Electronic Supplementary Material (ESI) for New Journal of Chemistry.

A coumarin-based reversible fluorescent probe for Cu^{2+} and S^{2-} and its applicability in *vivo* and organisms imaging

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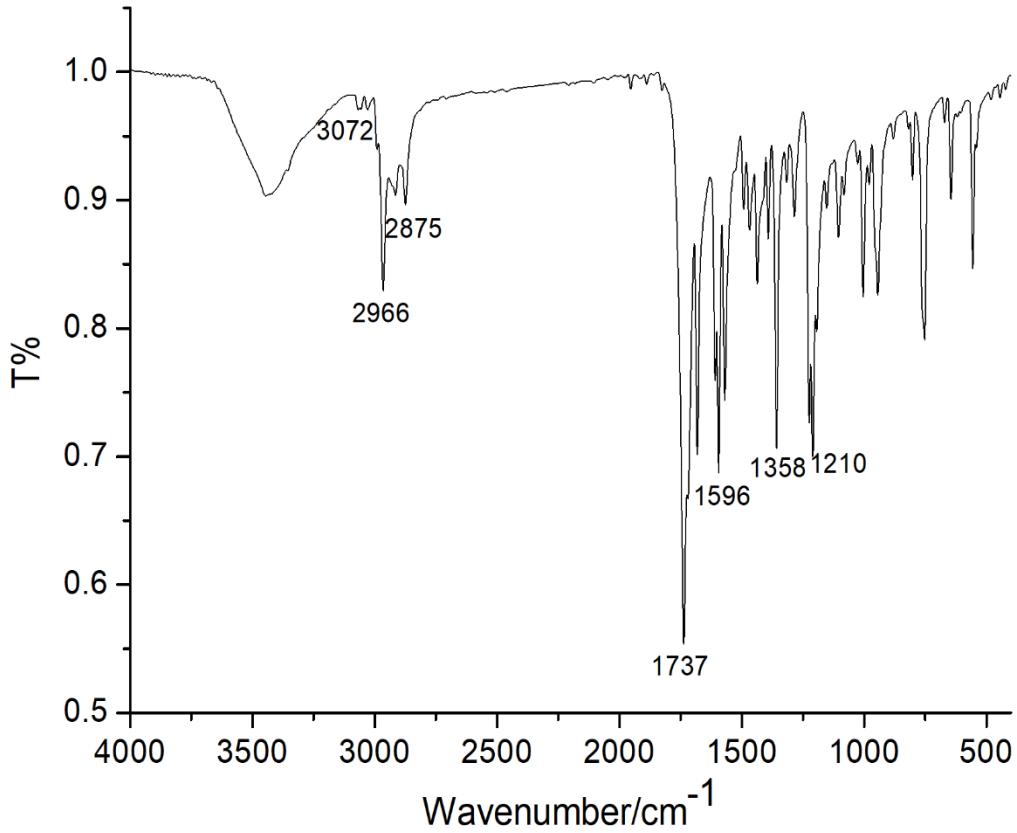


Fig. S1. IR spectrum of 3-acetyl-8-tert-butyl coumarin (**BuCAC**).

