Electronic Supplementary Material (ESI) for Analyst.

SUPPORTING INFORMATION

Inexpensive water soluble methyl methacrylate-functionalized hydroxyphthalimide: variations of the mycophenolic acid core for selective live cell imaging of free cysteine

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Contents

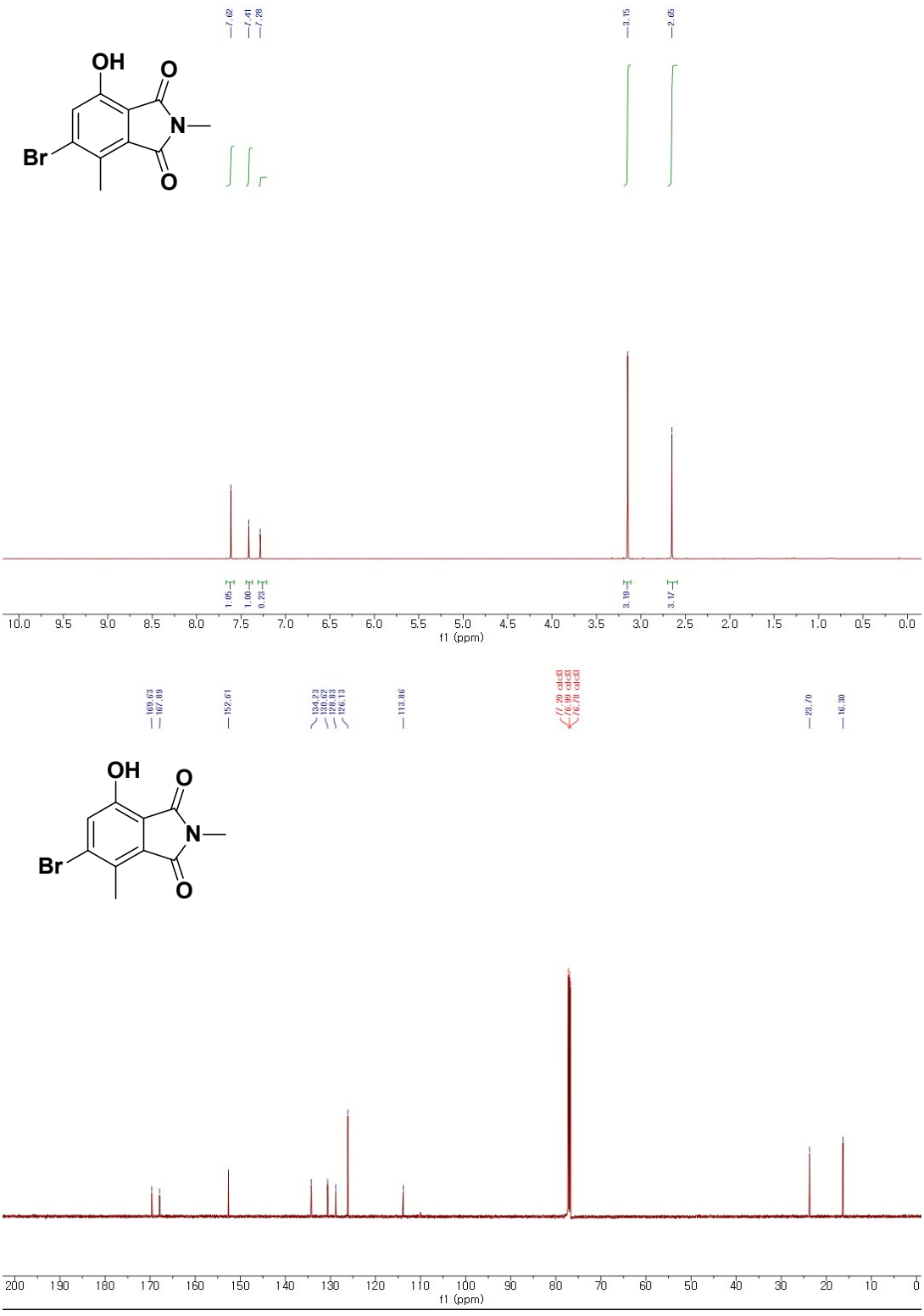


Fig. S1. (*top*) ^{1}H and (*bottom*) ^{13}C NMR spectrum of compound **Myco-OH**.

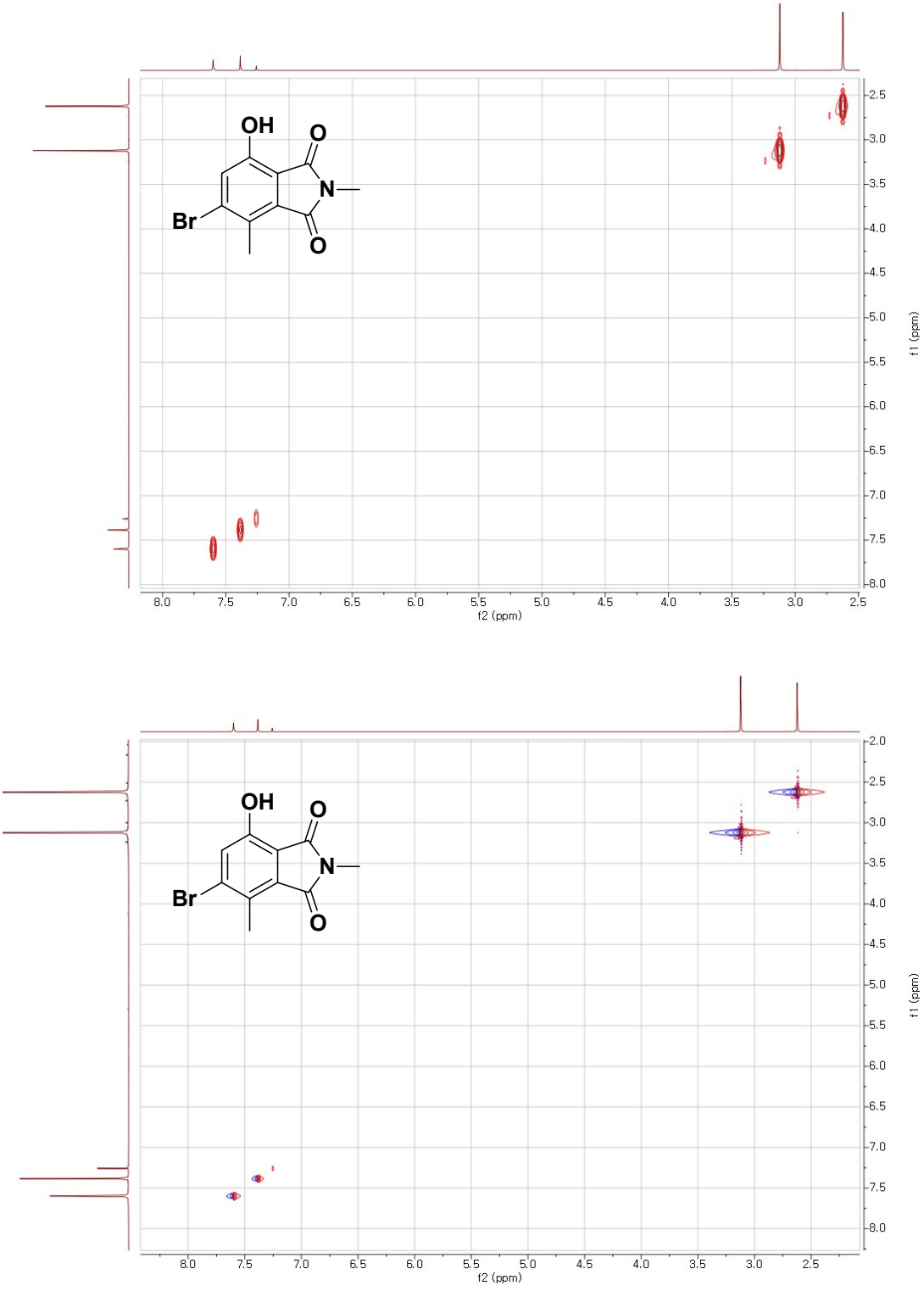
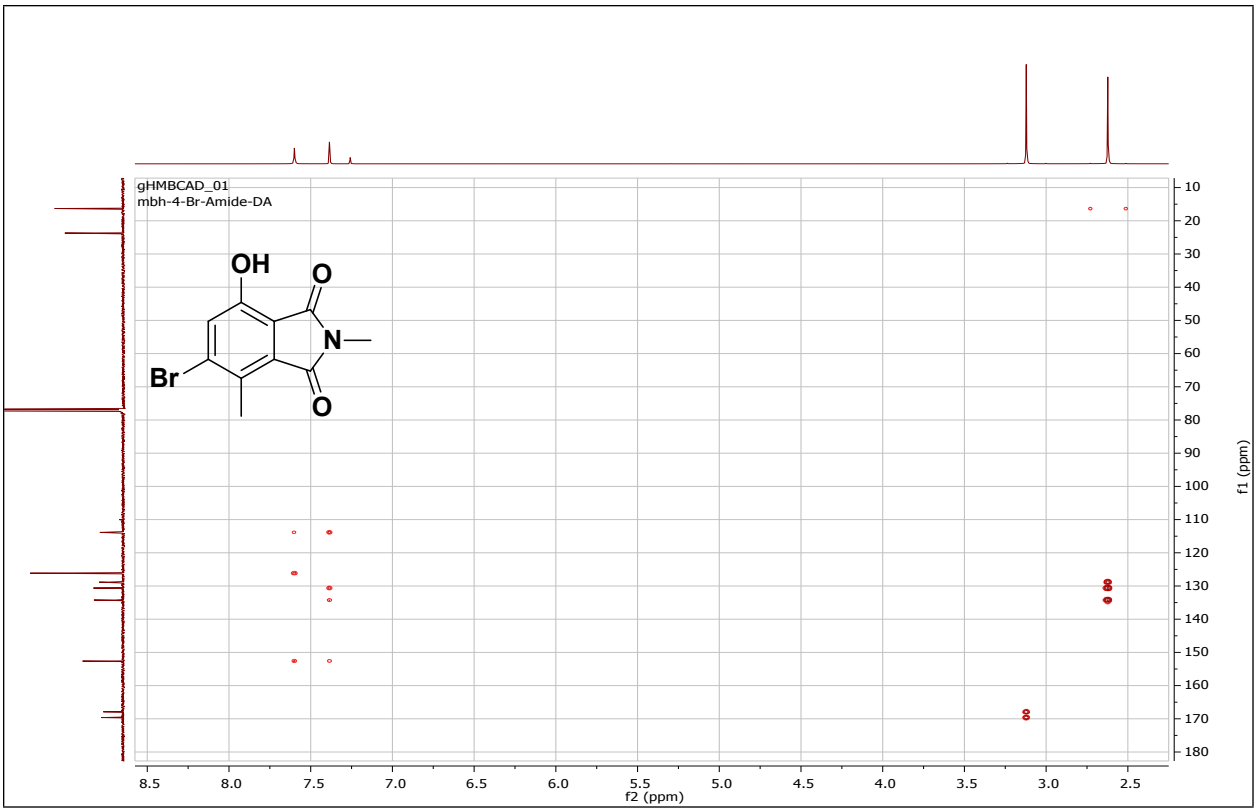


