

Electronic supporting information

Different view of solvents effect on the synthesis methods of Zeolitic Imidazolate Framework-8 to tuning the crystal structure and properties

Arezoo Akhundzadeh Tezerjani^a, Rouein Halladj^{a*}, Sima Askari^b

^a Department of Chemical Engineering, Amirkabir University of Technology, Tehran, Tel: 0098-2164543151, Fax: 0098-2166405847.

^b Department of Chemical Engineeringt, Science and Research Branch, Islamic Azad University, Tehran, Iran.

*Corresponding author: Dr. Rouein Halladj; E-mail address: halladj@aut.ac.ir

Table of Contents	Page
Experimental Section	S2
Fig. S1	S3
Fig. S2	S3
Fig. S3	S4
Fig. S4	S4
Fig. S5	S5
Fig. S6	S5
Fig. S7	S6
Fig. S8	S6
Fig. S9	S7
Table S1	S8
Product yield calculation	S8
Reference	S8

Experimental Section

Synthesis ZIF-8 by Mixing method

To prepare the ZIF-8 sample, First, 3 g zinc nitrate hexahydrate ($\text{Zn}(\text{NO}_3)_2$) and 6.6 g 2-methylimidazole (HMIM) were separately dissolved in 50 ml solvent (methanol, DMF, water) and stir until a clear solution was obtained. Then two solutions were stirred for 6 h at ambient temperature and pressure on the magnetic stirrer to give a milky solution. The resulting slurry solution was separated by centrifugation and washed 3 times with methanol to remove unreacted raw materials and impurities. Finally, to dry the resulting product, it was placed in the oven at 120 °C for 12 hours.

Synthesis ZIF-8 by Solvothermal method

To prepare the ZIF-8 sample, First, 3 g zinc nitrate hexahydrate ($\text{Zn}(\text{NO}_3)_2$) and 6.6 g 2-methylimidazole (HMIM) were separately dissolved in 50 ml solvent (methanol, DMF, water) and stir until a clear solution was obtained. Then the two solutions were loaded in 80ml Teflon lined stainless steel autoclave and autoclave was placed in convection oven at 140 °C for 24 hours. The resulting slurry solution was separated by centrifugation and washed 3 times with methanol to remove unreacted raw materials and impurities. Finally, to dry the resulting product, it was placed in the oven at 120 °C for 12 hours.

Synthesis ZIF-8 by Sonochemical method

To prepare the ZIF-8 sample, First, 3 g zinc nitrate hexahydrate ($\text{Zn}(\text{NO}_3)_2$) and 6.6 g 2-methylimidazole (HMIM) were separately dissolved in 50 ml solvent (methanol, DMF, water) and stir until a clear solution was obtained. Then the two solutions were blended and it was held under ultrasonic waves with frequency of 50 Hz and voltage of 200 V with 100% ultrasonic power intensity for one-hour period. Also, the synthesis temperature was maintained by placing the solution in a bath water. The resulting slurry solution was separated by centrifugation and washed 3 times with methanol to remove unreacted raw materials and impurities. Finally, to dry the resulting product, it was placed in the oven at 120 °C for 12 hours.

