Electronic Supplementary Material (ESI) for Analytical Methods.

Electronic Supporting Information

Structure property studies revealed a new indoylfuranone based bifunctional chemosensor for Cu^{2+} and Al^{3+}

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Spectral Data

2-(tert-butylamino)-3-(1H-indol-3-yl)furo[3,2-c]quinolin-4-ol (compound A)

Yield: 85% ; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm)1.60 (s, 9H), 3.93 (br s, 1H), 7.53 (td, 1H, *J* = 6.0 & 1.3 Hz), 7.56-7.65 (m, 4H), 7.68-7.74 (m, 2H), 7.92 (dd, 1H, *J* = 5.9 & 1.3 Hz), 8.16 (dd, 1H, *J* = 5.9 & 1.3 Hz), 8.93 (s, 1H), 9.71 (s, 1H). HRMS (ESI) m/z calcd.for $C_{23}H_{21}N_3O_2$ $[M+Na]^+$: 394.1532, found: 394.1528.

2-(cyclohexylamino)-1-(1H-indol-3-yl)-11H-benzo[h]furo[3,2-c]chromen-11-one (compound B)

Yield: 87% ; ^{1}H NMR (400 MHz, DMSO-d_6): δ (ppm)1.30-1.39 (m, 3H), 1.44 (sex, 2H, *J* = 2.4 Hz), 1.62-1.70 (m, 3H), 2.05 (sex, 2H, *J* = 2.5 Hz), 3.14 (quin, 1H, *J* = 2.3 Hz), 3.93 (br s, 1H), 7.20-7.28 (m, 2H), 7.37-7.43 (m, 3H), 7.53-7.58 (m, 2H), 7.68 (d, 1H, *J* = 6.0 Hz), 7.73 (td, 1H, *J* = 3.4 & 1.1 Hz), 7.88 (dd, 1H, *J* = 4.8 & 1.8 Hz), 8.05-8.10 (m, 1H), 8.93 (s, 1H). HRMS (ESI) m/z calcd.for $C_{29}H_{24}N_2O_3$ $[M+Na]^+$: 471.1685, found: 471.1676.

2-(tert-butylamino)-1-(1H-indol-3-yl)-11H-benzo[h]furo[3,2-c]chromen-11-one (compound C)

Yield: 85% ; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm)1.11 (s, 9H), 3.92 (br s, 1H), 6.54 (td, 1 H, *J* = 6.2 & 1.1 Hz), 6.68 (s, 1H), 7.08 (td, 1H, *J* = 6.0 & 1.1 Hz), 7.14-7.23 (m, 4H), 7.32 (dd, 1H, *J* = 6.0 & 1.1 Hz), 7.44 (d, 1H, *J* = 6.0 Hz), 7.49 (td, 1H, *J* = 3.6 & 1.2 Hz), 7.81-7.87 (m, 1H), 9.37 (s, 1H). HRMS (ESI) m/z calcd.for $C_{27}H_{22}N_2O_3$ $[M+Na]^+$: 445.1528, found: 445.1518.

2-(tert-butylamino)-3-(1H-indol-3-yl)naphtho[2,3-b]furan-4,9-dione (compound D)

Yield: 81%; ^{1}H NMR (400 MHz,$CDCl_3$): δ (ppm)1.08 (s, 9H), 3.92 (br s, 1H), 6.74 (td, 1H, *J* = 6.0 & 1.3 Hz), 6.81 (s, 1H), 7.29 (td, 1H, *J* = 6.0 & 1.1 Hz), 7.33 (dd, 1H, *J* = 5.8 & 1.1 Hz), 7.39 (td, 1H, *J* = 5.9 & 1.1 Hz), 7.44 (td, 1H, *J* = 5.9 & 1.1 Hz), 7.68 (dd, 1H, *J* = 6.0 & 1.1 Hz), 7.78 (dd, 1H, *J* = 6.0 & 1.1 Hz), 7.86 (dd, 1H, *J* = 5.9 & 1.1 Hz), 9.33 (s, 1H). ^{13}C NMR: (100 MHz, $CDCl_3$): δ (ppm) 29.7, 53.6, 98.1, 112.4, 121.8, 123.3, 124.8, 126.6, 126.9, 128.5, 132.3, 133.1, 133.8, 135.1, 138.1, 153.6, 172.9, 176.2, 182.1. HRMS (ESI) m/z calcd.for $C_{24}H_{20}N_2O_3$ $[M+Na]^+$: 407.1372, found: 407.1368.

