## Supporting Information

# A facile turn-on luminescence technique to trap hydrazine and its application in button mushroom (*Agaricus bisporus*)

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**CONTENT** **Page no.**

**$^{1}$H NMR of C1 in DMSO-$d_6$:**

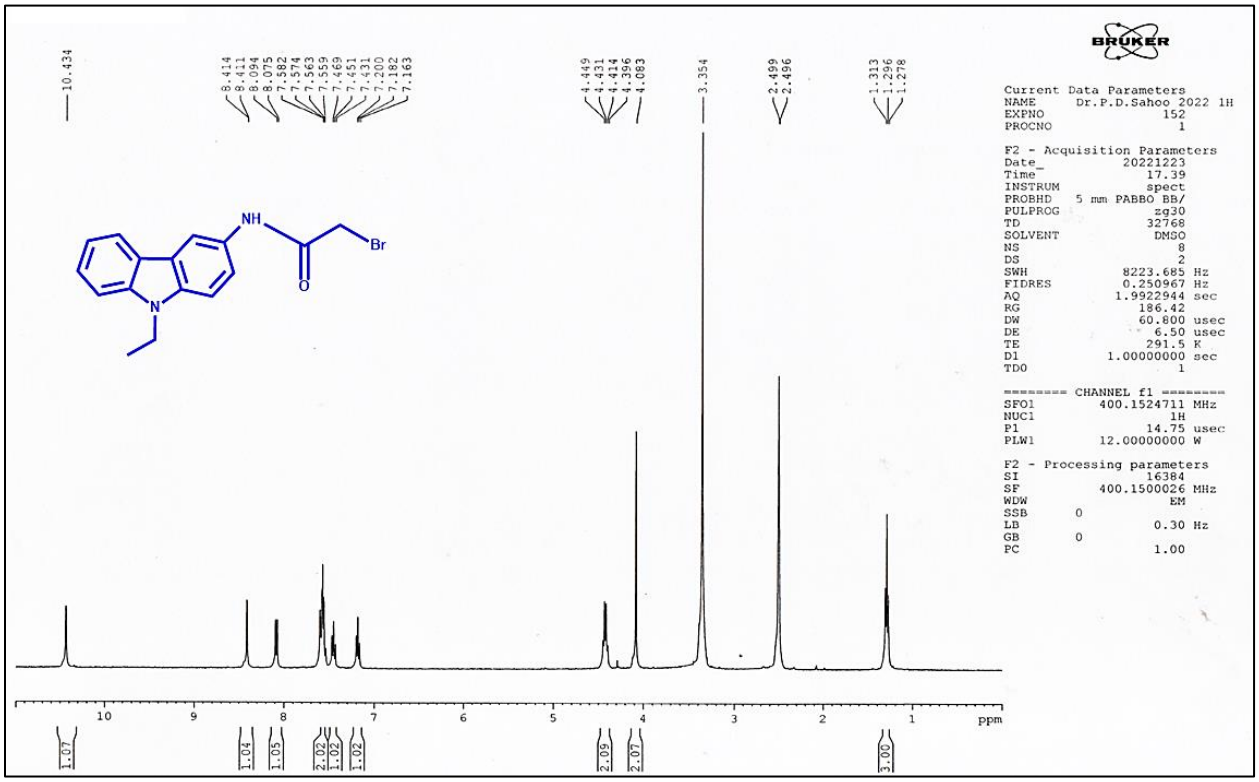



**Figure S1.** $^{1}$H NMR of **C1** in DMSO-$d_6$ (400 MHz).

**$^{13}$C NMR of C1 in DMSO-$d_6$:**

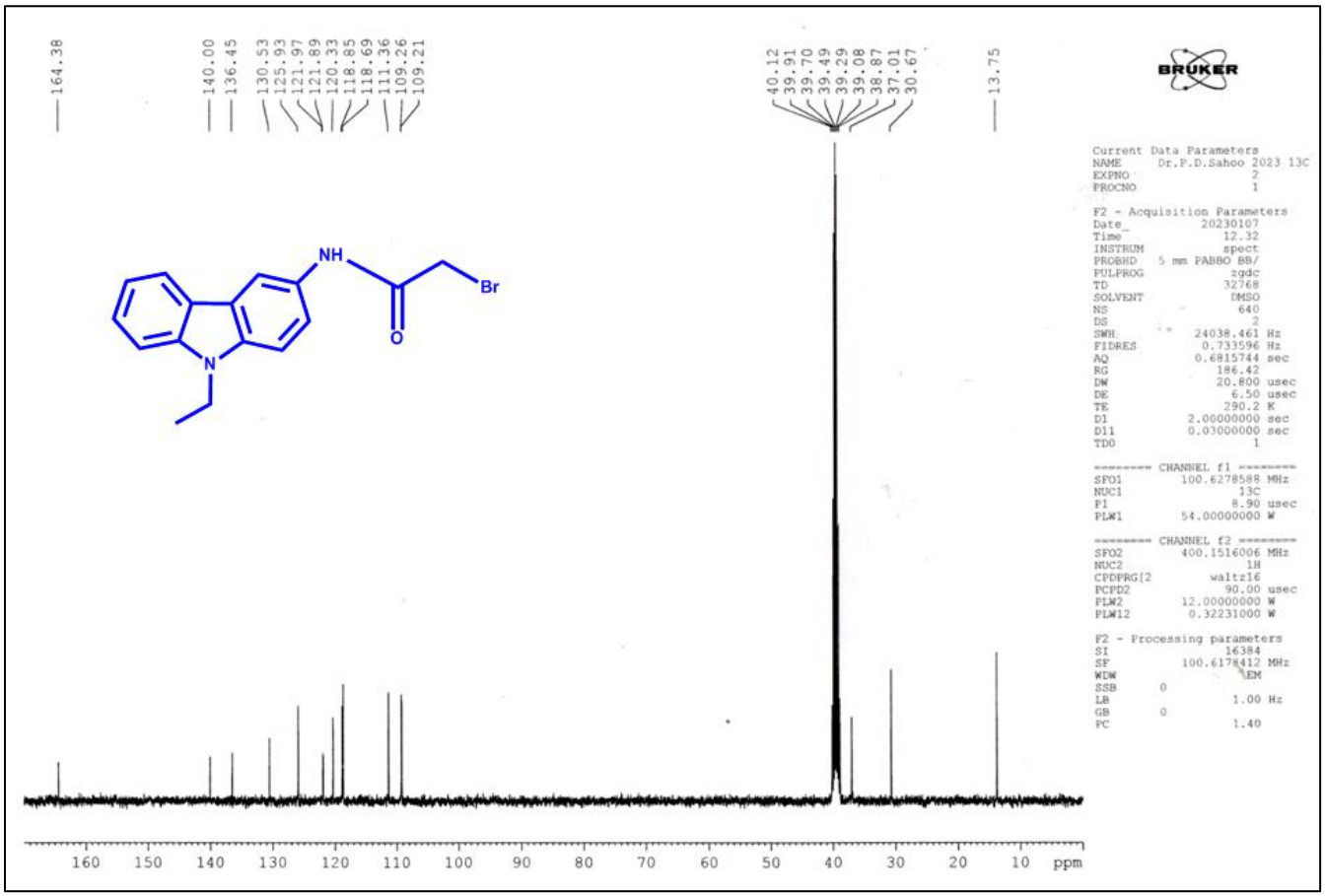



**Figure S2.** $^{13}$C NMR of **C1** in DMSO-$d_6$ (100 MHz).

**$^{1}$H NMR of CCF in DMSO-$d_6$**

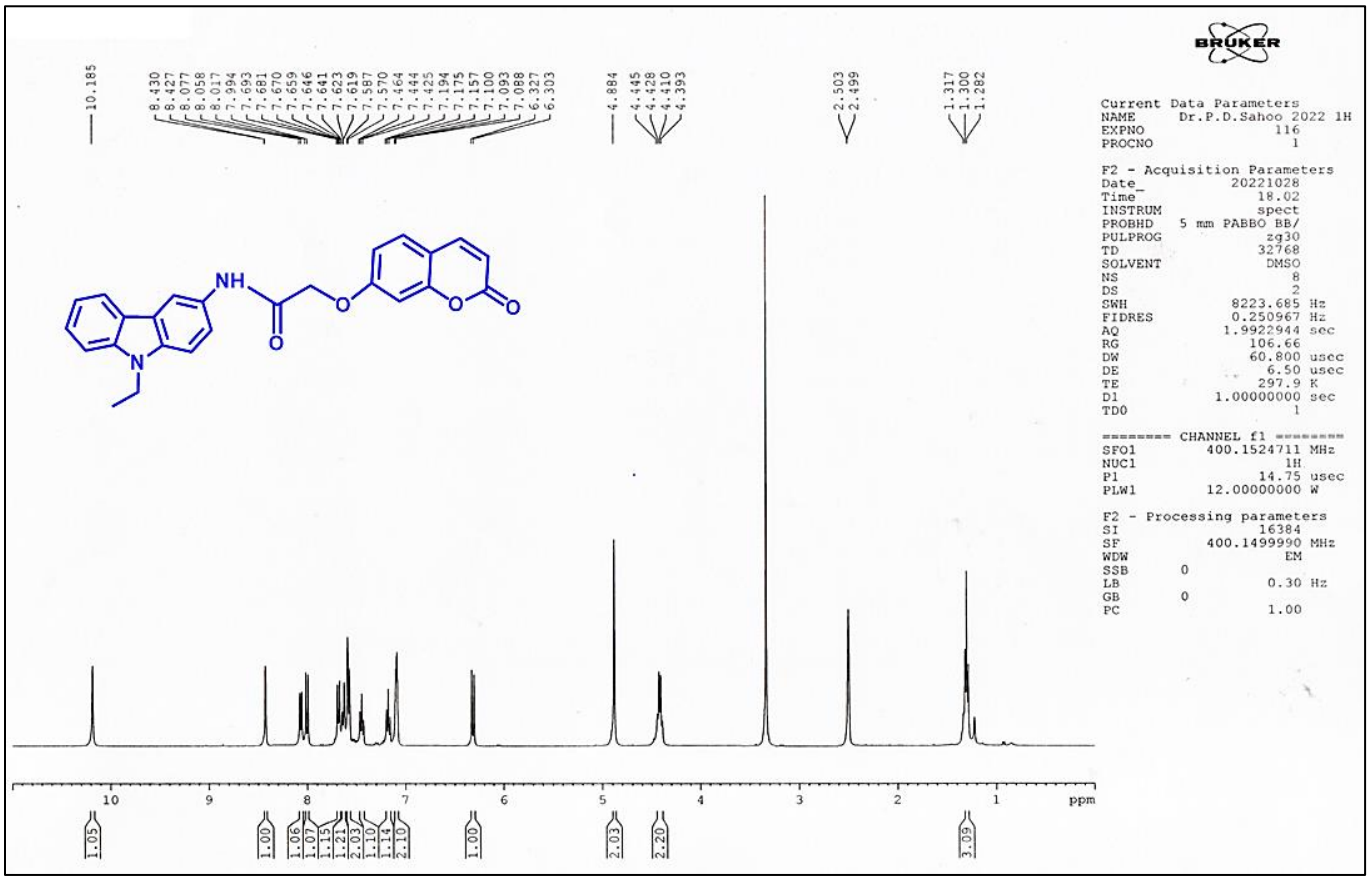



**Figure S3.** $^{1}$H NMR of **CCF** in DMSO-$d_6$ (400)

**$^{13}$C NMR of CCF in DMSO-$d_6$:**

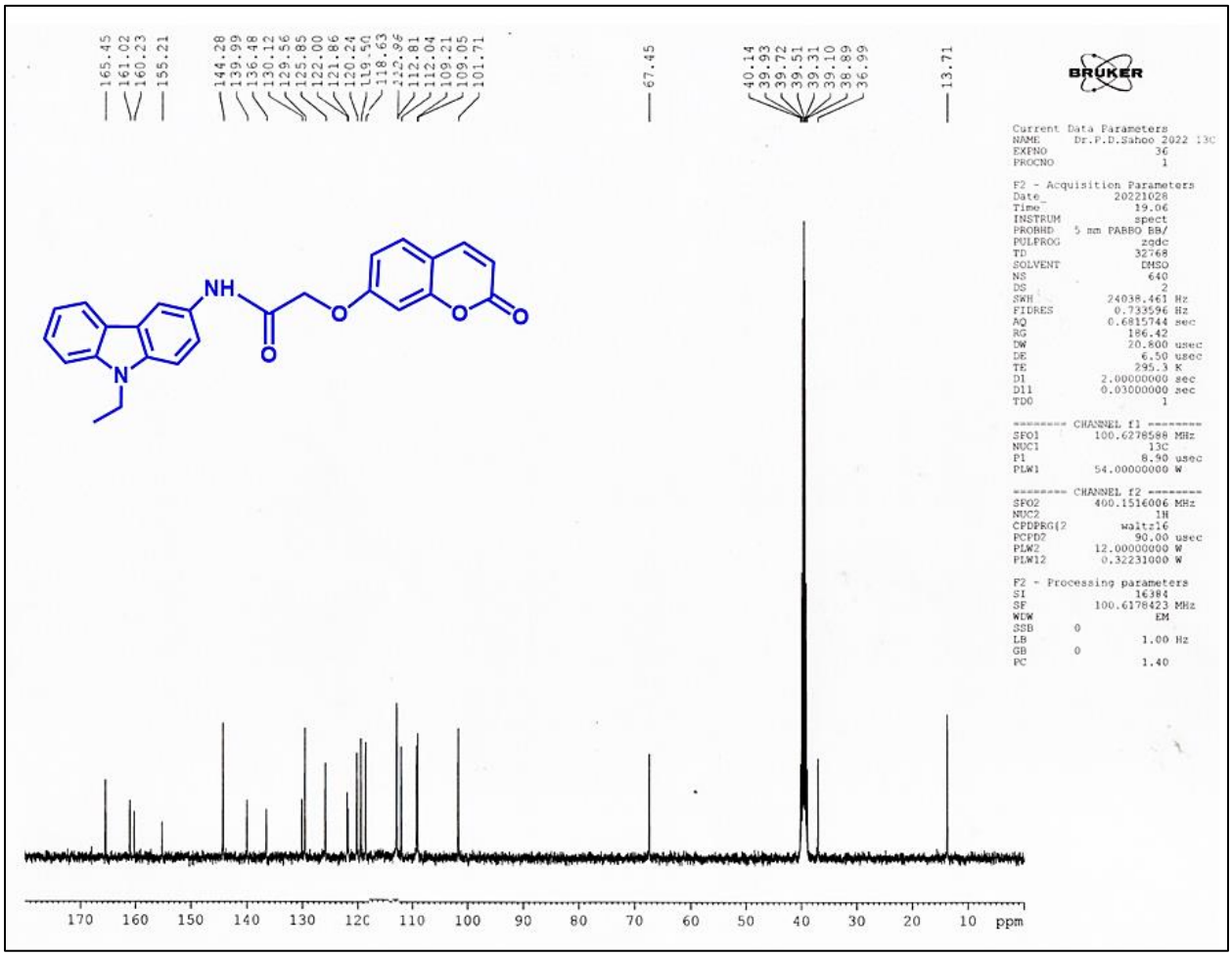



**Figure S4.** $^{13}$C NMR of **CCF** in DMSO-$d_6$ (100 MHz).

## 2. Selectivity Experiment

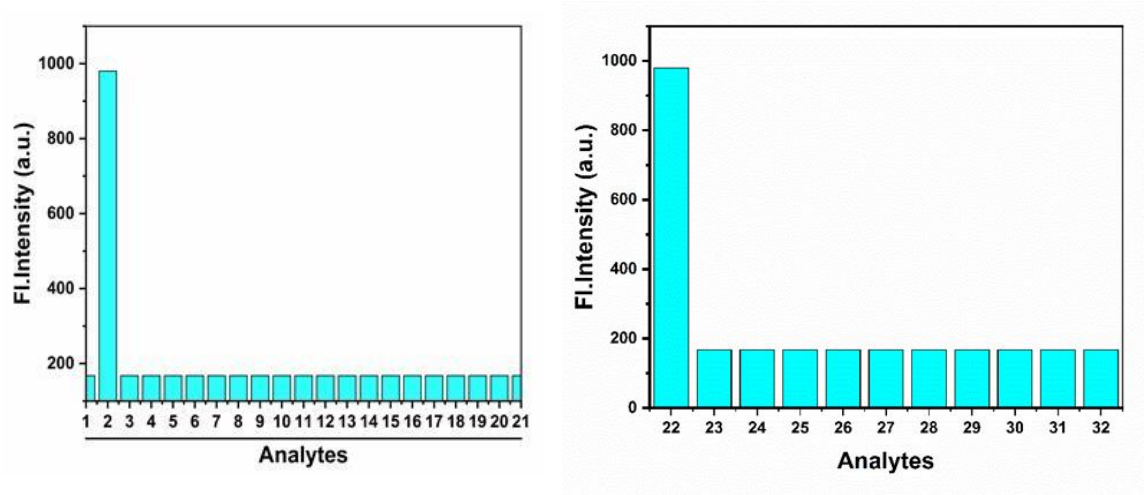