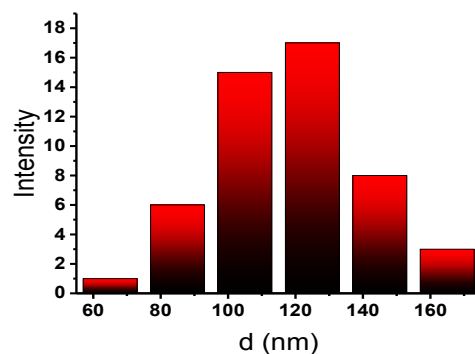
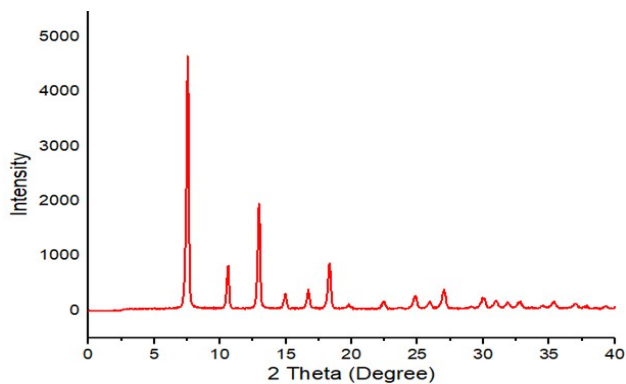
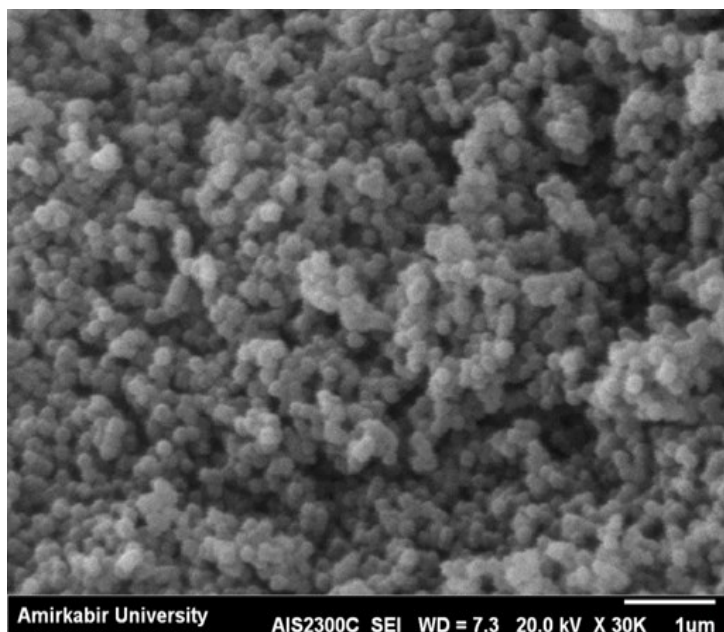


Fig. S1. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in methanol at mixing method.

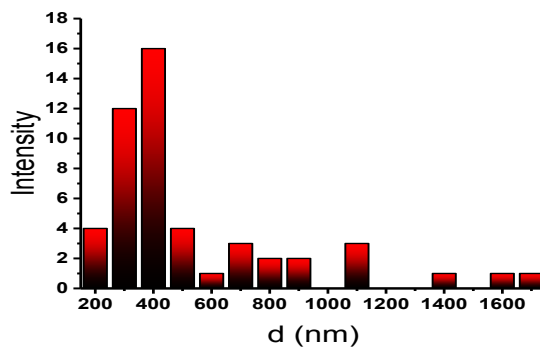
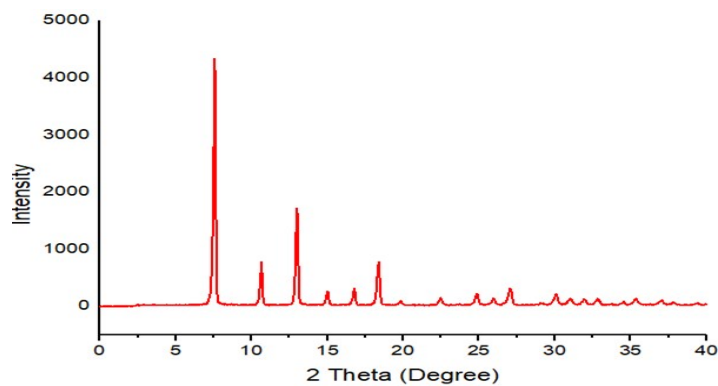
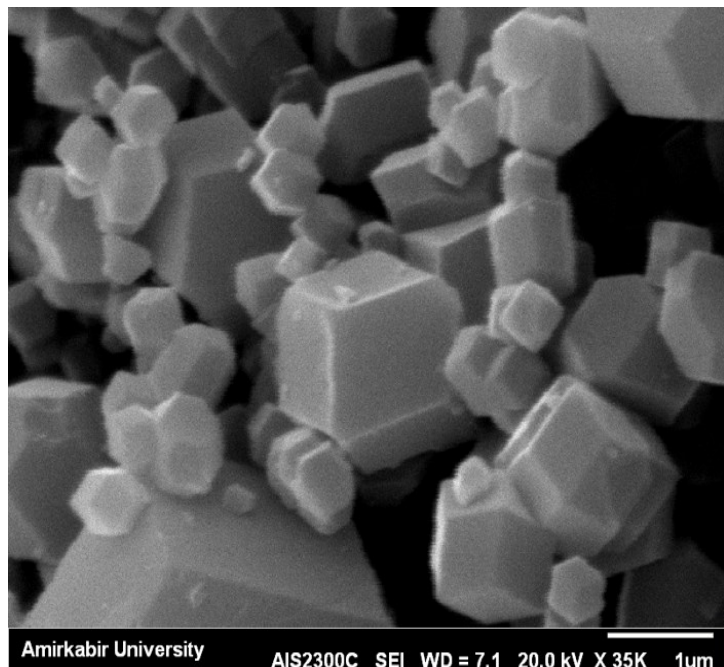