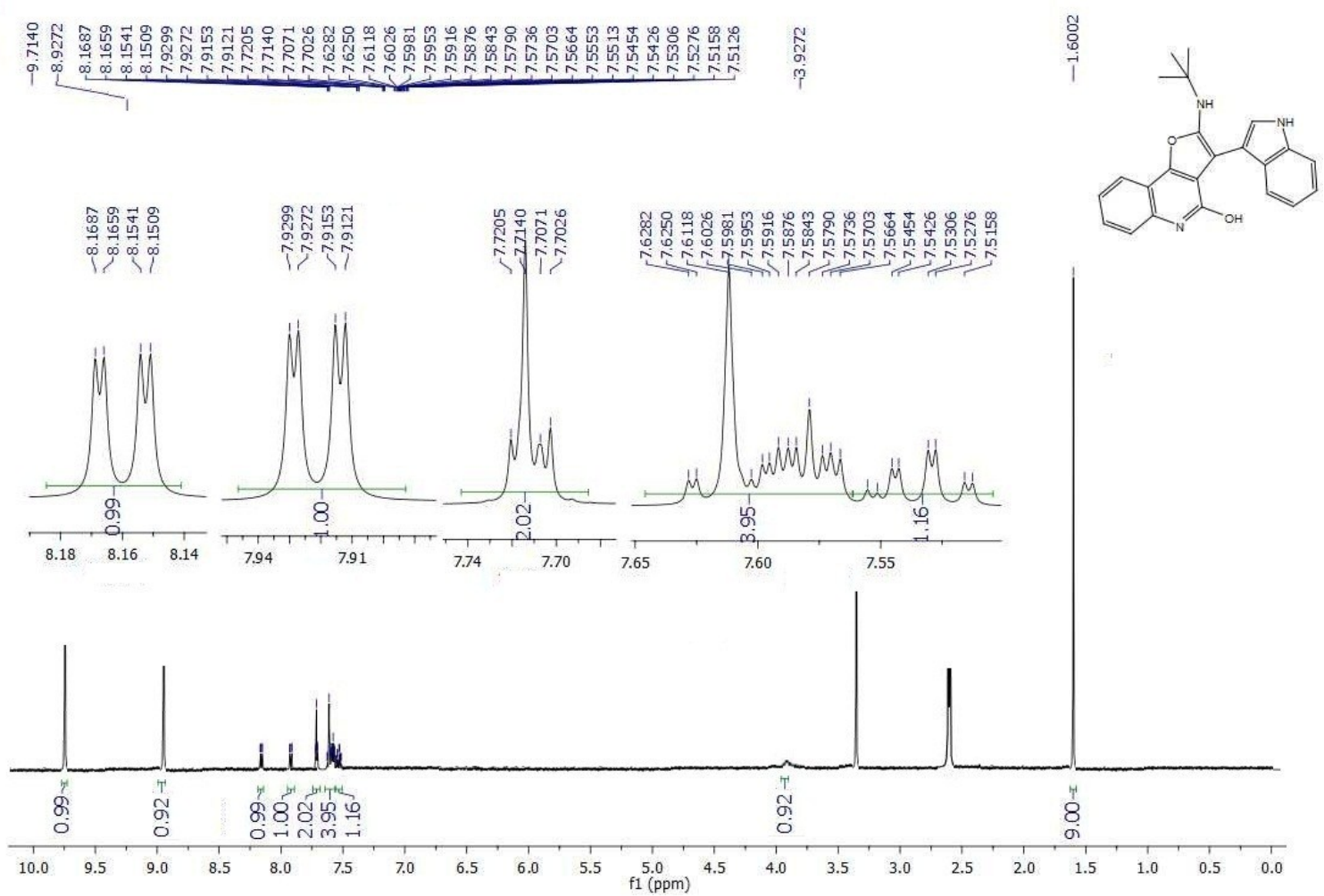
Compound **X**, **Y** and **Z** were synthesized according to literature described methods (1, 2 and 3 respectively).

(1) M. B. Teimouri and R. Bazhrang, *Monatsh Chem.*, 2008, **139**, 957–961.

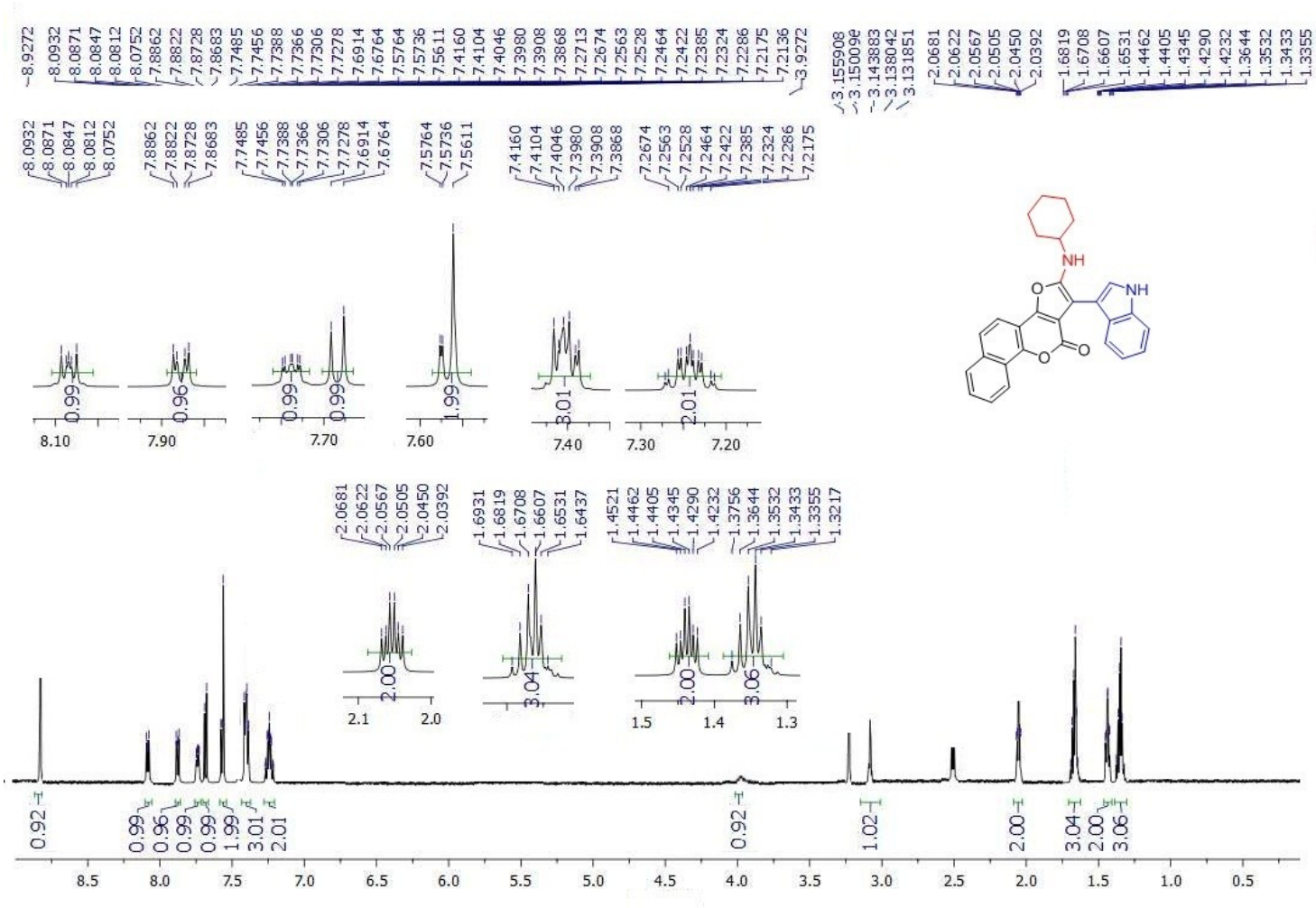
(2) M. Kumar, S. Bagchi and A. Sharma, *RSC Adv.*, 2015, **5**, 53592-53603.

