

SUPPORTING MATERIAL

Expanding the NUIG MOF Family: synthesis and characterization of new MOFs for selective CO₂ adsorption, metal ion removal from aqueous systems, and drug delivery applications

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Table S1: Crystallographic data for **1**•DMF

1 •DMF	
Formula	C ₃₆ H ₂₈ Co ₂ N ₂ O ₁₆
Mw	862.46
Crystal System	orthorhombic
Space group	<i>C</i> _{mca}
<i>a</i> / Å	26.2183(7)
<i>b</i> / Å	23.5289(10)
<i>c</i> / Å	15.3542(5)
<i>V</i> / Å ³	9471.8(6)
<i>Z</i>	8
<i>T</i> / K	100(2)
λ / Å	1.54184
<i>D</i> _c /g cm ⁻³	1.210
μ (Mo Ka)/mm ⁻¹	6.019
Reflections collected	11393
Independent reflections	4693 [Rint = 0.0245]
<i>R</i> ₁ ^a	0.0675
w <i>R</i> ₂ ^b	0.0832
Goodness of fit on <i>F</i> ²	1.078
$\Delta\rho$ max/min/e Å ⁻³	0.822/-0.569

^a $R_1 = \frac{\sum(|F_o| - |F_c|)}{\sum |F_o|}$; ^b $wR_2 = \frac{[\sum[w(F_o^2 - F_c^2)^2]]^{1/2}}{[\sum[wF_o^2]]^{1/2}}$

Table S2: Selected interatomic distances (Å) and angles for **1**•DMF.

Co1-O2	2.119(4)	Co2-O1	2.053(5)
Co1-O3	2.125(4)	Co2-O2	2.070(4)
Co1-O4	2.040(3)	Co2-O5	2.062(3)
Co1-O6	2.141(3)	Co2-O9	2.109(4)
O2-Co1-O3	177.50(15)	O1-Co2-O2	177.55(18)
O2-Co1-O4	93.34(11)	O2-Co2-O5	91.13(12)
O2-Co1-O6	90.53(11)	O5-Co2-O9	175.09(16)

Table S3: Fitting parameters of the metal adsorption data to the Langmuir model for **NUIG2** and **NUIG3**

	Metal ion	q_s (mg g ⁻¹)	K_L (10 ⁴ L mol ⁻¹)	R^2
NUIG2	Co ²⁺	135.1	10.57	0.9804
	Cu ²⁺	173.5	3.03	0.9064
NUIG3	Co ²⁺	148.5	1.49	0.9627
	Cu ²⁺	189.3	1.76	0.9555
	Ni ²⁺	134.6	1.45	0.9713

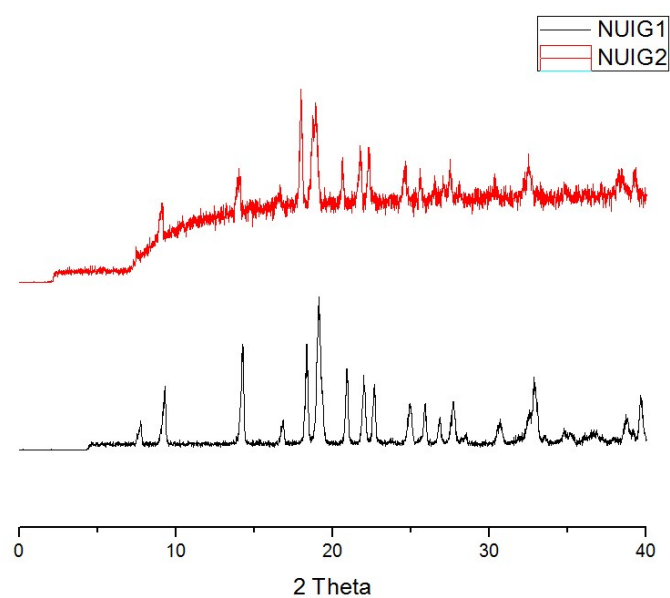


Fig. S1. Experimental pxd pattern for **NUIG2** (red) in comparison with the theoretical pxd pattern of the isostructural **NUIG1** (black).

