SUPPORTING INFORMATION

Novel antibacterial azelaic acid BioMOFs

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PXRD

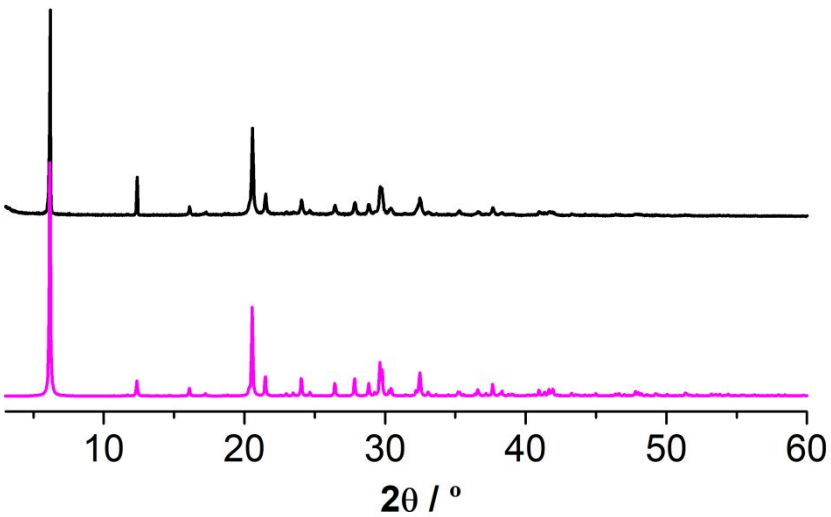

Figure S1 – PXRD patterns of the experimental (*top*) and simulated (*bottom*) compound **1**.

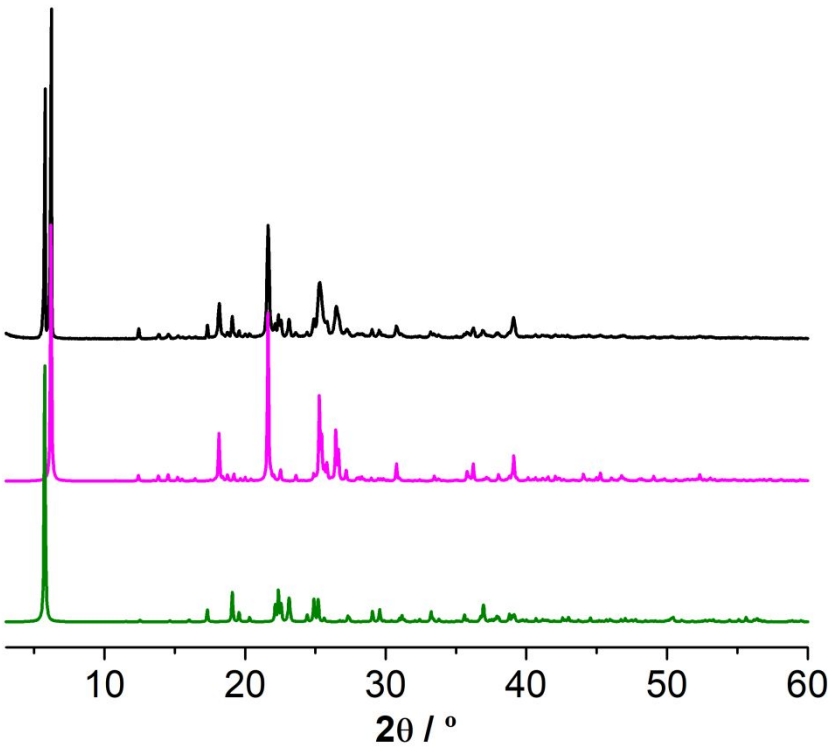

Figure S2 – PXRD patterns of the experimental compound **2** (*top*), and simulated compound **2** (*middle*) and **3** (*bottom*).

