

*Electronic Supplementary Information for*

**Sequential and cellular detection of copper and lactic acid by  
disaggregation and reaggregation of the fluorescent panchromatic fibers  
of anacylthiourea based sensor**

VivekshinhKshtriya<sup>[a]</sup>, Bharti Koshti<sup>[a]</sup>, Deepak K. Pandey<sup>[c]</sup>, Sumit Kharbanda<sup>[d]</sup>, Chandra  
KanthP<sup>[e]</sup>, Dheeraj K. Singh<sup>[c]\*</sup>, Dhiraj Bhatia<sup>[d]\*</sup>, Nidhi Gour<sup>[a, b] \*</sup>

[a] Department of Chemistry, Indrashil University, Kadi, Mehsana, Gujarat, India;E-mail:

[nidhi.gour@indrashiluniversity.edu.in](mailto:nidhi.gour@indrashiluniversity.edu.in); [gournidhi@gmail.com](mailto:gournidhi@gmail.com)

[b] Past affiliation: Department of Medicinal Chemistry, Indian Institute of Advanced Research,  
Gandhinagar, Gujarat, 382426, India;

[c]Department of Basic Sciences, Institute of Infrastructure Technology Research And  
Management, Ahmedabad, 380026; E-mail: [dheerajsingh@iitram.ac.in](mailto:dheerajsingh@iitram.ac.in)

[d] Biological Engineering Discipline and Center for Biomedical Research, Indian Institute of  
Technology Gandhinagar, Palaj 382355, Gandhinagar, India;E-mail: [dhiraj.bhatia@iitgn.ac.in](mailto:dhiraj.bhatia@iitgn.ac.in)

[e] Department of Science, School of Technology, Pandit Deendayal Petroleum University,  
Gandhinagar, Gujarat, India.

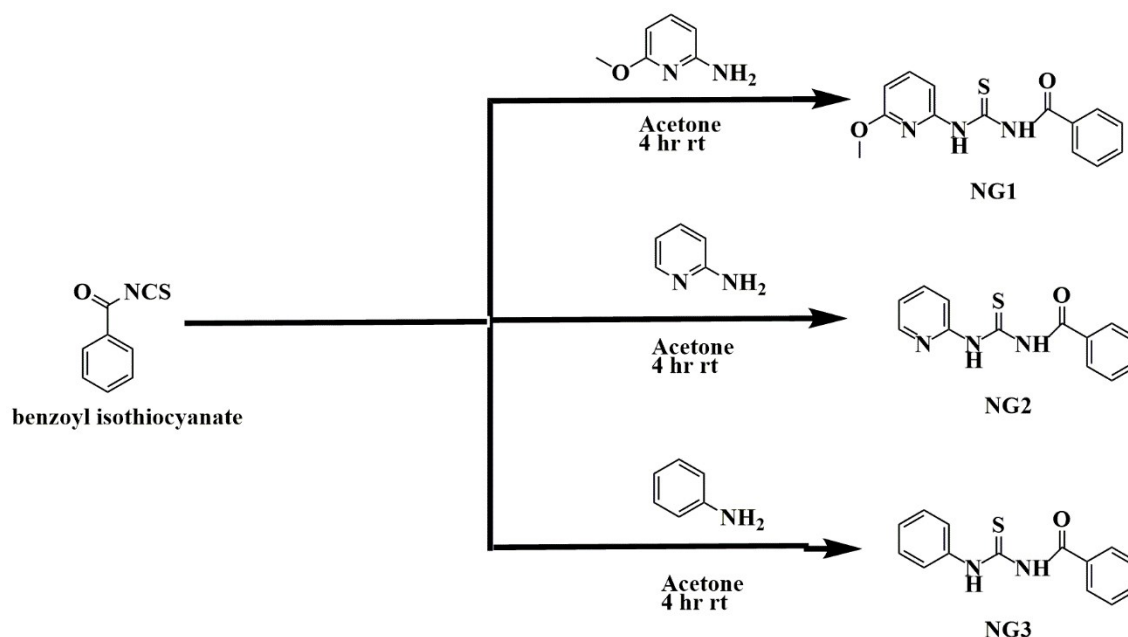
## Table of content

1. Scheme	<b>S1</b>
2. UV spectra of <b>NG2</b> and <b>NG3</b> with and without $\text{Cu}^{2+}$ at 50 ppm.....	<b>S1</b>
3. UV-visible spectra of <b>NG2</b> and <b>NG3</b> with $\text{Cu}^{2+}$ .....	<b>S2</b>
4. Optical microscopic images.....	<b>S3</b>
5. Optical microscopic images of <b>NG2</b> and <b>NG3</b> in different filter.....	<b>S4</b>
6. Optical microscopic images of <b>NG2</b> and <b>NG3</b> in with copper and Lactic acid.....	<b>S5</b>
7. Vial images of <b>NG1</b> with $\text{Cu}^{2+}$ ions and other metals showing yellow colour and selectivity for $\text{Cu}^{2+}$ ions.....	<b>S6</b>
8. LOD at the wavelength 410 nm.....	<b>S7</b>
9. FTIR spectra of Copper nitrate hemihydrate and <b>NG1</b> - $\text{Cu}^{2+}$ complex.....	<b>S8</b>
10. Bar graph of the relative intensity of <b>NG1</b> at 410 nm upon treatment with various metal ions.....	<b>S9</b>
11. Vials images of <b>NG1</b> at different pH.....	<b>S10</b>
12. UV visible spectra of colour change on sequential addition of $\text{Cu}^{2+}$ and Lactic acid.....	<b>S11</b>
13. Powdered XRD graph of <b>NG1</b> assembled, <b>NG1</b> Non-assembled and <b>NG1</b> + $\text{Cu}^{2+}$ ....	<b>S12</b>
14. Fluorescence spectra of <b>NG1</b> , <b>NG1</b> + $\text{Cu}^{2+}$ at 353nm.....	<b>S13</b>
15. Fluorescence spectra of <b>NG1</b> at different excitation wavelength at 390, 420 and 450 nm.....	<b>S14</b>
16. $^1\text{H}$ -NMR spectra of <b>NG1</b> , <b>NG2</b> and <b>NG3</b> .....	<b>S15</b>
17. $^{13}\text{C}$ NMR spectra <b>NG1</b> .....	<b>S16</b>
18. $^{13}\text{C}$ NMR spectra <b>NG3</b> .....	<b>S17</b>
19. LCMS spectra of <b>NG1</b> .....	<b>S18</b>
20. HPLC spectra of <b>NG1</b> .....	<b>S19</b>
21. Optical microscopic images of <b>NG1</b> A) <b>NG1</b> alone; B) <b>NG1</b> + $\text{Cu}^{2+}$ ; C) <b>NG1</b> + $\text{Cu}^{2+}$ + EDTA.....	<b>S20</b>
22. <b>NG1</b> : $\text{Cu}^{2+}$ complex in presence of Aspartic acid, Glutamic acid, Cysteine, Phenyl alanine.....	<b>S21</b>

## Material and methods:

All the starting materials for **NG1**, **NG2** and **NG3** synthesis were obtained from commercial suppliers and used as received. 2-Amino-6-methoxypyridine and Benzoyl isothiocyanate were purchased from Combi-Blocks, USA. 2-amino pyridine purchased from TCI chemicals, India, Aniline purchased from spectrochem, India. Acetone, THF, Sodium sulphate was purchased from Sisco Research Laboratories (SRL), India. Moisture sensitive reactions were performed under an atmosphere of dry Nitrogen. All the solvents used for the reactions were distilled prior to use. The R<sub>f</sub> was recorded in Analytical TLC Silica Gel 60F<sub>254</sub> purchased from Merck (Germany). The melting point of **NG1**, **NG2** and **NG3** were recorded in Visual Melting Range Apparatus (MR-VIS) provided by LABINDIA. <sup>1</sup>H NMR (400 MHz) and <sup>13</sup>C NMR (100 MHz) spectra were recorded on an Avance III 400 NMR spectrometer instrument. Proton chemical shifts were reported in parts per million. HPLC was done using the Waters E2695 machine. HPLC was performed using ammonium bicarbonate buffer (ABC) 27 minutes run time and water:ACN as mobile phase in C-18 Column. LC-MS was obtained on a Waters 2690 LC-MS instrument. The method used was Ammonium bicarbonate Buffer (ABC); 7 minutes run time and water: ACN as mobile phase in C-18 Column. UV-visible spectra were recorded on a Shimadzu UV-Vis Spectrophotometer 1900 with 10 mm quartz cell at 25 °C. Fluorescence Spectra were recorded on Horiba Jobin Yvon Fluorolog-3 spectrometer. XRD was recorded in powder mode on D8 DISCOVER (Bruker) Model.