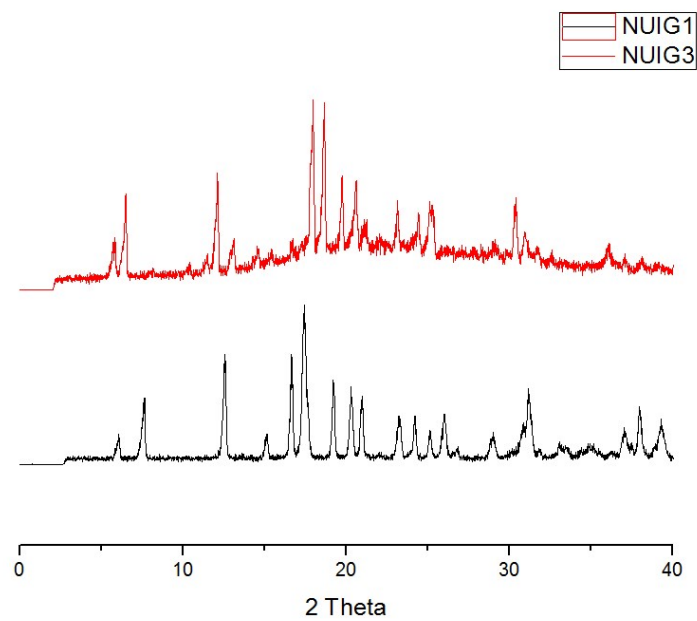


Fig. S2. Experimental pxd pattern for **NUIG3** (red) in comparison with the theoretical pxd pattern of the isostructural **NUIG1** (black).

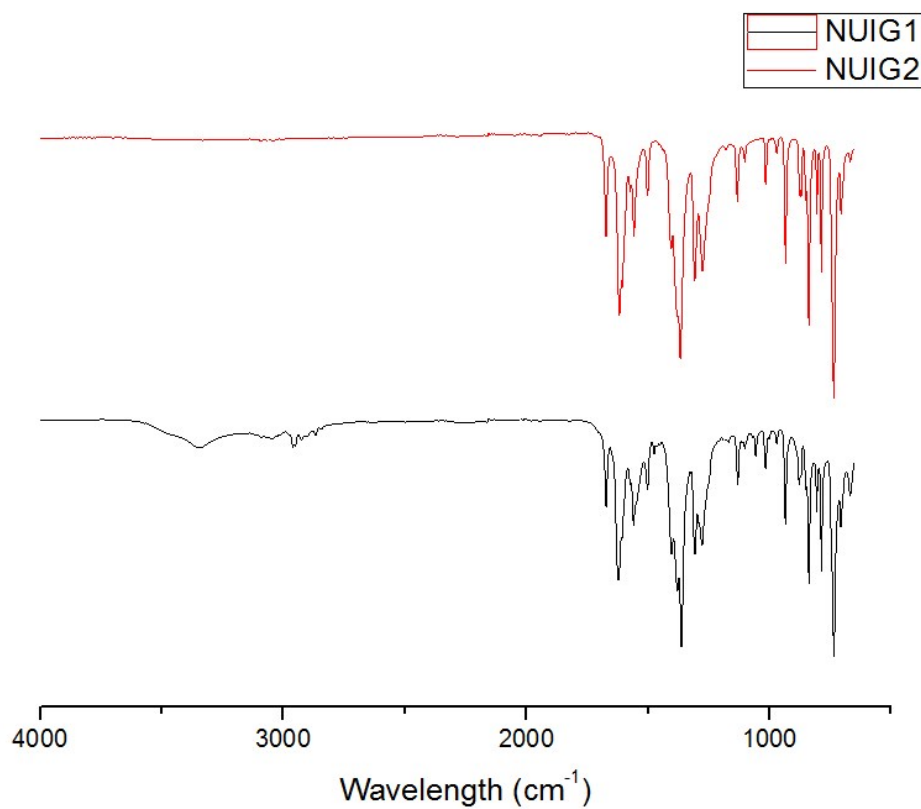


Fig. S3. IR spectra of **NUIG2** (red) and **NUIG1** (black).

