A new chloro-substituted dicyanoisophorone-based near-infrared fluorophore with largre Stokes shift and its application for detecting cysteine in cells and *in vivo*

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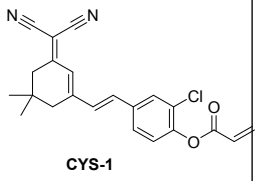
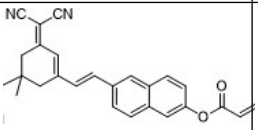
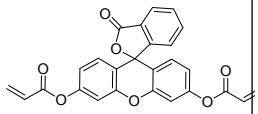
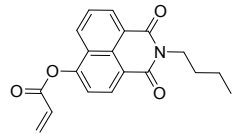
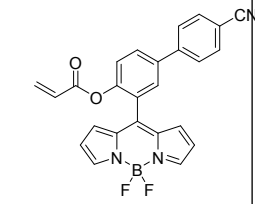
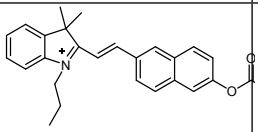
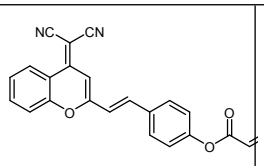
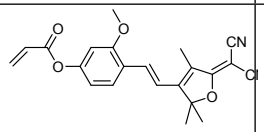
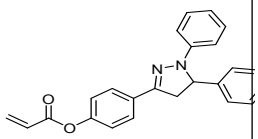
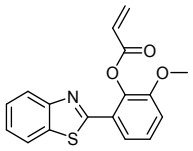
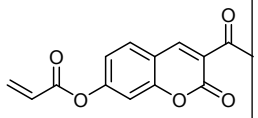
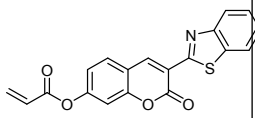
Contents

Table S1. Some similar acrylate-functionalized probes for the detection of cysteine.

	Probe	Solvent (pH=7.4)	Time (min)	Stokes shift（nm）	Analyte	Detection Limit (μM)	Reference
1	 CYS-1 $\lambda_{ex/em}$=490/655 nm	PBS	25	165	Cys	0.173	**This work**
2	 $\lambda_{ex/em}$=503/631 nm	DMSO-PBS (1/1,v/v)	15	128	Cys	0.26	[1]
3	 $\lambda_{ex/em}$=450/520 nm	EtOH-water (2/3, v/v)	60	70	Cys Hcy	0.50	[2]
4	 $\lambda_{ex/em}$=452/547 nm	DMSO-PBS (containing 0.2% DMSO)	7	95	Cys Hcy	1.8	[3]
5	 $\lambda_{ex/em}$=503/525 nm	CH_3CN-H_2O (1:1,v/v)	150	22	Cys	0.037	[4]
6	 $\lambda_{ex/em}$=410/595 nm	DMSO-PBS (containing 0.2%DMSO)	10	185	Cys	0.95	[5]

7	 $\lambda_{ex/em}$=560/676 nm	DMSO-PBS (1/1,v/v)	20	116	Cys Hcy	0.081	[6]
8	 $\lambda_{ex/em}$=585/635 nm	DMSO-PBS (1/1,v/v)	30	50	Cys Hcy	0.3	[7]
9	 $\lambda_{ex/em}$=370/474 nm	EtOH-PBS (3/7, v/v)	no date	104	GSH	0.082	[8]
10	 $\lambda_{ex/em}$=377/487 nm	EtOH-H_2O (2:8, v/v)	40	110	Cys Hcy	o date	[9]
11	 $\lambda_{ex/em}$=420/454 nm	EtOH-HEPES (2:8, v/v)	40	34	Cys GSH	0.657	[10]
12	 $\lambda_{ex/em}$=458/498 nm	DMSO-PBS (1/1,v/v)	15	40	Cys Hcy GSH	0.02	[11]

