Supplementary Information (SI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2026

Structural Features and Antibacterial Activity of Ni(II) Thiosemicarbazones in a Zirconium Metal Organic Framework Composite

Edward Loukopoulos[a,b], David Fabra[a], Jorge Melones-Herrero[c], Ana I Matesanz[a], Carmen Viciana[a], Ana E Platero-Prats[d*]. Isabel Sanchez Pérez[c,e,f*], Adoracion G. Quiroga[a,g*]

*[a]Inorganic Chemistry department. Universidad Autonoma de Madrid(UAM), [b] Condensed Matter Physics Center (IFIMAC), [c]Department of Biochemistry. Medicine School, UAM, [d]Instituto de Investigaciones Biomédicas "Sols-Morreale" IIBM-CSIC-UAM.[e] Institute of Catalysis and Petrochemistry CSIC [e]BIOPAC-IRYCIS [g]IadChem-UAM. 28049 Madrid, Spain. *adoracion.gomez@uam.es, is.pere@uam.es; ana.platero@icp.csic.es*

SUPPLEMENTARY MATERIAL

Content

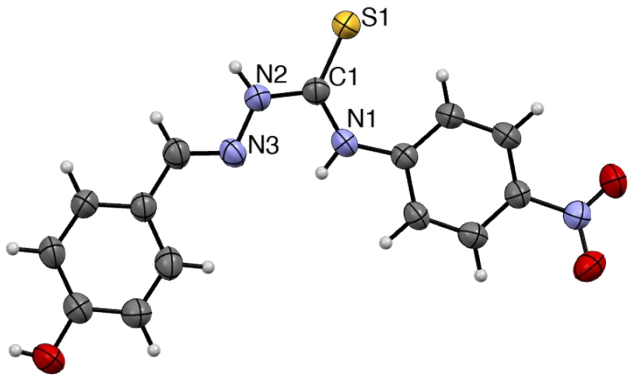

Figure S 1. SC-XRD of the ligand L2. CCDC number : 2477479

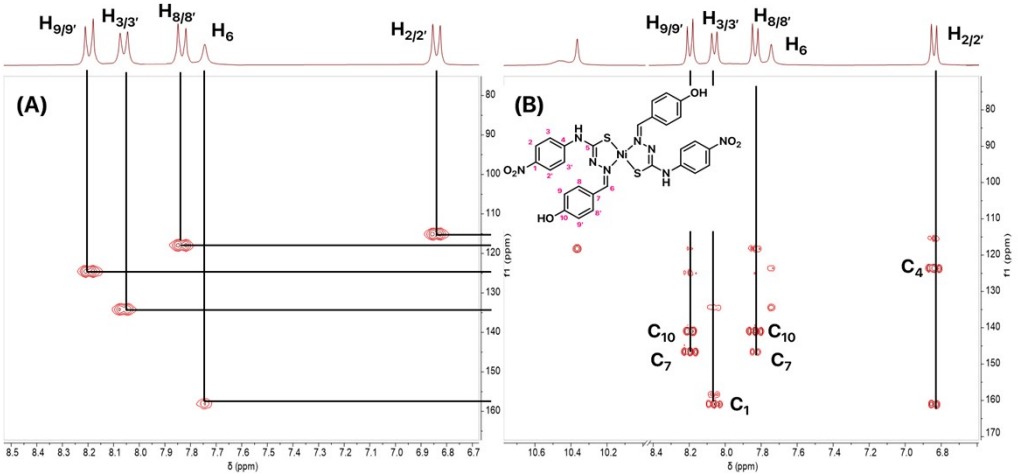

Figure S 2. Aromatic area of the 2D [1H, 13C] NMR. (a) HSQC and (B) HMBC spectra of Ni2