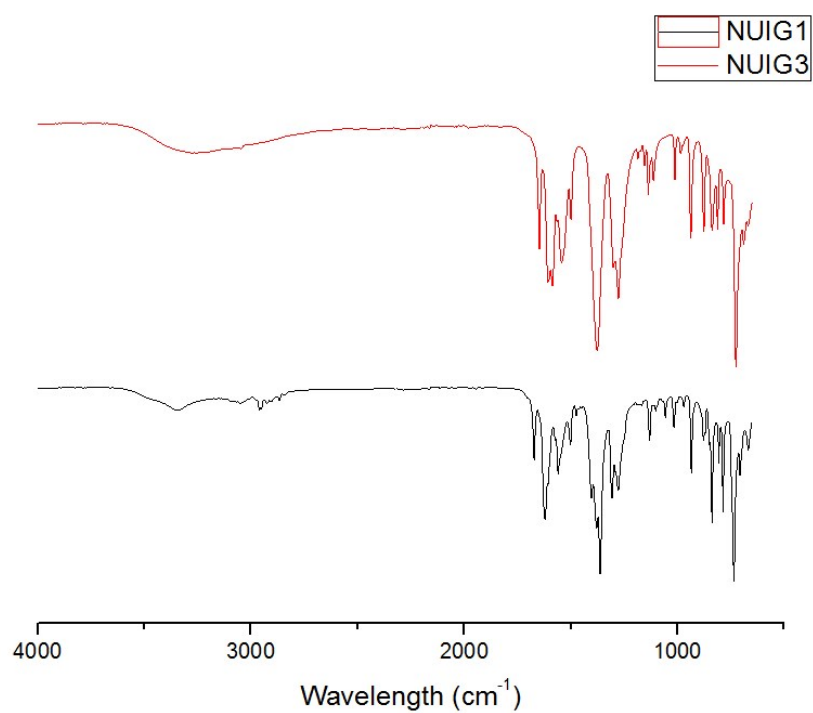


Fig. S4. IR spectra of **NUIG3** (red) and **NUIG1** (black).