Fig. S2. (*top*) COSY and (*bottom*) NOESY NMR spectrum of compound **Myco-OH**.



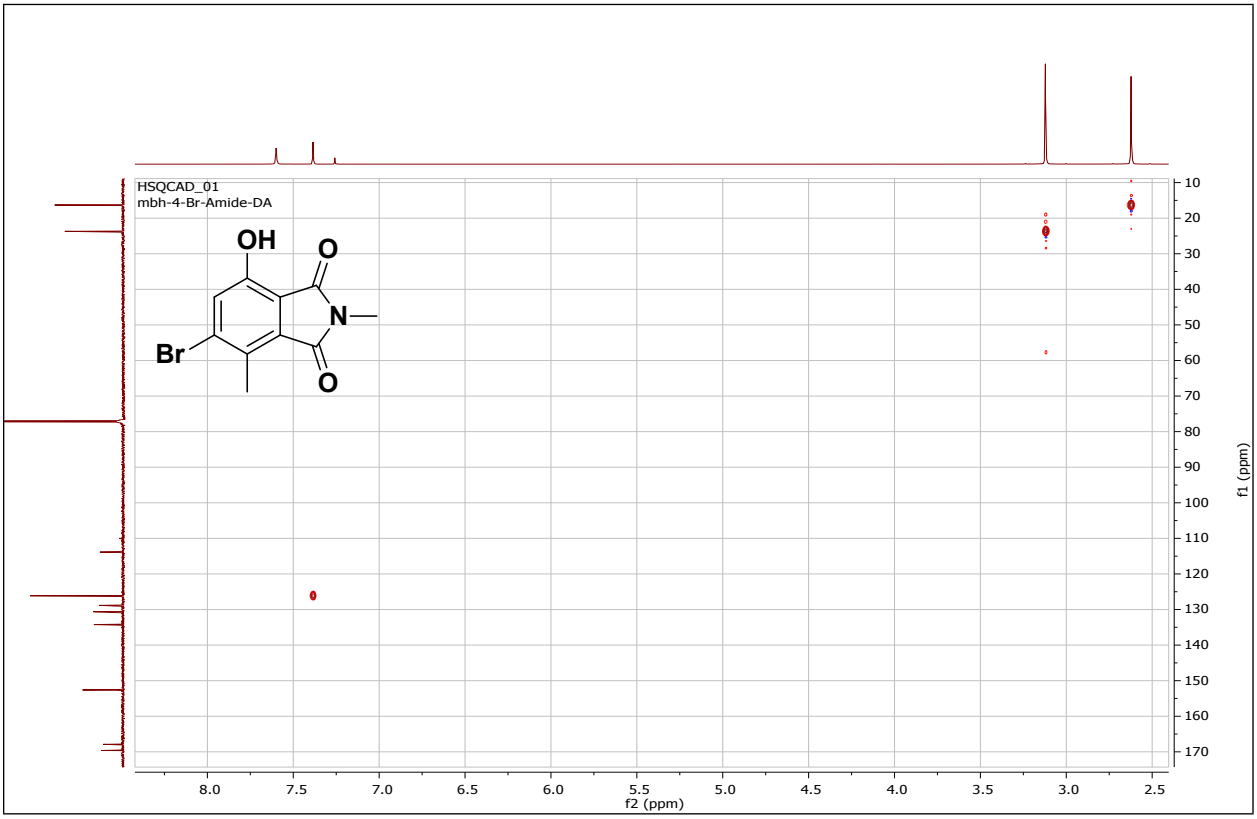


Fig. S3. (*top*) HMBC and (*bottom*) HSQC NMR spectrum of compound **Myco-OH**.

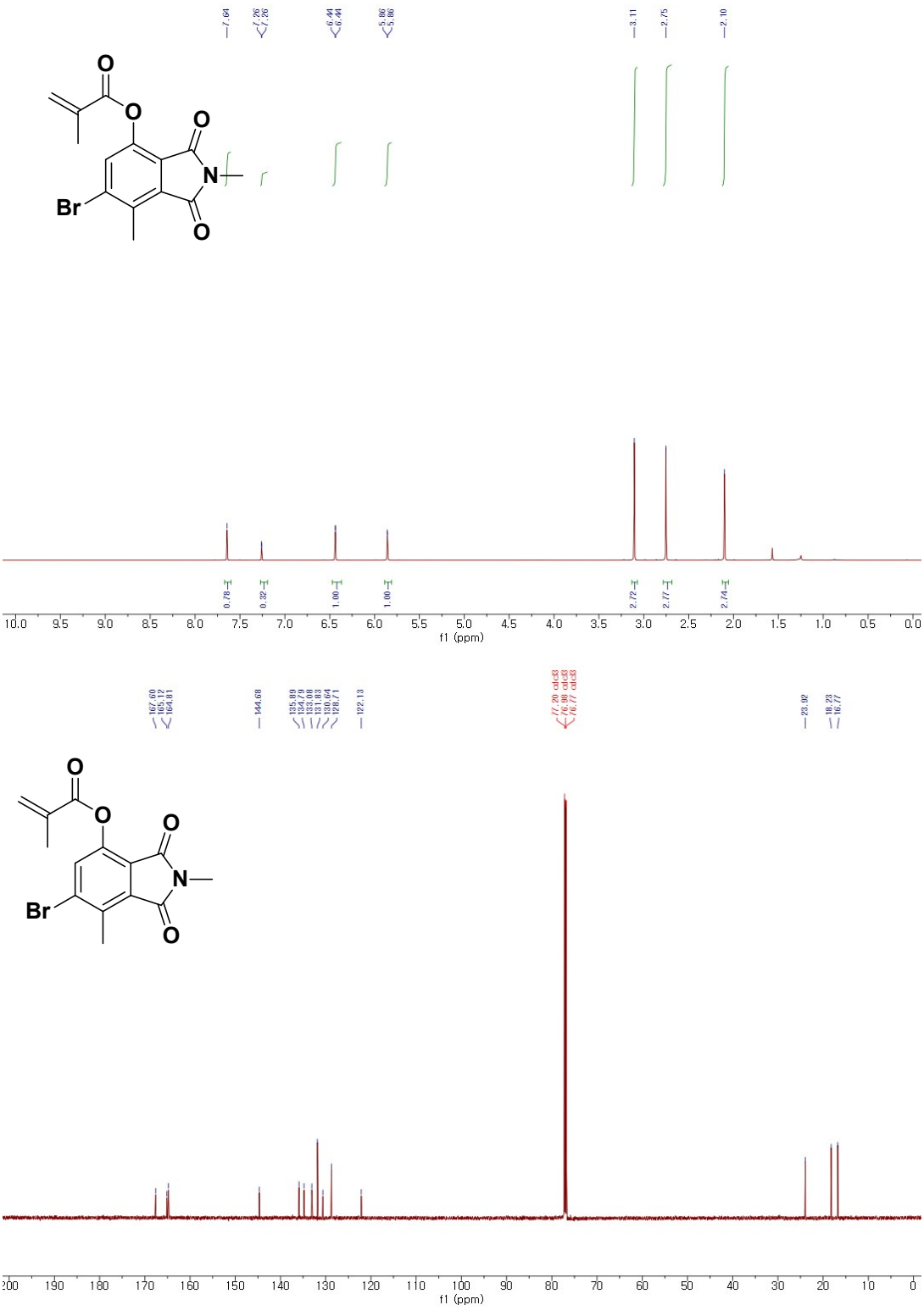


Fig. S4. (*top*) ^{1}H and (*bottom*) ^{13}C NMR spectrum of compound **Myco-Cys**.

