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

SUPPORTING INFORMATION

Nerve Agent Simulant Diethyl Chlorophosphate Detection Using Cyclization Reaction Approach with High Stokes Shift System

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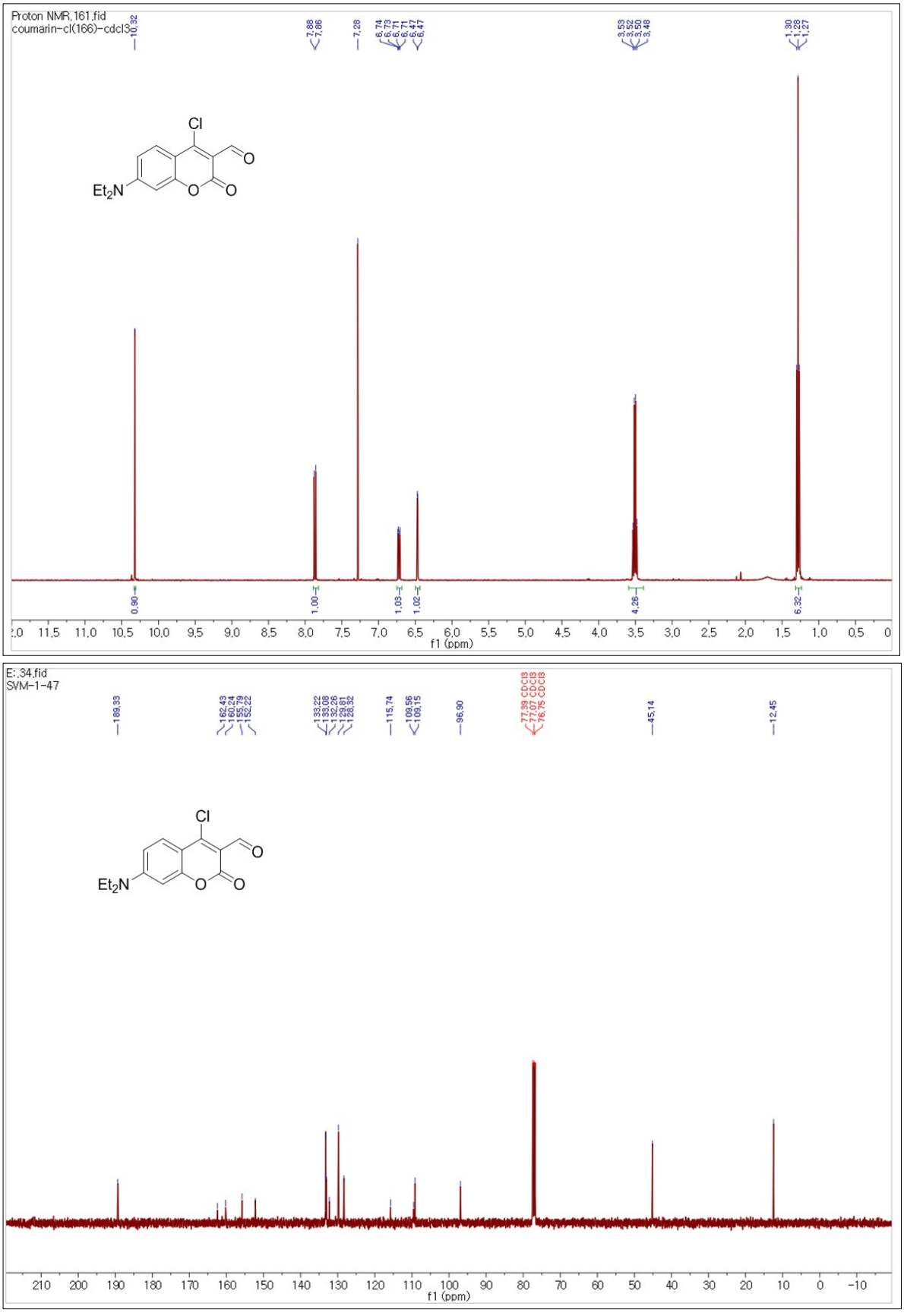


