Supplementary Materials: Synthesis and Sensing Applications of Fluorescent 3-Cinnamoyl Coumarins

Preeti Yadav, Hardeep Singh Gill, Karam Chand, Lian Li, Jayant Kumar and Sunil K. Sharma

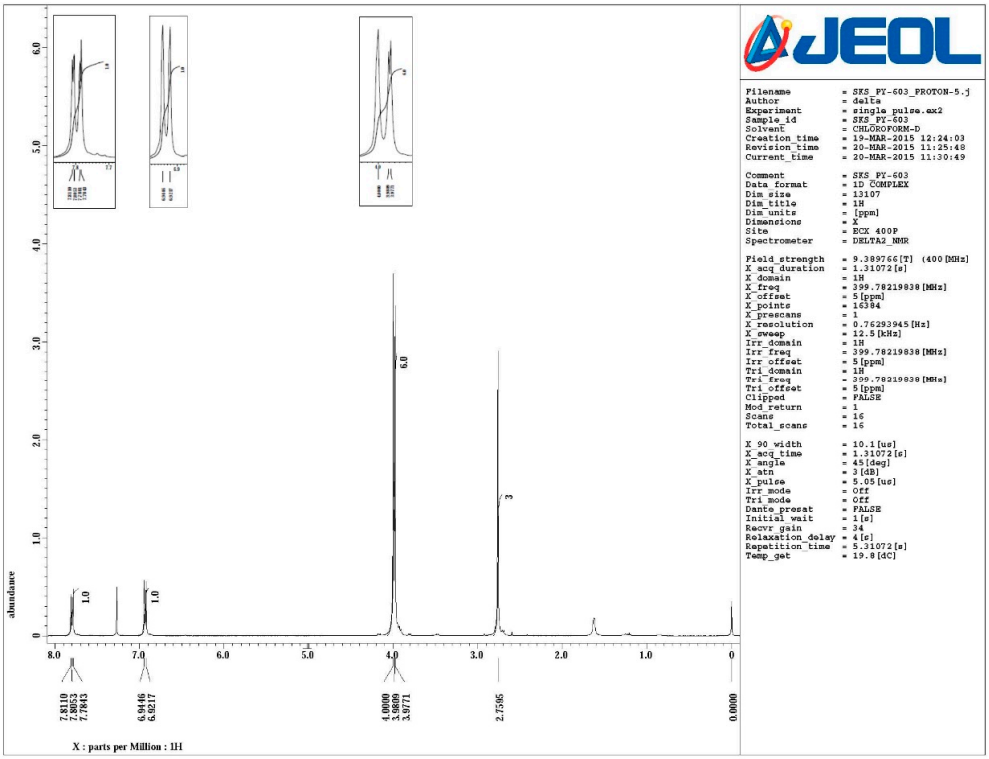

Figure S1. 1H-NMR of 3-acetyl-4-hydroxy-7,8-dimethoxy-2H-chromen-2-one (**6**).

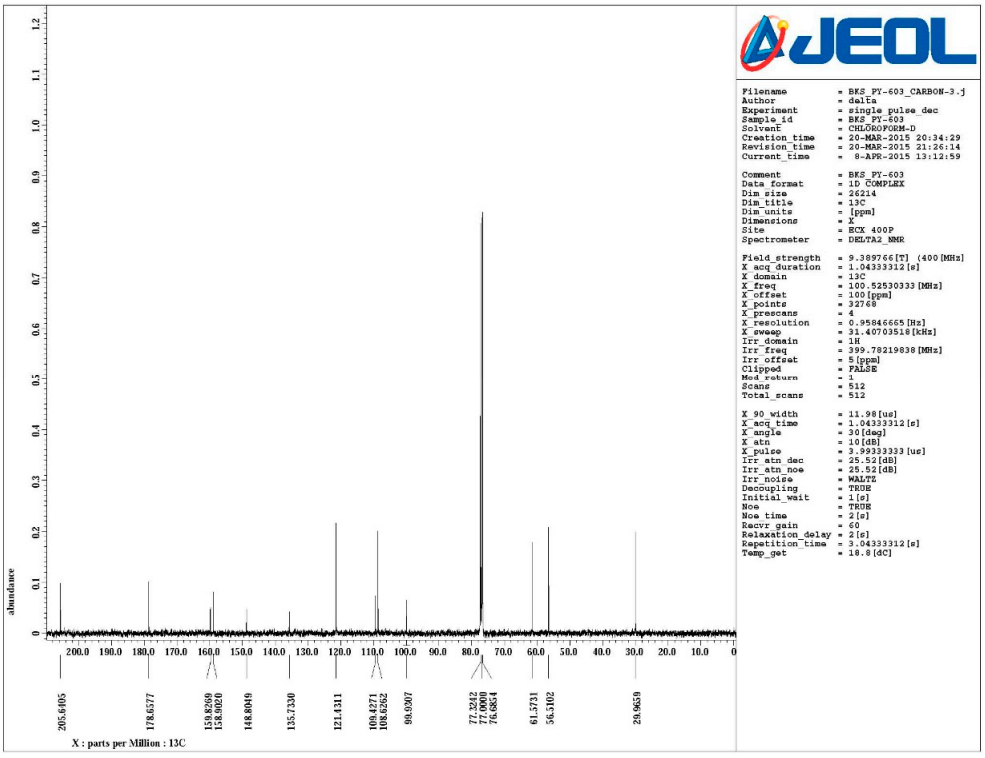

Figure S2. 13C-NMR of 3-acetyl-4-hydroxy-7,8-dimethoxy-2H-chromen-2-one (**6**).