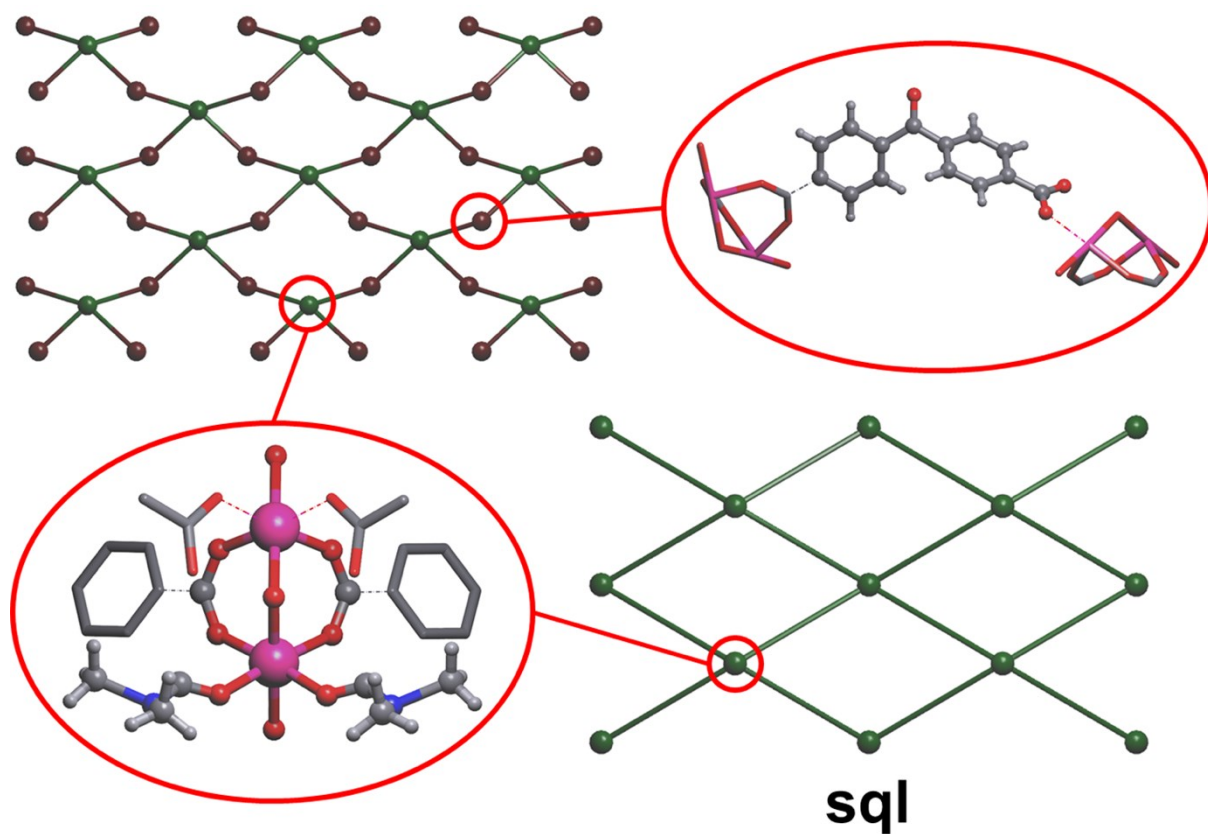


Fig. S5. Representation of the **sql** topological type in **1•DMF**.

