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Supporting Information

Effective Removal of Chemical Warfare Agent Simulants Using Water Stable Metal-Organic Frameworks: Mechanistic Study and Structure-Property Correlation

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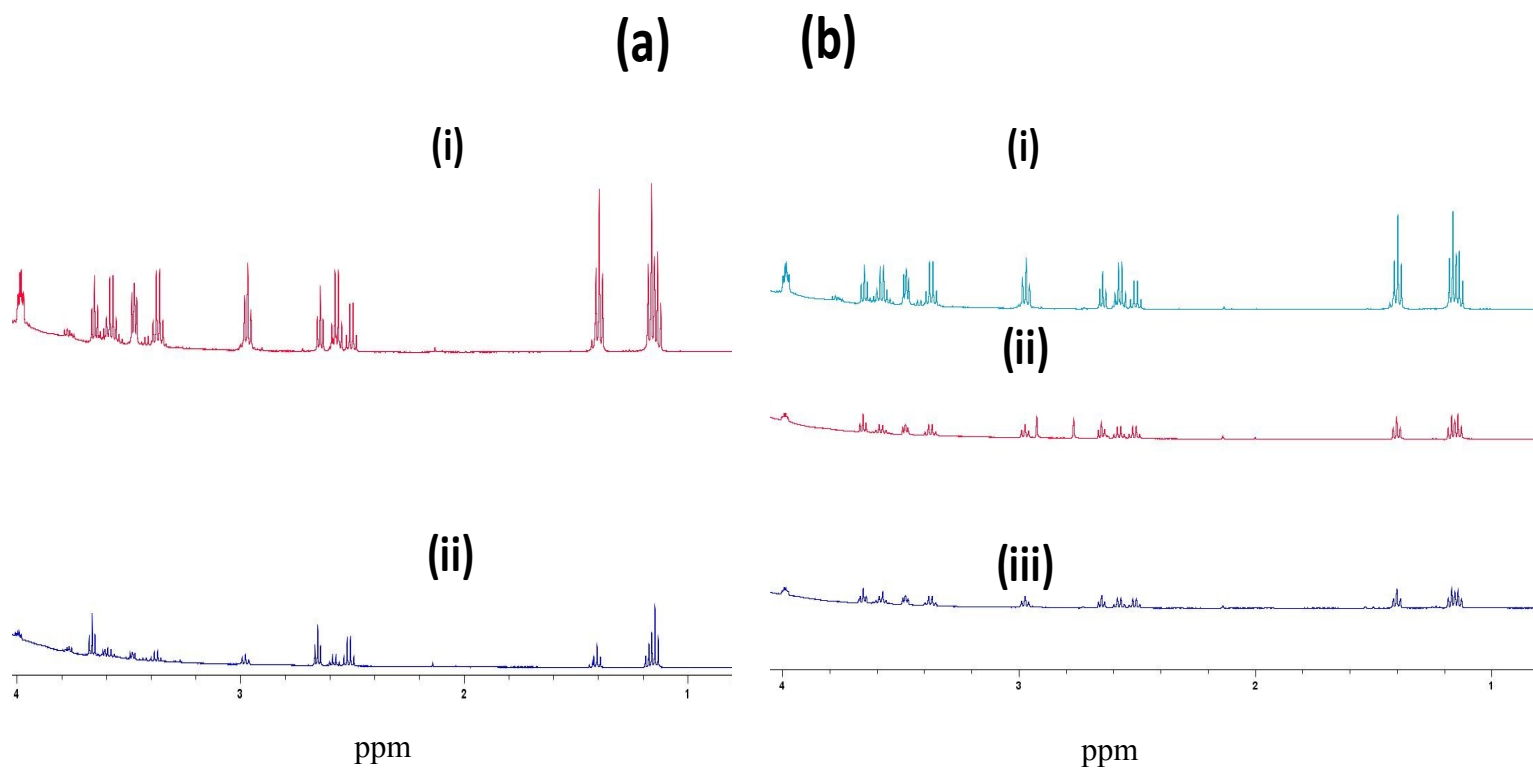
Figure S1. ^{1}H NMR data showing the adsorption of 2-CEES and/or its hydrolysis products in water

(a) (i) Before adsorption with NU-1000 (ii) 30 minutes after the process of adsorption, intensity of every peak decreased considerably.

(b)(i) Before adsorption with UiO-67 (ii) 30 minutes after the process of adsorption .The new peaks may corresponds to the hydrolysis products of 2-CEES (iii) 1 hour after the adsorption process
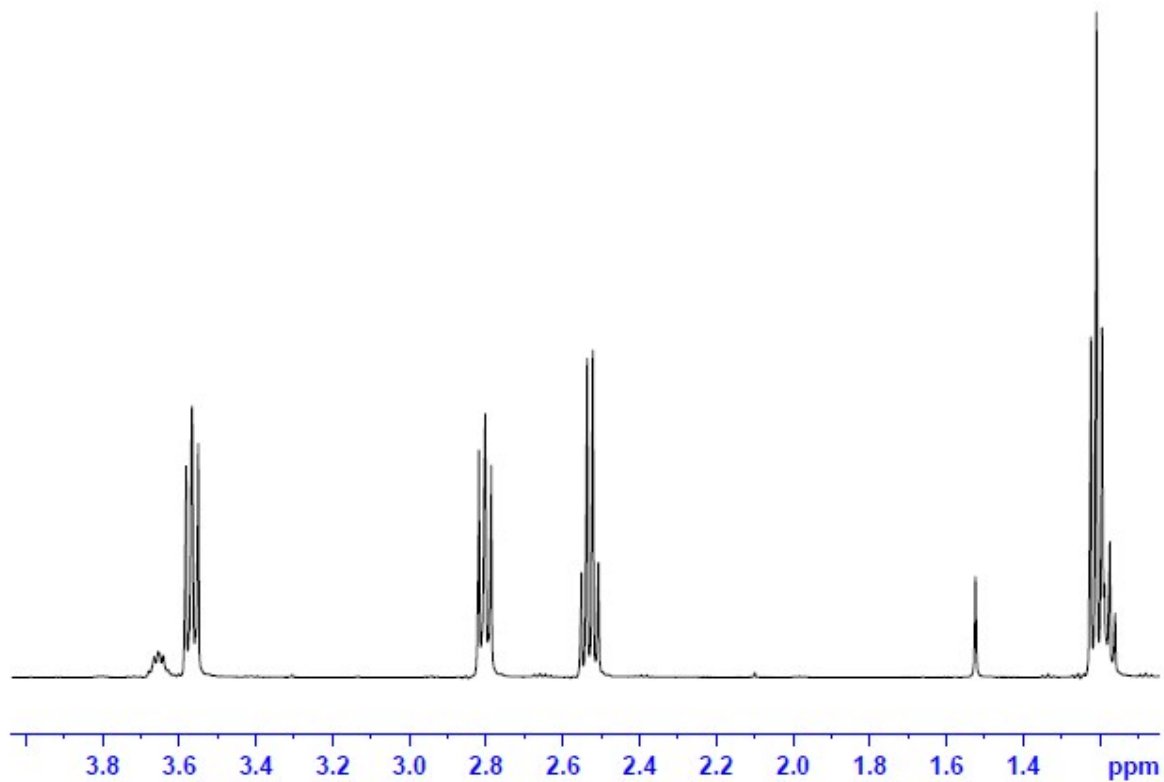
Figure S2. ^{1}H NMR spectrum of 2-CEES in $CHCl_3$ solvent. Note that 2-CEES was not hydrolyzed in $CHCl_3$ solvent