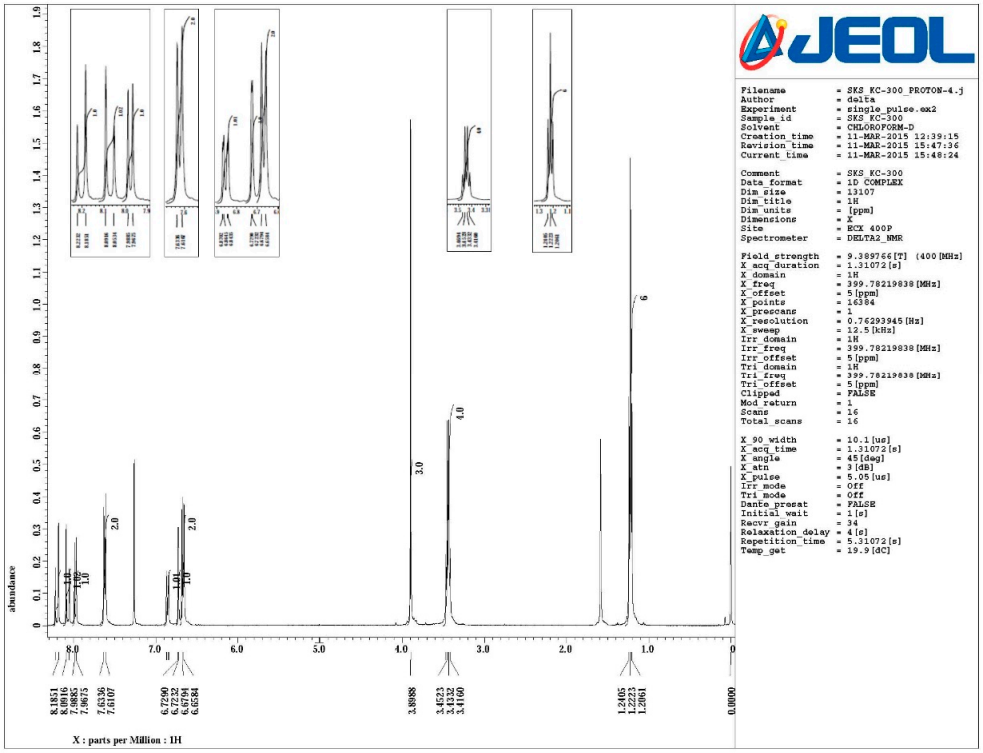

Figure S3. 1H-NMR of (E)-3-[3-(4-(diethylaminophenyl)acryloyl]-4-hydroxy-7-methoxy-2H-chromen-2-one (**7**).

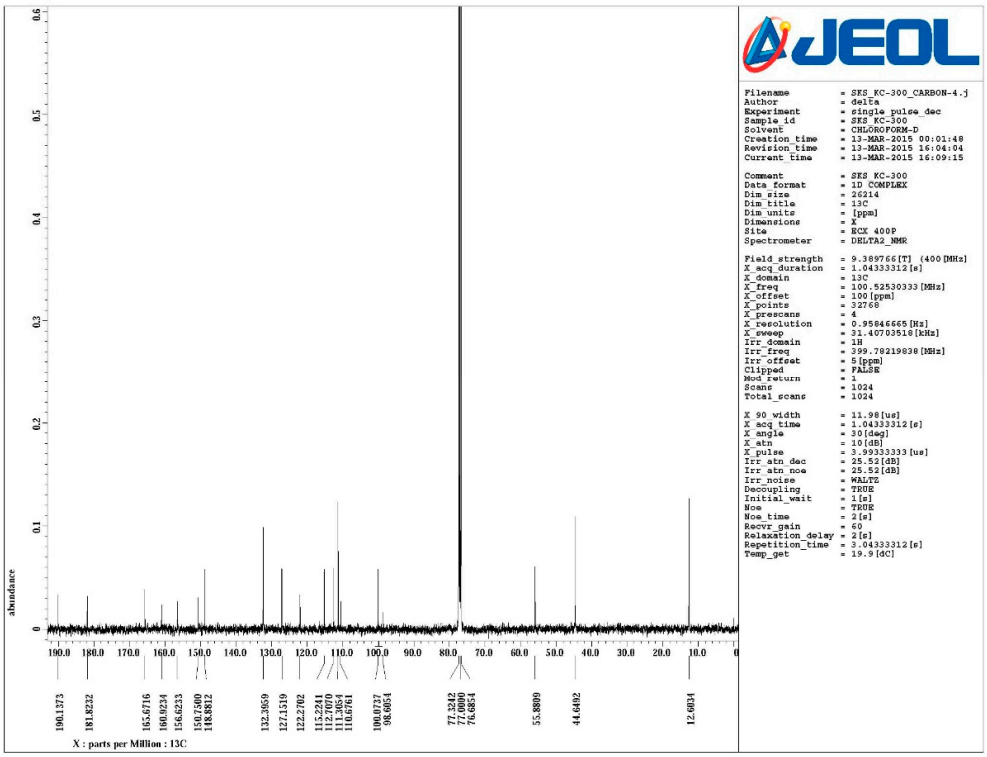

Figure S4. 13C-NMR of (E)-3-[3-(4-(diethylaminophenyl)acryloyl]-4-hydroxy-7-methoxy-2H-chromen-2-one (**7**).