**Figure S5.** Fluorescence spectra of **CCF** in presence of different analytesat452 nm ($\lambda_{ex}$= 332 nm) in $H_2O$-$CH_3CN$ (4:1, v/v) at neutral pH.1) Blank, 2) $N_2H_4$, 3) $Zn^{2+}$, 4) $Cu^{2+}$, 5) $Pb^{2+}$, 6) $Al^{3+}$, 7) $OCl^-$, 8) $CN^-$, 9) $NO_3^-$, 10) $H_2PO_4^-$, 11) $NH_4OH$ 12) Pyridine, 13) n-Butylamine and 14) Ethylenediamine, 15) lysine, 16) histidine, 17) aniline, 18) cysteine, 19) $SCN^-$, 20) $H_2O_2$ , 21)$CH_3NH_2$ , 22) $N_2H_4$, 23) $Cl^-$ , 24) $F^-$ , 25) alanine, 26) tryptophan, 27) leucine, 28) glycine , 29) $ClO_4^-$ , 30) $N_3^-$ , 31) $NO_3^-$ , 32) arginine.

## 3. Competitive selectivity in presence of other analytes

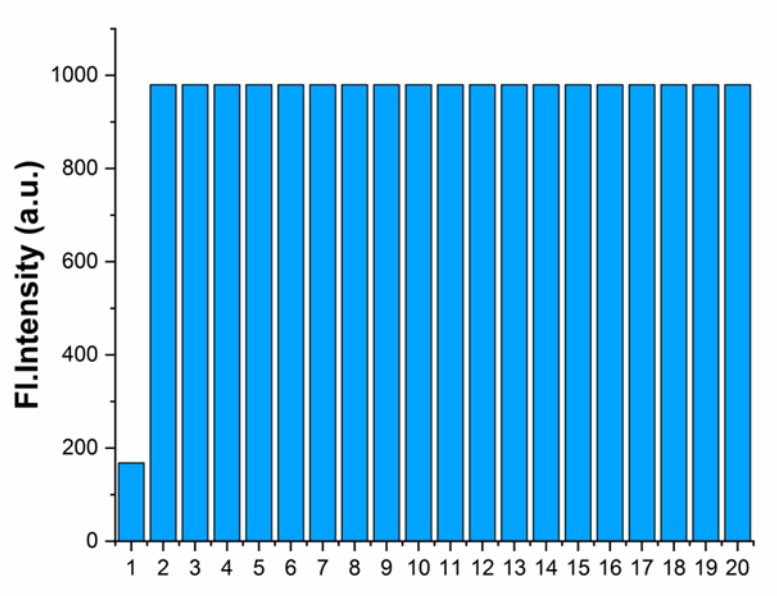



**Figure S6.** Histogram representing competitive fluorescence spectra of CCF+ $N_2H_4$ in presence of different analytes at 452 nm ($\lambda_{ex}$= 332 nm) in $H_2O$-$CH_3CN$ (4:1, v/v) at neutral pH. [1) Blank, 2) $N_2H_4$, 3) $N_2H_4$+$Zn^{2+}$, 4) $N_2H_4$+$Cu^{2+}$, 5) $N_2H_4$+$Pb^{2+}$, 