### Synthesis of NG1, NG2, and NG3:

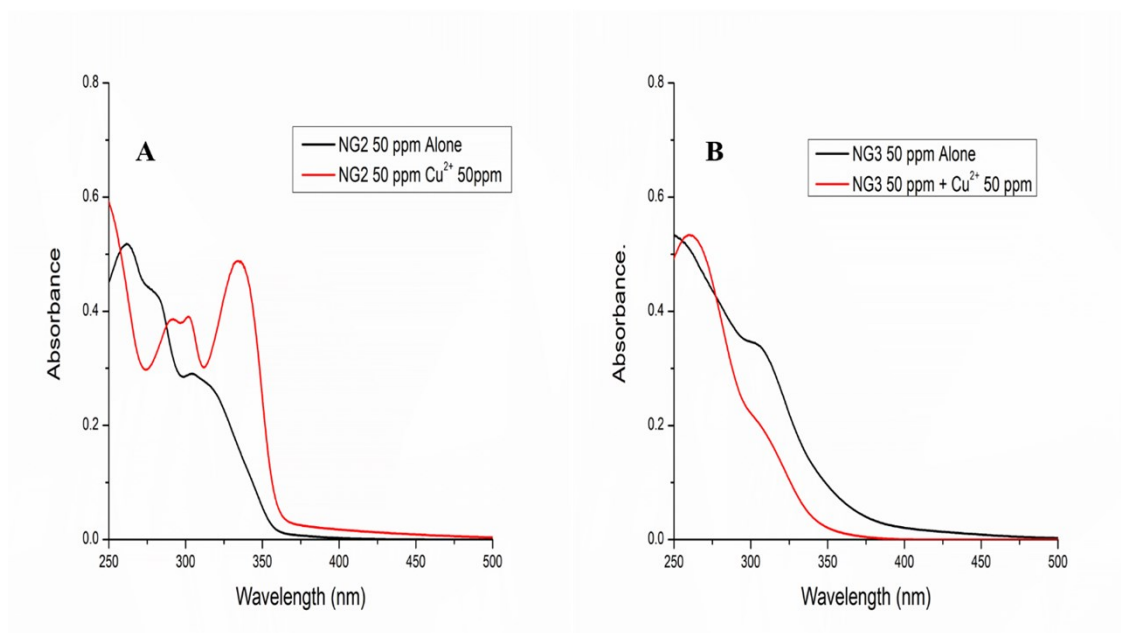


**SchemeS1:** Synthesis of **NG1**, **NG2**&**NG3**

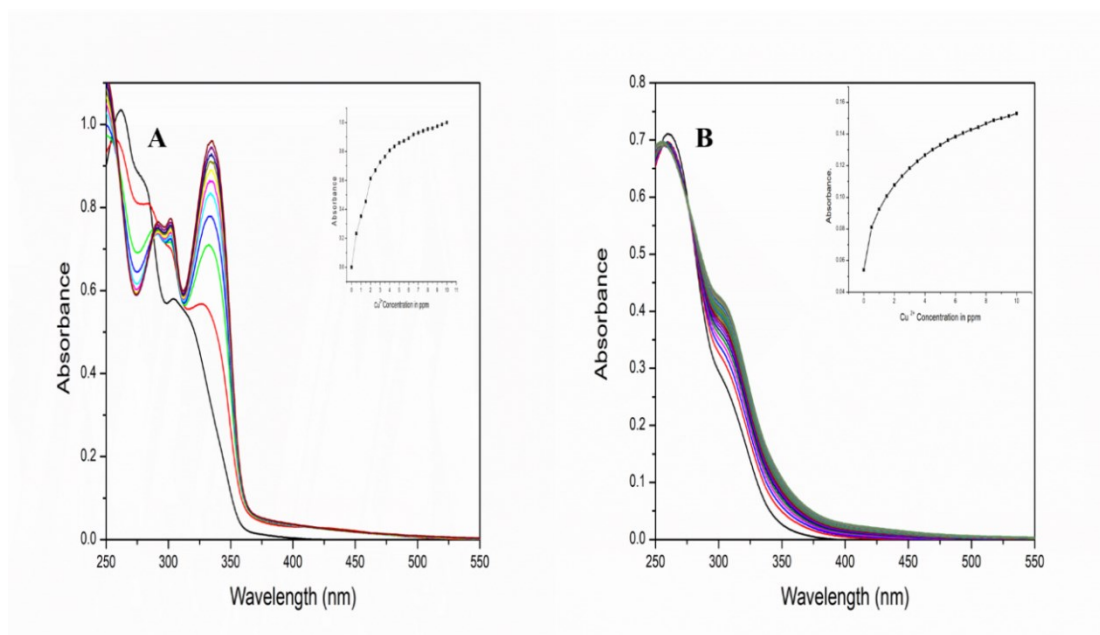
**Synthesis of NG1:** In a three-necked round bottom flask-fitted with a dropping funnel filled with 50 mL of dry acetone- 5.0g (27 mmol) of 2-Amino 6-Methoxy pyridine was placed followed by dropwise addition of dry acetone under N<sub>2</sub> atmosphere during constant stirring of the reaction mixture. Next, 7.2 g (44 mmol) of benzoyl isothiocyanate was added and the reaction mixture was then allowed to stir for another 2h at room temperature. The progress of the reaction was monitored by analytical TLC by using the ethyl acetate-hexane (3:7) solvent mixture. After the completion of the reaction, the reaction mixture was then poured carefully with stirring into 500 mL of cold water and the resulting yellow precipitate of (N-((6-methoxypyridin-2-yl)carbamothioyl)benzamide) is separated by suction filtration followed by washing of precipitate with water (3x100 mL). The filtrate was further purified by vacuum distillation which yielded the desired product (10.0 g, 34mmol, Yields 86 %) as solid light of white material. M.P. 136 °C R<sub>f</sub> 0.53. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, 25°C, TMS) δ(ppm) = 13.14 (s, 1H), 11.70 (s, 1H), 8.36 (s, 1H) 7.97 (t, J=8.8 Hz, 2H), 7.80 (t, J=8.0 Hz, 1H), 7.664 (m, 1), 7.53 (t, J=8.0 Hz, 2H), 6.71 (d, J=8.4 Hz, 1H), 3.83 (s, 3H), <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, 25 °C, TMS) δ(ppm)= 177.52, 162.54, 140.86, 140.85, 133.23, 128.75, 128.44, 107.68, 53.32. LCMS: obtained m/z value is 286.8 and, the calculated m/z value is 286.3 for the chemical formula: C<sub>14</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>S.

**Synthesis of NG2:** In a three-necked round bottom flask-fitted with a dropping funnel filled with 50mL of dry acetone- 5.0g (27 mmol) of 2-Amino pyridine was placed followed by dropwise addition of dry acetone under N<sub>2</sub> atmosphere during constant stirring of the reaction mixture. Next, 6.5 g (42 mmol) of benzoyl isothiocyanate was added and the reaction mixture was then allowed to stir for another 2h at room temperature<sup>1</sup>. The progress of the reaction was monitored by analytical TLC by using the ethyl acetate-hexane (3:7) solvent mixture. After the completion of the reaction, the reaction mixture was then poured carefully with stirring into 500 mL of cold water and the resulting yellow precipitate of N-(pyridine-2-ylcarbamothioyl)benzamide is separated by suction filtration followed by washing of precipitate with water (3x100 mL). The filtrate was further purified by vacuum distillation which yielded the desired product (9.6 g, 34 mmol, Yields 86 %) as solid light yellow material. M.P. 136 °C R<sub>f</sub> 0.53. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, 25°C, TMS) δ(ppm) = 13.28 (s, 1H), 11.71 (s, 1H), 8.78 (s, 1H) 8.43-8.42 (d, J=2.4 Hz, 1H), 7.98-7.89 (m, 3H), 7.67 (d, J=6.0 Hz, 1H), 7.55 (t, J=10.8 Hz, 2H), 7.27 (s, 1H).

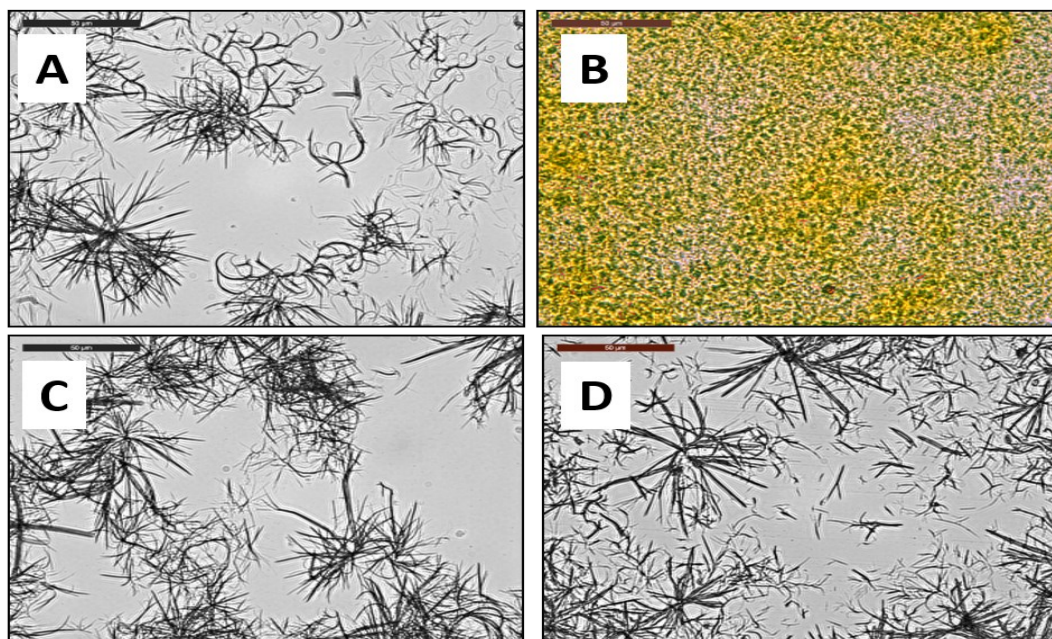
**Synthesis of NG3:** In a three-necked round bottom flask- fitted with a dropping funnel filled with 50mL of dry acetone- 5.0g (27 mmol) of 2-Amino 6-Methoxy pyridine was placed followed by dropwise addition of dry acetone under N<sub>2</sub> atmosphere during constant stirring of the reaction mixture. Next, 7.2 g (44 mmol) of benzoyl isothiocyanate was added and the reaction mixture was then allowed to stir for another 2h at room temperature<sup>1</sup>. The progress of the reaction was monitored by analytical TLC by using the ethyl acetate-hexane (3:7) solvent mixture. After the completion of the reaction, the reaction mixture was then poured carefully with stirring into 500 mL of cold water and the resulting yellow precipitate of N-(phenylcarbamothioyl)benzamide is separated by suction filtration followed by washing of precipitate with water (3x100 mL). The filtrate was further purified by vacuum distillation which yielded desired product (10.0 g, 34mmol, Yields 86 %) as solid light yellow material. M.P. 136 °C R<sub>f</sub> 0.53 (This material was used in next step without any further purification. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, 25°C, TMS) δ(ppm) = 12.59 (s, 1H), 11.56 (s, 1H), 7.96 (t, J=5.6 Hz, 2H) 7.69-7.64 (m, 3H), 7.53 (t, J=12.4 Hz, 2H), 7.42 (t, J=12.4 Hz, 2H), 7.26 (s, 1H), <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, 25 °C, TMS) δ(ppm)= 179.59, 168.76, 138.48, 133.60, 129.16, 128.92, 126.80, 124.79.



