Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information For:

A MOF chemosensor for highly sensitive and ultrafast detection of folic acid in biofriendly medium, paper strips and real samples

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1.1. Materials and Characterization Methods

All the reagents and solvents were procured from commercial sources and used without purification, except the 2-((5-(dimethylamino)naphthalene)-1-sulfonamido) terephthalic acid (H_2BDC-NH-dansyl) linker. The notations used for characterization of the bands are broad (br), strong (s), very strong (vs), medium (m), weak (w) and shoulder (sh). PXRD data were collected by using Rigaku Smartlab X-ray diffractometer with Cu-*K*α radiation (λ = 1.54056 Å), 50 kV of operating voltage and 100 mA of operating current. The Attenuated Total Reflectance Infrared (ATR-IR) spectra were recorded using PerkinElmer UATR Two at ambient condition in the region 400-4000 cm^{-1}. Thermogravimetric analysis (TGA) was carried out with a TG 209 F1 Libra Netzsch, thermogravimetric analyser in the temperature range of 25-700 °C in an N_2 atmosphere at the rate of 10 °C min^{-1}. N_2 sorption isotherms were recorded by using Quantachrome Autosorb iQ-MP volumetric gas adsorption equipment at −196 °C. Before the sorption analysis, the degassing of the compound was carried out at 100 °C under a high vacuum for 12 h. Fluorescence sensing studies were performed with a HORIBA JOBIN YVON Fluoromax-4 spectrofluorometer. FE-SEM images were captured with a Zeiss (Zemini) scanning electron microscope. A BrukerAvance III 600 NMR spectrometer was used for recording 1H NMR spectra at 500 MHz. Mass spectra were recorded with an Agilent 6520 QTOF high-resolution mass spectrometer (HR-MS). UPS work was performed with PHI-5000 Versaprobe III (ULVAC-PHI Inc.) using He(I) (21.22 eV) excitation. Fluorescence lifetimes were measured using Picosecond Time-resolved and Steady State Luminescence Spectrometer on an Edinburg Instruments Lifespec II & FSP 920 instrument. Pawley refinement was carried out using Materials Studio software.

1.2. Analysis of band gap:

For UiO@Dansyl:

E_g = 2.83 eV (calculated from the Tauc plot Fig. S48a, ESI†)

E_{VB} = Width of the He I UPS spectra from the excitation energy (21.22 eV)

$$E_{VB} = 21.22 – (14.64\text{-}0.13)$$

$$= 6.71 \text{ eV}$$

$$E_{CB} = E_{VB} - E_g$$

$$= 3.88 \text{ eV}$$

With respect to RHE:

$$E_{VB} = 6.71 - 4.44 = 2.27 \text{ V}$$

$$E_{CB} = 3.88 - 4.44 = -0.56 \text{ V}$$

For FA:

E_g = 2.83 eV (calculated from the Tauc plot Fig. S48b, ESI†)

$$E_{VB} = 21.22 – (13.58 - 0.37)$$

$$= 8.01 \text{ eV}$$

$$E_{CB} = E_{VB} - E_g$$

$$= 5.63 \text{ eV}$$

With respect to RHE:

$$E_{VB} = 6.71 - 4.44 = 3.57 \text{ V}$$

$$E_{CB} = 3.88 - 4.44 = 1.19 \text{ V}$$

Ultraviolet photoelectron spectroscopy was done to estimate the exact position of valance band (VB) and conduction band (CB) with minimum error (± 0.1 eV). Excitation source is used He I (excitation energy 21.22 eV). All the values (in eV) are got with respect to the vacuum. Values are converted in electrochemical energy (Volts) by subtracting 4.44. According to the literature 0 V vs RHE (Reversible Hydrogen Electrode) = -4.44 eV vs vacuum level.[1]

1.3. Synthesis of H_2BDC-NH-dansyl linker:

Dimethyl 2-aminoterephthalate (209 mg, 1 mmol) and 5-(dimethylamino)naphthalene-1-sulfonyl chloride (269 mg, 1 mmol) were added in a 50 mL round bottom flask containing 20 mL of dry DCM under N_2 atmosphere. Afterwards, 1 mL of pyridine was added dropwise in the reaction mixture and kept it for 24 h at a temperature of 60 ºC. Then, the reaction mixture was extracted with DCM, water (3 × 20 mL) and saturated NaCl solution. The solvent was evaporated under reduced pressure and the product was used in the next step.

The product was dissolved in 20 mL solution of THF and ethanol (1 : 1). Thereafter, 10 mL of aqueous solution of LiOH (1 M) was added and the mixture was left for 3 h at 65 ºC. Then, the organic part was evaporated under reduced pressure and the lemon yellow coloured solid product was obtained by neutralising with HCl (1 M). The precipitate was filtered out, washed several times with water and kept in an oven for overnight at 100 ºC. Yield: 309 mg (75%). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 11.56 (br, 1H), 8.48 (d, 1H), 8.30 (d, 1H), 8.18 (d, 1H), 8.01 (s, 1H), 7.94 (d, 1H), 7.63 (m, 2H), 7.54 (d, 1H), 7.26 (d, 1H), 2.80 (s, 6H). ^{13}C NMR (100 MHz, DMSO-d_6): δ =169.29, 165.89, 150.94, 140.43, 139.69, 135.66, 133.52, 131.90, 130.88, 130.21, 128.70, 128.54, 123.72, 123.23, 119.44, 118.23, 117.93, 115.92, 45.10. ESI-MS (m/z): Calculate mass [M - H^+] (m/z): 413.088, obtained mass [M - H^+] (m/z): 413.104.

1.4. Fluorescence detection of folic acid in PBS buffer:

At first, activated **UiO@Dansyl** (3 mg) was taken in a Falcon tube. After that, **UiO@Dansyl** was dispersed in 3 mL of PBS buffer solution and sonicated for 15 min. To obtain a stable suspension of **UiO@Dansyl**, it was kept overnight at room temperature.

Aliquot (25 µL) of the resulting suspension in PBS buffer was taken as a probe and mixed well with 2975 µL of PBS buffer in a quartz fluorescence cuvette. In all the fluorescence titrations, excitation wavelength was 324 nm. The selectivity study was executed with a 5 mM PBS buffer solution of the analytes, prepared by proper dilution. During titration

experiments, sequential addition of 5 mM buffer solution of all the analytes was performed in 3 mL PBS buffer suspension of **UiO@Dansyl**. Quenching efficiency was calculated by the formula: $\left(1-\frac{I}{I_0}\right)\times 100\%$, where I_0 refers to the initial fluorescence emission intensity of the probe and I refers to the emission fluorescence intensity after the addition of the analyte.

1.5. Fluorescence detection of folic acid in human blood serum samples:

From the right arm vein of a completely healthy individual (blood group: A^+), 10 mL of blood sample was taken out and centrifuged at 10000 rpm for 15 min to separate out the blood plasma. The pale-yellow coloured blood serum was collected in a Falcon tube and kept in a refrigerator at -20 ºC. For fluorescence detection experiments, aliquots of different concentrations of folic acid were spiked into the human blood serum sample, which contained PBS buffer suspension of the probe.

1.6. Fluorescence detection of folic acid in human urine samples:

From a completely healthy individual, 10 mL of first early morning urine sample was collected and 500 µL of HNO_3 was poured into the sample to eliminate all the interfering living organisms. The sample was centrifuged at 8000 rpm for 10 min. The supernatants were taken for the experiments. For fluorescence detection experiments, different aliquots of folic acid were spiked in the urine sample containing PBS buffer suspension of the probe.

1.7. Fluorescence detection of folic acid in pig liver:

A fresh pig liver sample was collected from a meat shop (Guwahati, India) and washed with distilled water to remove the blood stain. Then, the sample was cut into small pieces and 10 g of sample was taken. It was poured in 20 mL of PBS buffer solution in a Falcon tube and purged with nitrogen. Then, the solution was sonicated for 2 h and the sample was kept in water bath for 15 min at 40 ºC. Then, the sample was centrifuged at 8000 rpm for 15 min. The supernatant was collected and taken for further experiments. For fluorescence detection experiments, different aliquots of the supernatant were spiked in the PBS buffer suspension of the probe.

1.8. Fluorescence detection of folic acid in food supplements and folic acid tablets:

For detection of the folic acid in orange and green gram dal (pulse), fresh samples were collected from the local market (Guwahati, India). The orange sample was squished and 1 mL of the orange juice was collected. It was diluted with 9 mL of PBS buffer, centrifuged at 8000 rpm and the supernatant was collected for the further experiments.

Fresh green gram dal was dried in sunlight for 1 day and then it was crushed into powder. 1 gm of powder sample was collected, poured into 10 mL of PBS buffer solution and sonicated

for 1 hour. The solution was centrifuged at 8000 rpm for 10 min and supernatant was collected for the next experiments.

Folic acid tablets FOLVITE® (Pfizer Ltd.) were collected from a local medical shop (Guwahati, India). Two tablets were crushed into powder before the addition of 4 mL of PBS buffer solution. The solution was sonicated to get homogeneous solution, which was followed by centrifugation at 8000 rpm for 5 min. The supernatant was collected for further experiments.

1.9. Fluorescence detection of folic acid in different aqueous media:

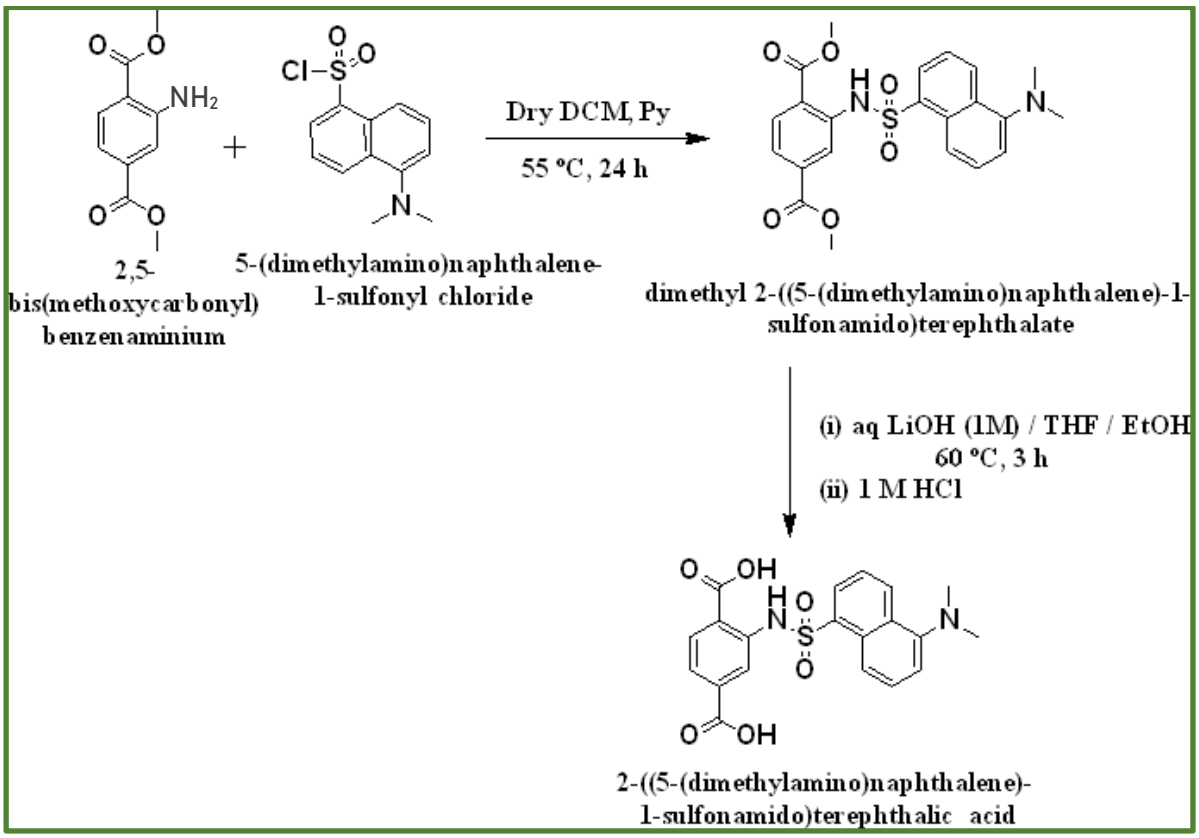
At first, activated **UiO@Dansyl** (3 mg) was taken in a Falcon tube. After that, **UiO@Dansyl** was dispersed in 3 mL of PBS buffer solution and sonicated for 15 min. To obtain a stable suspension of **UiO@Dansyl**, it was kept overnight at room temperature.

Aliquot (25 µL) of the resulting suspension in PBS buffer was taken as a probe and mixed well with 2975 µL of different water sample (Lake water, river water, tap water, distilled water) in a quartz fluorescence cuvette. In all the fluorescence titrations, excitation wavelength was 324 nm. The fluorescent titration study was executed with a 5 mM FA acid solution in different water sample was prepared by proper dilution. Aliquot of the resulting suspension in PBS buffer was taken as a probe and mixed well with 2975 µL of different water sample.

2.0. Comparison of concentration of FA by fluorescence and UV-Vis method:

Previously in many literatures, UV-Vis spectroscopy technique was used as a tool for quantification of FA. FA is UV active molecule. It shows its absorption maxima at $\lambda = 354$ nm. With increasing concentration of the FA, absorbance at λ_{max} increases. Here, we have added 25 µL aliquot of FA of different concentrations to water (2975 µL) in UV cuvette and recorded the absorbance value at λ_{max}. Calibration plot (Fig. S47, ESI†) was drawn taking the concentration of FA in *x* axis and absorbance value at λ_{max} in *y* axis. Calibration curve of fluorometric titration (Figure S32, ESI†) was previously obtained by plotting the concentration of FA in *x* axis and fluorescence intensity value in *y* axis.

Further, few samples of FA with different concentrations were prepared in water. The concentration of FA for all the samples were determined by both UV and fluorescence titrations using the respective calibration curves. The results of FA detection by both methods are documented in Table S4 (ESI†). The recovery of FA by fluorescence method was found 97.4-100.2%. The results demonstrate that the concentrations of FA found by both the techniques are comparable.



Scheme S1. Scheme for synthesis of H_2BDC-NH-dansyl linker.

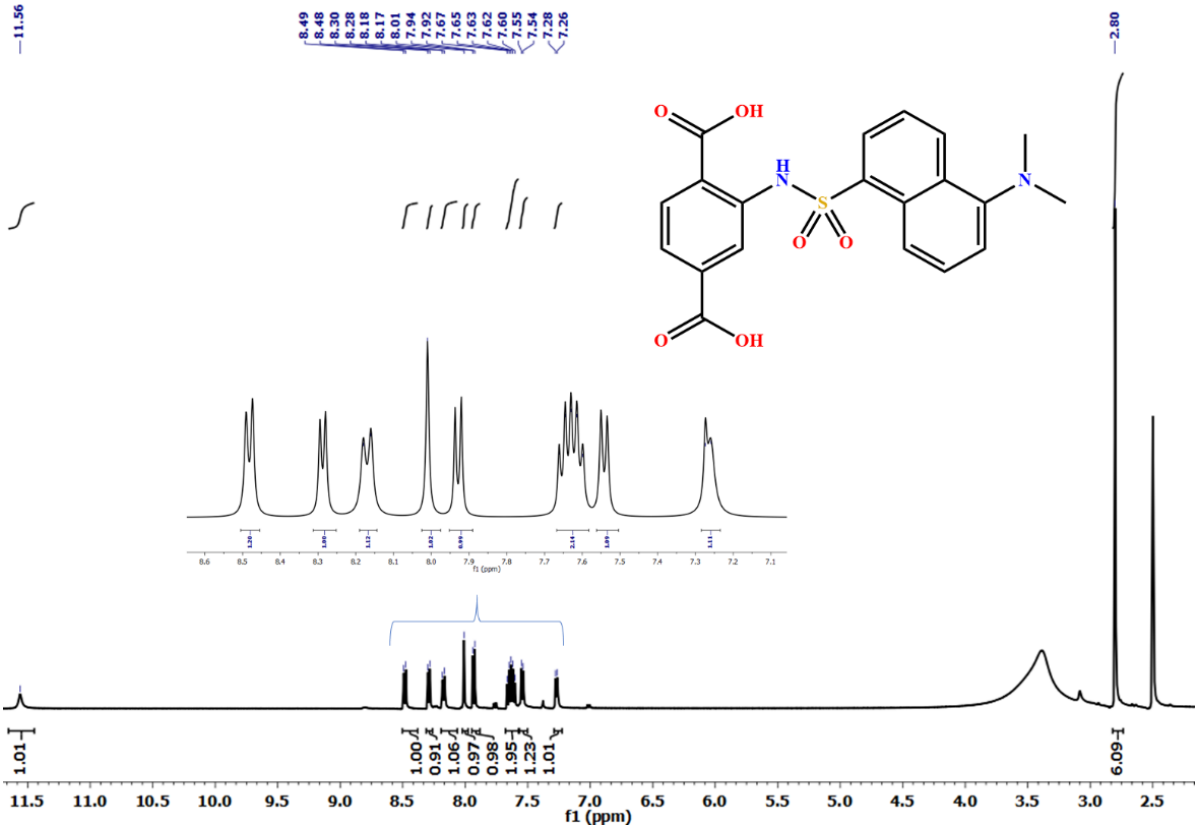


Figure S1. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of H_2BDC-NH-dansyl linker.