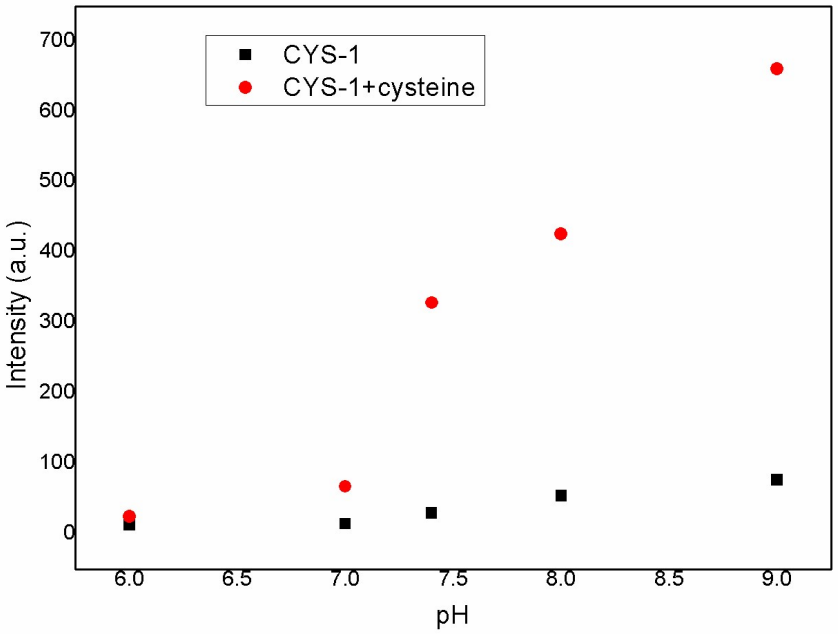


Figure S1. Fluorescence intensity at different pH conditions. (λ_{ex} = 490 nm, λ_{em} = 655 nm).

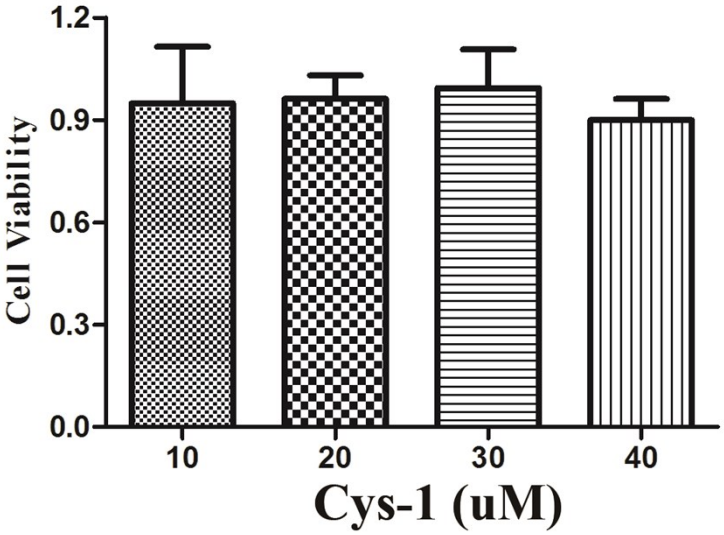


Figure S2. The MTT assay

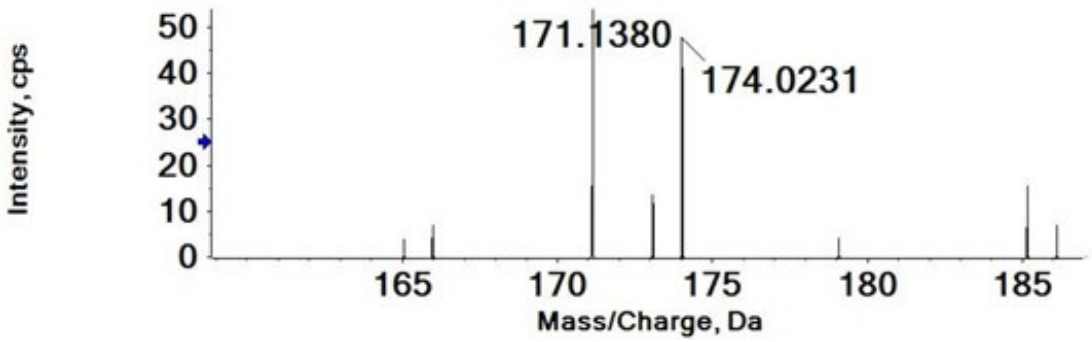


Figure S3. ESI-MS analysis the product of **CYS-1** with cysteine.