6) $N_2H_4$+$Mg^{2+}$, 7) $N_2H_4$+$Ca^{2+}$, 8) $N_2H_4$+$Na^{+}$, 9) $N_2H_4$+$K^{+}$, 10) $N_2H_4$+$F^{-}$, 11) $N_2H_4$+$Cl^{-}$,12) $N_2H_4$+$ClO_4^{-}$, 13) $N_2H_4$+$CN^{-}$, 14) $N_2H_4$+$NO_3^{-}$, 15) $N_2H_4$+$H_2PO_4^{-}$, 16) $N_2H_4$+$N_3^{-}$, 17) $N_2H_4$+$NH_4OH$ 18) $N_2H_4$+Pyridine, 19) $N_2H_4$+n-Butylamine and 20) $N_2H_4$+Ethylenediamine]

## 4. UV-vis and fluorescence titration studies

### UV-vis spectral studies:

A stock solution of **CCF** ($1 \times 10^{-5}$ M) was prepared in water-acetonitrile (4:1, v/v). **$N_2H_4$** solution of concentration $1 \times 10^{-4}$ M was prepared in Millipore water. All experiments were carried out in an aqueous medium at neutral pH. During the titration, each time a $1 \times 10^{-5}$ M solution of **CCF** was filled in a quartz optical cell of 1 cm optical path length and **$N_2H_4$** stock solution was added into the quartz optical cell gradually by using a micropipette.