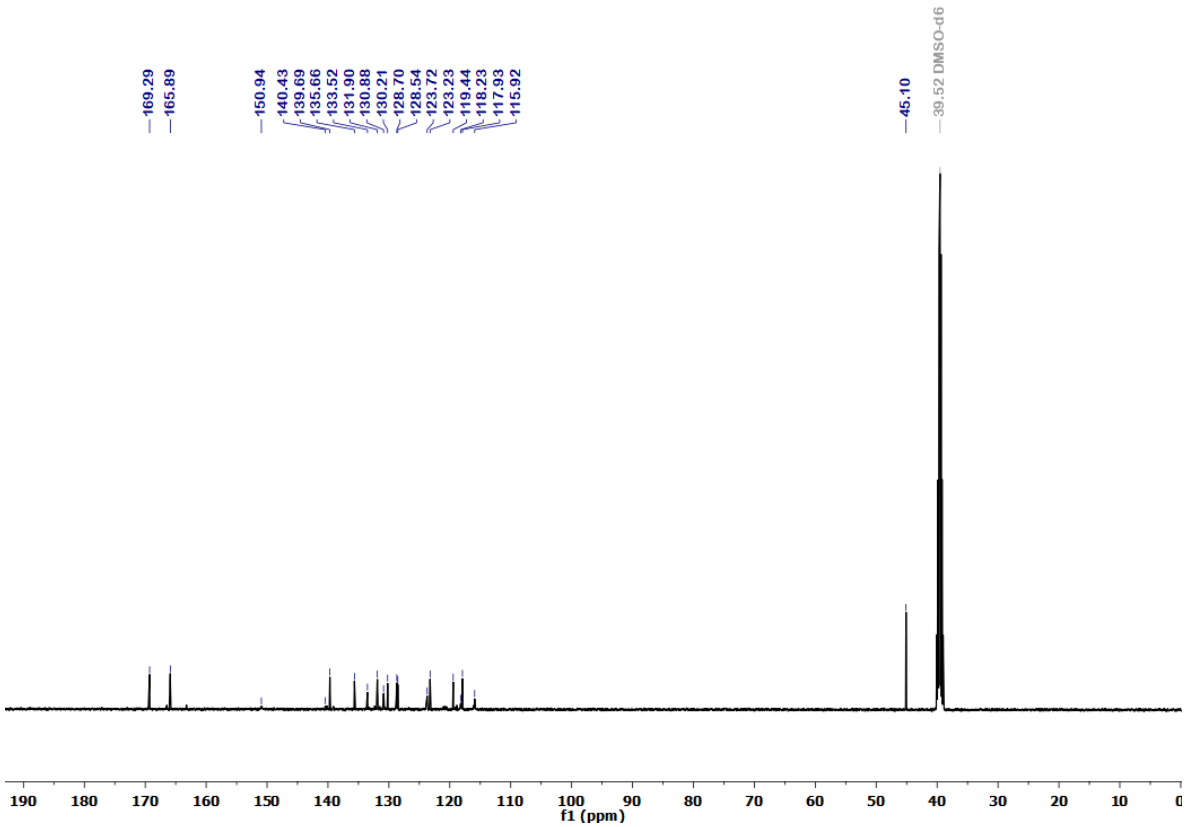


Figure S2. ^{13}C NMR spectrum (500 MHz, DMSO-d_6) of H_2BDC-NH-dansyl linker.

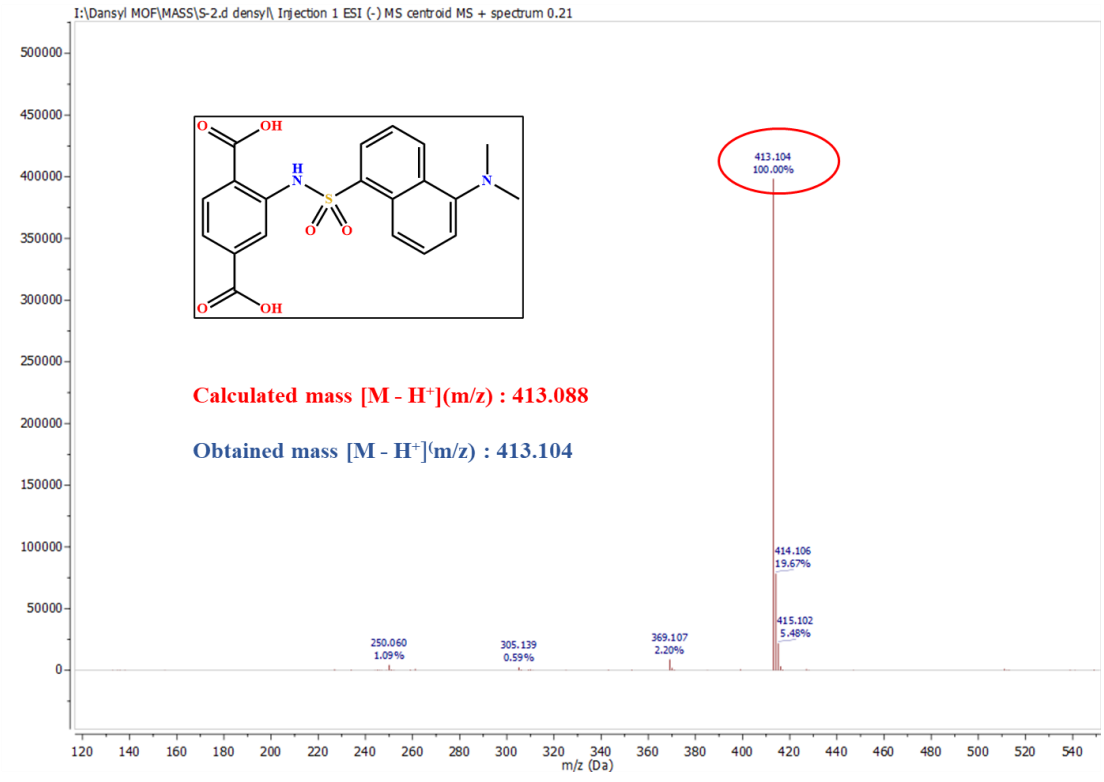


Figure S3. ESI-MS spectrum of H_2BDC-NH-dansyl linker.

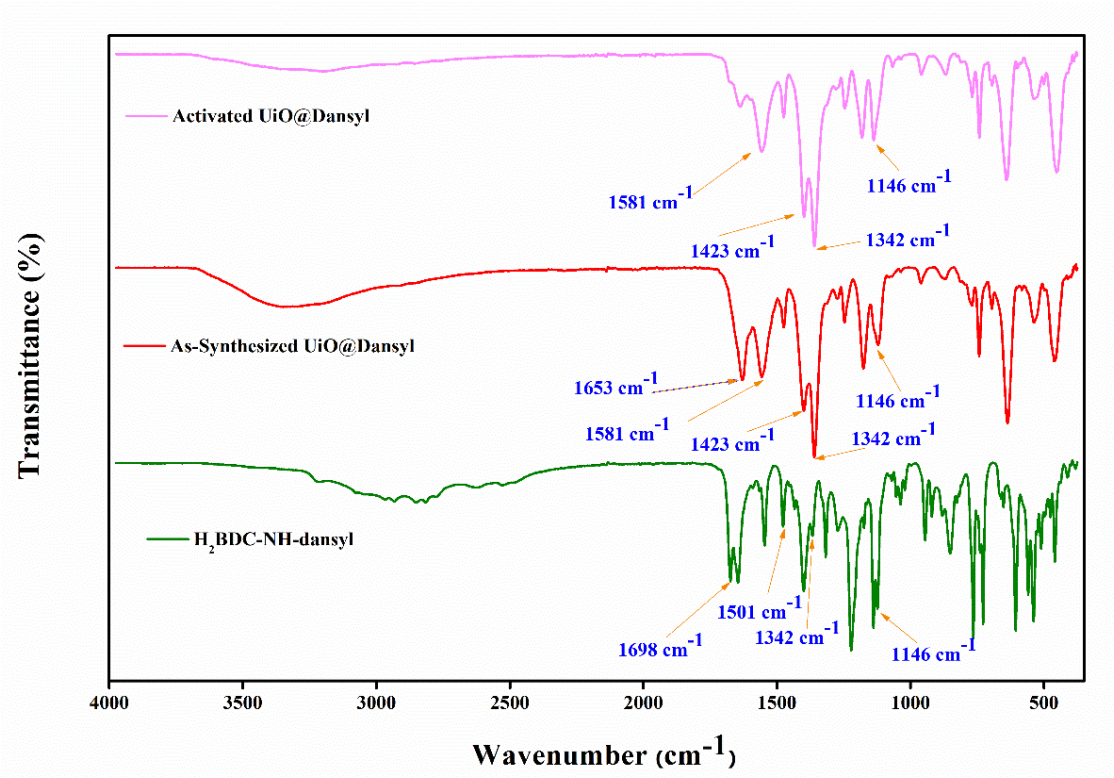


Figure S4. IR spectra of H_2BDC-NH-dansyl linker (green), as-synthesized **UiO@Dansyl** (red), activated **UiO@Dansyl** (pink).

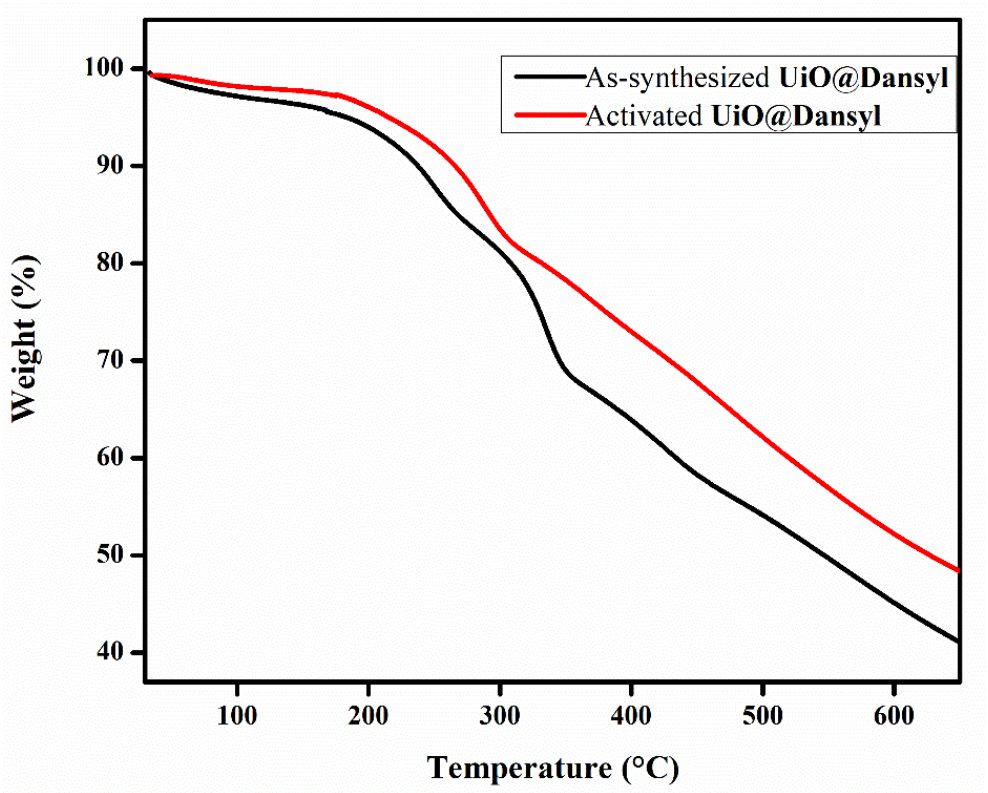


Figure S5. TGA curves of as-synthesized **UiO@Dansyl** (black), activated **UiO@Dansyl** (red) recorded in the temperature range of 30-700 °C with a heating rate of 4 °C min^{-1}.

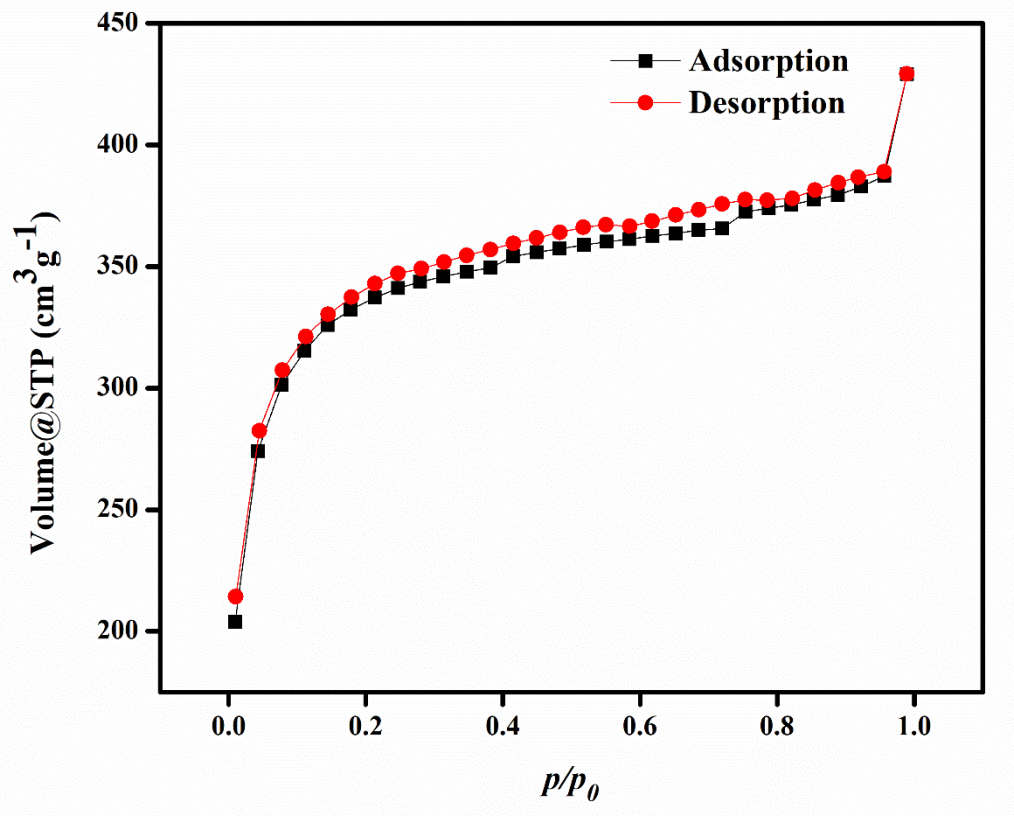


Figure S6. N_2 sorption isotherms of activated **UiO@Dansyl** (recorded at 77 K).

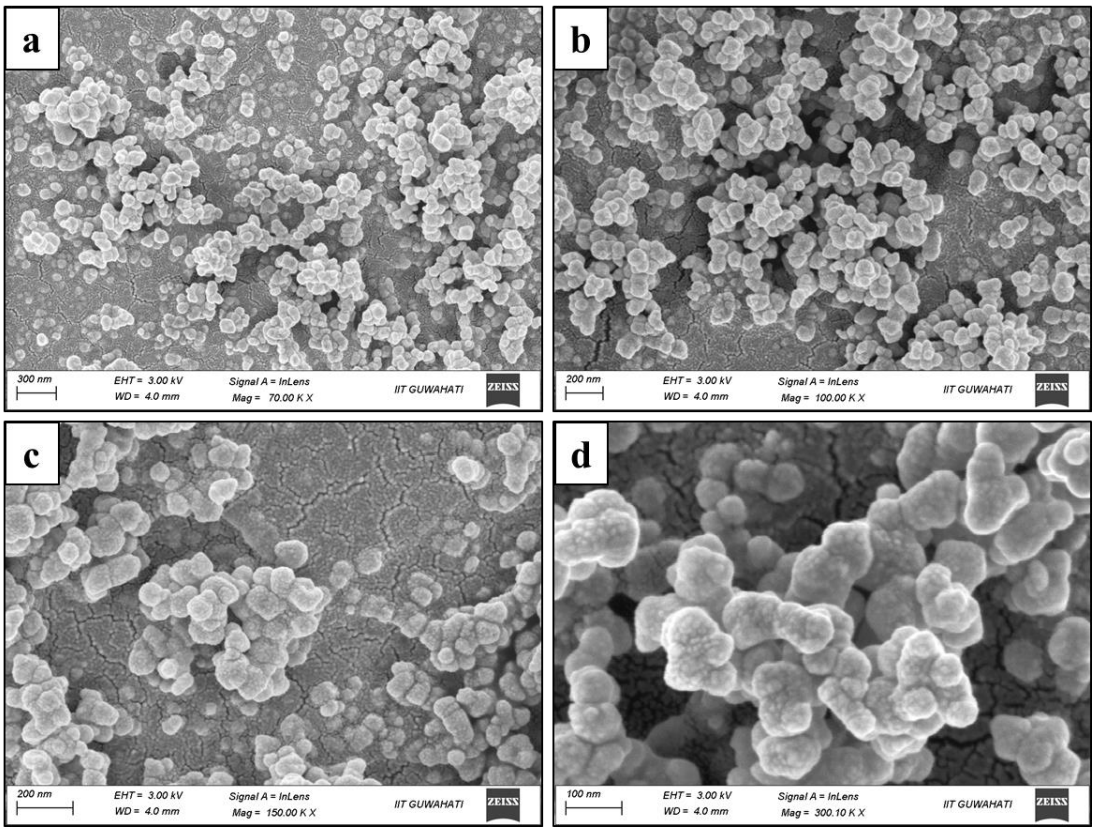


Figure S7. FE-SEM images of **UiO@Dansyl** under different magnifications.

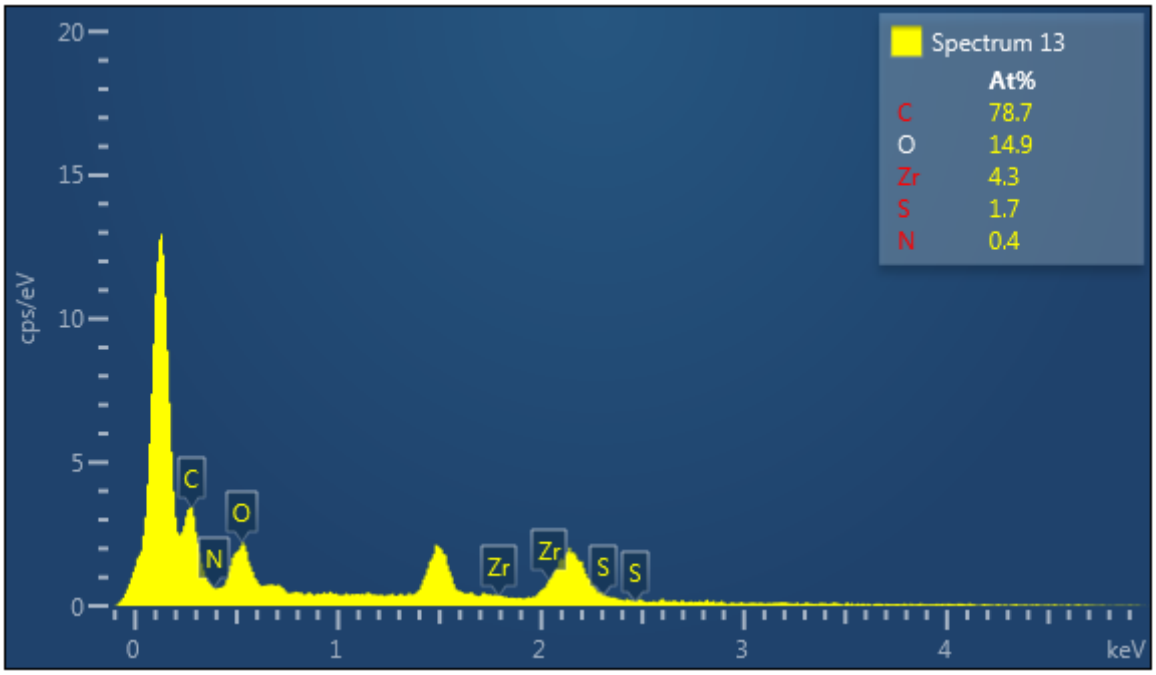


Figure S8. EDX spectrum of **UiO@Dansyl**.