(3) R. Zhang, D. Xu and J. Xie, *Chin. J. Chem.*, 2012, **30**, 1690-1694.

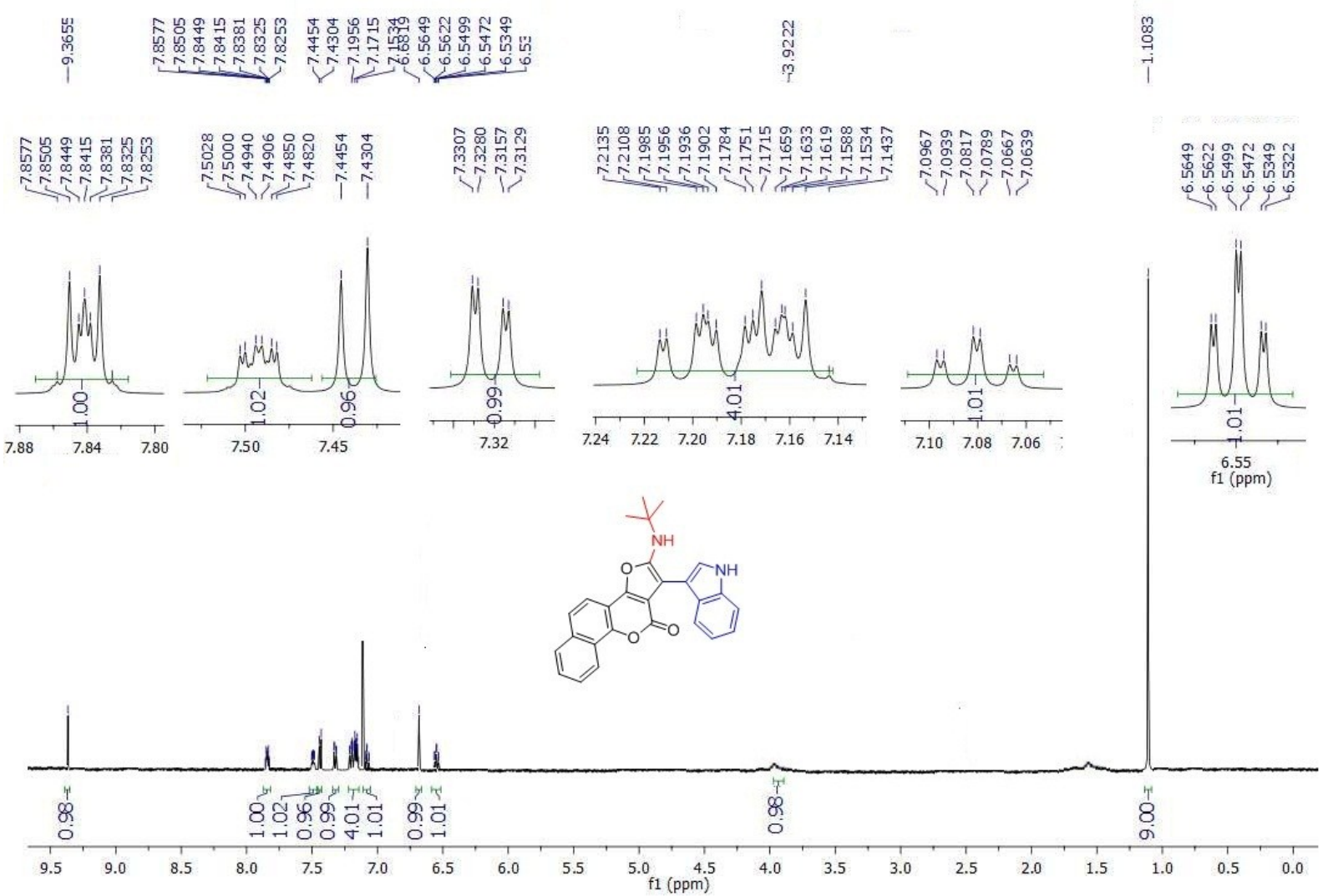
[1]HNMR Spectra of compound **A**



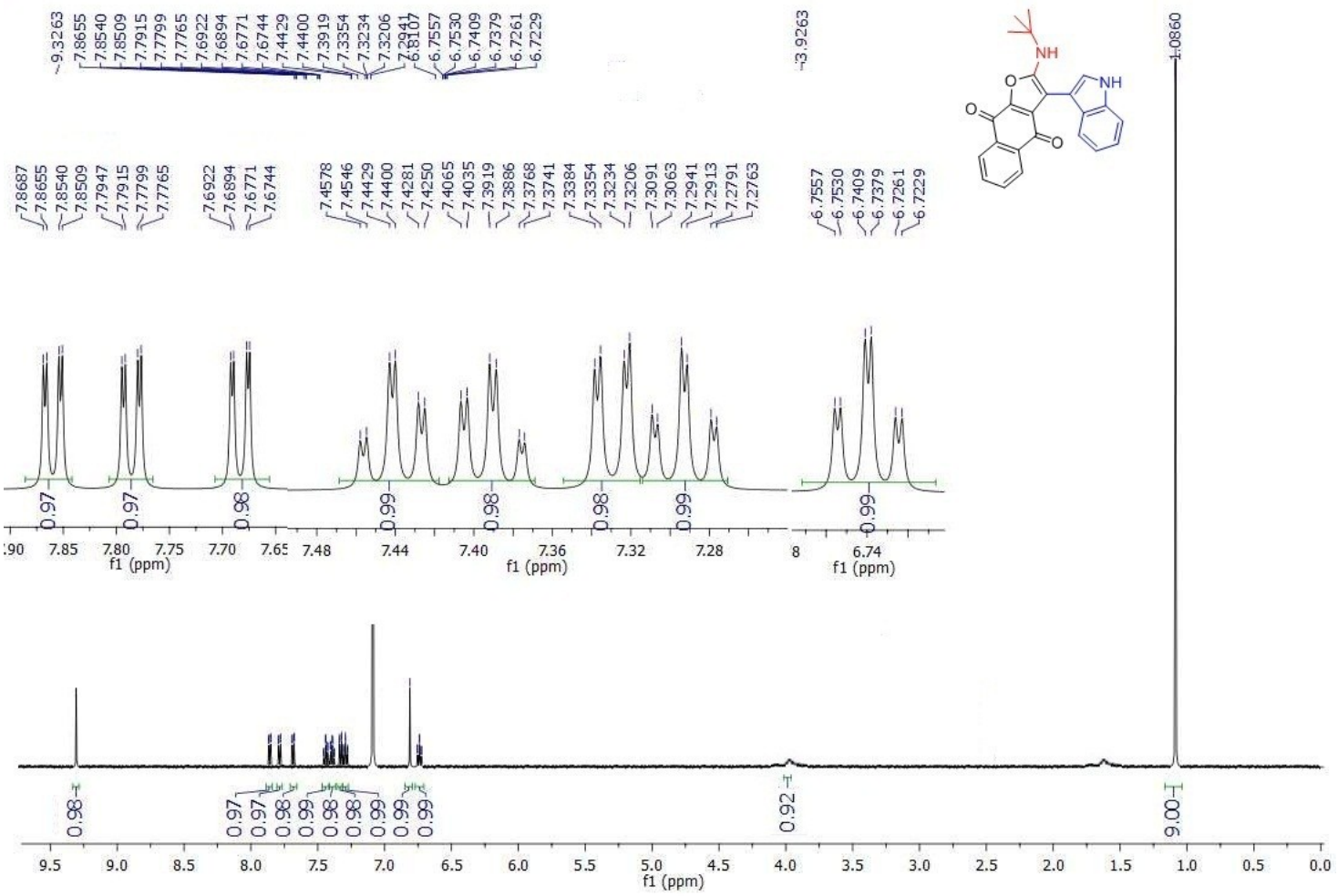
[1]HNMR Spectra of compound **B**



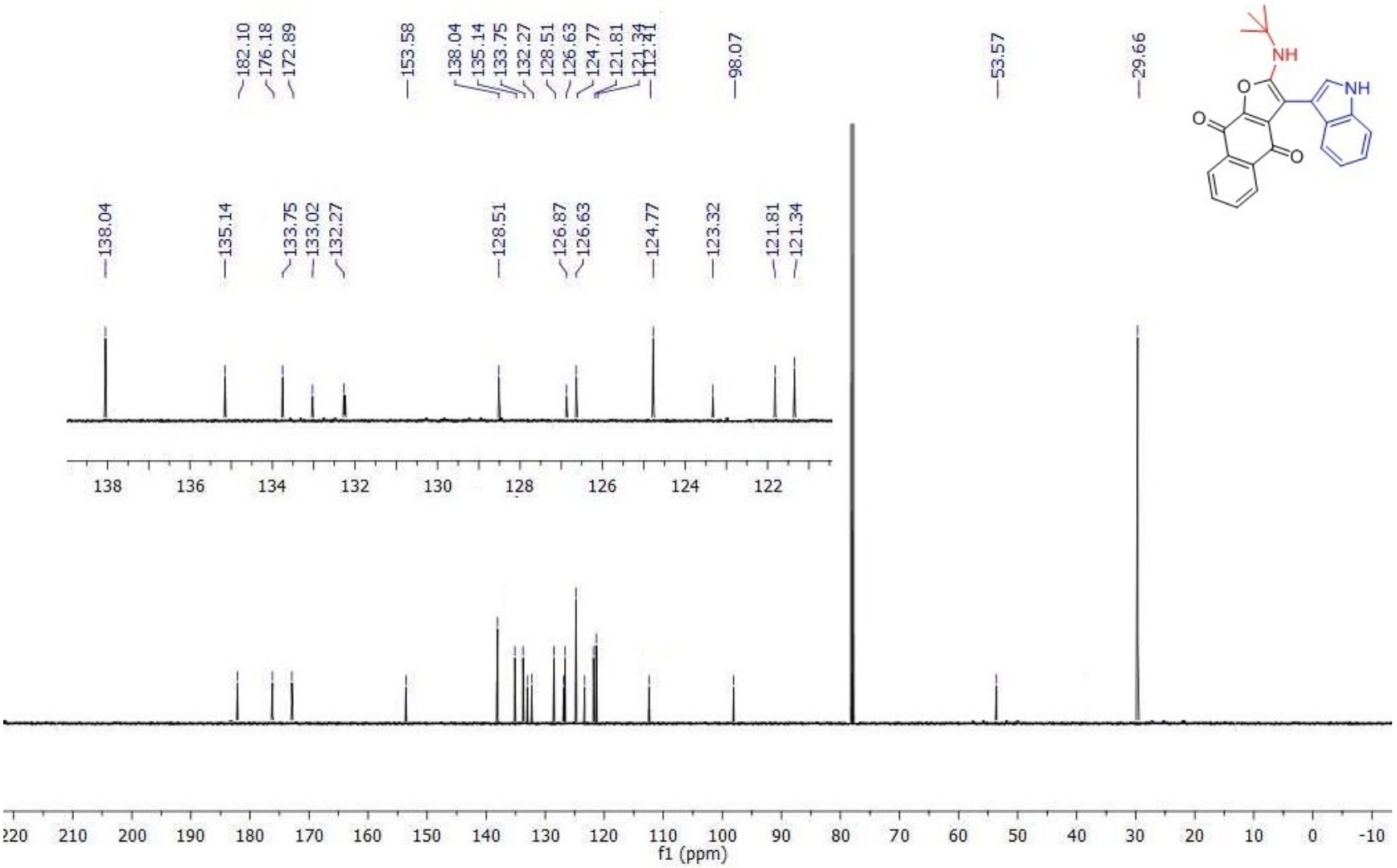