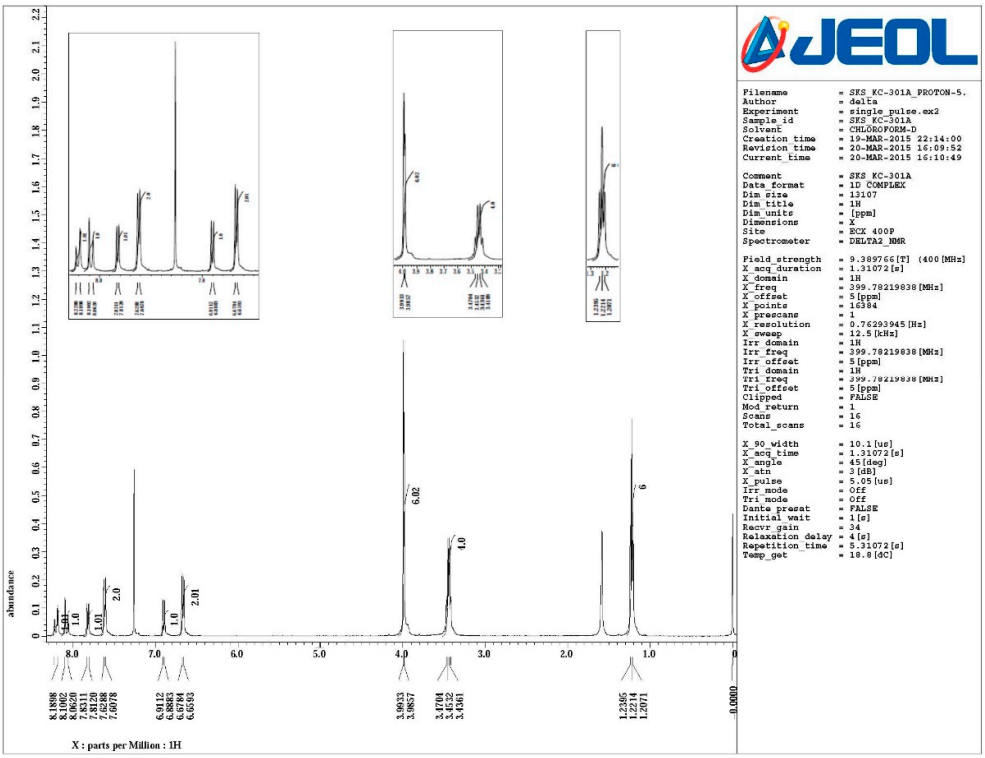

Figure S5. 1H-NMR of (E)-3-[3-(4-(diethylaminophenyl)acryloyl]-4-hydroxy-7,8-dimethoxy-2H-chromen-2-one (**8**).

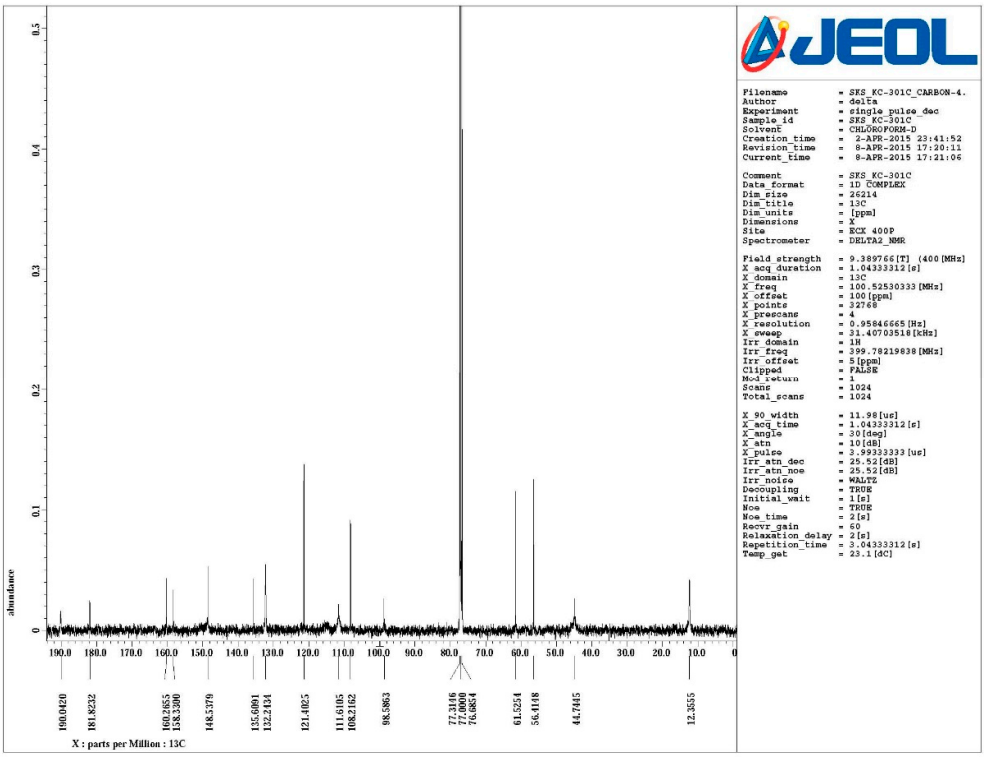

Figure S6. 13C-NMR of (E)-3-[3-(4-(diethylaminophenyl)acryloyl]-4-hydroxy-7,8-dimethoxy-2H-chromen-2-one (**8**).

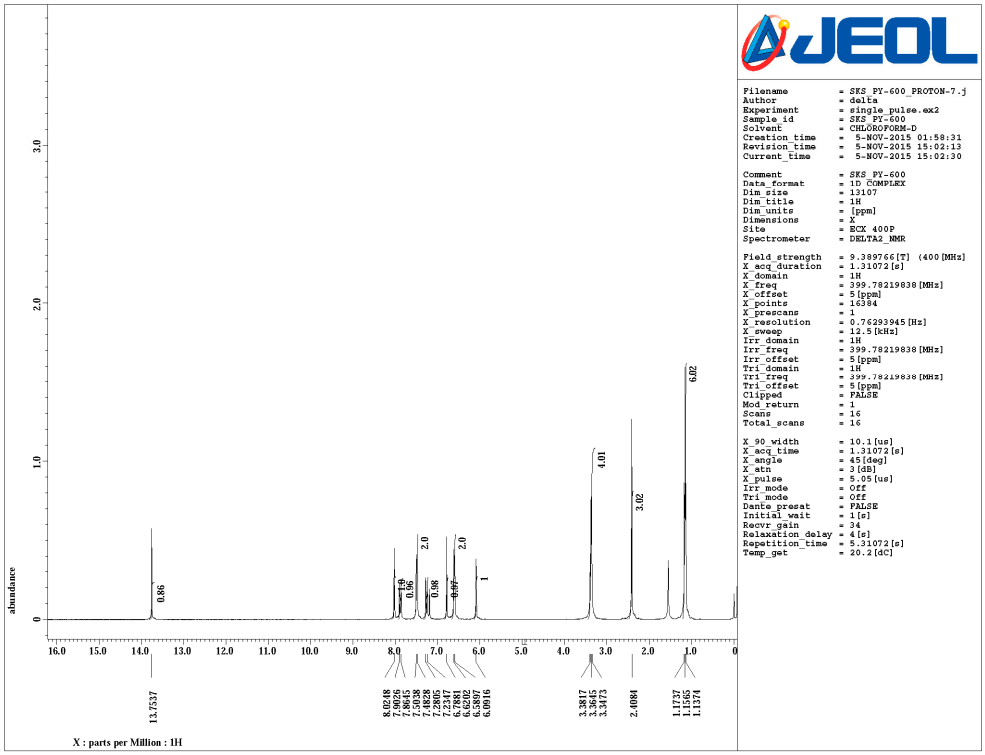

Figure S7. 1H-NMR of (E)-6[(3-(4-diethylaminophenyl)acryloyl]-7-hydroxy-4-methyl-2H-chromen-2-one (**12**).