**FigureS1 (A)**UV spectra **NG2** with and without Cu<sup>2+</sup> 50 ppm;**(B)** UV spectra of **NG3**with and without Cu<sup>2+</sup> at 50 ppm

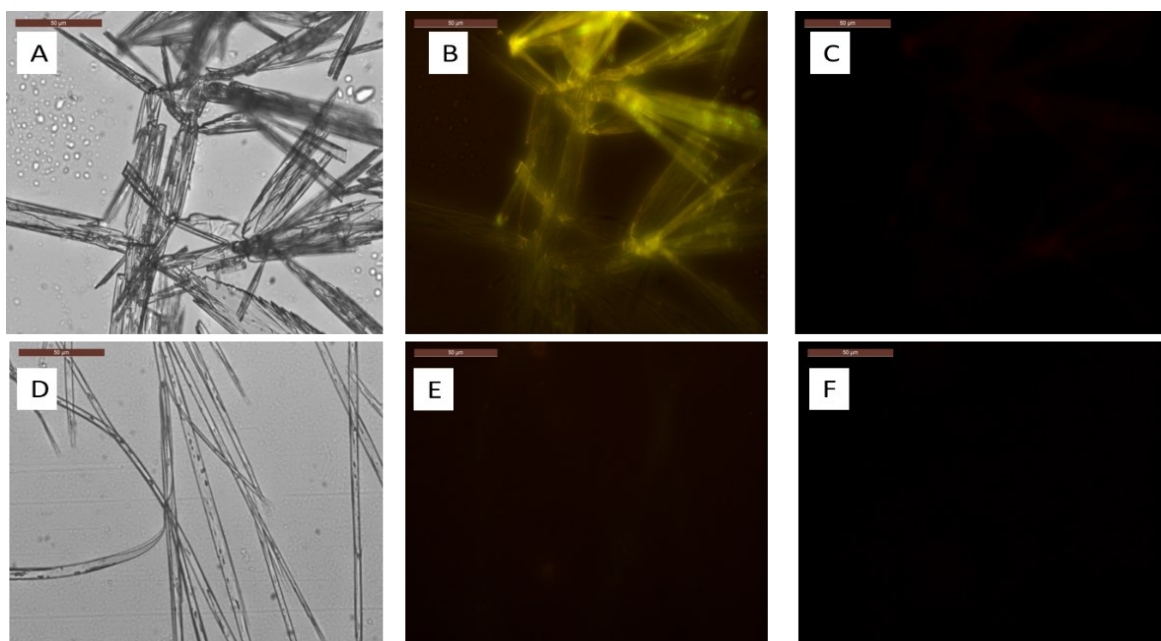


**FigureS2(A)** UV spectra of **NG2** with varying concentration of  $\text{Cu}^{2+}$  ions from 0 to 50 ppm;  
**(B)** UV Spectra of **NG3** with varying concentration of  $\text{Cu}^{2+}$  ions from 0 to 50 ppm

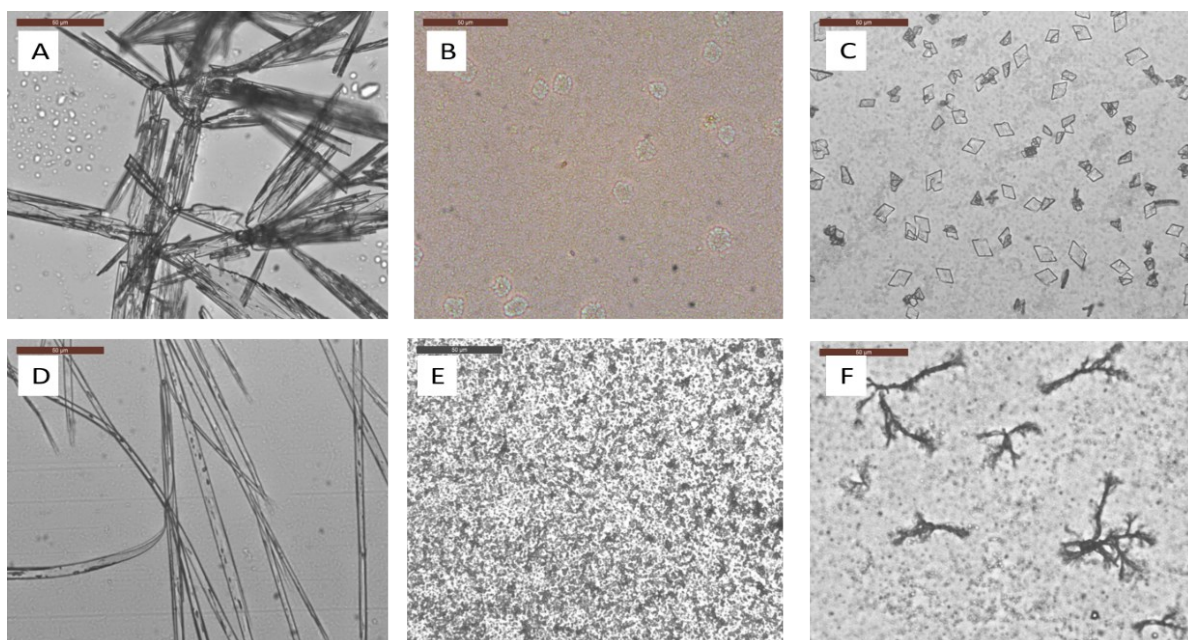


**FigureS3**Optical microscopic images of **A)** **NG1** at 1 mM concentration in bright field at 40X;  
**B)** **NG1**+ $\text{Cu}^{2+}$  complex at 1:1 ratio in bright field at 40X; **C)** **NG1**+ $\text{Zn}^{2+}$  complex at 1:1 ratio  
in bright field at 40X; **D)** **NG1**+ $\text{Mg}^{2+}$  complex at 1:1 ratio in bright field at 40X.





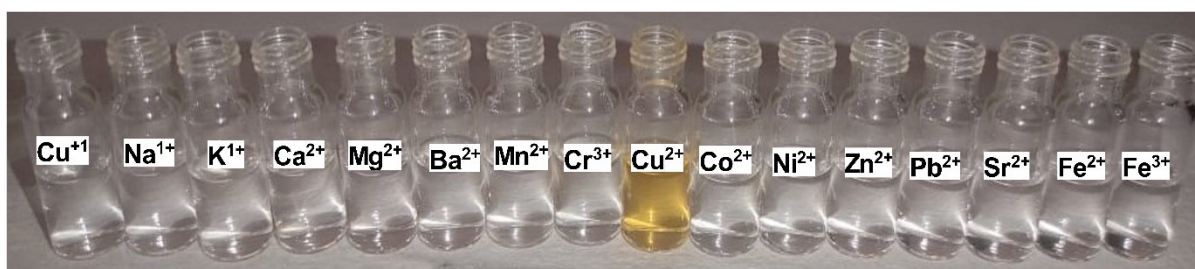
**FigureS4** Optical microscopic images of **A)** NG2 at1 mM concentration in bright field at 40X; **B)** NG2+Cu<sup>2+</sup>complex at 1:1 ratio in green filter at 40X; **C)** NG2+Cu<sup>2+</sup> complex at 1:1 red filter at 40X; **D)** NG3 at1 mM concentration in bright field at 40X; **E)** NG3+Cu<sup>2+</sup>complex at 1:1 ratio in green filter at 40X; **F)** NG3+Cu<sup>2+</sup> complex at 1:1 red filter at 40X.



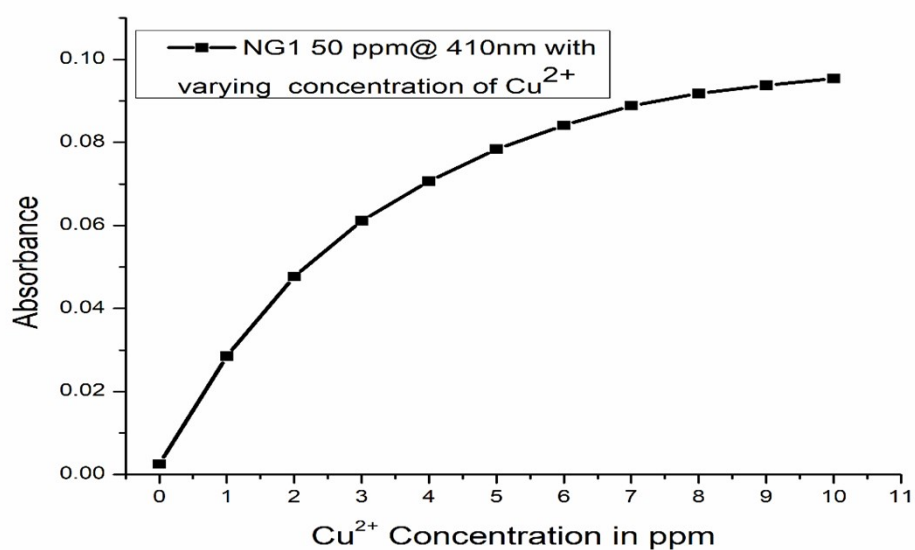
**FigureS5** Optical microscopic images of **A)** NG2 at1 mM concentration in bright field at 40X; **B)** NG2+Cu<sup>2+</sup>complex at 1:1 ratio in Bright field at 40X; **C)** NG1+Cu<sup>2+</sup>+ Lactic acid



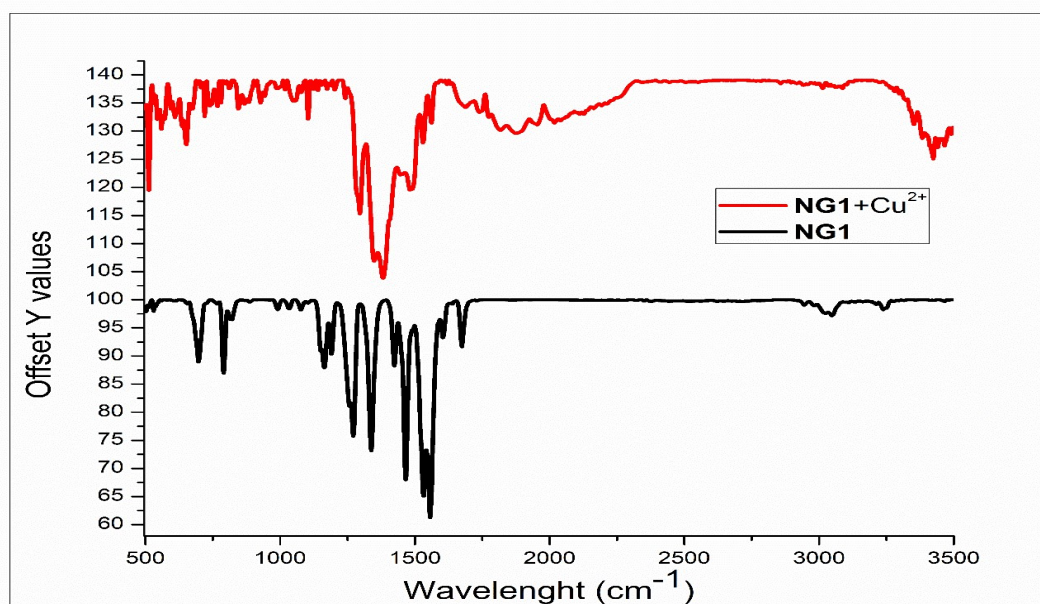
complex at 1:1 Bright field at 40X;**D)** **NG3** at1 mM concentration in bright field at 40X; **B)** **NG3**+ $\text{Cu}^{2+}$ complex at 1:1 ratio in Bright field at 40X; **C)** **NG3**+ $\text{Cu}^{2+}$ + Lactic acid complex at 1:1 Bright field at 40X.