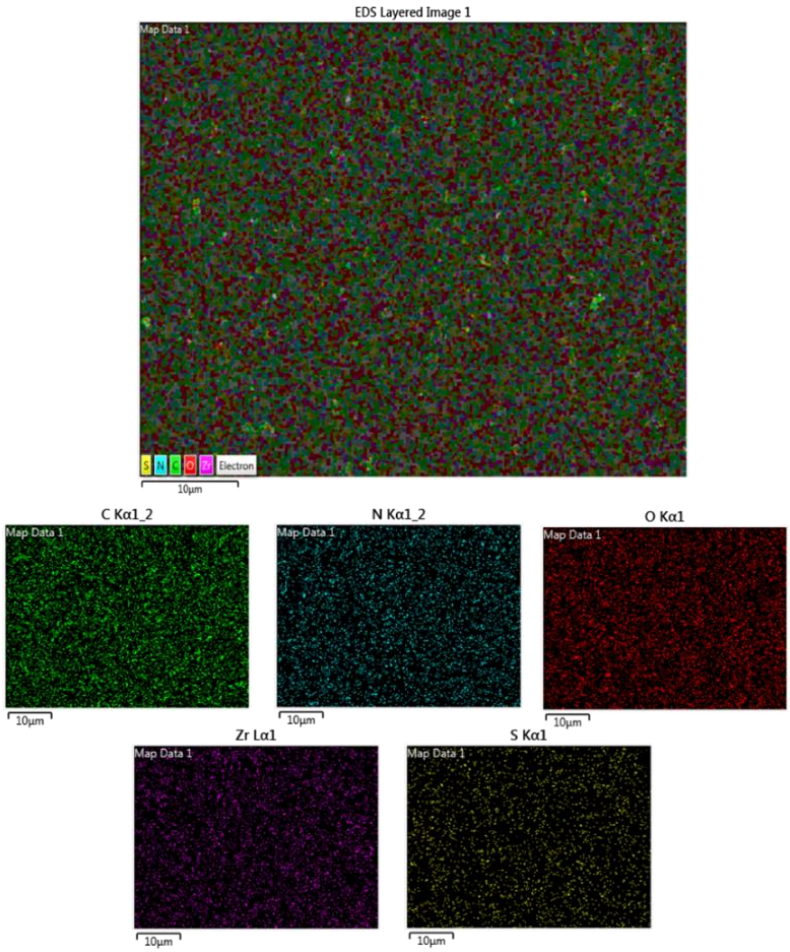


Figure S9. EDX elemental mapping of **UiO@Dansyl**.

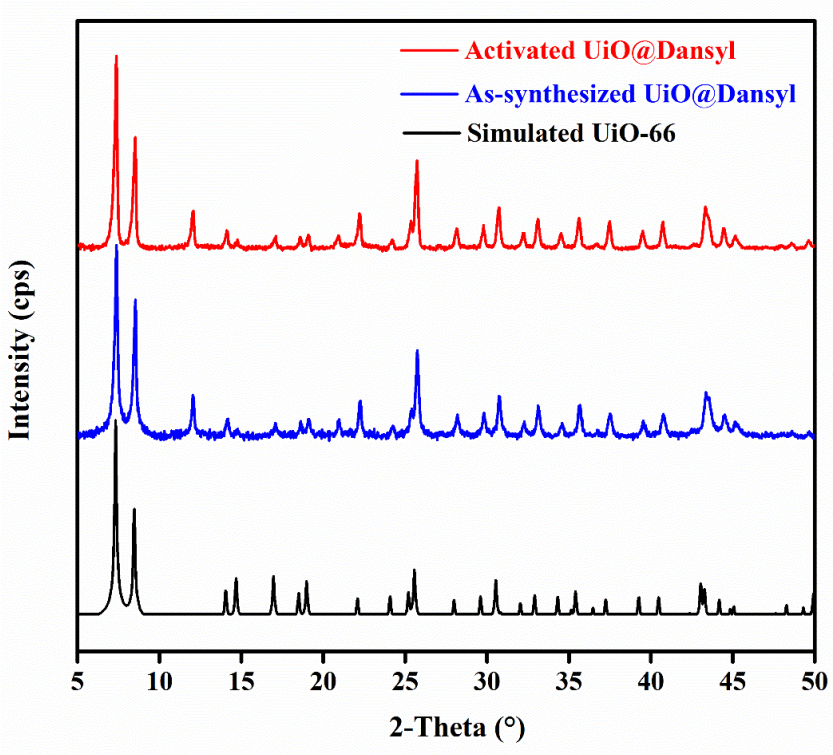


Figure S10. PXRD patterns of simulated **UiO-66** (black), as-synthesized **UiO@Dansyl** (blue), activated **UiO@Dansyl** (red).

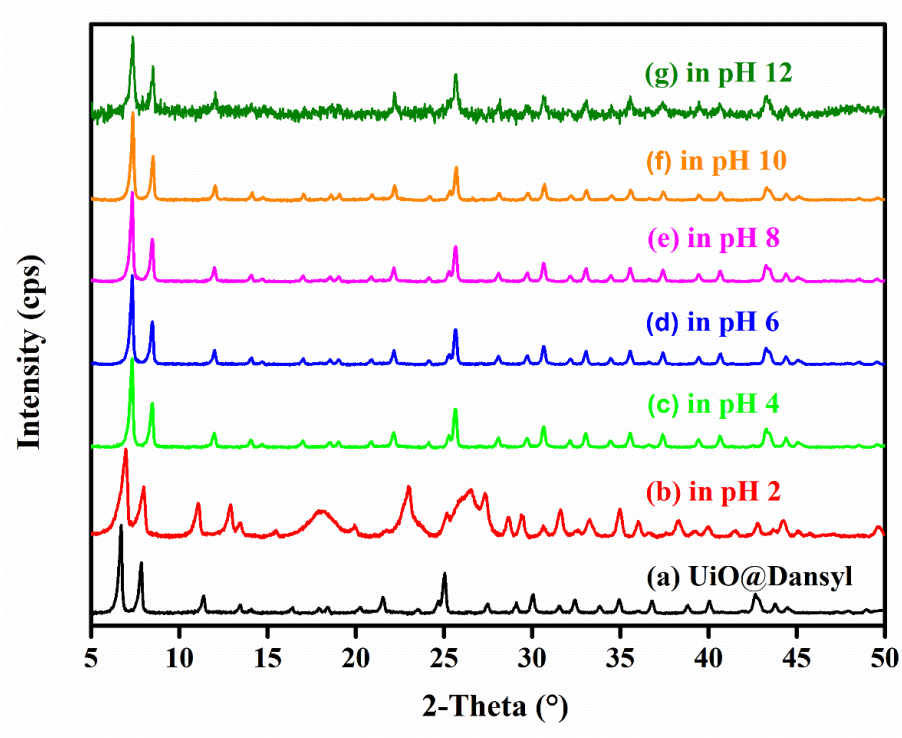


Figure S11. PXRD patterns of (a) activated **UiO@Dansyl** (black), after stirring in (b) pH 2 (red), (c) pH 4 (green), (d) pH 6 (blue), (e) pH 8 (pink), (f) pH 10 (orange) and (g) pH 12 (olive green) solutions.

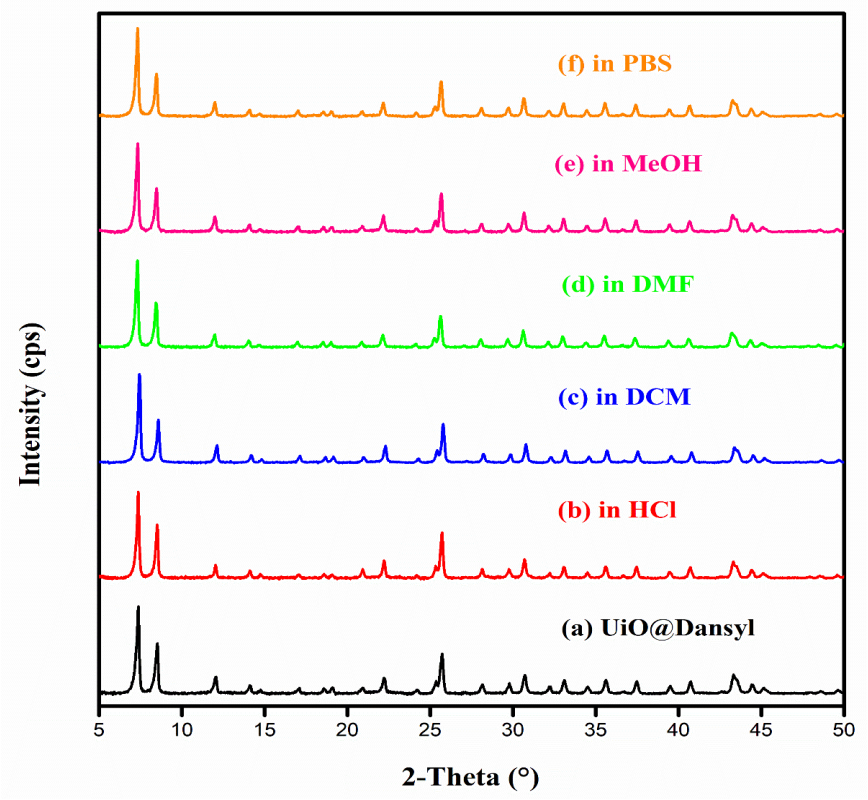


Figure S12. PXRD patterns of (a) activated **UiO@Dansyl** (black), after stirring in (b) 1M HCl (red), (c) DCM (blue), (d) DMF (green), (e) MeOH (pink) and (f) PBS (pH = 7.4) buffer (orange) solutions.

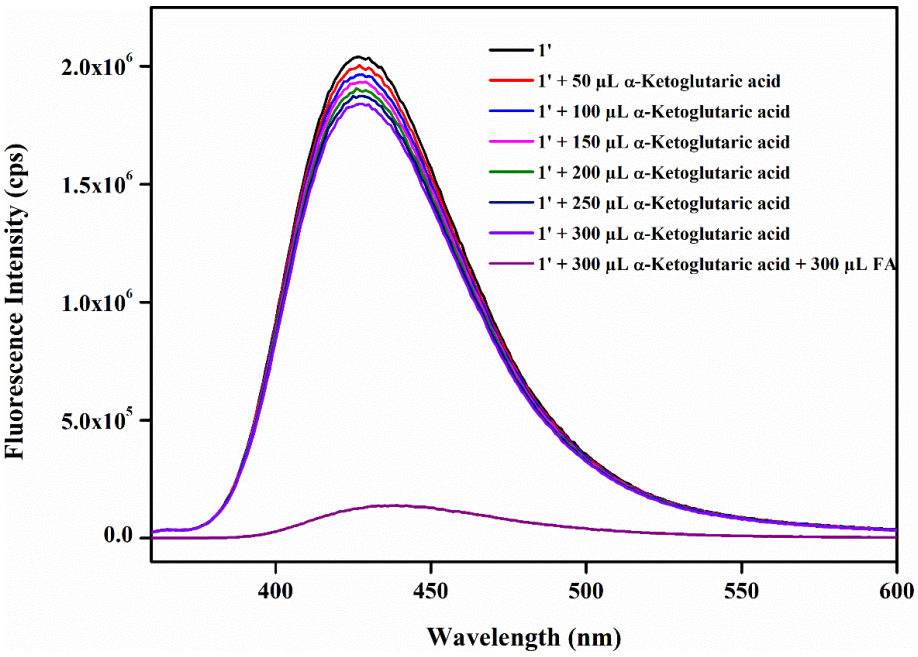


Figure S13. Change in fluorescence emission intensity of activated **UiO@Dansyl** (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM α-ketoglutaric acid solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

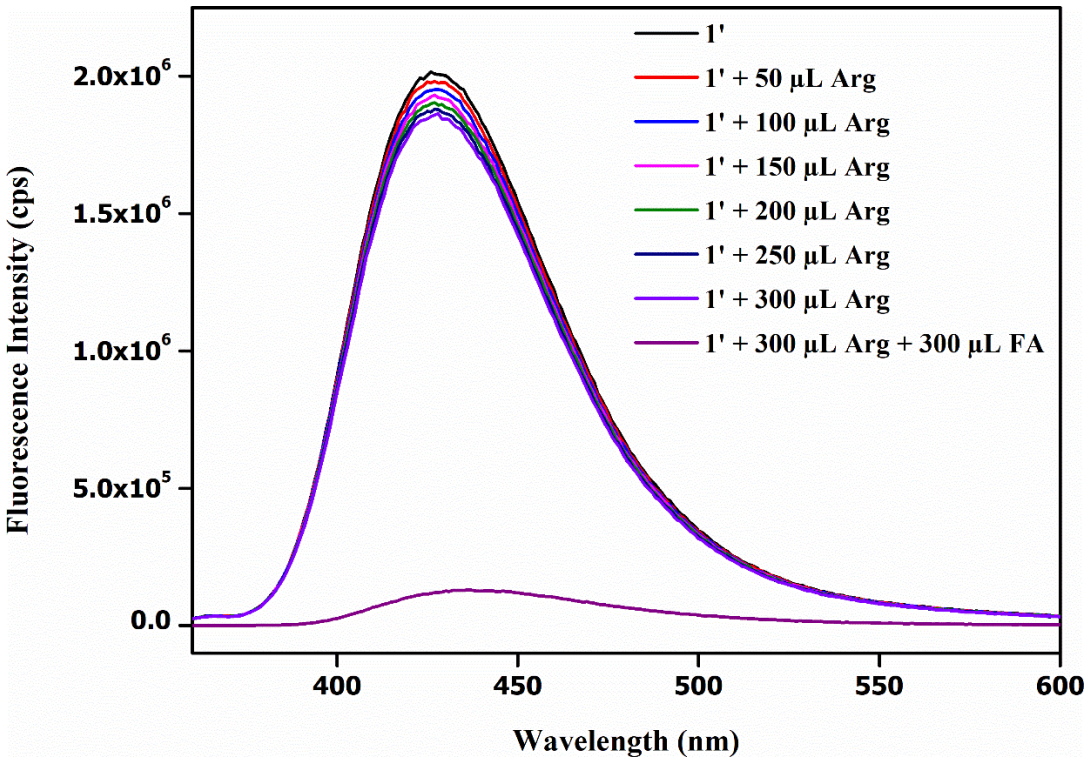


Figure S14. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM arginine (Arg) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

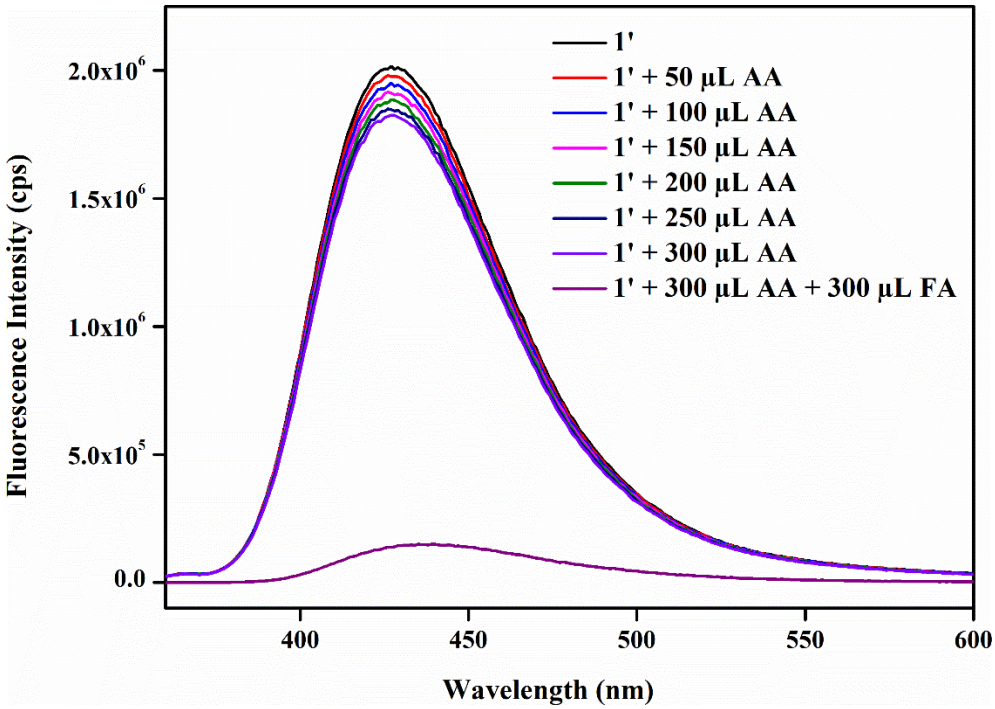


Figure S15. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM ascorbic acid (AA) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