Fig. S1. (*top*) ^{1}H and (*bottom*) ^{13}C NMR spectrum of compound **1.**

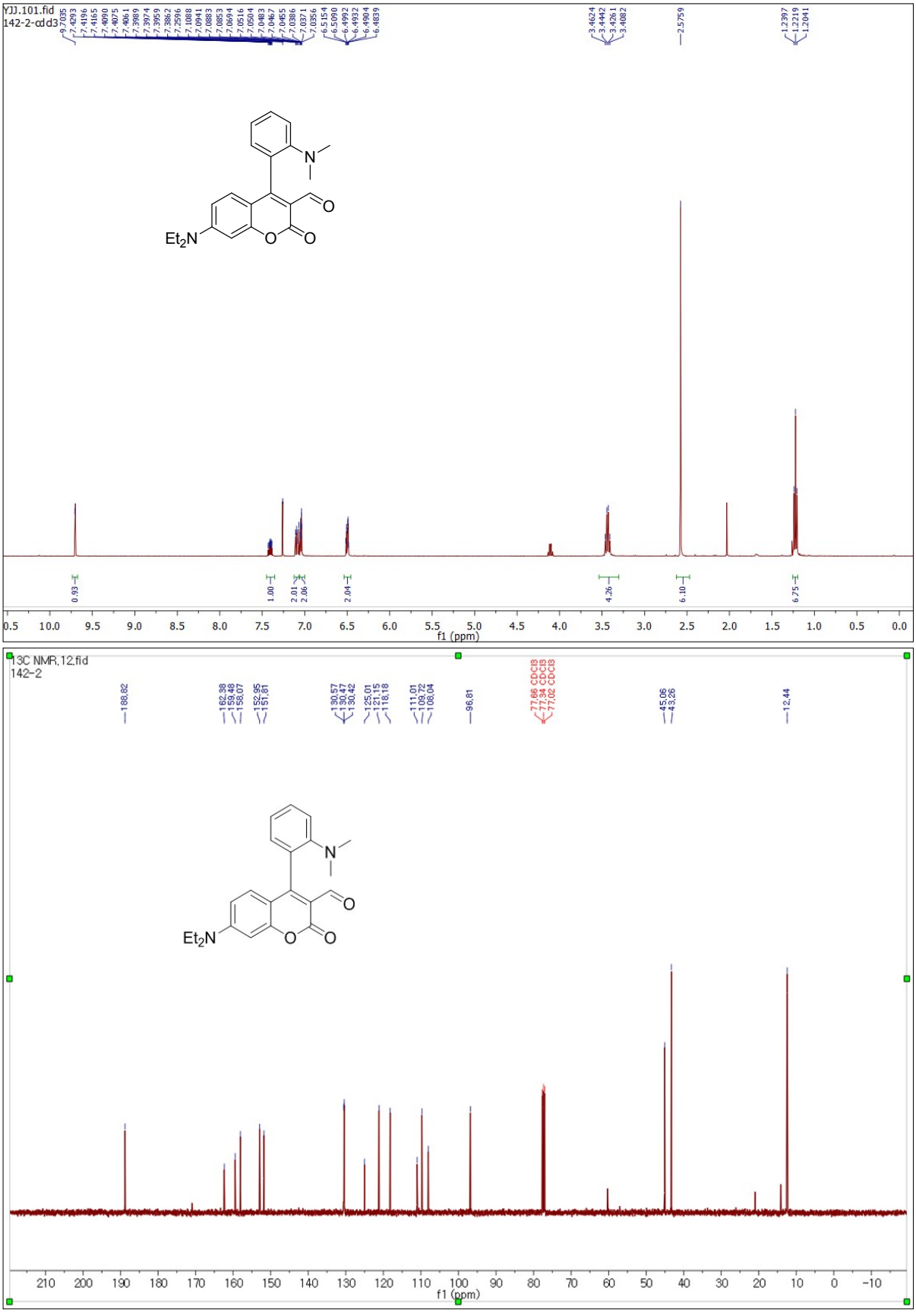


Fig. S2. (*top*) ^{1}H and (*bottom*) ^{13}C NMR spectrum of compound **2.**

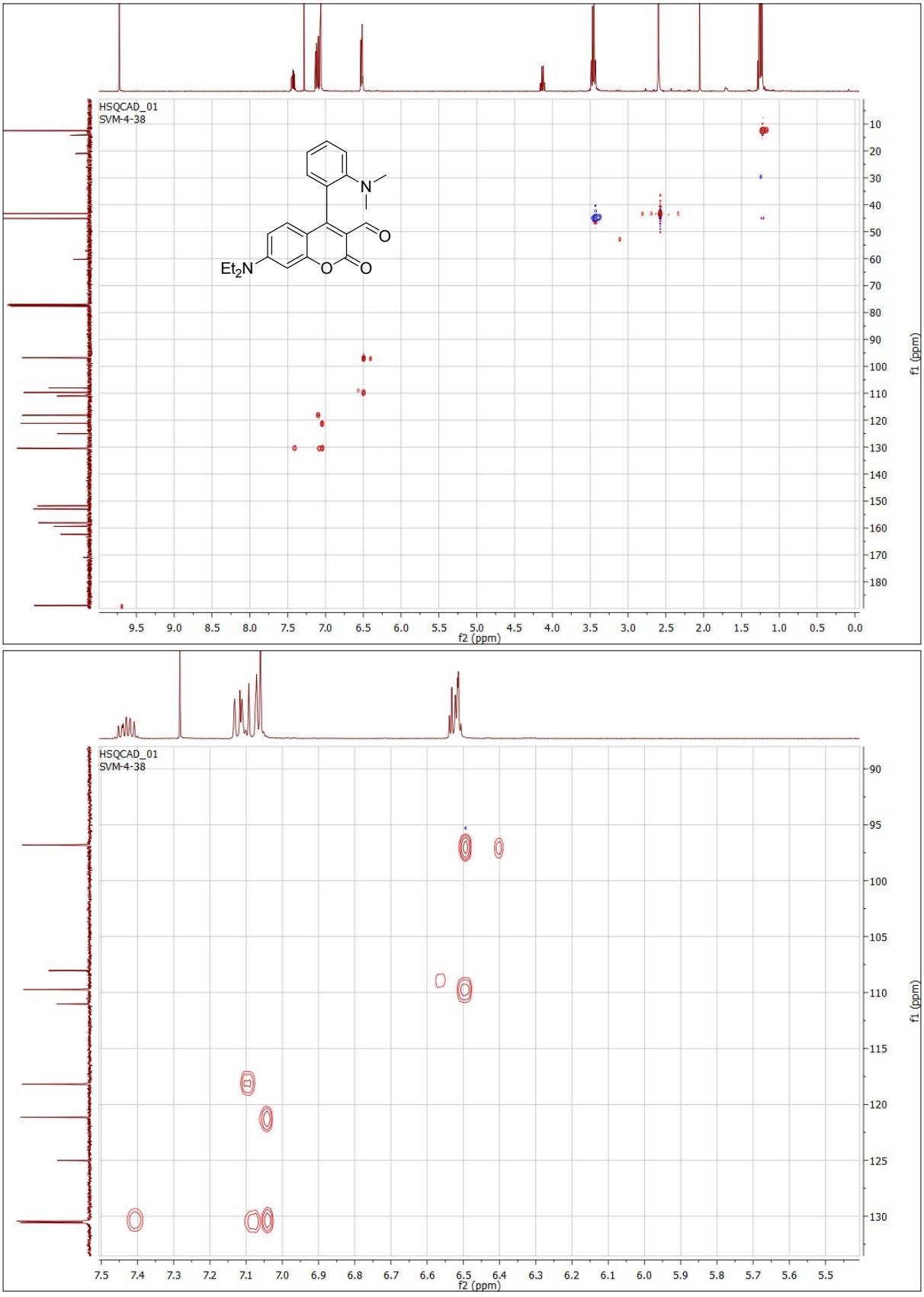


Fig. S3. (*top*) ^{1}H-^{13}C HSQC NMR spectrum of compound **2** and (*bottom*) expanded aromatic region.

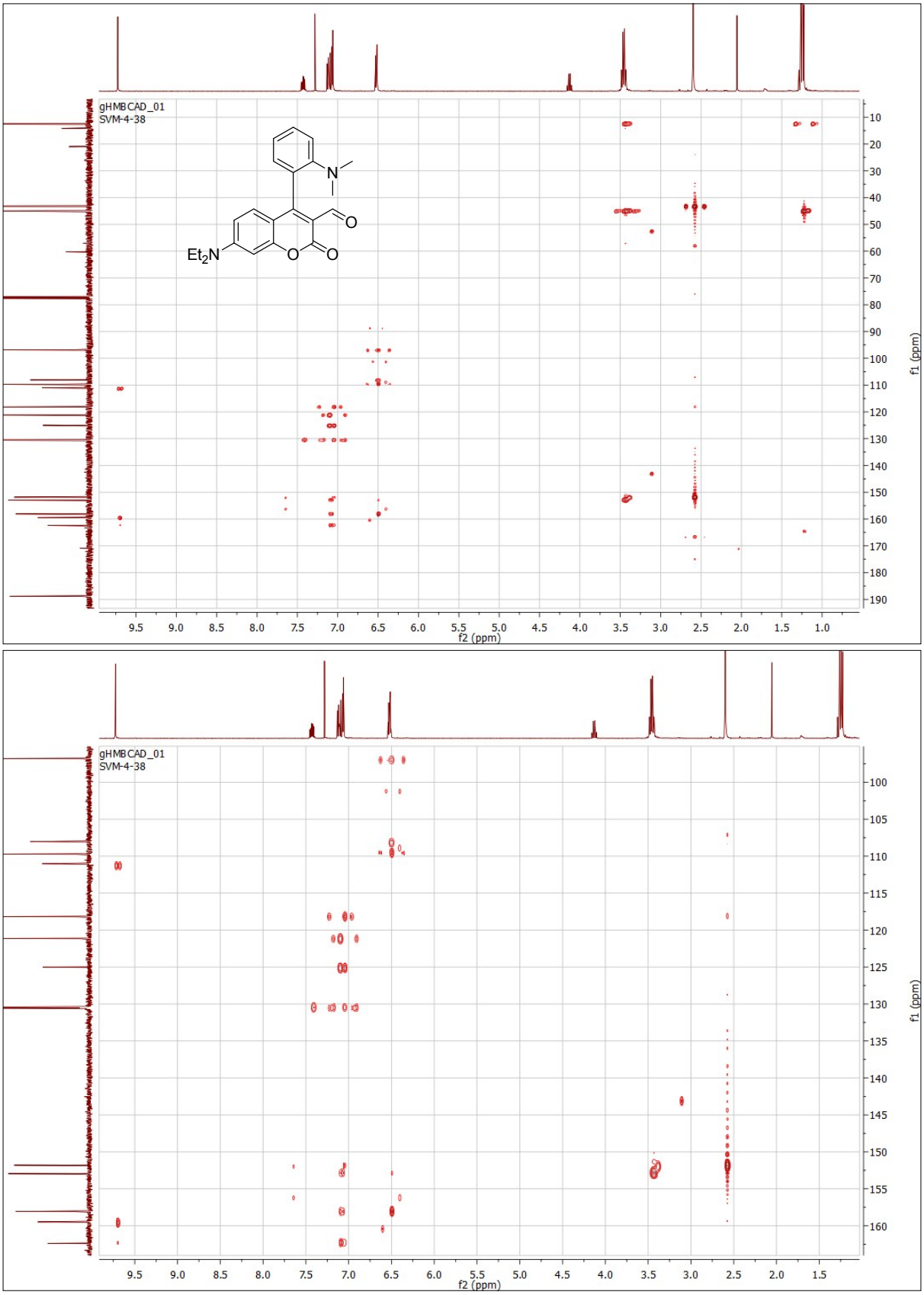
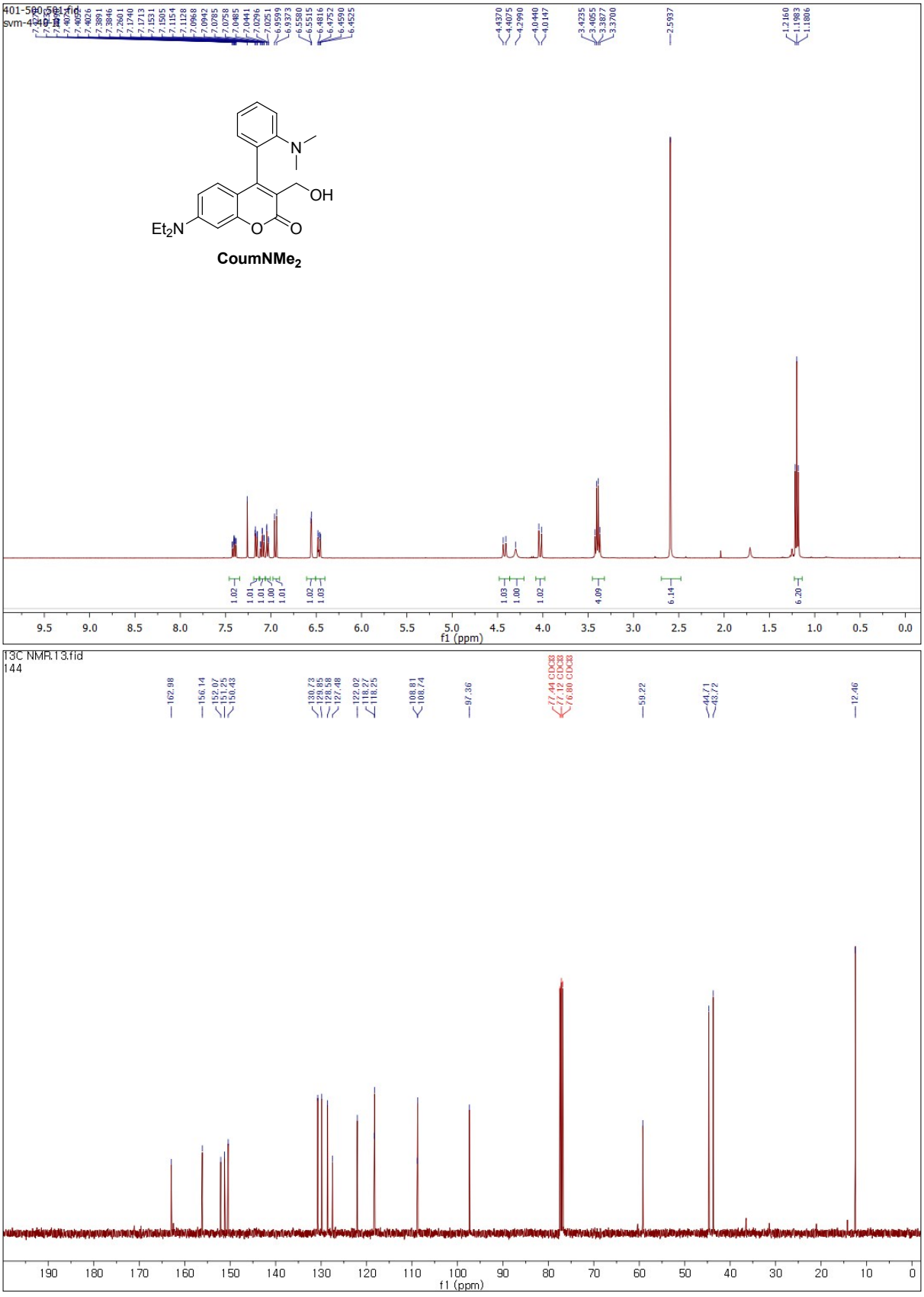