[1]HNMR Spectra of compound **C**



[1]HNMR Spectra of compound **D**



^{13}CNMR Spectra of compound **D**



HRMSof compounds **A** to **D**

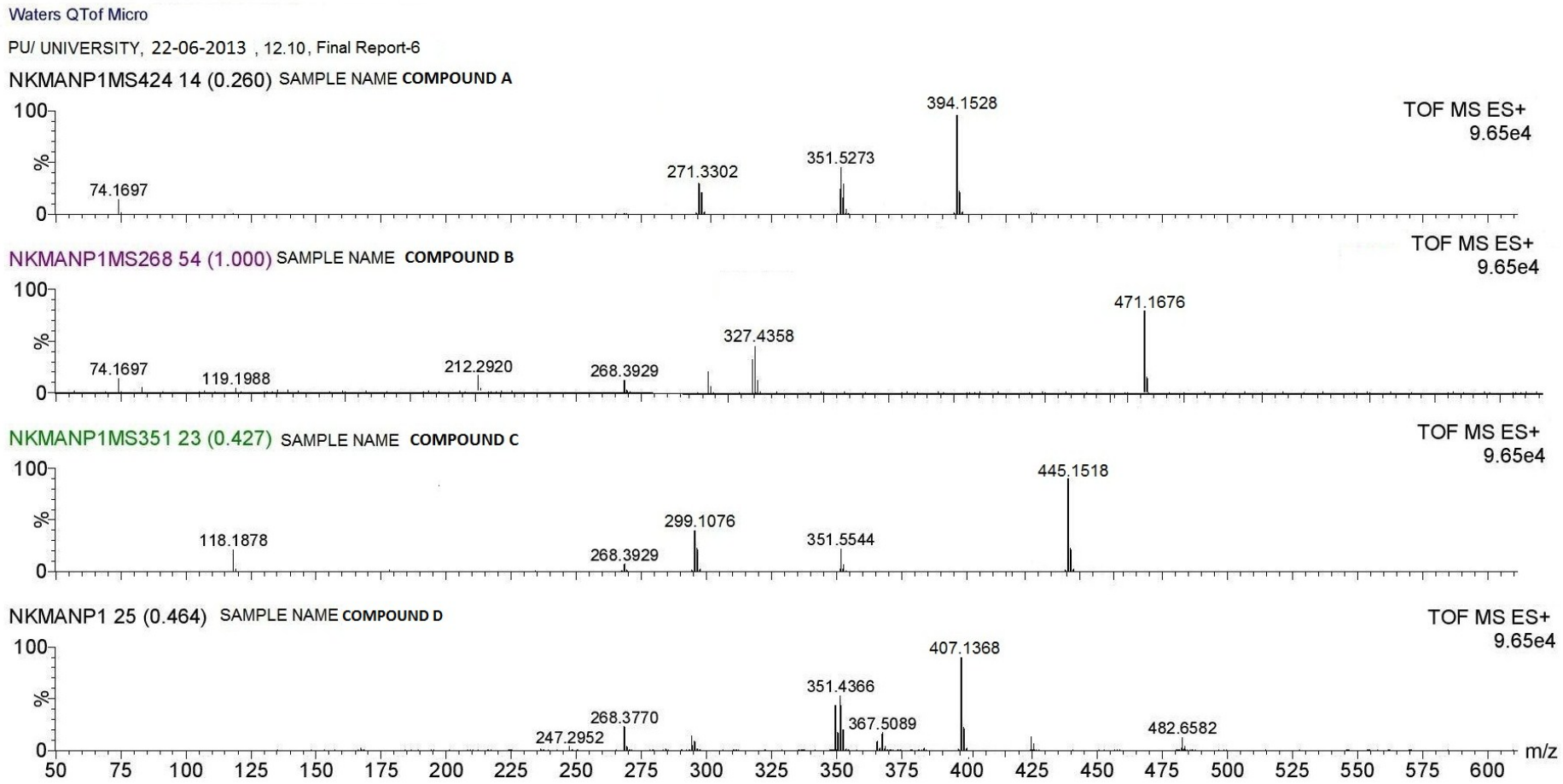


Figure SS1 Benesi-Hilderbrand plots between $1/I-I_0$ (at 574 nm) and $1/[Cu^{2+}]$.

