Comparison of reactive sites in 2(1*H*)-quinolone derivatives for the detection of biologically important sulfur compounds

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Supplementary Information

Contents

6. **Fig. S9** Fluorescence intensity of **Q4** (20 μM) at different pH values in the absence/presence of HSO_3^- (1 mM)
7. **Fig. S10** ^{1}H-NMR spectra of **Q3** in the presence of excess ME (2-mercaptoethanol) in dimethyl sulphoxide-d_6
8. **Fig. S11** ESI mass spectrum of **Q3** (10 μM) with 2-mercaptoethanol (1000 μM)
9. **Fig. S12** Fluorescence intensity of **Q1** (10 μM), **Q2** (6 μM), **Q3** (10 μM) in 0.1 M phosphate buffer with CH_3CN (20%, v/v, pH=7.4) in the presence of biothiols (1 mM), NEM (1 mM)

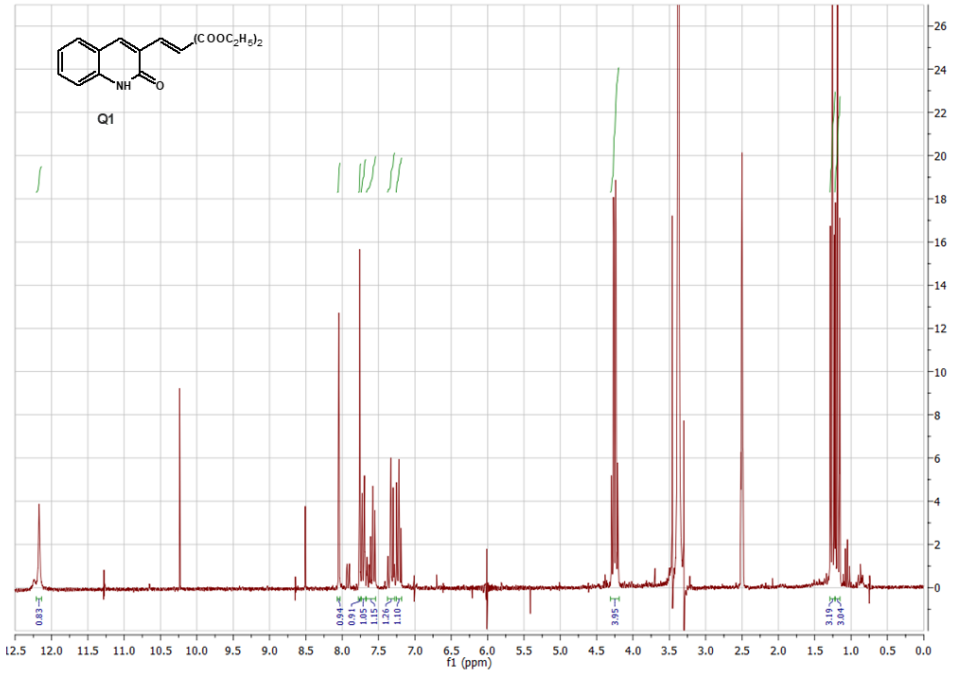


Figure S1 ^{1}H NMR spectrum of **Q1** in DMSO-d_6

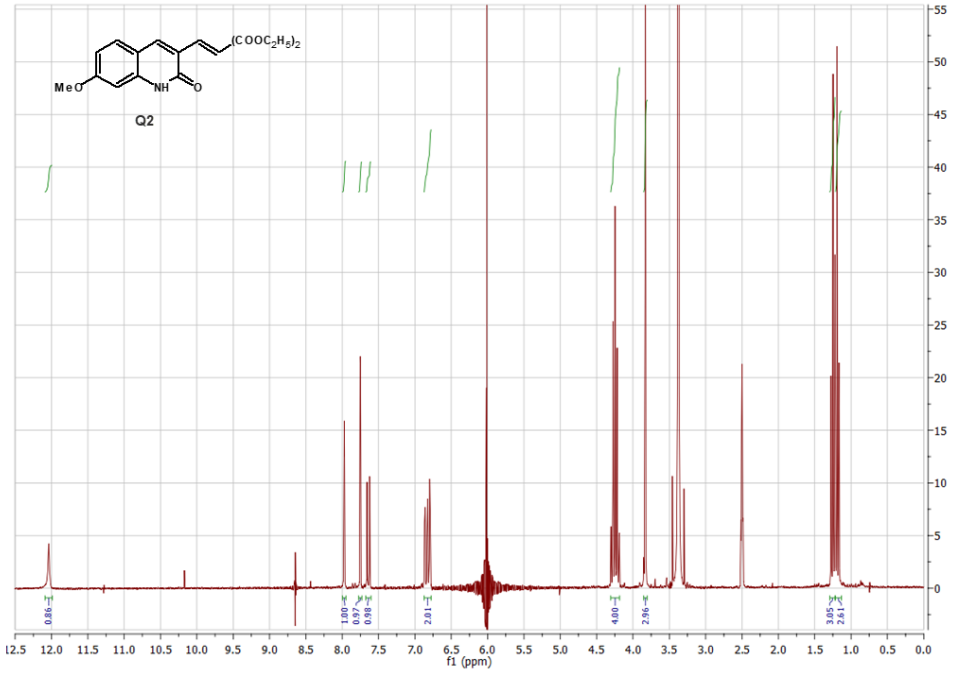


Figure S2 ^{1}H NMR spectrum of **Q2** in DMSO-d_6

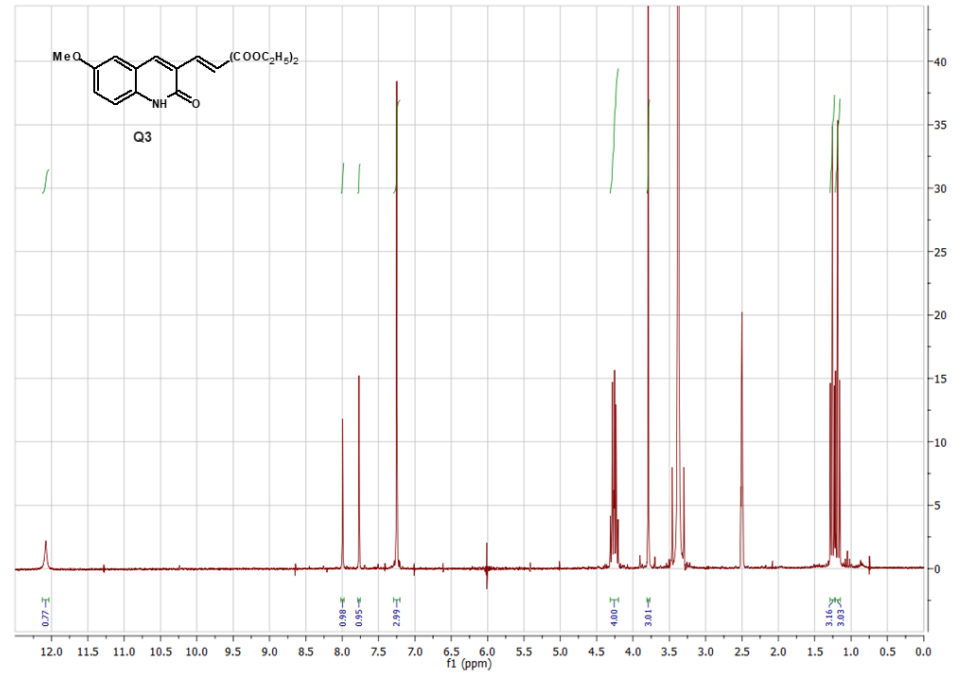
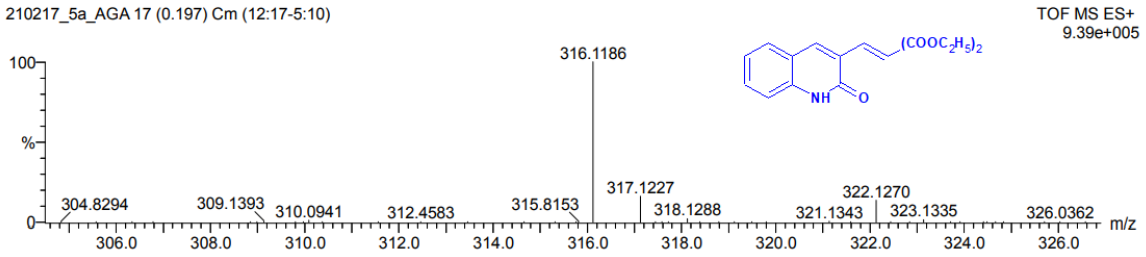


