Supplementary Information

A Zn azelate MOF: combining antibacterial effect

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1. Crystallographic data

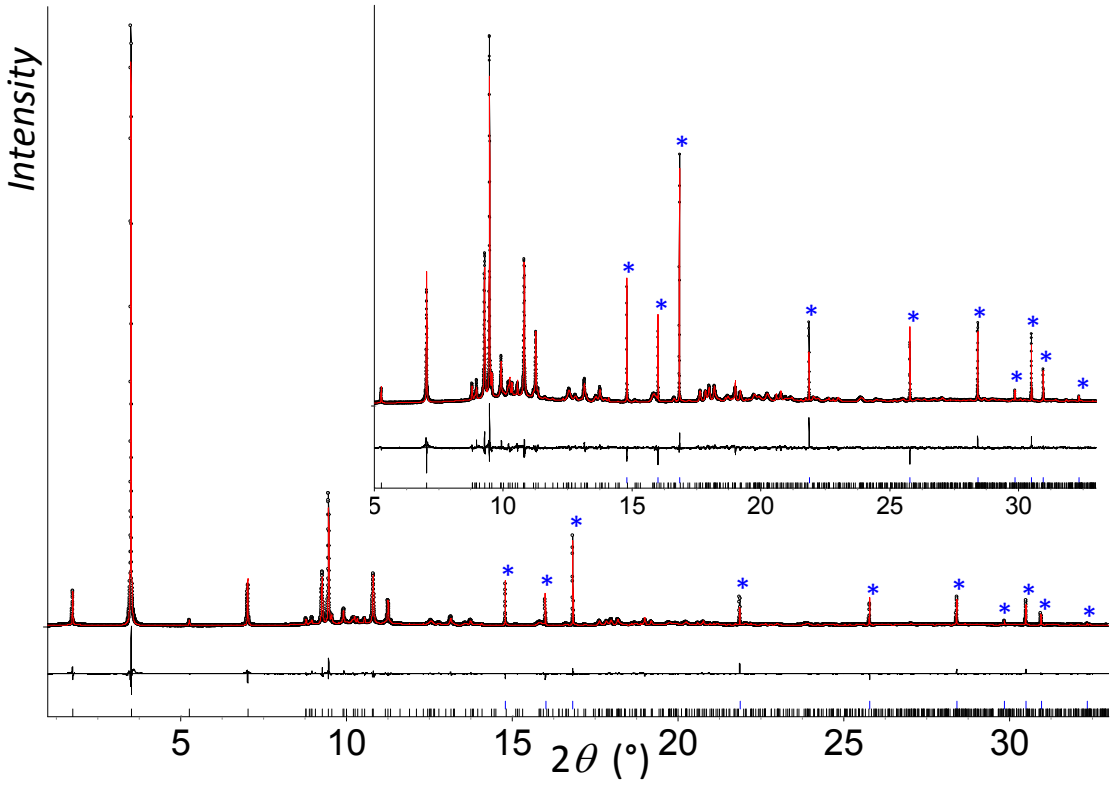

Fig. S1 Final Rietveld plot of BioMIL-5 showing observed (black circles), calculated (red line), and difference (black line) curves. A zoom at high angles is shown as inset. Blue marked lines and stars correspond to ZnO impurity. (λ=0.72528 Å)

Tab. S1 Crystallographic data and Rietveld refinement parameter for BioMIL-5 or $Zn[C_9O_4H_{14}]$.

Empirical formula	$C_9H_{14}O_4Zn$
M_r	251.595
Crystal system	Orthorhombic
Space group	*Pcca*
a (Å)	47.288(1)
b (Å)	4.7297(2)
c (Å)	9.3515(3)
V (Å^3)	2091.5(1)
Z	8
λ (Å)	0.72518
Number of reflections	555
No. of fitted structural parameters	47
Number of soft restraints	31
R_p, R_{wp}	0.076, 0.104
R_{Bragg}, *GoF*	0.029, 2.94