**Figure S6** Vial images of **NG1** with  $\text{Cu}^{2+}$  ions and other metals showing yellow colour and selectivity for  $\text{Cu}^{2+}$  ions



**FigureS7** LOD at the wavelength 410 nm



**FigureS8 (A)** FTIR spectra of Copper nitrate hemihydrate and **NG1**-Cu<sup>2+</sup> complex.

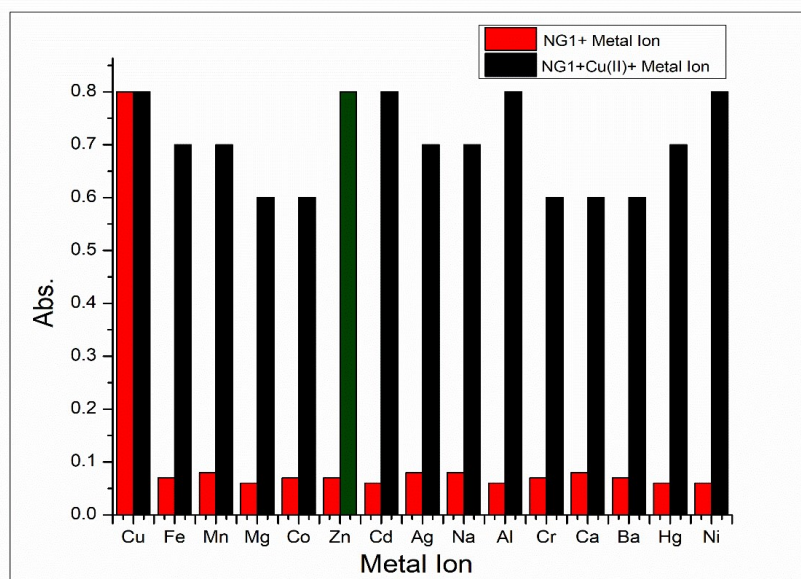
FTIR spectra of Copper nitrate hydrated alone revealed 1043 and 798 cm<sup>-1</sup> bands which may be attributed to NO<sup>3-</sup> bands. The main IR bands of **NG1** have been identified to show five absorption bands, namely,  $\nu(\text{N-H})$ ,  $\nu(\text{C-H})$ ,  $\nu(\text{C=O})$ ,  $\nu(\text{C-N})$ , and  $\nu(\text{C=S})$ . The first absorption band can be assigned as the secondary amine N-H which could be observed at 3241.36 cm<sup>-1</sup> as a medium intensity absorption band. In most thiourea derivatives, N-H stretching band appears at above 3200 cm<sup>-1</sup> due to the influence of strong intramolecular hydrogen bond between N-H...O=C which led to the formation of the broad and weak absorption band of N-H stretching. Meanwhile, C-H alkane stretching bands could be observed in the region of 2974 to 3037 cm<sup>-1</sup> as aromatic and alkyl type of CH groups were present in their molecular structures. In addition, in a range of 1555 cm<sup>-1</sup>, the high intensity of  $\nu(\text{C-N})$  absorption band could be observed. Strong absorption band observed at 1606 to 1675 cm<sup>-1</sup> in both spectra may be assigned to C=O absorption band. The C=O stretch in all the synthesized compounds were found at lower wavenumber compared with the expected carbonyl stretching at around 1700 cm<sup>-1</sup> as most carbonyl thiourea derivatives were stabilized by the formation of intramolecular hydrogen bond between C=O...H-N which lead to emergence of pseudo-six-membered ring. Consequently, the formation of the intramolecular hydrogen bond interaction led to an increase in its polarity making the double bond character to be weaker and shifting the band to a lower wavenumber region. The absorption band of C=S stretch for all synthesized compounds appear as medium bands within range of 739 to 741 cm<sup>-1</sup>. The FTIR

spectrum of the **NG1** shows a broad vibration band at 3241 cm<sup>-1</sup> which corresponds to the N–H group. The most intense band observed at 1675 cm<sup>-1</sup> was ascribed to the stretching vibration of the carbonyl group. After the complexation reaction, the vibration band of the carbonyl group shifted to lower wavenumber (1675 to 1620 cm<sup>-1</sup>). The stretching vibration band of the C=S group in the ligand was observed at 1382 cm<sup>-1</sup>. The shifted vibration band of the C=S group in the complexes cannot be observed because of overlapping with the other bands in that region. Complexation reaction is confirmed by the shifting of the N–H band, C=O, and C=S bands.

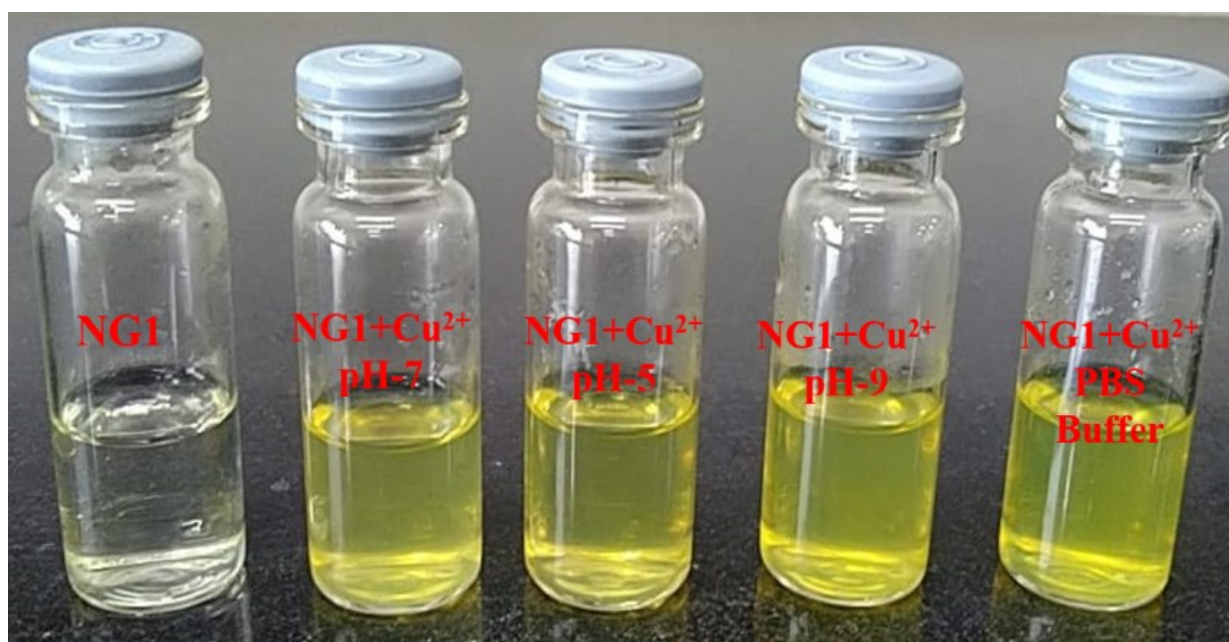
	Optimized Energy (Hartree)	Position 1 with Cu (Hartree)	Position 2 with Cu (Hartree)	With Lactic Acid (Hartree)
<b>NG2</b>	-1139.9170	-2780.4292 {-25.06}	-2780.4032 {-8.73}	-3124.1970 {-120.91}
<b>NG3</b>	-1123.8654	-2764.3567 {-11.97}	-2764.3385 {-0.55}	-3108.1511 {-124.46}

The binding energies in kcal/mol are provided in curly braces.

**Table 1.** Optimized energy (in Hartree) and binding energy (in kcal/mol) of the Complex **NG2** and **NG3**

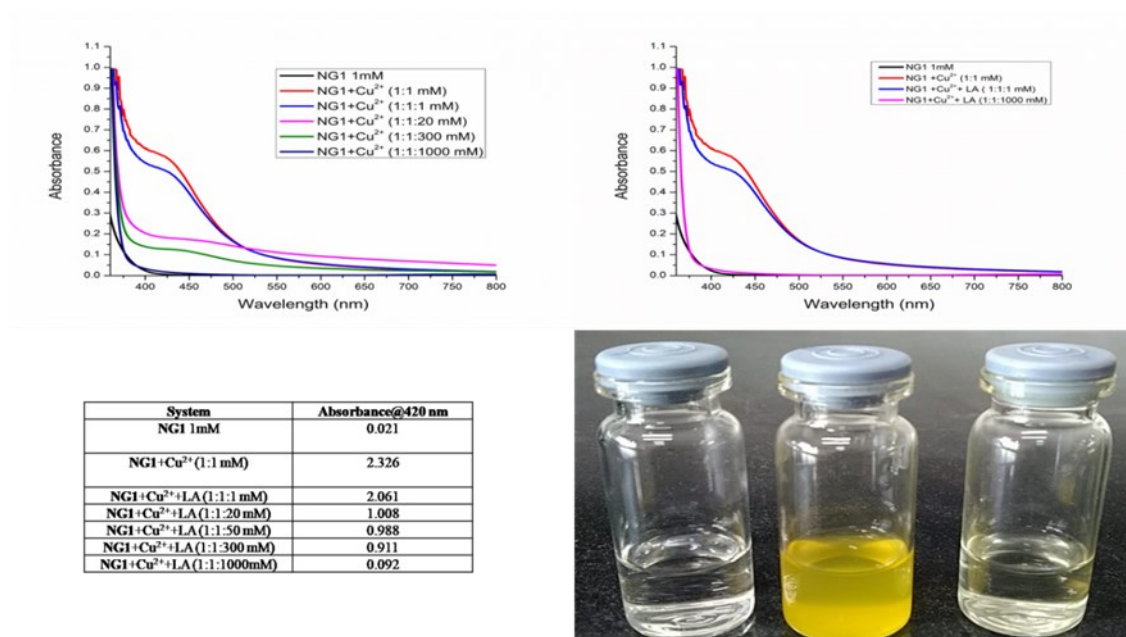


**Figure S9.** (a) Bar graph representing the change of the relative intensity of **NG1** at 410 nm upon treatment with various metal ions.