(a)   (b)

(i)   (i)

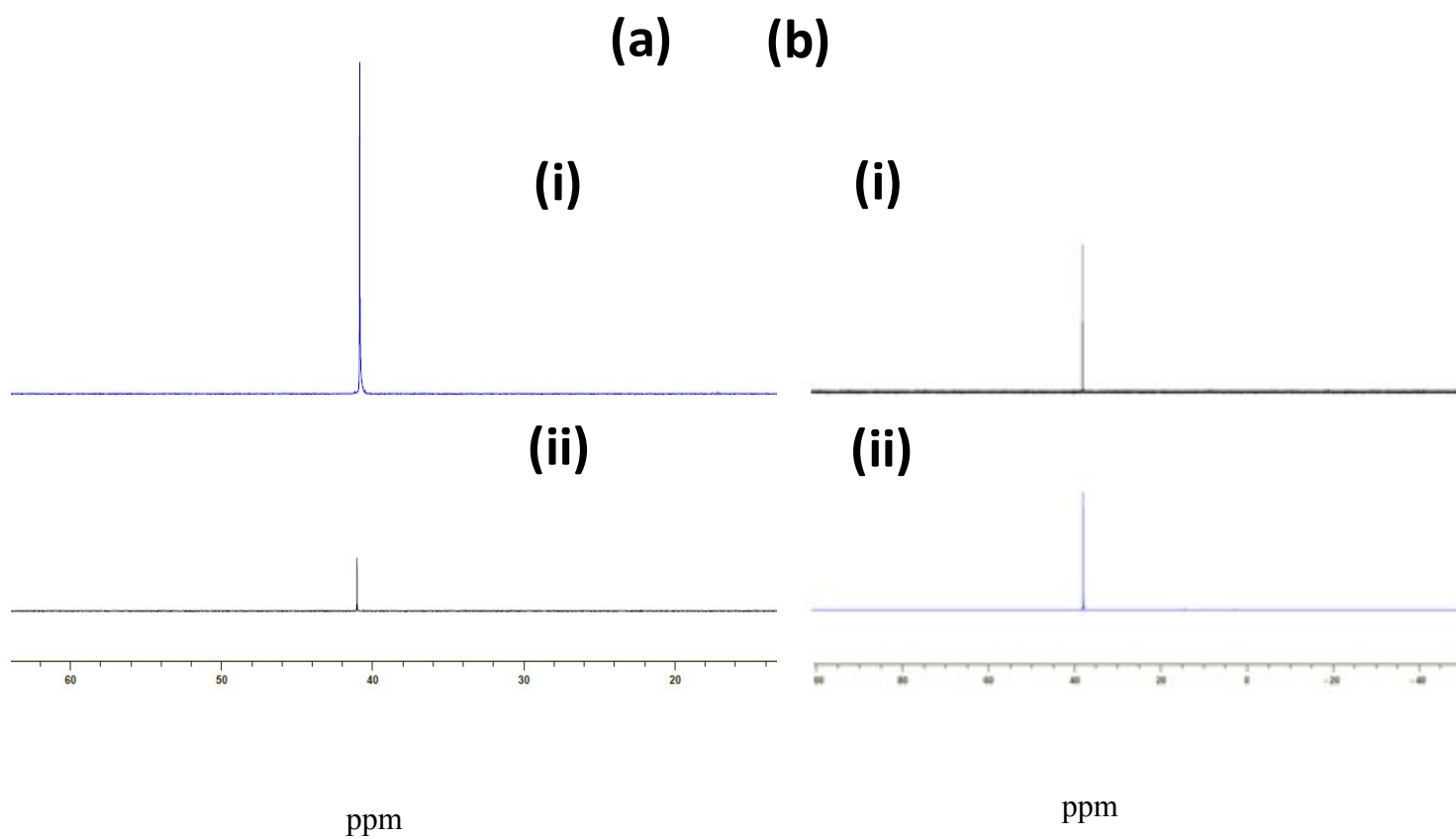**(ii)   (ii)**

ppm   ppm

Figure S3. ^{31}P NMR data of DMMP in water (a) (i) before adsorption with NU-1000; (ii) 30minutes after the process of adsorption; (b) (i) before adsorption with UiO-67; (ii) 30minutes after the process of adsorption
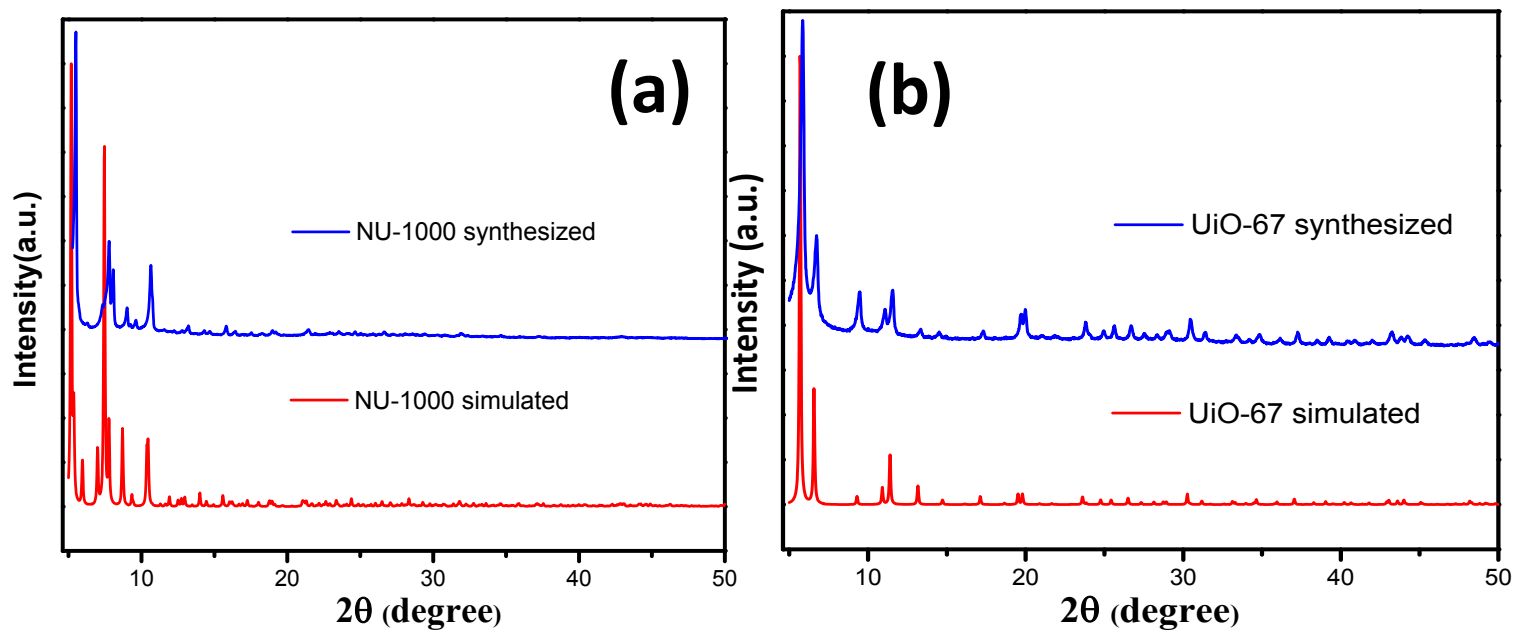
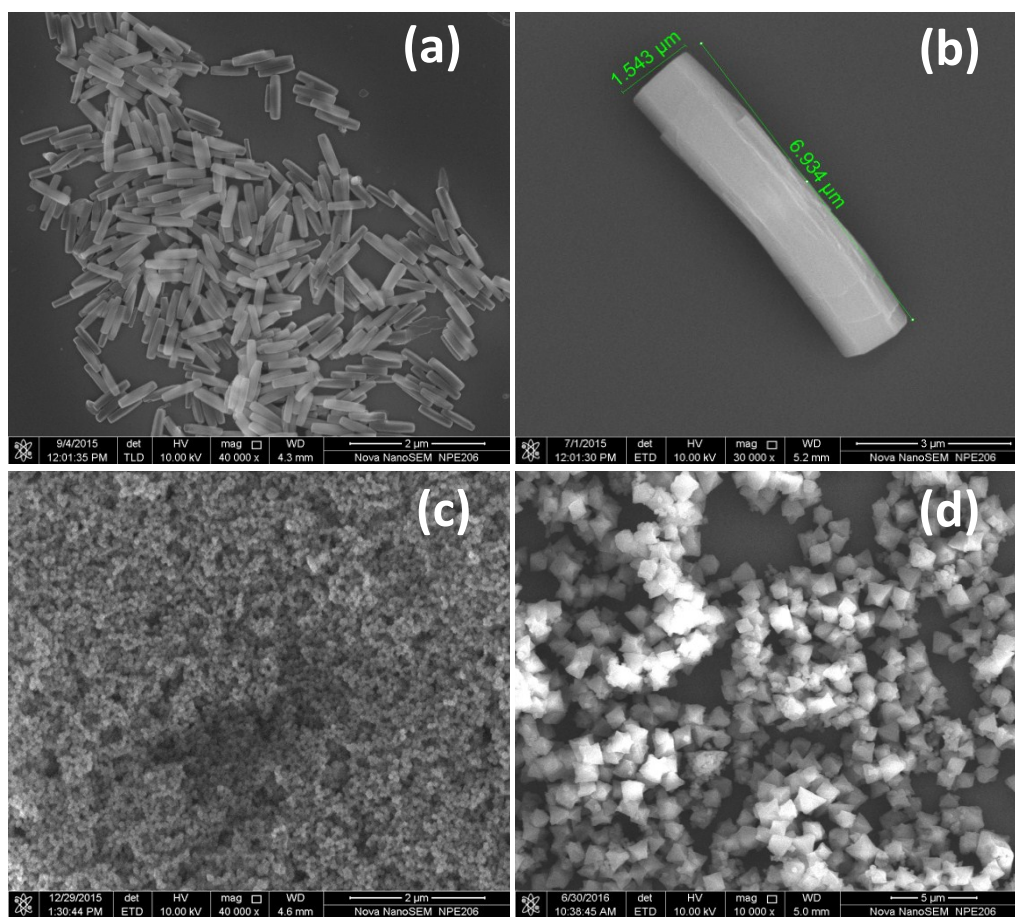**Figure S4.** PXRD plots showing the purity of (a) NU-1000 and (b) UiO-67

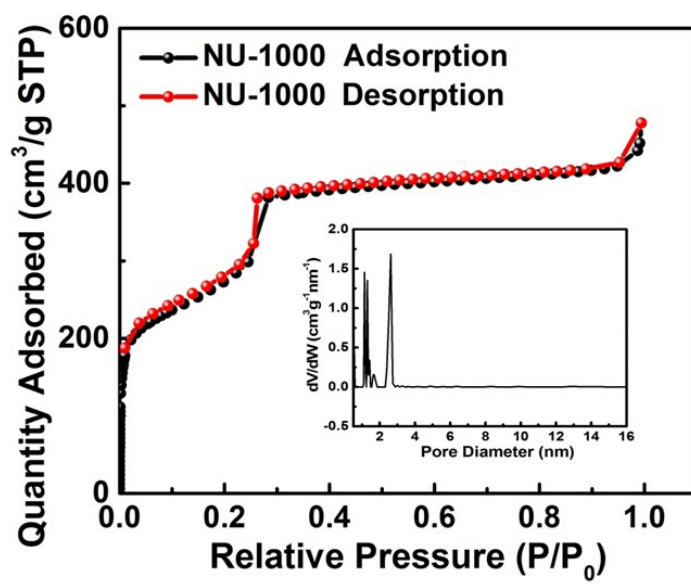**Figure S5.** SEM images of (a) & (b) NU-1000 and (c) & (d) UiO-67 showing their uniform particle sizes