Fig. S2. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in methanol at solvothermal method.

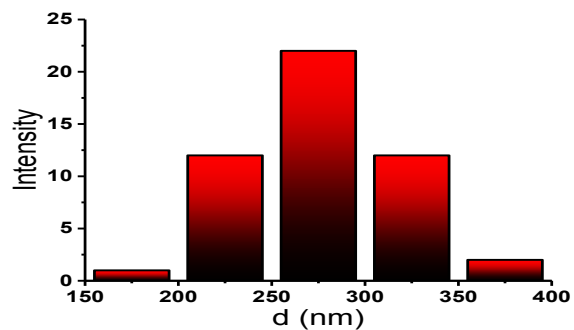
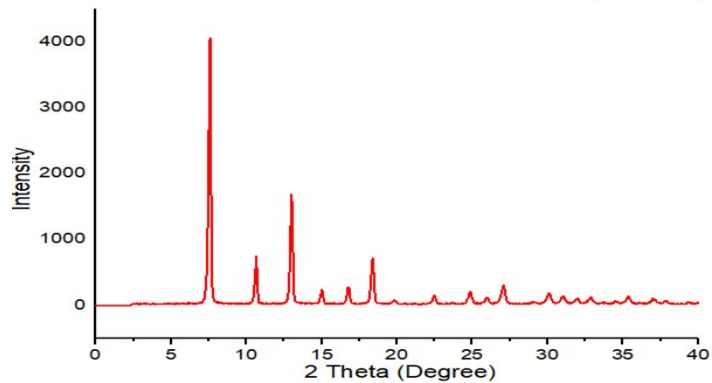
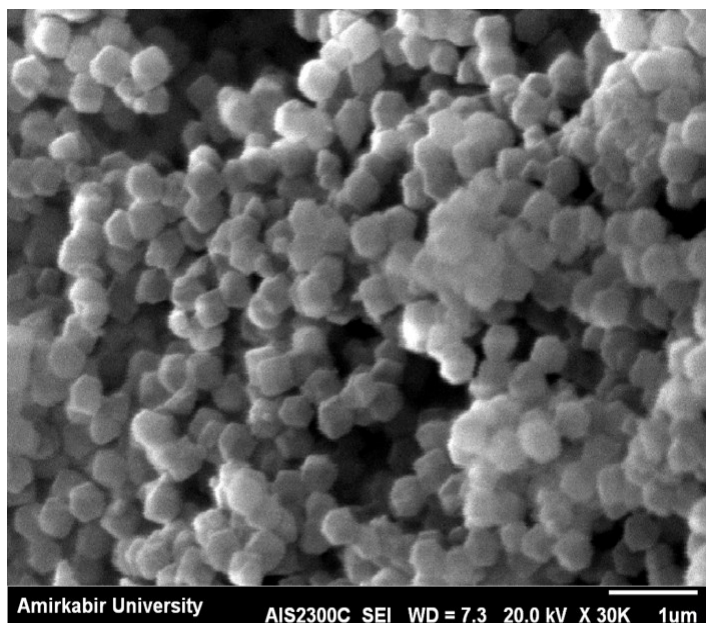


Fig. S3. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in methanol at sonochemical method.