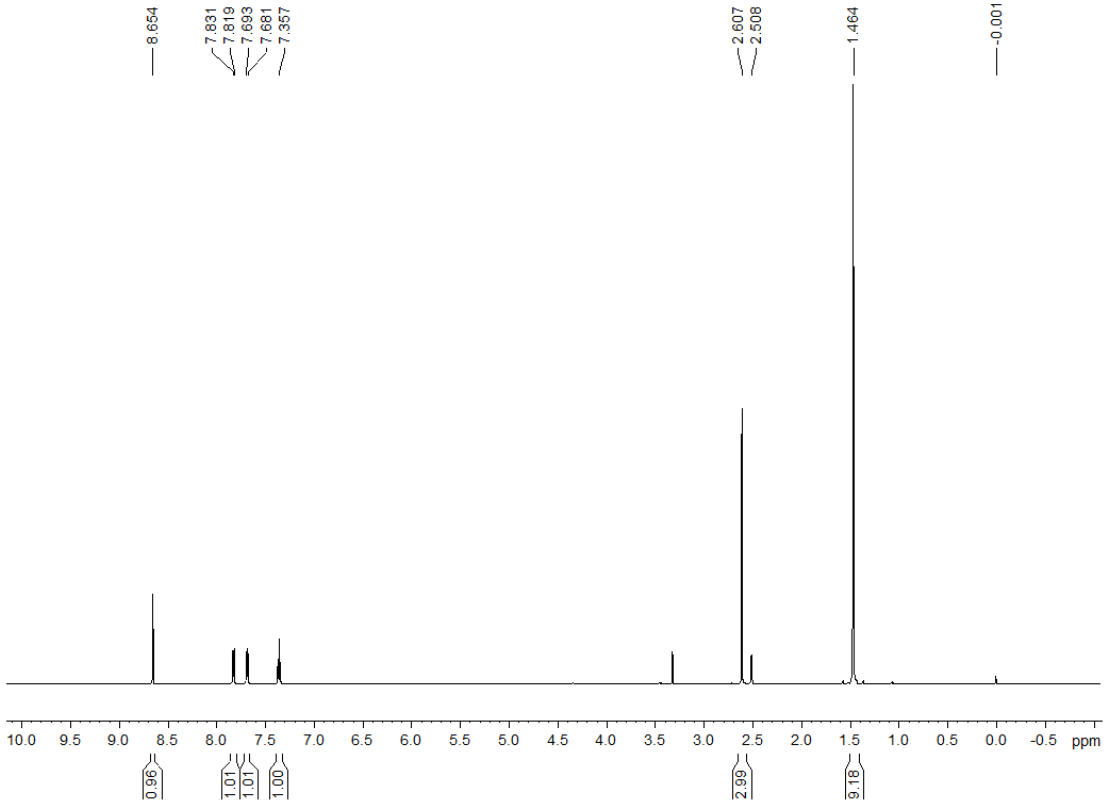


Fig. S2. ^{1}H NMR spectrum of 3-acetyl-8-tert-butyl coumarin (**BuCAC**).

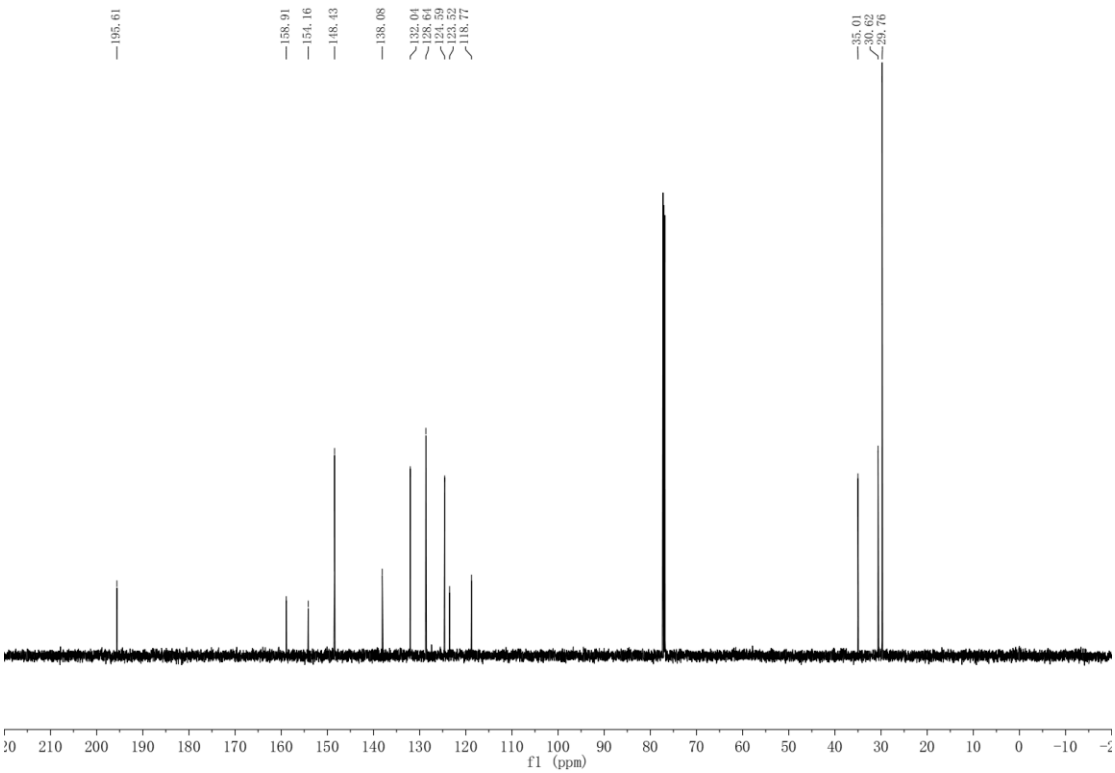


Fig. S3. ^{13}C NMR spectrum of 3-acetyl-8-tert-butyl coumarin (**BuCAC**).