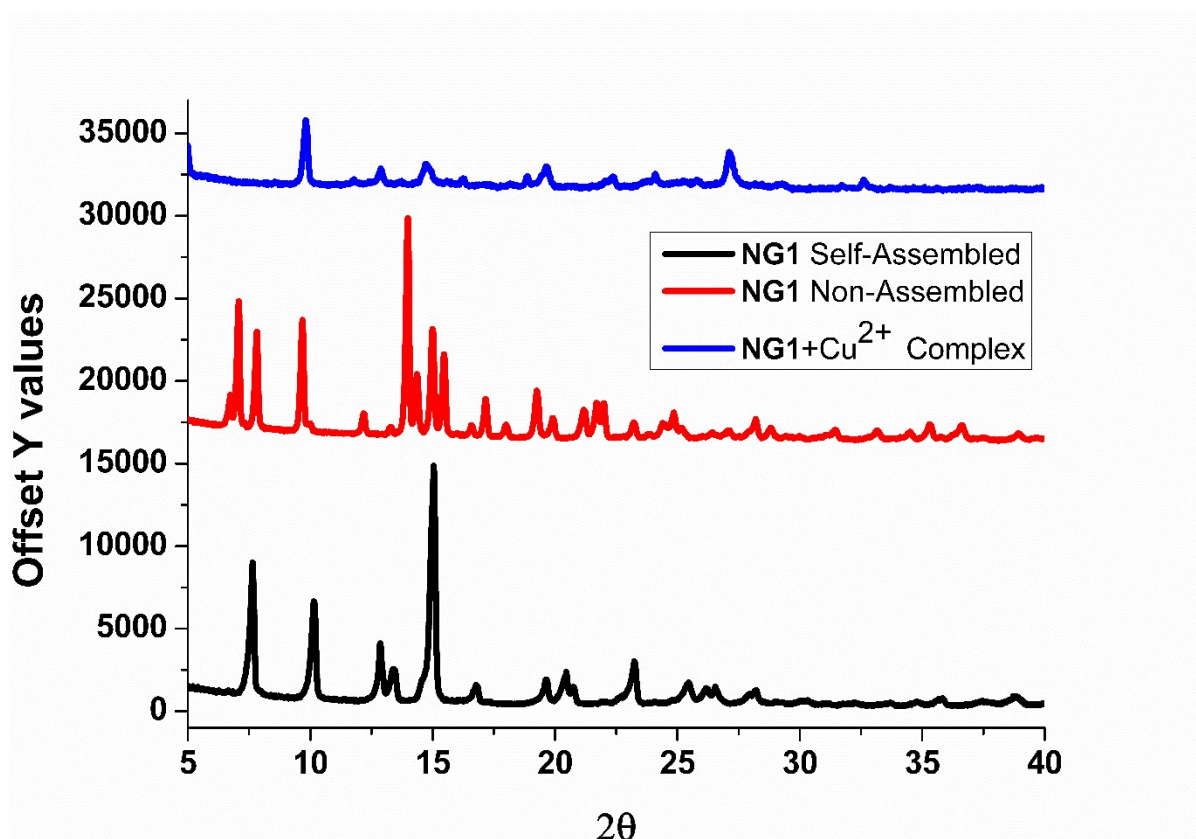


**Figure S10.** Image of vials capturing **NG1** at different pH. **NG1** pH was made acidic till pH 5.0 and also basic pH 9.0. Also, **NG1** was dissolved in PBS buffer pH 7.4 and subsequently  $\text{Cu}^{2+}$  was added. In all of these vials **NG1** was able to sense  $\text{Cu}^{2+}$  and produced yellow colour, indicating pH does not affect the sensing properties.