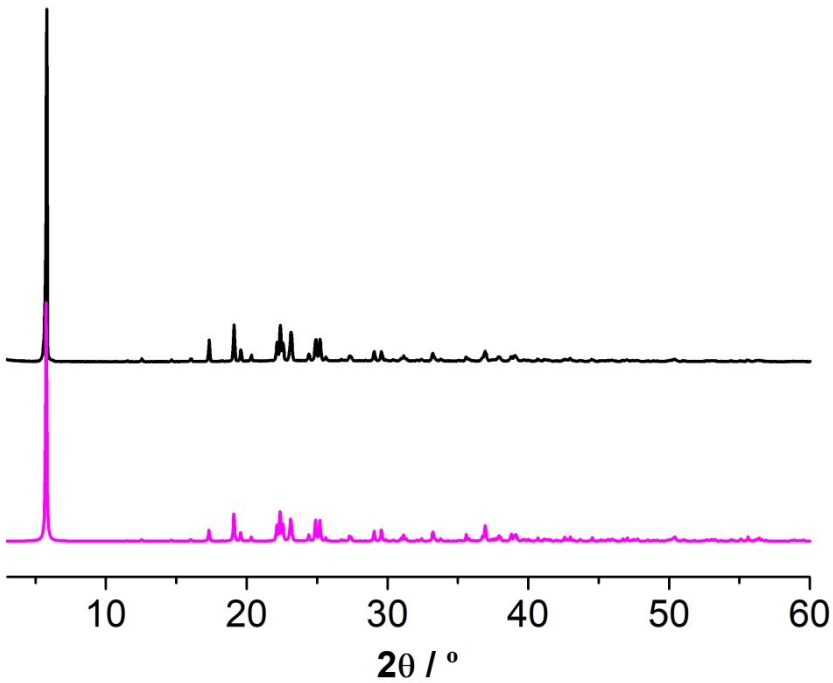

Figure S3 – PXRD patterns of the experimental (*top*) and simulated (*bottom*) compound **3**.

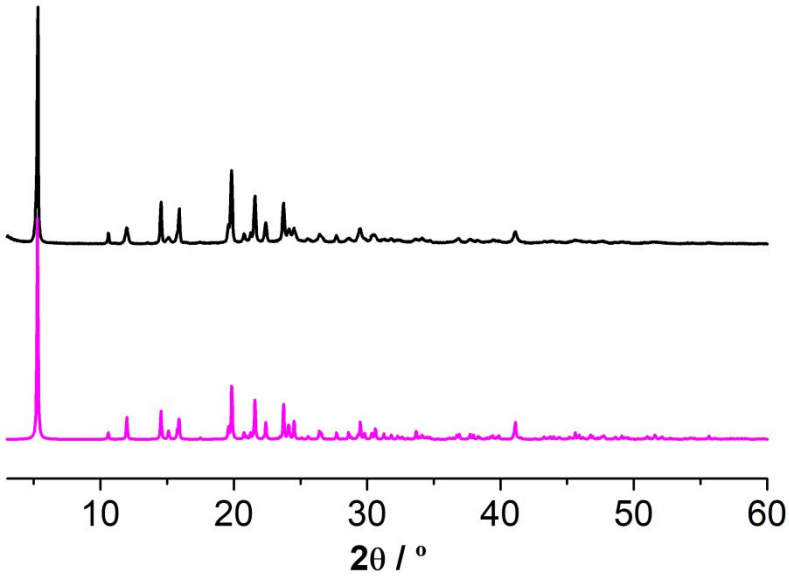

Figure S4 – PXRD patterns of the experimental (*top*) and simulated (*bottom*) compound **4**.

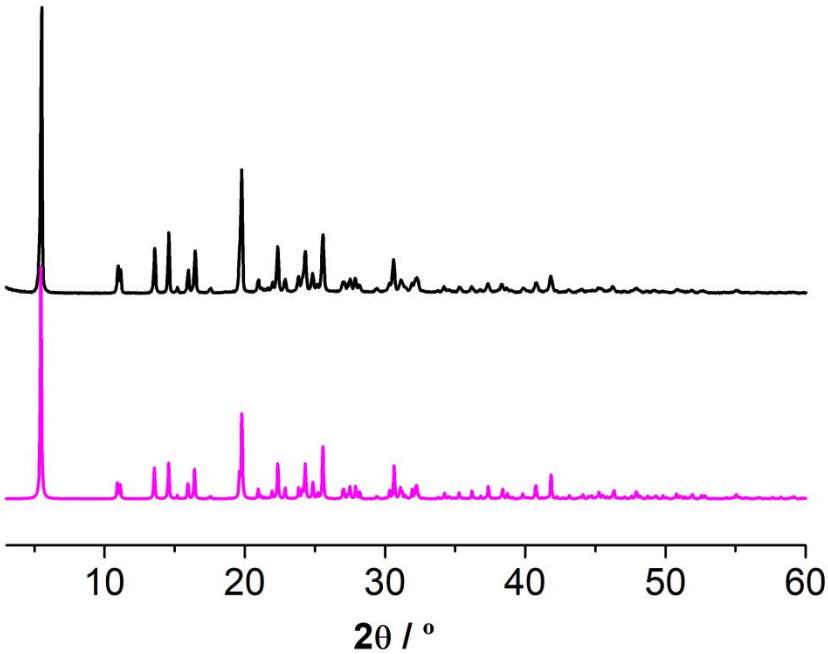

Figure S5 – PXRD patterns of the experimental (*top*) and simulated (*bottom*) compound **5**.