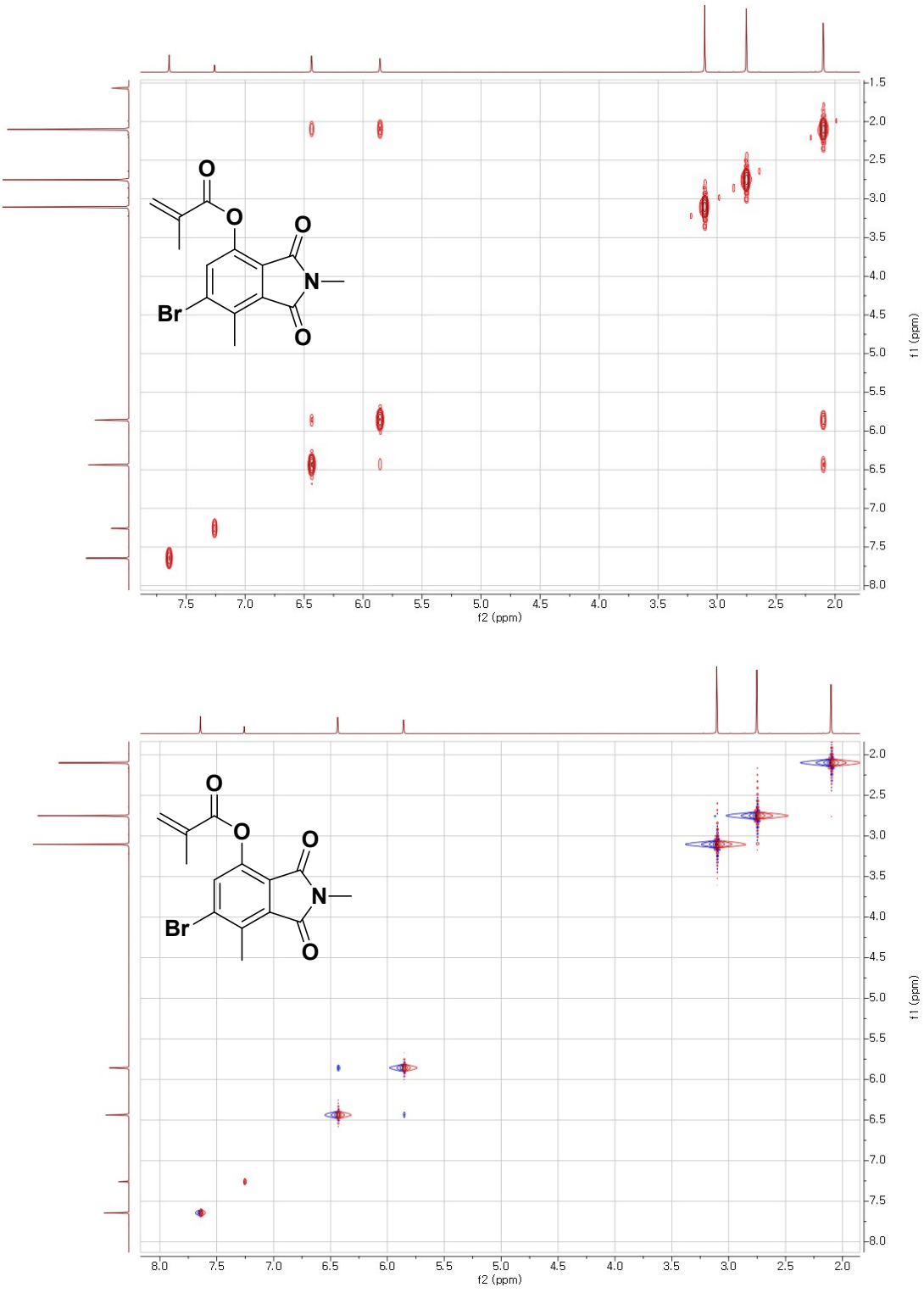


Fig. S5. (*top*) COSY and (*bottom*) NOESY NMR spectrum of compound **Myco-Cys**.

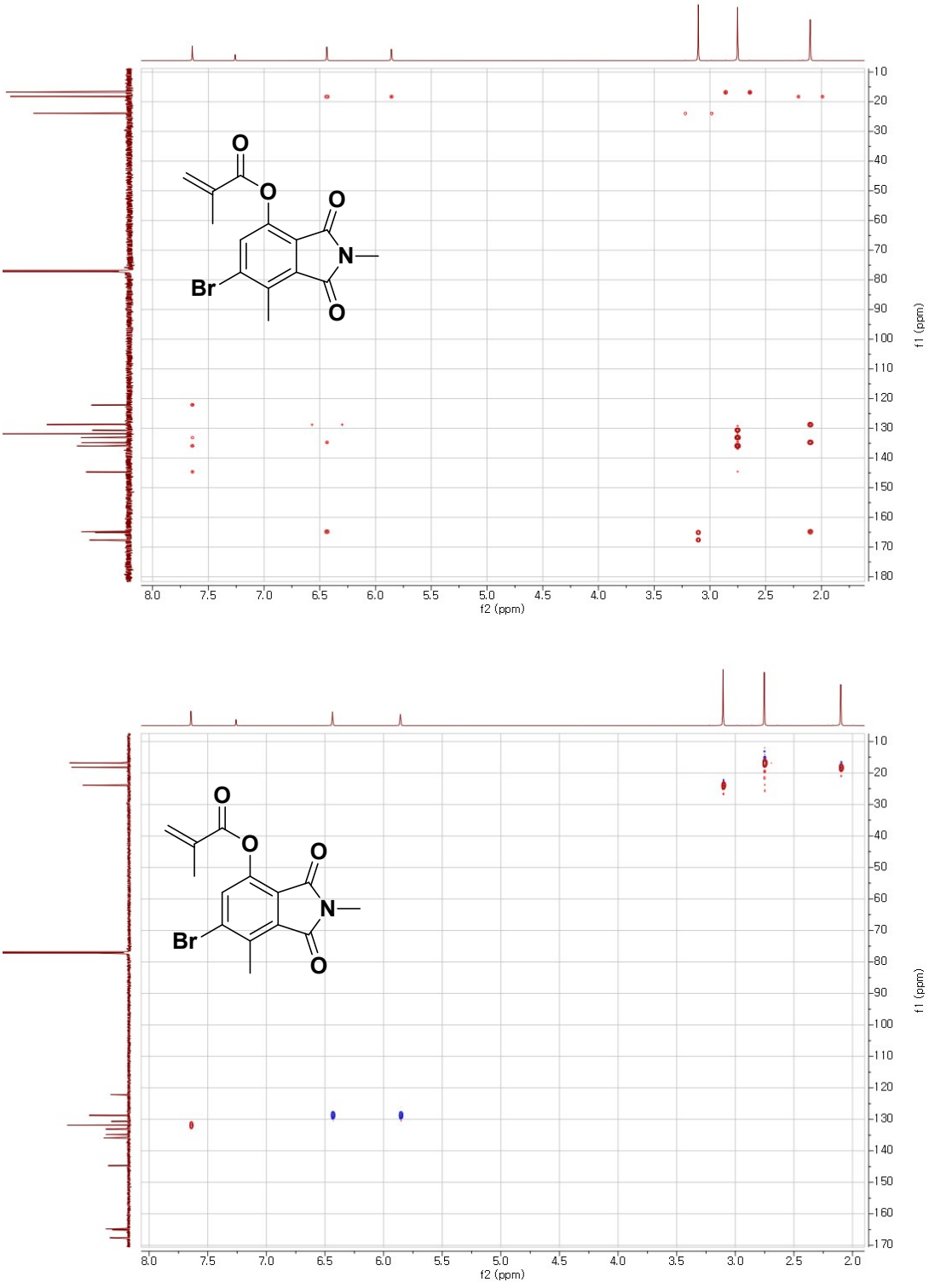


Fig. S6. (*top*) HMBC and (*bottom*) HSQC NMR spectrum of compound **Myco-Cys**.