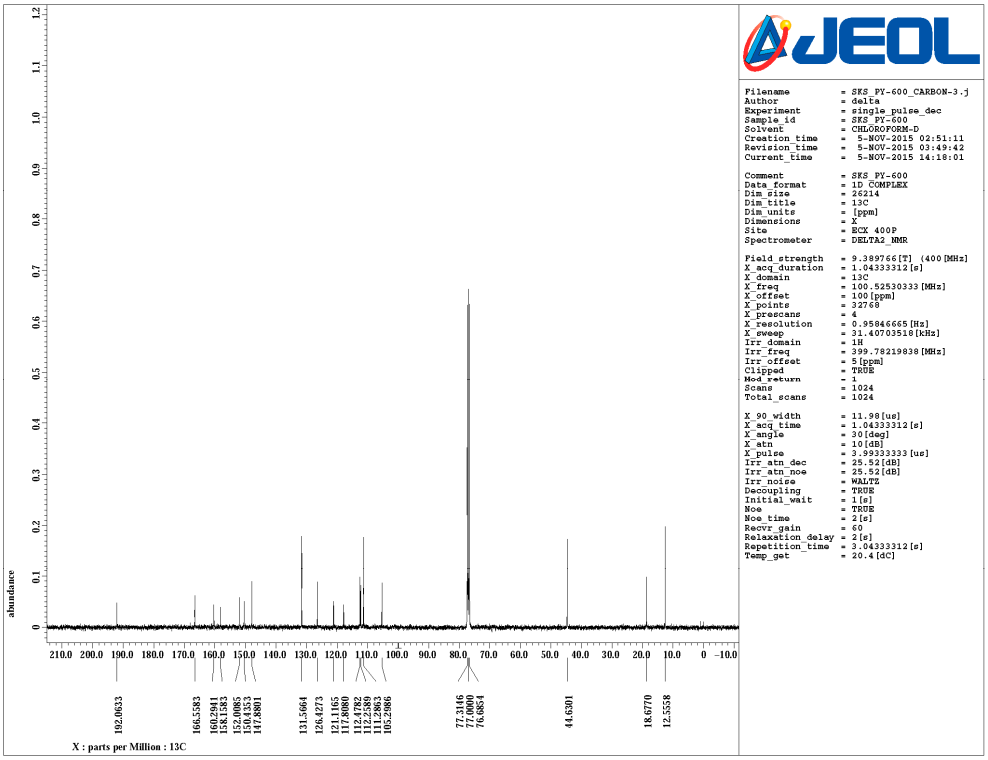

Figure S8. 13C-NMR of (E)-6[(3-(4-diethylaminophenyl)acryloyl]-7-hydroxy-4-methyl-2H-chromen-2-one (**12**).

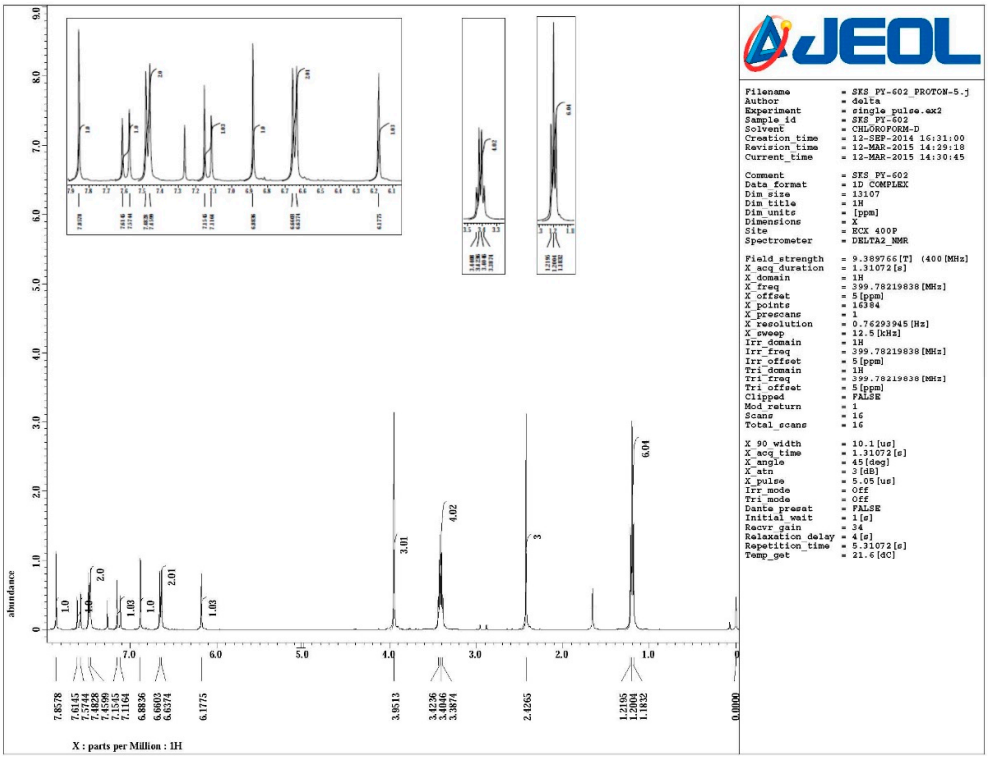

Figure S9. 1H-NMR of (E)-6[(3-(4-diethylaminophenyl)acryloyl]-7-methoxy-4-methyl-2H-chromen-2-one (**13**).