Crystallographic Studies

Table S1 – Selected bond lengths (Å) and angles (°C) for **1**.

K(1) - O(1)	2.837(2)	O(1) - K(1) - O(5)	78.51(7)	O(8) - K(2) - O(3)j	97.02(7)
K(1) - O(3)	2.784(2)	O(1) - K(1) - O(7)	127.58(7)	O(5)d - K(2) - O(7)d	64.93(6)

K(1) - O(5)	2.820(2)	O(1) - K(1) - O(2)h	157.17(6)	O(5)d - K(2) - O(1)j	116.86(7)
K(1) - O(7)	3.039(2)	O(1) - K(1) - O(6)i	103.00(8)	O(5)d - K(2) - O(3)j	81.66(7)
K(1) - O(2)h	2.805(2)	O(1) - K(1) - O(8)i	70.46(7)	O(7)d - K(2) - O(1)j	70.29(6)
K(1) - O(6)i	3.058(3)	O(3) - K(1) - O(5)	93.96(7)	O(7)d - K(2) - O(3)j	96.70(7)
K(1) - O(8)i	2.835(3)	O(3) - K(1) - O(7)	81.16(7)	O(1)j - K(2) - O(3)j	61.72(6)
K(2) - O(2)	2.897(2)	O(3) - K(1) - O(2)h	137.29(6)	K(1) - O(1) - K(2)i	79.23(5)
K(1) - O4h	3.136(3)	O(3) - K(1) - O(6)i	67.40(8)	K(2) - O(2) - K(1)g	97.53(7)
K(2) - O(4)	2.963(3)	O(3) - K(1) - O(8)i	98.68(7)	K(1) - O(3) - K(2)i	81.38(6)
K(2) - O(6)	2.968(3)	O(5) - K(1) - O(7)	64.57(6)	K(1) - O(5) - K(2)e	96.49(7)
K(2) - O(8)	2.781(2)	O(5) - K(1) - O(2)h	100.80(7)	K(2) - O(6) - K(1)j	76.02(6)
K(2) - O(5)d	2.848(2)	O(5) - K(1) - O(6)i	157.56(7)	K(1) - O(7) - K(2)e	89.07(6)
K(2) - O(7)d	2.989(2)	O(4) - K(2) - O(8)	83.98(8)	K(2) - O(8) - K(1)j	82.74(7)
K(2) - O(1)j	2.982(2)	O(4) - K(2) - O(5)d	99.55(8)	O(1) - C(1) - O(2)	122.5(3)
K(2) - O(3)j	2.908(3)	O(4) - K(2) - O(7)d	70.17(7)	O(3) - C(6) - O(4)	122.7(3)
O(1) - C(1)	1.233(5)	O(4) - K(2) - O(1)j	104.63(6)	O(5) - C(11) - O(6)	123.1(3)
O(2) - C(1)	1.296(4)	O(4) - K(2) - O(3)j	164.34(6)	O(7) - C(16) - O(8)	121.8(2)
O(3) - C(6)	1.294(4)	O(6) - K(2) - O(8)	63.09(7)	Symmetry transformations used to generate equivalent atoms:	
O(4) - C(6)	1.208(5)	O(6) - K(2) - O(5)d	109.03(7)	h = 3/2-x,1/2-y,1/2+z	
O(5) - C(11)	1.292(4)	O(6) - K(2) - O(7)d	163.74(7)	i = 3/2-x,-1/2+y,z	
O(6) - C(11)	1.214(5)	O(6) - K(2) - O(1)j	101.73(7)	d = x,1-y,-1/2+z	
O(7) - C(16)	1.229(4)	O(6) - K(2) - O(3)j	67.13(7)	j = 3/2-x,1/2+y,z	
O(8) - C(16)	1.295(3)	O(8) - K(2) - O(5)d	171.63(6)	g = 3/2-x,1/2-y,-1/2+z	
		O(8) - K(2) - O(7)d	123.44(6)	e = x,1-y,1/2+z	
O(1) - K(1) - O(3)	65.04(6)	O(8) - K(2) - O(1)j	69.08(7)		

Table S2 – Selected bond lengths (Å) and angles (°C) for **2**.