### Fluorescence spectral studies:

A stock solution of **CCF** ($1 \times 10^{-5}$ M) was prepared in water-acetonitrile(4:1, v/v). **$N_2H_4$** solution of concentration $1 \times 10^{-4}$ M was prepared in Millipore water. All experiments were carried out in aqueous medium at neutral pH. During titration, each time a $1 \times 10^{-5}$ M solution of **CCF** was filled in a quartz optical cell of 1 cm optical path length and **$N_2H_4$** stock solution was added into the quartz optical cell gradually by using a micropipette. For all fluorescence measurements, excitations were provided at 332 nm, and emissions were collected from 350 to 580 nm.

## 5. Job's plot

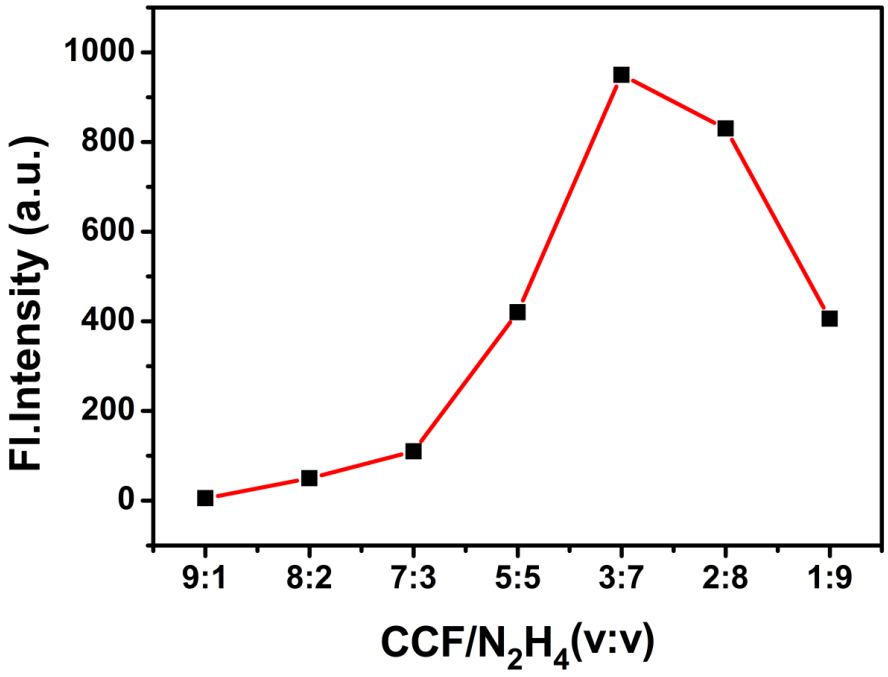



**Figure S7.** Job's plot of **CCF** (10μM) with **$N_2H_4$** in acetonitrile-water (1:4, v/v), at neutral pH, by fluorescence method, which indicate 1:2 stoichiometry for **CCF** with **$N_2H_4$**. Standard deviations are represented by error bar (n=3).

## 6. Calculation of limit of detection (LOD) of CFC with $N_2H_4$:

The detection limit of the chemosensor **CCF** for **$N_2H_4$** was calculated on the basis of fluorescence titration. To determine the standard deviation for the fluorescence intensity, the emission intensity of four individual receptors without **$N_2H_4$** was measured by 10 times and the standard deviation of blank measurements was calculated.

The limit of detection (LOD) of **CCF** for sensing **$N_2H_4$** was determined from the following equation:

$$LOD = K \times SD/S$$

Where K = 2 or 3 (we take 3 in this case); SD is the standard deviation of the blank receptor solution; S is the slope of the calibration curve.

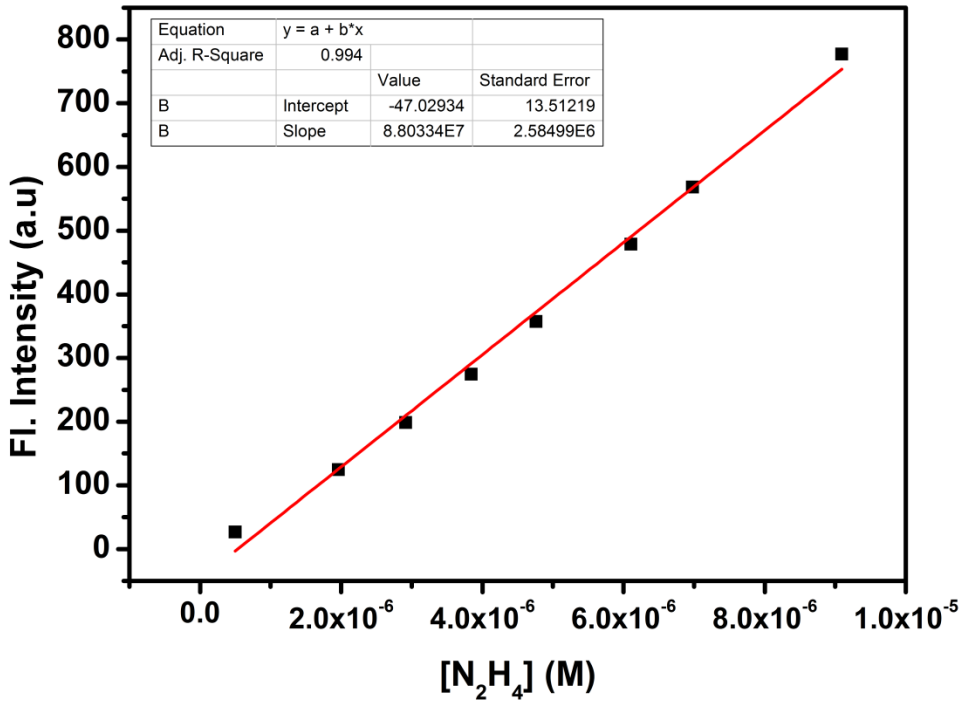



**Figure S8.** Linear fit curve of **CCF** at 452 nm with respect to **$N_2H_4$** concentration

For **CCF** with **$N_2H_4$:**

From the linear fit graph, we get slope = $8.80334 \times 10^7$, and SD value is 0.3852.

Thus, using the above formula, we get the Limit of Detection = $1.312 \times 10^{-8}$ M. Therefore **CCF** can detect **$N_2H_4$** up to this very lower concentration by fluorescence technique.