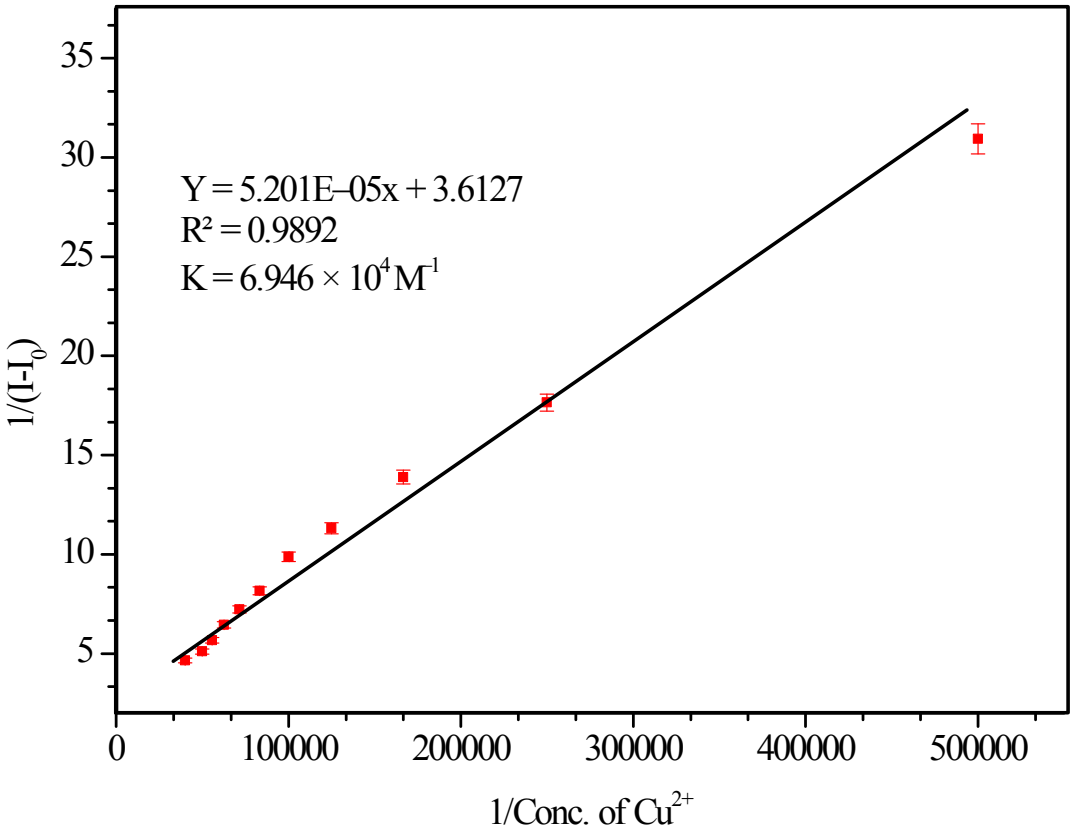


Figure SS2 Job's plot (absorption) of probe **D** with Cu^{2+} in ($MeOH/H_2O$, 2/8, v/v). (Total concentration of probe and metal was kept constant at the level of 20 μM).