Fig. S4. (*top*) ^{1}H-^{13}C HMBC NMR spectrum of compound **2** and (*bottom*) expanded aromatic region.



CoumNMe$_2$

Fig. S5. (*top*) ^{1}H and (*bottom*) ^{13}C NMR spectrum of **CoumNMe$_2$**.

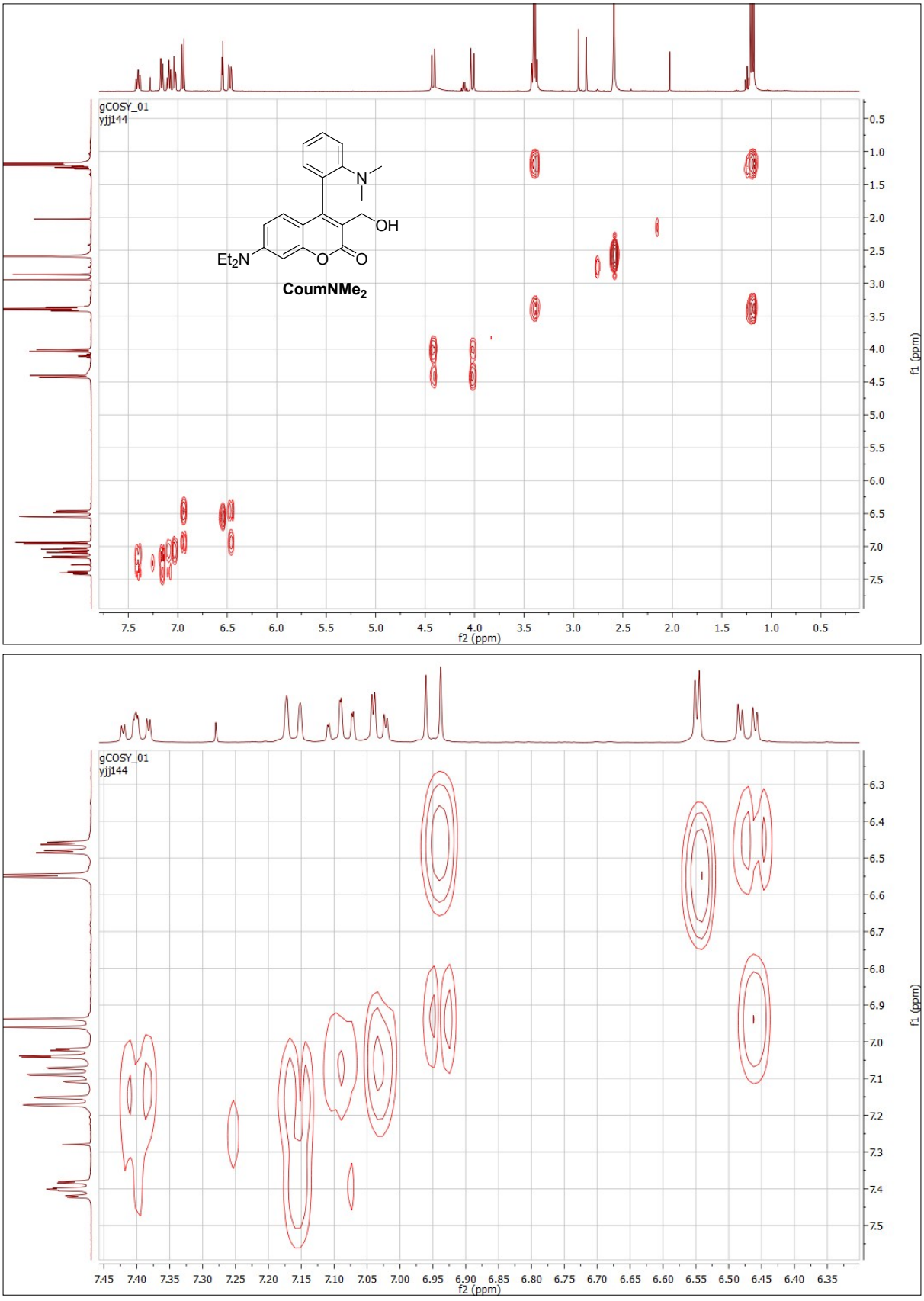


Fig. S6. (*top*) COSY NMR spectrum of **CoumNMe$_2$** and (*bottom*) expanded aromatic region.

