

Supporting Information for:

Fluoresceinylcarbonate-based fluorescent probe for the rapid and sensitive detection of biothiols in a HEPES buffer and its cellular expression

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1. NMR spectra

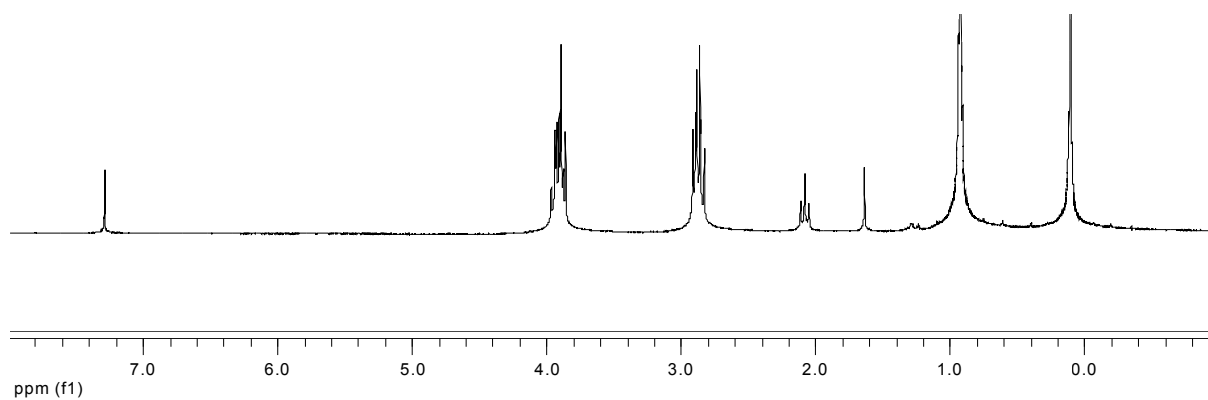


Figure S1. ¹H spectra of compound **3** in CDCl₃.

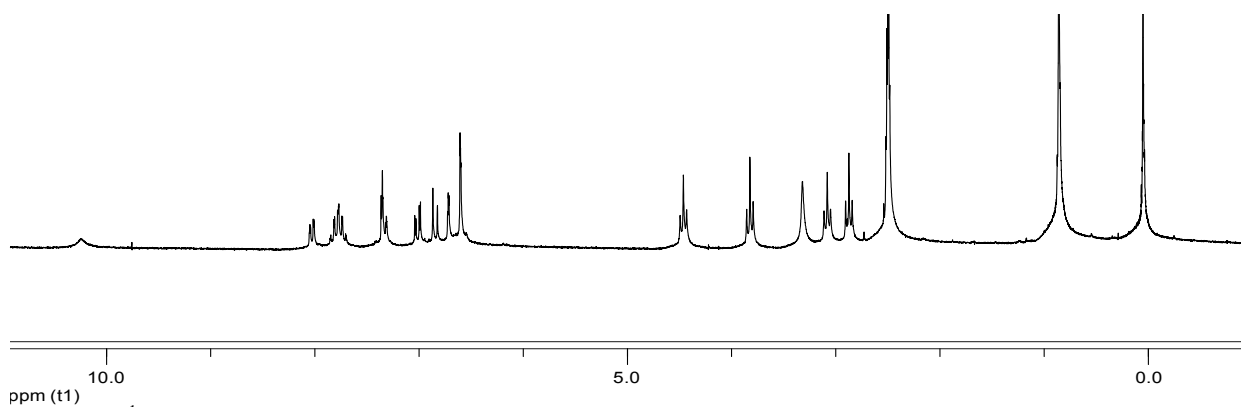


Figure S2. ¹H spectra of compound **5** in DMSO-*d*₆.