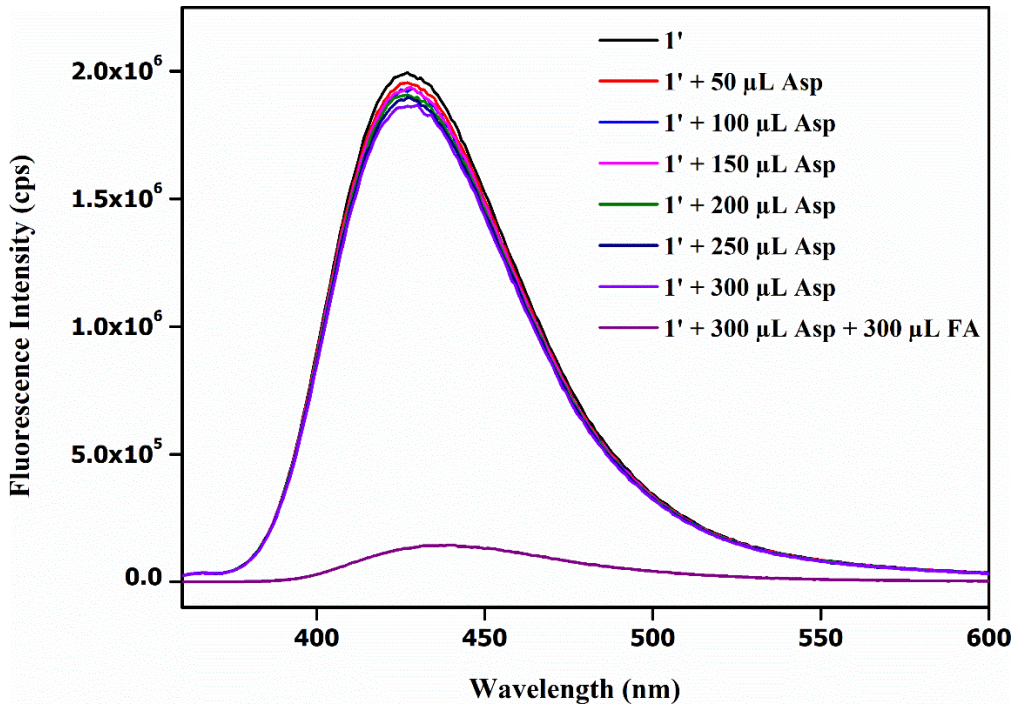


Figure S16. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM aspartic acid (Asp) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

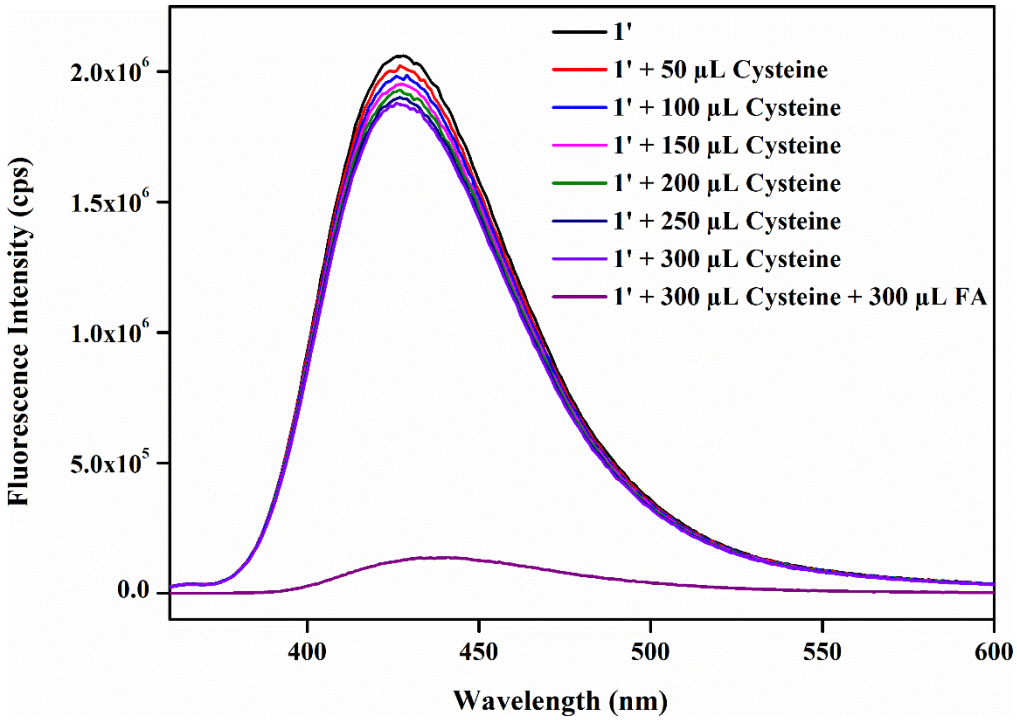


Figure S17. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM cysteine solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

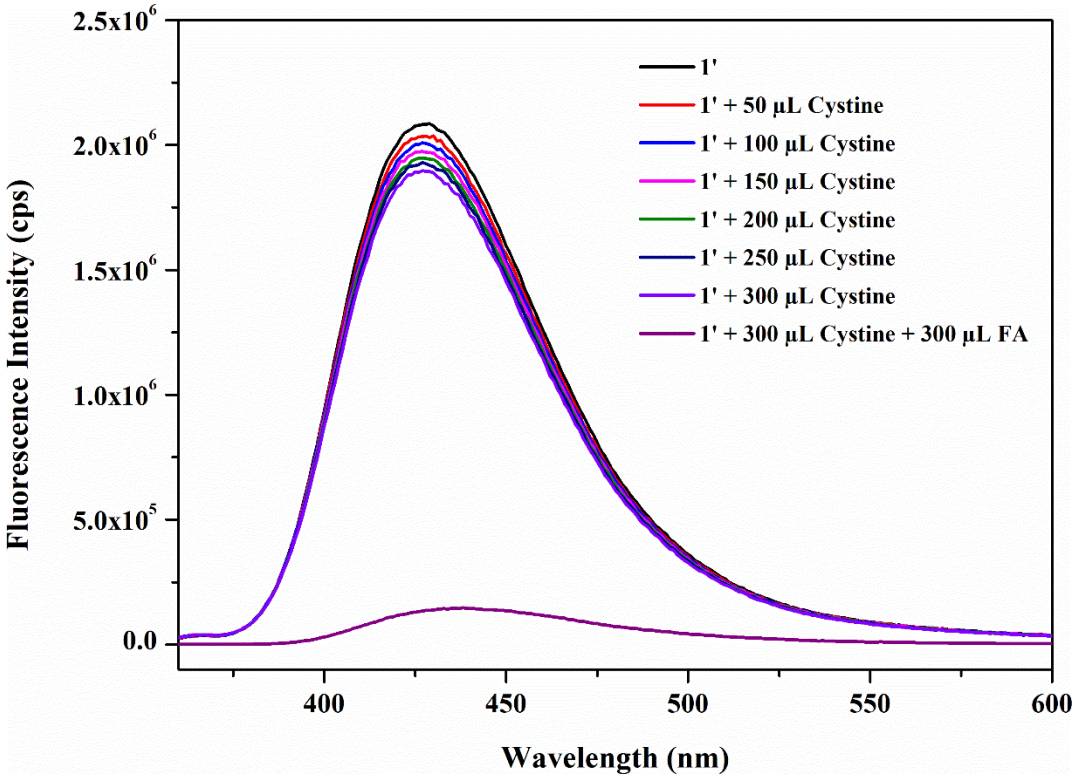


Figure S18. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM cysteine solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

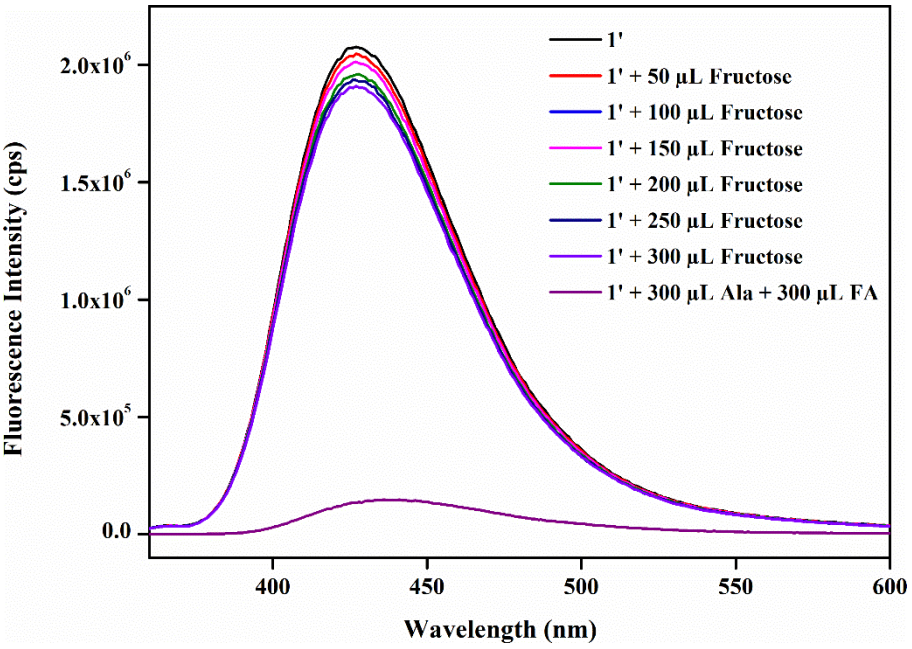


Figure S19. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM fructose solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

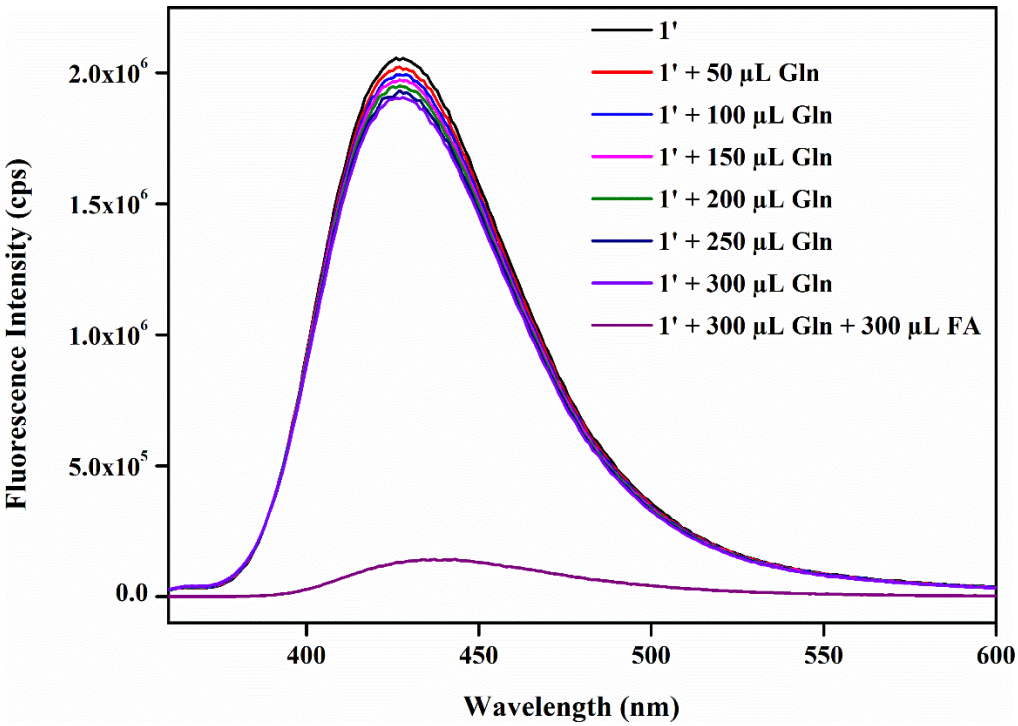


Figure S20. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM glutamine (gln) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

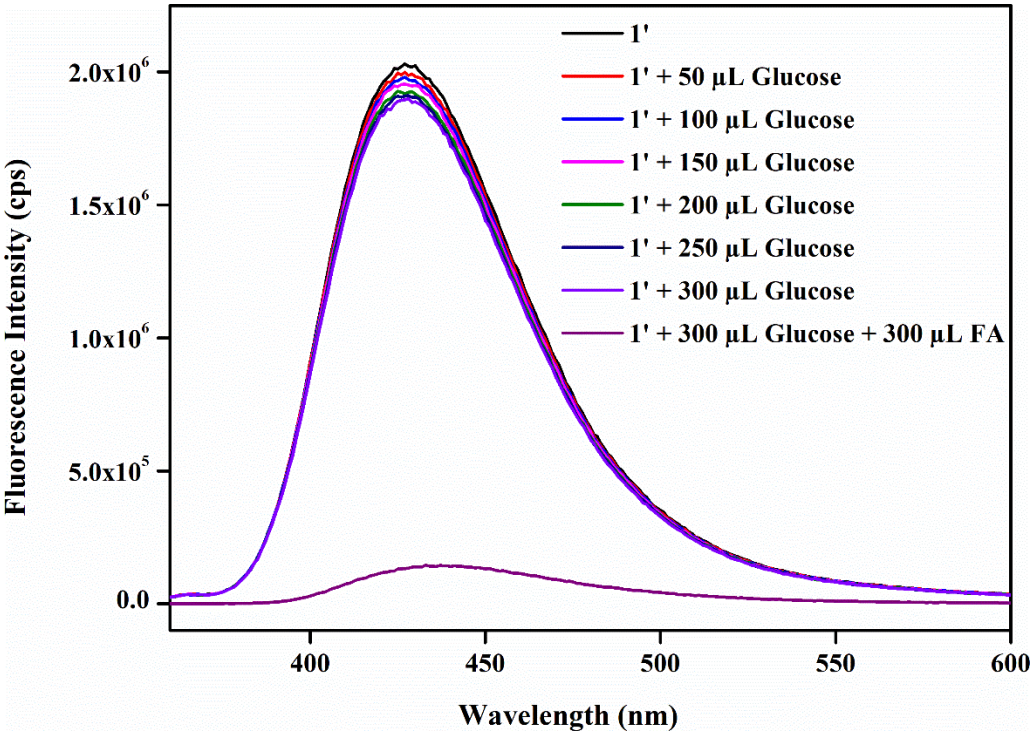


Figure S21. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM glucose solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

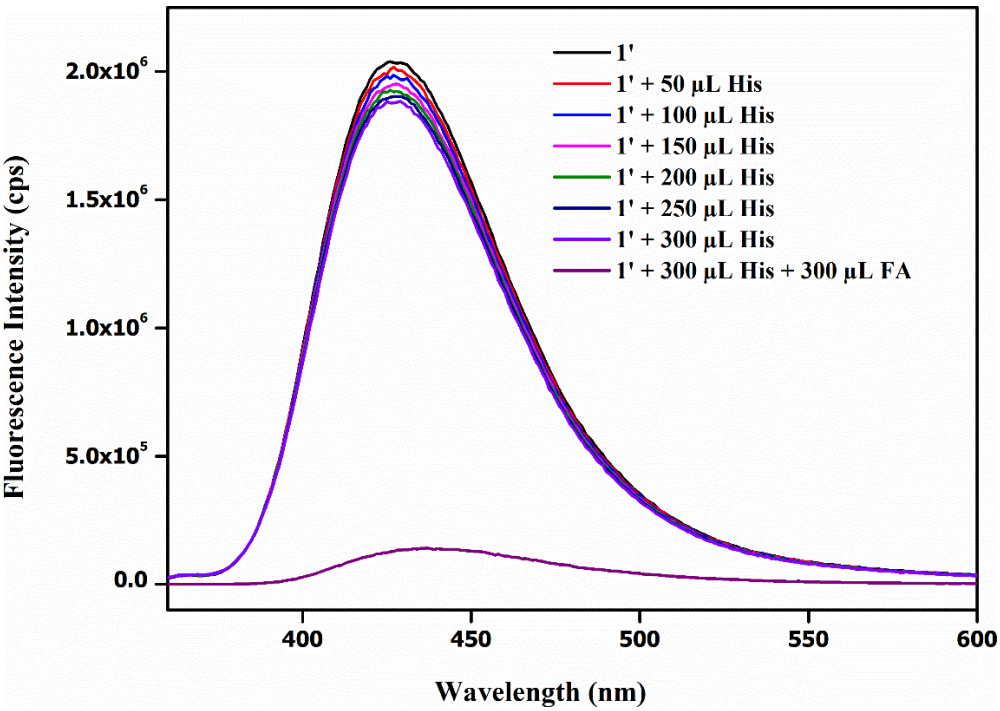


Figure S22. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM folic acid in presence of 300 µL of 5 mM histidine (his) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

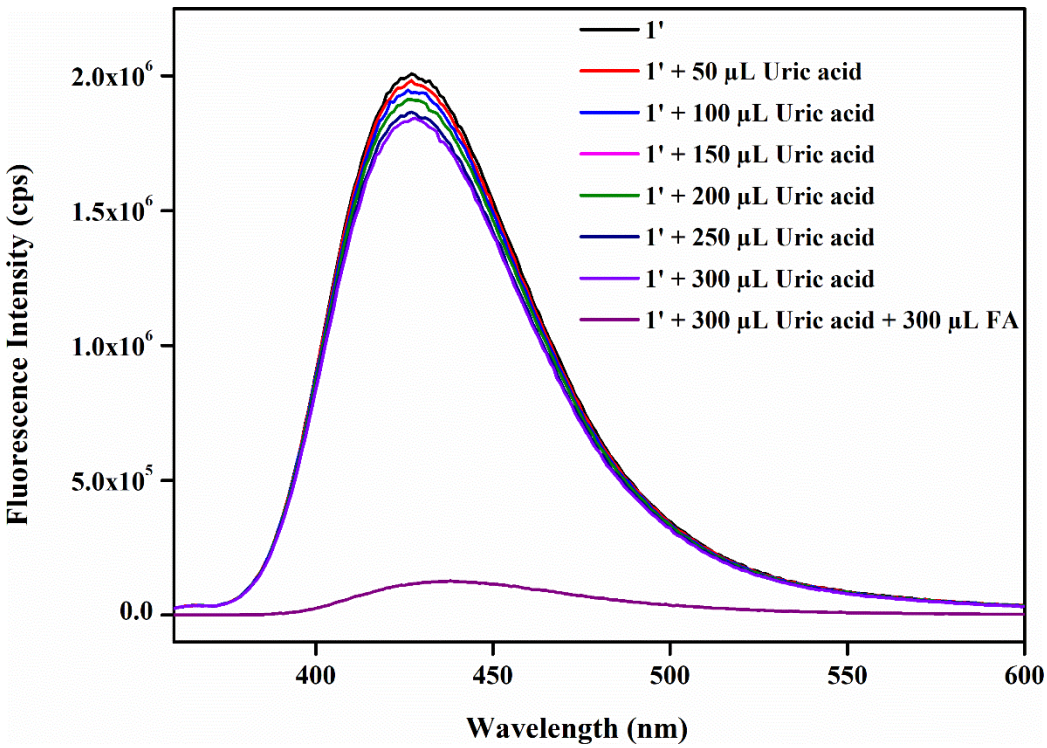


Figure S23. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM FA in presence of 300 µL of 5 mM Uric acid solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