Figure S6. Surface properties measurement of NU-1000

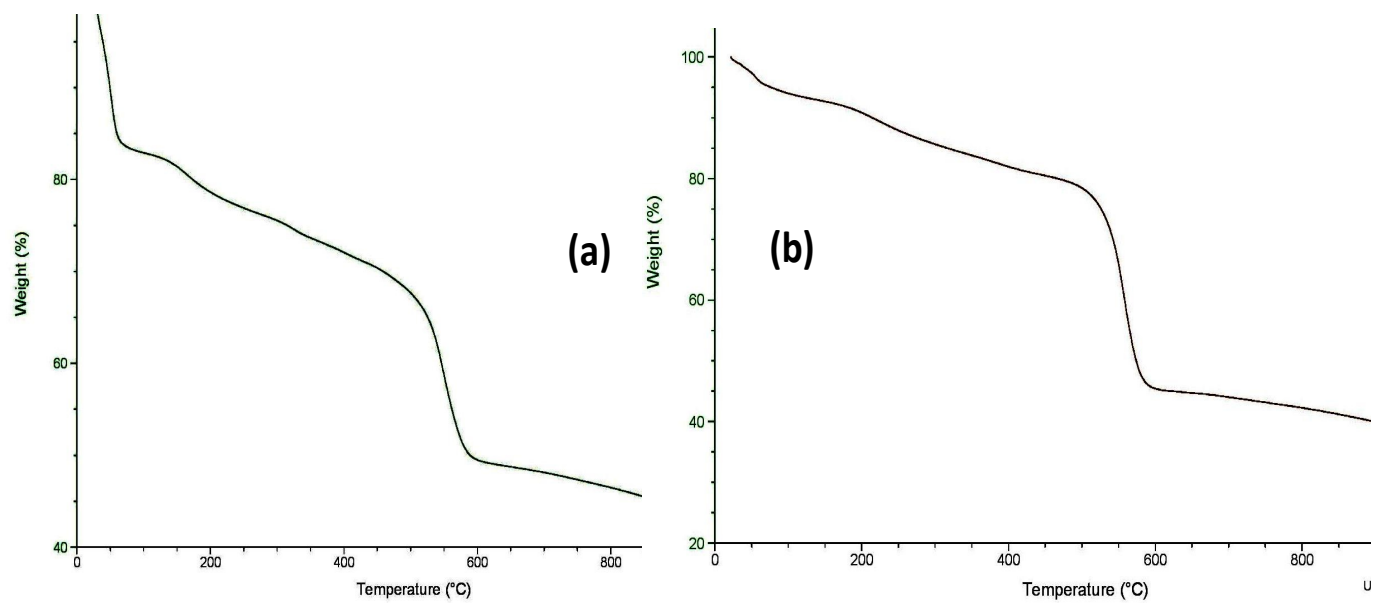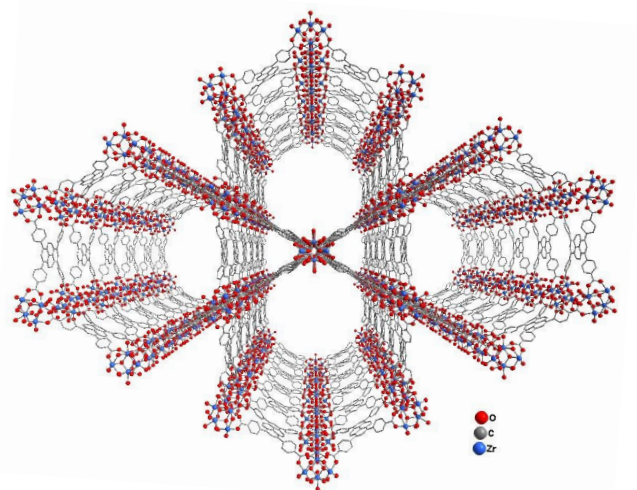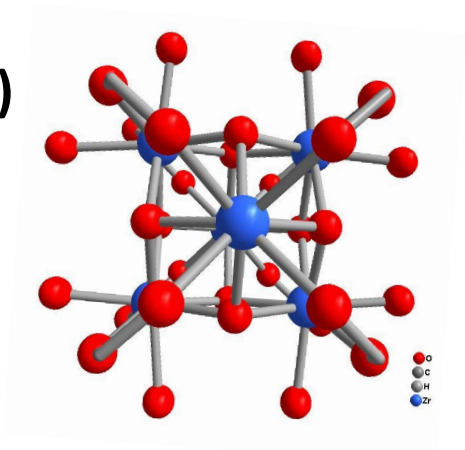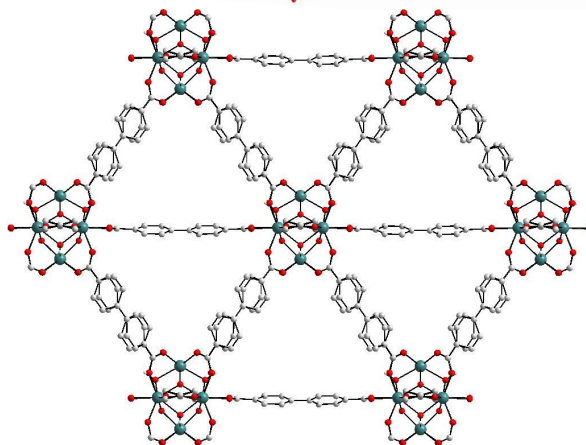**Figure S7.** TGA plots of (a) NU-1000 and (b) UiO-67
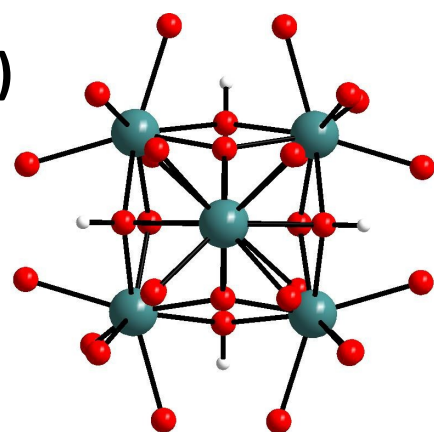
Figure S8. Pictorial representation showing the cluster node and three dimensional structures of (a) NU-1000 and (b) UiO-67
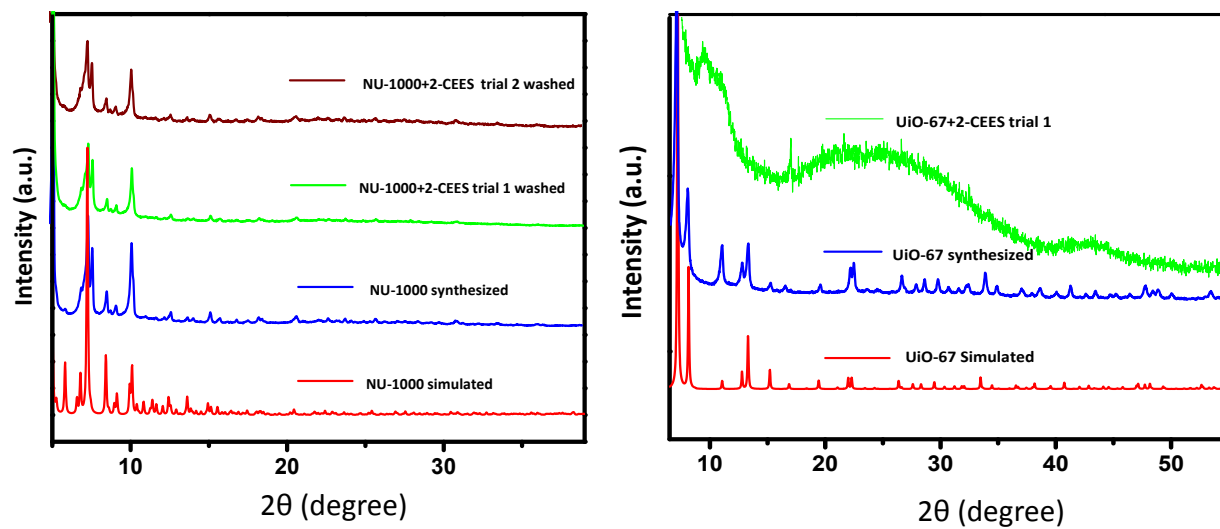
Figure S9. PXRD data of (a) NU-1000 and (b) UiO-67 after adsorption of 2-CEES.
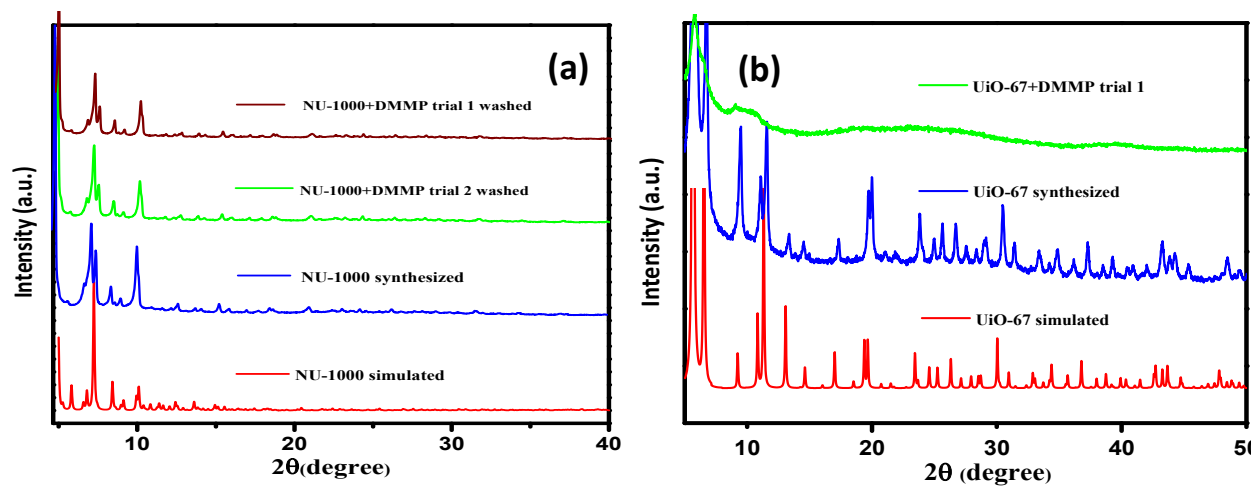