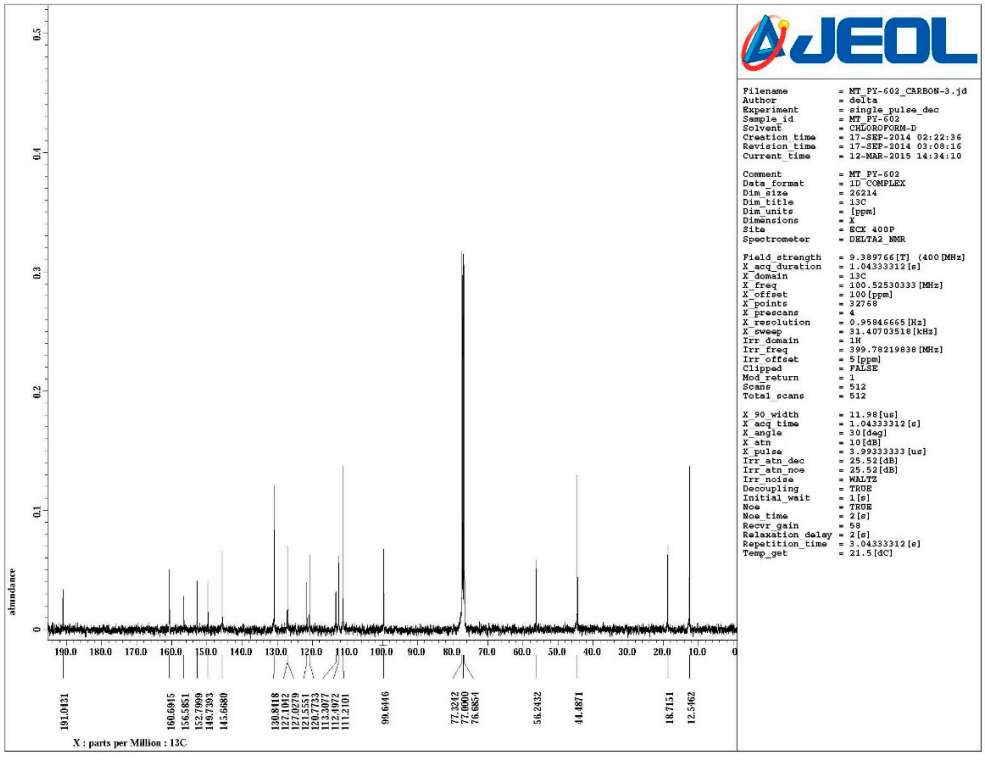

Figure S10. 1H-NMR of (E)-6[(3-(4-diethylaminophenyl)acryloyl]-7-methoxy-4-methyl-2H-chromen-2-one (**13**).

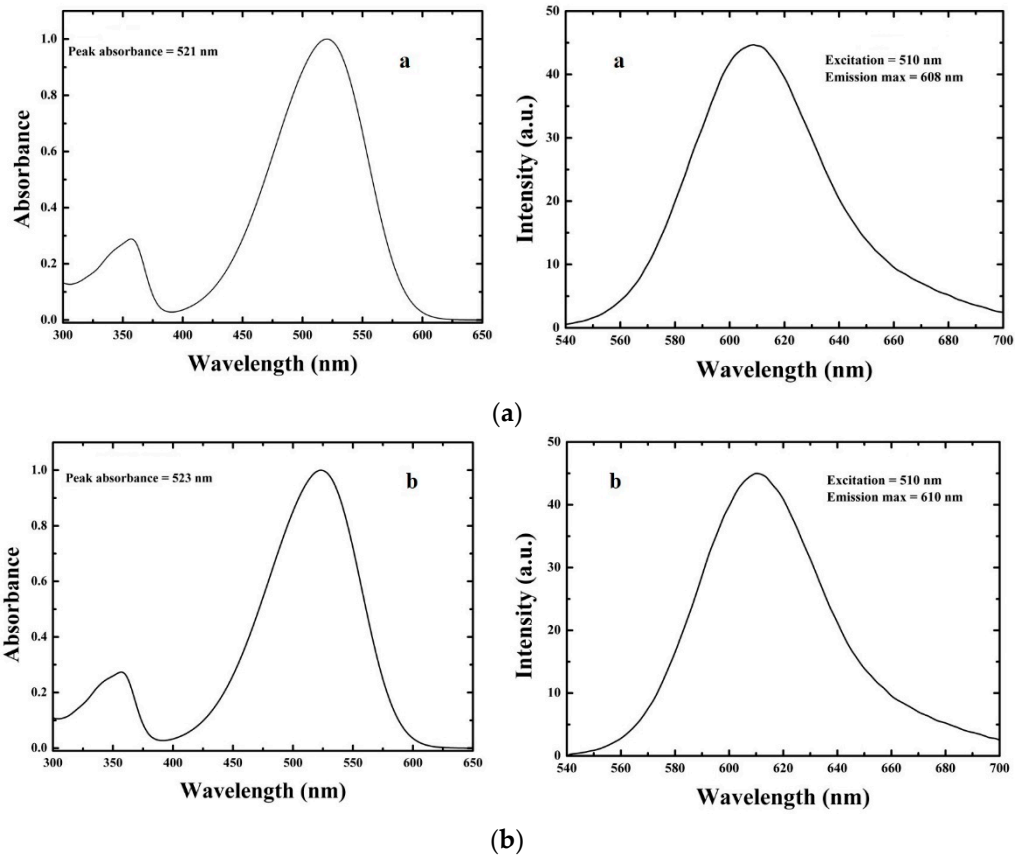

Figure S11. Normalized one-photon absorption and fluorescence spectra of compounds **7** (**a**) and **8** (**b**) in DMSO.