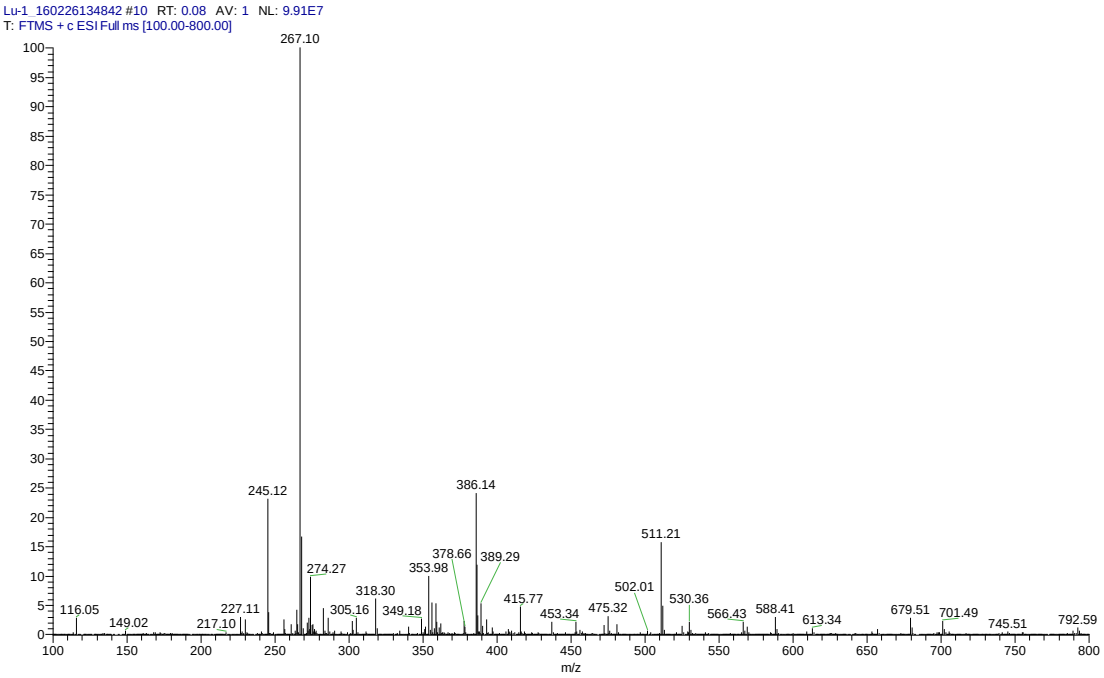


Fig. S4. 3-acetyl-8-tert-butyl coumarin (**BuCAC**).