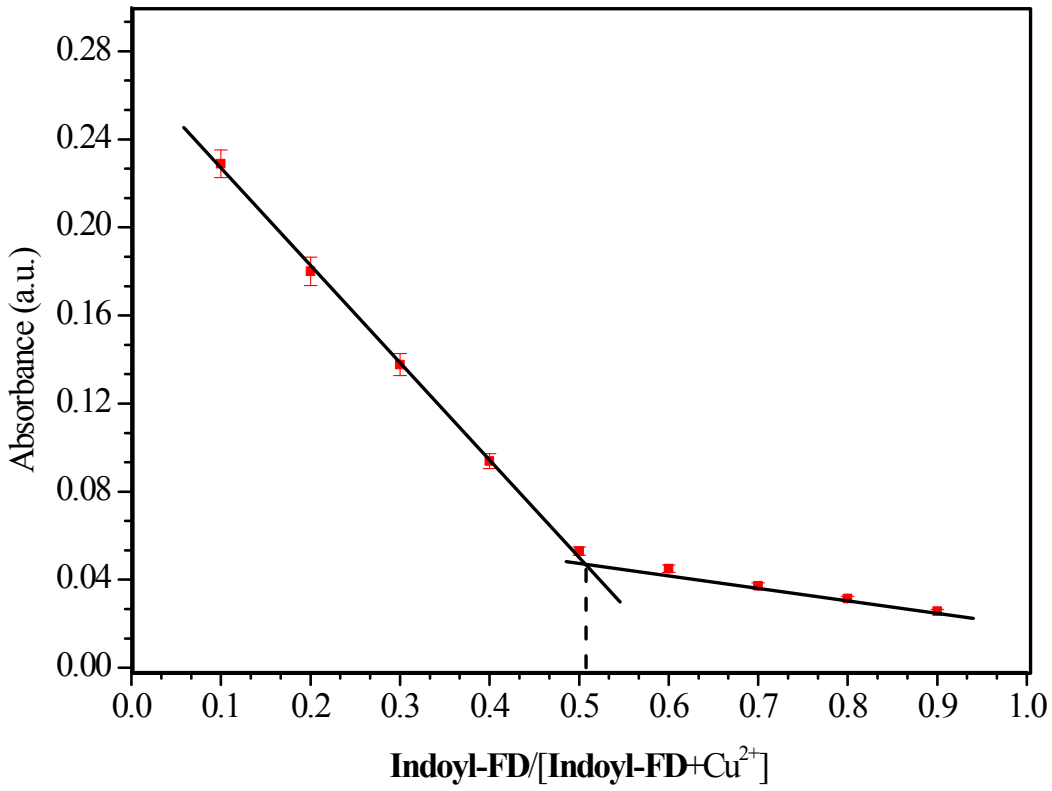


Figure SS3 Benesi-Hilderbrand plots between $1/I-I_0$ (at 598 nm) and $1/[Al^{3+}]$.

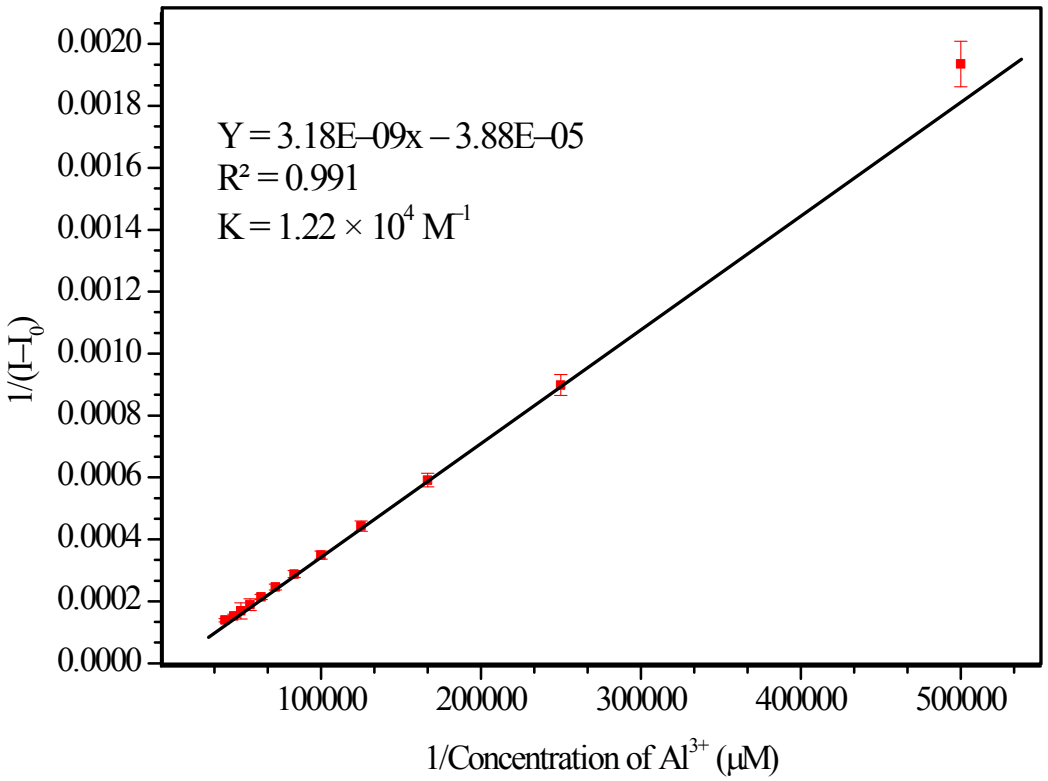


Figure SS4 Job's plot (emission) of probe **D** with Al^{3+} in ($MeOH/H_2O$, 2/8, v/v). (Total concentration of probe and metal is kept constant at the level of 20 μM).