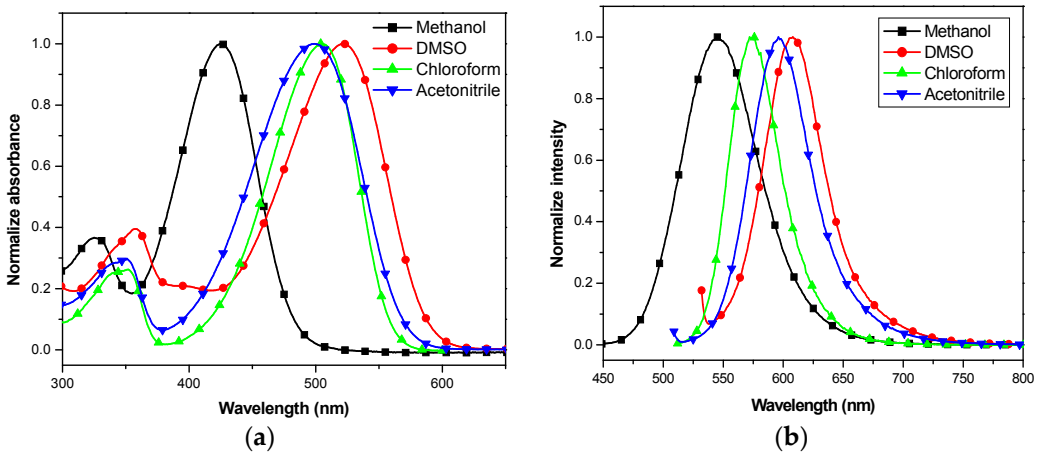

Figure S12. Effect of solvent on the absorption and fluorescence spectra of compound **8**.

Table S1. Stokes shift in different solvents for compound **8**.

Solvent	Relative Polarity[1]	Compd. 8		
		λab. (nm)	λem. (nm)	Stokes Shift (nm)
Methanol	0.762	425	546	121
Acetonitrile	0.460	499	597	98
Dimethyl sulfoxide	0.444	522	608	86
Chloroform	0.259	505	572	67

[1] Christian R. *Solvents and Solvent Effects in Organic Chemistry*; Wiley-VCH Publishers: Weinheim, Germany, 2003.

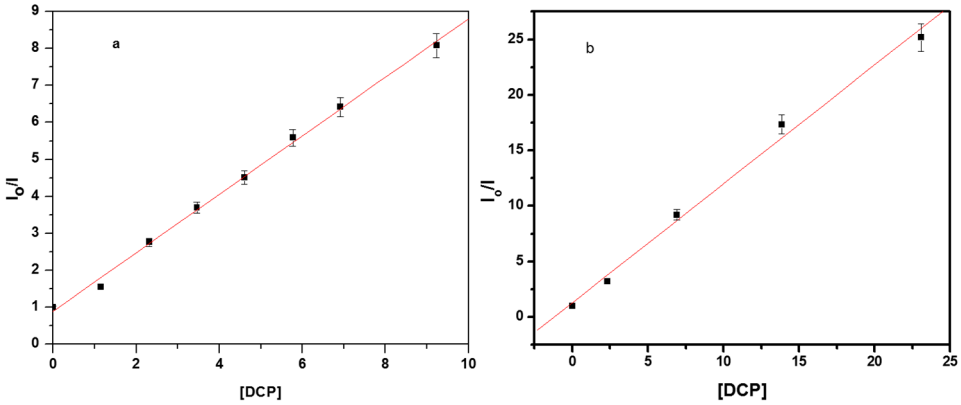

Figure S13. Stern-Volmer plot for compounds **7** (**a**) and **8** (**b**) upon DCP addition.

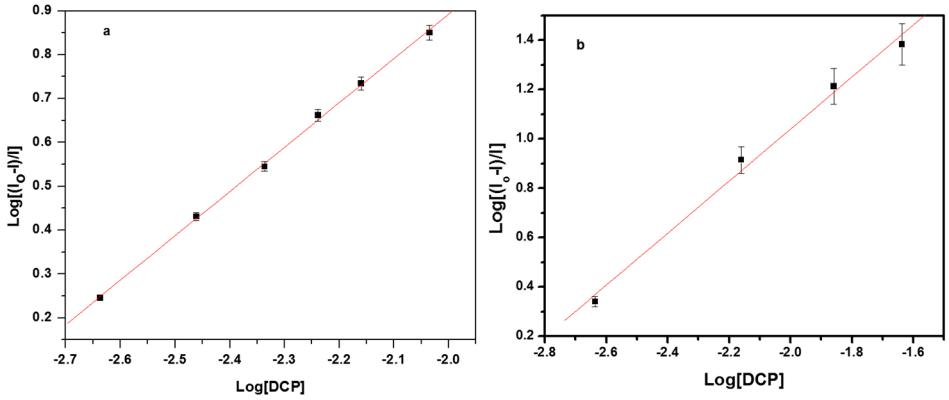

Figure S14. Plot for calculation of binding constant (K) and binding sites (n) for compounds **7** (**a**) and **8** (**b**) on increasing concentration of DCP.

Table S2. The Stern-Volmer constants of the 6-(4-dialkylaminocinnamoyl) coumarins with DCP in chloroform.

S.No.	Structure	Ksv(M^{-1})
7		791
8		1070
11		214
12		208
13		253

Stern-Volmer constant was calculated from the fluorescence titration data of compounds (0.02 mM) 3 mL in a cuvette.

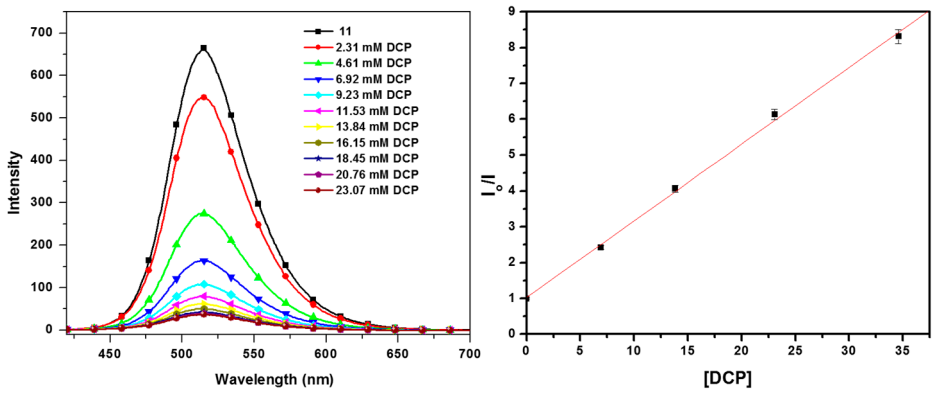

Figure S15. Fluorescence spectra for titration of compound **11** with DCP and Stern-Volmer plot.