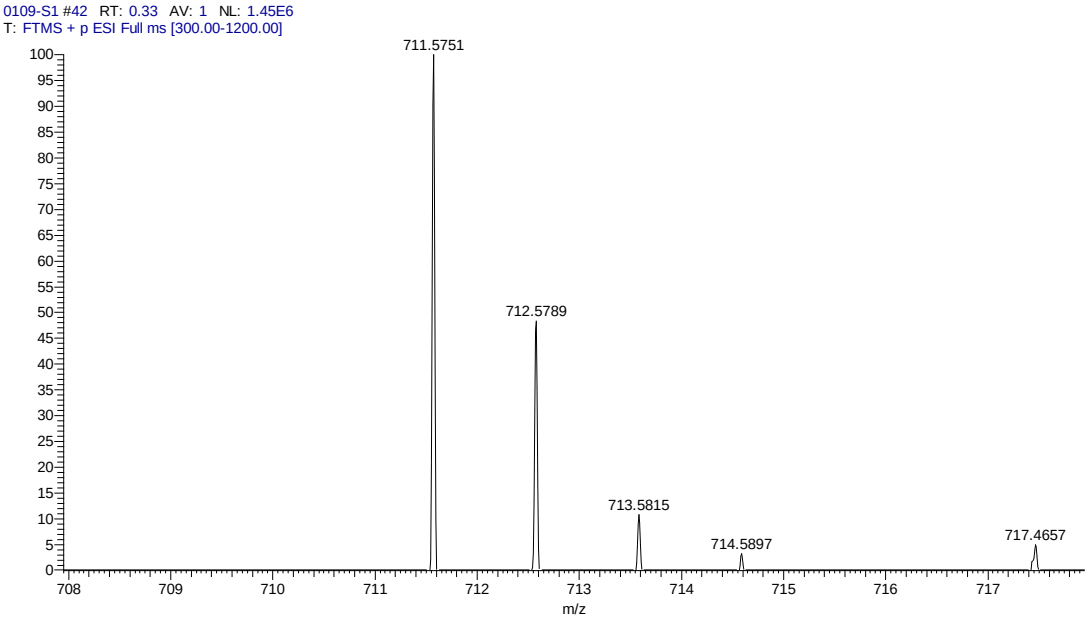


Fig. S5. Experimental mass spectrum of **BuCAC-Cu^{2+}**.

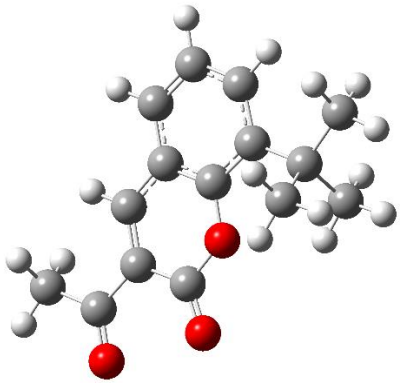


Fig. S6 The optimized molecular structure of **BuCAC.**

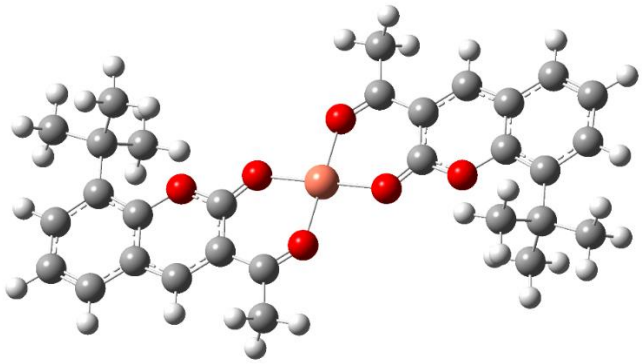
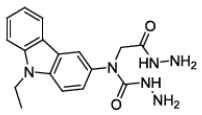
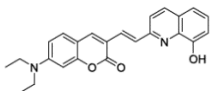
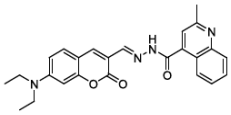
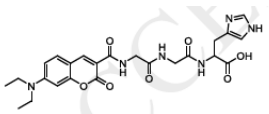
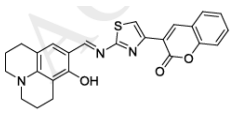
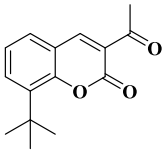


Fig. S7 The optimized molecular structure of **BuCAC-Cu^{2+}.**

Table S1 Compared with other currently reported probe for Cu^{2+} and S^{2-}.

Structure	Limit of detection		Ref
	Cu^{2+}	S^{2-}	
	6.5×10^{-8}M	2.9×10^{-7}M	39
	1.1×10^{-7}M	2.2×10^{-7}M	40
	3.1×10^{-7}M	1.9×10^{-7}M	41
	1.9×10^{-7}M	4.4×10^{-7}M	42
	1.5×10^{-6}M	No data	43
	3.03×10^{-7}M	1.7×10^{-7}M	This work

T**able S2** The HOMO and LUMO distributions of **BuCAC** and **BuCAC**-Cu^{2+}**.**

	BuCAC	**BuCAC-Cu^{2+}**	
		α orbital	β orbital
LUMO (eV)	-2.636	-8.743	-9.449
HOMO (eV)	-6.826	-12.248	-12.245
Gap(eV)	4.190	3.505	2.796

Ethical Statement of Animal Experiment

All animal procedures were performed in accordance with the Guidelines for Care and Use of Laboratory Animals of " Nanjing Forestry " University and experiments were approved by the Animal Ethics Committee of " Nanjing Forestry University ".