Figure S10. Powder XRD data of (a) NU-1000 and (b) UiO-67 on adsorption of DMMP.
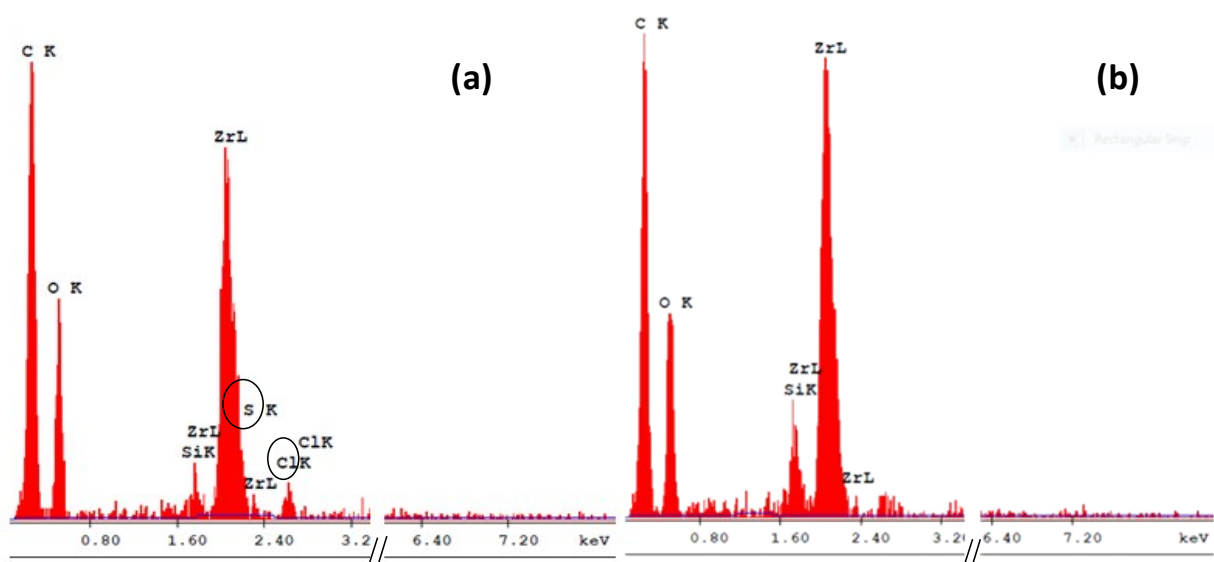
Figure S11. SEM-EDX data of adsorption of 2-CEES and/or its hydrolysis products on NU-1000 (a) after adsorption study and (b) after removal
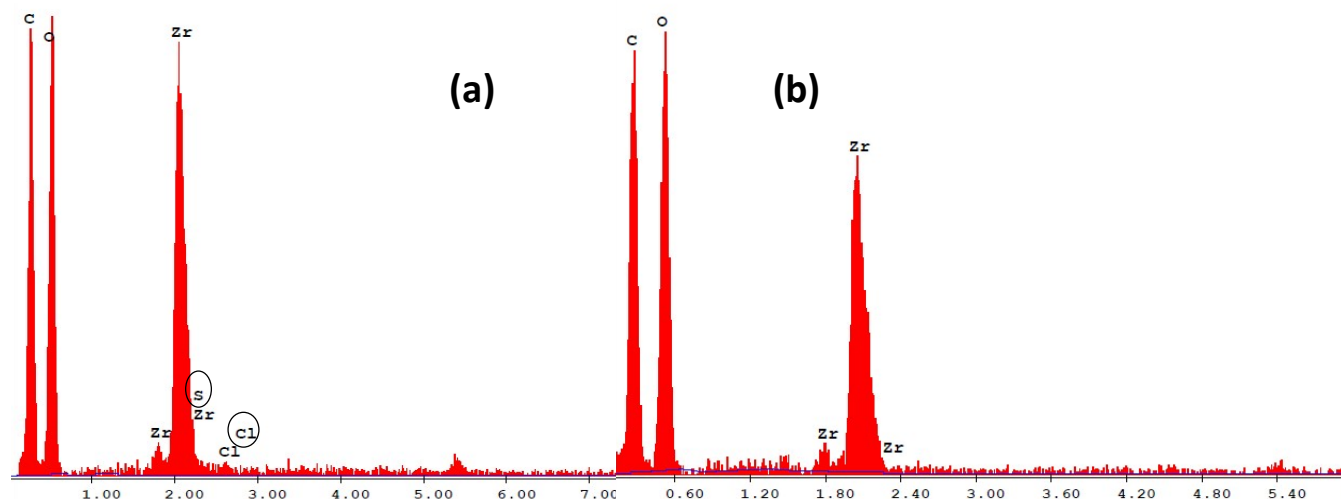
Figure S12. SEM-EDX data of adsorption of 2-CEES and/or its hydrolysis products on UiO-67 (a) after adsorption study and (b) after removal
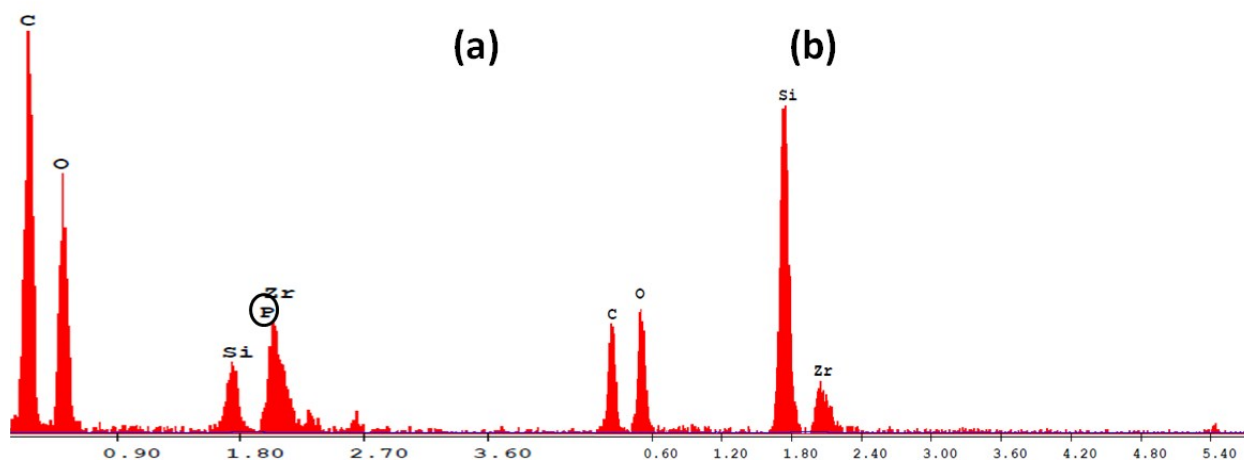
Figure S13. SEM-EDX data of DMMP on NU-1000 (a) after adsorption study and (b) after removal
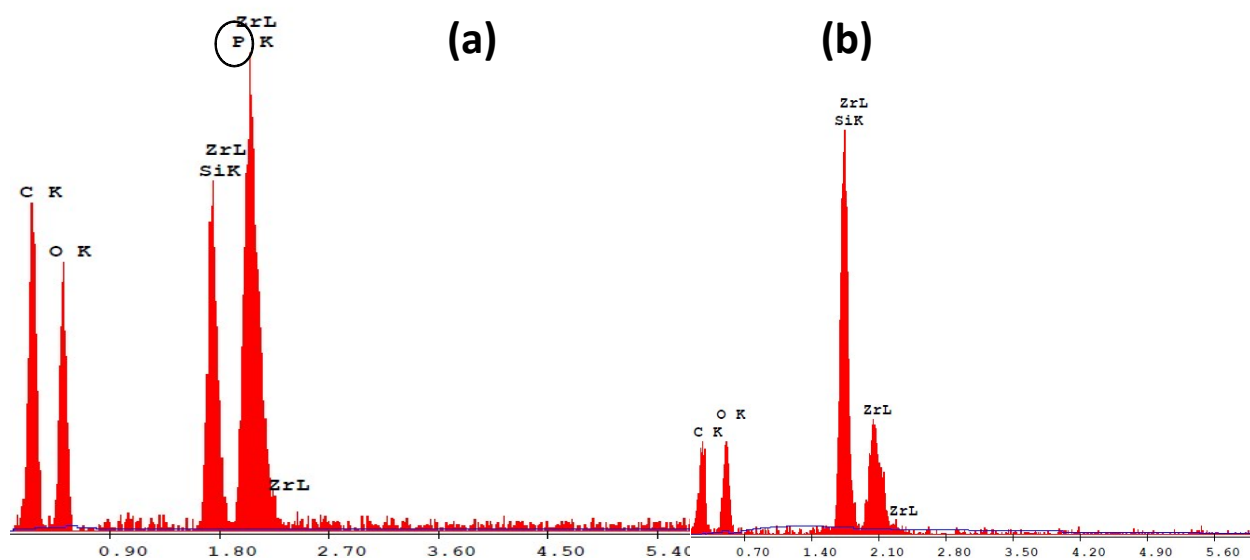