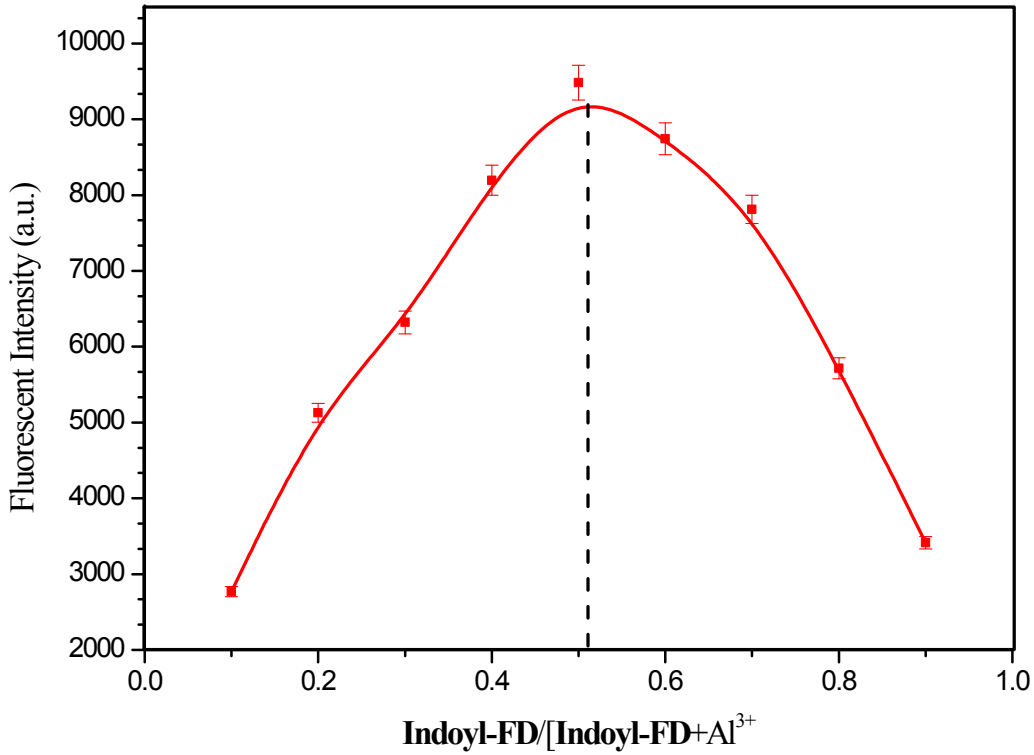


Figure SS5 Dependence of fluorescence response of furandione**D**–Cu^{2+} over pH of the medium (MeOH/Water, 2/8, v/v) was used as a solvent.

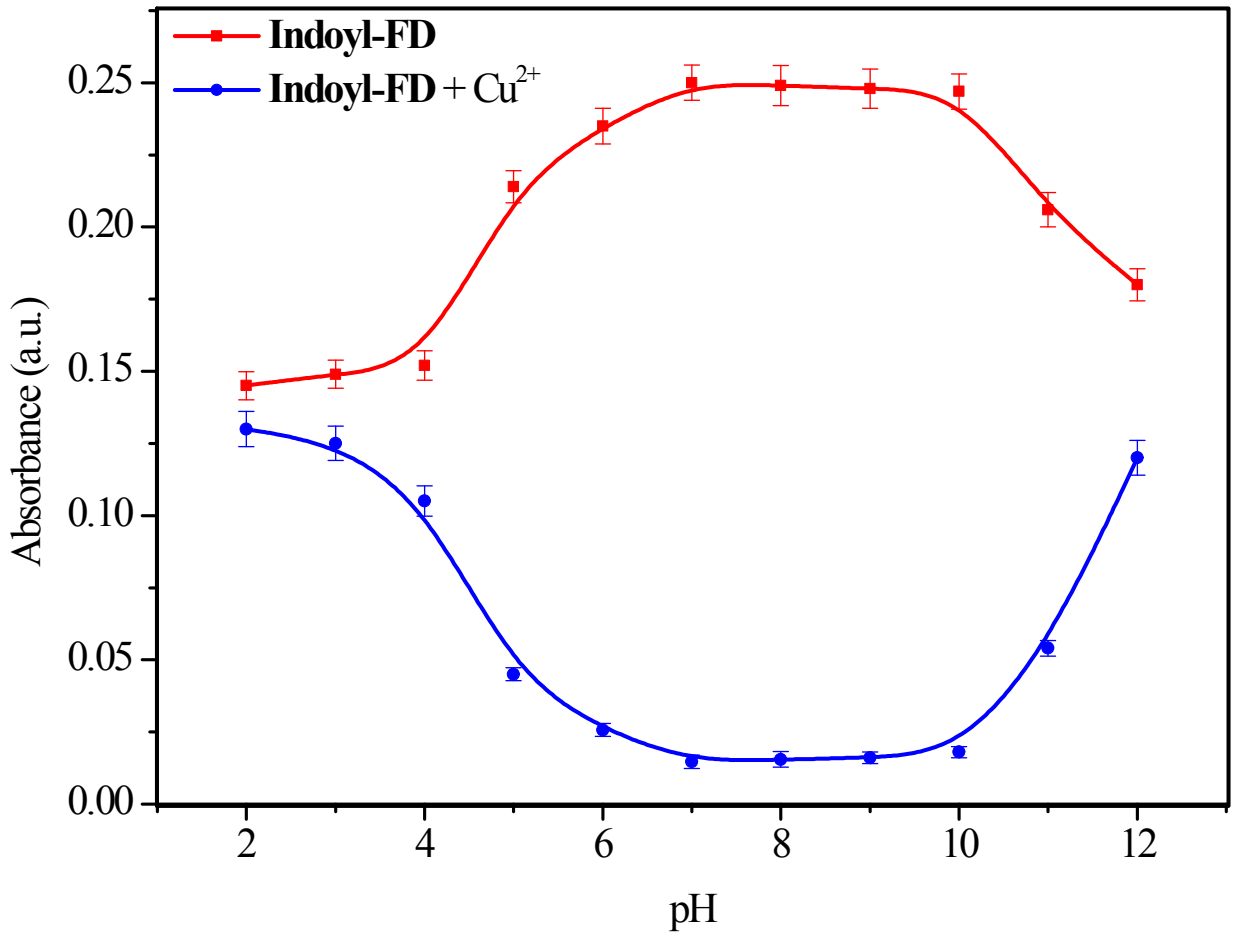


Figure SS6 Dependence of fluorescence response of furandione**D**–Al^{3+} over pH of the medium (MeOH/Water, 2/8, v/v) was used as a solvent.