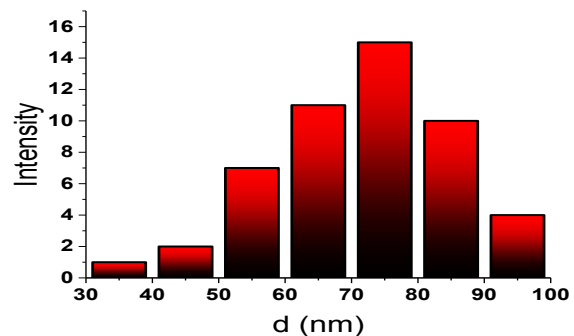
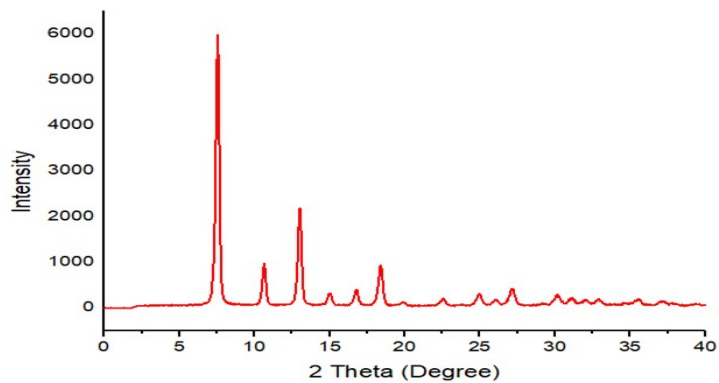
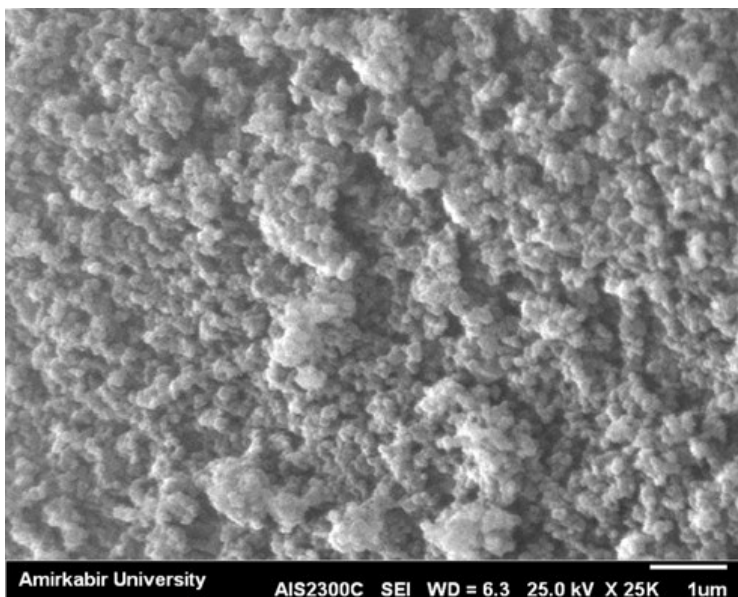


Fig. S4. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in DMF at mixing method.