Figure S14. SEM-EDX data of adsorption of DMMP on UiO-67 (a) after adsorption study and (b) after removal
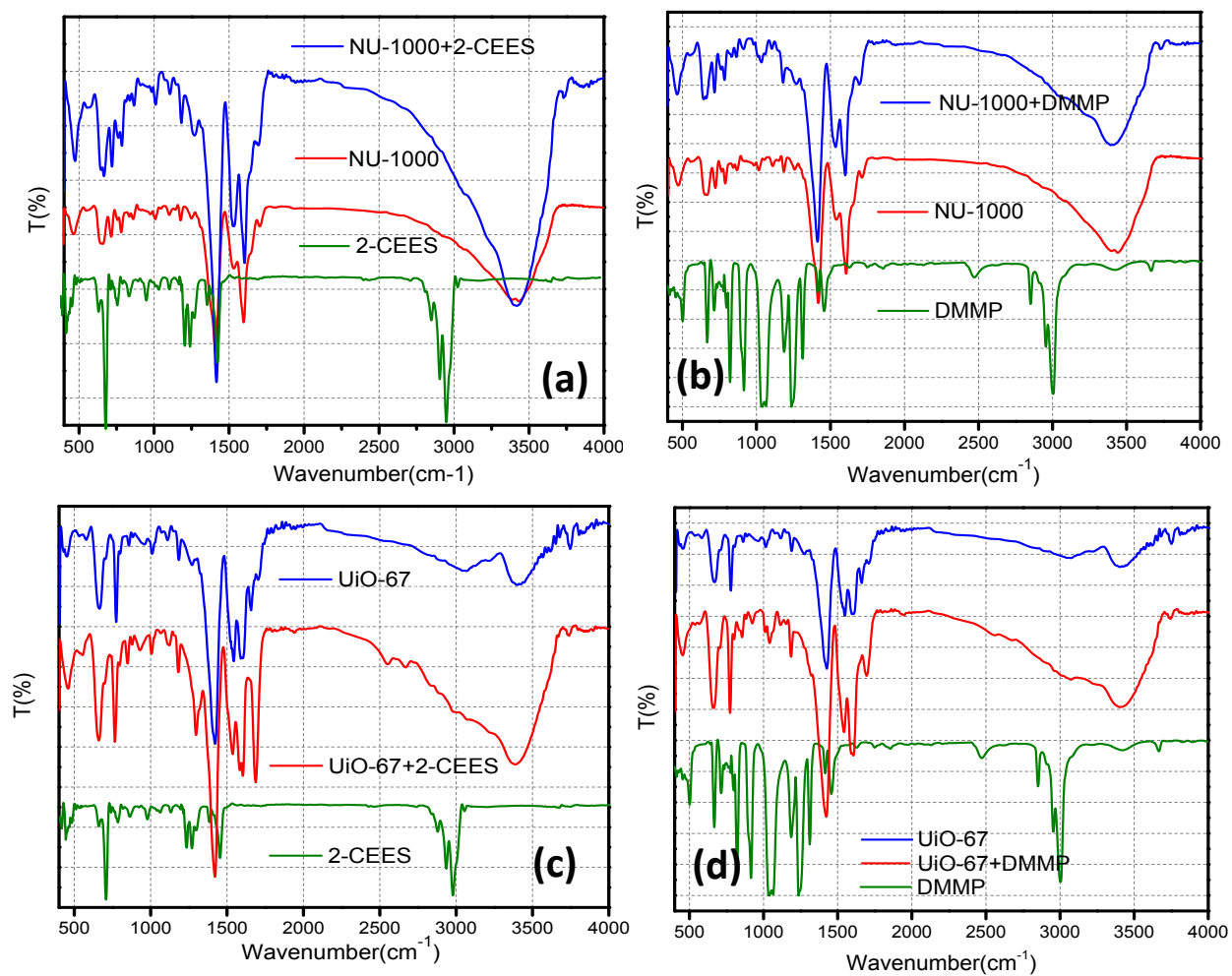
Figure S15. FT-IR spectra of the combinations (a) NU-1000-2-CEES; (b) NU-1000-DMMP; (c) UiO-67- 2-CEES and (d) UiO-67-DMMP
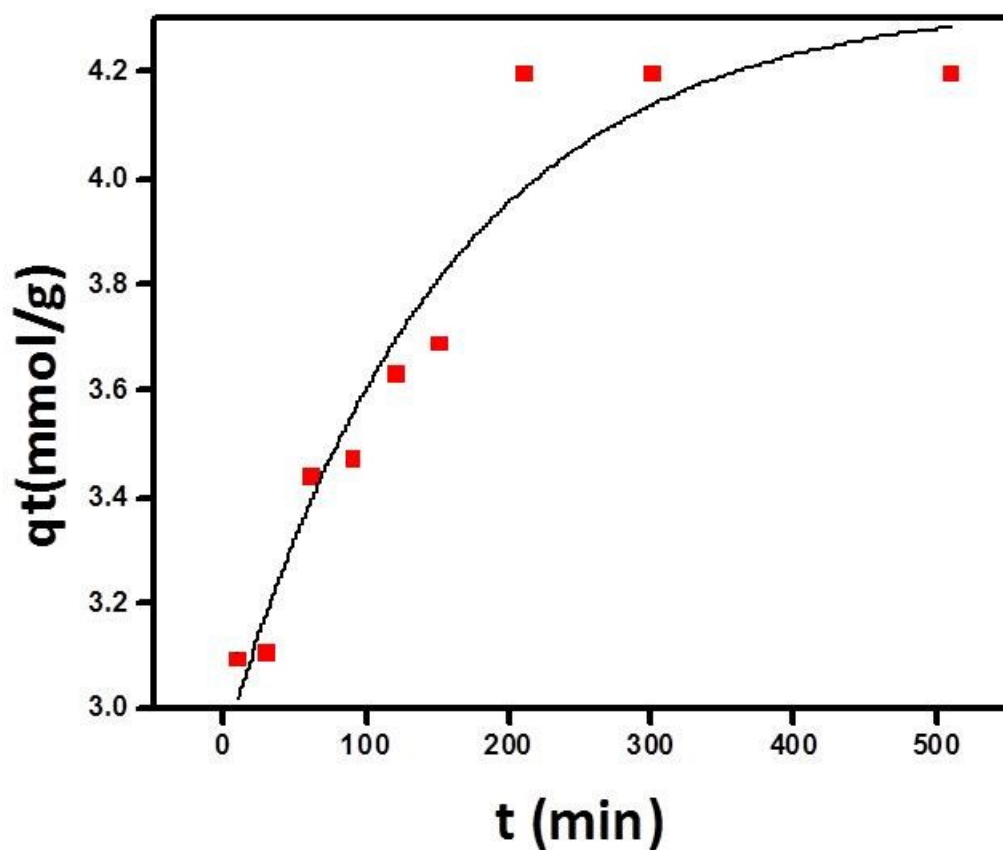
Figure S16. q_t *vs.* t graph for the adsorption of 2-CEES on NU-1000 MOF
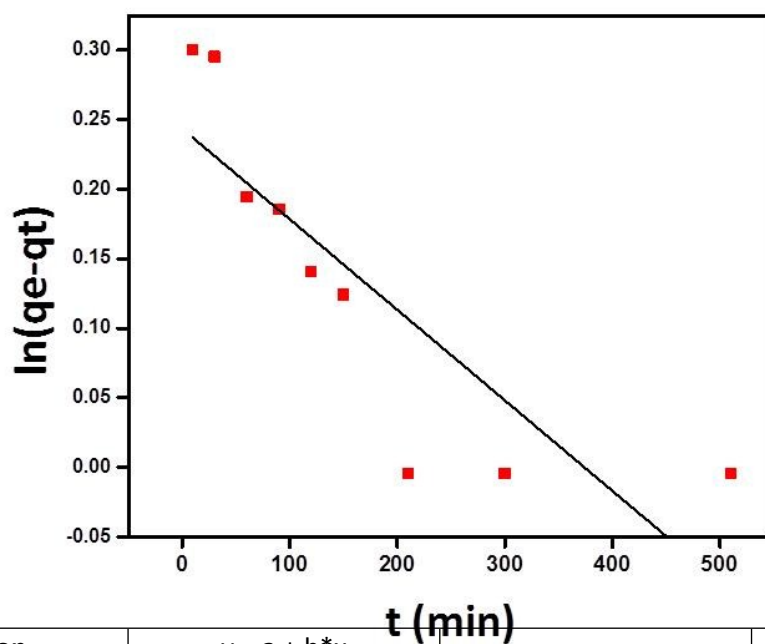
Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	0.03245		
Pearson's r	-0.85075		
Adj. R-Square	0.68432		
		Value	Standard Error
B	Intercept	0.24358	0.03377
	Slope	-6.51348E-4	1.52085E-4