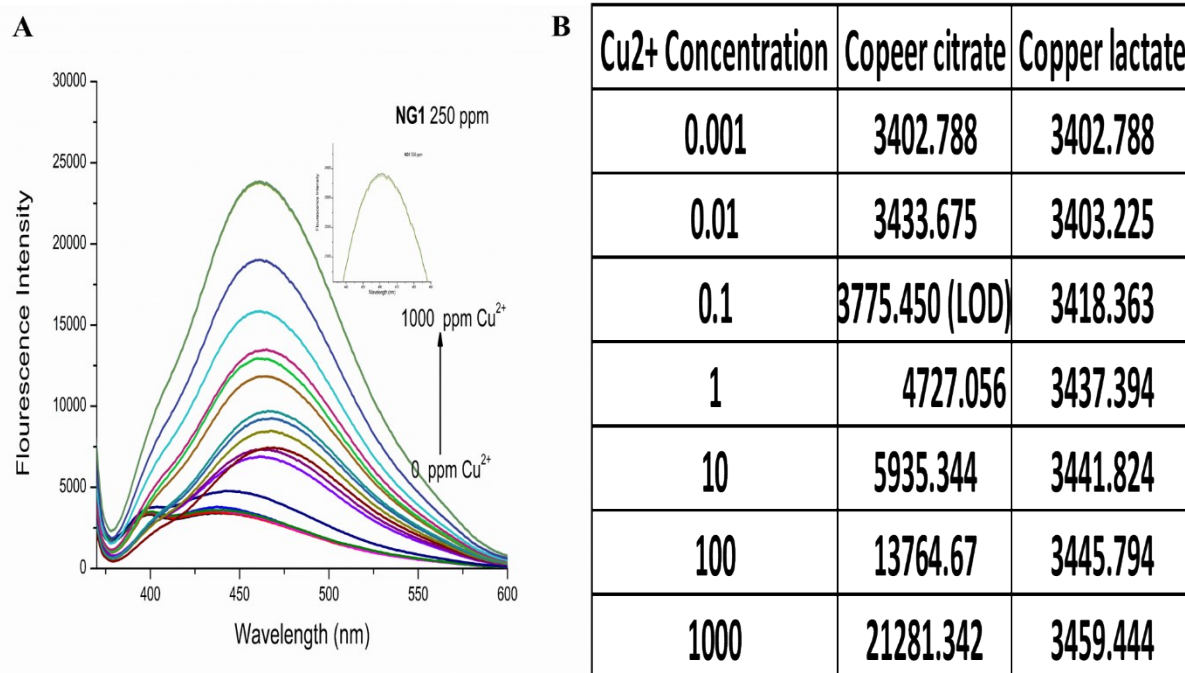




**Figure S11.** UV visible spectra of colour change on sequential addition of Cu<sup>2+</sup> and Lactic acid.

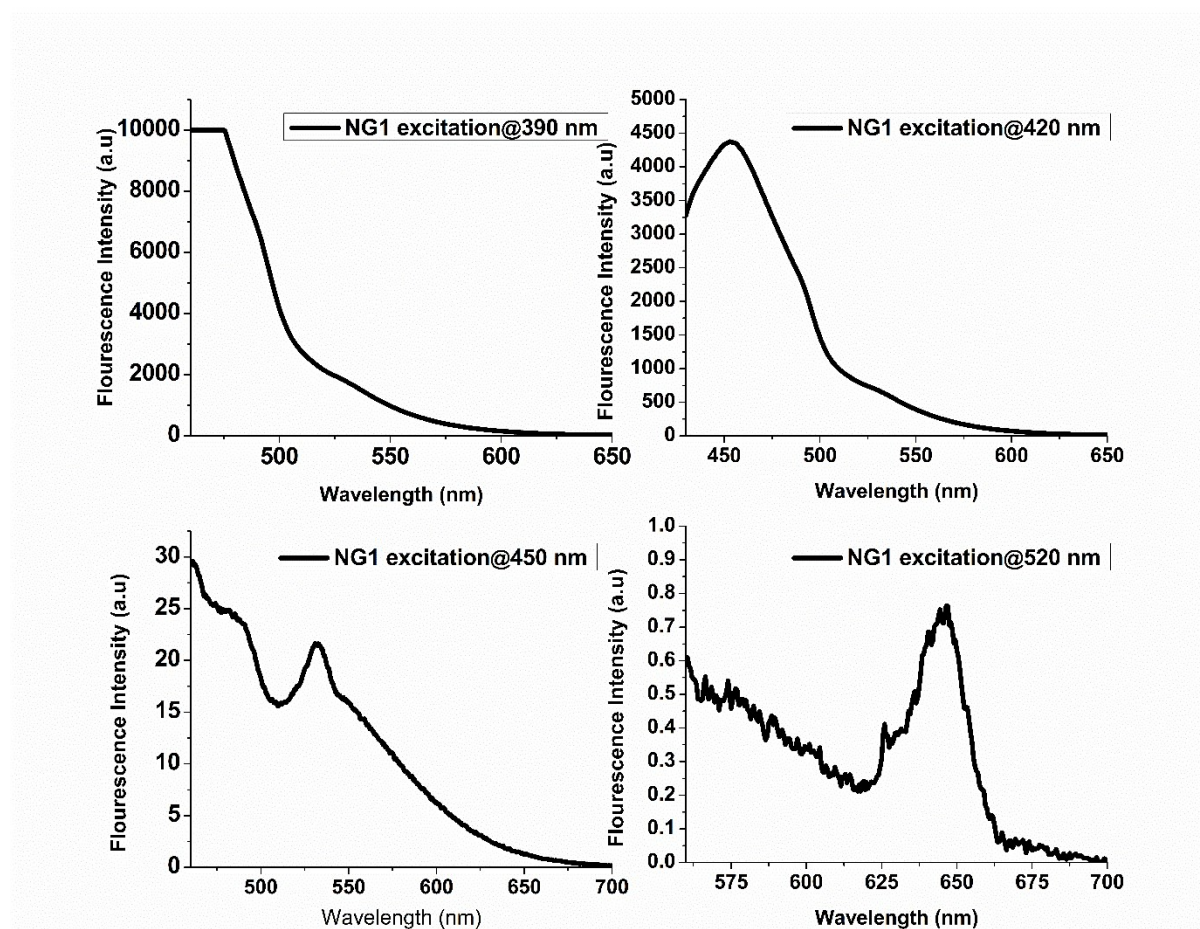


**Figure S12** Powder XRD Offset graph of Non-assembled NG1, Assembled NG1 and NG1+Cu<sup>2+</sup> complex.



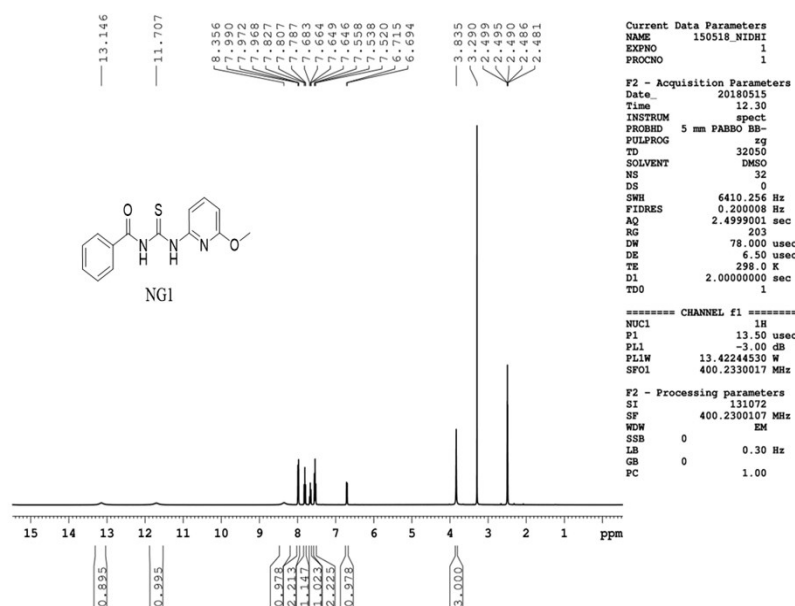
**Figure S13.** Fluorescence spectra of **NG1**, **NG1**+Cu<sup>2+</sup> recorded using excitation wavelength 353nm; A) Fluorescence spectra with increasing concentration of Cu<sup>2+</sup> from 0 to 100 ppm; B) Fluorescence intensity of Copper citrate complex and copper lactate with increasing concentration of Cu<sup>2+</sup> ions.