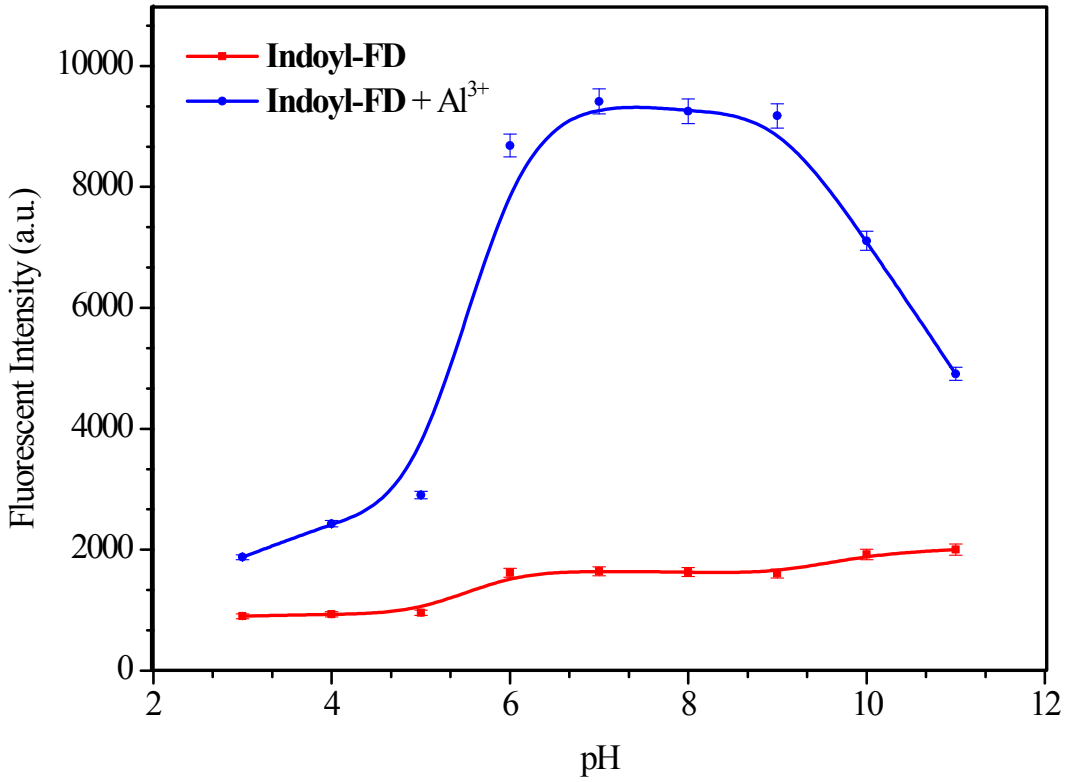


Figure SS7 Reversibility and reusability test of furandione **D**-Cu^{2+} in the presence of EDTA.

Compound **D**(20 μM in MeOH) with equimolar concentration of EDTA and Cu^{2+}.

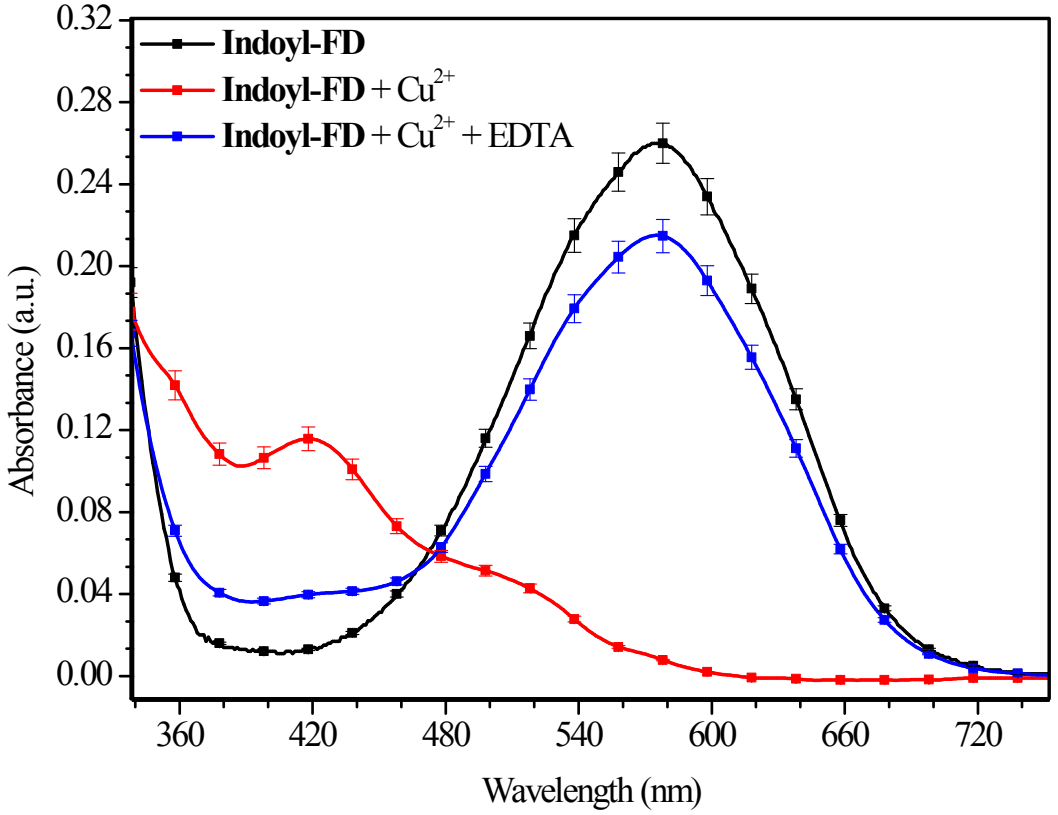


Figure SS8 Reversibility and reusability test of furandione**D-**Al^{3+}in the presence of EDTA. Compound **D**(20 μM in MeOH) with equimolar concentration of EDTA and Al^{3+}.