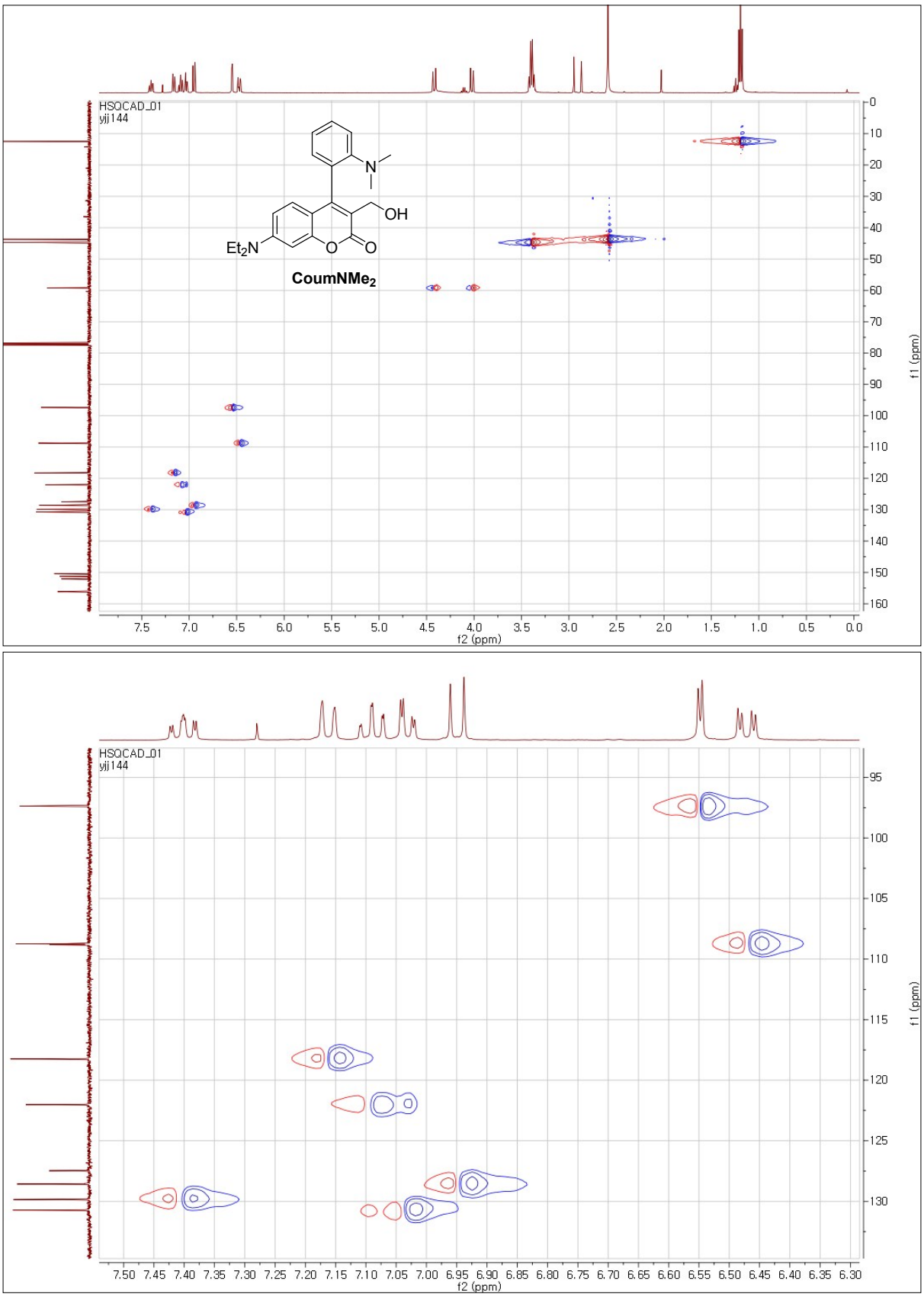


Fig. S7. (*top*) ^{1}H-^{13}C HSQC NMR spectrum of **CoumNMe$_2$** and (*bottom*) expanded aromatic region.

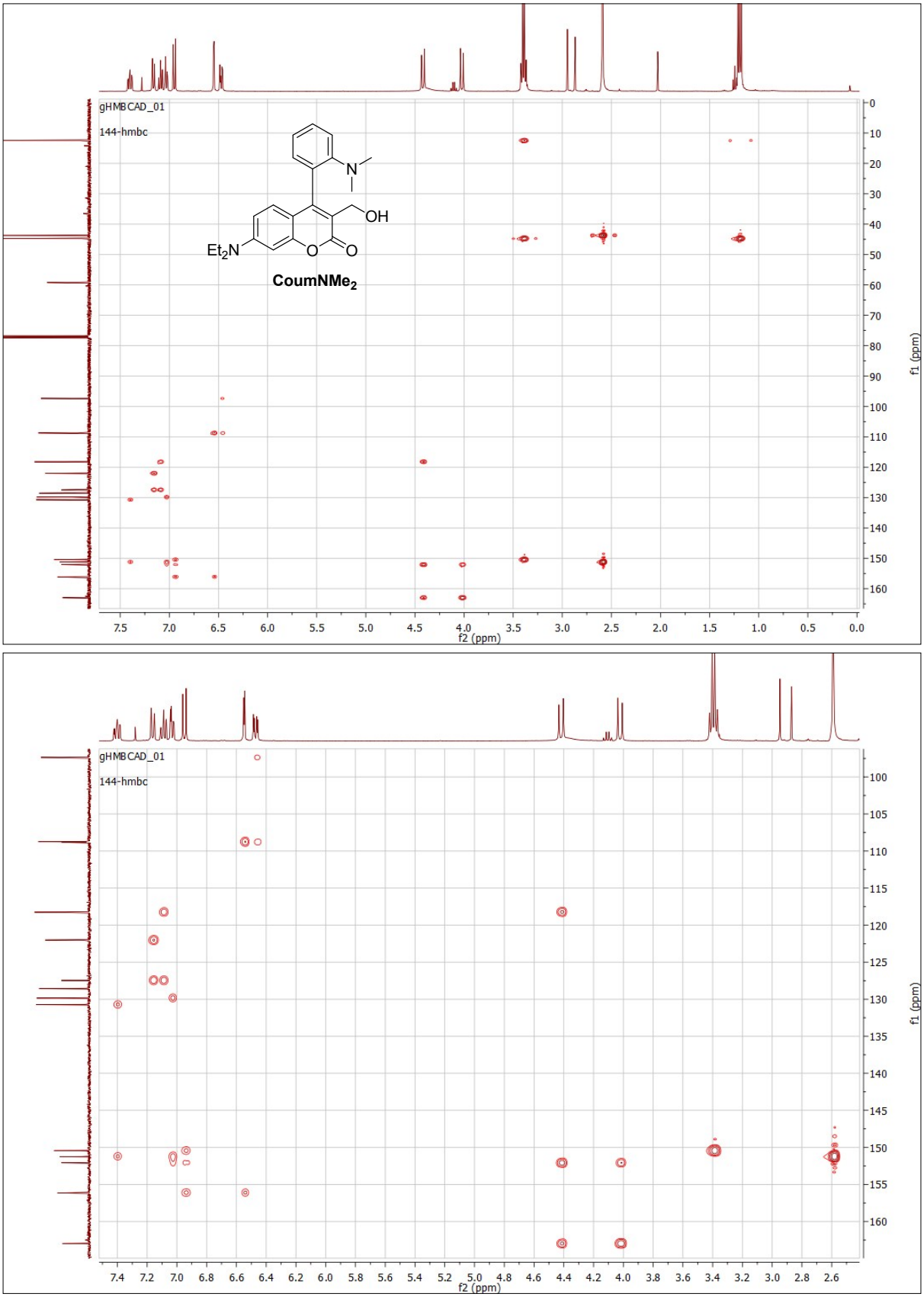


Fig. S8. (*top*) ^{1}H-^{13}C HMBC NMR spectrum of **CoumNMe$_2$** and (*bottom*) expanded aromatic region.