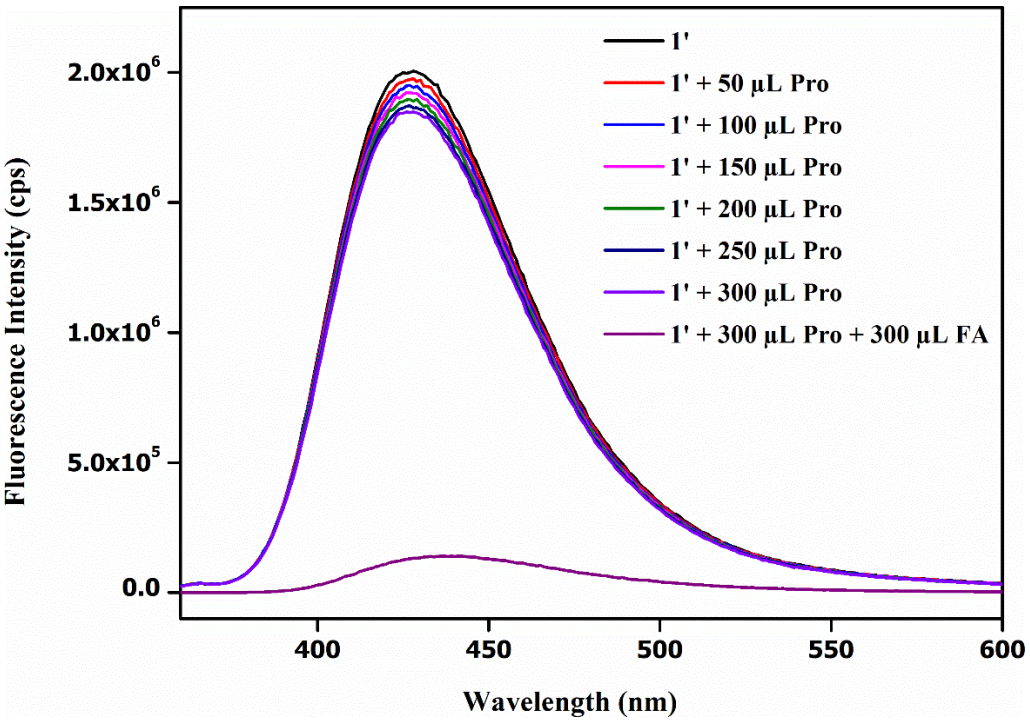


Figure S24. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM FA in presence of 300 µL of 5 mM proline (pro) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

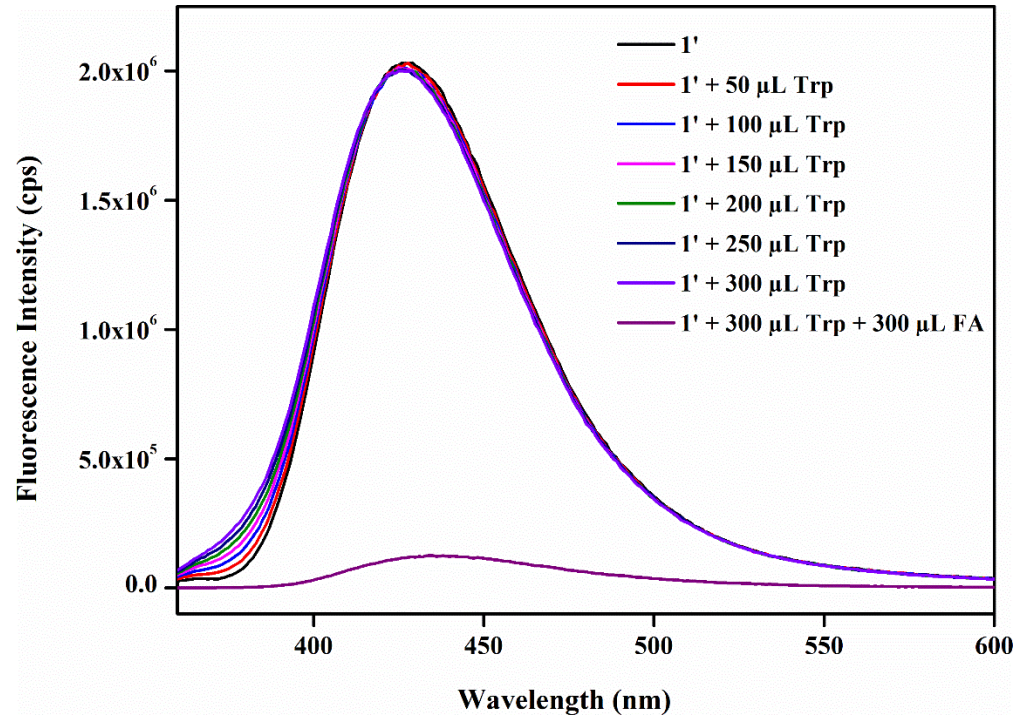


Figure S25. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM FA in presence of 300 µL of 5 mM tryptophan (trp) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

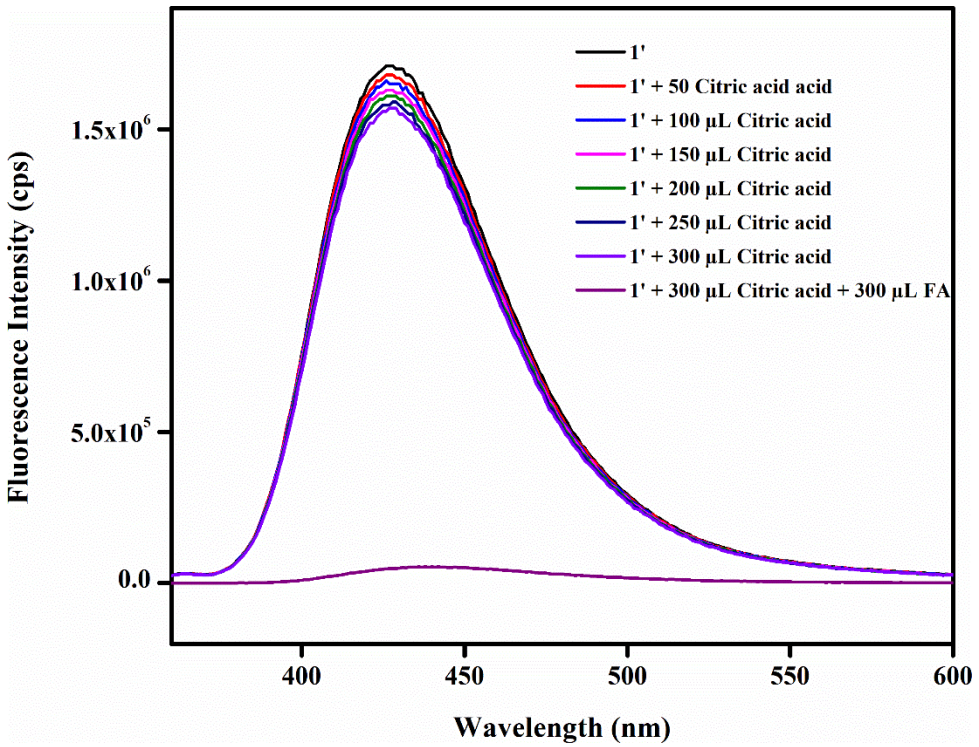


Figure S26. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM FA in presence of 300 µL of 5 mM citric acid solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

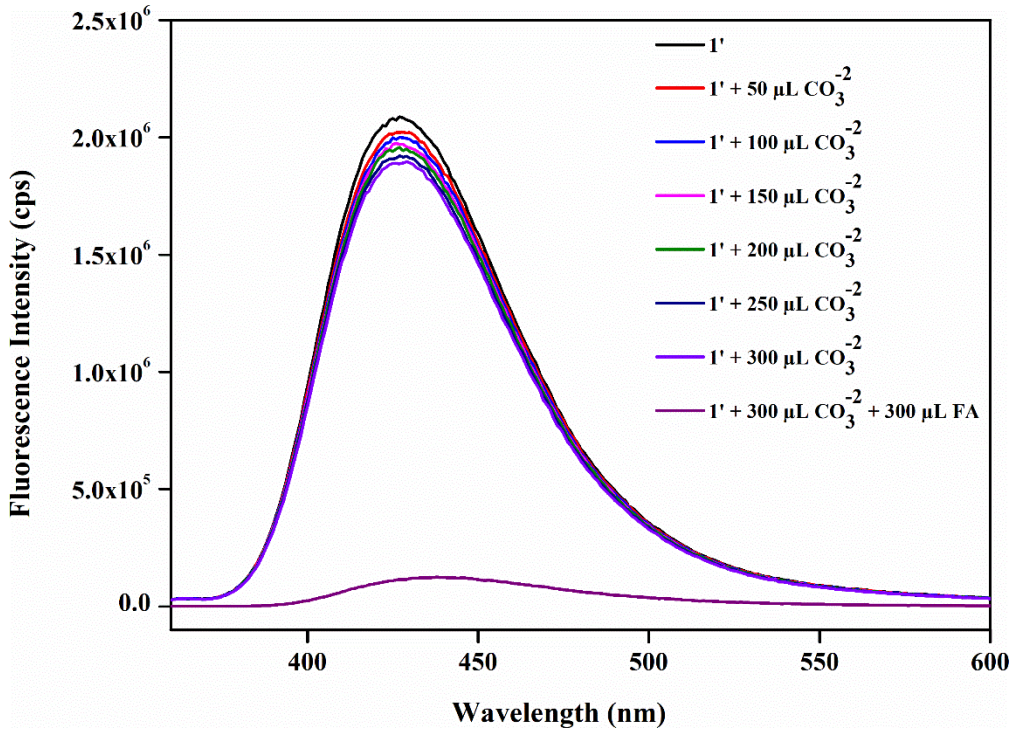


Figure S27. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM FA in presence of 300 µL of 5 mM carbonate (CO_3^{2-}) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

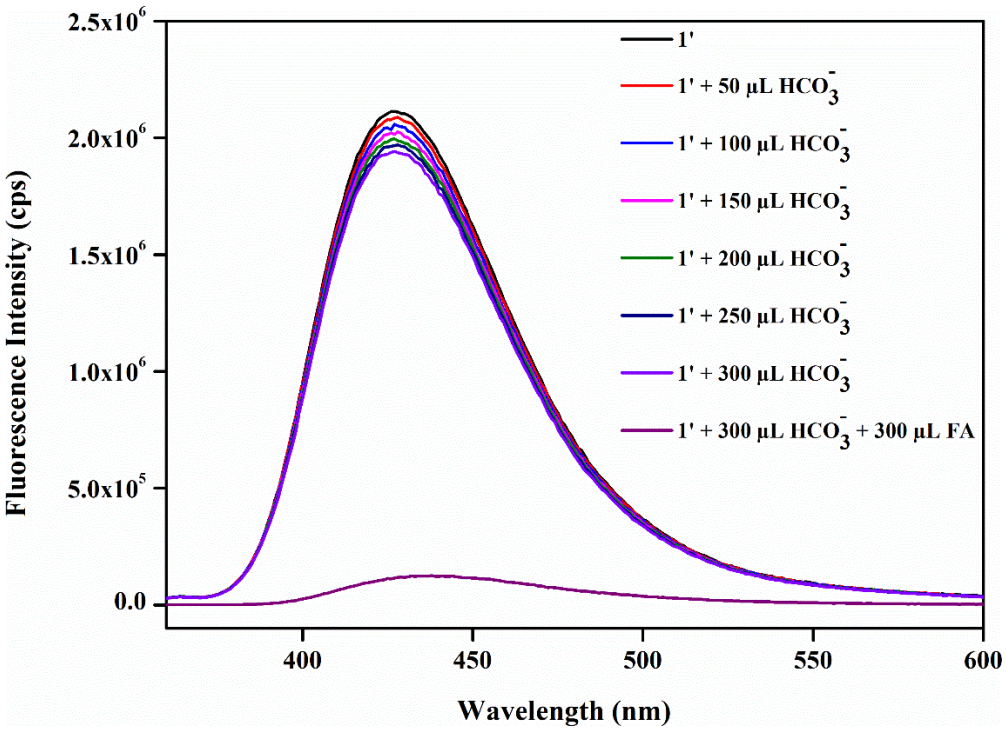


Figure S28. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM FA in presence of 300 µL of 5 mM bicarbonate (HCO_3^-) solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

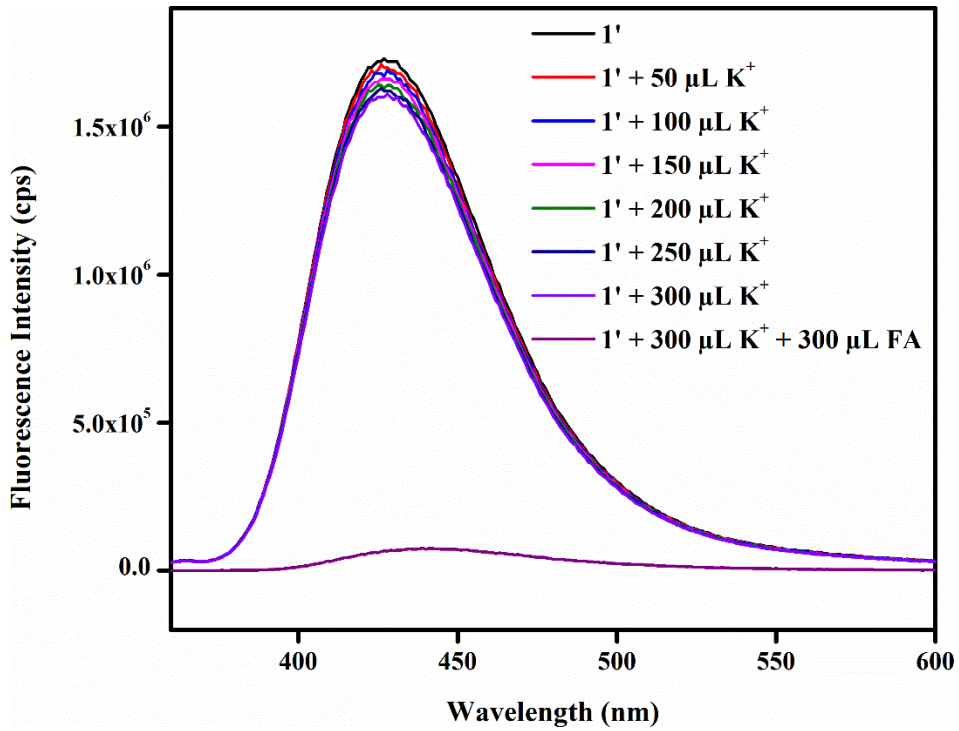


Figure S29. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM FA in presence of 300 µL of 5 mM K^+ solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

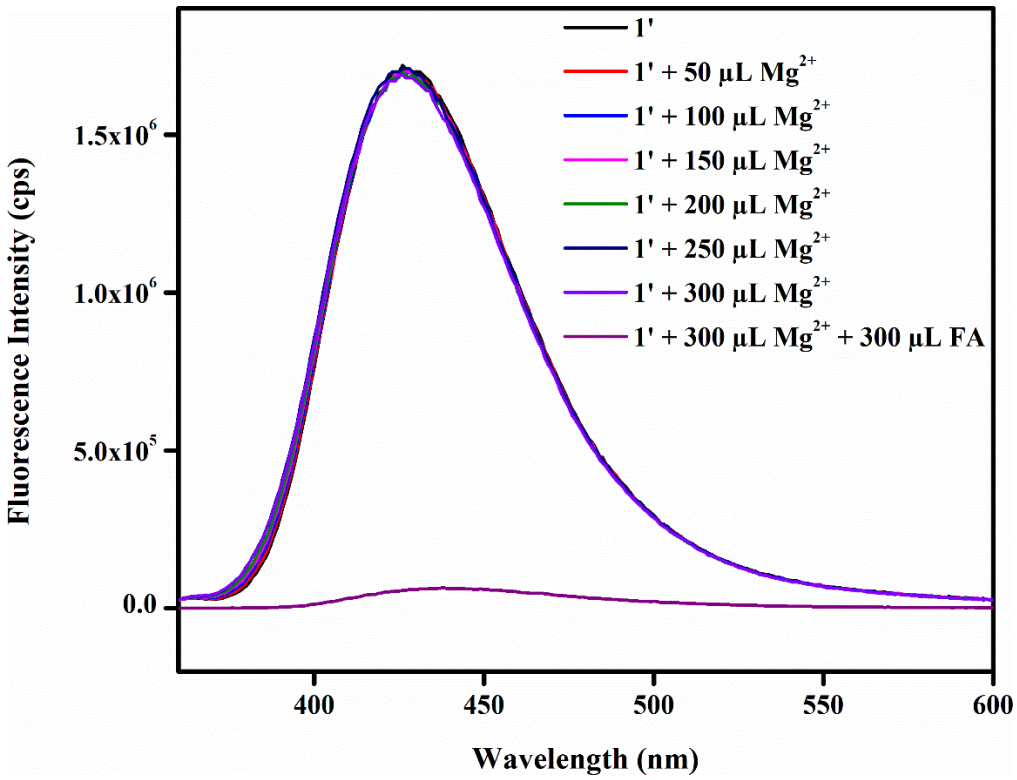


Figure S30. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon addition of 300 µL of 5 mM FA in presence of 300 µL of 5 mM Mg^{2+} solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

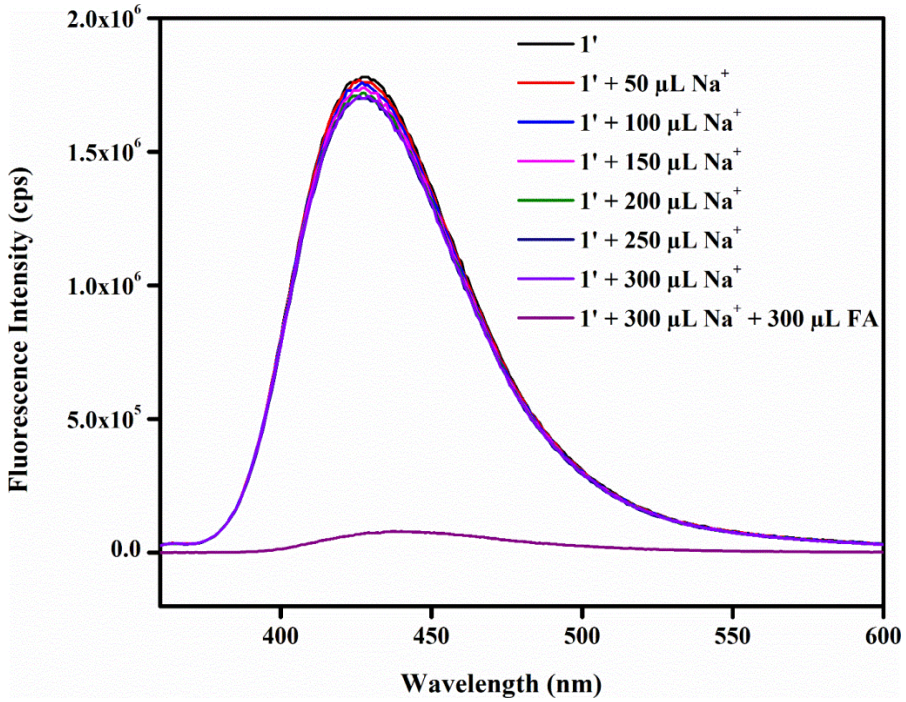


Figure S31. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon of 300 µL of 5 mM FA in presence of 300 µL of 5 mM Na^{+} solution (λ_{ex} = 325 nm and λ_{em} = 428 nm).