Na(1) - O(1)	2.403(5)	O(11) - C(27)	1.227(7)	O(6)d - Na(3) - O(13)d	103.36(17)
Na(1) - O(7)	2.388(5)	O(12) - C(27)	1.292(7)	O(12) - Na(4) - O(13)	107.79(19)

Na(1) - O(14)d	2.439(5)	O(13) - C(28)	1.238(7)	O(12) - Na(4) - O(2)e	157.5(2)
Na(1) - O(5)h	2.417(5)	O(14) - C(28)	1.287(7)	O(12) - Na(4) - O(10)e	80.98(17)
Na(1) - O(16)k	2.344(5)	O(15) - C(36)	1.224(7)	O(12) - Na(4) - O(3)j	88.97(17)
Na(2) - O(4)	2.352(5)	O(16) - C(36)	1.306(7)	O(13) - Na(4) - O(2)e	94.53(18)
Na(2) - O(5)	2.720(6)			O(13) - Na(4) - O(10)e	86.88(17)
Na(2) - O(11)	2.355(5)	O(7) - Na(1) - O(16)k	88.93(17)	O(13) - Na(4) - O(3)j	102.08(17)
Na(2) - O(9)e	2.354(5)	O(14)d - Na(1) - O(5)h	104.28(17)	O(2)e - Na(4) - O(10)e	103.59(17)
Na(2) - O(1)g	2.402(5)	O(14)d - Na(1) - O(16)k	147.2(2)	O(2)e - Na(4) - O(3)j	83.47(16)
Na(2) – O(6)b	2.869(6)	O(5)h - Na(1) - O(16)k	80.90(16)	O(10)e - Na(4) - O(3)j	168.3(2)
Na(3) - O(8)	2.323(5)	O(5) - Na(2) - O(6)b	175.97(16)	Na(1) - O(1) - Na(2)h	100.43(18)
Na(3) - O(15)	2.369(5)	O(4) - Na(2) - O(5)	99.22(17)	O(7) - C(18) - O(8)	122.9(5)
Na(3) - O(10)a	2.622(6)	O(4) - Na(2) - O(11)	94.46(17)	O(9) - C(19) - O(10)	124.1(5)
Na(3) - O(6)d	2.402(5)	O(4) - Na(2) - O(9)e	160.7(2)	O(1) - C(1) - O(2)	124.2(5)
Na(3) - O(13)d	2.395(5)	O(4) - Na(2) - O(1)g	82.24(16)	O(11) - C(27) - O(12)	122.1(5)
Na (3) – O(9)	2.994(6)	O(5) - Na(2) - O(11)	90.34(16)	O(13) - C(28) - O(14)	123.3(5)
Na(4) - O(12)	2.315(5)	O(5) - Na(2) - O(9)e	99.86(18)	O(3) - C(9) - O(4)	123.3(5)
Na(4) - O(13)	2.421(5)	O(5) - Na(2) - O(1)g	80.64(16)	O(5) - C(10) - O(6)	122.6(5)
Na(4) - O(2)e	2.399(5)	O(11) - Na(2) - O(9)e	82.85(16)	O(15) - C(36) - O(16)	122.4(5)
Na(4) - O(10)e	2.433(5)	O(11) - Na(2) - O(1)g	169.72(19)		
Na(4) - O(3)j	2.384(5)	O(9)e - Na(2) - O(1)g	103.43(17)		
O(1) - C(1)	1.243(8)	O(8) - Na(3) - O(15)	94.87(17)		
O(2) - C(1)	1.271(8)	O(8) - Na(3) - O(10)a	102.79(18)		
O(3) - C(9)	1.208(7)	O(8) - Na(3) - O(6)d	154.8(2)		
O(4) - C(9)	1.304(7)	O(8) - Na(3) - O(13)d	80.03(16)		
O(5) - C(10)	1.239(8)	O(15) - Na(3) - O(10)a	91.87(17)		
O(6) - C(10)	1.295(8)	O(15) - Na(3) - O(6)d	83.92(16)		
O(7) - C(18)	1.212(7)	O(15) - Na(3) - O(13)d	171.95(19)		
O(8) - C(18)	1.302(7)	O(10)a - Na(3) - O(6)d	102.41(18)		
O(9) - C(19)	1.279(8)	O(10)a - Na(3) - O(13)d	83.27(16)		

Symmetry transformations used to generate equivalent atoms:

h = 3/2-x,y,1/2+z

k = 1/2+x,-y,z

e = 1-x,1-y,-1/2+z

g = 3/2-x,y,-1/2+z

j = -1/2+x,1-y,z

a = x,-1+y,z

d = 1-x,-y,1/2+z

b = x, y+1, z

O(10) - C(19) 1.233(8)	O(10)a - Na(3) - O(9) 175.36(16)	

Table S3 – Selected bond lengths (Å) and angles (°C) for **3**.

