# **Supporting Information**

Synthesis of C<sub>3</sub>-symmetric Triazine based Derivatives: Study their AIEE, Mechanochromic Behaviours, Detection of Picric acid and Uric acid in Aqueous Medium

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### **Experimental section**

### **Materials and Methods**

All the chemicals and reagents used in this work were analytical grade. 4-Methoxy phenylboronic acid and 4-bromo thiophenol were purchased from the spectrochem, trifluoromethanesulfonic acid purchased from Sigma Aldrich, bis(pinacolato)diboron, 4-bromo aniline, 4-bromo benzonitrile, purchased from Alfa Aesar and all the other dry solvents purchased from Merck. The <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded on Brucker (Avance) 300 and 400 MHz NMR instrument using TMS as an internal standard, CDCl<sub>3</sub> as a solvent. Chemical shifts are given in parts per million ( $\delta$ -scale) and the coupling constants are given in Hertz. Silica gel-G plates (Merck) were used for TLC analysis with a mixture of n-hexane and ethyl acetate as an eluent. The HPLC spectra were recorded on SHIMADZU instrument, solvent mixture is acetonitrile and methanol (90:10), dual pump mode, flow rate 1 ml/ min. Column chromatography was carried out in silica gel (60-120 mesh) using n-hexane and ethyl acetate as an eluent. UV-Vis spectrum of the synthesized compounds was recorded in JASCO (V-630) spectrophotometer and emission spectra were obtained by JASCO (F-8500) fluorescence spectrophotometer. The sample was kept in a 3ml quartz cuvette to get the emission spectra. The stock solution (10<sup>-3</sup> M) of the synthesized compounds were prepared in a 3ml of individual solvents (polar and non-polar solvents) after that 20µL of the stock solution was taken into 2ml of solvents placed in a 3ml cuvette, and the total concentration of samples were 10µM for the solvatochromism spectra in both absorbance and emission spectroscopy. In aggregation studies, the stock solution (10<sup>-3</sup>M) of the **TZNET** was prepared by taking 0.0028g in 2ml of THF solvent. THF and water fraction were used in the aggregation studies, 20µL of stock solution was taken into 2ml of total THF and water fraction, and the final concentration of the solution is 10μM. Then, the experiment was carried out in selectivity and competitive studies of 1 equiv. of the probe and 3 equiv. of analyte.

### General procedure for Suzuki Miyaura coupling and trimerization reaction

Aromatic halide (1 equiv.), boronate ester compound (1.2 equiv.), Pd(PPh<sub>3</sub>)<sub>4</sub> (0.05 equiv.), K<sub>2</sub>CO<sub>3</sub> (2 equiv.) was dissolved in DMF/H<sub>2</sub>O and heated the reaction mixture to 90°C and maintained for about overnight. After completion of the reaction, the resulting mixture was

passed through the celite bed, washed with ethyl acetate and water. The organic layer was further washed with a saturated brine solution and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography using petroleum ether/ethyl acetate as an eluent. Two necked RB flask containing aromatic cyano compound in chloroform stirring at 0°C under a nitrogen atmosphere and then dropwise addition of trifluoromethanesulfonic acid into the solution, once the addition was completed the mixture was warmed into the room temperature and stirred for about overnight. After the completion of the reaction, the mixture was poured into solid ice cubes, neutralized with ammonium hydroxide to form a precipitate. The precipitate was filtered and washed with water and diethyl ether three times. Then the product was dried in a vacuum oven at 55°C to afford the desired product.

## Synthetic procedure of triazine based fluorophores

Scheme S1. Synthetic route of target TZOME.

**Reagent and Conditions:** (a) Pd(PPh<sub>3</sub>)<sub>4</sub>, K<sub>2</sub>CO<sub>3</sub>, DMF/H<sub>2</sub>O (1:1), 80°C, (b) triflic acid, CHCl<sub>3</sub>, RT.

Scheme S2. Synthetic route of target TZSET

**Reagent and Conditions:** (a) bromoethane, DMF, K<sub>2</sub>CO<sub>3</sub>, 60°C, (b) Bis(pinacolato) diboron, Pd(dppf)Cl<sub>2</sub>. CH<sub>2</sub>Cl<sub>2</sub>, 1,4 dioxane, KOAc, 80°C, overnight, (c) Pd(PPh<sub>3</sub>)<sub>4</sub>, K<sub>2</sub>CO<sub>3</sub>, DMF/H<sub>2</sub>O (1:1), 80°C, (d) triflic acid, CHCl<sub>3</sub>, RT.

Scheme S3. Synthetic route of target TZNET

**Reagent and Conditions:** (a) bromoethane, DMF, K<sub>2</sub>CO<sub>3</sub>, 60°C, (b) Bis(pinacolato) diboron, Pd(dppf)Cl<sub>2</sub>. CH<sub>2</sub>Cl<sub>2</sub>, 1,4 dioxane, KOAc, 80°C, overnight, (c) Pd(PPh<sub>3</sub>)<sub>4</sub>, K<sub>2</sub>CO<sub>3</sub>, DMF/H<sub>2</sub>O (1:1), 80°C, (d) triflic acid, CHCl<sub>3</sub>, RT.