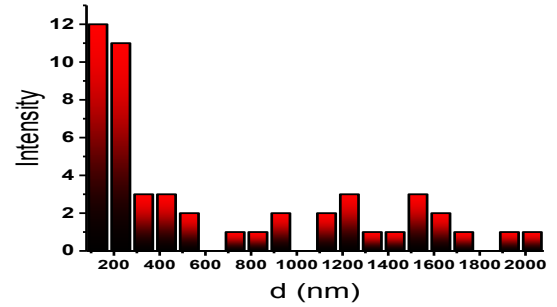
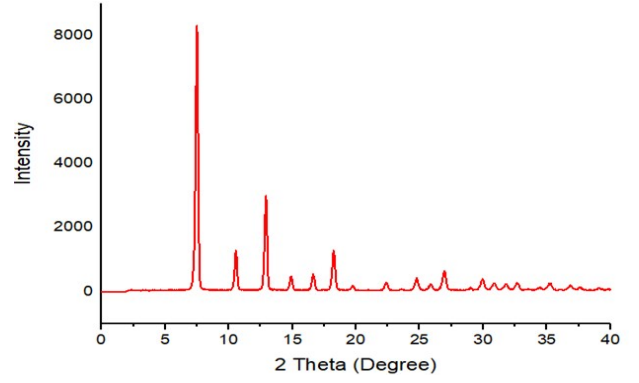
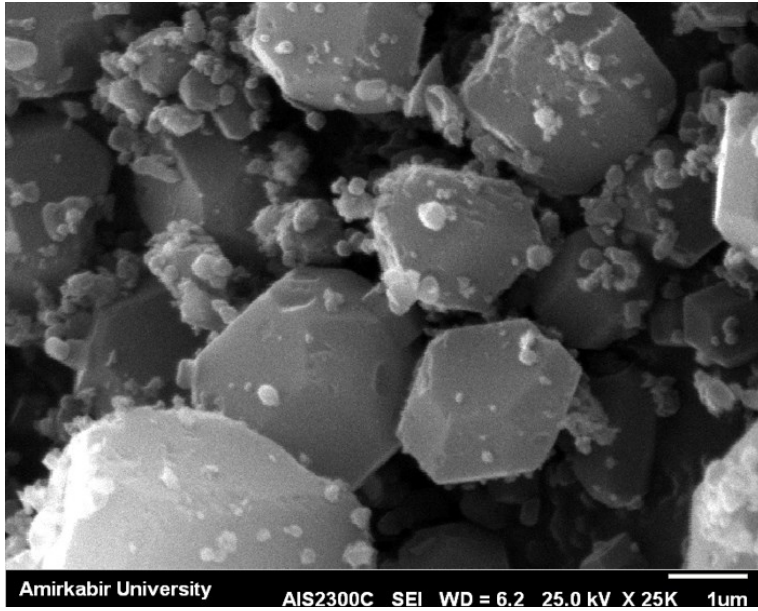


Fig. S5. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in DMF at solvothermal method.

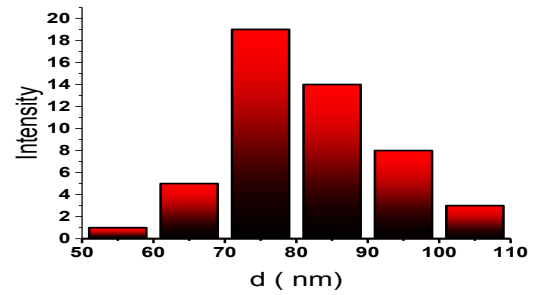
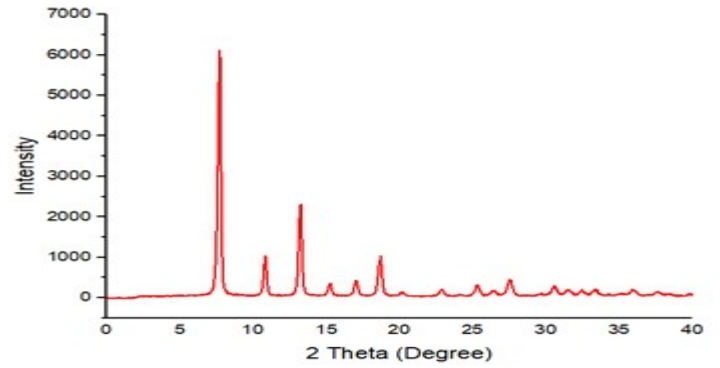
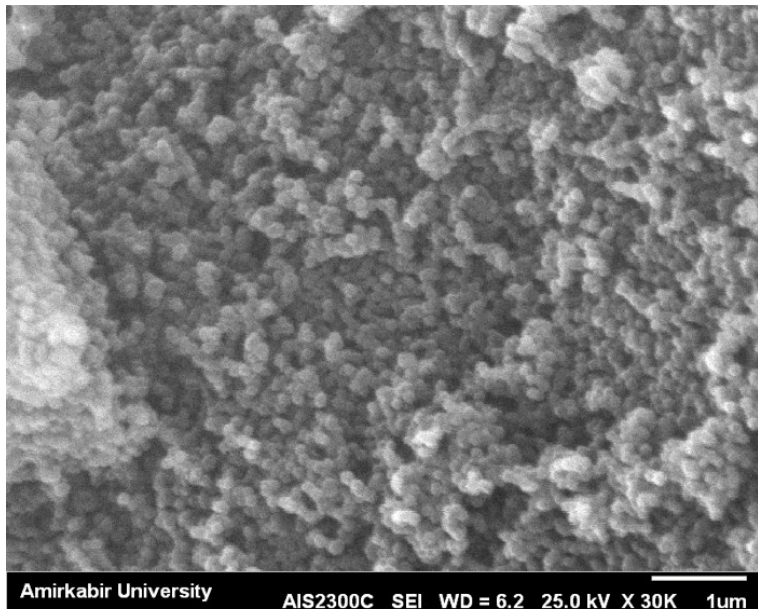


