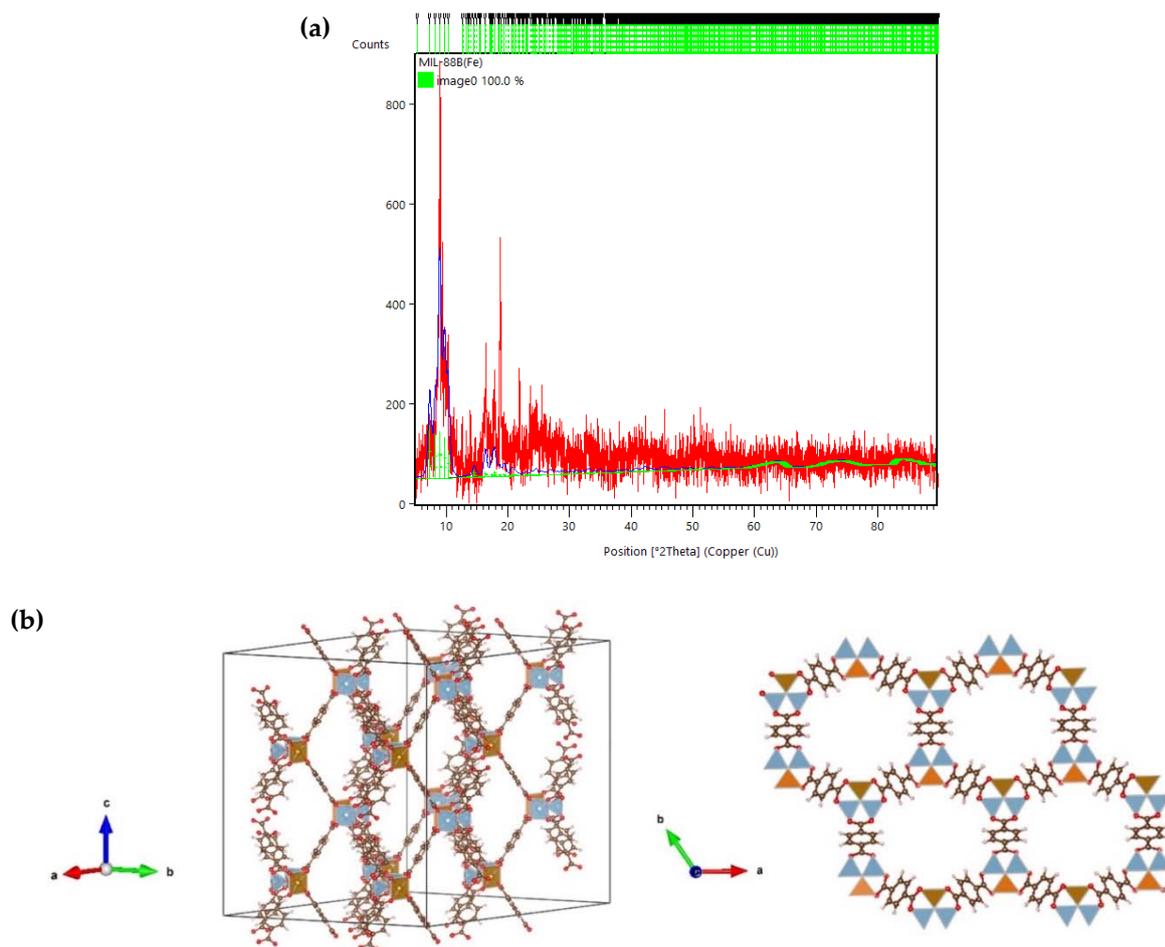


## S1. Rietveld refinement on the XRD pattern of MIL-88B(Fe)



**Figure S1.** (a) Rietveld refinement on the XRD pattern of MIL-88B(Fe) based on the triclinic structure with  $P-1$  space group, and (b) Predicted crystal structure of MIL-88B(Fe), with goodness of fit (defined by  $G = \chi^2$ ) is found at 1.068.

## S2. EDX Spectrum of MIL-88B(Fe)

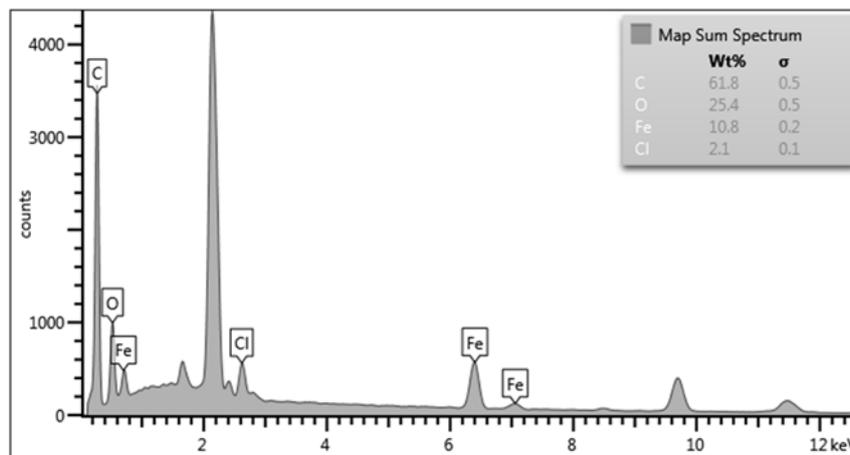
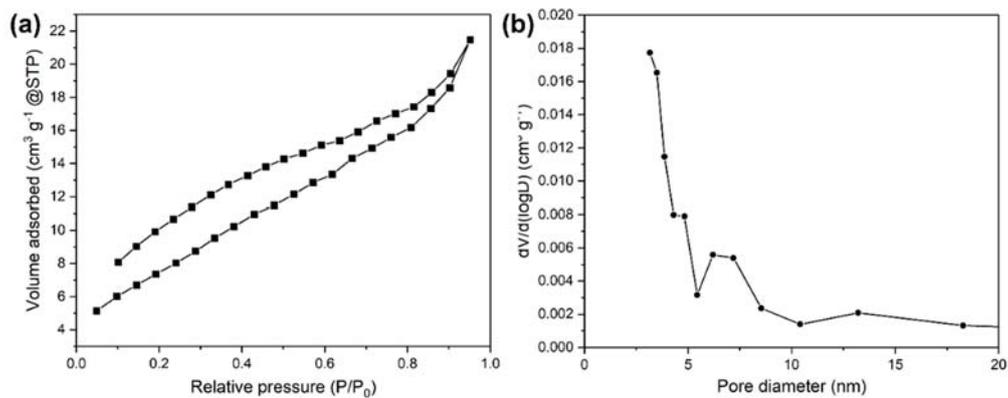