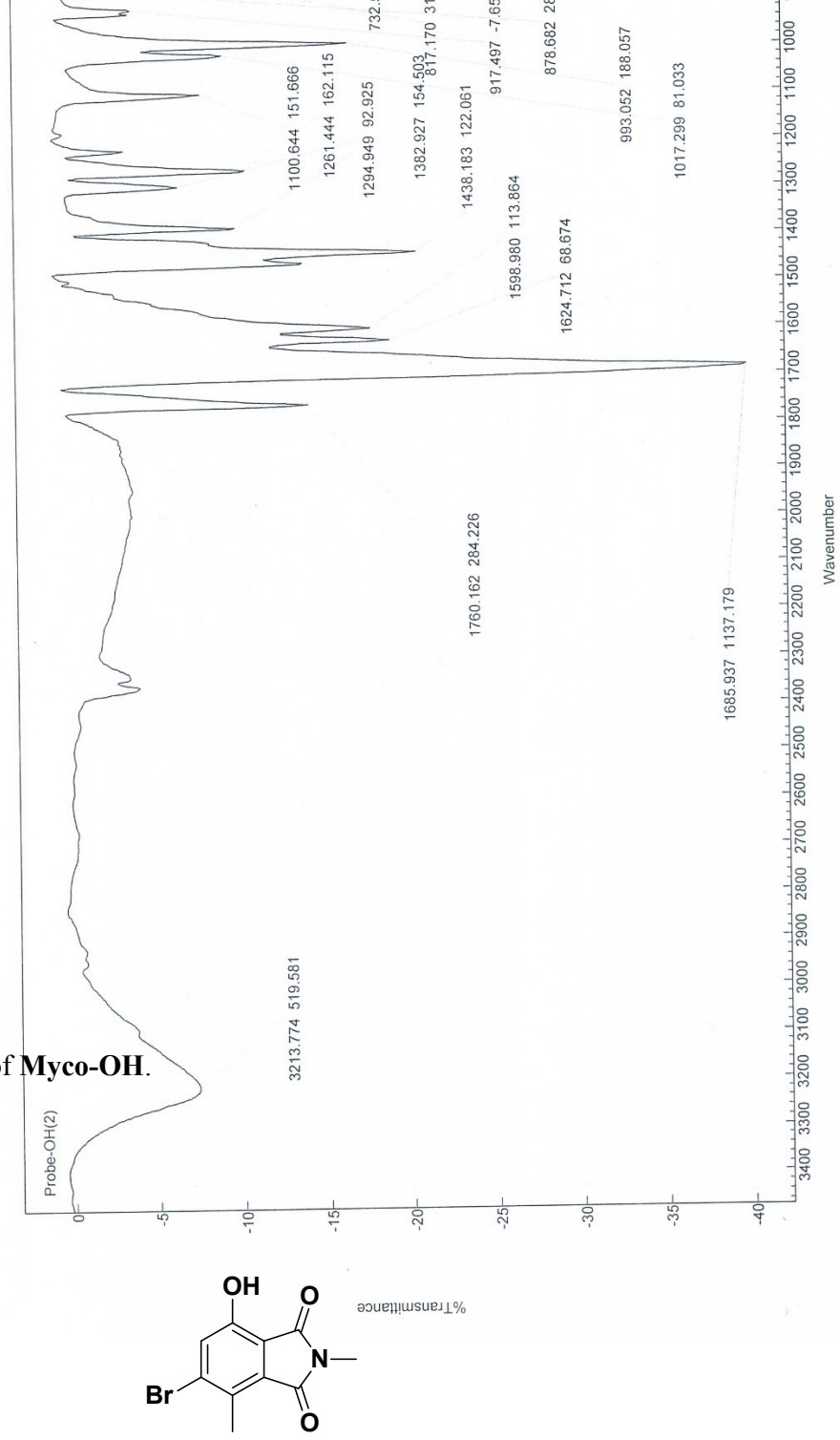


Fig. S7. FT-IR spectrum of **Myco-OH**.

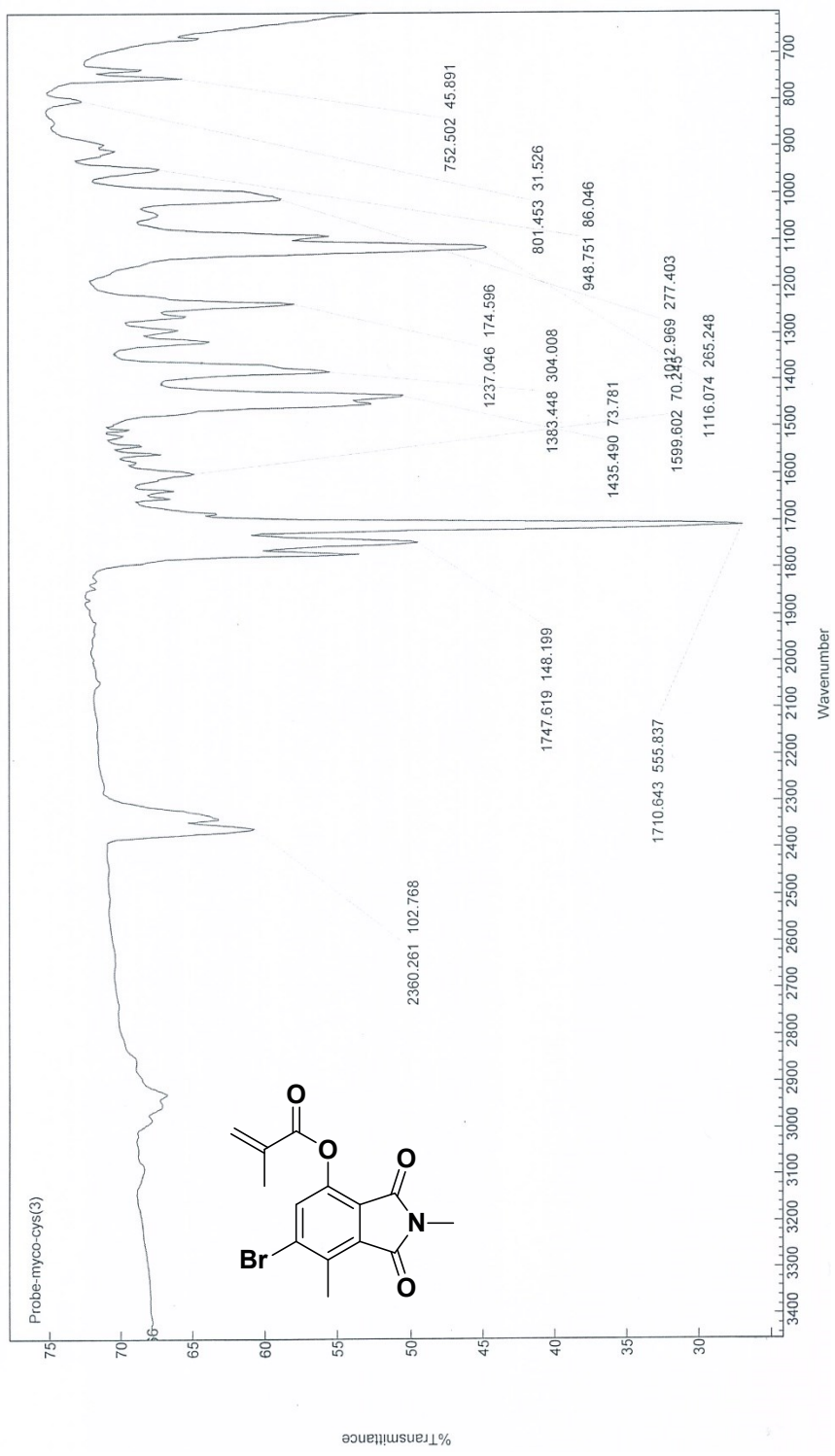
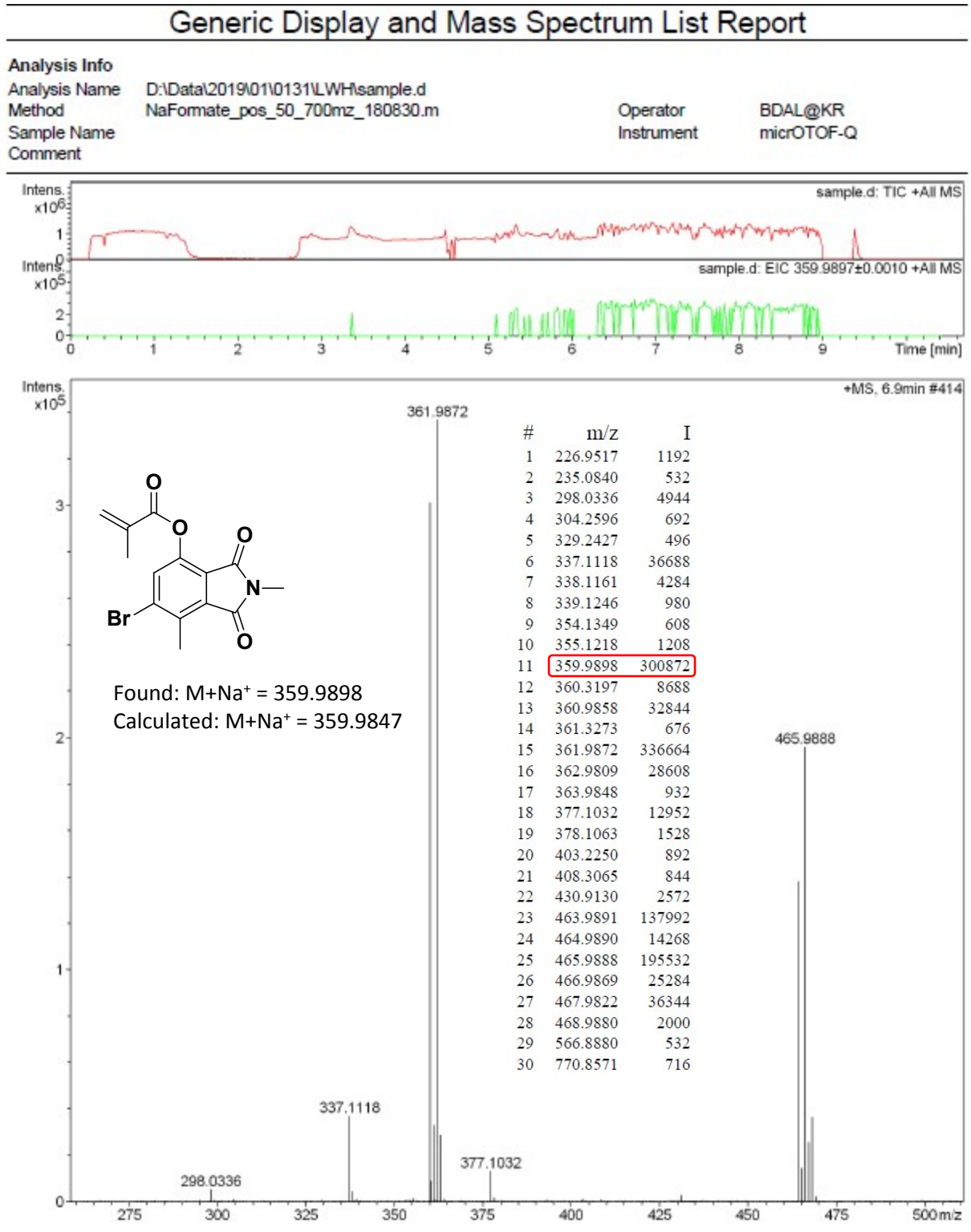