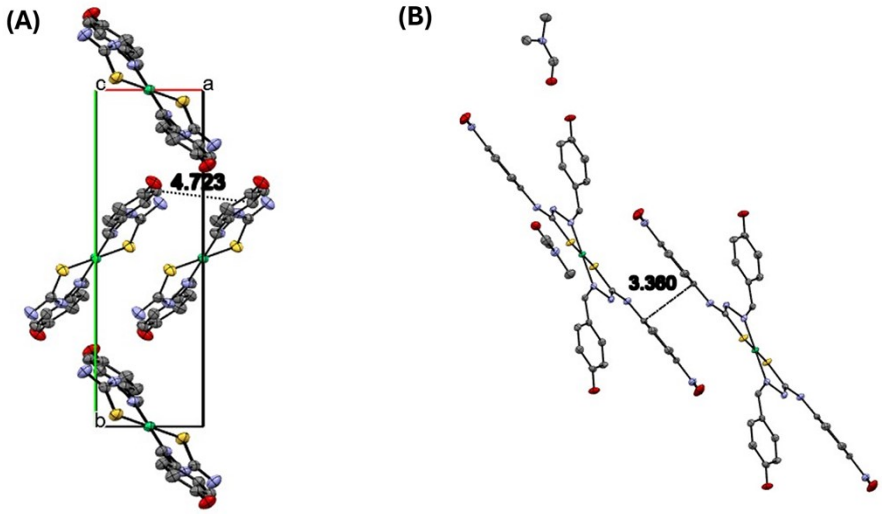

Figure S 3. Partial view of supramolecular association in Ni1 (A) and Ni2 (B)

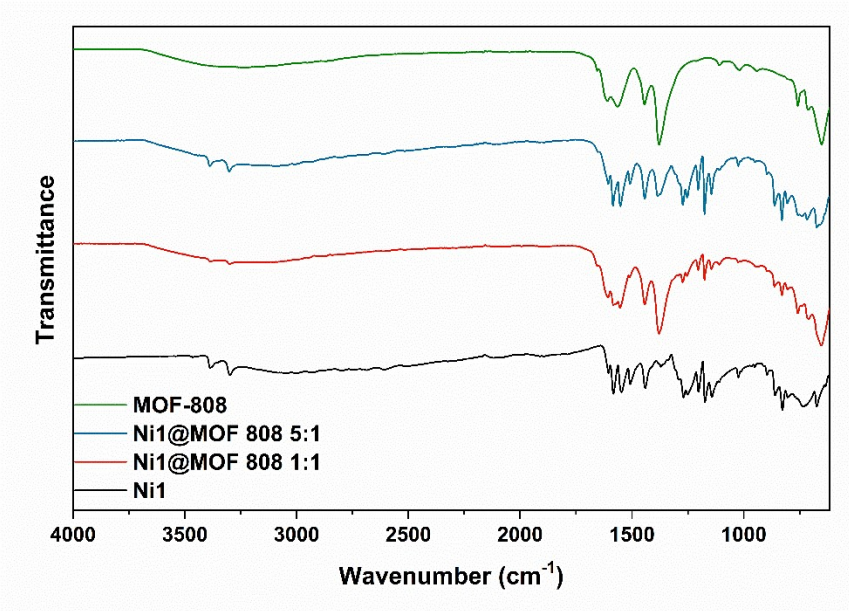

Figure S 4. Detailed FT-IR spectra for pristine MOF-808 and the composite materials of this study.

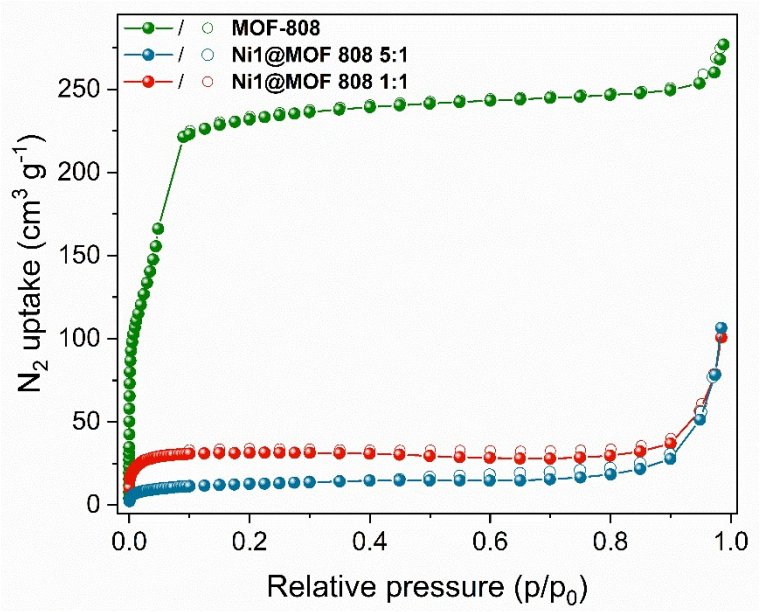

Figure S 5. N_2 isotherm (linear scale) for pristine MOF-808 and Ni1@MOF-808 composites, recorded at 77 K.