Fig. S6. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in DMF at sonochemical method.

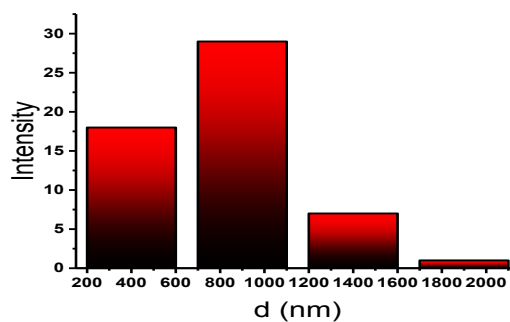
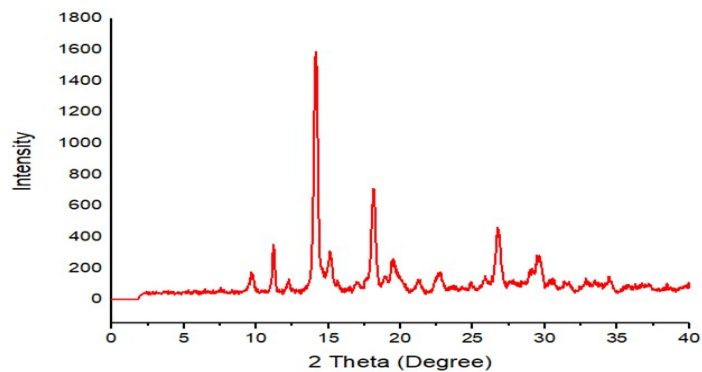
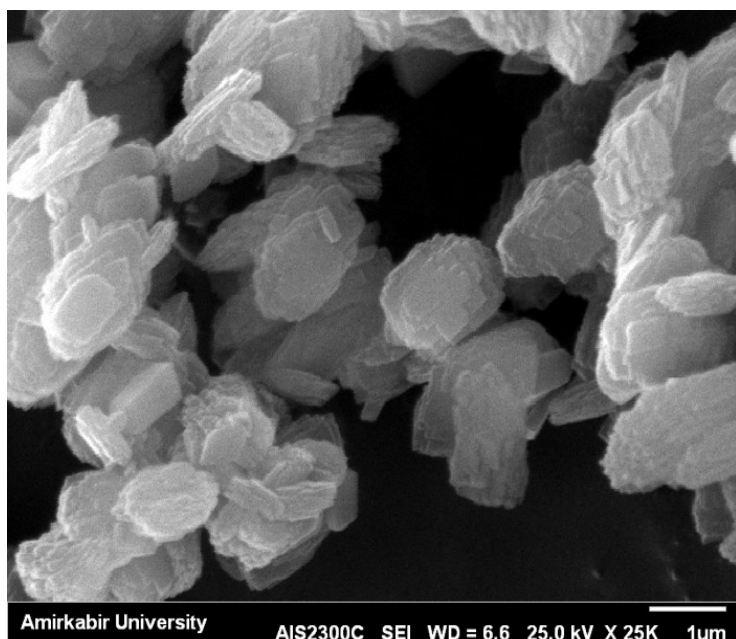


Fig. S7. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in water at mixing method.