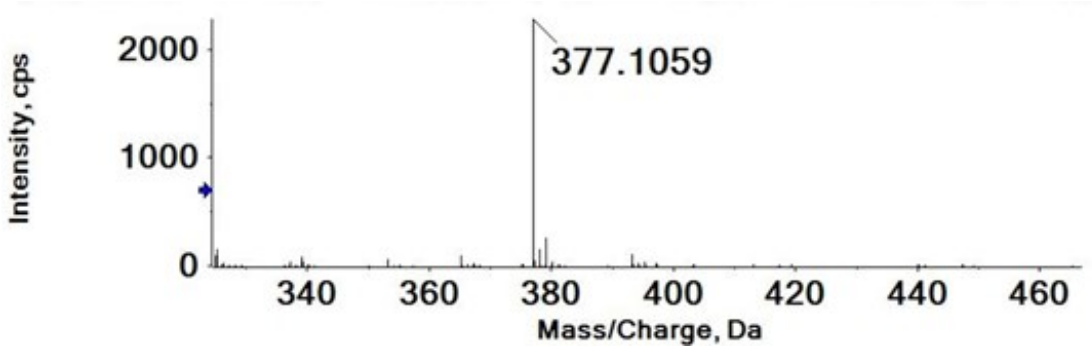


Figure S4. ESI-MS analysis the product of **CYS-1** with cysteine.

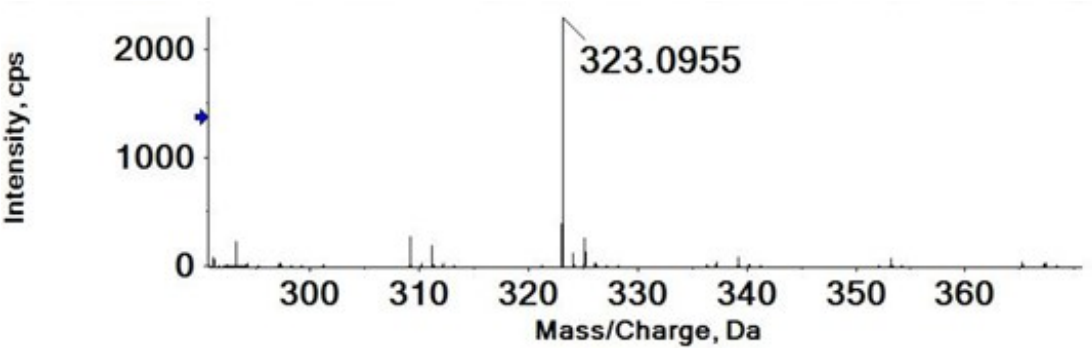


Figure S5. ESI-MS analysis the product of **CYS-1** with cysteine.

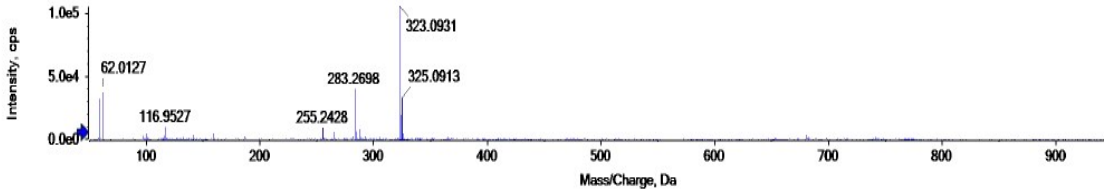


Figure S6. ESI-MS analysis of **DCM-COH**.