# Synthetic procedures for triazine based fluorophores Synthesis of 2,4,6-tris(4'-methoxy-[1,1'-biphenyl]-4-yl)-1,3,5-triazine (TZOME)

To a Schlenck tube containing 4-bromobenzonitrile 0.50g (2.7 mmol), 4-methoxyphenylboronic acid 0.50g (3.2 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> 32mg (0.02 mmol), K<sub>2</sub>CO<sub>3</sub> 0.57g (4.12 mmol) were dissolved in DMF/H<sub>2</sub>O and heated the reaction mixture to 90°C and maintained for overnight. After completion of the reaction, the resulting mixture was passed through the celite bed, washed with ethyl acetate and water. The organic layer was further washed with a saturated brine solution and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography using petroleum ether/ethyl acetate as an eluent. The white color solid powder was obtained. The yield is 80%. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.70 (d, J = 8.6 Hz, 2H), 7.64 (d, J = 8.7 Hz, 2H), 7.55 (d, J = 8.9 Hz, 2H), 7.01 (d, J = 8.9 Hz, 2H), 3.87 (s, 3H). Two neck RB containing compound 1 0.5g (2.38 mmol) in 10 ml of chloroform stirring at 0°C under a nitrogen

atmosphere and then dropwise addition of trifluoromethanesulfonic acid (1 mL) into the solution, an addition was completed, the mixture was warmed into the room temperature and stirred for overnight. After the completion of the reaction, the mixture was poured into solid ice cubes, neutralized with ammonium hydroxide to form a precipitate. The precipitate was filtered and washed with water and diethyl ether. Hereafter the product was dried in a vacuum oven at 55°C to afford the product. Yield is 85%. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.74 (d, J = 8.3 Hz, 2H), 7.78 (d, J = 8.4 Hz, 2H), 7.64 (d, J = 8.6 Hz, 2H), 7.01 (d, J = 8.6 Hz, 2H), 3.88 (s, 3H). <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ : 160.73, 145.63, 132.87, 131.95, 128.68, 127.46, 119.28, 115.02, 110.65, 55.75. HR-MS m/z (TZOME + NH<sub>4</sub>) calcd. 645.2866, found 645.2889.

### Synthesis of 2,4,6-tris(4'-(ethylthio)-[1,1'-biphenyl]-4-yl)-1,3,5-triazine (TZSET)

4-Bromothiophenol 1.0g (5.28 mmol), bromoethane 0.7g (0.67 mmol), potassium carbonate 1.0g (7.88 mmol) were added to the Schlenck tube and dissolved in dry DMF (5 ml) and it was heated at 100°C for about 7 hrs. After the completion of the reaction, the mixture was poured into the solid ice, extracted with ethyl acetate and washed with brine, dried over sodium sulphate and concentrated, finally purified by column chromatography using n-hexane as an eluent. Colourless liquid was obtained with 90% of yield. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.39 (d, J = 8.6 Hz, 2H), 7.17 (d, J = 8.6 Hz, 2H), 2.91 (q, J = 7.4 Hz, 2H), 1.30 (t, J = 7.4 Hz, 3H).

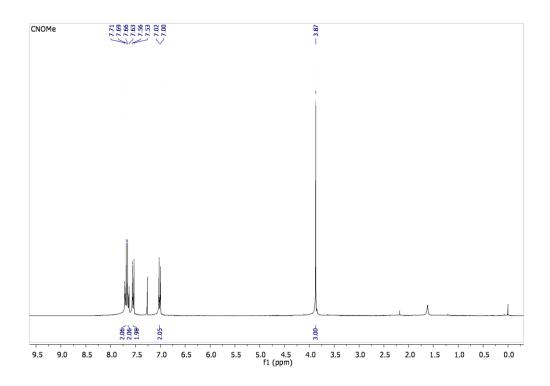
To a Schlenck tube containing (4-bromophenyl)(ethyl)sulfane 1.0g (4.60 mmol), bis (pinacolato)diboron 2.3g (9.21 mmol), Pd(dppf)Cl<sub>2</sub>. CH<sub>2</sub>Cl<sub>2</sub> 75 mg (0.09 mmol), was dissolved in dioxane (7 ml) and then potassium acetate 1.14g (11 mmol) was added as a base and heated the reaction mixture to 80°C and maintained for overnight. After completion of the reaction, the resulting mixture was passed through the celite bed, washed with ethyl acetate and water. The organic layer was further washed with a saturated brine solution and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The crude material was purified by column chromatography using petroleum ether/ethyl acetate as an eluent. The white color solid powder was obtained with a yield of 65%. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.71 (d, J = 8.3 Hz, 2H), 7.27 (d, J = 8.1 Hz, 2H), 2.98 (q, J = 7.3 Hz, 2H), 1.33 (s, 12H), 1.26 (t, J = 7.1 Hz, 3H).

The compound **5** was synthesized by following a procedure similar to the compound **1** synthesis. White color solid powder product obtained with 75% of yield. <sup>1</sup>H NMR (300 MHz,

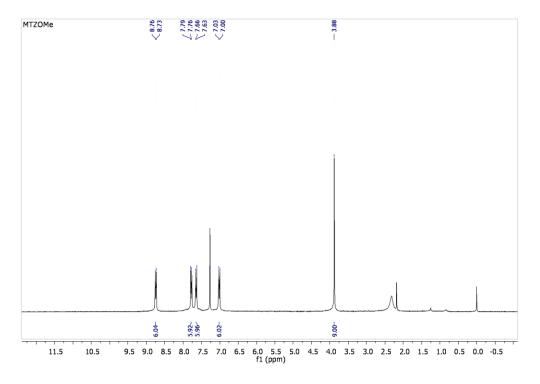
CDCl<sub>3</sub>)  $\delta$ : 7.72 (d, J = 8.5 Hz, 2H), 7.66 (d, J = 8.5 Hz, 2H), 7.52 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.5 Hz, 2H), 3.01 (q, J = 7.4 Hz, 2H), 1.37 (t, J = 7.4 Hz, 3H). **TZSET** was synthesized by following the procedure similar to **TZOME**. The pale green solid product was obtained with the yield of 80%. <sup>1</sup>H NMR (300 MHz, DMSO + CDCl<sub>3</sub>)  $\delta$ : 8.76 (d, J = 8.1 Hz, 6H), 7.81 (d, J = 8.3 Hz, 6H), 7.65 (d, J = 7.8 Hz, 6H), 7.37 (d, J = 8.1 Hz, 6H), 2.98 (q, J = 7.3 Hz, 6H), 1.29 (t, J = 7.2 Hz, 9H). <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ : 148.52 (s), 146.01 (s), 132.87 (s), 128.47 (s), 126.47 (s), 112.21 (s), 44.80 (s), 12.98 (s). HRMS m/z (TZSET+Na) calcd 740.2204, found 740.2189.