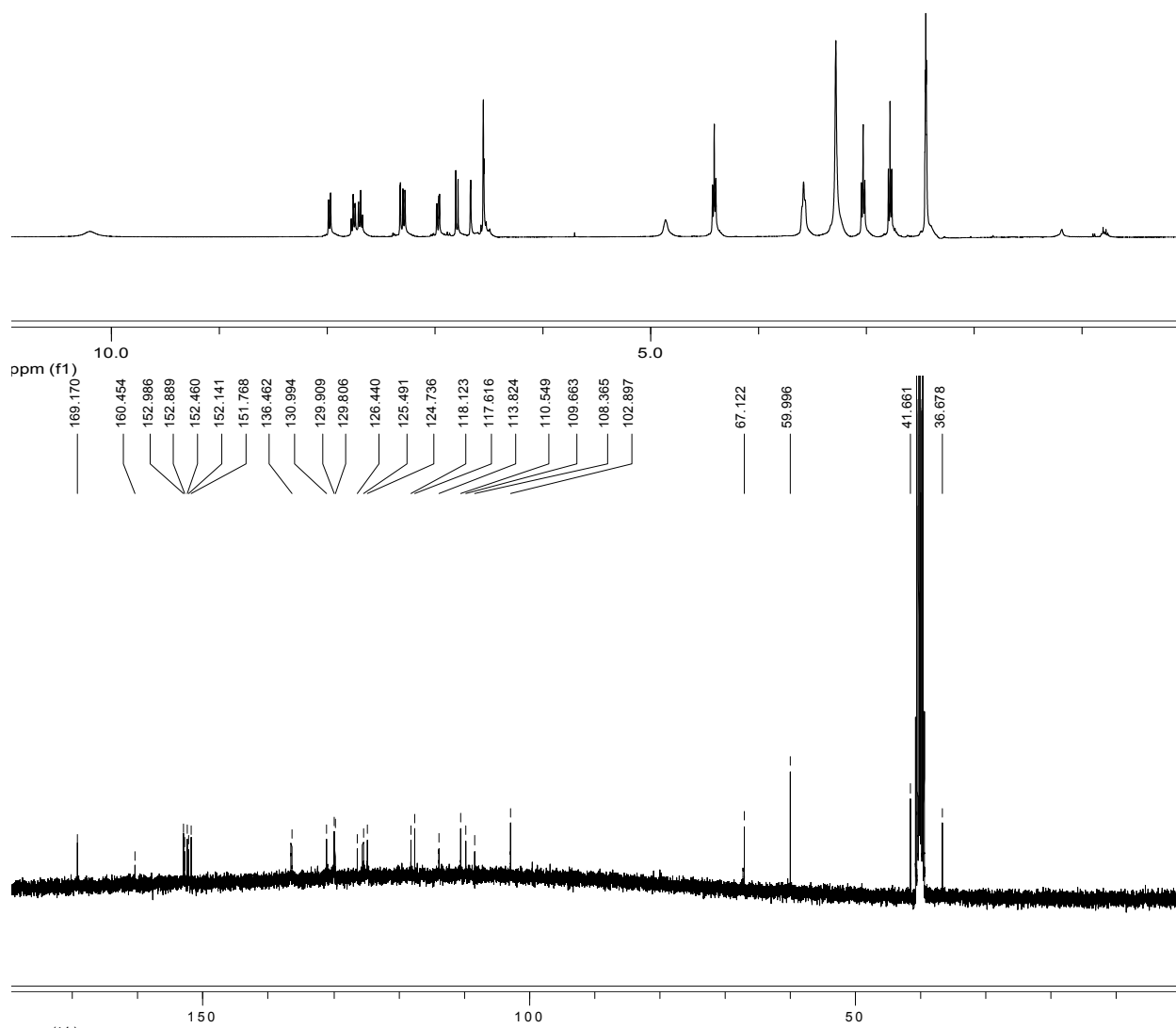
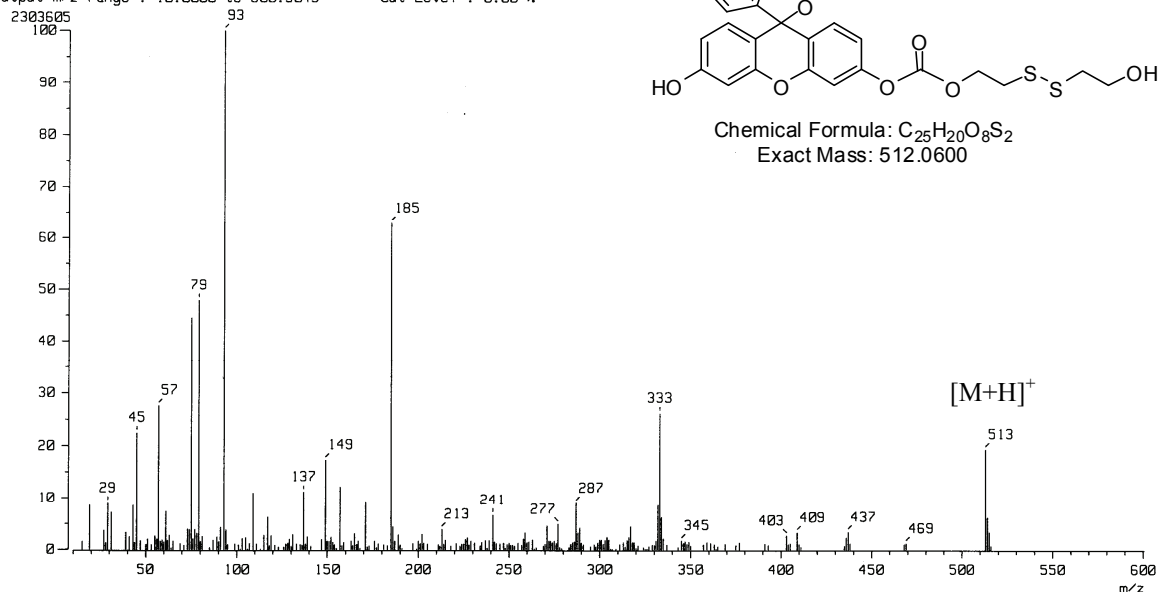