Figure S3 ^{1}H NMR spectrum of **Q3** in DMSO-d_6

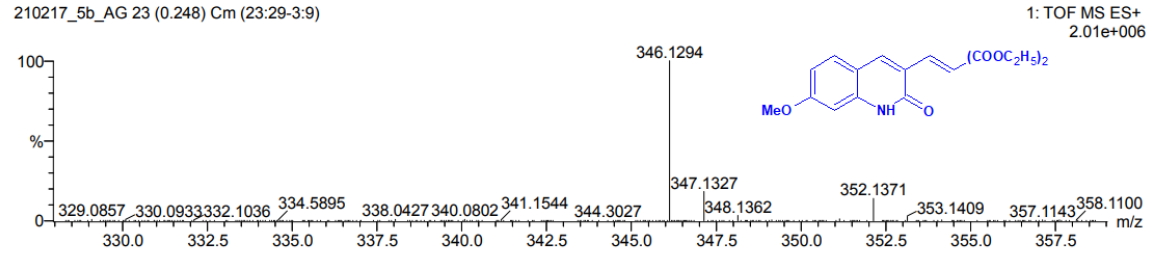
Monoisotopic Mass, Even Electron Ions
58 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-35 H: 0-60 N: 0-1 O: 0-6
210217_5a_AGA 17 (0.197) Cm (12:17-5:10)



Minimum:				-1.5				
Maximum:		5.0	5.0	80.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
316.1186	316.1185	0.1	0.3	9.5	193.7	n/a	n/a	C17 H18 N O5

Figure S4 HRMS spectrum of **Q1**

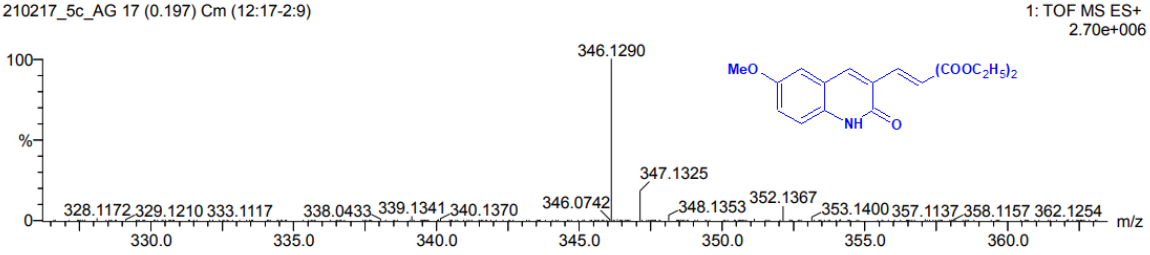
Monoisotopic Mass, Even Electron Ions
121 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-35 H: 0-60 N: 0-1 O: 0-6 Na: 0-1
210217_5b_AG 23 (0.248) Cm (23:29-3:9)



Minimum:				-1.5				
Maximum:		5.0	5.0	80.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
346.1294	346.1291	0.3	0.9	9.5	952.6	n/a	n/a	C18 H20 N O6

Figure S5 HRMS spectrum of **Q2**

Monoisotopic Mass, Even Electron Ions
121 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-35 H: 0-60 N: 0-1 O: 0-6 Na: 0-1
210217_5c_AG 17 (0.197) Cm (12:17-2:9)



Minimum:				-1.5				
Maximum:		5.0	5.0	80.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
346.1290	346.1291	-0.1	-0.3	9.5	735.1	n/a	n/a	C18 H20 N O6