### 4',4''',4''''-(1,3,5-triazine-2,4,6-triyl)tris(N,N-diethyl-[1,1'-biphenyl]-4-amine) (TZNET)

The compound **5** was synthesized by following the procedure similar to compound **2**. Colourless liquid was attained by 90% of yield.  $^{1}$ H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.68 (d, J = 9.0 Hz, 2H), 6.66 (d, J = 9.0 Hz, 2H), 3.33 (q, J = 7.1 Hz, 4H), 1.16 (t, J = 7.1 Hz, 6H). The compound **6** was synthesized by following the procedure similar to compound **3**. White color solid was obtained with the yield of 60%.  $^{1}$ H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.45 (d, J = 9.0 Hz, 2H), 6.47 (d, J = 9.0 Hz, 2H), 3.42 (q, J = 7.1 Hz, 4H), 1.32 (s, 12H), 1.19 (t, J = 7.1 Hz, 6H). The compound **7** was synthesized by following the procedure similar to compound **1** to get white color solid with the yield of 80%.  $^{1}$ H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$ : 7.64 (d, 4H), 7.51 (d, J = 9.0 Hz, 2H), 6.76 (d, J = 9.0 Hz, 2H), 3.45 (q, J = 7.1 Hz, 4H), 1.23 (t, J = 7.1 Hz, 6H). The compound **TZNET** was synthesized by following a procedure similar to the compound **TZOME** to get red color solid product with 80% of yield.  $^{1}$ H NMR (400 MHz, DMSO)  $\delta$ : 8.85 (d, J = 11.6 Hz, 6H), 8.00 (d, J = 8 Hz, 12H), 7.54 (d, J = 8 Hz, 6H), 3.47 (q, 12H), 1.06 (t, J = 6.9 Hz, 18H).  $^{13}$ C NMR (100 MHz, DMSO)  $\delta$ : 153.38, 146.14, 133.58, 133.21, 128.80, 120.71, 114.85, 112.83, 97.65, 44.18, 12.89. HRMS m/z (TZSET+H) calcd 751.4488, found 751.4408.



**Figure S1.** <sup>1</sup>H NMR spectrum of compound 1.



**Figure S2.** <sup>1</sup>H NMR spectrum of TZOME.

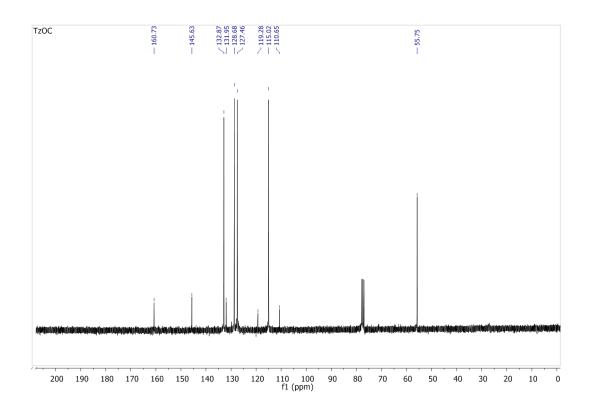
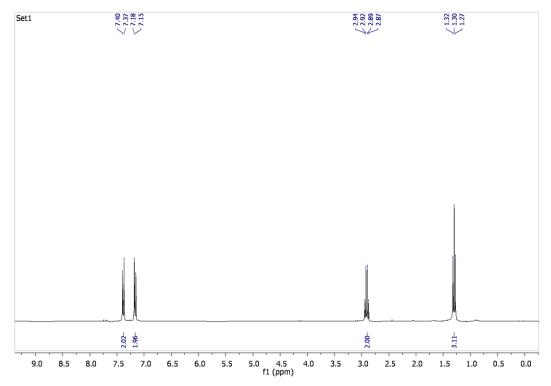
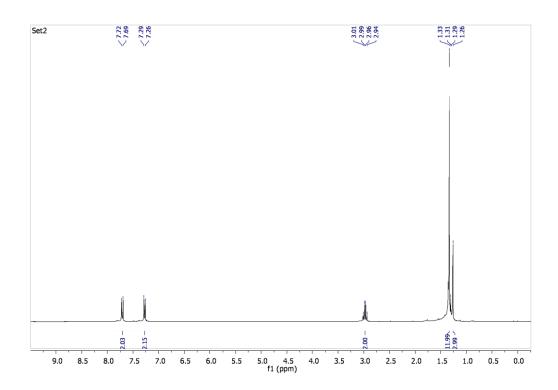


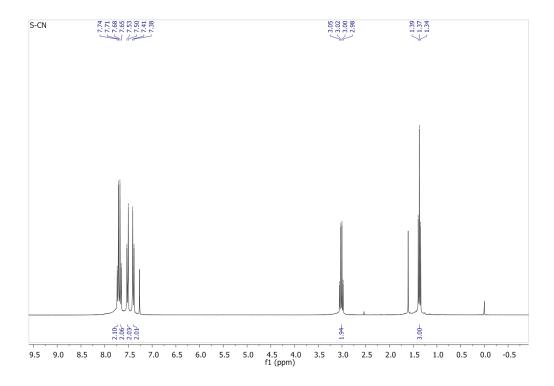
Figure S3. <sup>13</sup>C NMR spectrum of TZOME



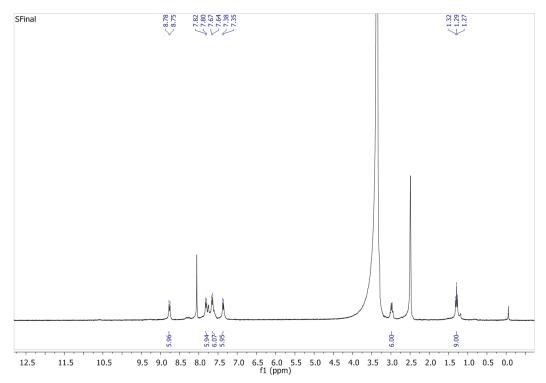
**Figure S4.** <sup>1</sup>H NMR spectrum of compound 2.