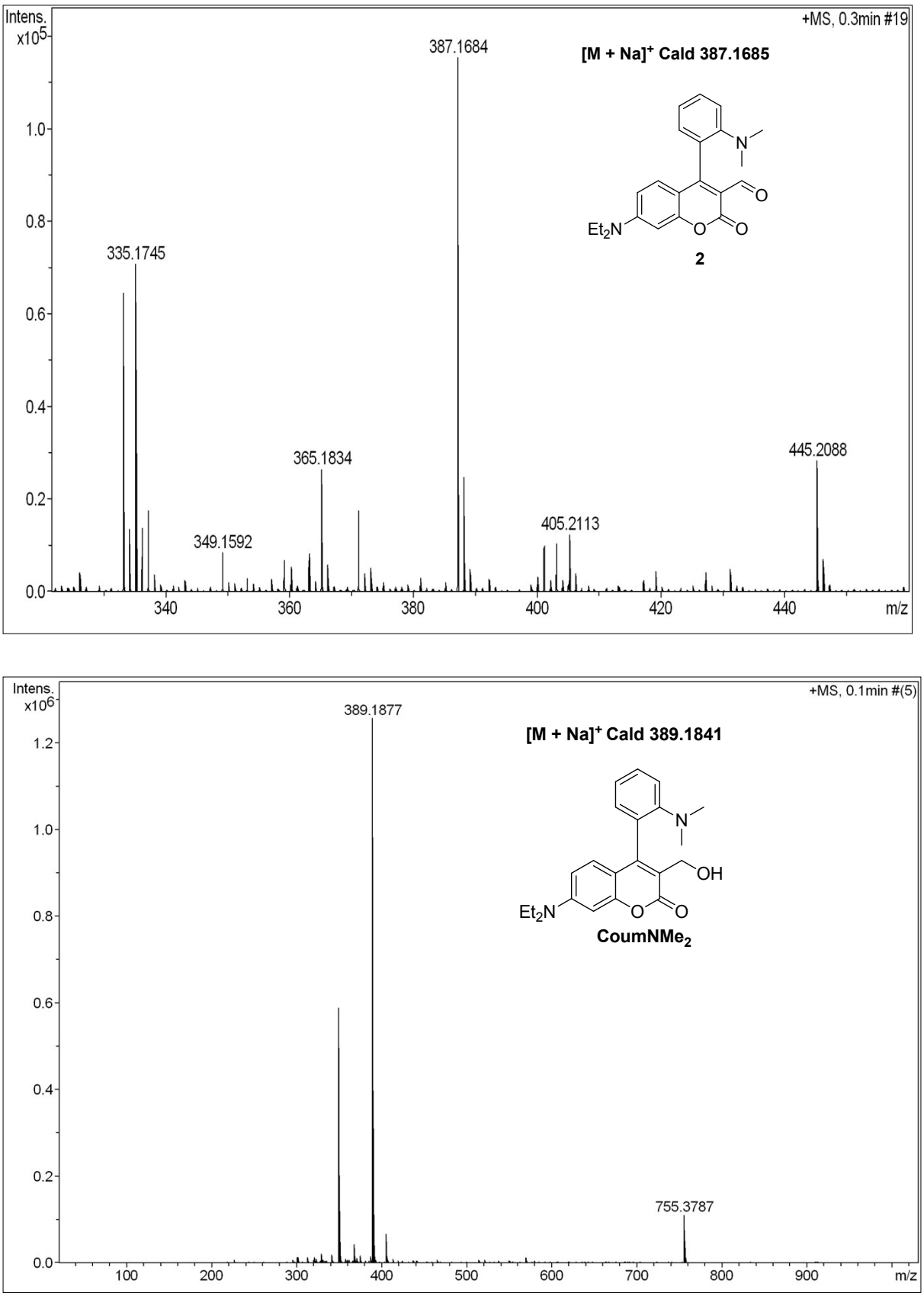


Fig. S9. (*top*) HR-MS (ESI) spectrum of compound **2** and (*bottom*) **CoumNMe$_2$**.

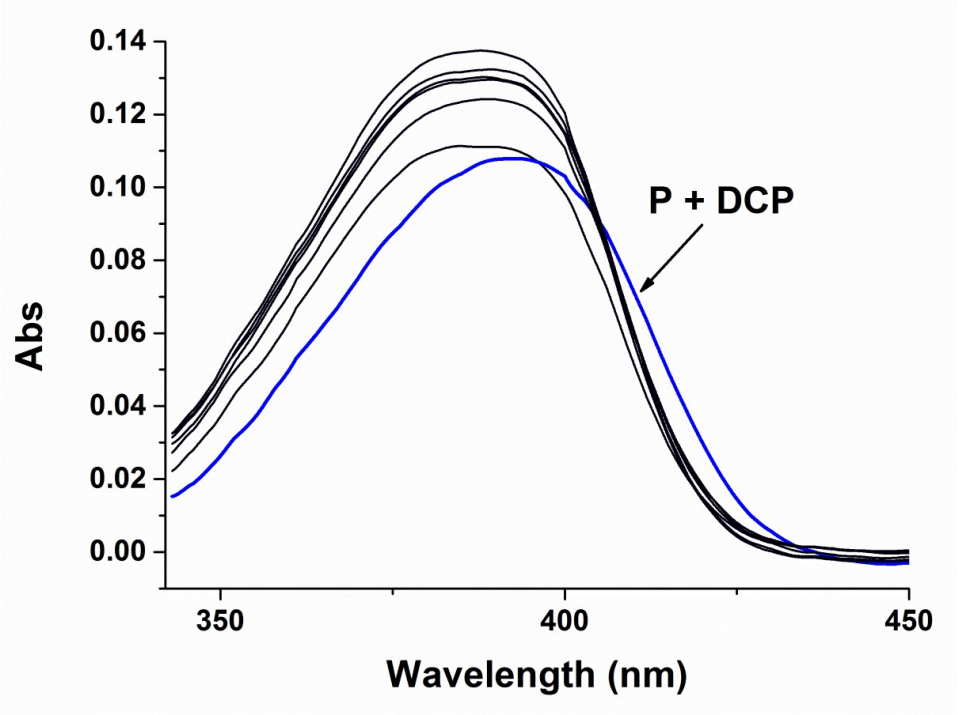


Fig. S10. Absorbance spectra of **CoumNMe$_2$** (10 μM) with 0.5 mM of DCP (blue) and other analytes (DCEP, DEMP, TEPP, TFA and HCl) in $CHCl_3$, incubated for 5.0 min at room temperature.

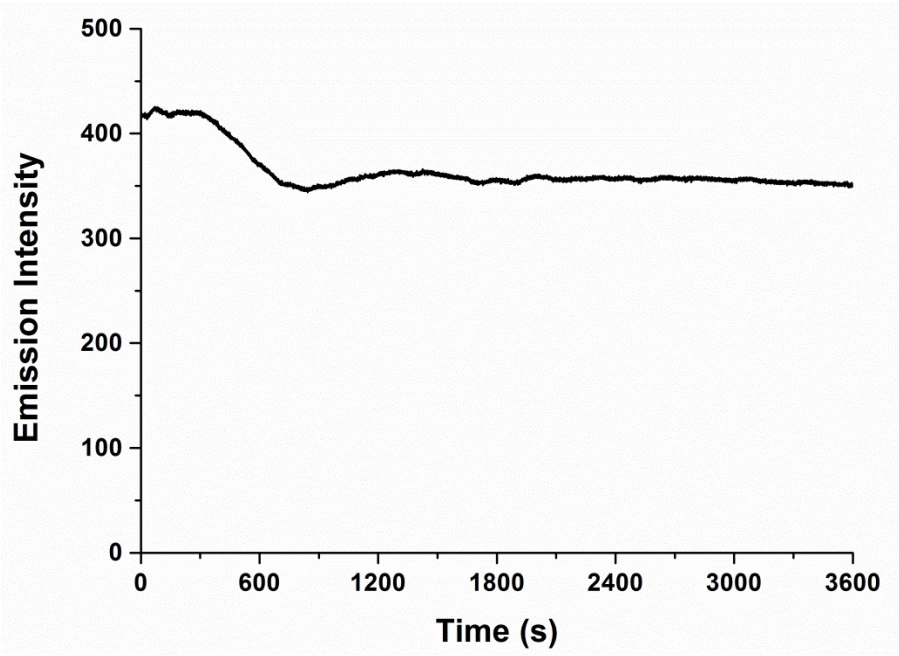


Fig. S11. Time-dependent emission spectral changes of **CoumNMe$_2$** (10 μM) with 0.5 mM DCP in $CHCl_3$, λ_{ex} = 388 nm, λ_{em} = 460 nm.