## 7. pH titration study:

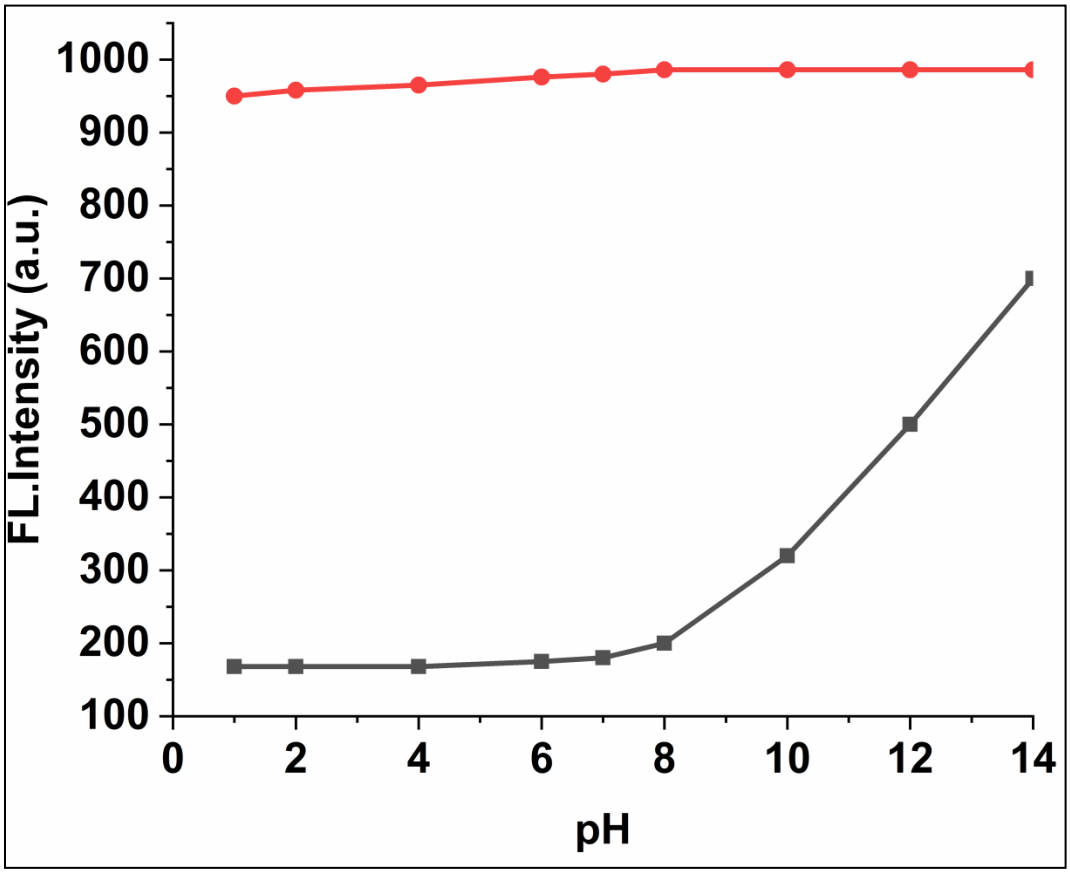



**Figure S9.** Effect of pH on the fluorescence intensity of **CCF** ($10^{-5}$M) in the absence of $N_2H_4$ (blackline) and in the presence of $N_2H_4$ ($10^{-4}$M, red line).

## 8. DFT study

**Table S1. Details of the geometry optimization in Gaussian 09 program**

| Details | CCF | F1 moiety | F2 moiety |
|---|---|---|---|
| **Calculation method** | B3LYP | B3LYP | B3LYP |
| **Basis set** | 6-31G** | 6-31G** | 6-31G** |
| **E(CAM-B3LYP) (a.u.)** | -1375.20 | -651.50 | -947.49 |
| **Charge, Multiplicity** | 0, 1 | 0, 1 | 0, 1 |
| **Solvent (CPCM)** | Water | Water | Water |

## TDDFT- Calculations

**Table S2.** Selected electronic excitation energies (eV), oscillator strengths (f), main configurations of the low-lying excited states of CPLC. The data were calculated by TDDFT//B3LYP/6-31G(d,p) based on the optimized ground state geometries.

| Molecules | Electronic Transition | Excitation Energy[a] | f[b] | Composition[c](%) |
|---|---|---|---|---|
| **CCF** | $S_0 \rightarrow S_4$ | 4.0781eV304.03 nm | 0.5287 | H -2→ L (68.7%) |

[a]Only selected excited states were considered. The numbers in parentheses are the excitation energy in wavelength. [b]Oscillator strength. [c]H stands for HOMO and L stands for LUMO.