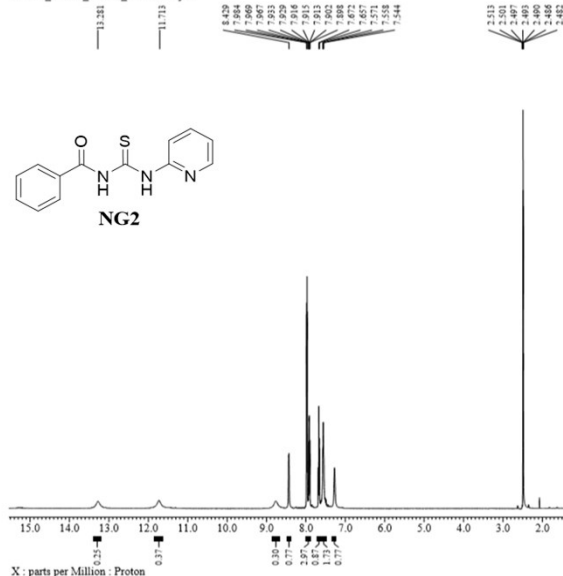


**Figure S14:** Fluorescence spectra of NG1 recorded at different excitation wavelength

**FigureS15:**  $^1\text{H}$ -NMR spectra of NG1, NG2 and NG3

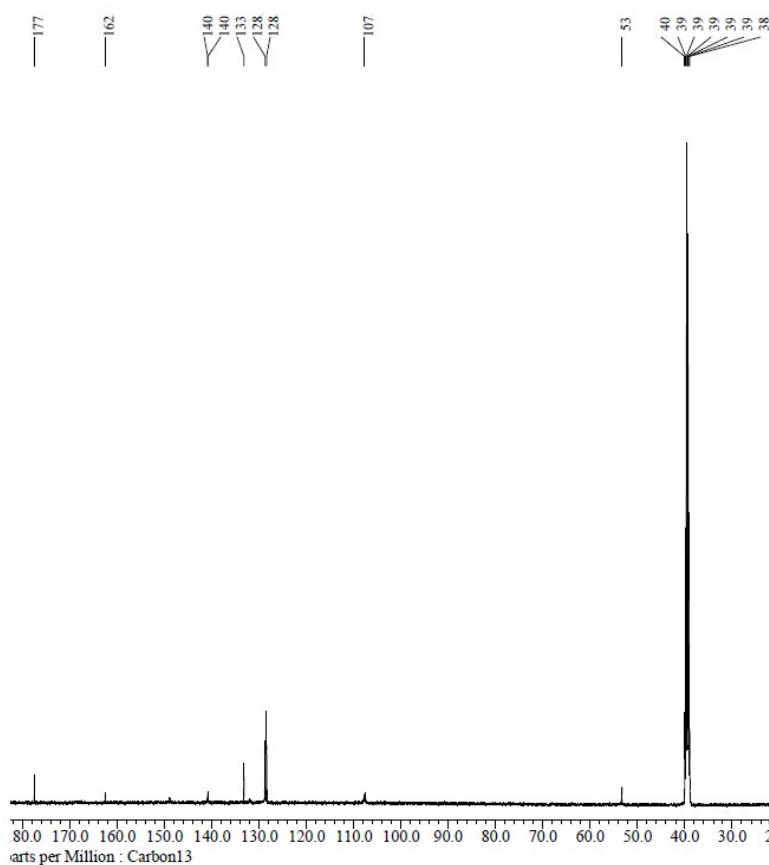


060119\_NIDHI\_Probe2\_Proton-1-2.jdf



<b>JEOL</b>	
Filename	= 060119_NIDHI_Probe2
Author	= delta
Experiment	= proton_2p
Sample_ID	= 060119_NIDHI_Probe2
Solvent	= DMSO-d6
AcqStart_Time	= 6-JUN-2019 21:58:14
AcqStop_Time	= 6-JUN-2019 22:58:10
Comment	= single_pulse
Data_Format	= 1D_1H_NMR
Dir_Exp	= 104858
Dir_Main	= Proton
Dir_Title	= Proton
Dir_Unit	= ppm
Dimensions	= 2
Spectrometer	= DELTA2_500
Field_Strength	= 11.7473797(T) (500)
AcqDuration	= 2.27359712(s)
AcqIn	= 18
AcqOut	= 800.15991521(MHz)
AcqOffset	= 7.5(ppm)
AcqPhase	= 270deg
AcqPulse	= 0
AcqPulse2	= 0.20564485(Hz)
AcqPulse3	= 10.01402544(MHz)
AcqPulse4	= 0.01202551(MHz)
AcqPulse5	= 800.15991521(MHz)
AcqPulse6	= 3.31703615(ppm)
AcqPulse7	= Proton
AcqPulse8	= 800.15991521(MHz)
AcqPulse9	= 7.5(ppm)
AcqPulse10	= 0(s)
AcqPulse11	= 0(s)
AcqPulse12	= 0(s)
AcqPulse13	= 0(s)
AcqPulse14	= 0(s)
AcqPulse15	= 0(s)
AcqPulse16	= 0(s)
AcqPulse17	= 0(s)
AcqPulse18	= 0(s)
AcqPulse19	= 0(s)
AcqPulse20	= 0(s)
AcqPulse21	= 0(s)
AcqPulse22	= 0(s)
AcqPulse23	= 0(s)
AcqPulse24	= 0(s)
AcqPulse25	= 0(s)
AcqPulse26	= 0(s)
AcqPulse27	= 0(s)
AcqPulse28	= 0(s)
AcqPulse29	= 0(s)
AcqPulse30	= 0(s)
AcqPulse31	= 0(s)
AcqPulse32	= 0(s)
AcqPulse33	= 0(s)
AcqPulse34	= 0(s)
AcqPulse35	= 0(s)
AcqPulse36	= 0(s)
AcqPulse37	= 0(s)
AcqPulse38	= 0(s)
AcqPulse39	= 0(s)
AcqPulse40	= 0(s)
AcqPulse41	= 0(s)
AcqPulse42	= 0(s)
AcqPulse43	= 0(s)
AcqPulse44	= 0(s)
AcqPulse45	= 0(s)
AcqPulse46	= 0(s)
AcqPulse47	= 0(s)
AcqPulse48	= 0(s)
AcqPulse49	= 0(s)
AcqPulse50	= 0(s)
AcqPulse51	= 0(s)
AcqPulse52	= 0(s)
AcqPulse53	= 0(s)
AcqPulse54	= 0(s)
AcqPulse55	= 0(s)
AcqPulse56	= 0(s)
AcqPulse57	= 0(s)
AcqPulse58	= 0(s)
AcqPulse59	= 0(s)
AcqPulse60	= 0(s)
AcqPulse61	= 0(s)
AcqPulse62	= 0(s)
AcqPulse63	= 0(s)
AcqPulse64	= 0(s)
AcqPulse65	= 0(s)
AcqPulse66	= 0(s)
AcqPulse67	= 0(s)
AcqPulse68	= 0(s)
AcqPulse69	= 0(s)
AcqPulse70	= 0(s)
AcqPulse71	= 0(s)
AcqPulse72	= 0(s)
AcqPulse73	= 0(s)
AcqPulse74	= 0(s)
AcqPulse75	= 0(s)
AcqPulse76	= 0(s)
AcqPulse77	= 0(s)
AcqPulse78	= 0(s)
AcqPulse79	= 0(s)
AcqPulse80	= 0(s)
AcqPulse81	= 0(s)
AcqPulse82	= 0(s)
AcqPulse83	= 0(s)
AcqPulse84	= 0(s)
AcqPulse85	= 0(s)
AcqPulse86	= 0(s)
AcqPulse87	= 0(s)
AcqPulse88	= 0(s)
AcqPulse89	= 0(s)
AcqPulse90	= 0(s)
AcqPulse91	= 0(s)
AcqPulse92	= 0(s)
AcqPulse93	= 0(s)
AcqPulse94	= 0(s)
AcqPulse95	= 0(s)
AcqPulse96	= 0(s)
AcqPulse97	= 0(s)
AcqPulse98	= 0(s)
AcqPulse99	= 0(s)
AcqPulse100	= 0(s)
AcqPulse101	= 0(s)
AcqPulse102	= 0(s)
AcqPulse103	= 0(s)
AcqPulse104	= 0(s)
AcqPulse105	= 0(s)
AcqPulse106	= 0(s)
AcqPulse107	= 0(s)
AcqPulse108	= 0(s)
AcqPulse109	= 0(s)
AcqPulse110	= 0(s)
AcqPulse111	= 0(s)
AcqPulse112	= 0(s)
AcqPulse113	= 0(s)
AcqPulse114	= 0(s)
AcqPulse115	= 0(s)
AcqPulse116	= 0(s)
AcqPulse117	= 0(s)
AcqPulse118	= 0(s)
AcqPulse119	= 0(s)
AcqPulse120	= 0(s)
AcqPulse121	= 0(s)
AcqPulse122	= 0(s)
AcqPulse123	= 0(s)
AcqPulse124	= 0(s)
AcqPulse125	= 0(s)
AcqPulse126	= 0(s)
AcqPulse127	= 0(s)
AcqPulse128	= 0(s)
AcqPulse129	= 0(s)
AcqPulse130	= 0(s)
AcqPulse131	= 0(s)
AcqPulse132	= 0(s)
AcqPulse133	= 0(s)
AcqPulse134	= 0(s)
AcqPulse135	= 0(s)
AcqPulse136	= 0(s)
AcqPulse137	= 0(s)
AcqPulse138	= 0(s)
AcqPulse139	= 0(s)
AcqPulse140	= 0(s)
AcqPulse141	= 0(s)
AcqPulse142	= 0(s)
AcqPulse143	= 0(s)
AcqPulse144	= 0(s)
AcqPulse145	= 0(s)
AcqPulse146	= 0(s)
AcqPulse147	= 0(s)
AcqPulse148	= 0(s)
AcqPulse149	= 0(s)
AcqPulse150	= 0(s)
AcqPulse151	= 0(s)
AcqPulse152	= 0(s)
AcqPulse153	= 0(s)
AcqPulse154	= 0(s)
AcqPulse155	= 0(s)
AcqPulse156	= 0(s)
AcqPulse157	= 0(s)
AcqPulse158	= 0(s)
AcqPulse159	= 0(s)
AcqPulse160	= 0(s)
AcqPulse161	= 0(s)
AcqPulse162	= 0(s)
AcqPulse163	= 0(s)
AcqPulse164	= 0(s)
AcqPulse165	= 0(s)
AcqPulse166	= 0(s)
AcqPulse167	= 0(s)
AcqPulse168	= 0(s)
AcqPulse169	= 0(s)
AcqPulse170	= 0(s)
AcqPulse171	= 0(s)
AcqPulse172	= 0(s)
AcqPulse173	= 0(s)
AcqPulse174	= 0(s)
AcqPulse175	= 0(s)
AcqPulse176	= 0(s)
AcqPulse177	= 0(s)
AcqPulse178	= 0(s)
AcqPulse179	= 0(s)
AcqPulse180	= 0(s)
AcqPulse181	= 0(s)
AcqPulse182	= 0(s)
AcqPulse183	= 0(s)
AcqPulse184	= 0(s)
AcqPulse185	= 0(s)
AcqPulse186	= 0(s)
AcqPulse187	= 0(s)
AcqPulse188	= 0(s)
AcqPulse189	= 0(s)
AcqPulse190	= 0(s)
AcqPulse191	= 0(s)
AcqPulse192	= 0(s)
AcqPulse193	= 0(s)
AcqPulse194	= 0(s)
AcqPulse195	= 0(s)
AcqPulse196	= 0(s)
AcqPulse197	= 0(s)
AcqPulse198	= 0(s)
AcqPulse199	= 0(s)
AcqPulse200	= 0(s)
AcqPulse201	= 0(s)
AcqPulse202	= 0(s)
AcqPulse203	= 0(s)
AcqPulse204	= 0(s)
AcqPulse205	= 0(s)
AcqPulse206	= 0(s)
AcqPulse207	= 0(s)
AcqPulse208	= 0(s)
AcqPulse209	= 0(s)
AcqPulse210	= 0(s)
AcqPulse211	= 0(s)
AcqPulse212	= 0(s)
AcqPulse213	= 0(s)
AcqPulse214	= 0(s)
AcqPulse215	= 0(s)
AcqPulse216	= 0(s)
AcqPulse217	= 0(s)
AcqPulse218	= 0(s)
AcqPulse219	= 0(s)
AcqPulse220	= 0(s)
AcqPulse221	= 0(s)
AcqPulse222	= 0(s)
AcqPulse223	= 0(s)
AcqPulse224	= 0(s)
AcqPulse225	= 0(s)
AcqPulse226	= 0(s)
AcqPulse227	= 0(s)
AcqPulse228	= 0(s)
AcqPulse229	= 0(s)
AcqPulse230	= 0(s)
AcqPulse231	= 0(s)
AcqPulse232	= 0(s)
AcqPulse233	= 0(s)
AcqPulse234	= 0(s)
AcqPulse235	= 0(s)
AcqPulse236	= 0(s)
AcqPulse237	= 0(s)
AcqPulse238	= 0(s)
AcqPulse239	= 0(s)
AcqPulse240	= 0(s)
AcqPulse241	= 0(s)
AcqPulse242	= 0(s)
AcqPulse243	= 0(s)
AcqPulse244	= 0(s)
AcqPulse245	= 0(s)
AcqPulse246	= 0(s)
AcqPulse247	= 0(s)
AcqPulse248	= 0(s)
AcqPulse249	= 0(s)
AcqPulse250	= 0(s)
AcqPulse251	= 0(s)
AcqPulse252	= 0(s)
AcqPulse253	= 0(s)
AcqPulse254	= 0(s)
AcqPulse255	= 0(s)
AcqPulse256	= 0(s)
AcqPulse257	= 0(s)
AcqPulse258	= 0(s)
AcqPulse259	= 0(s)
AcqPulse260	= 0(s)
AcqPulse261	= 0(s)
AcqPulse262	= 0(s)
AcqPulse263	= 0(s)
AcqPulse264	= 0(s)
AcqPulse265	= 0(s)
AcqPulse266	= 0(s)
AcqPulse267	= 0(s)
AcqPulse268	= 0(s)
AcqPulse269	= 0(s)
AcqPulse270	= 0(s)
AcqPulse271	= 0(s)
AcqPulse272	= 0(s)
AcqPulse273	= 0(s)
AcqPulse274	= 0(s)
AcqPulse275	= 0(s)
AcqPulse276	= 0(s)
AcqPulse277	= 0(s)
AcqPulse278	= 0(s)
AcqPulse279	= 0(s)
AcqPulse280	= 0(s)
AcqPulse281	= 0(s)
AcqPulse282	= 0(s)
AcqPulse283	= 0(s)
AcqPulse284	= 0(s)
AcqPulse285	= 0(s)
AcqPulse286	= 0(s)
AcqPulse287	= 0(s)
AcqPulse288	= 0(s)
AcqPulse289	= 0(s)
AcqPulse290	= 0(s)
AcqPulse291	= 0(s)
AcqPulse292	= 0(s)
AcqPulse293	= 0(s)
AcqPulse294	= 0(s)
AcqPulse295	= 0(s)
AcqPulse296	= 0(s)
AcqPulse297	= 0(s)
AcqPulse298	= 0(s)
AcqPulse299	= 0(s)
AcqPulse300	= 0(s)
AcqPulse301	= 0(s)
AcqPulse302	= 0(s)
AcqPulse303	= 0(s)
AcqPulse304	= 0(s)
AcqPulse305	= 0(s)
AcqPulse306	= 0(s)
AcqPulse307	= 0(s)
AcqPulse308	= 0(s)
AcqPulse309	= 0(s)
AcqPulse310	= 0(s)
AcqPulse311	= 0(s)
AcqPulse312	= 0(s)
AcqPulse313	= 0(s)
AcqPulse314	= 0(s)
AcqPulse315	= 0(s)
AcqPulse316	= 0(s)
AcqPulse317	= 0(s)
AcqPulse318	= 0(s)
AcqPulse319	= 0(s)
AcqPulse320	= 0(s)
AcqPulse321	= 0(s)
AcqPulse322	= 0(s)
AcqPulse323	= 0(s)
AcqPulse324	= 0(s)
AcqPulse325	= 0(s)
AcqPulse326	= 0(s)
AcqPulse327	= 0(s)
AcqPulse328	= 0(s)
AcqPulse329	= 0(s)
AcqPulse330	= 0(s)
AcqPulse331	= 0(s)
AcqPulse332	= 0(s)
AcqPulse333	= 0(s)
AcqPulse334	= 0(s)
AcqPulse335	= 0(s)
AcqPulse336	= 0(s)
AcqPulse337	= 0(s)
AcqPulse338	= 0(s)
AcqPulse339	= 0(s)
AcqPulse340	= 0(s)
AcqPulse341	= 0(s)
AcqPulse342	= 0(s)
AcqPulse343	= 0(s)
AcqPulse344	= 0(s)
AcqPulse345	= 0(s)
AcqPulse346	= 0(s)
AcqPulse347	= 0(s)
AcqPulse348	= 0(s)
AcqPulse349	= 0(s)
AcqPulse350	= 0(s)
AcqPulse351	= 0(s)
AcqPulse352	= 0(s)
AcqPulse353	= 0(s)
AcqPulse354	= 0(s)
AcqPulse355	= 0(s)
AcqPulse356	= 0(s)
AcqPulse357	= 0(s)
AcqPulse358	= 0(s)
AcqPulse359	= 0(s)
AcqPulse360	= 0(s)
AcqPulse361	= 0(s)
AcqPulse362	= 0(s)
AcqPulse363	= 0(s)
AcqPulse364	= 0(s)
AcqPulse365	= 0(s)
AcqPulse366	= 0(s)
AcqPulse367	= 0(s)
AcqPulse368	= 0(s)
AcqPulse369	= 0(s)
AcqPulse370	= 0(s)
AcqPulse371	= 0(s)
AcqPulse372	= 0(s)
AcqPulse373	= 0(s)
AcqPulse374	= 0(s)
AcqPulse375	= 0(s)
AcqPulse376	= 0(s)
AcqPulse377	= 0(s)
AcqPulse378	= 0(s)
AcqPulse379	= 0(s)
AcqPulse380	= 0(s)
AcqPulse381	= 0(s)
AcqPulse382	= 0(s)
AcqPulse383	= 0(s)
AcqPulse384	= 0(s)
AcqPulse385	= 0(s)
AcqPulse386	= 0(s)
AcqPulse387	= 0(s)
AcqPulse388	= 0(s)
AcqPulse389	= 0(s)
AcqPulse390	= 0(s)
AcqPulse391	= 0(s)
AcqPulse392	= 0(s)
AcqPulse393	= 0(s)
AcqPulse394	= 0(s)
AcqPulse395	= 0(s)
AcqPulse396	= 0(s)
AcqPulse397	= 0(s)
AcqPulse398	= 0(s)
AcqPulse399	= 0(s)
AcqPulse400	= 0(s)
AcqPulse401	= 0(s)
AcqPulse402	= 0(s)
AcqPulse403	= 0(s)
AcqPulse404	= 0(s)
AcqPulse405	= 0(s)
AcqPulse406	= 0(s)
AcqPulse407	= 0(s)
AcqPulse408	= 0(s)
AcqPulse409	= 0(s)
AcqPulse410	= 0(s)
AcqPulse411	= 0(s)
AcqPulse412	= 0(s)
AcqPulse413	= 0(s)
AcqPulse414	= 0(s)
AcqPulse415	= 0(s)
AcqPulse416	= 0(s)
AcqPulse417	= 0(s)
AcqPulse418	= 0(s)
AcqPulse419	= 0(s)
AcqPulse420	= 0(s)
AcqPulse421	= 0(s)
AcqPulse422	= 0(s)
AcqPulse423	= 0(s)
AcqPulse424	= 0(s)
AcqPulse425	= 0(s)
AcqPulse426	= 0(s)
AcqPulse427	= 0(s)
AcqPulse428	= 0(s)
AcqPulse429	= 0(s)
AcqPulse430	= 0(s)
AcqPulse431	= 0(s)
AcqPulse432	= 0(s)
AcqPulse433	= 0(s)
AcqPulse434	= 0(s)
AcqPulse435	= 0(s)
AcqPulse436	= 0(s)
AcqPulse437	= 0(s)
AcqPulse438	= 0(s)
AcqPulse439	= 0(s)
AcqPulse440	= 0(s)
AcqPulse441	= 0(s)
AcqPulse442	= 0(s)
AcqPulse443	= 0(s)
AcqPulse444	= 0(s)
AcqPulse445	= 0(s)
AcqPulse446	= 0(s)
AcqPulse447	= 0(s)
AcqPulse448	= 0(s)
AcqPulse449	= 0(s)
AcqPulse450	= 0(s)
AcqPulse451	= 0(s)
AcqPulse452	= 0(s)
AcqPulse453	= 0(s)
AcqPulse454	= 0(s)
AcqPulse455	= 0(s)
AcqPulse456	= 0(s)
AcqPulse457	= 0(s)
AcqPulse458	= 0(s)
AcqPulse459	= 0(s)
AcqPulse460	= 0(s)
AcqPulse461	= 0(s)
AcqPulse462	= 0(s)
AcqPulse463	= 0(s)
AcqPulse464	= 0(s)
AcqPulse465	= 0(s)
AcqPulse466	= 0(s)
AcqPulse467	= 0(s)
AcqPulse468	= 0(s)
AcqPulse469	= 0(s)
AcqPulse470	= 0(s)
AcqPulse471	= 0(s)
AcqPulse472	= 0(s)
AcqPulse473	= 0(s)
AcqPulse474	= 0(s)
AcqPulse475	= 0(s)
AcqPulse476	= 0(s)
AcqPulse477	= 0(s)
AcqPulse478	= 0(s)
AcqPulse479	= 0(s)
AcqPulse480	= 0(s)
AcqPulse481	= 0(s)
AcqPulse482	= 0(s)
AcqPulse483	= 0(s)
AcqPulse484	= 0(s)
AcqPulse485	= 0(s)
AcqPulse486	= 0(s)
AcqPulse487	= 0(s)
AcqPulse488	= 0(s)
AcqPulse489	= 0(s)
AcqPulse490	= 0(s)
AcqPulse491	= 0(s)
AcqPulse492	= 0(s)
AcqPulse493	= 0(s)
AcqPulse494	= 0(s)
AcqPulse495	= 0(s)
AcqPulse496	= 0(s)