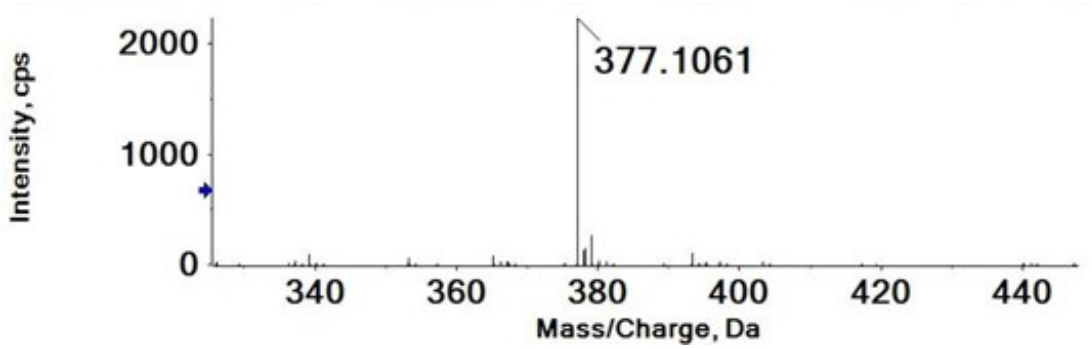


Figure S7. ESI-MS analysis of **CYS-1**.

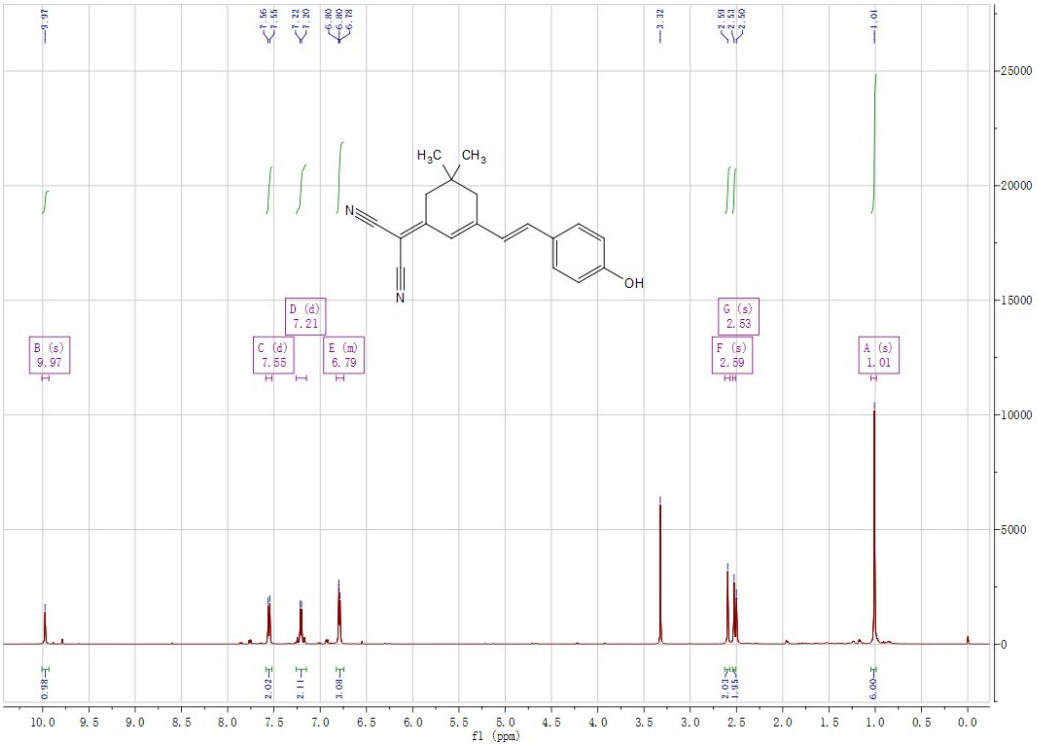


Figure S8. ^{1}H NMR spectra (500 MHz) of compound **DCI-OH** in DMSO.