**Top view of energy optimized geometry:**

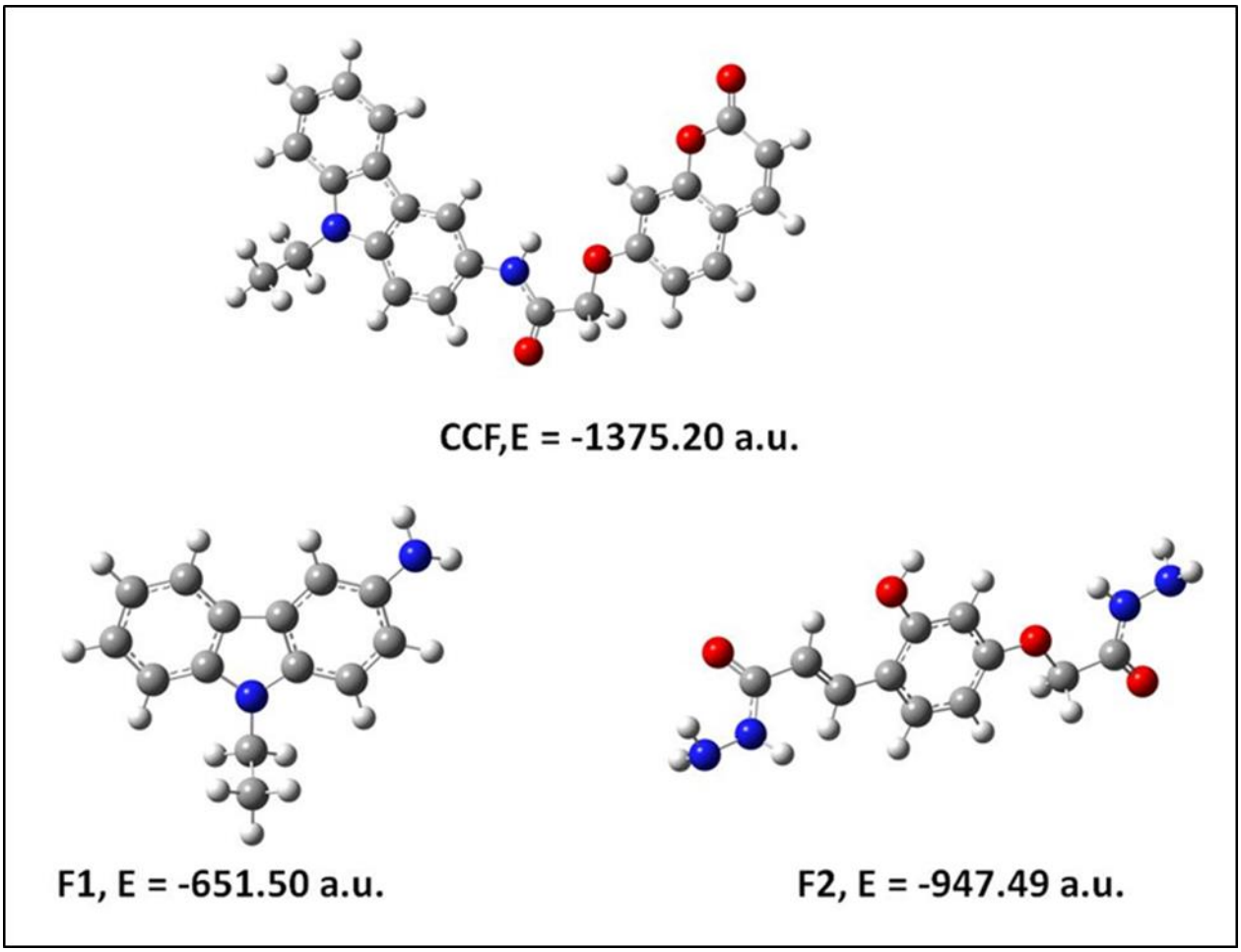



**Figure S10.** Optimized structures of CCF, F1 and F2 moiety with their corresponding energies.

## 9. IR Spectroscopy Study

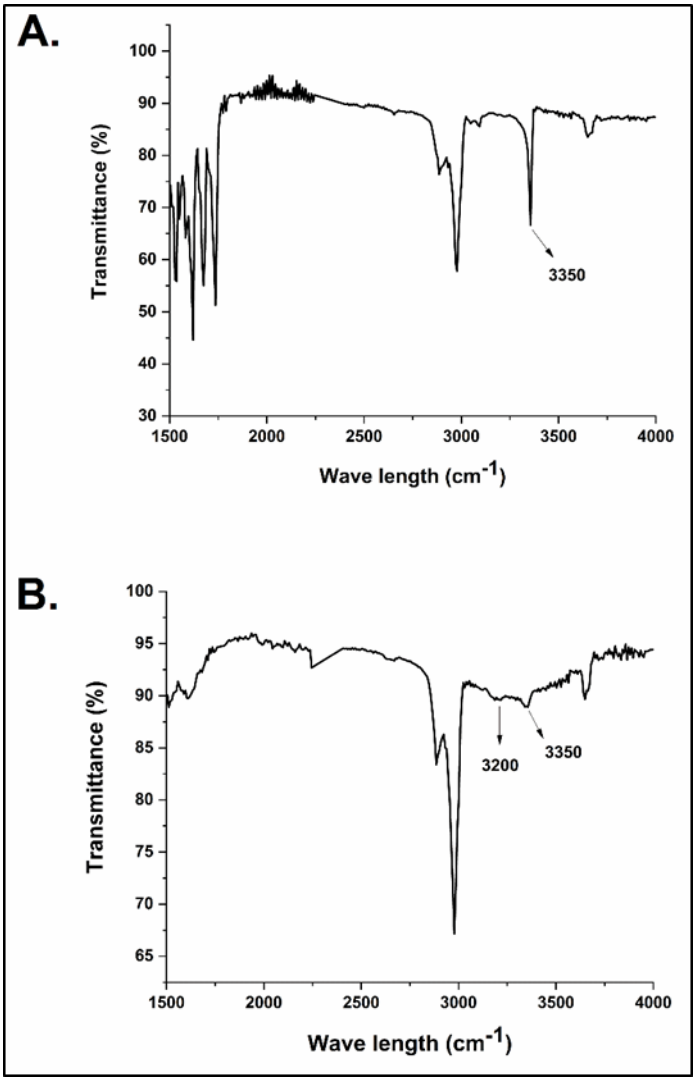



**Figure S11**. (A) IR spectrum of CCF and (B) IR spectrum of CCF + $N_2H_4$, 3350 $cm^{-1}$ and 3200 $cm^{-1}$ indicates amide and O-H bond respectively.