Fig. S8. FT-IR spectrum of **Myco-Cys**.



#	m/z	I
1	226.9517	1192
2	235.0840	532
3	298.0336	4944
4	304.2596	692
5	329.2427	496
6	337.1118	36688
7	338.1161	4284
8	339.1246	980
9	354.1349	608
10	355.1218	1208
11	359.9898	300872
12	360.3197	8688
13	360.9858	32844
14	361.3273	676
15	361.9872	336664
16	362.9809	28608
17	363.9848	932
18	377.1032	12952
19	378.1063	1528
20	403.2250	892
21	408.3065	844
22	430.9130	2572
23	463.9891	137992
24	464.9890	14268
25	465.9888	195532
26	466.9869	25284
27	467.9822	36344
28	468.9880	2000
29	566.8880	532
30	770.8571	716

Fig. S9. ESI-MS spectrum of **Myco-Cys**

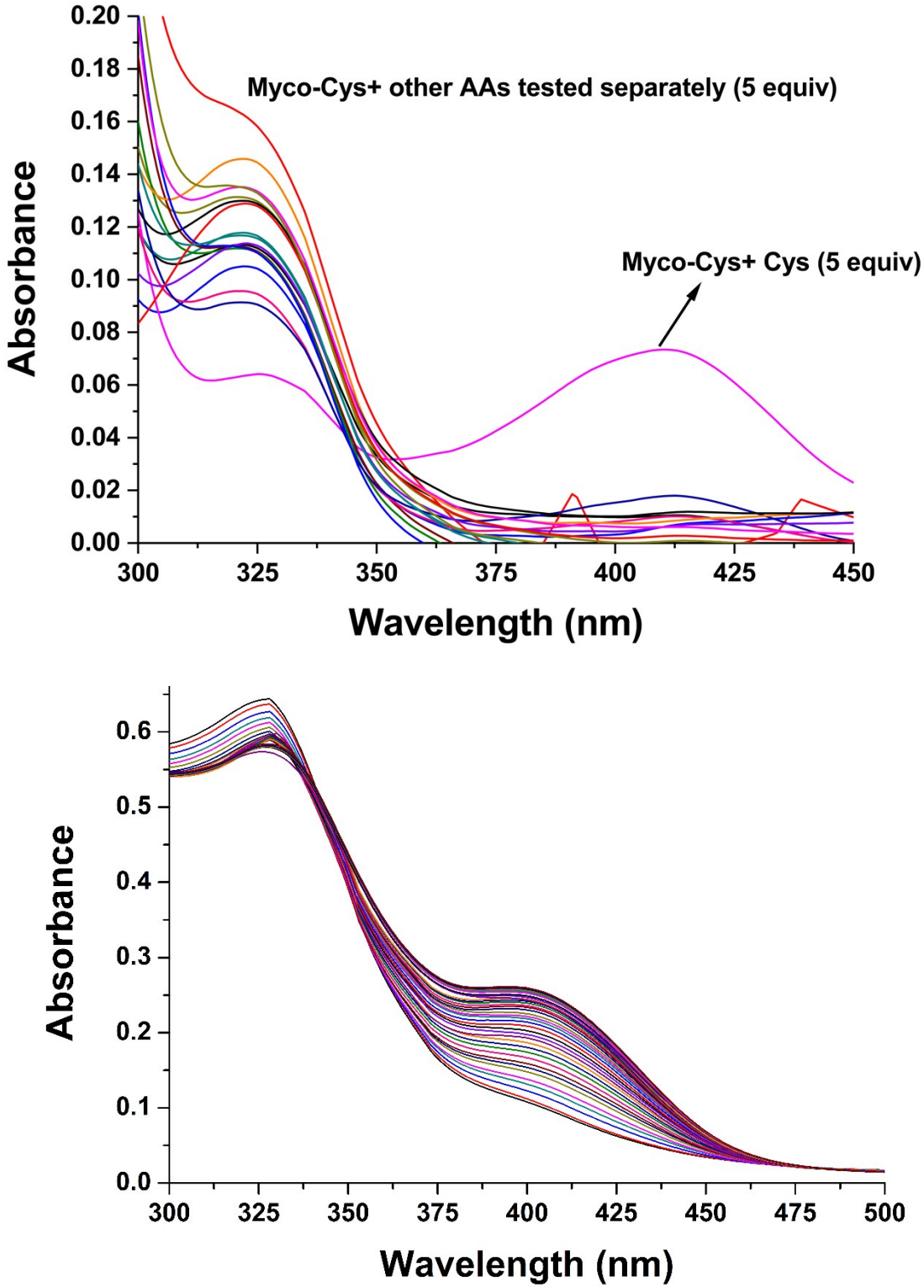


Fig. S10. (top) Comparison of UV-vis absorption spectra **Myco-Cys**+Cys (5 equiv) and **Myco-Cys**+other AAs (5 equiv); (bottom) Time dependent UV-vis absorption spectrum between **Myco-Cys**+Cys (5 equiv); incubation time 3600 seconds (Data was taken every 1 minute).

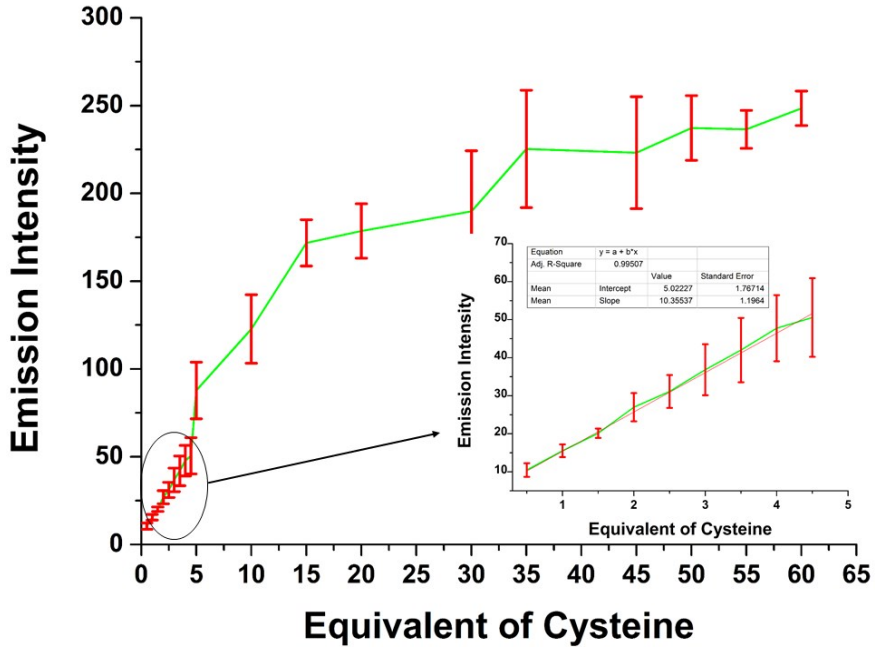


Fig. S11. Plot for the calculation of the limit of detection from the emission of **Myco-Cys** (10.0 μM) in the solution of PBS (pH 7.4); incubated for 30 minutes with increasing concentration of Cys (0.0 to 55.0 equiv) λ_{ex}= 417 nm and λ_{em} = 517 nm; slit width (3 nm/3 nm) at rt (error bars are reflecting error based on taking the average three experiments).