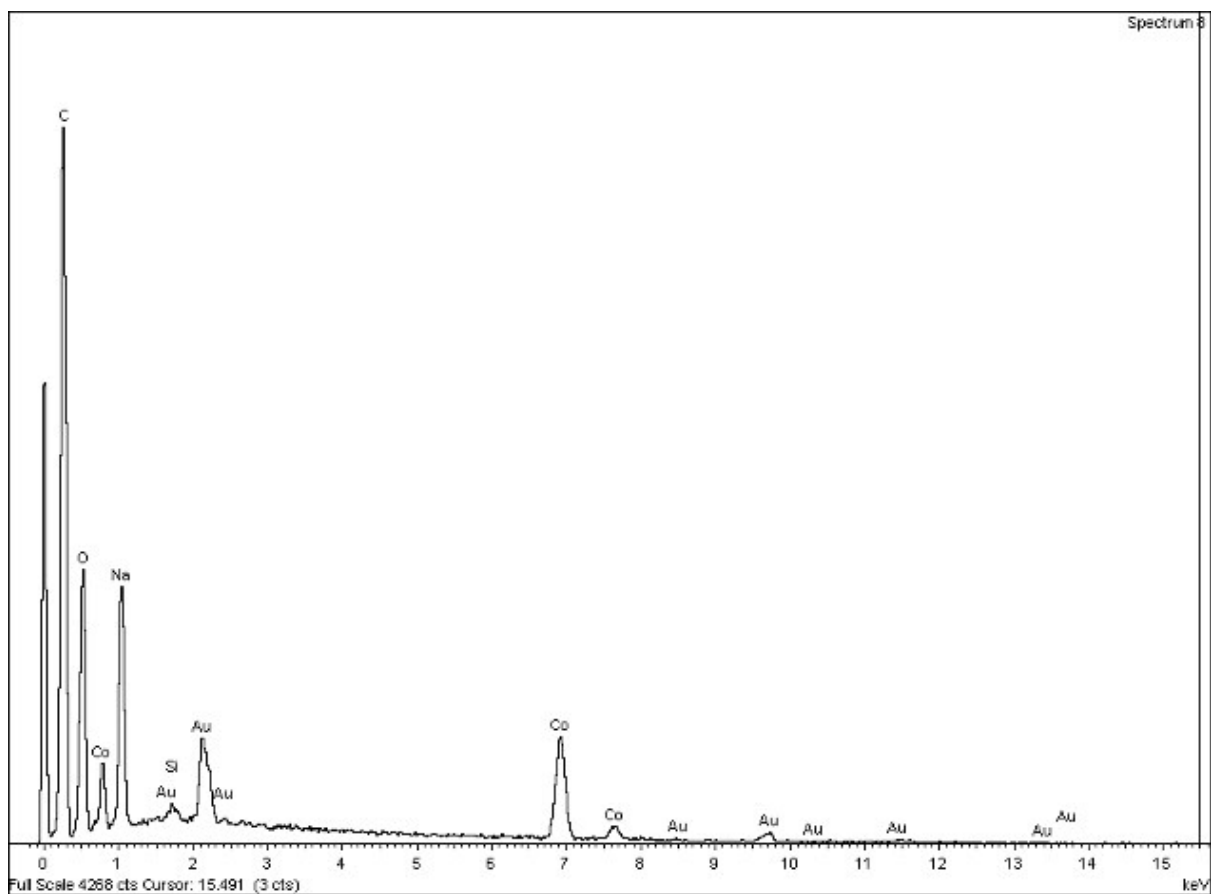


Fig S6. EDX spectrum for NUIG2.

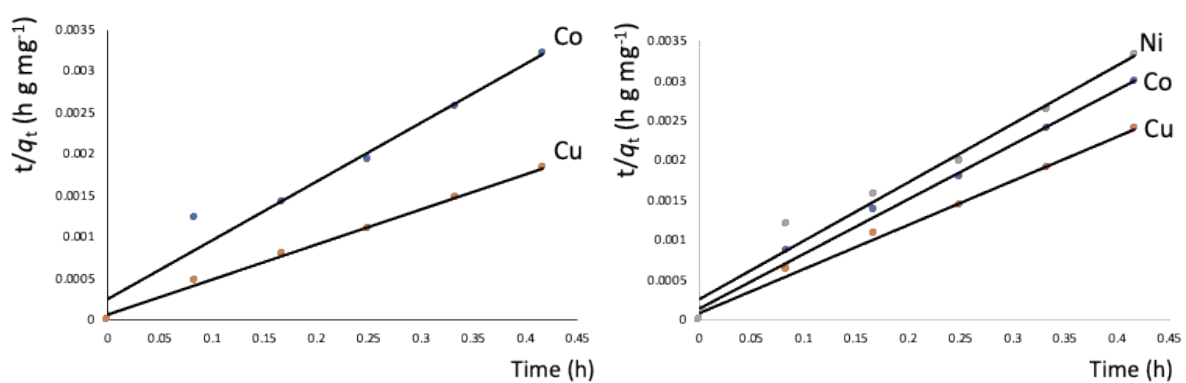


Fig. S7. Simulation of the experimental data to the pseudo-second order kinetic model for NUIG2 (left) and NUIG3 (right); the solid lines represent the fitting of the data.

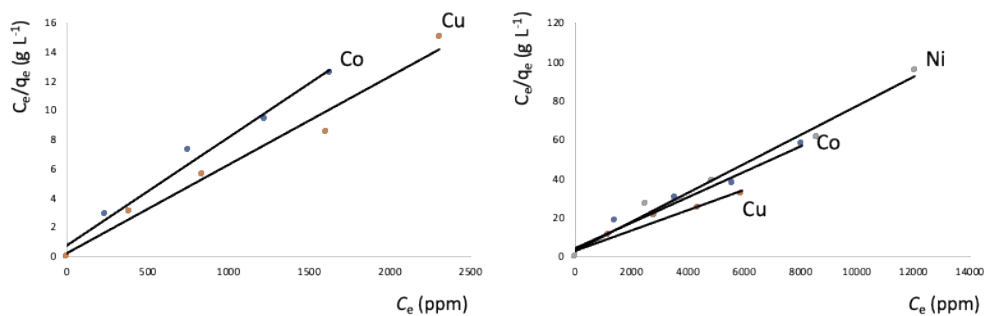


Fig. S8. Fitting of the metal adsorption data to the Langmuir model for **NUIG2** (left) and **NUIG3** (right).