Figure S6 HRMS spectrum of **Q3**

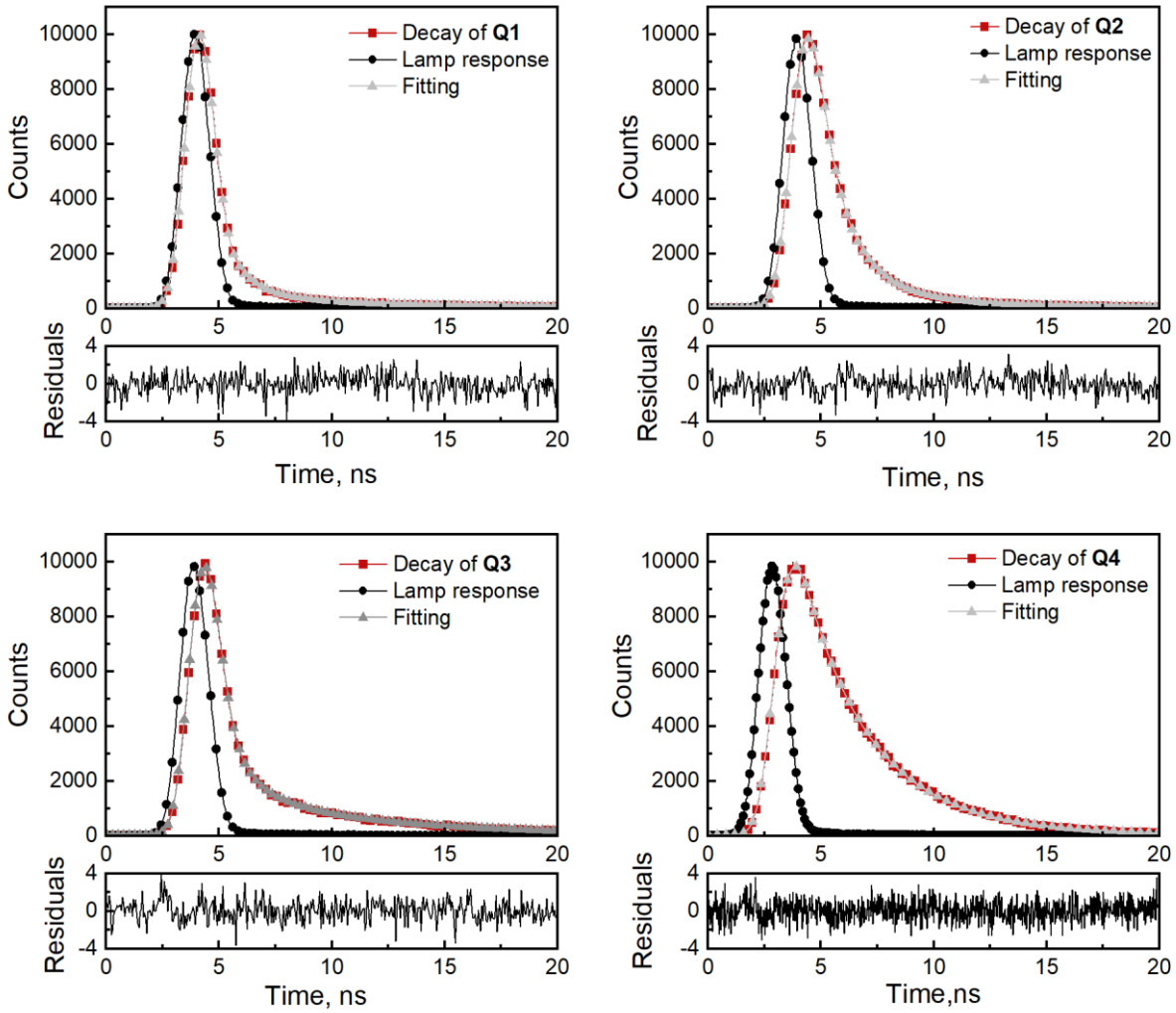


Figure S7 The fluorescence decay profiles of the compounds **Q1**-**Q4** in acetonitrile with excitation at 376.2 nm. Lamp response was determined using Ludox. The fitting of the decay profiles to a three-exponential function. Residuals are shown versus time

Table S1 The fluorescence lifetimes, quantum yields, and rate constant for radiative and non-radiative decay in acetonitrile

	Φ_{em} (–)	τ (ns)	k_r ($10^9 s^{-1}$)	k_{nr} ($10^9 s^{-1}$)	k_r/ k_{nr}
Q1	0.0020	1.25	0.0016	0.7984	0.0020
Q2	0.0019	1.86	0.0010	0.5366	0.0019