**10. NMR spectra of C2, C3**

**$^{1}$H NMR of C2 in DMSO-$d_6$:**

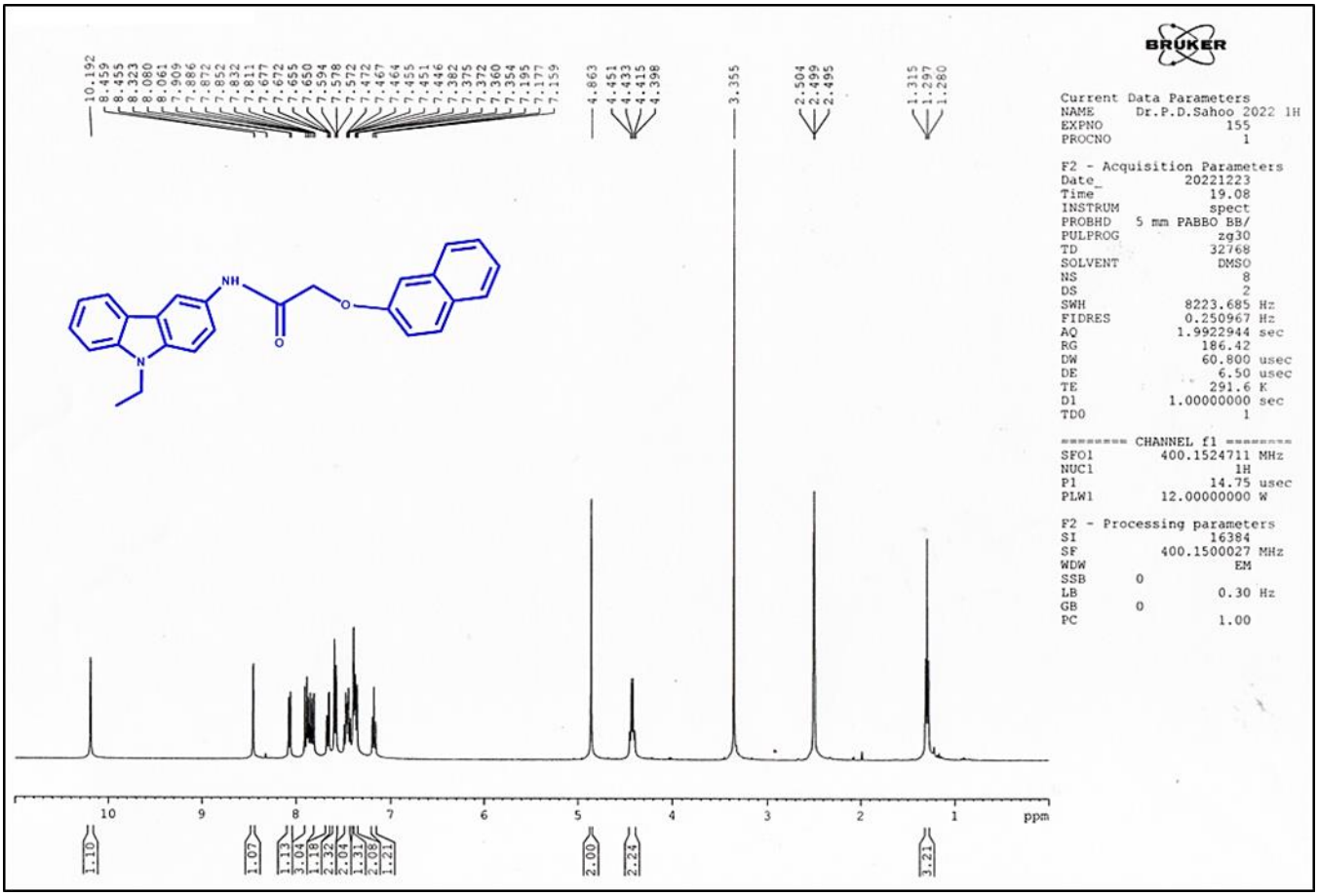



**Figure S12.** $^{1}$H NMR of **C2** in DMSO-$d_6$ (400 MHz).

**$^{1}$H NMR of C3 in DMSO-$d_6$:**

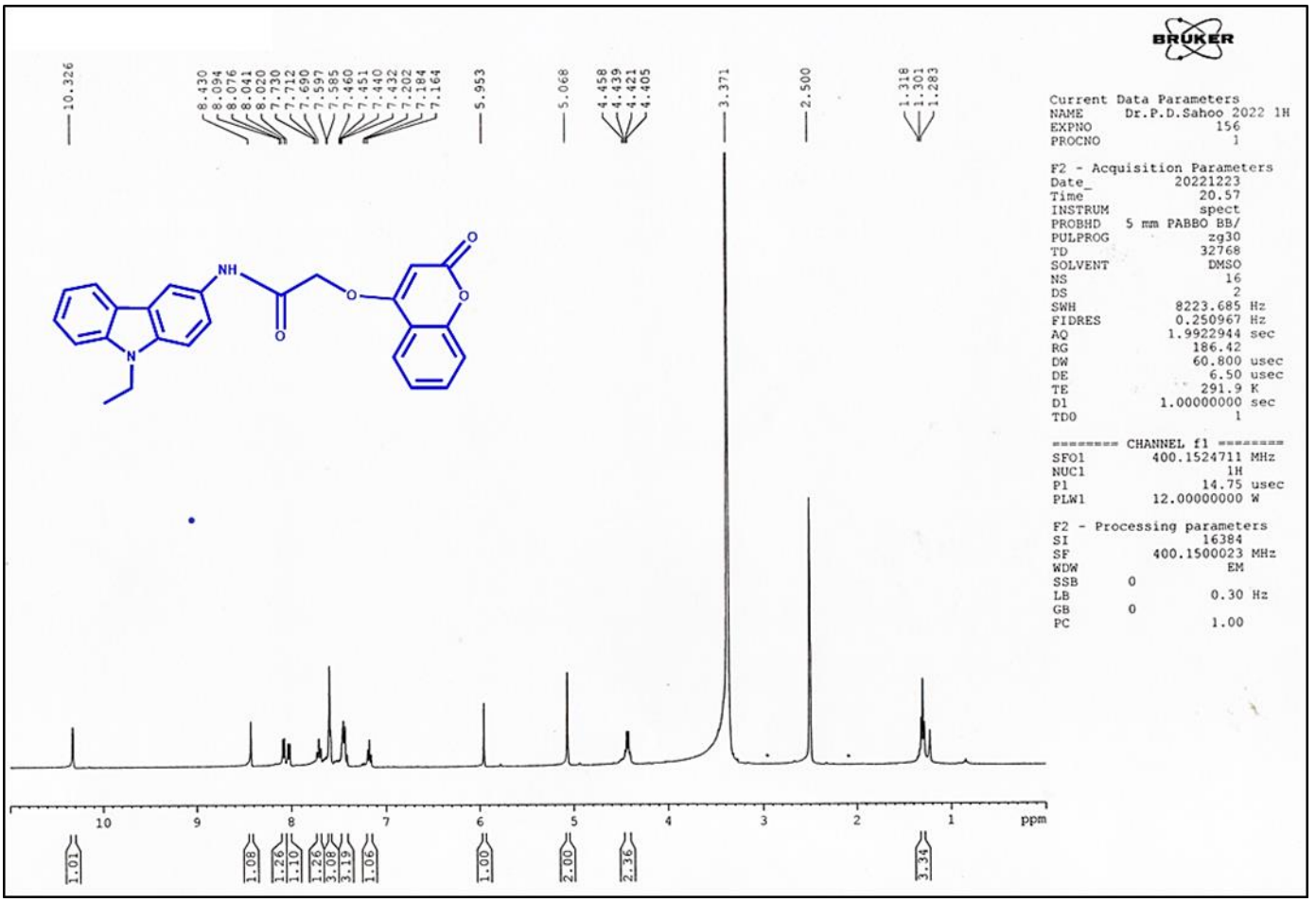
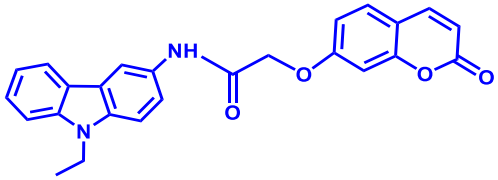
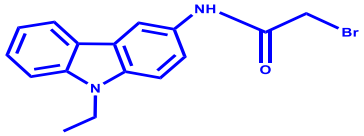
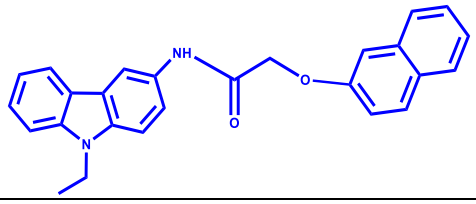
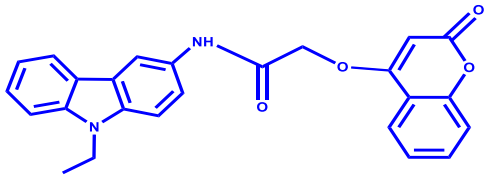



**Figure S13.** $^{1}$H NMR of **C3** in DMSO-$d_6$ (400 MHz).

**11. Table S3. Comparative Fluorescence study of CCF with C1,C2,C3 in presence of $N_2H_4$**

| CHEMOSENSOR | ANALYTE | EXICTATION | Maximum EMISSION at |
|---|---|---|---|
| CCF  | $N_2H_4$ | 332 nm | 452 nm |
| C1  | $N_2H_4$ | 281 nm | 372nm, 392nm |
| C2  | $N_2H_4$ | 330 nm | 372nm, 392nm |
| C3  | $N_2H_4$ | 360 nm | 372nm, 392nm |