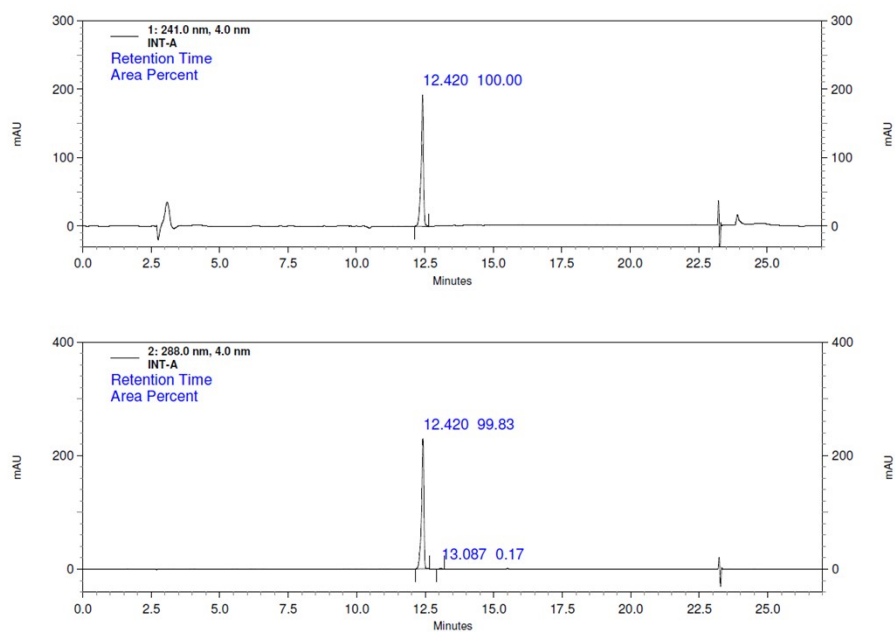
19\_NIDHI\_Probe1\_Carbon-1-2.jdf



<b>JEOL</b>	
Filename	= 060119_NIDHI_Pro
Author	= delta
Experiment	= carbon_jup
Sample Id	= 060119_NIDHI_Pro
Solvent	= DMSO-D6
Actual_Start_Time	= 6-JAN-2019 20:4
Revision_Time	= 6-JAN-2019 22:4
Comment	= single pulse dec
Data Format	= 1D COMPLEX
Dim Size	= 104858
X Domain	= Carbon13
Dim Title	= Carbon13
Dim Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field Strength	= 11.7473579 [T] (5
X Acq_Duration	= 0.82837504 [s]
X Domain	= 13C
X Freq	= 125.76529768 [MHz]
X Offset	= 100 [ppm]
X Points	= 32768
X Prescans	= 4
X Resolution	= 1.20716268 [Hz]
X Sweep	= 39.55696203 [kHz]
X Sweep_Clip	= 31.64556962 [kHz]
Irr Domain	= Proton
Irr Freq	= 500.15991521 [MHz]
Irr Offset	= 5.0 [ppm]
Blanking	= 15 [us]
Clipped	= FALSE
Scans	= 1024
Total Scans	= 1024
Relaxation Delay	= 3 [s]
Recvx Gain	= 56
Temp Get	= 24.3 [dC]
X 90_Width	= 11.82 [us]
X Acq_Time	= 0.82837504 [s]
X Angle	= 90 [deg]
X Atn	= 10.5 [dB]
X Pulse	= 11.82 [us]
Irr_Atn_Dec	= 23.465 [dB]
Irr_Atn_Dec_Calc	= 23.465 [dB]
Irr_Atn_Dec_Default_Calc	= 23.465 [dB]
Irr_Atn_Noe	= 26.46 [dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087 [kHz]
Irr_Dec_Bandwidth_Ppm	= 11.9526989 [ppm]
Irr_Dec_Freq	= 500.15991521 [MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr-Decoupling	= TRUE
Irr_Moe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5 [ppm]
Irr_Pwidth	= 92 [us]
Irr_Pwidth_Default	= 92 [us]
Irr_Pwidth_Default_Calc	= 92 [us]
Irr_Pwidth_Temp1	= 92 [us]
Irr_Wurst	= FALSE
Decimation Rate	= 0
Initial_Wait	= 1 [s]
Noe_Time	= 3 [s]
Noe_Time_Flag	= FALSE

FigureS16: C-13 NMR spectra NG1

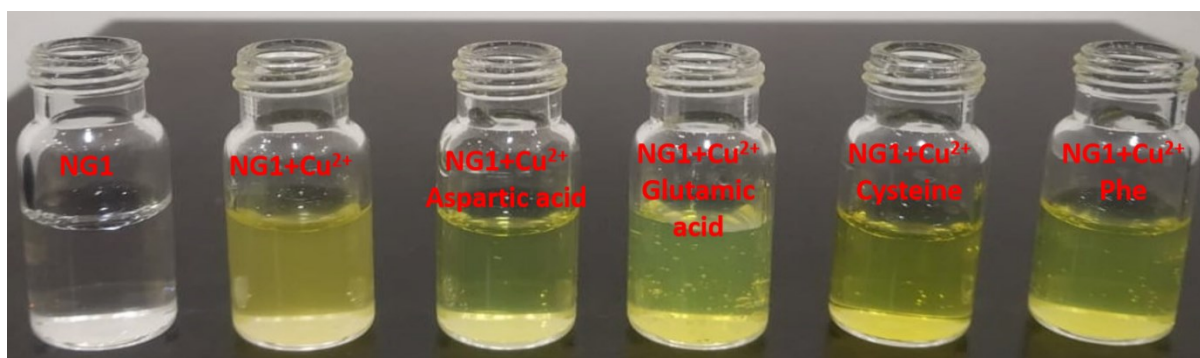




**FigureS19:**HPLC spectra of NG1



**FigureS20**Optical microscopic images of NG1 A) NG1alone; B) NG1+Cu<sup>2+</sup>; C) NG1+Cu<sup>2+</sup>+EDTA



**Figure S21**depicts the NG1:Cu<sup>2+</sup>complex does notshows any colour changes effects in presence of Aspartic acid, Glutamicacid, Cysteine, and Phenylalanine.