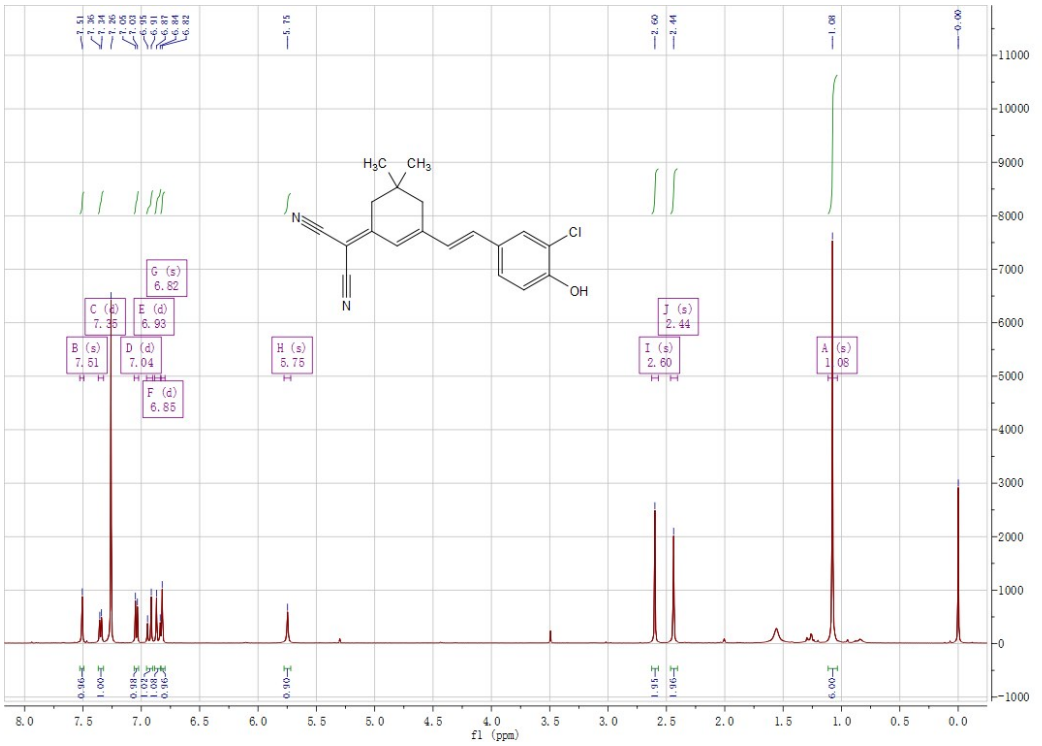


Figure S9. [1]H NMR spectra (500 MHz) of compound **DCM-COH** in DMSO.