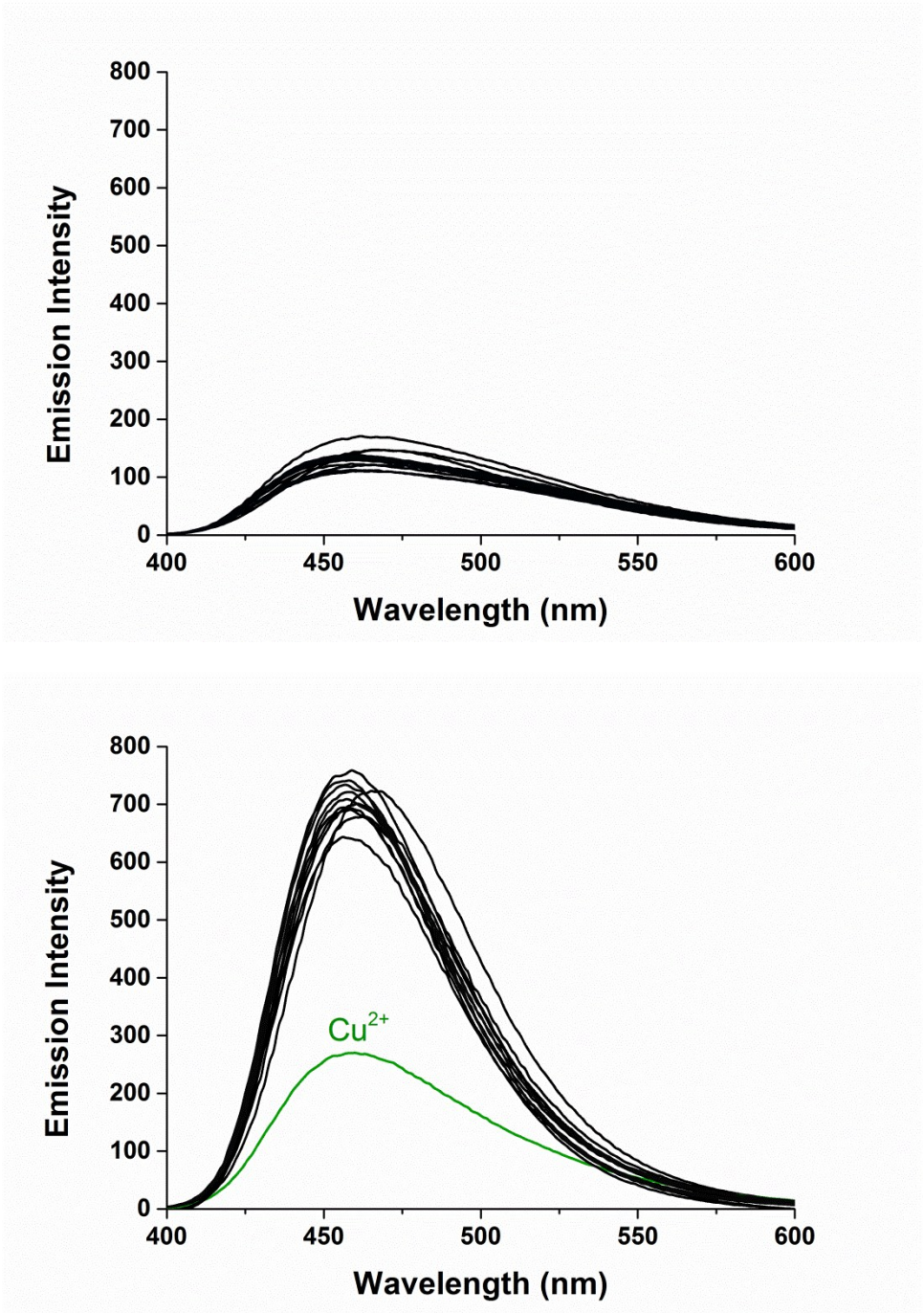


Fig. S12. (*top*) Emission spectra of **CoumNMe$_2$** (10 μM) with excess amount of metal ions (*vide infra*) in $CHCl_3$; (*bottom*) Emission spectra of **CoumNMe$_2$** (10 μM) with excess amount of metal ions (Li^+, Na^+, K^+, Cd^{2+}, Ce^+, Co^{2+}, Cu^{2+}, Fe^{3+}, Fe^{2+}, Hg^{2+}, Mg^{2+}, Mn^{2+}, Pb^{2+}, Zn^{2+}) followed by addition of DCP (0.5 mM), in $CHCl_3$, λ_{ex} = 388 nm, λ_{em} = 460 nm, slit width 3.0 nm/3.0 nm; (herein respective metal perchlorate salts were used as sources of the matal ion).

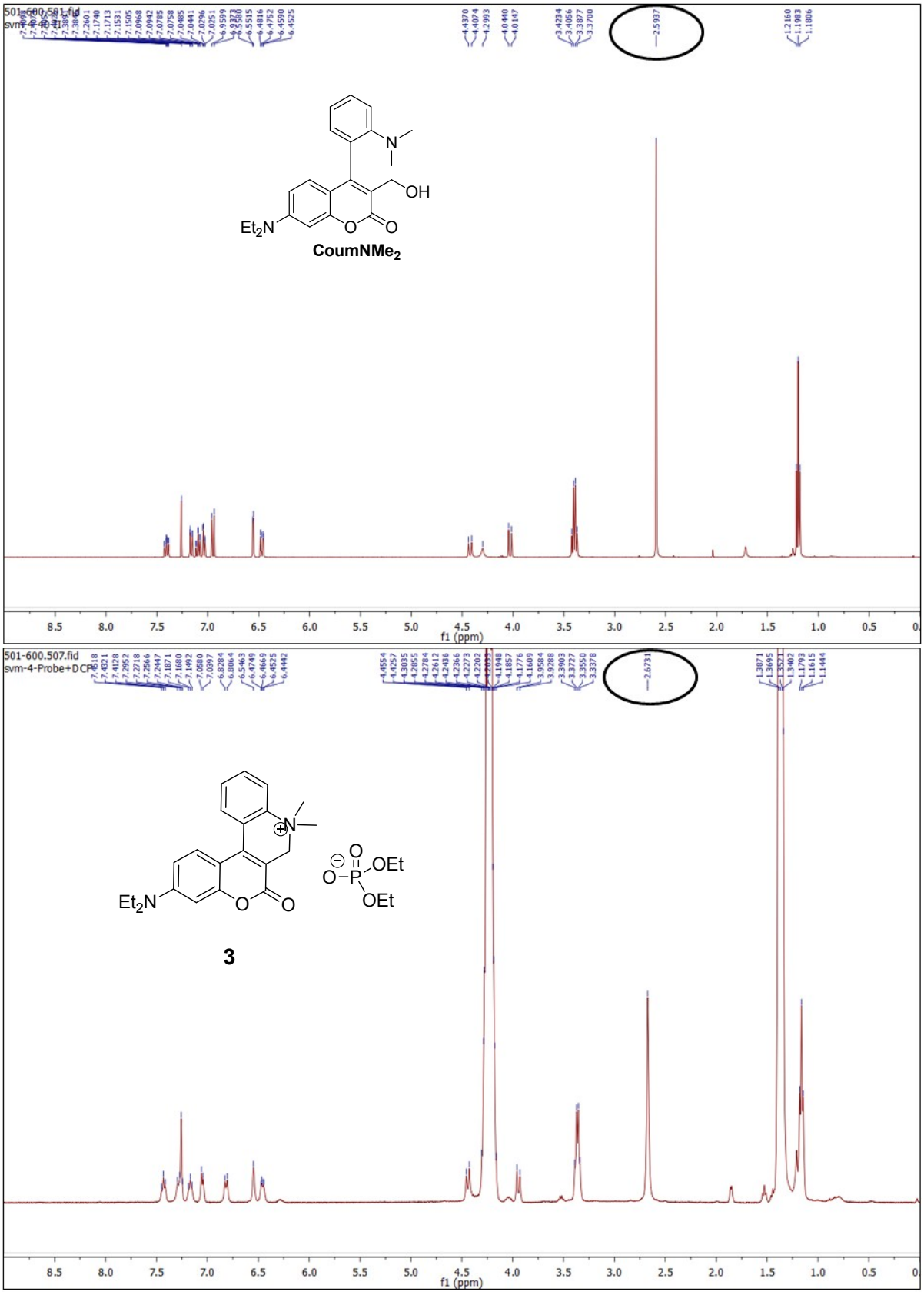


Fig. S13. (*top*) ^{1}H NMR spectra of **CoumNMe$_2$**, and (*bottom*) **CoumNMe$_2$** with DCP in $CDCl_3$ at room temperature.