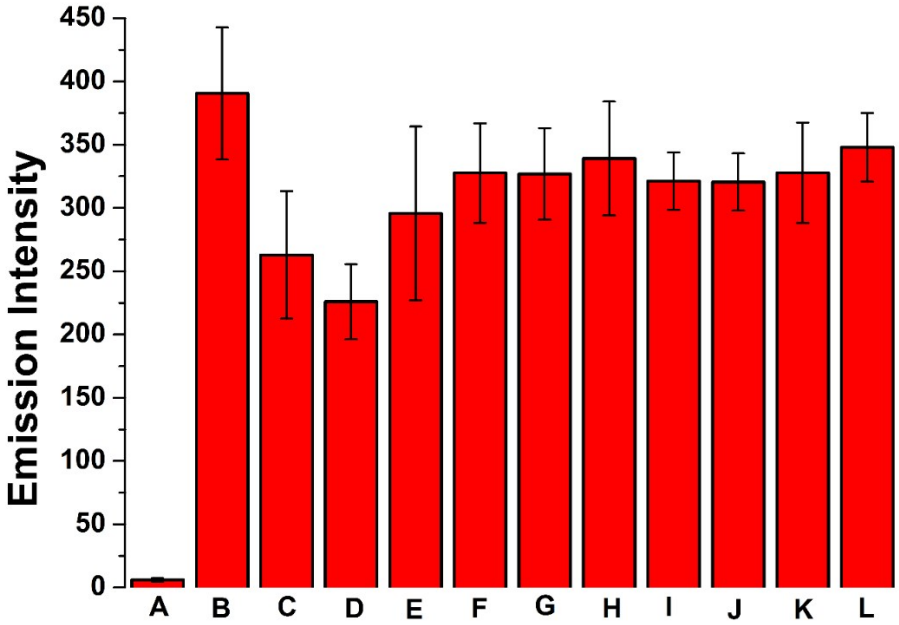


Fig. S12. Interference study of **Myco-Cys** (10 μM) with various soluble metal ions in a PBS solution (10 mM, pH 7.4); A; **Myco-Cys**; B: **Myco-Cys**+Cys; C: **Myco-Cys**+Cys+Cd; D: **Myco-Cys**+Cys+Co; E: **Myco-Cys**+Cys+Cs; F: **Myco-Cys**+Cys+Cu; G:**Myco-Cys**+Cys+Fe(II); H: **Myco-Cys**+Cys+Fe(III); I: **Myco-Cys**+Cys+Li; J: **Myco-Cys**+Cys+Mg; K: **Myco-Cys**+Cys+Mn; L: **Myco-Cys**+Cys+Pb; incubated for 30 min; λ_{ex}= 417 nm and λ_{em} = 519 nm; slit width (3 nm/3 nm); (bottom) at rt (error bars are the average three experiments).

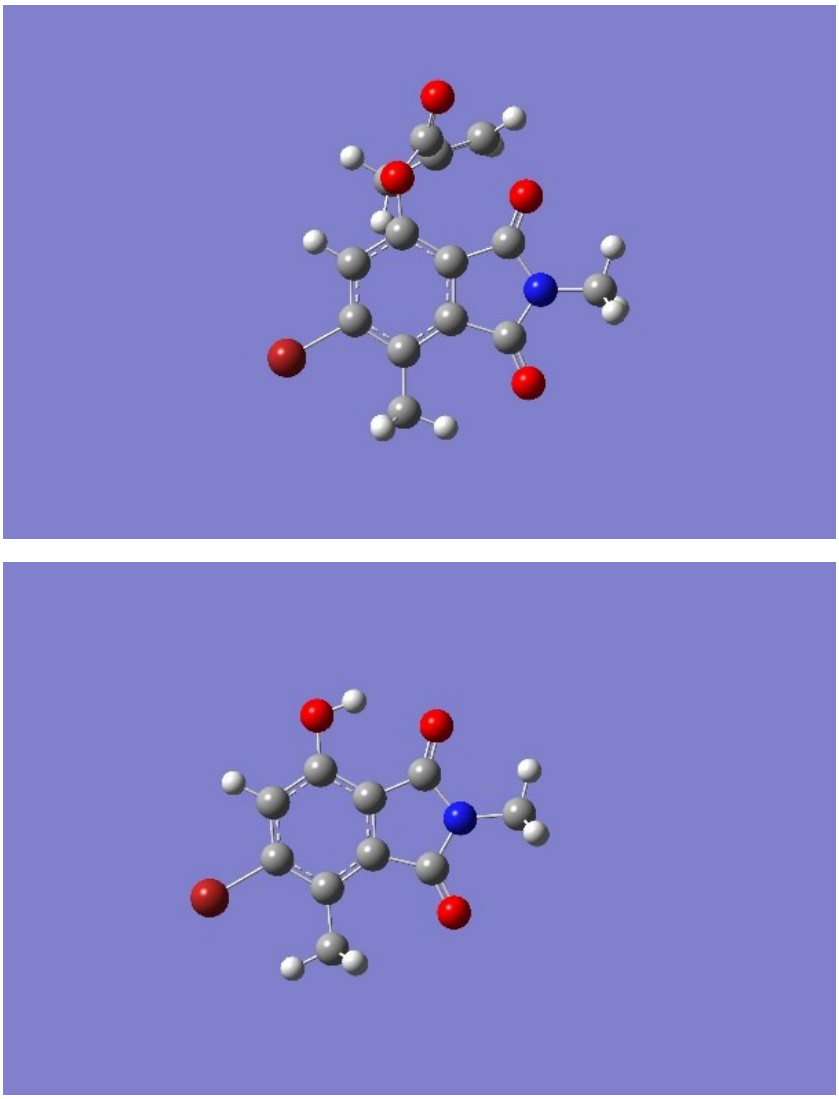


Fig. S13. DFT-optimized geometries of **Myco-Cys** (top), and **Myco-OH**(bottom) (B3LYP/6-31g* basis set, G09).

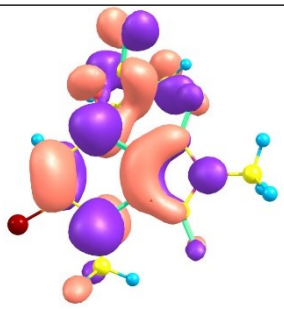
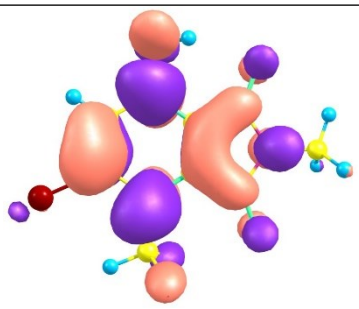
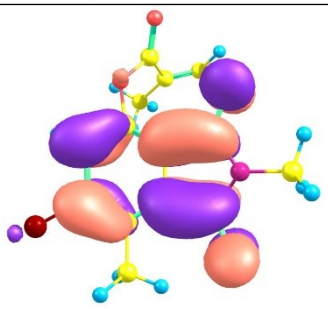
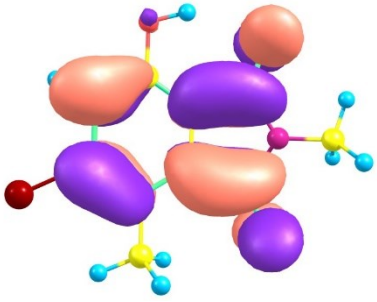
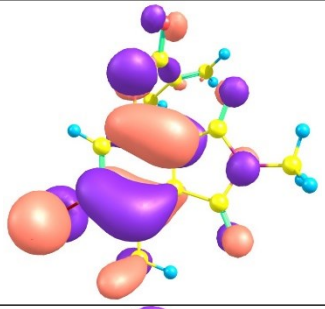
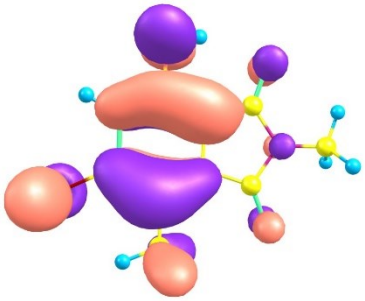
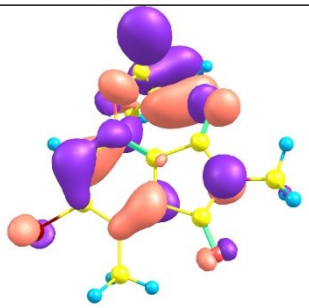
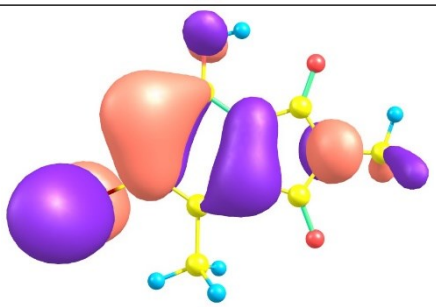
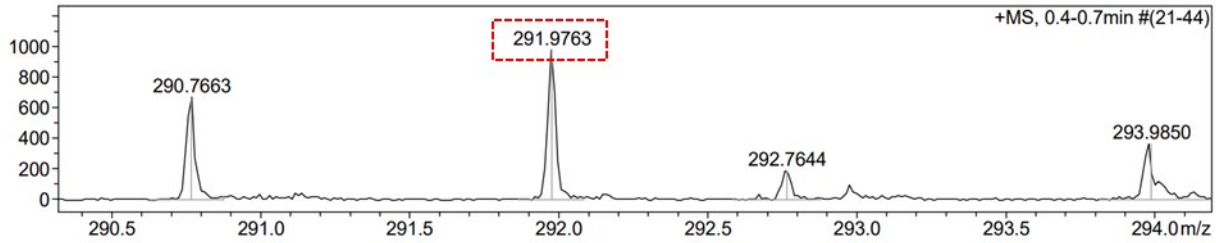
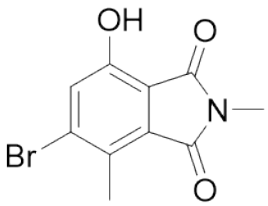
	Cys Probe	Fluorophore core
LUMO+1		
LUMO		
HOMO		
HOMO-1		

Fig. S14. HOMO-LUMO of DFT-optimized geometries of **Myco-Cys** and **Myco-OH**(B3LYP/6-31g* basis set and 6-311g* only for Se, G09).