Q3	0.0242	3.09	0.0078	0.3157	0.0248
Q4	0.0930	3.12	0.0298	0.2907	0.1025

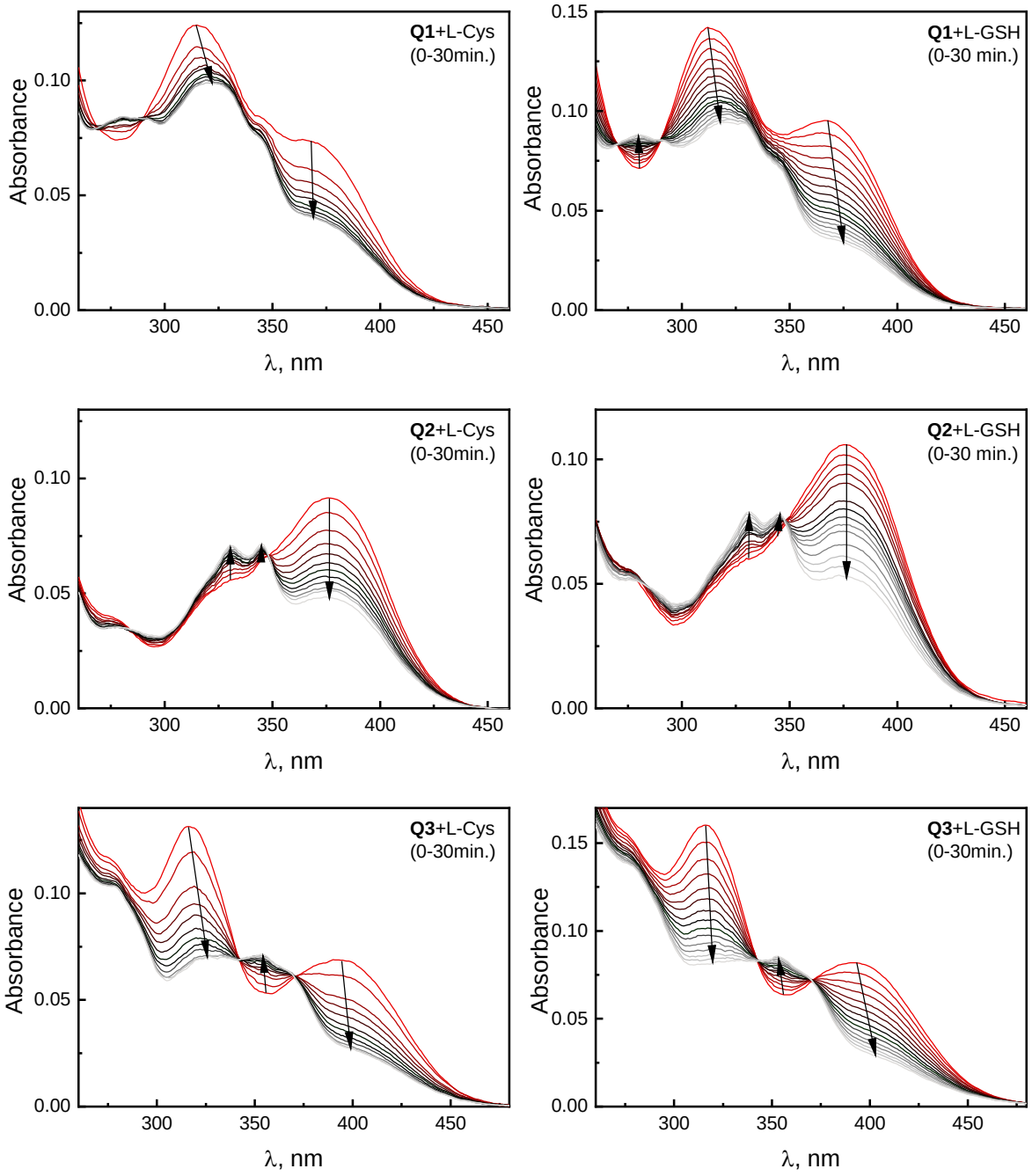


Figure S8 Changes in the absorption spectra of **Q1** (10 μM), **Q2** (6 μM), **Q3** (10 μM)

over time toward L-Cys and L-GSH (100 μM) in 0.1 M phosphate buffer with CH_3CN (20%, v/v, pH=7.4)