Figure S3. ¹H and ¹³C NMR spectra of **1** in DMSO-*d*₆.

2. Mass spectra

[Mass Spectrum]
 Date : 11-Jun-2013 16:43
 Sample: Fluo_monodisulfide
 Note : m-NBA
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.50 min Scan# : (2,7)
 BP : m/z 93.0000 Int. : 219.69
 Output m/z range : 10.0000 to 600.5045 Cut Level : 0.00 %



[Elemental Composition]

Date : 11-Jun-2013 16:55
 Sample: Fluo_monodisulfide
 Note : Glycerol + DMSO
 Inlet : Direct Ion Mode : FAB+
 RT : 0.07 min Scan# : (3,5)
 Elements : C 100/0, H 150/0, O 10/0, S 3/0
 Mass Tolerance : 1000ppm, 3mmu if m/z < 3, 5mmu if m/z > 5
 Unsaturation (U.S.) : 0.0 - 50.0

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Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
513.0677	100.0	-5.2 / -2.7	38.5	C 42 H 9
		+6.5 / +3.3	21.5	C 28 H 17 O 8 S
		-0.1 / +0.0	17.5	C 25 H 21 O 8 S 2
		+4.8 / +2.5	22.5	C 29 H 21 O 3 S 3
		-6.6 / -3.4	13.5	C 22 H 25 O 8 S 3

[Theoretical Ion Distribution]

Molecular Formula : C₂₅ H₂₁ O₈ S₂
 (m/z 513.0678, MW 513.5689, U.S. 17.5)
 Base Peak : 513.0678, Averaged MW : 513.5635(a), 513.5648(w)

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m/z	INT.
513.0678	100.0000
514.0709	29.6892
515.0675	14.7114
516.0692	3.4260
517.0679	0.8415
518.0688	0.1509
519.0692	0.0245
520.0702	0.0034
521.0713	0.0004