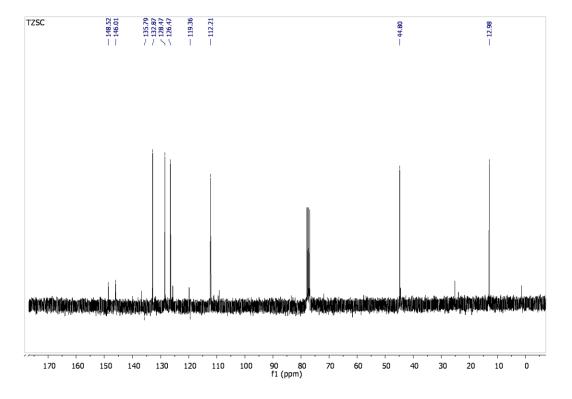
**Figure S5.** <sup>1</sup>H NMR spectrum of compound 3.



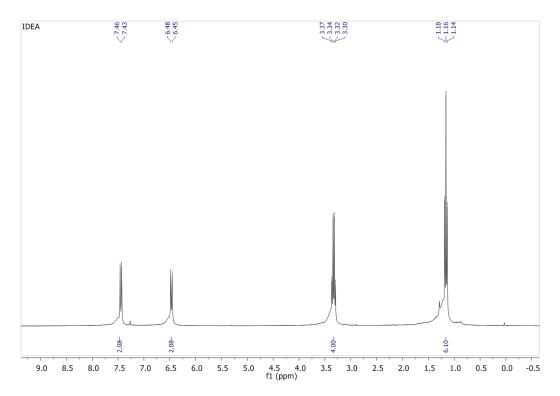
**Figure S6.** <sup>1</sup>H NMR spectrum of compound 4.



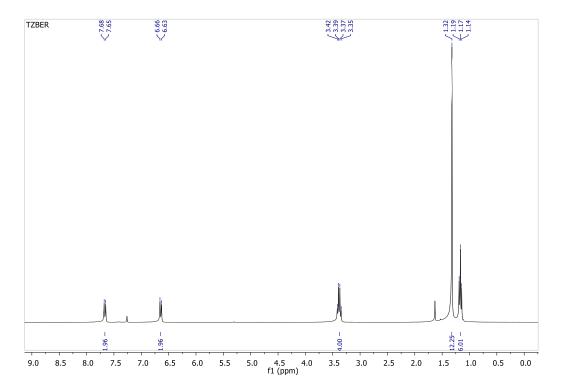
**Figure S7.** <sup>1</sup>H NMR spectrum of TZSET.



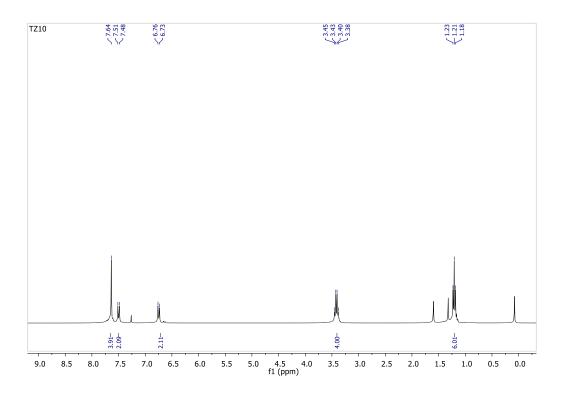
**Figure S8.** <sup>13</sup>C NMR spectrum of TZSET.



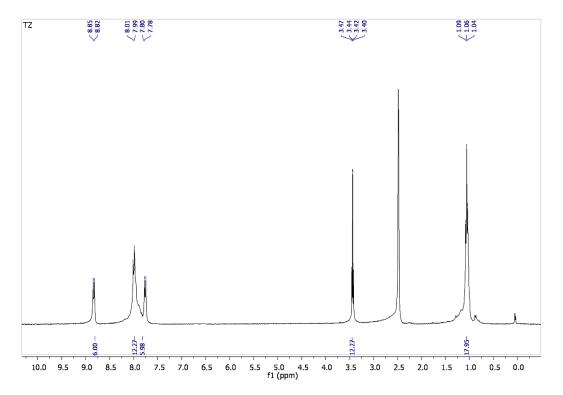
**Figure S9.** <sup>1</sup>H NMR spectrum of compound 5.



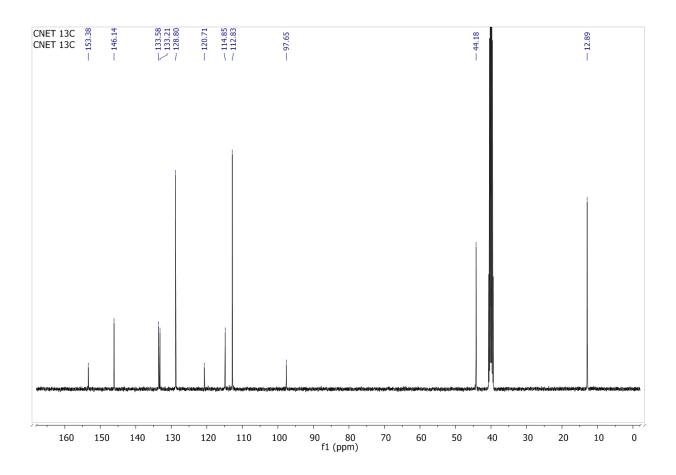
**Figure S10.**  $^{1}$ H NMR spectrum of compound 6