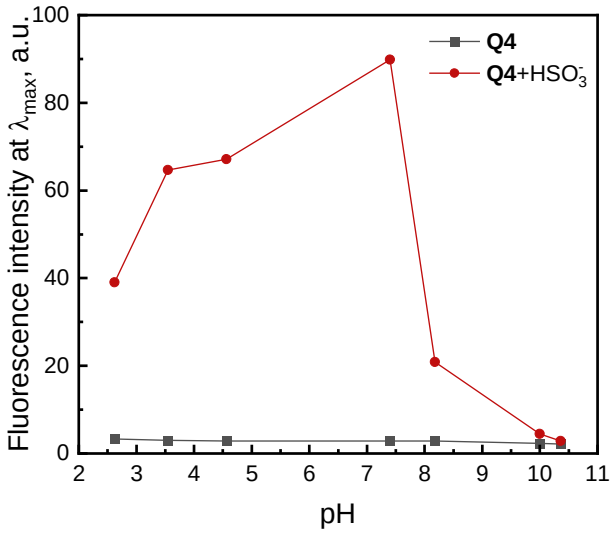
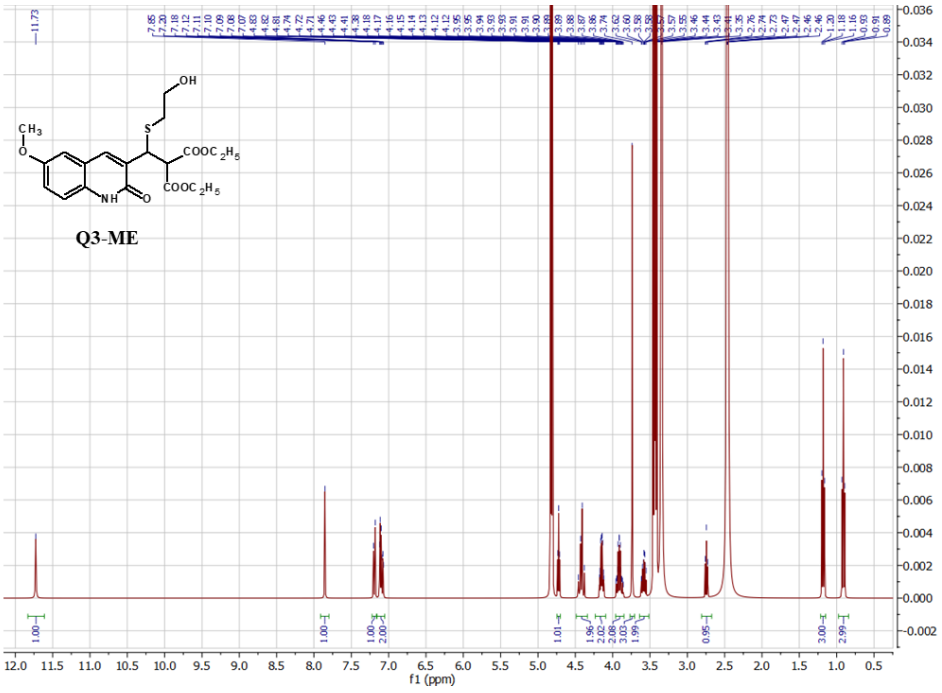


Figure S9 Fluorescence intensity of **Q4** (20 μM) at different pH values in the absence/presence of HSO_3^- (1 mM)



DMSO-*d*$_6$

Figure S10 ^{1}H-NMR spectra of **Q3** in the presence of excess ME (2-mercaptoethanol) in dimethyl sulphoxide-d_6