Table S 1. Nitrogen uptake, pore volume (calculated at $p/p_0 = 0.95$) and BET surface area values for pristine MOF-808 and the composite materials of this study, as calculated from the N_2 isotherms.

Material	Uptake ($cm^3\ g^{-1}$)	Pore volume ($cm^3\ g^{-1}$)	BET surface area ($m^2\ g^{-1}$)
MOF-808	276.9	0.43	1235.4±30.6
Ni1@MOF-808 (5:1)	78.2	0.09	45.5±0.5
Ni1@MOF-808 (1:1)	78.7	0.16	105.8±1.5

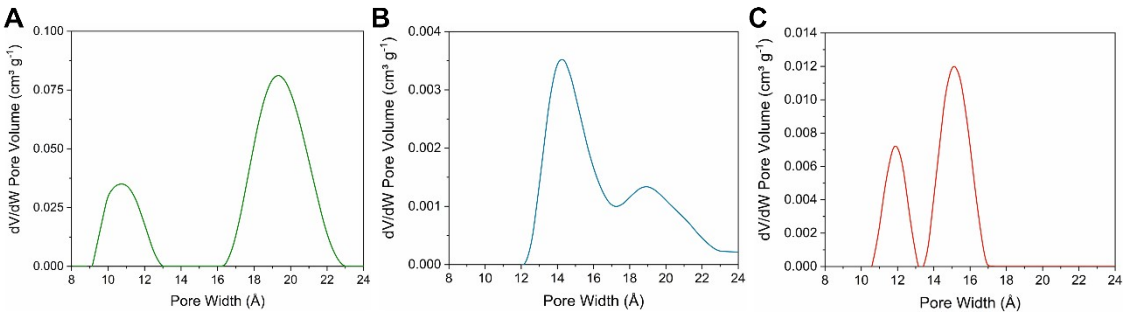

Figure S 6. Corresponding pore-size-distribution curves for MOF-808 (**A**), Ni1@MOF-808 5:1 (**B**) and Ni1@MOF-808 1:1 (**C**), obtained from the recorded N_2 adsorption isotherms. A non-local density functional theory (NLDFT) method for a cylinder pore in pillared clays was applied.