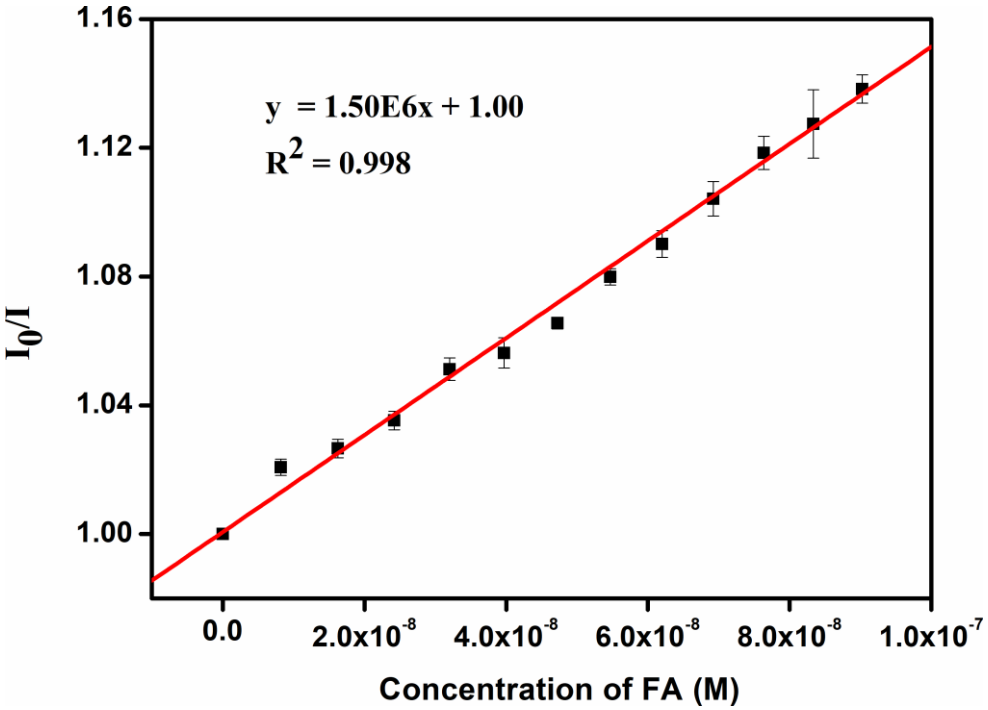


Figure S32. Stern-Volmer plot for fluorescence quenching of activated **UiO@Dansyl** in PBS medium against increasing concentration of FA.

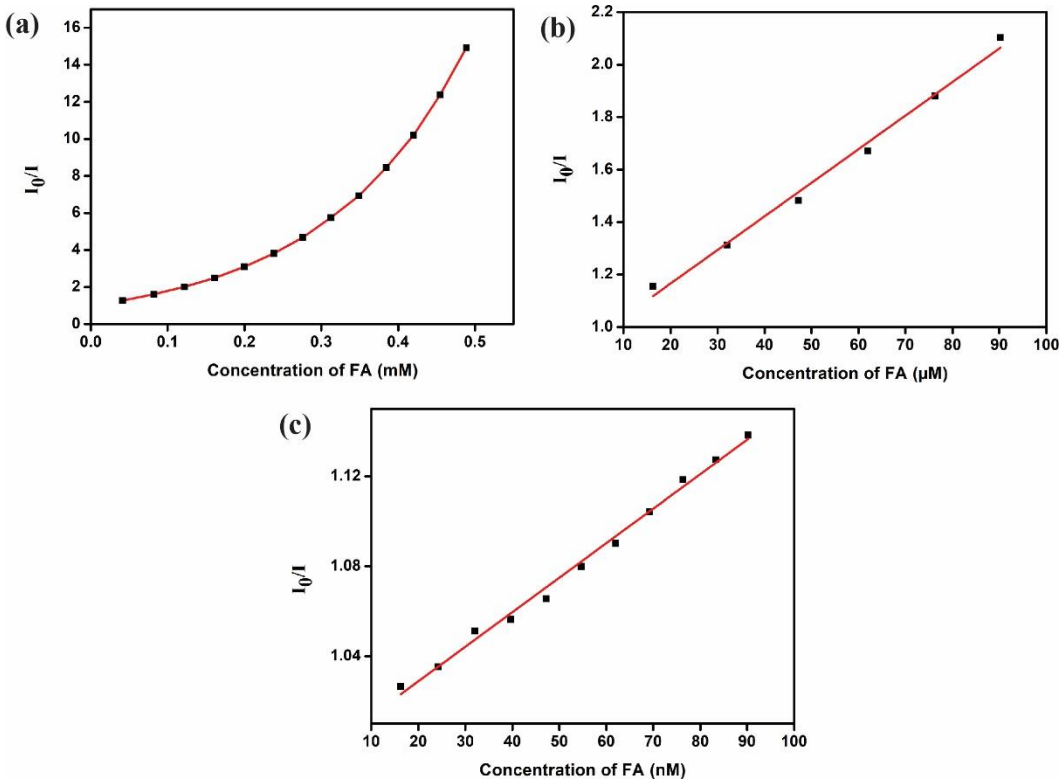


Figure S33. Stern-Volmer plot for fluorescence quenching of activated **UiO@Dansyl** in PBS medium against increasing different concentrations of FA: (a) milli molar, (b) micro molar and (c) nano molar.

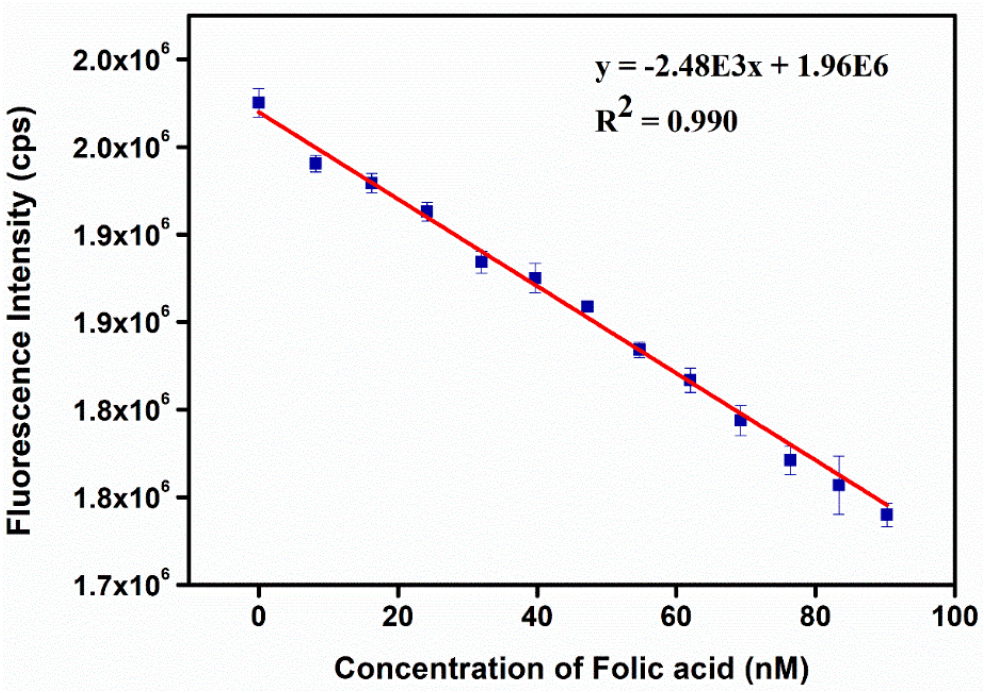


Figure S34. Change in fluorescence emission intensity of activated **UiO@Dansyl** in PBS medium as a function of FA concentration.

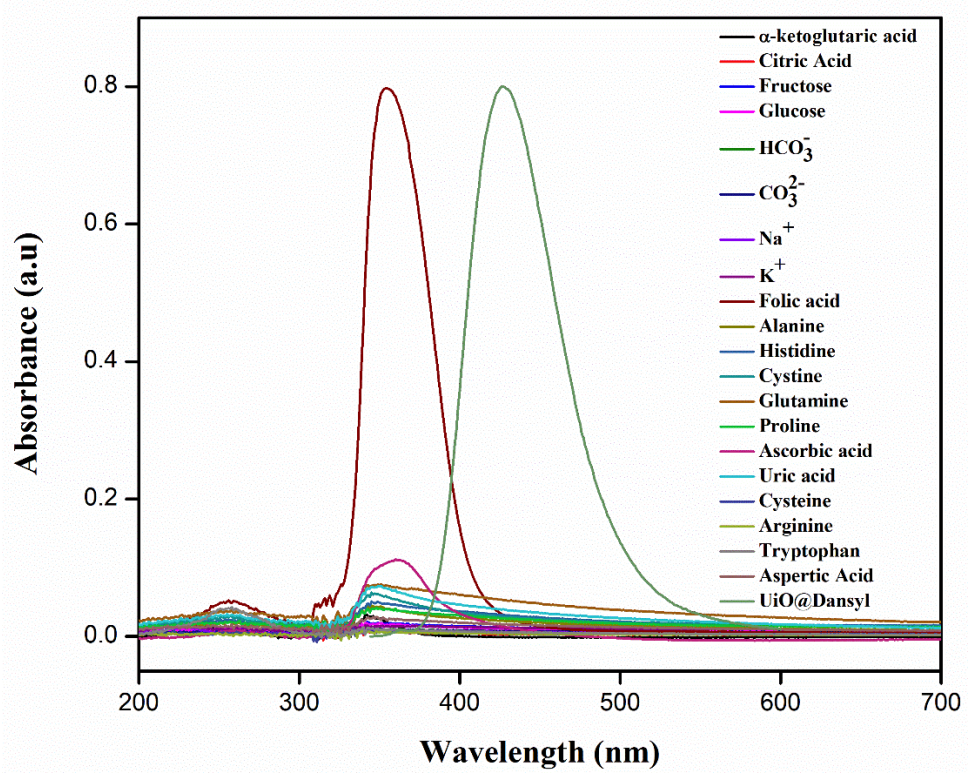


Figure S35. UV-absorption spectra of all analytes and emission spectra of **UiO@Dansyl** MOF.

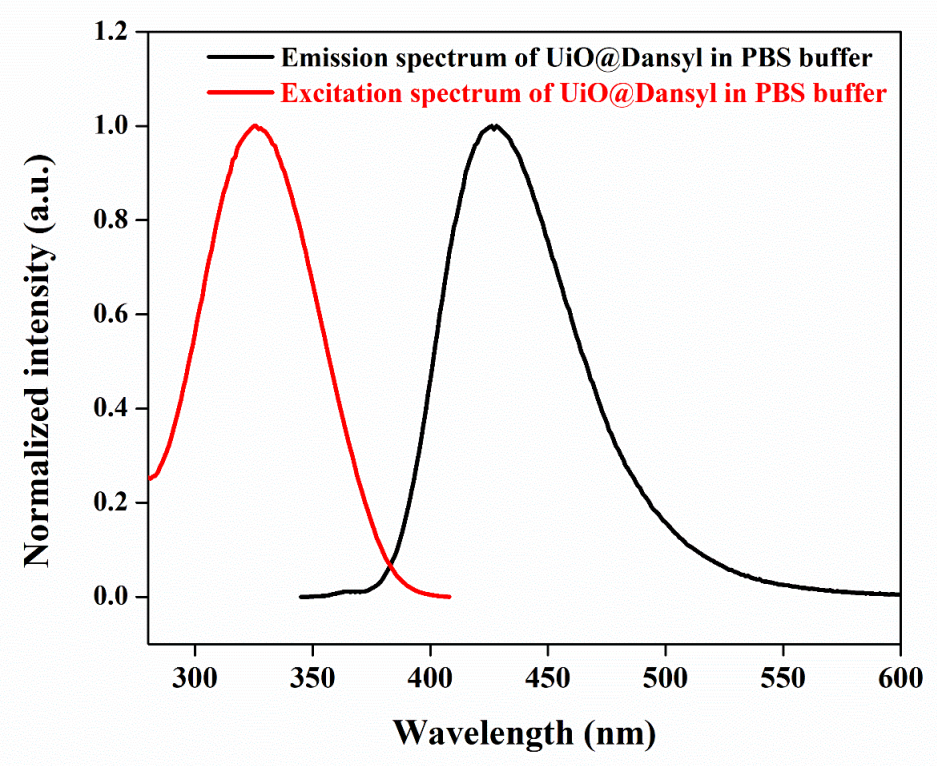


Figure S36. Excitation (red) and emission (black) spectra of **UiO@Dansyl** in PBS buffer medium.

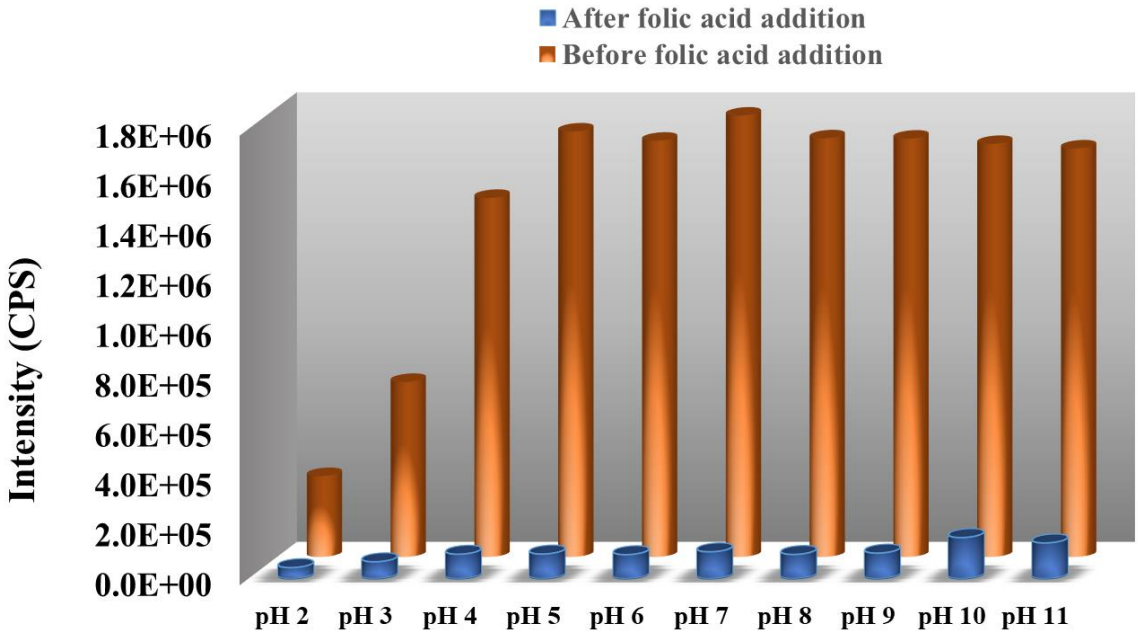


Figure S37. Quenching of fluorescence emission intensity of activated **UiO@Dansyl** with introduction of FA (5 mM, 300 µL) in different pH media.

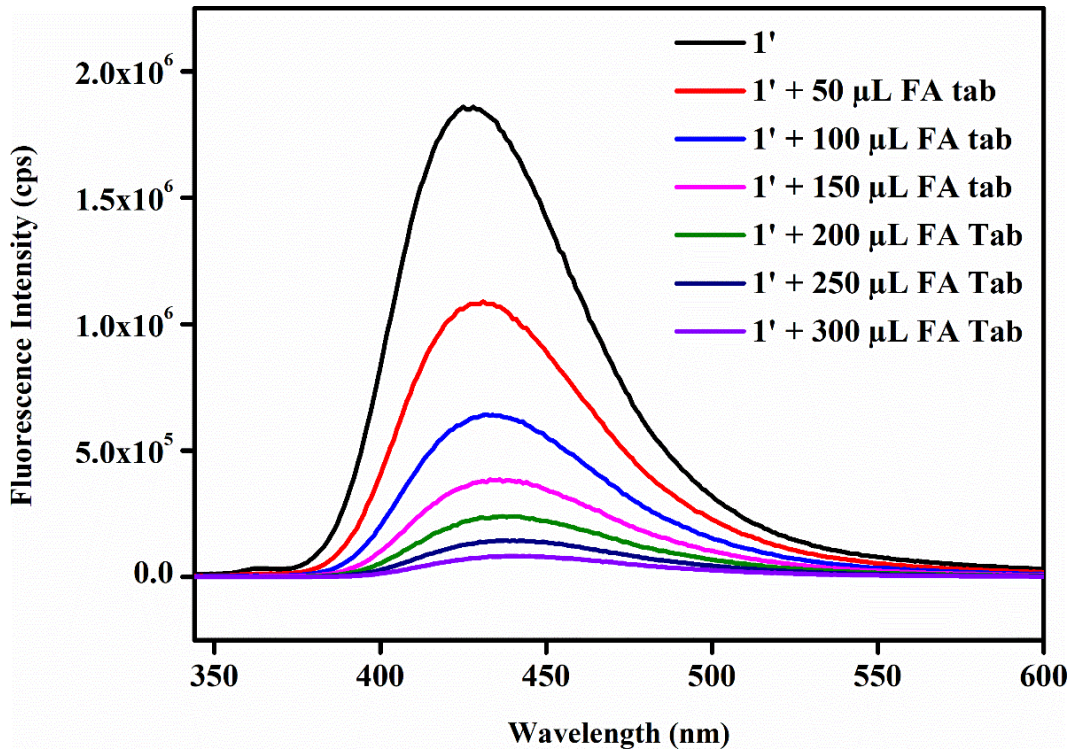


Figure S38. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon incremental addition of FA tablet extract (FA Tab) (λ_{ex} = 325 nm and λ_{em} = 428 nm).