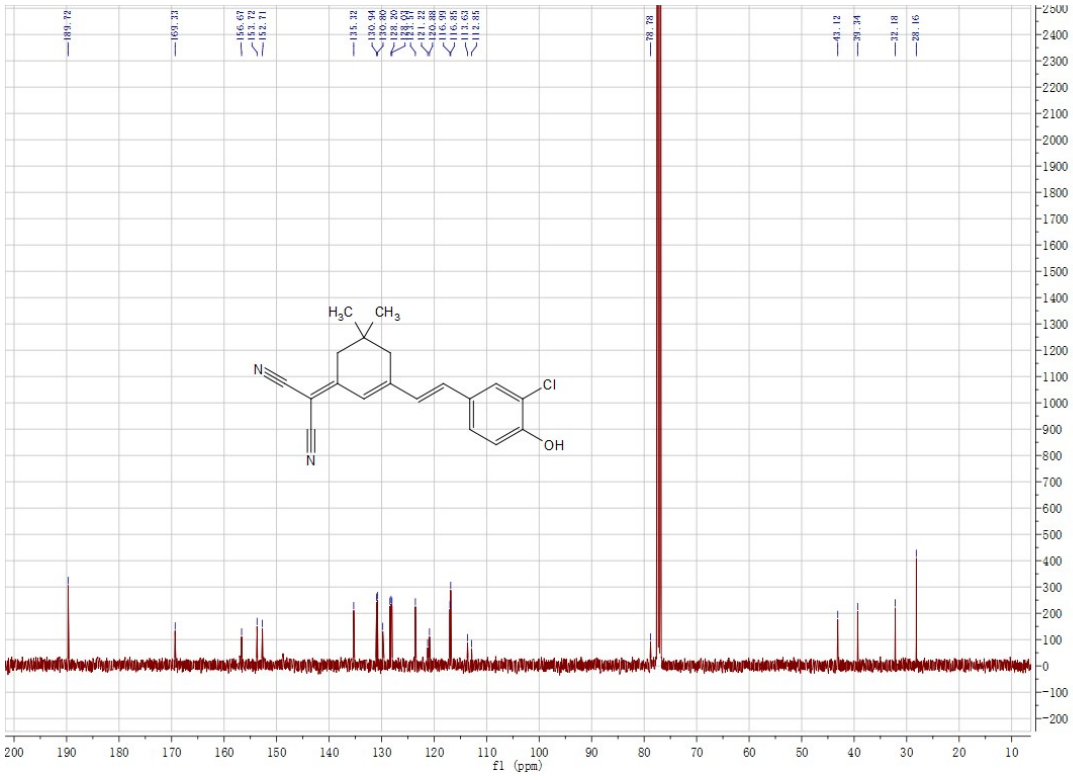


Figure S10. [1]H NMR spectra (101 MHz) of compound **DCM-COH** in $CDCl_3$.

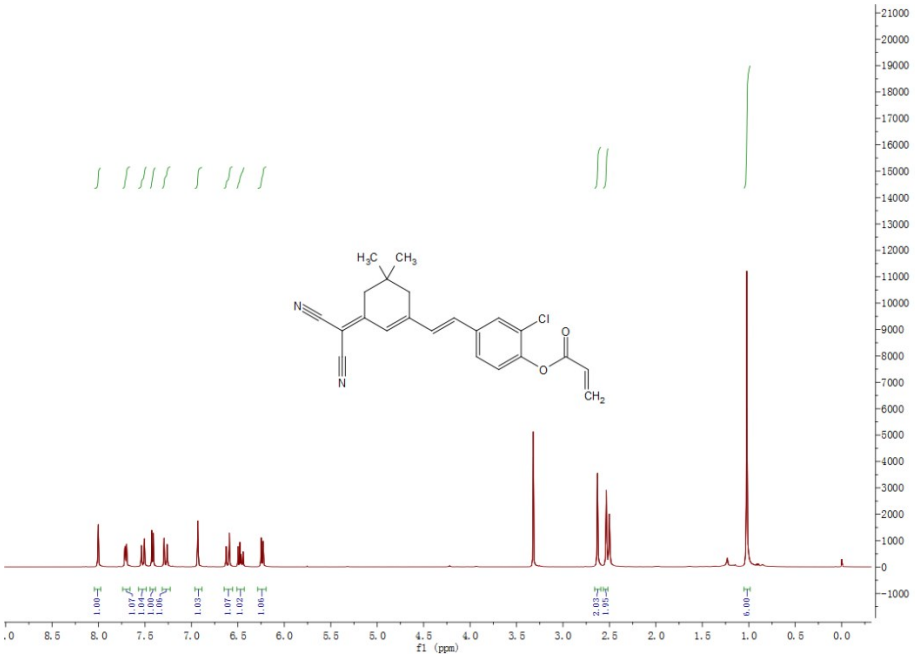


Figure S11. ^{1}H NMR spectra (500 MHz) of compound **CYS-1** in DMSO.