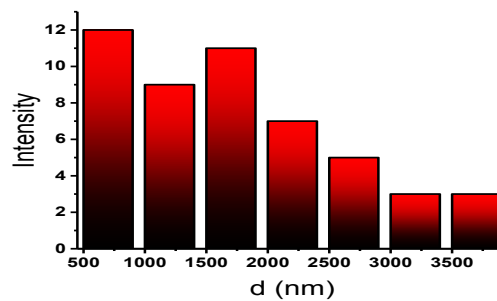
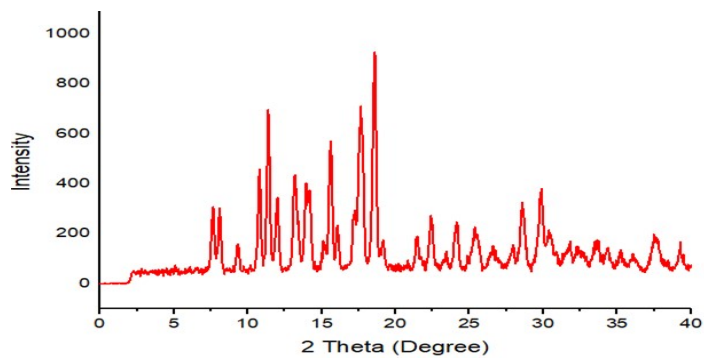


Fig. S8. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in water at solvothermal method.

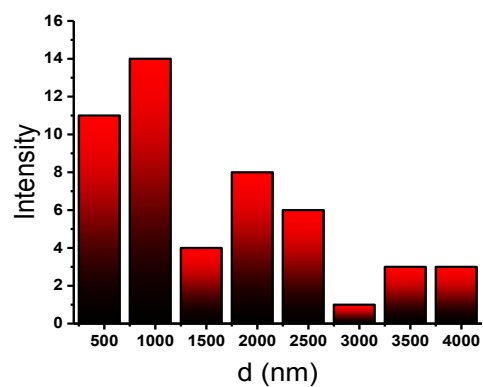
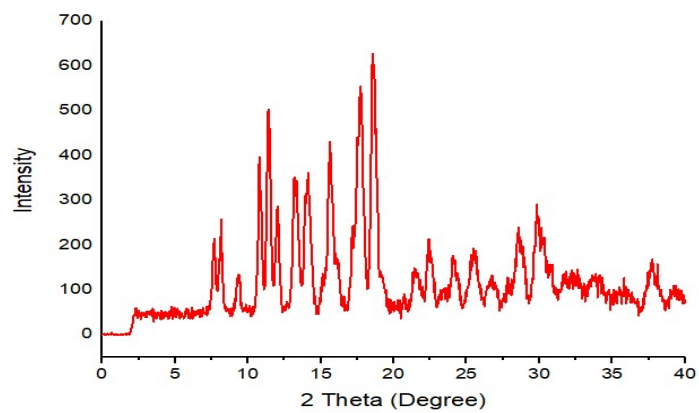


Fig. S9. Sem image, XRD pattern and particle size distribution of ZIF-8 sample synthesized in water at sonochemical method.

Table S1. Dielectric constant, dipole moment, and van der Waals volume for solvents[1].

Solvent	Dielectric constant	Dipole moment(D)	Van der waals volume (cm ³ mol ⁻¹)
MeOH	33	1.70	21.71
DMF	38	3.82	47.67
Water	80	1.85	11.44

Product yield calculation

The product yield is the ratio of the amount of product obtained from experiment to the amount of reactants, according to the following equation:

$$\text{percent of product yield} = \frac{\text{amount of product}}{\text{amount of reactants}} \times 100$$

Reference

- 1- C.-P. Li and M. Du, "Role of solvents in coordination supramolecular systems," Chemical Communications, vol. 47, no. 21, pp. 5958-5972, 2011.