Found: M+Na$^+$ = 291.9580

Calculated: M+Na$^+$ = 291.9763

Fig. S15. ESI-MS spectrum of the reaction product of **Myco-Cys** and cysteine.

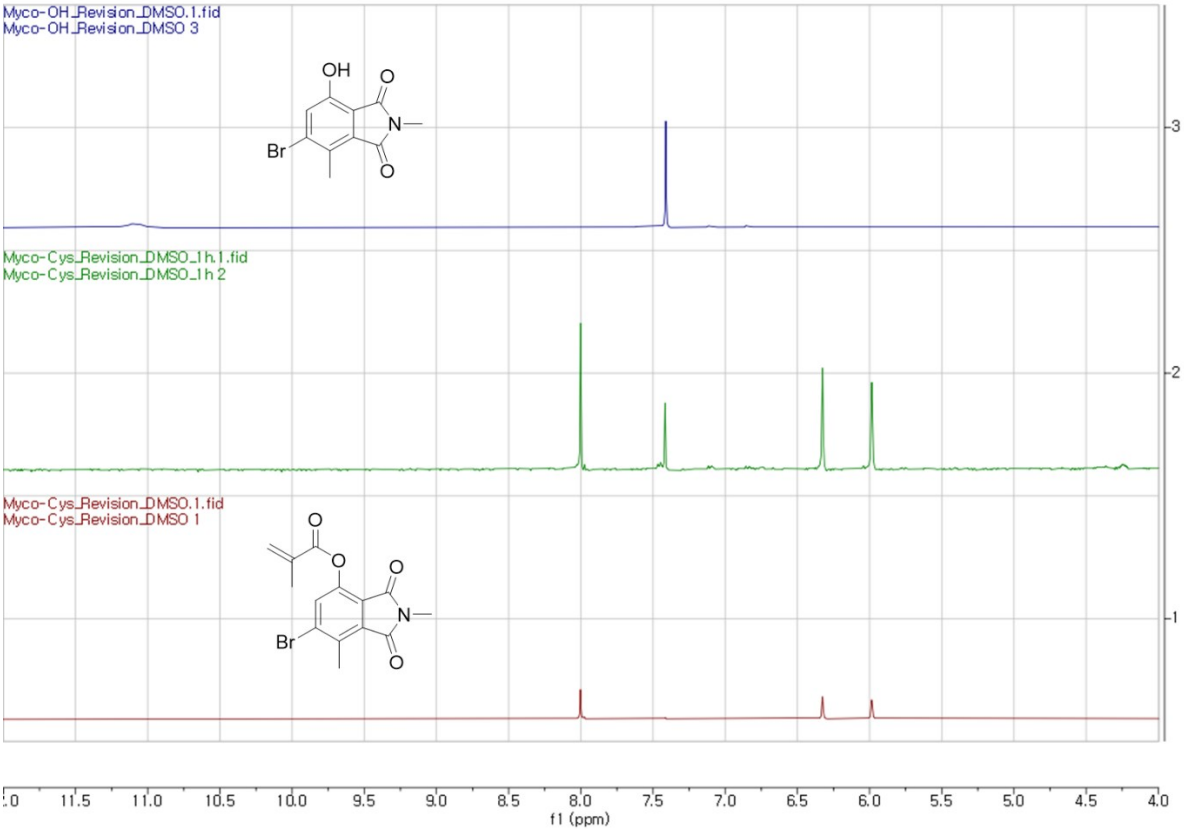


Fig. S16. ^{1}H NMR spectrum of **Myco-OH**, **Myco-Cys**+cysteine, **Myco-Cys** in DMSO-d6.

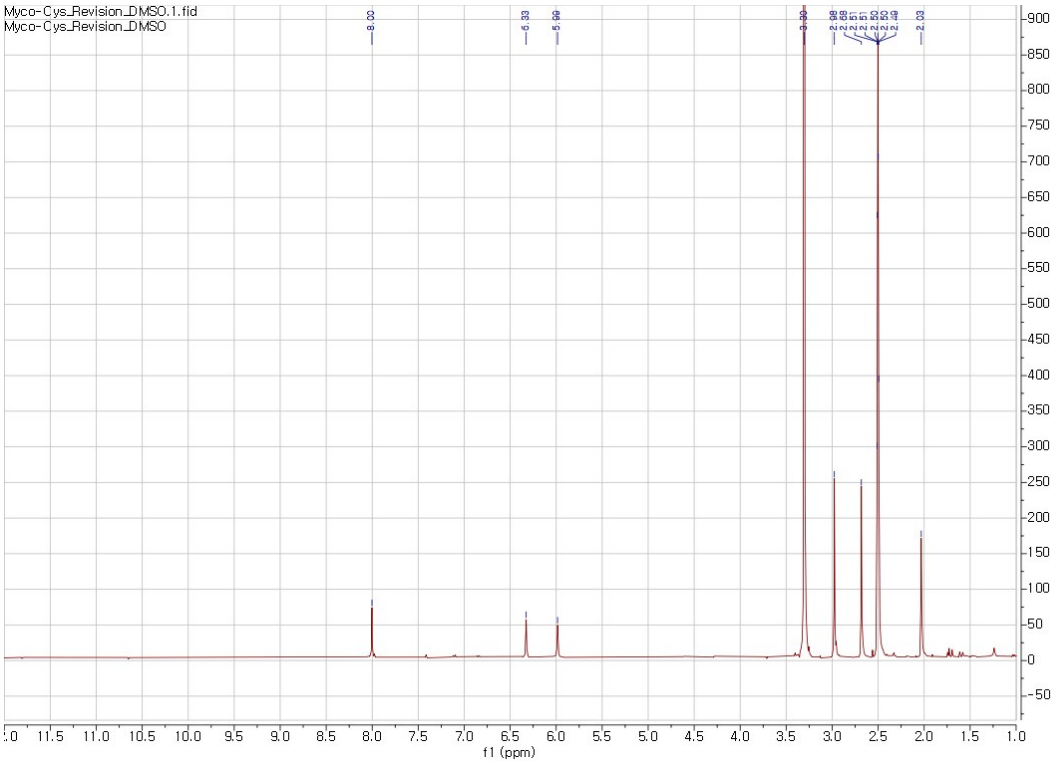


Fig. S17. [1]H NMR spectrum of **Myco-Cys** in DMSO-d6.

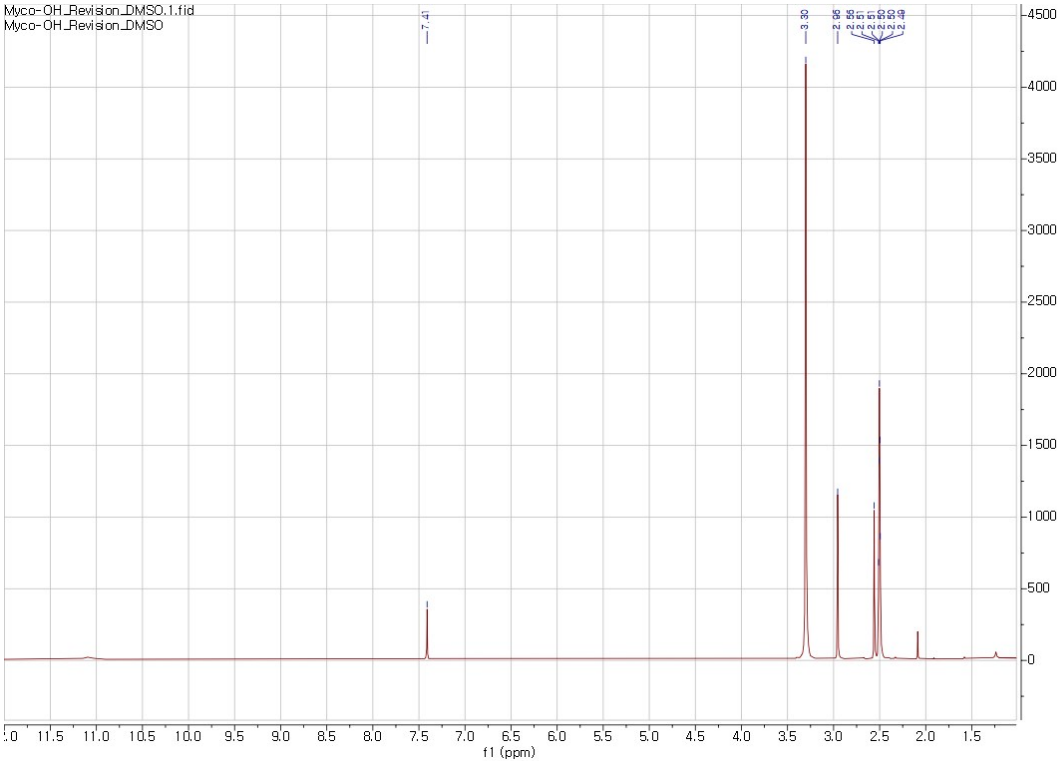


Fig. S18. [1]H NMR spectrum of **Myco-OH** in DMSO-d6.