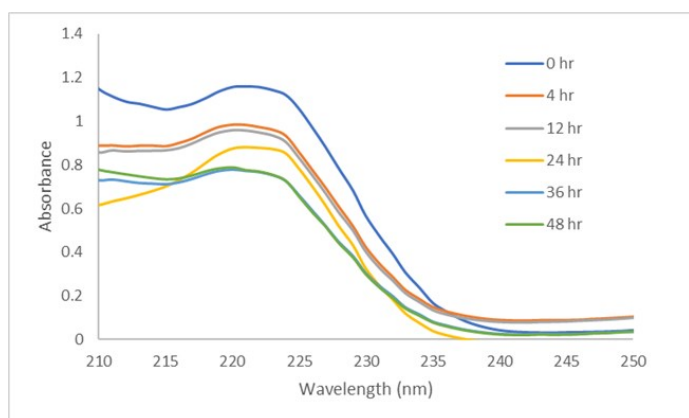


Fig. S9. UV Vis data for the ibuprofen uptake by **NUIG2**.

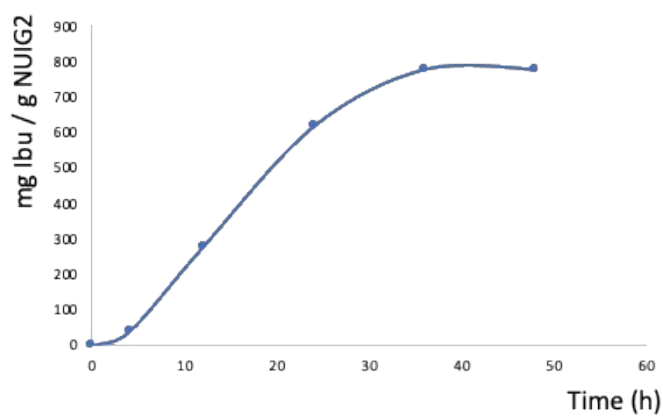


Fig. S10. The ibu uptake kinetics of **NUIG2**.

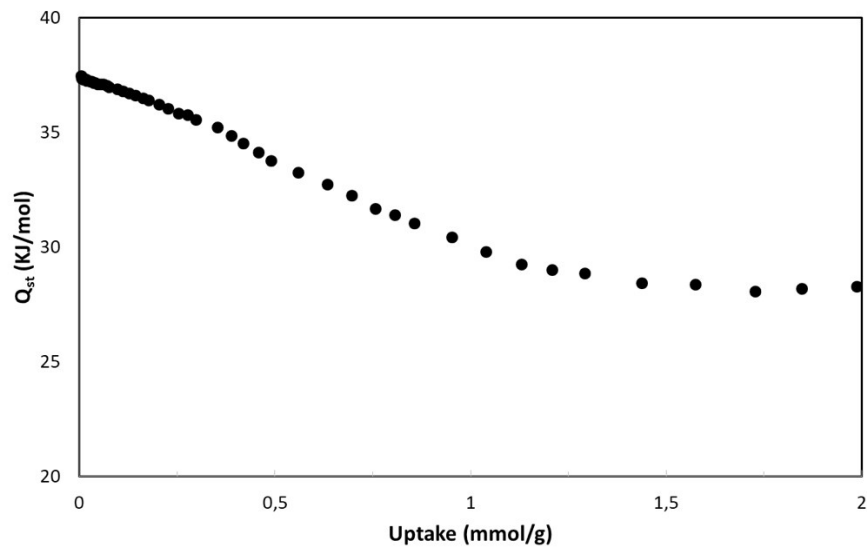


Fig. S11. Isosteric heat of CO₂ adsorption by NUIG1 at 298 K.