Figure S17. Pseudo first order kinetic plot and the corresponding data for the adsorption of 2-CEES on NU-1000 MOF
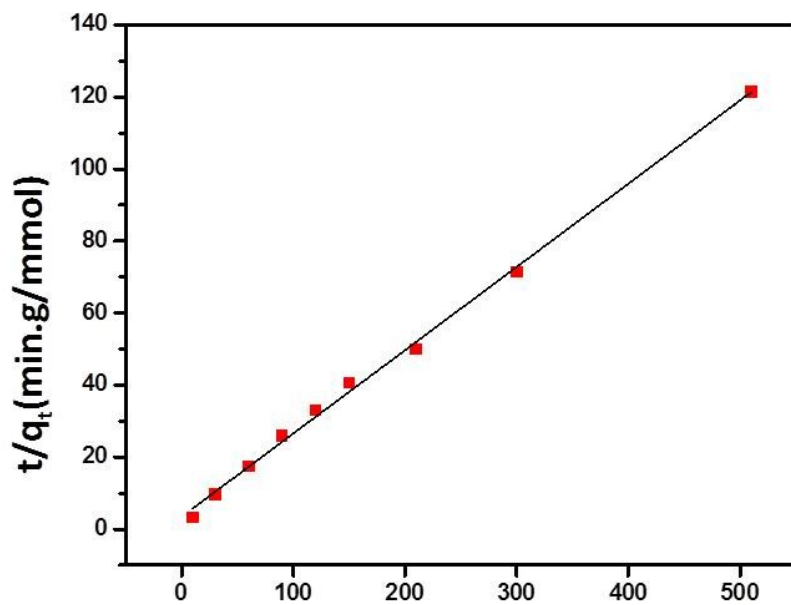
Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	25.26525		
Pearson's r	0.99882		
Adj. R-Square	0.99731		
		Value	Standard Error
B	Intercept	3.41053	0.94235
	Slope	0.23129	0.00424