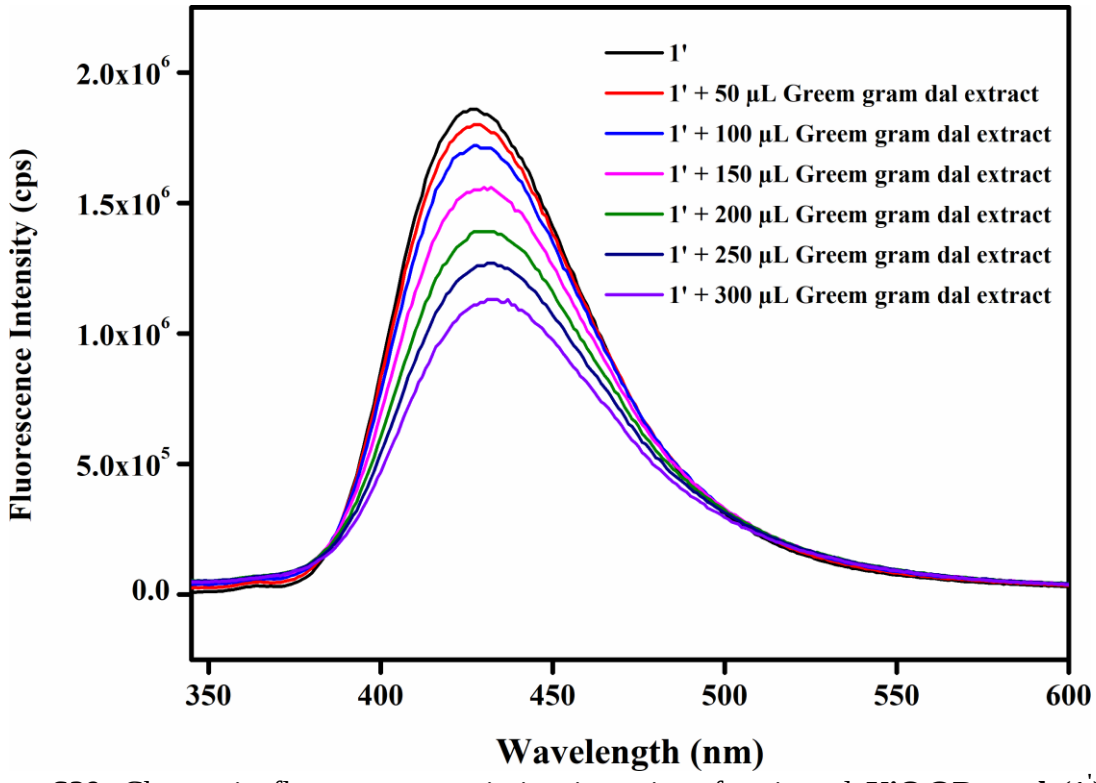


Figure S39. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon incremental addition of green gram dal extract (FA Tab) (λ_{ex} = 325 nm and λ_{em} = 428 nm).

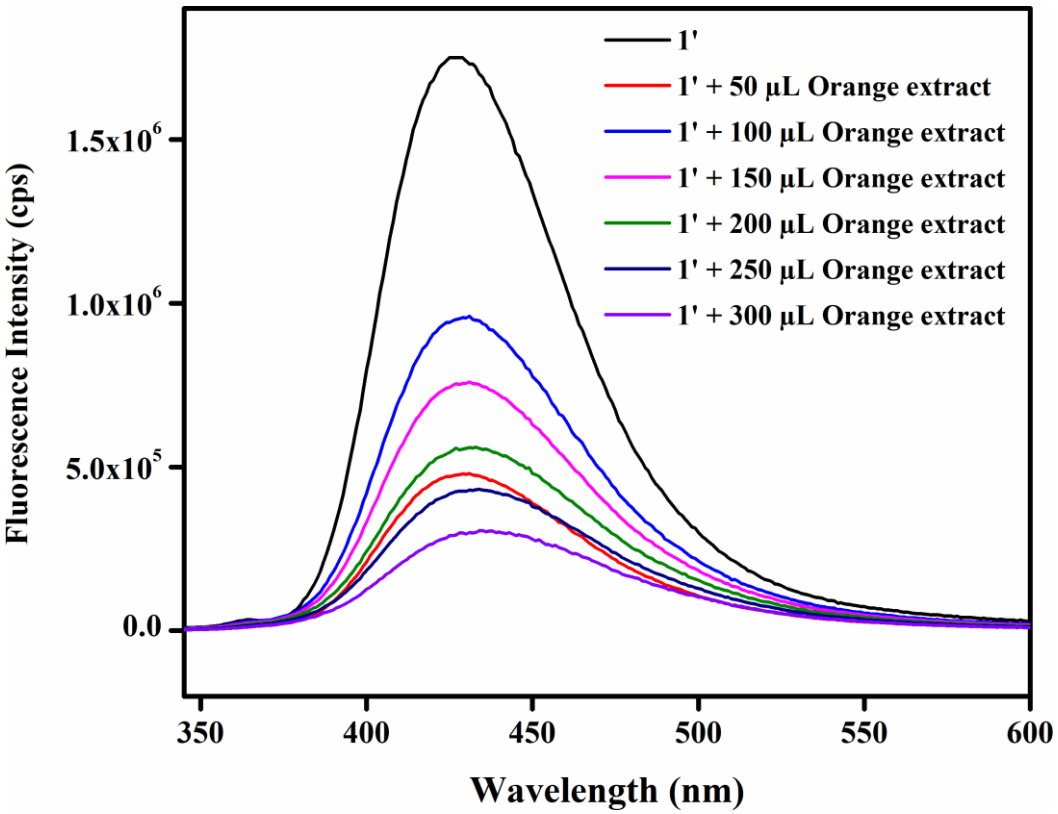


Figure S40. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon incremental addition of orange extract (FA Tab) (λ_{ex} = 325 nm and λ_{em} = 428 nm).

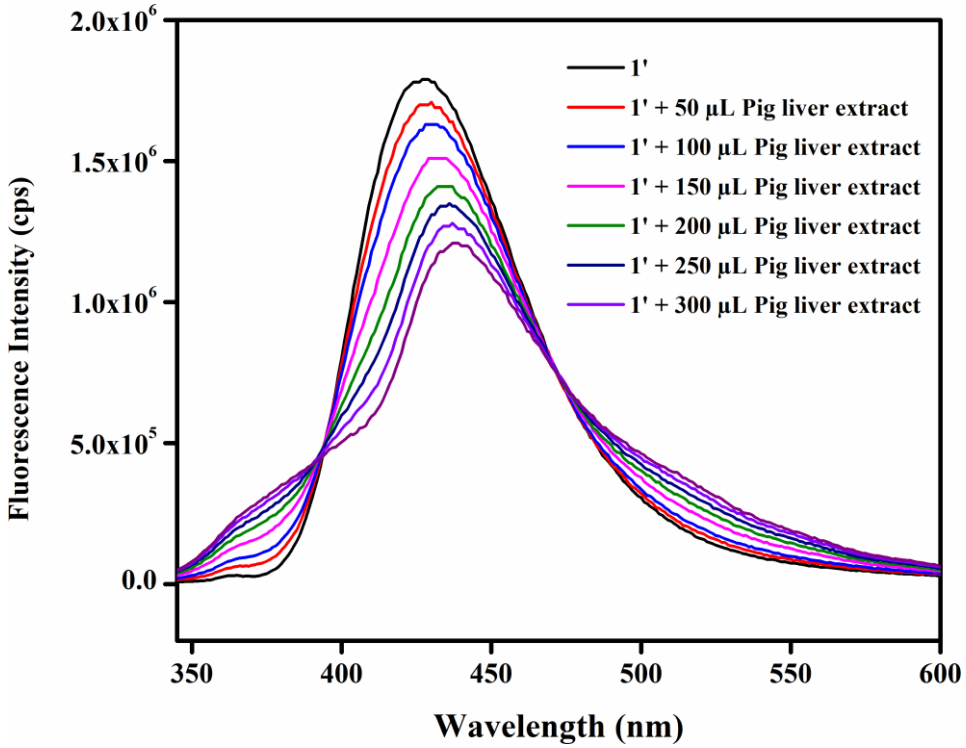


Figure S41. Change in fluorescence emission intensity of activated **UiO@Dansyl** (**1**') (in PBS medium) upon incremental addition of pig liver extract (FA Tab) (λ_{ex} = 325 nm and λ_{em} = 428 nm).

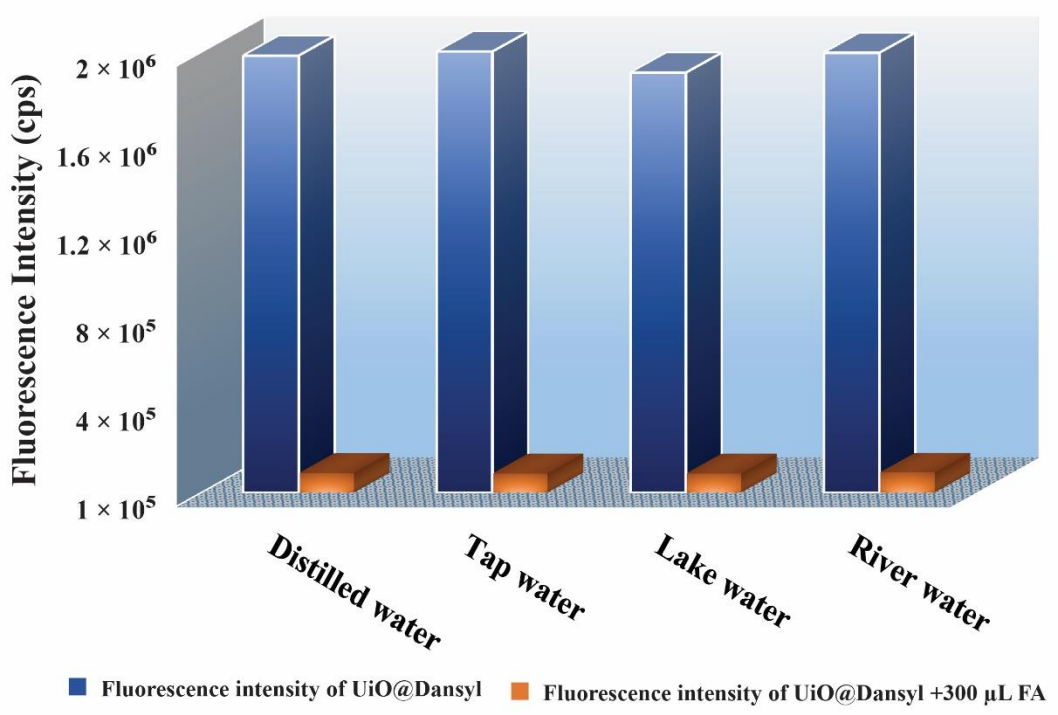


Figure S42. Quenching of fluorescence emission intensity of activated **UiO@Dansyl** with introduction of FA (5 mM, 300 µL) in different aqueous media.

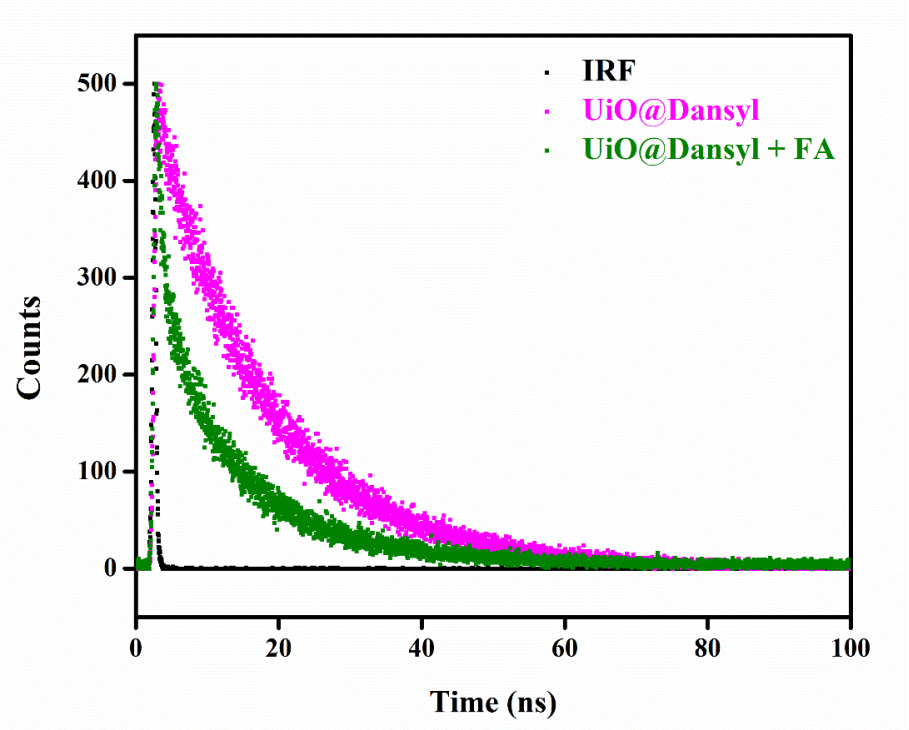


Figure S43. Lifetime decay profile of **UiO@Dansyl** in presence and absence of FA (λ_{ex} = 336 monitored at 429 nm).

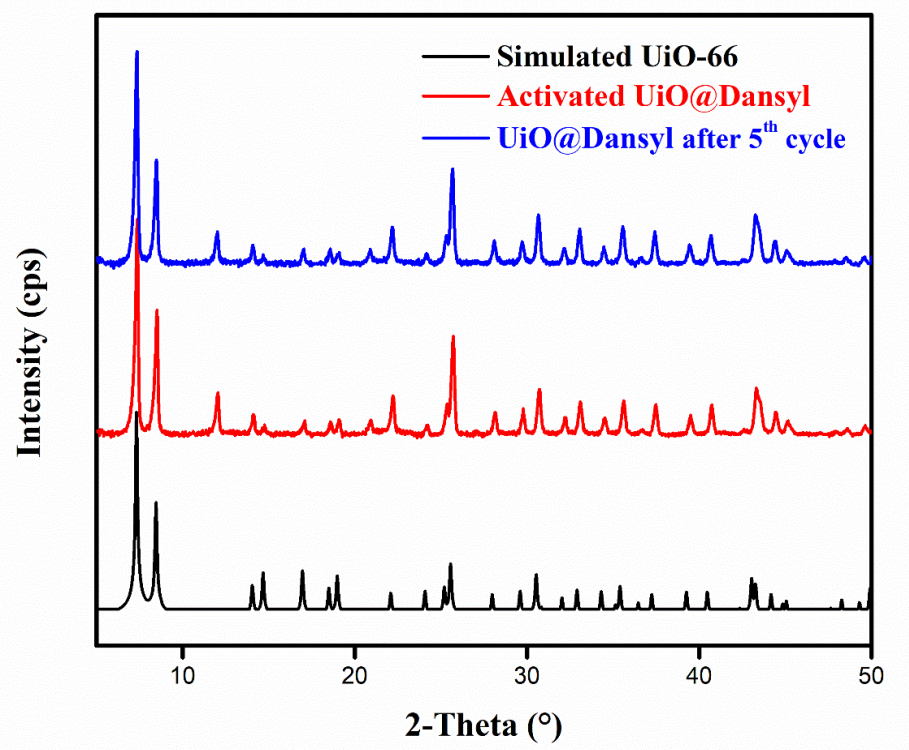


Figure S44. PXRD pattern comparison between activated **UiO@Dansyl** (red) and **UiO@Dansyl** after 5th cycle of recyclability (blue).

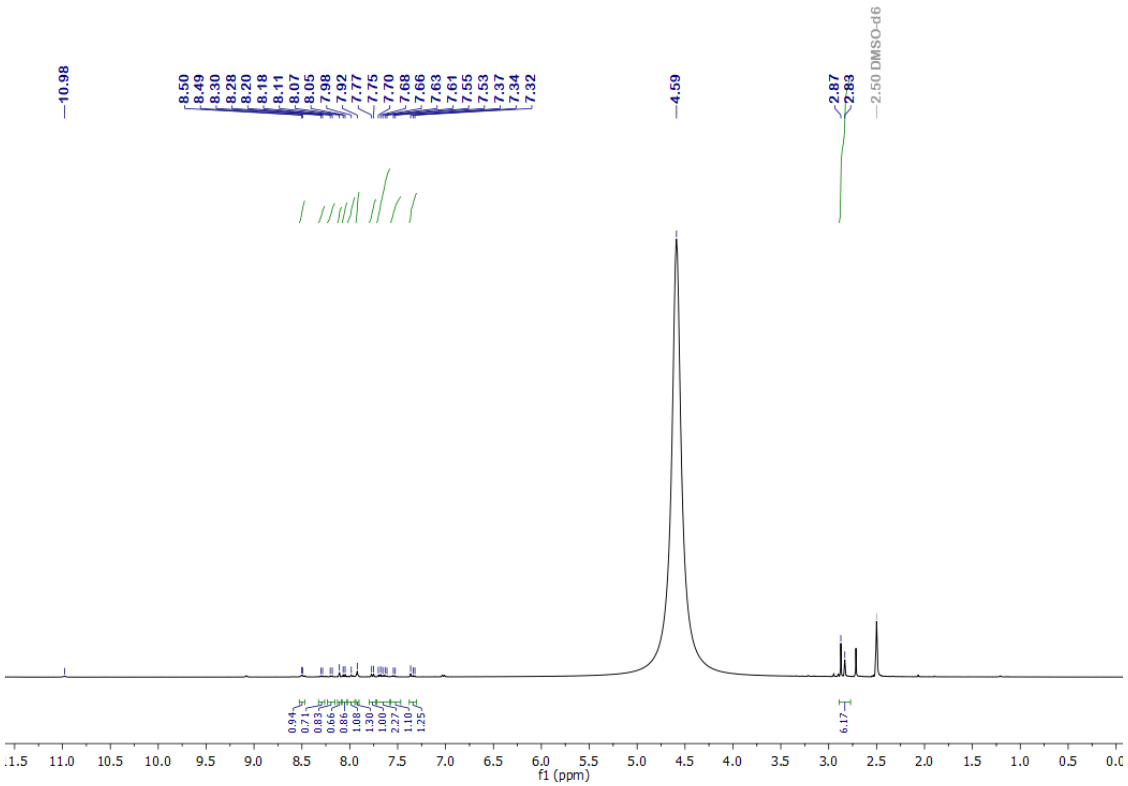


Figure S45. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of **UiO@Dansyl** MOF after 5th cycle of recyclability (digested with minimum amount of HF).