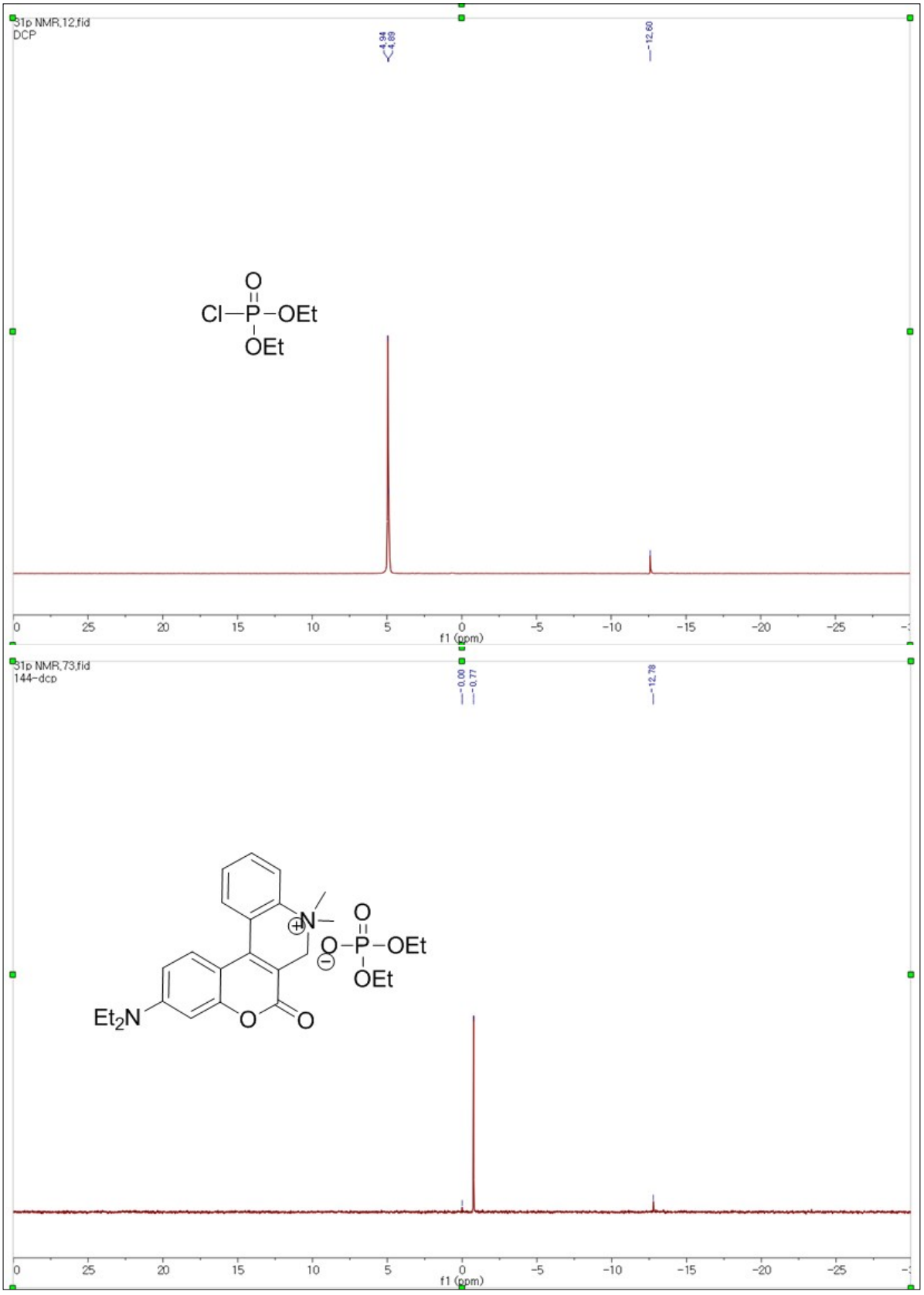


Fig. S14. (*top*) ^{31}P NMR spectra of DCP, and (*bottom*) **CoumNMe$_2$** with DCP in $CDCl_3$ at room temperature.

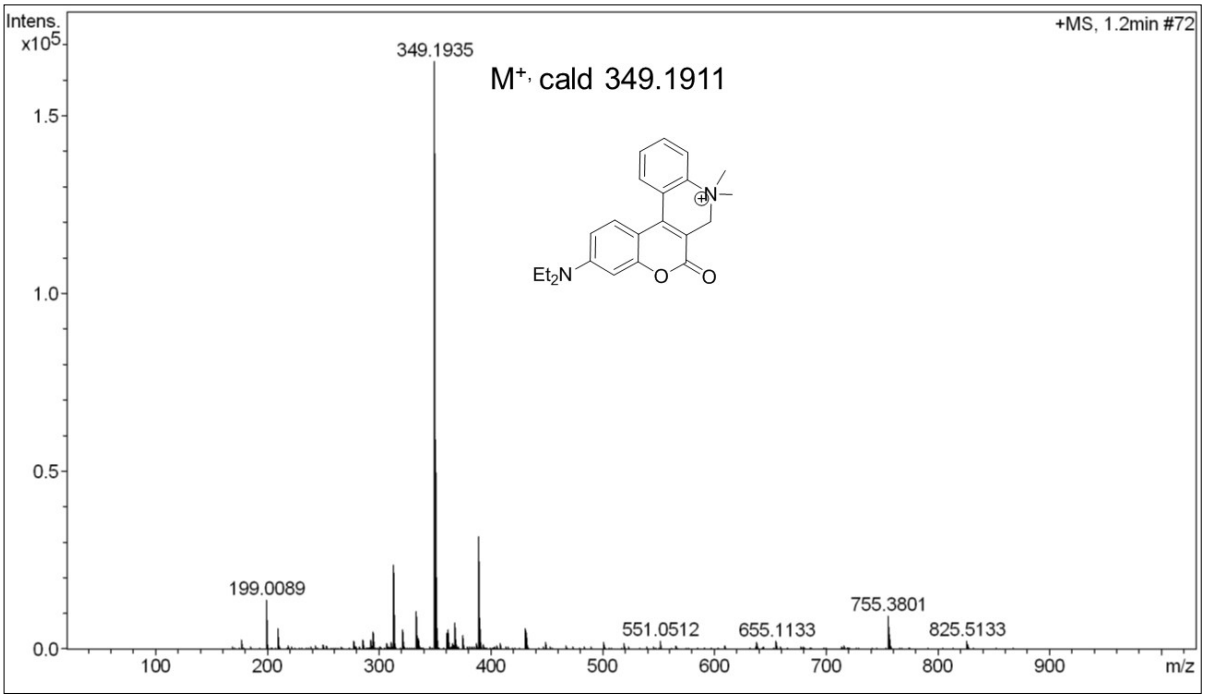
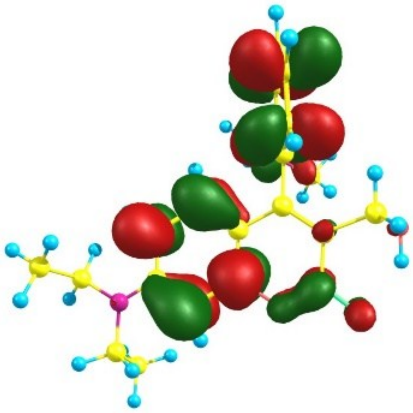
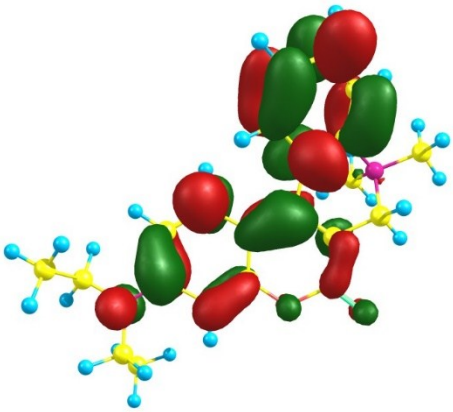
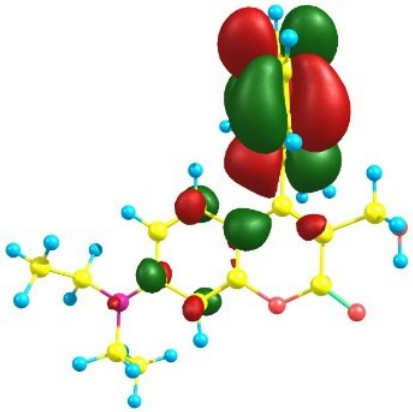
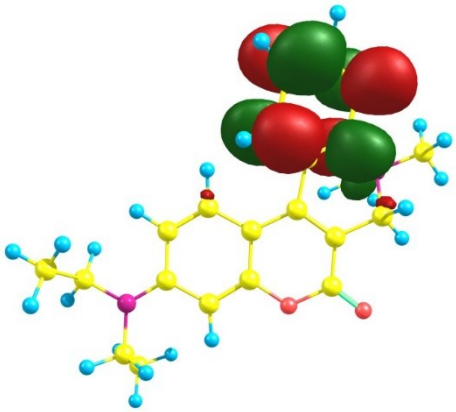
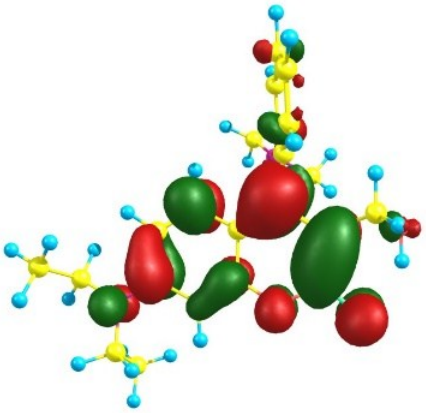
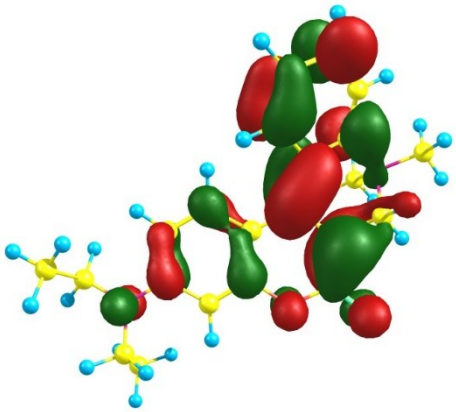
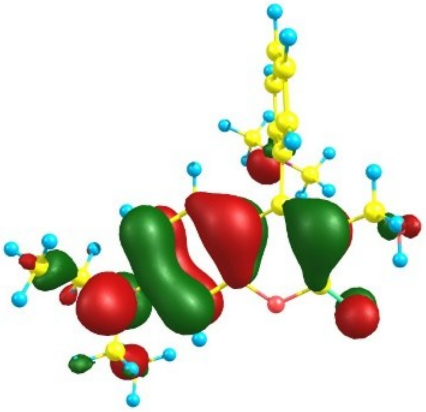
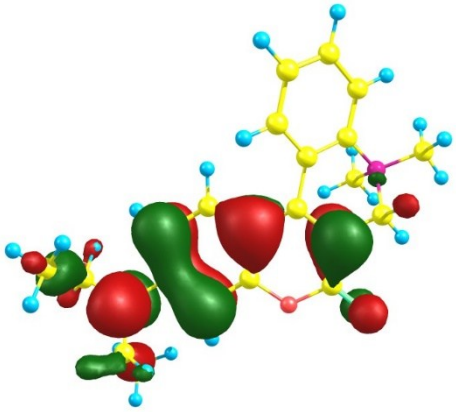


Fig. S15. HR-MS spectrum (ESI) of compound **3**.