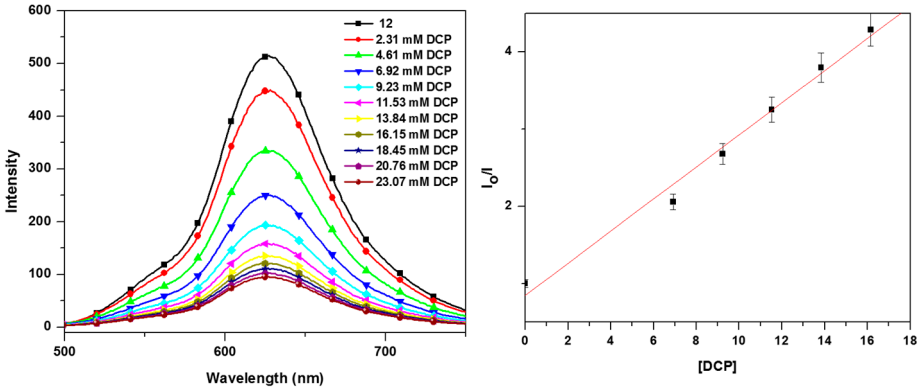

Figure S16. Fluorescence spectra for titration of compound **12** with DCP and Stern-Volmer plot.

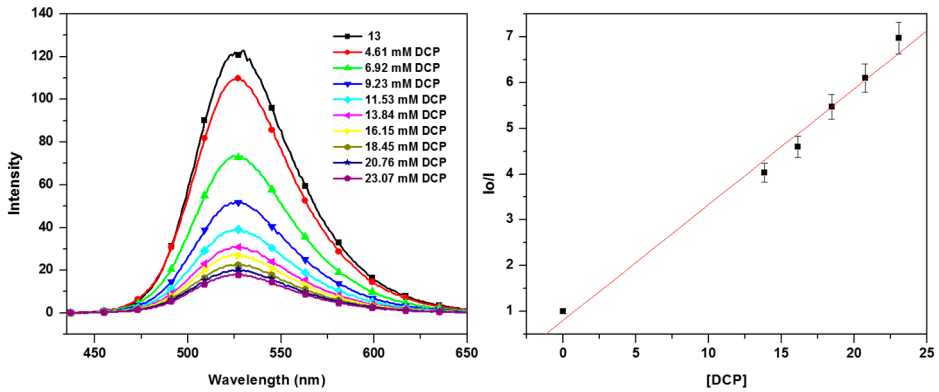

Figure S17. Fluorescence spectra for titration of compound **13** with DCP and Stern-Volmer plot.

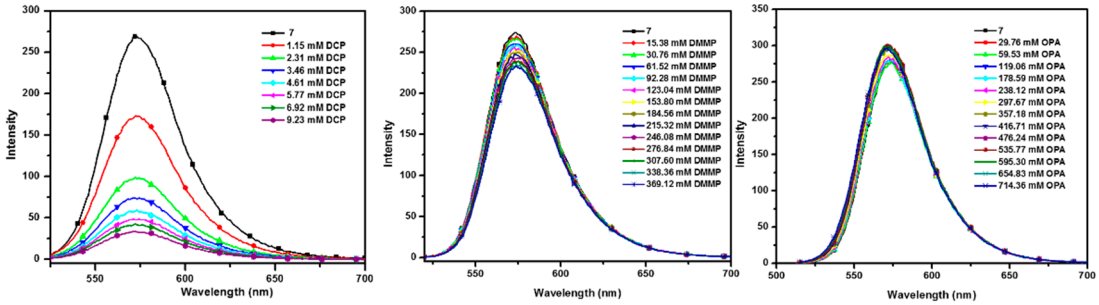

Figure S18. Fluorescence spectra for titration of compounds **7** with DCP, DMMP (dimethyl methylphosphonate) and o-phosphoric acid (OPA).

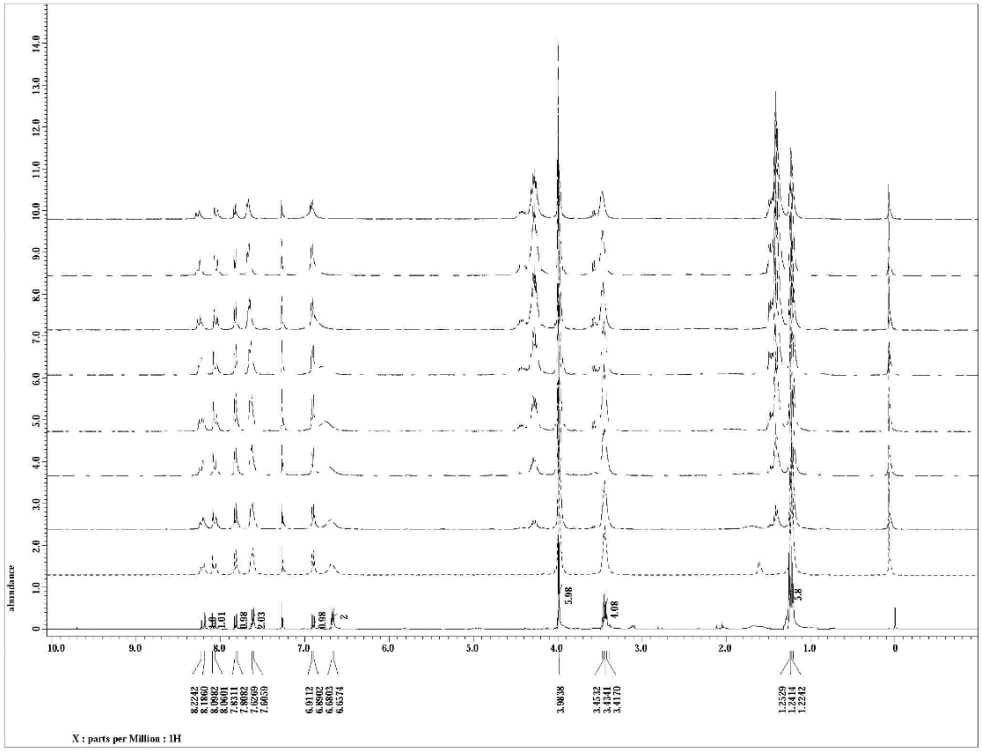

Figure S19. 1H-NMR titration plot of compound **8** on addition of DCP (0–4 eq.) in $CDCl_3$.