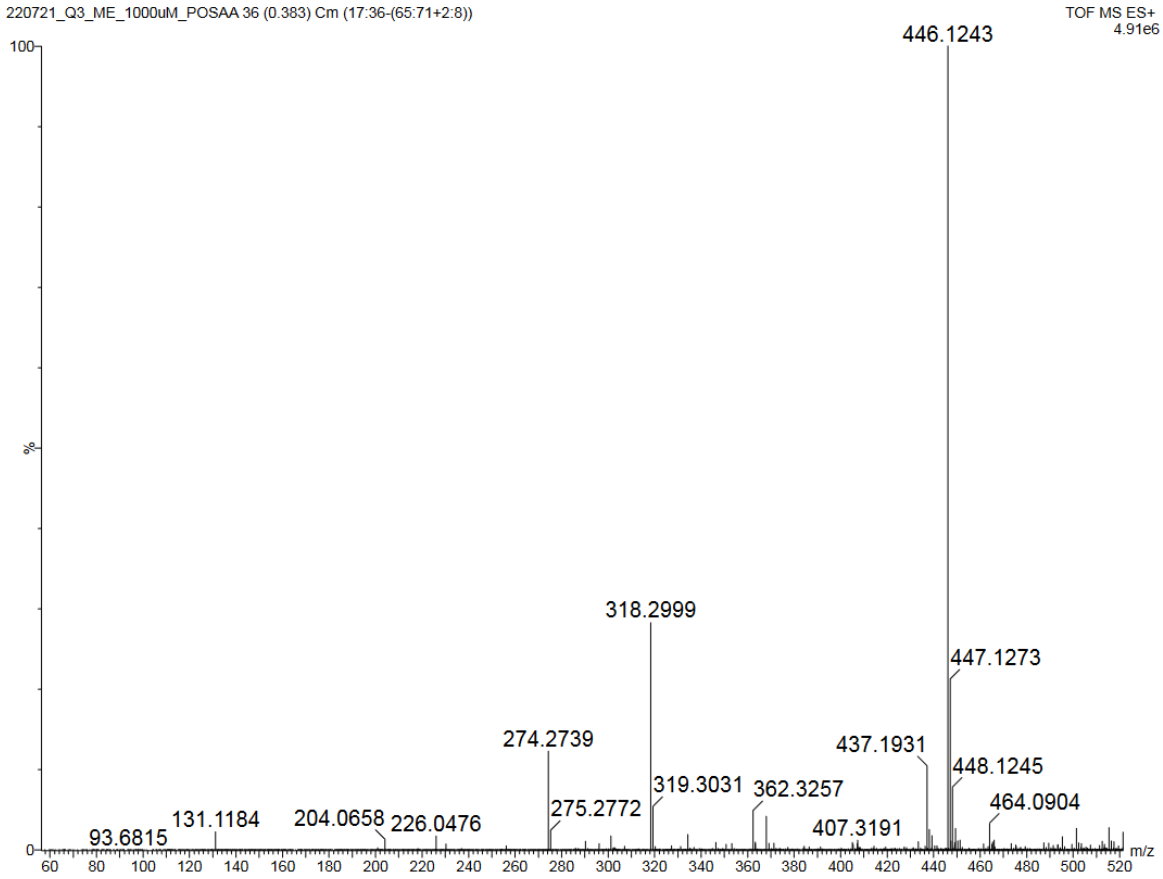


Figure S11 ESI mass spectrum of **Q3** (10 μM) with 2-mercaptoethanol (1000 μM)

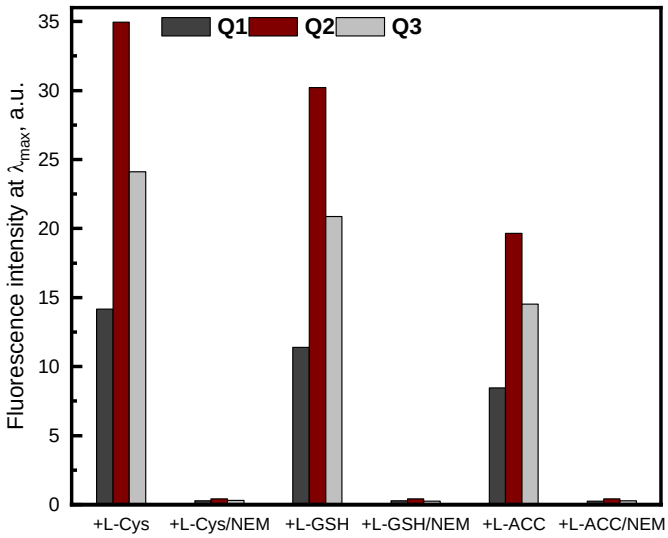


Figure S12 Fluorescence intensity of **Q1** (10 μM), **Q2** (6 μM), **Q3** (10 μM) in 0.1 M phosphate buffer with CH_3CN (20%, v/v, pH=7.4) in the presence of biothiols (1 mM), NEM (1 mM)