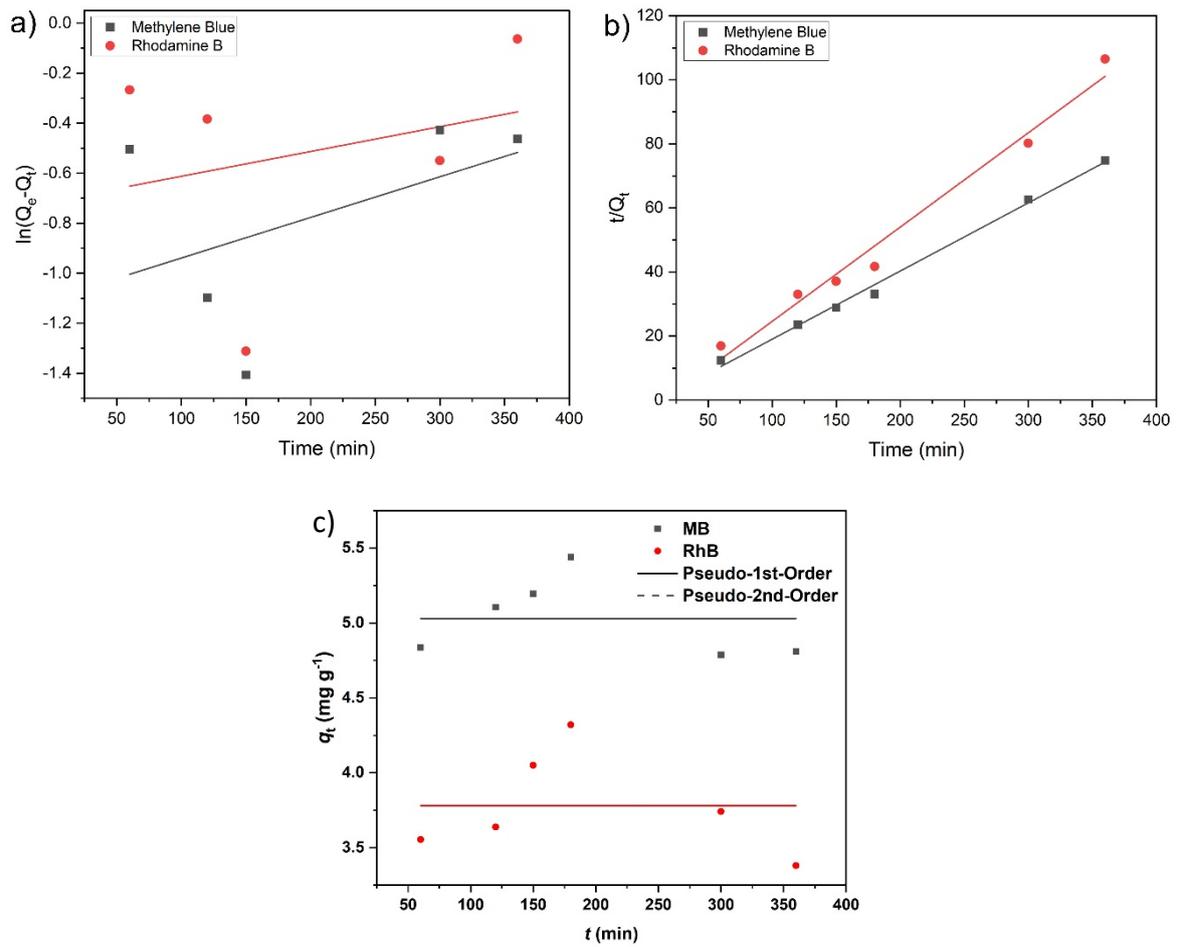
Figure S2. EDX spectrum of MIL-88B(Fe) polycrystalline crystals.

### S3. N<sub>2</sub> physisorption Graphs



**Figure S3.** N<sub>2</sub> physisorption (a) adsorption-desorption isotherm and (b) pore size distribution of MIL-88B(Fe).

#### S4. Comparison between linear and non-linear fitting of the adsorption kinetics



**Figure S3.** The linear-fitting kinetics by pseudo-first order (a) and pseudo-second order (b); also non-linear-fitting kinetics by pseudo-first and pseudo-second order of MB and RhB.