**Figure S11.** <sup>1</sup>H NMR spectrum of compound 7.



**Figure S12.** <sup>1</sup>H NMR spectrum of TZNET



**Figure S13.** <sup>13</sup>C NMR spectrum of TZNET

		Display	Report		
Analysis Info				Acquisition Date 5/19/201	9 1:06:57 PM
Method Sample Name Comment	tune_wide.m TZOME			Operator IIT_R Instrument maXis Impact	000000.00000
Acquisition Par	rameter				
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus Scan Begin	Not active 50 m/z	Set Capillary Set End Plate Offset	4500 V -500 V	Set Dry Heater Set Dry Gas	180 °C 4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C

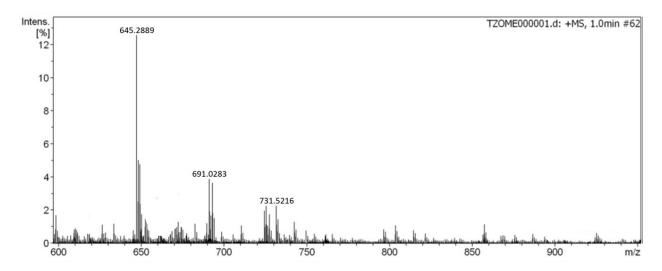


Figure S14. HR-MS spectrum of TZOME

		Display	Report		
Analysis Info				Acquisition Date 5/19/2019	9 12:42:57 PM
Method Sample Name Comment	tune_wide.m TZSET			Operator IIT_R Instrument maXis Impact	000000.00000
Acquisition Par	rameter				
Source Type Focus Scan Begin Scan End	ESI Not active 50 m/z 3000 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 0 V 0 nA	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	0.4 Bar 180 °C 4.0 l/min Source 0 °C

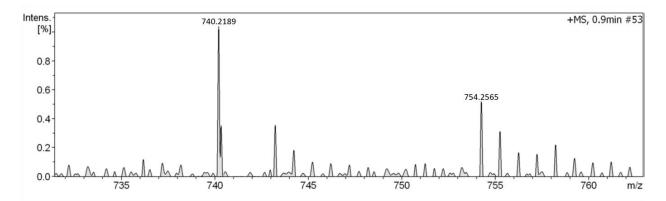


Figure S15. HR-MS spectrum of TZSET

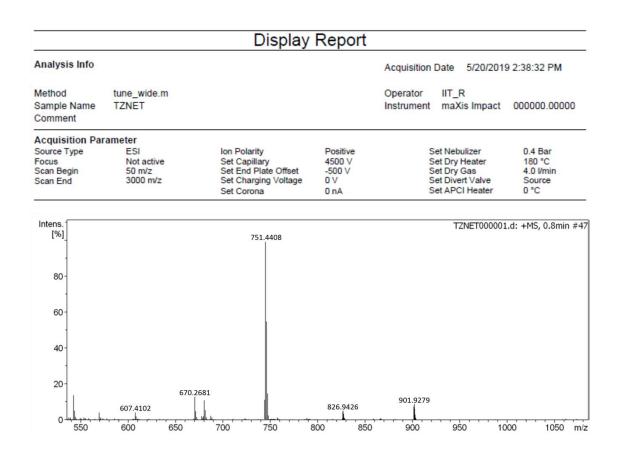


Figure S16. HR-MS spectrum of TZNET

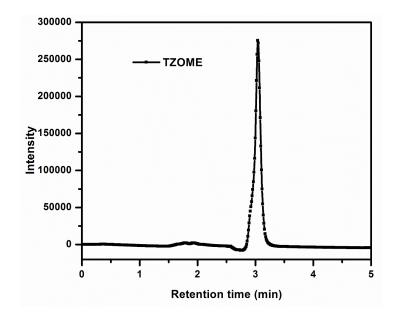


Figure S17. HPLC chromatogram of TZOME

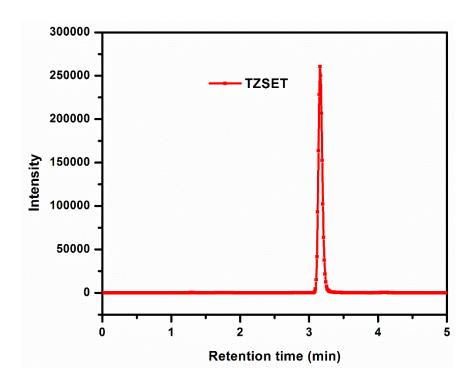
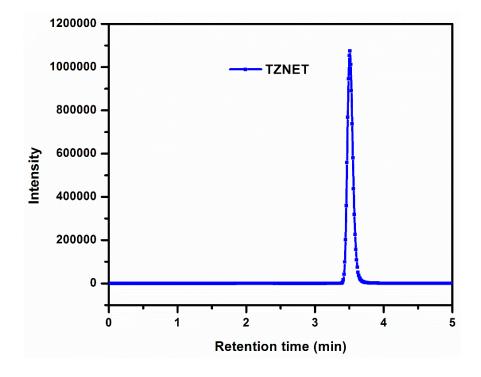


Figure S18. HPLC chromatogram of TZSET



 $\textbf{Figure S19.} \ \textbf{HPLC} \ \textbf{chromatogram} \ \textbf{of} \ \textbf{TZNET}$ 

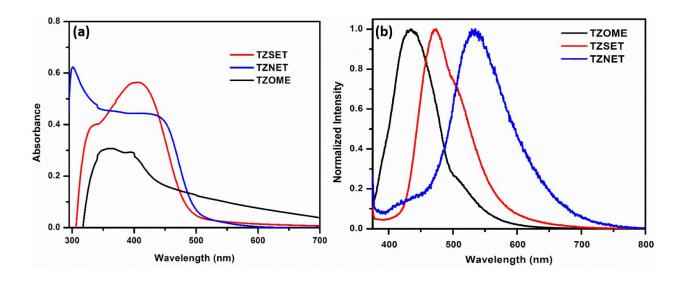


Figure S20. (a) Absorption and (b) emission spectra of triazine based materials in film phase.