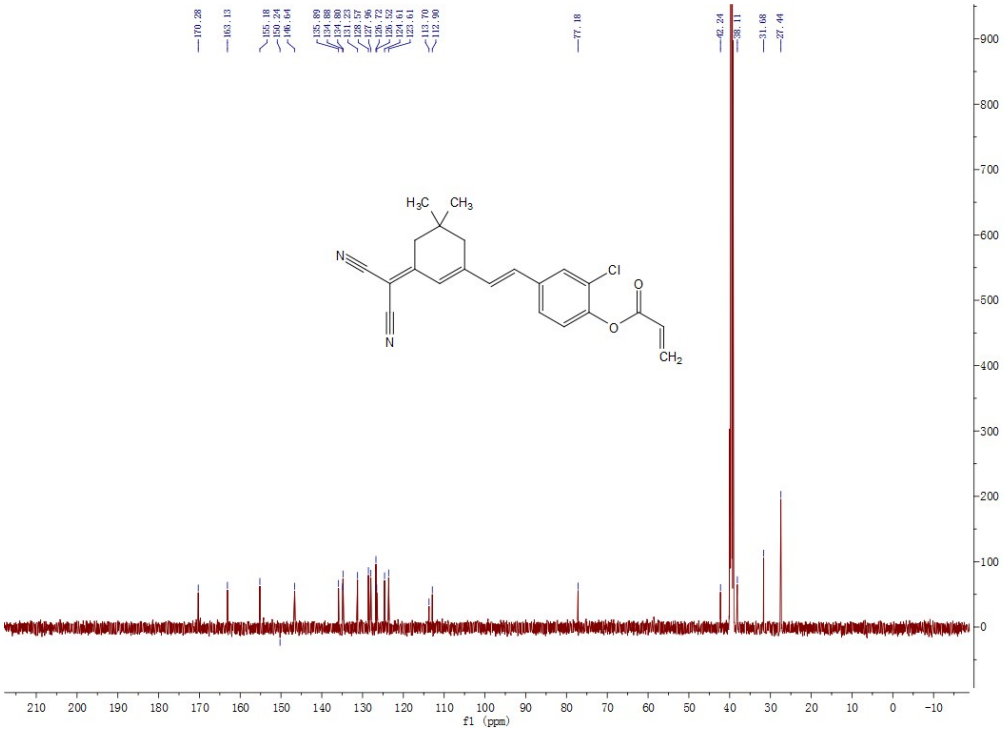


Figure S12. ^{13}C NMR spectra (500 MHz) of compound **CYS-1** in DMSO.

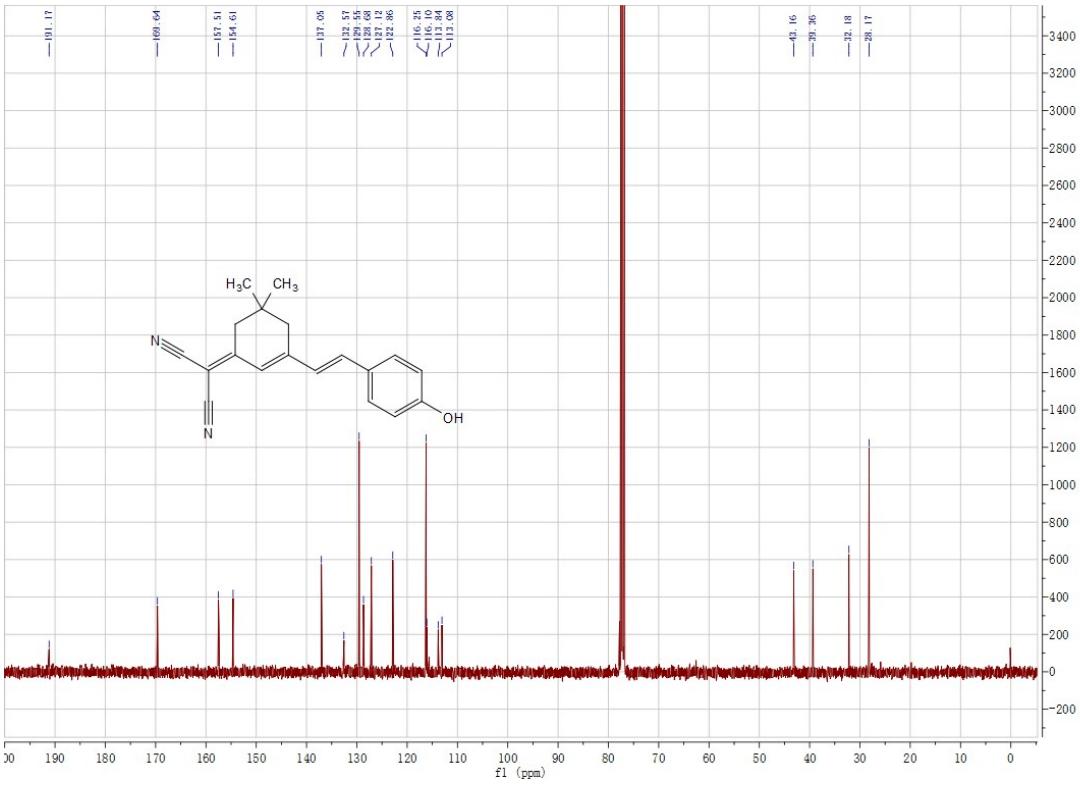


Figure S13. ^{13}C NMR spectra (101 MHz) of compound **DCI-COH** in $CDCl_3$.

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