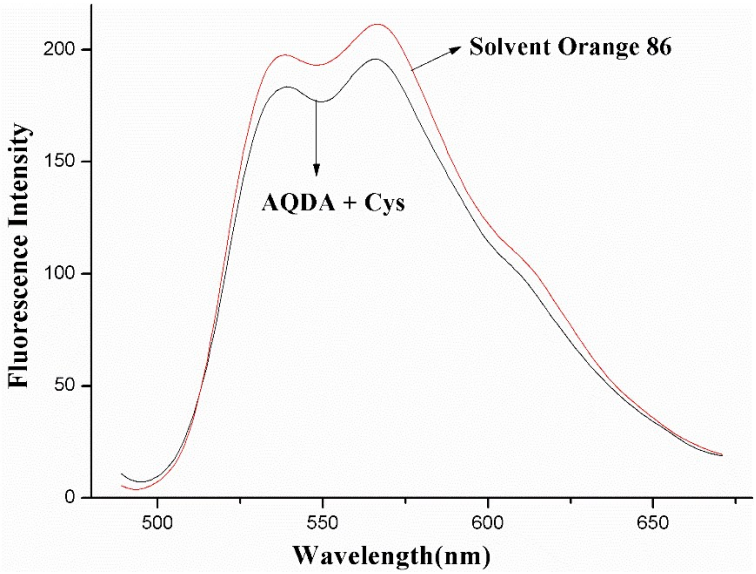

Figure S6 Fluorescence spectra of AQDA (1×10^{-5} M) with Cys (5 equiv.) and compound **3** (1×10^{-5} M) in HEPES buffer solution (ACN/HEPES = 2:8, pH 7.4, λ_{ex} = 470 nm, slit: 5.0 nm/5.0 nm).

Table 1: Summary of fluorescent probes for Cys

Probe	$\lambda_{ex}/\lambda_{em}$	LOD	Ref.
-	420/492	0.9 μM	[16c]
-	440/525	7.62 μM	[16d]
NQ	370/536	0.5 μM	[18c]
ACA	420/456	0.657 μM	[18e]
CAA	380/490	0.192 μM	[20]
AQDA	470/565	0.16 μM	this work

Table 2: Electron transition configurations, excitation energies, and oscillator strengths (f) for main band of **Compound 5** and **AQDA**

	State	Marjor contrib.[a]	Energy	f	Exp
	$S_0 \rightarrow S_1$	H→L (99.3%)	485/2.55	0.3170	470
Compound 3	$S_0 \rightarrow S_2$	H-2→L (97.2%)	341/3.63	0.0938	370
	$S_1 \rightarrow S_0$	L→H (100%)	572/2.17	0.3140	565
	$S_0 \rightarrow S_1$	H→L (66.2%)	422/2.94	0.0030	410
AQDA	$S_0 \rightarrow S_2$	H-1→L (33.7%)	354/3.50	0.2488	340
	$S_1 \rightarrow S_0$	L→H (96.2%)	479/2.59	0.0004	-

[a] 'H' means HOMO and 'L' means LUMO