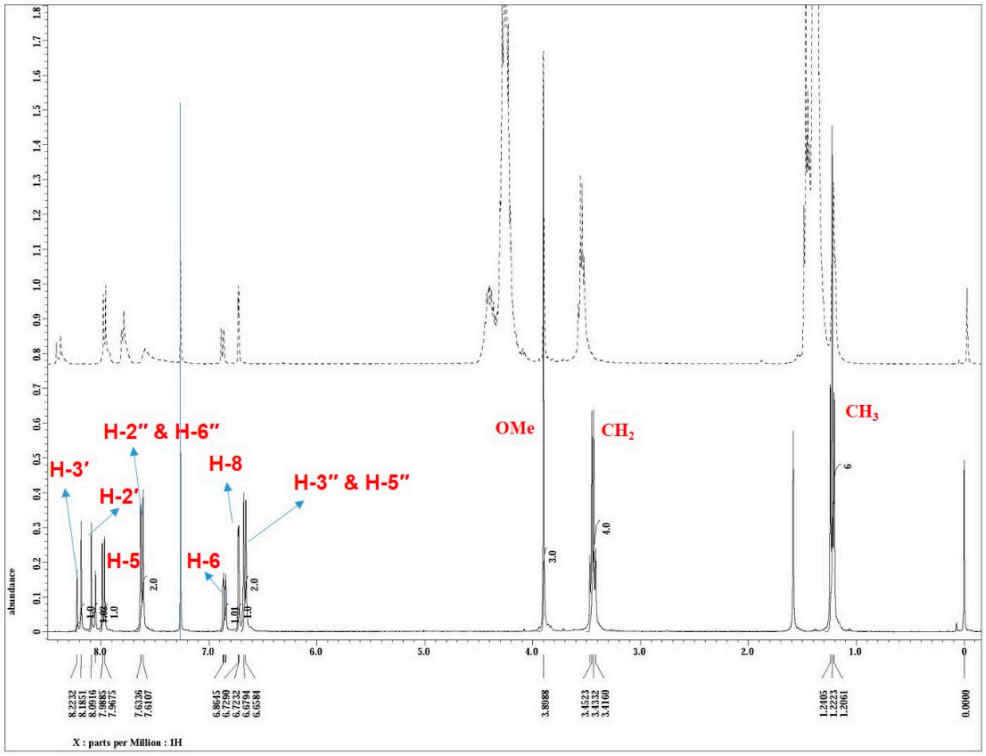

Figure S20. 1H-NMR of compound **7** on addition of DCP (4 eq.) in $CDCl_3$.

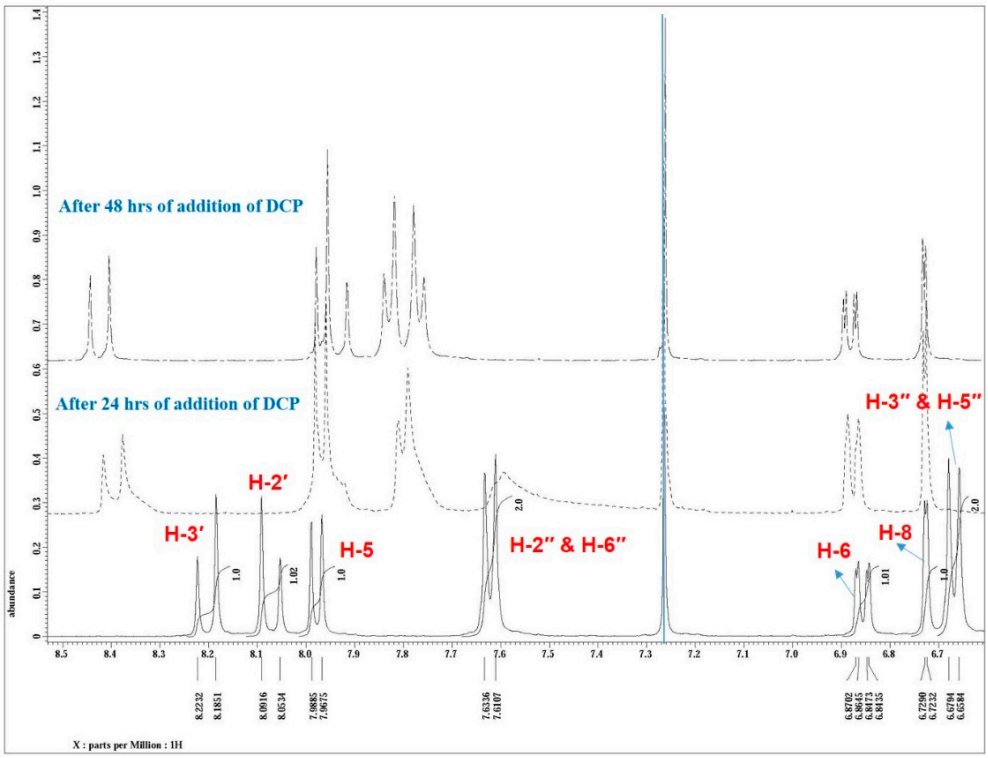

Figure S21. 1H-NMR (aromatic region) of compound **7** on addition of DCP (4 eq.) in $CDCl_3$ after 24 and 48 h.