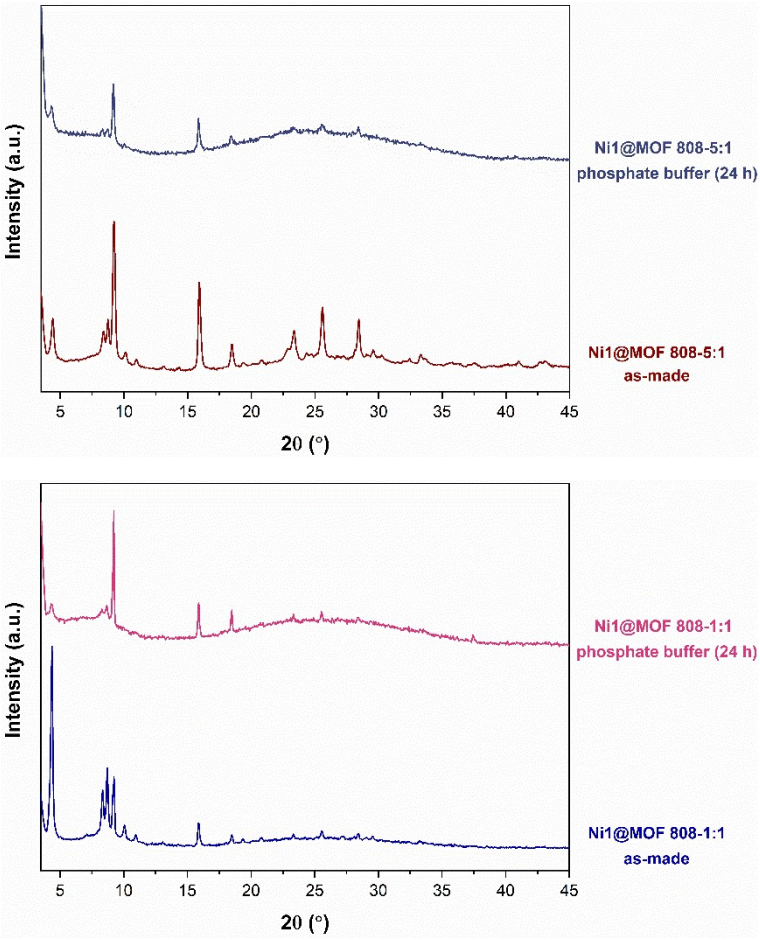

Figure S 7. Stability of Ni1@MOF 5:1 and Ni1@MOF 1:1 in phosphate buffer (20 mM), as determined by PXRD.

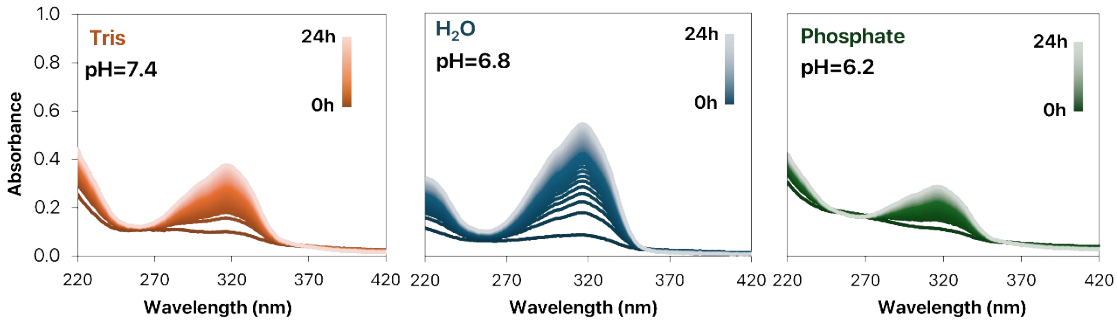

Figure S 8. UV-Visible spectra of Ni1@MOF 1:1 in Tris-HCl (orange), water (blue) and phosphate buffer(green)

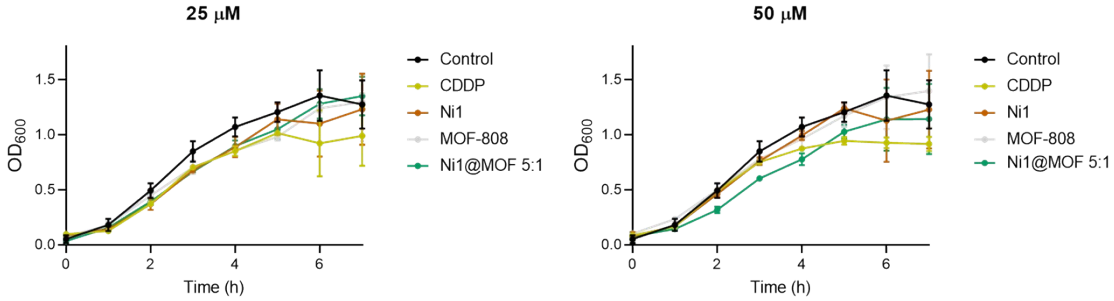

Figure S 9. OD_{600} evolution of DH5α treated with cisplatin, MOF-808, Ni1, and Ni1@MOF 5:1 at 25 and 50 μM

Table S 2. Crystal data and structure refinement results for ligand L2H.

		HL2
Chemical formula		$C_{16}H_{18}N_6O_2S_2$
Formula weight (g mol^{-1})		390.48
Temperature (K)		250(2)
Crystal system		Triclinic
Wavelength (Å)		0.71073
Space group		P -1
Crystal size (mm)		0.176 × 0.227 × 0.290
Crystal habit		Intense yellow-green needle
Cell unit dimensions	*a* (Å)	4.06720(10)
	b (Å)	10.8484(4)
	c (Å)	20.5829(6)
	α (º)	85.0576(13)
	β (º)	89.4170(13)
	γ (º)	80.0585(13)
Volume (Å^3)		891.20(5)
Z		2
Density, calculated (g cm^{-3})		1.455
Absorption coefficient (mm^{-1})		0.324