Table S1. Absorption energies with largest oscillator strength for **CoumNMe$_2$** and **3** (B3LYP/6-31g* basis set, G09).

	f	Composition	CI (%)
CoumNMe$_2$	0.2927	HOMO-1 → LUMO HOMO → LUMO	48.5 48.7
3	0.2422	HOMO → LUMO	98.3

	CoumNMe$_2$	**3**
LUMO+2		
LUMO+1		
LUMO		
HOMO		

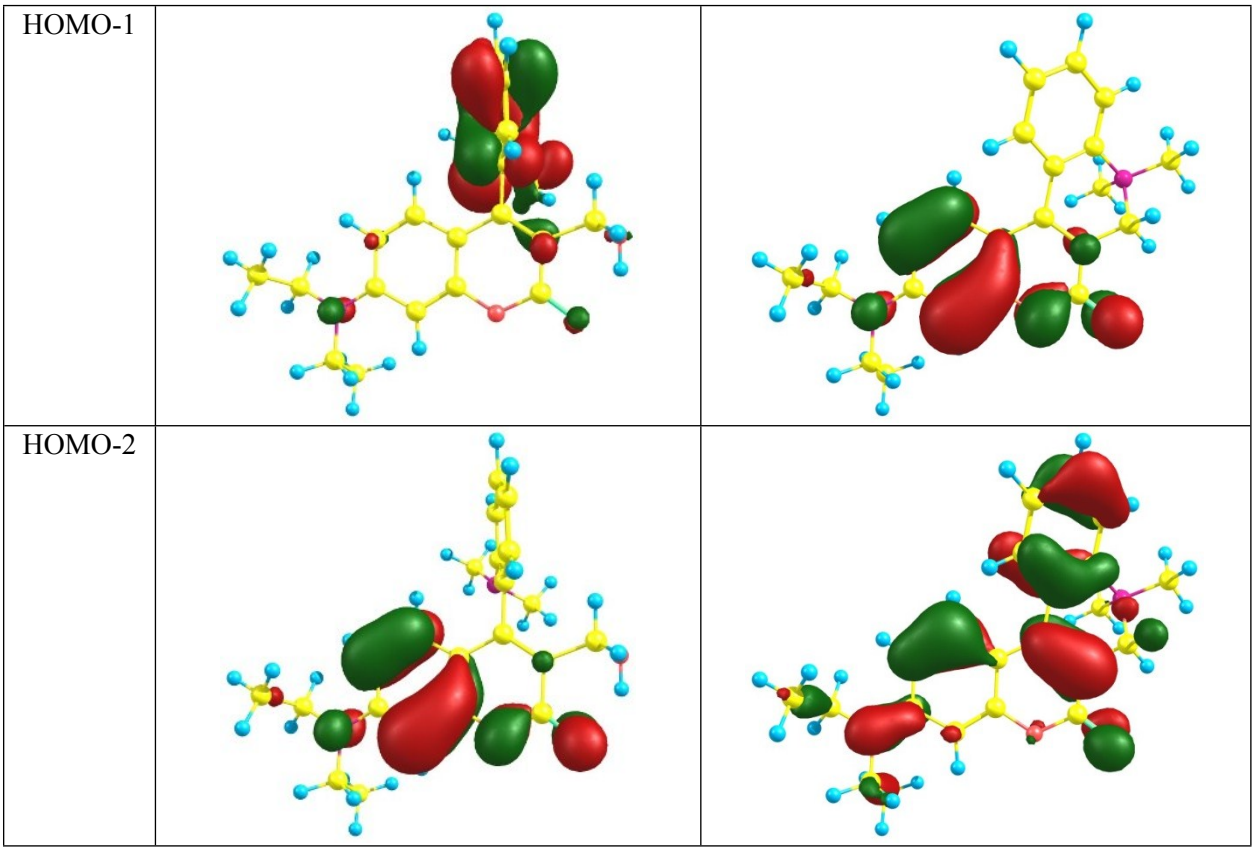


Fig. S16. DFT calculations of **CoumNMe$_2$** and compound **3**.

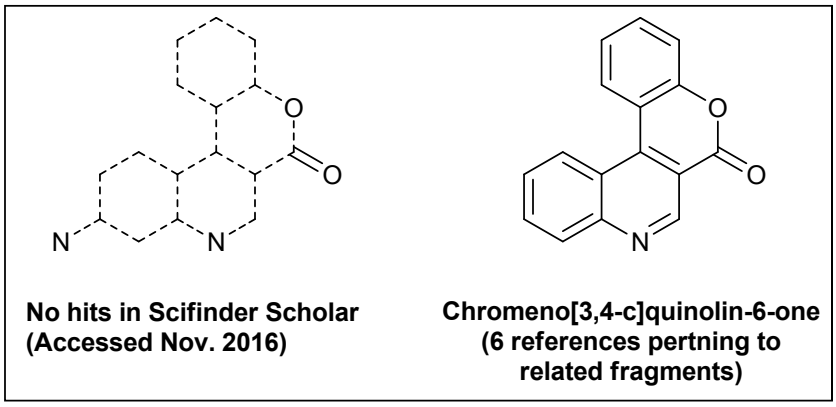


Fig. S17. Previously published research related to the skeleton of the chrominoquinoline core.

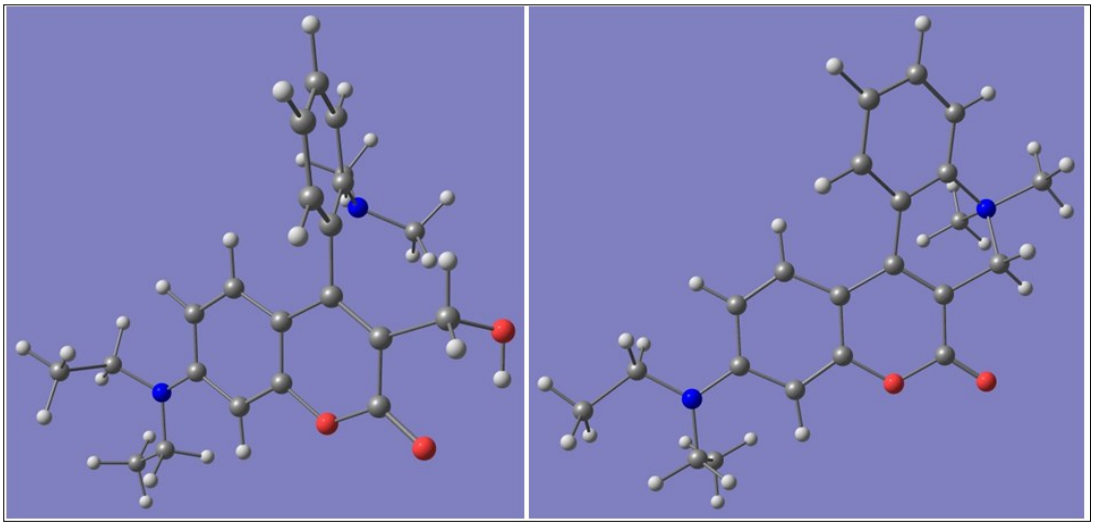


Fig. S18. DFT-optimized geometries of (*left*) **CoumNMe$_2$**, and (*right*) compound **3** (B3LYP/6-31g* basis set, G09).

Information of the **CoumNMe$_2$** and **3** calculated through 'molinspiration property engine v2011.04' at the website, http://www.molinspiration.com.

Properties (CoumNMe$_2$) (NOTE: abbreviation same as website)	**Value**
milogP	3.89
TPSA	56.91
Natom	27
MW	364.46
nON	5
nOHNH	1
nviolations	0
nrotb	6
volume	358.23

Properties (3) (NOTE: abbreviation same as website)	**Value**
milogP	-0.20
TPSA	29.54
Natom	26
MW	351.47
nON	4
nOHNH	0
nviolations	0
nrotb	3
volume	341.4

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