2. Thermogravimetric Analysis (TGA)

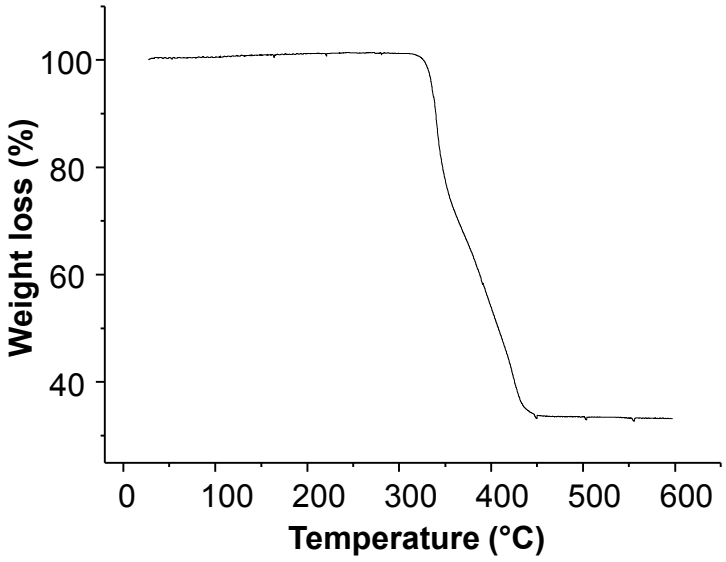

Fig. S2 Thermogravimetric analysis of BioMIL-5.

3. Thermal stability

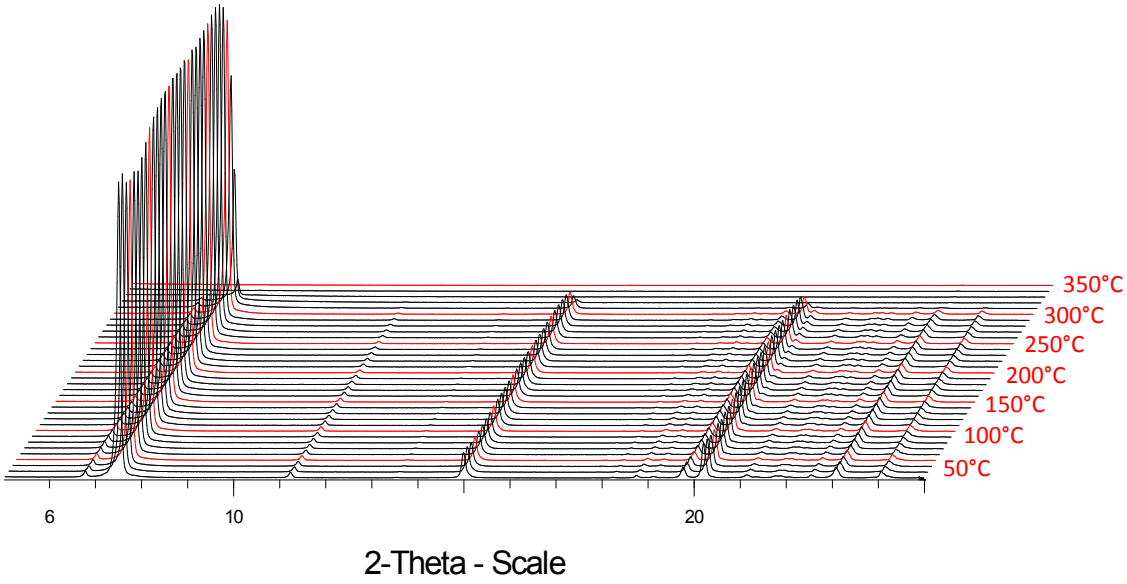

Fig. S3 X ray thermodiffraction patterns (λCu = 1.5405 Å) under air atmosphere of the BioMIL-5. Each red pattern corresponds to a multiple of 50°C. X-ray powder thermodiffractometry (XRTD) was performed using a Bruker D8 Advance diffractometer (θ –θ mode, Cu radiation) equipped with a LYNXEYE XE detector. Data were collected in the 2θ range 5-25° with a 0.02° step width, in the temperature range of 20-400°C at 10°C intervals.