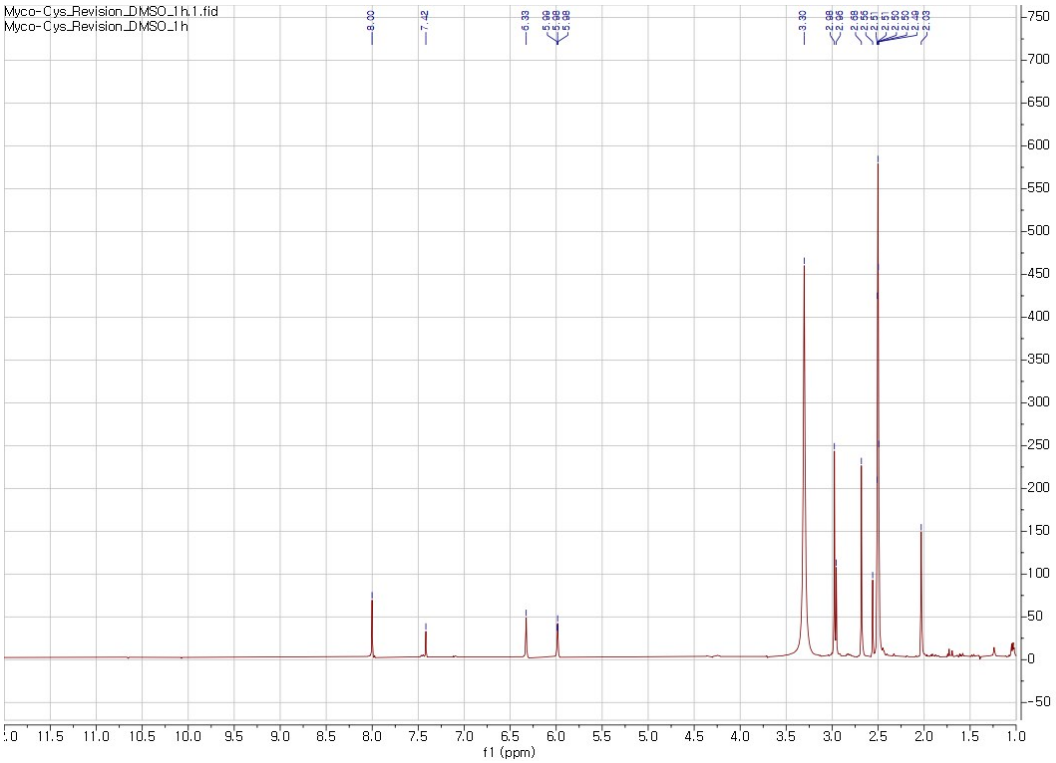


Fig. S19. ^{1}H NMR spectrum of **Myco-Cys**+cysteine in DMSO-d6.

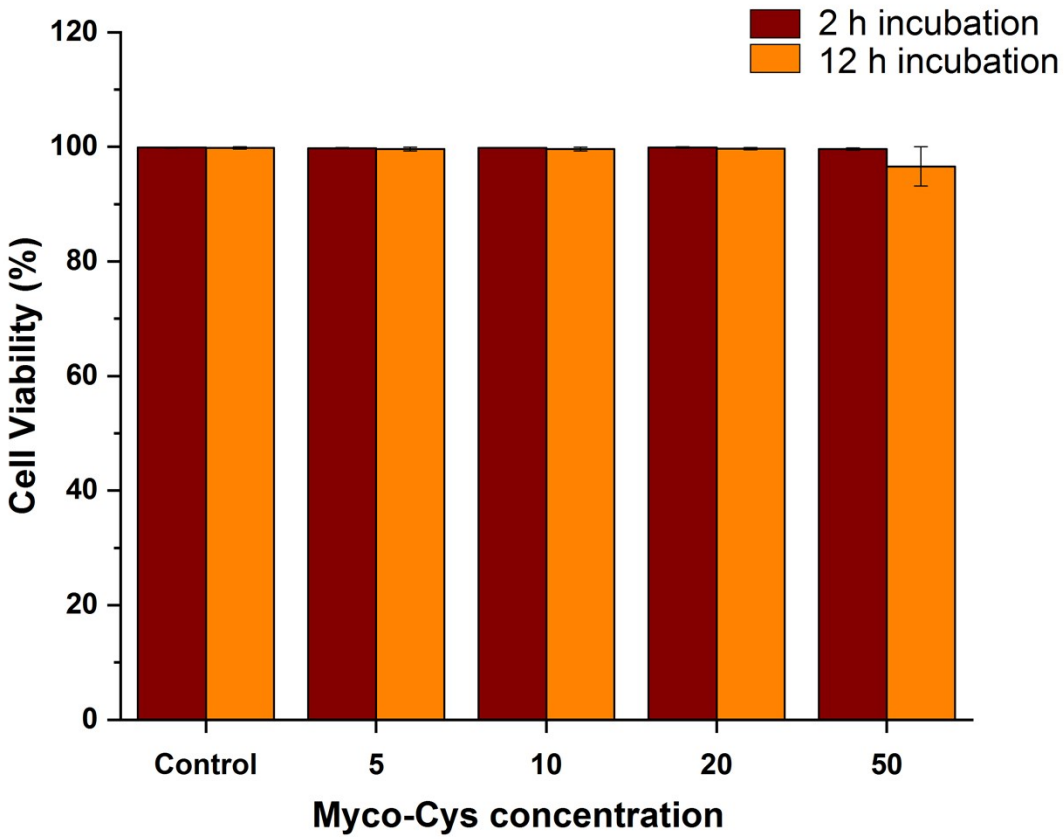


Fig. S20. Concentration-dependent cell viability assays with LIVE/DEAD® viability/cytotoxicity kit. A549 cells were incubated with various concentrations (0, 5, 10, 20, 50 μM) of **Myco-Cys** for 2 h and 12 h.

	f	Composition	CI(%)
Myco-Cys	**0.0629**	HOMO-1 → LUMO	13.1
		HOMO → LUMO	**76.6**
	0.0207	**HOMO-1 → LUMO**	**69.6**
		HOMO → LUMO	9.73
Myco-OH	**0.1164**	**HOMO → LUMO**	**87.8**

Table S1. Absorption energies with largest oscillator strength for **Myco-Cys** and **Myco-OH** (B3LYP/6-31g* basis set and 6-311g* only for Se, G09)

C_1	V	A	$\bar{A}$	C_2	P	Log P
1.3×10^{-5}	3.5	0.0399 0.0491 0.0454	0.0415	1.24×10^{-5}	1.89	0.276
1.6×10^{-5}	4.8	0.0475 0.0429 0.0461	0.0455	1.36×10^{-5}	6.96	0.842
2.0×10^{-5}	6.0	0.0439 0.0409 0.0440	0.0428	1.28×10^{-5}	22.20	1.34

Table S2. Results of experimental determination of log P value by the shake flask method for the **Myco-Cys**

※ C_1 = Concentration (mol L^{-1}) of the stock solution in *n*-octanol before partition; V = volume (μL) of stock solution; A = absorbance in buffer solution after the partition (λ = 500 nm); $\bar{A}$ = arbitrary absorbance in buffer solution after partitioning (λ = 500 nm); C_2 = concentration (mol L^{-1}) in buffer solution after partitioning; P = partition coefficient; log P = logarithm of the partition coefficient.

Properties (NOTE: abbreviation same as website)	Value (Myco-OH)	Value (Myco-Cys)
milogP	**1.77**	**2.52**
TPSA	**59.30**	**65.38**
Natom	**15**	**20**
MW	**270.08**	**338.16**
nON	**4**	**5**
nOHNH	**1**	**0**
nviolations	**0**	**0**
nrotb	**0**	**3**
volume	**182.98**	**247.22**

Table S3. Information of the **Myco-OH** and **Myco-Cys** calculated through 'molinspiration property engine v2011.04' at the website, http://www.molinspiration.com.

References:

1. C. A. Lipinski, F. Lombardo, B. W. Dominy, P. J. Feeney, *Adv. Drug Del. Rev.*, **1997**, *23*, 3-25.

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