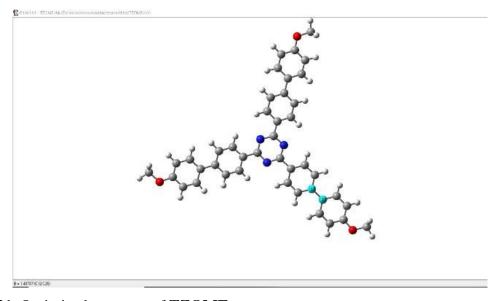


Figure S21. Optimized structure of TZOME

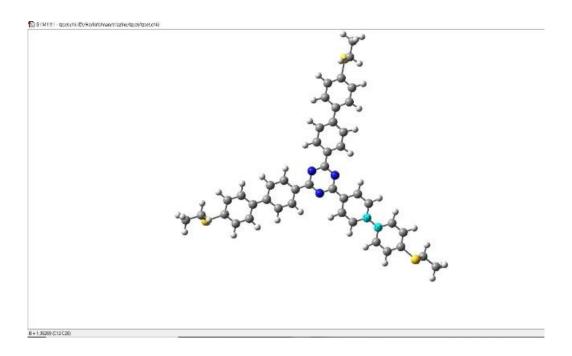


Figure S22. Optimized structure of TZSET

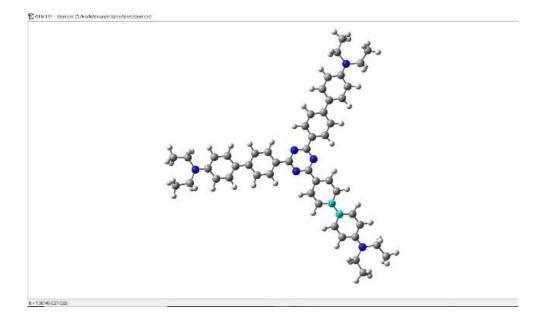


Figure S23. Optimized structure of TZNET

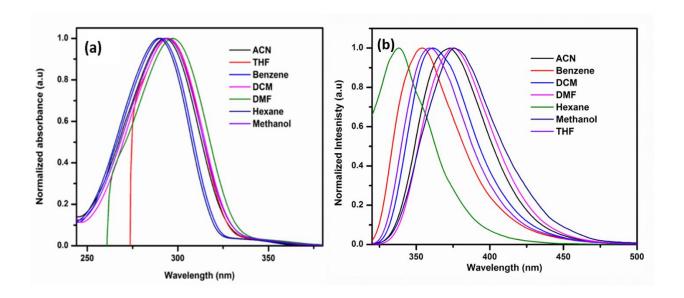


Figure S24. Solvent variation of TZOME in (a) absorbance (b) emission spectra.

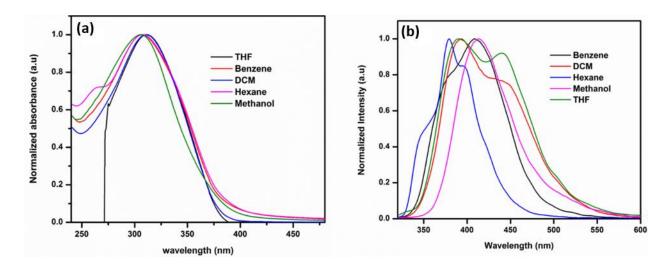


Figure S25. Solvent variation of TZSET in (a) absorbance (b) emission spectra.

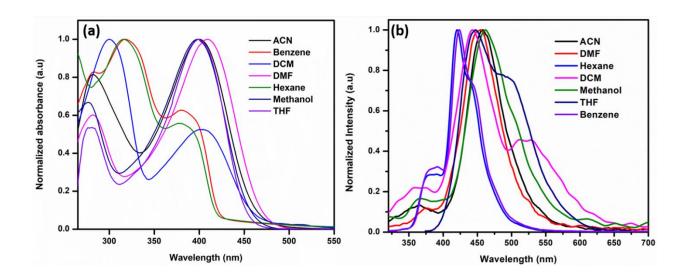


Figure S26. Solvent variation of TZNET in (a) absorbance (b) emission spectra.

Table S1. Photophysical Properties of triazine derivatives in solution and solid phase

S. No	compounds	Solution phase		Film phase		
		$\lambda_{max} (nm)$	$\lambda_{emi}\left(nm\right)$	$\lambda_{max}\left(nm\right)$	$\lambda_{emi} (nm)$	
1.	TZOME	295	358	350	434	
2.	TZSET	312	392	395	472	
3.	TZNET	398	448	441	533	

Table S2. Solvent effect of TZOME

S. No	Solvent	$\lambda_{max} (nm)$	$\lambda_{emi}\left(nm\right)$	Stokes shift (cm <sup>-1</sup> )
1.	Hexane	290	338	4895
2.	Benzene	292	354	6000
3.	ACN	293	372	7240
4	THF	295	358	5960
5.	DCM	296	361	6080
6.	DMF	297	374	6940
7.	Methanol	294	376	7415

Table S3. Solvent effect of TZSET

S. No	Solvent	$\lambda_{max}$ (nm)	$\lambda_{emi} (nm)$	Stokes shift (cm <sup>-1</sup> )
1.	Hexane	308	379	6080
2.	Benzene	307	382	6390
3	THF	312	392	6540
4.	DCM	310	393	6810
5.	Methanol	306	414	8530

Table S4. Solvent effect of TZNET

S. No	Solvent	$\lambda_{max} (nm)$	$\lambda_{max} (nm)$	Stokes shift (cm <sup>-1</sup> )
1.	Hexane	382	419	2310
2.	Benzene	384	422	2342
3.	ACN	401	458	3110
4	THF	398	448	2800
5.	DCM	401	444	2370
6.	DMF	409	455	2470
7.	Methanol	399	463	3460