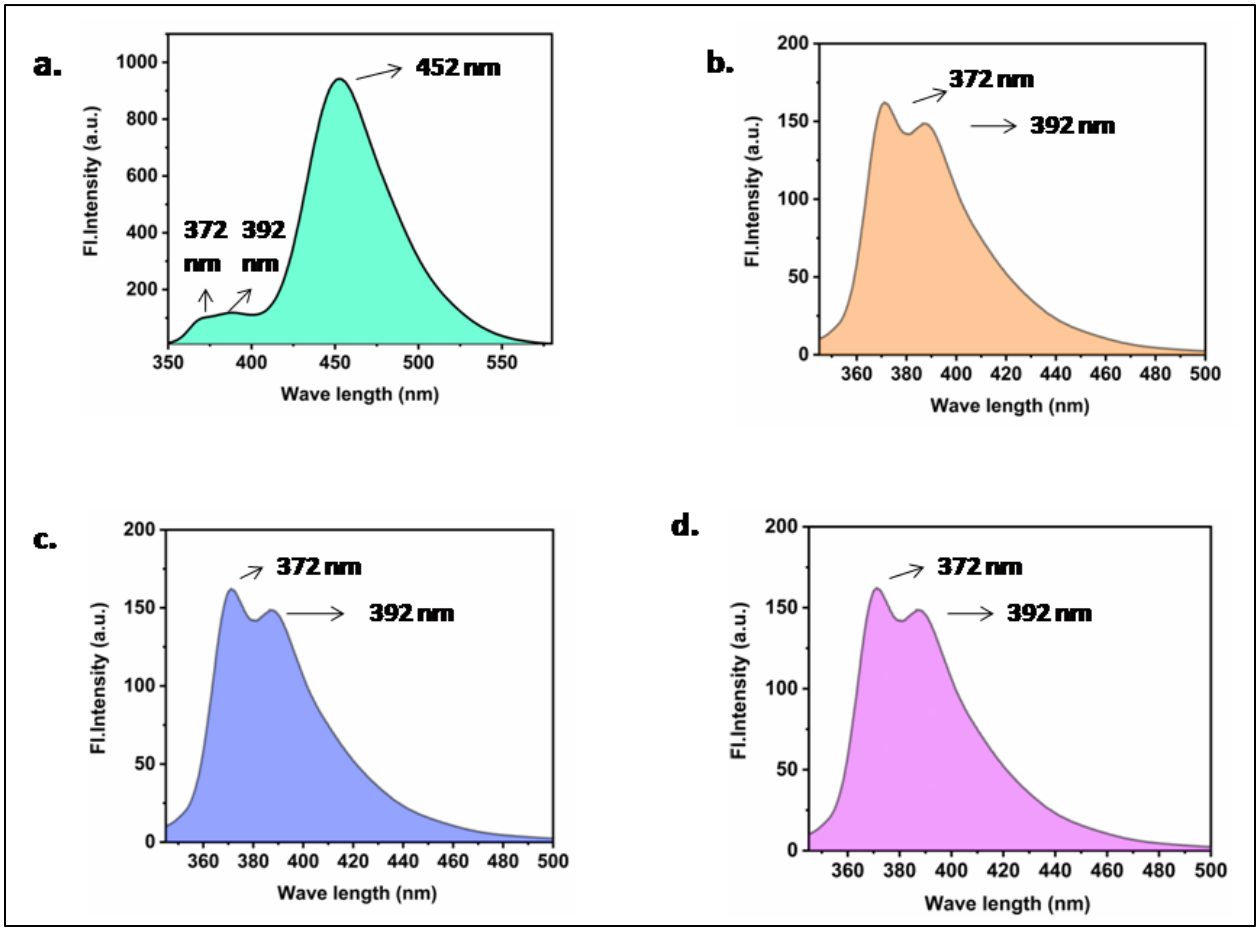



**Figure S14.** Comparative Fluorescence studies of **(**a) CCF vs$N_2H_4$ (b) C1 vs $N_2H_4$ (c) C2 vs $N_2H_4$ (d) C3 vs $N_2H_4$ at 452 nm excitation at 332 nm, 280 nm, 330 nm, 360 nm respectively.

## 12. Quantitative analysis of hydrazine in button mushroom

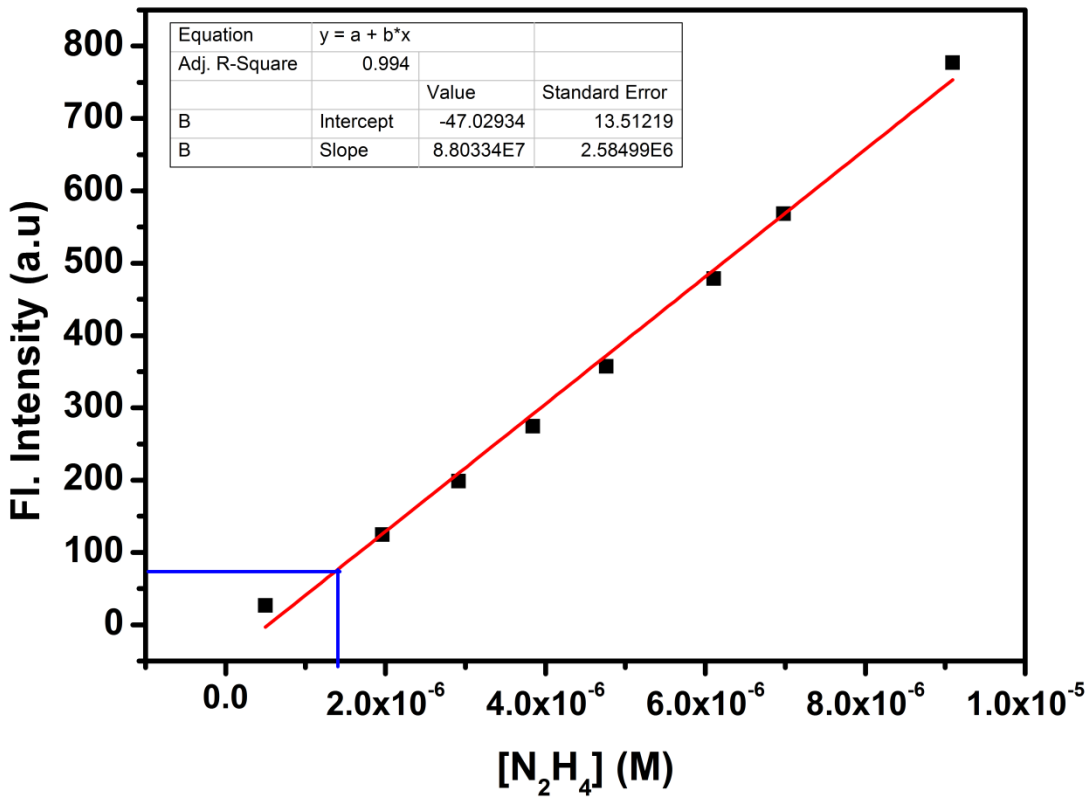



**Figure S15**. Estimation of unknown concentration of hydrazine (blue line) in the gills extract of button mushroom fromthe standard fluorescence curve.