Figure S18. Pseudo second order kinetic plot and the corresponding data for the adsorption of 2-CEES on NU-1000 MOF
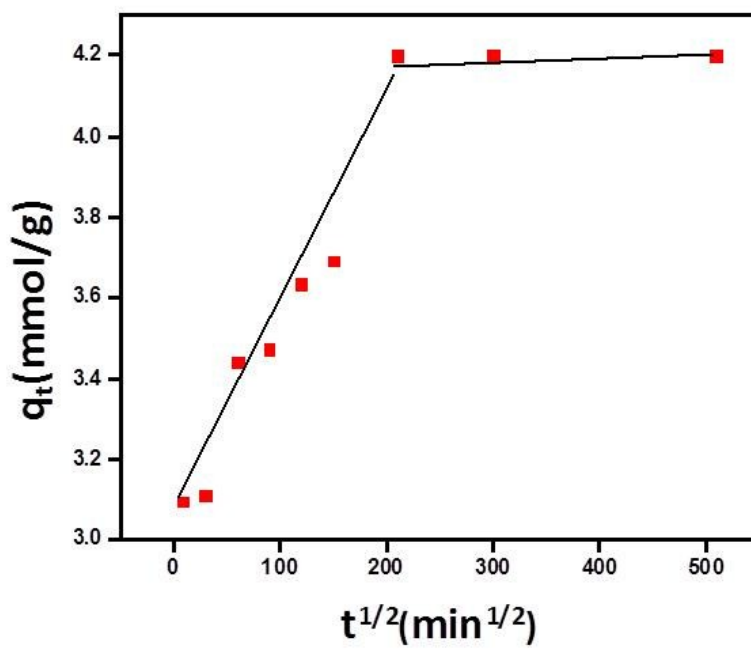
Figure S19. Intra-particle diffusion model for the adsorption of 2-CEES on NU-1000 MOF
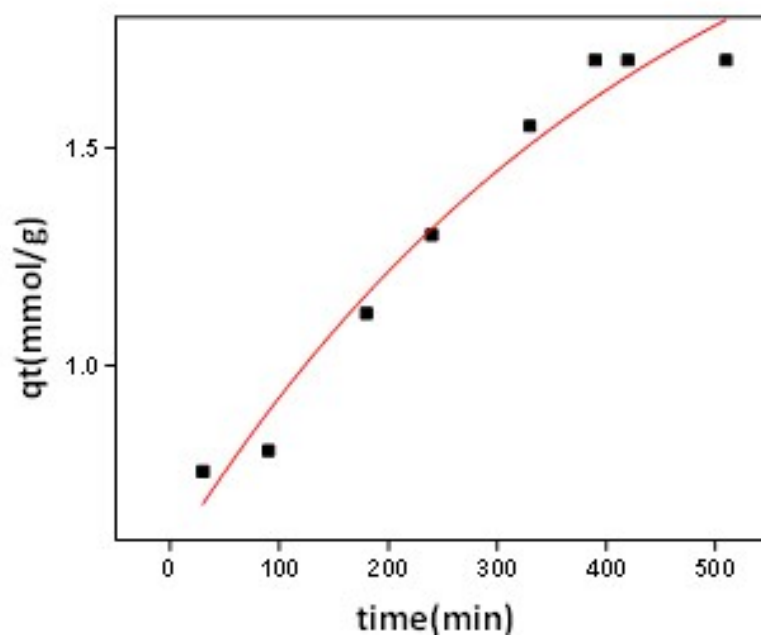
Figure S20. q_t *vs*. t graph for the adsorption of DMMP on NU-1000 MOF

Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	0.06283		
Pearson's r	-0.9592		
Adj. R-Square	0.90674		
		Value	Standard Error
B	Intercept	0.81651	0.07275
	Slope	-0.00192	2.30563E-4

Figure S21. Pseudo first order kinetic plot and the corresponding data for the adsorption of DMMP on NU-1000 MOF

Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	1905.84048		
Pearson's r	0.97948		
Adj. R-Square	0.95261		
		Value	Standard Error
B	Intercept	54.90239	12.67057
	Slope	0.47802	0.04016

Figure S22. Pseudo second order kinetic plot and the corresponding data for the adsorption of DMMP on NU-1000 MOF

Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	0.05111		
Pearson's r	0.97664		
Adj. R-Square	0.94613		
		Value	Standard Error
B	Intercept	0.29595	0.09838
	Slope	0.06619	0.00595

Figure S23. Intra-particle diffusion model and the corresponding data for the adsorption of DMMP on NU-1000 MOF

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Table S1. Decrease in concentration of 2-CEES and/or C and DMMP on adsorption with NU-1000 and UiO-67 and in the control experiments without the MOFs (ICP-AES data)

Sl.No	Time(s)	Conc. of S/Zr (mg/L)					Time(s)	Conc. of P/Zr (mg/L)				
		2-CEES						DMMP				
		NU-1000		UiO-67		Control		NU-1000		UiO-67		Control
		S	Zr	S	Zr			P	Zr	P	Zr	
1	0	316.78	0	316.78	0	315.26	0	128.42	0	128.42	0	127.01
2	10	85.31	-	-	-	-	30	71.97	-	-	-	-
3	30	83.96	-	-	-	-	90	71.79	-	-	-	-
4	60	59.3	-	-	-	-	180	70.29	-	-	-	-
5	90	57.23	-	-	-	-	240	70.24	-	-	-	-
6	120	45.69	-	-	-	-	330	68.47	-	-	-	-
7	150	40.65	-	-	-	-	390	1.55	-	-	-	125.95
8	210	2.95	-	-	-	316.21	420	1.55	-	-	-	-
9	300	2.93	-	-	-	-	510	1.55	0	5.72	0	125.57
10	510	2.93	0	17.30	0	310.13						

Table S2. Reusability of NU-1000 in adsorbing 2-CEES and/or C and DMMP (ICP-AES data)

		Conc. of S in 2-CEES(mg/L)		Conc. of P in DMMP(mg/L)	
		Time(min)		Time(min)	
		0	510	0	510
NU-1000	Trial 1	316.78	2.93	316.78	1.55
	Trial 2	316.78	7.79	316.78	3.15
	Trial 3	316.78	77.79	316.78	19.17