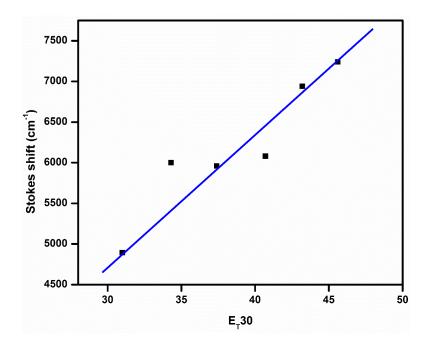


Figure S27. D-R plot of TZOME

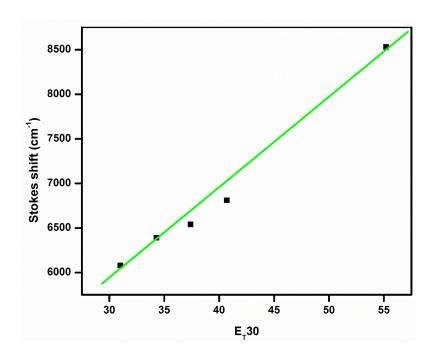


Figure S28. D-R plot of TZSET

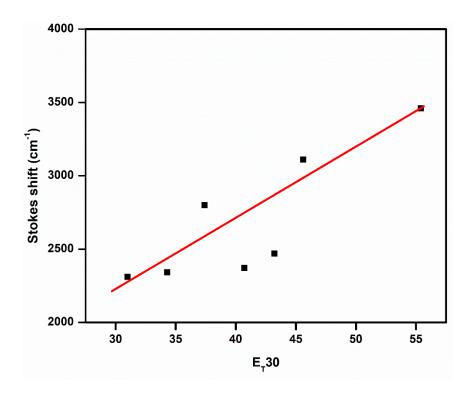


Figure S29. D-R plot of TZNET

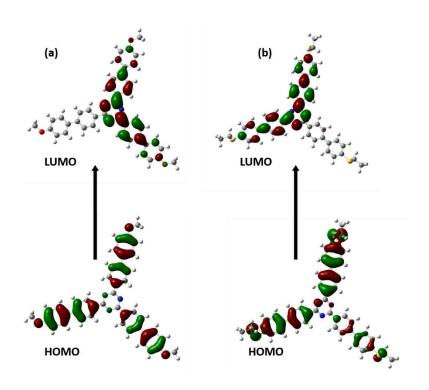


Figure S30. Frontier orbital of the (a) TZOME and (b) TZSET compound

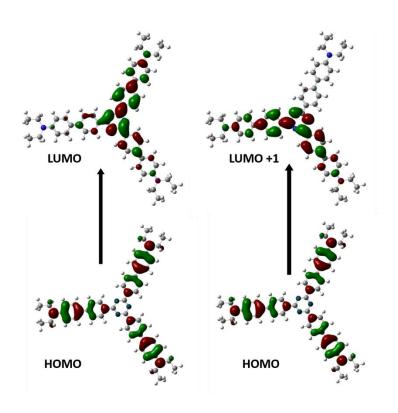


Figure S31. Frontier orbital of the TZNET

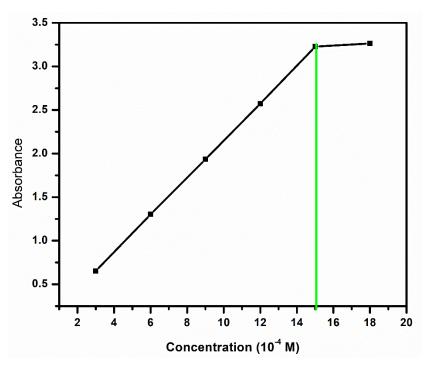


Figure S32. Various concentration of TZOME in THF solvent

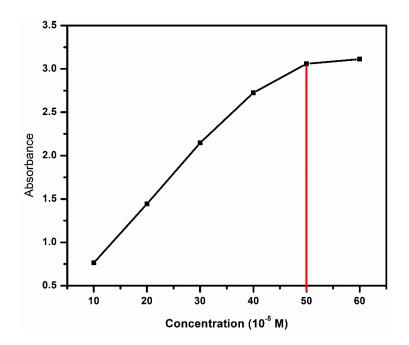


Figure S33. Various concentration of TZSET in THF solvent

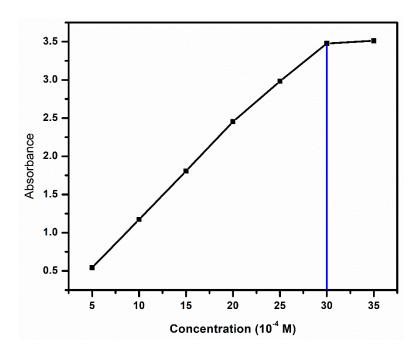


Figure S34. Various concentration of TZNET in THF solvent

# **Limit of Detection (LOD)**

We calculate the limit of detection from emission titration and calculated on the basis of the equation LOD =  $3\sigma/K$  Where K is the slope and slope was derived from a titration curve,  $\sigma$  is the standard division of the blank solutions