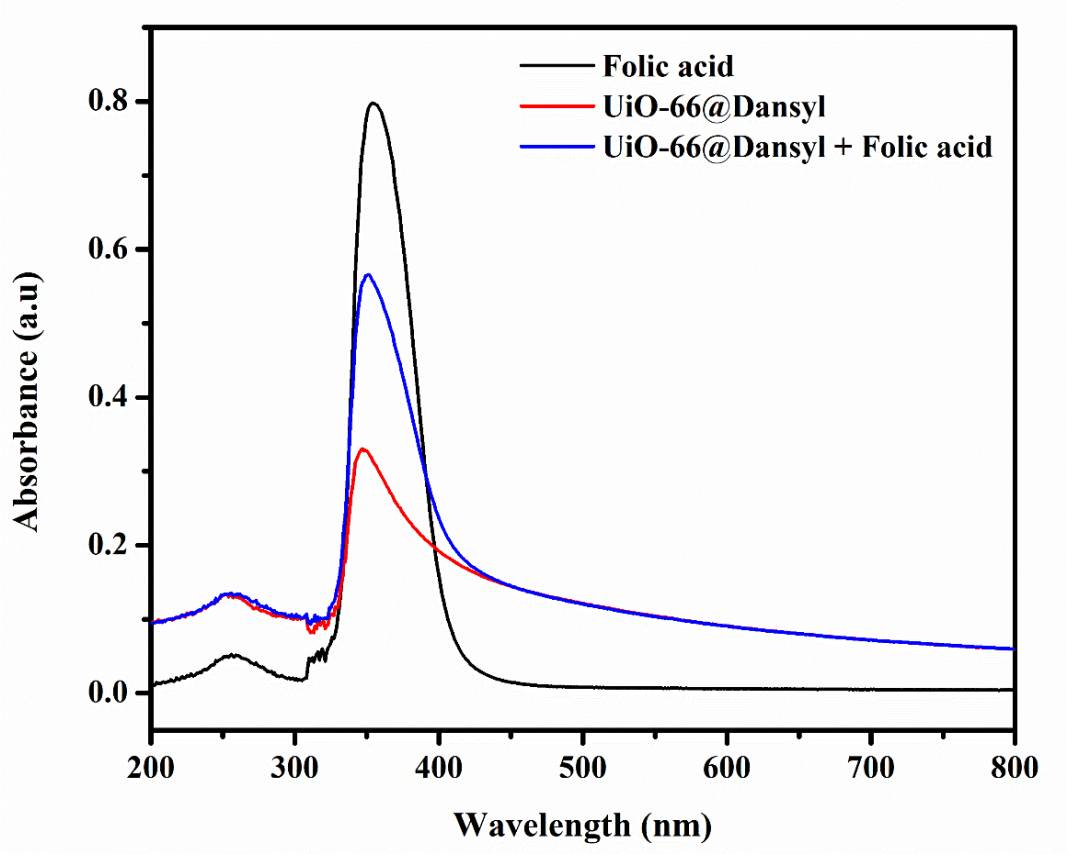


Figure S46. UV-Vis spectra of FA and **UiO@Dansyl** MOF.

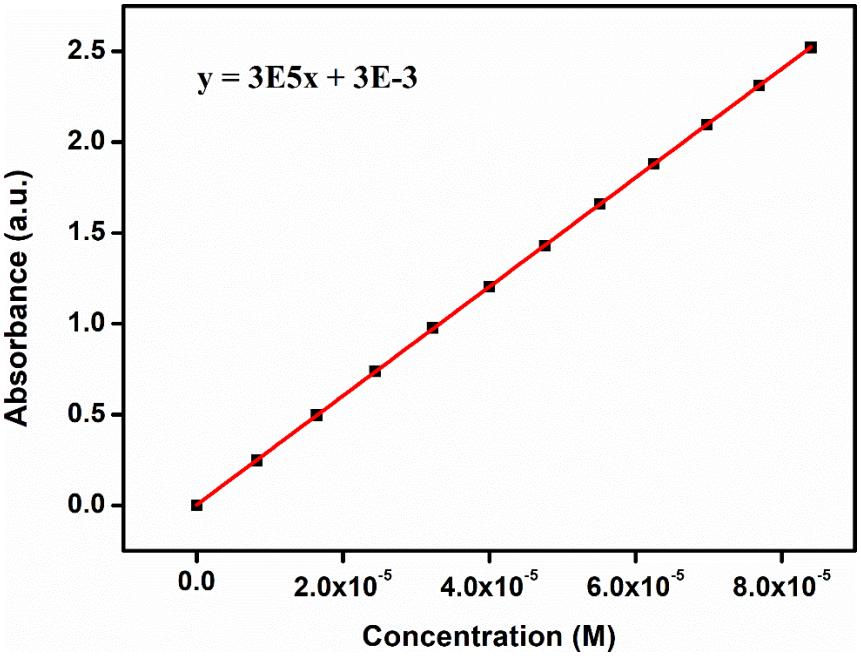


Figure S47. Calibration curve obtained from UV-Vis spectra for FA in water (absorption maxima was taken at 354 nm).

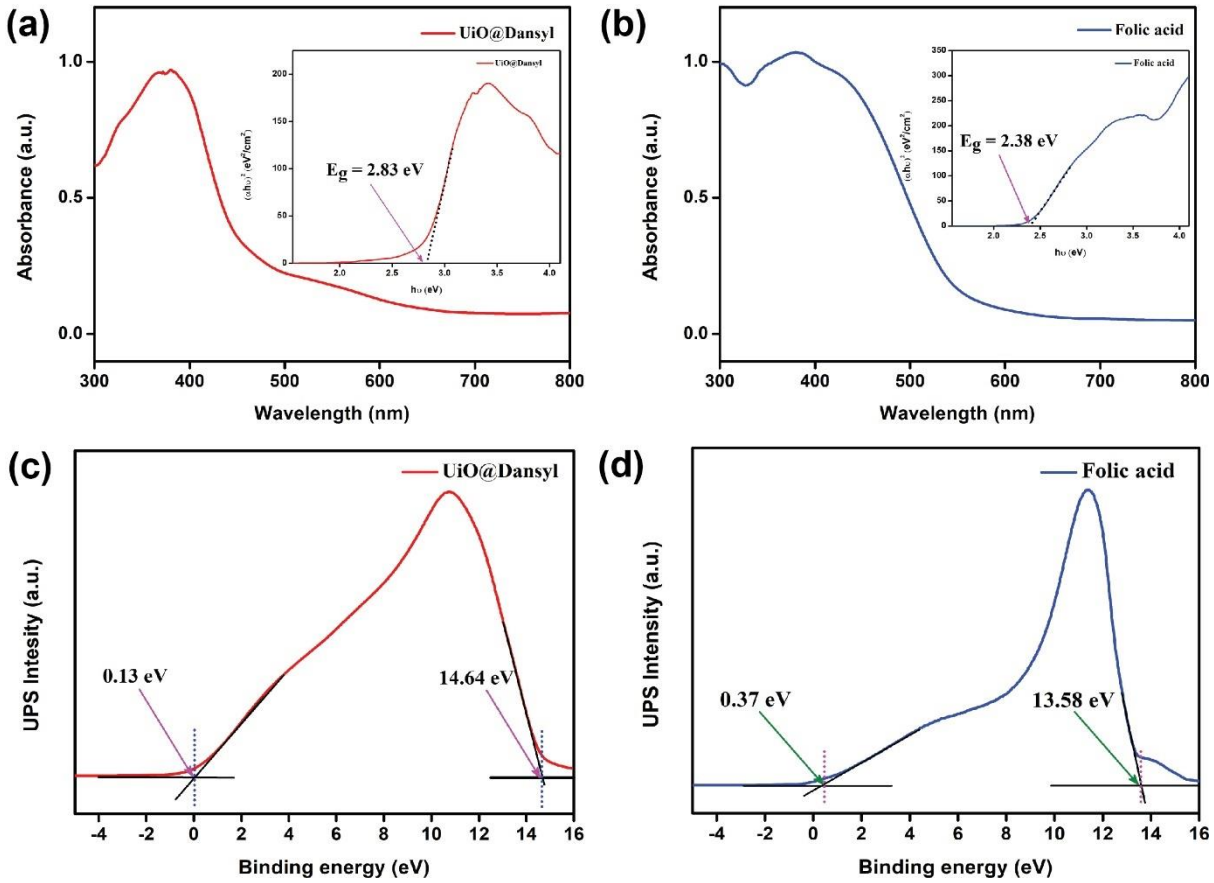


Figure S48. (a) UV-DRS spectrum of **UiO@Dansyl** (Tauc plot is shown inset). (b) UV-DRS spectrum of folic acid (Tauc plot was shown inset). (c) UPS spectrum of **UiO@Dansyl**. (d) UPS spectrum of folic acid.

Table S1. Detection of FA in human serum samples.

Background (mol L^{-1})	**FA Spiked (mol L^{-1})**	**FA Found (mol L^{-1})***	**Recovery (%)**	**RSD (%) (n=3)**
2.09×10^{-6}	8.0×10^{-5}	7.63	95.4	0.54
	1.5×10^{-5}	1.6×10^{-5}	101.3	1.56
	1.6×10^{-6}	1.7×10^{-6}	108.2	6.74

* Excluding background.

Table S2. Detection of FA in human urine samples.

Background (mol L^{-1})	**FA Spiked (mol L^{-1})**	**FA Found (mol L^{-1})***	**Recovery (%)**	**RSD (%) (n=3)**
1.22×10^{-6}	8.0×10^{-5}	8.1×10^{-5}	101.00	0.42
	1.5×10^{-5}	1.6×10^{-5}	106.7	1.31
	1.6×10^{-6}	1.7×10^{-6}	106.2	6.58

* Excluding background.

Table S3. Fluorescence lifetime of **UiO@Dansyl** before and after addition of FA (λ_{ex} = 336 nm), pulsed diode laser).

Volume of FA (μL)	a_1	a_2	τ_1 (ns)	τ_2 (ns)	$< \tau >^*$ (ns)	χ^2
0	0.555	0.944	2.033	14.634	14.942	1.121
300	0.139	0.860	0.929	10.926	9.525	1.093

Average lifetime $< \tau >^* = a_1\tau_1 + a_2\tau_2$

Table S4. Comparison of FA concentration obtained by UV-Vis and fluorescence spectroscopy.

Sl. No.	**FA Spiked (mol L^{-1})**	**Concentration of FA Found by UV-Vis Spectroscopy (mol L^{-1})***	**Concentration of FA Found by Fluorescence Spectroscopy (mol L^{-1})**	**Recovery (%) of FA by Fluorescence Spectroscopy**
1	6.49×10^{-5}	6.53×10^{-5}	6.47×10^{-5}	99.6
2	4.42×10^{-5}	4.44×10^{-5}	4.31×10^{-5}	97.4
3	2.26×10^{-5}	2.27×10^{-5}	2.26×10^{-5}	100.2

Table S5. Calculated HOMO and LUMO energy of Linker and all competitive analytes.

Analyte	**HOMO (eV)**	**LUMO (eV)**
H_2BDC-NH-SO_2-dansyl	-2.405759874	-6.211818392
Folic acid	-2.526306376	-6.344610024
Tryptophan	-0.037551732	-6.316310168
Arginine	0.656066854	-7.458372626
Proline	-0.320278178	-7.66273024
Aspertic acid	0.148030016	-7.580007584
Cystine	-0.456607292	-7.073875544
Cysteine	-0.431844918	-6.852374748
Glutamine	-0.268848632	-6.77291746
Histidine	-0.102586978	-7.215919052
Ascorbic acid	-0.25306602	-7.452930346
Alpha keto glutaric acid	-0.980154628	-7.74844615
Citric acid	-0.865594634	-7.594973854
Uric acid	-0.943963466	-7.338642466
Glucose	7.161768366	-8.123691356
Fructose	7.477420606	-7.98110362

Table S6. Comparison of various probes previously reported in the literature for the detection of folic acid.

Sl. No.	Sensor Material	Analytical Method	Sample	Response Time	LOD	Linear Range	Reusability	Ref.
1	**UiO@Dansyl**	**fluorometric**	**tablets, serum, urine**	**< 5 s**	**1.20 nM**	**2×10^{5}-8.2 nM**	**yes**	**this work**
2	Fe_3O_4–ZnS:Mn^{2+}/SiO_2–NH_2	fluorometric	serum	10 min	21.70 nM	0.2-11.3 μM	no	2
3	MOF-$AgClO_4$-abtz	fluorometric	serum, plasma	5 min	49 nM	0.1–30 μM	no	3
4	MIP on dual-color CdTe QDs	fluorometric	blood plasma	3 min	32.00 nM	0.5–20 μM	no	4
5	Au/Ag NCs	fluorometric	serum, urine and tablet	5 min	0.47 nM	1–100 μM	no	5
6	Eu-MOF	fluorometric	tablet	-	0.30 μM	0.25–12.5 μM	no	6
7	Aconitic acid derived carbon dots	fluorometric	tablet, Food supplements	1 min	0.04 μM	1–100 μM	no	7
8	Ultrasonic extraction	capillary electrophoresis with chemiluminescence	tablets, apple juices, human urine	-	20.00 nM	10-0.005 μM	-	8
9	ion pair-based dispersive liquid−liquid microextraction	high performance liquid chromatography	flour, egg yolk, orange juice	-	4.53-9.2 nM	2.2−453 nM	no	9
10	Mn-SnO_2/GCE	electrochemical	tablets	-	0.079 μM	0.5-500 μM	yes	10
11	$NiTiO_3$/CPE	electrochemical	tablets, urine	-	2.90 nM	0.01–10.69 μM	no	11
12	Graphene modified electrode	electrochemical	tablets, urine	-	0.025 μM	0.90–8.52 μM	no	12
13	MB/ERGO/GCE	electrochemical	tablets	-	0.5 μM	4.00–167 μM	no	13
14	Pt:Co/IL/CPE	electrochemical	tablet, food supplements	-	40.0 nM	0.1–500 μM	no	14
15	CuONs/MWCNTs/GCE	electrochemical	tablet	450 s	15.0 nM	0.01–0.90 μM	no	15

References:

1. X. She, J. Wu, H. Xu, J. Zhong, Y. Wang, Y. Song, K. Nie, Y. Liu, Y. Yang and M. T. F. Rodrigues, High efficiency photocatalytic water splitting using 2D α-Fe2O3/g-C3N4 Z-scheme catalysts, *Adv. Energy Mater.*, 2017, **7**, 1700025.
2. X. Li and L. Chen, Fluorescence probe based on an amino-functionalized fluorescent magnetic nanocomposite for detection of folic acid in serum, *ACS Appl. Mater. Interfaces*, 2016, **8**, 31832-31840.
3. B. Yang, X. Li, L. Wang, J. An, T. Wang, F. Zhang, B. Ding and Y. Li, A water-stable MOF-AgClO4-abtz as fluorescent sensor for detection of folic acid based on inner filter effect, *Talanta*, 2020, **217**, 121019.
4. A. A. Ensafi, P. Nasr-Esfahani and B. Rezaei, Simultaneous detection of folic acid and methotrexate by an optical sensor based on molecularly imprinted polymers on dual-color CdTe quantum dots, *Anal. Chim. Acta*, 2017, **996**, 64-73.
5. S. L. Fereja, P. Li, J. Guo, Z. Fang, Z. Zhang, Z. Zhuang, X. Zhang, K. Liu and W. Chen, Silver-enhanced fluorescence of bimetallic Au/Ag nanoclusters as ultrasensitive sensing probe for the detection of folic acid, *Talanta*, 2021, **233**, 122469.
6. K. F. Kayani and K. M. Omer, A red luminescent europium metal organic framework (Eu-MOF) integrated with a paper strip using smartphone visual detection for determination of folic acid in pharmaceutical formulations, *New J. Chem.*, 2022, **46**, 8152-8161.
7. J. Qian, F. Quan, F. Zhao, C. Wu, Z. Wang and L. Zhou, Aconitic acid derived carbon dots: Conjugated interaction for the detection of folic acid and fluorescence targeted imaging of folate receptor overexpressed cancer cells, *Sens. Actuators B Chem.*, 2018, **262**, 444-451.
8. S. Zhao, H. Yuan, C. Xie and D. Xiao, Determination of folic acid by capillary electrophoresis with chemiluminescence detection, *J. Chromatogr. A*, 2006, **1107**, 290-293.
9. Y. Nojavan, M. Kamankesh, F. Shahraz, M. Hashemi and A. Mohammadi, Ion pair-based dispersive liquid–liquid microextraction followed by high performance liquid chromatography as a new method for determining five folate derivatives in foodstuffs, *Talanta*, 2015, **137**, 31-37.
10. N. Lavanya, E. Fazio, F. Neri, A. Bonavita, S. Leonardi, G. Neri and C. Sekar, Electrochemical sensor for simultaneous determination of ascorbic acid, uric acid and folic acid based on Mn-SnO2 nanoparticles modified glassy carbon electrode, *J. Electroanal. Chem.*, 2016, **770**, 23-32.
11. M. Mollaei, S. M. Ghoreishi and A. Khoobi, Electrochemical investigation of a novel surfactant for sensitive detection of folic acid in pharmaceutical and biological samples by multivariate optimization, *Measurement*, 2019, **145**, 300-310.
12. E. Senthilkumar, A. M. Shanmugharaj, R. Suresh Babu, G. Sivagaami Sundari, K. Thileep Kumar, S. Raghu and R. Kalaivani, Development of constructed nanoporous graphene-modified electrode for electrical detection of folic acid, *J. Mater. Sci. Mater. Electron.*, 2019, **30**, 13488-13496.
13. D. Zhang, X. Ouyang, W. Ma, L. Li and Y. Zhang, Voltammetric determination of folic acid using adsorption of methylene blue onto electrodeposited of reduced graphene oxide film modified glassy carbon electrode, *Electroanalysis*, 2016, **28**, 312-319.
14. T. Jamali, H. Karimi-Maleh and M. A. Khalilzadeh, A novel nanosensor based on Pt: Co nanoalloy ionic liquid carbon paste electrode for voltammetric determination of vitamin B9 in food samples, *LWT - Food Sci. Technol.*, 2014, **57**, 679-685.

15. X. Wang, Z. You, Y. Cheng, H. Sha, G. Li, H. Zhu and W. Sun, Application of nanosized gold and graphene modified carbon ionic liquid electrode for the sensitive electrochemical determination of folic acid, *J. Mol. Liq.*, 2015, **204**, 112-117.