4. Stability in solution

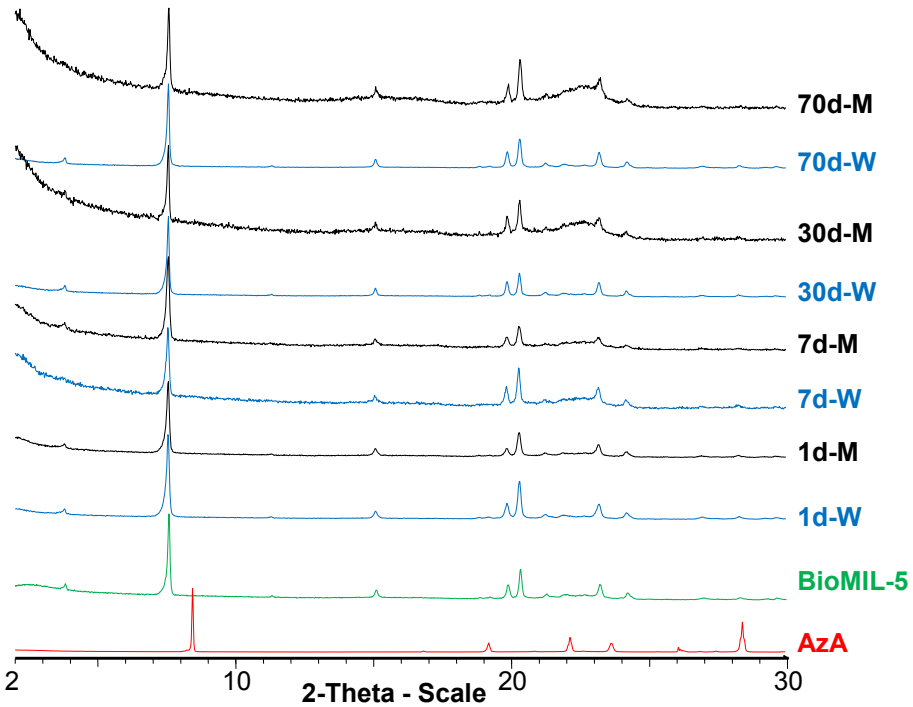

Fig. S4 XRPD patterns of azelaic acid (AzA; red), BioMIL-5 (green) and degradation samples after 1, 7, 30 and 70 days in water (W; blue) and in Mueller Hinton Cation Adjusted Broth medium or MHCA (M; black). X-ray powder diffraction (XRPD) patterns obtained during sample degradation were measured using a high-throughput Bruker D8 Advance diffractometer working on transmission mode and equipped with a focusing Göbel mirror producing CuKα radiation (λ=1.5418 Å) and a LYNXEYE detector. Data were collected at room temperature (RT), in the 2θ range 3–30˚, with a 0.02˚ step width.

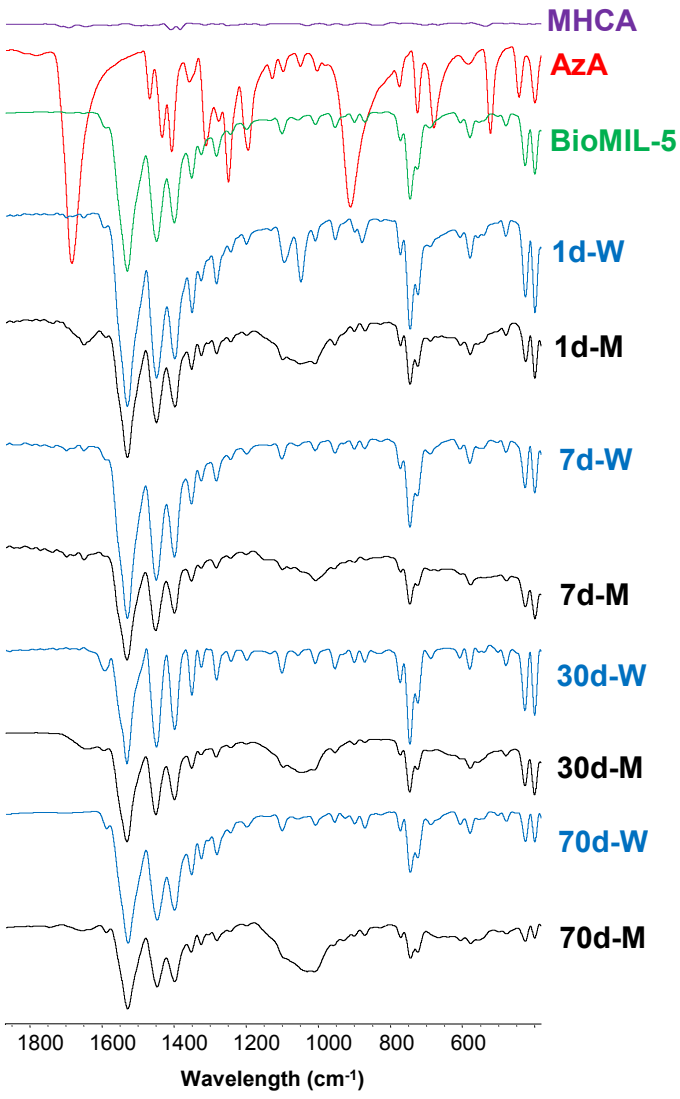

Fig. S5 FTIR spectra of azelaic acid (AzA; red), BioMIL-5 (green), degradation samples after 1, 7, 30 and 70 days in water (W; blue) and in MHCA (M; black).

FTIR spectrum showed the absence of the ν(C=O) band at 1700 cm^{-1} confirmed the absence of free-remaining azelaic ligand. For the degradation samples, the presence of phosphates ν(P-O) was observed at 1000 cm^{-1}.