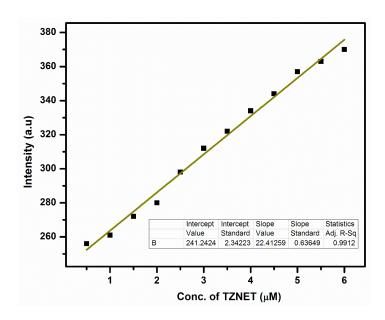


Figure S35. Linear fit of the TZNET

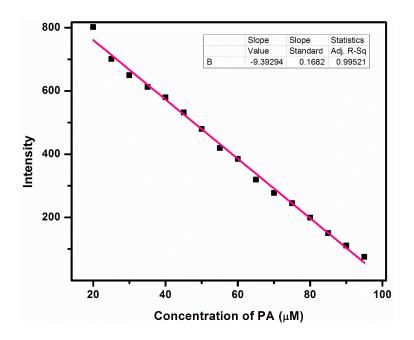


Figure S36. Linear fit of TZNET with PA

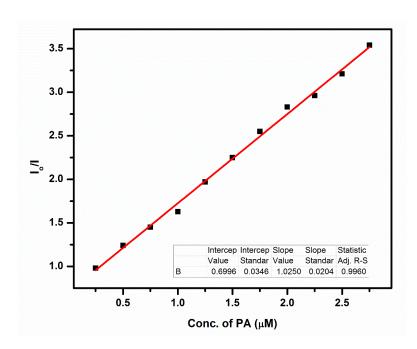


Figure S37. Determination of Stern-Volmer quenching constant of PA with TZNET

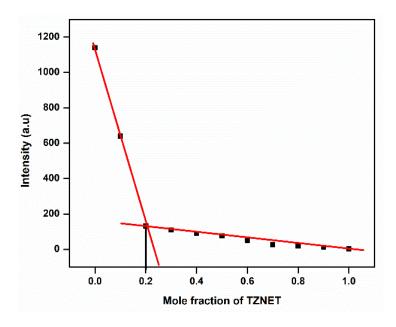


Figure S38. Job's plot of the receptor with PA.

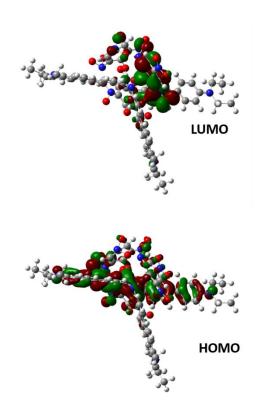
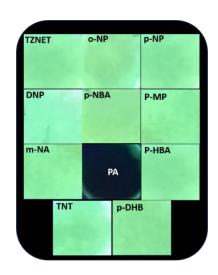
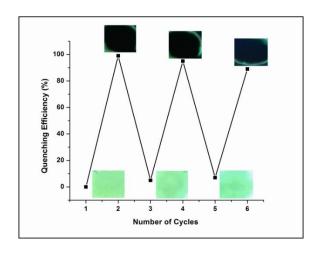


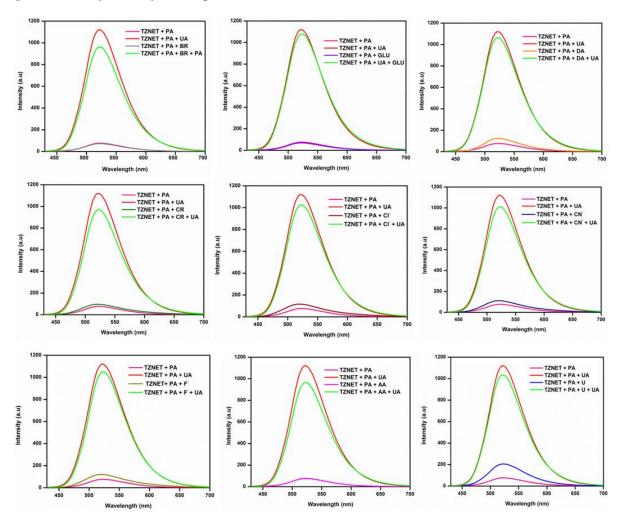
Figure S39. Frontier molecular orbital of TZNET-PA



**Figure S40.** Test strips photograph for the selective sensing of picric acid under 365 nm UV light.



**Figure 41**. Recyclability of the probe with PA



**Figure S42.** Competitive study of **TZNET-PA-UA** with various anions and biomolecules in emission spectra.

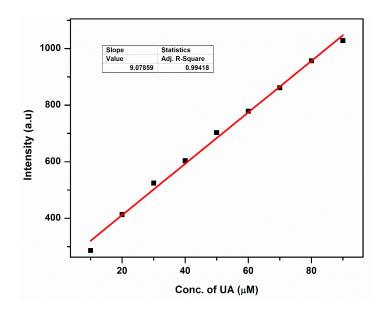


Figure S43. Linear fit of TZNET-PA with UA

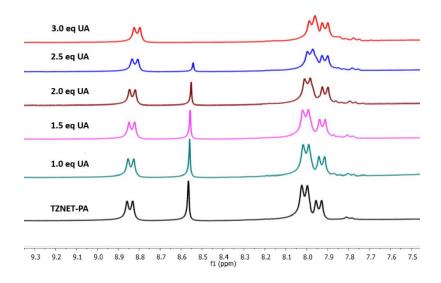


Figure S44. NMR titration spectra of TZNET-PA (10mM: 30mM) with 0 to 30mM of uric acid



Figure S45. Photographic image of grinding and treated with DCM under 365 nm

Table S5. Truth table for receptor with analyte

S. No.	Input TZNET-PA	Input TZNET-PA-UA	Output $\lambda_{\rm emi}$ = 532 nm
1	0	0	0
2	1	0	0
3	0	1	1
4	1	1	1

Table S6. Comparison study of the picric acid with recently reported materials

S.No.	Materials	LOD (nM)	Reference
1	Zn(II)-Coordination Polymer	120	1
2	Zinc(II) based MOF	1820	2
3	Europium(III) based MOF	4890	3
4	Polymer Nanoparticles	26	4
5	Cucurbit[8]uril based MOF	3580	5
6	Supramolecular naphthalimide	12	6
7	Hydrazone-Based	12	7
8	Dy(III)-Based MOF	710	8
9	Triazine based AIEE material	203	This work

**Table S7.** Comparison study of the uric acid with recently reported materials

S.No.	Compounds	LOD (nM)	Reference
1	Pyrene-Functionalized MOF	1400	9
2	MoS <sub>2</sub> based	1170	10
3	Biomimetic MOF	1800	11
4	Phosphonate MOF	1600	12
5	Gold Nanoclusters	1700	13
6	Triazine based AIEE material	209	This work

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