Na(1) - O(1) 2.2787(17)	O(1W) - Na(1) - O(4)d 92.16(6)	O(3)g - Na(2) - O(2)i 126.17(6)
Na(1) - O(1W) 2.3123(19)	O(1W) - Na(1) - O(3)h 83.87(6)	Na(1) - O(1W) - Na(2)b 79.01(6)
Na(1) - O(4)d 2.3382(18)	O(1W) - Na(1) - O(2)j 85.00(6)	Na(1) - O(1W) - Na(2)f 87.78(6)
Na(1) - O(3)h 2.3656(15)	O(4)d - Na(1) - O(3)h 82.65(6)	Na(2)b - O(1W) - Na(2)f 157.44(8)
Na(1) - O(2)j 2.4211(15)	O(4)d - Na(1) - O(2)j 93.58(6)	Na(2) - O(2) - Na(2)i 88.87(5)
Na(2) - O(2) 2.4005(17)	O(3)h - Na(1) - O(2)j 168.09(6)	Na(2) - O(2) - Na(1)k 113.68(6)
Na(2) - O(1W)a 2.4894(18)	O(2) - Na(2) - O(1W)a 171.17(6)	Na(2)i - O(2) - Na(1)k 92.34(5)
Na(2) - O(4)c 2.4632(17)	O(2) - Na(2) - O(4)c 100.15(6)	Na(2)g - O(3) - Na(1)h 79.30(5)
Na(2) - O(1W)e 2.7228(19)	O(2) - Na(2) - O(1W)e 84.20(5)	Na(1)c - O(4) - Na(2)d 79.06(5)
Na(2) - O(3)g 2.4256(17)	O(2) - Na(2) - O(3)g 94.98(6)	O(1) - C(1) - O(2) 124.10(19)
Na(2) - O(2)i 2.4352(16)	O(2) - Na(2) - O(2)i 91.13(5)	O(3) - C(9) - O(4) 124.35(18)
O(1) - C(1) 1.246(3)	O(1W)a - Na(2) - O(4)c 85.12(6)	Symmetry transformations used to generate equivalent atoms:
O(2) - C(1) 1.265(3)	O(1W)a - Na(2) - O(1W)e 103.86(6)	d = 1-x,1/2+y,1/2-z
O(3) - C(9) 1.269(2)	O(1W)a - Na(2) - O(3)g 78.99(6)	h = 1-x,2-y,1-z
O(4) - C(9) 1.252(2)	O(1W)a - Na(2) - O(2)i 87.35(6)	j = x,3/2-y,-1/2+z
	O(4)c - Na(2) - O(1W)e 79.03(6)	a = x,-1+y,z
O(1) - Na(1) - O(1W) 110.53(6)	O(4)c - Na(2) - O(3)g 78.89(5)	c = 1-x,-1/2+y,1/2-z
O(1) - Na(1) - O(4)d 156.37(7)	O(4)c - Na(2) - O(2)i 151.75(6)	e = 2-x,-1/2+y,1/2-z
O(1) - Na(1) - O(3)h 92.98(6)	O(1W)e - Na(2) - O(3)g 157.40(6)	g = 1-x,1-y,1-z
O(1) - Na(1) - O(2)j 94.86(6)	O(1W)e - Na(2) - O(2)i 76.43(5)	i = 2-x,1-y,1-z

Table S4 – Selected bond lengths (Å) and angles (°C) for **4**.

Mg(1) - O(1)	1.9983(13)	O(1) - Mg(1) - O(1W)	84.29(5)	O(2W) - Mg(1) - O(3)c	171.23(5)
Mg(1) - O(1W)	2.1350(12)	O(1) - Mg(1) - O(2W)	89.39(5)	O(3W) - Mg(1) - O(4)b	94.94(6)
Mg(1) - O(2W)	2.1552(13)	O(1) - Mg(1) - O(3W)	168.14(6)	O(3W) - Mg(1) - O(3)c	90.39(6)
Mg(1) - O(3W)	2.0923(14)	O(1) - Mg(1) - O(4)b	91.77(6)	O(4)b - Mg(1) - O(3)c	95.87(5)
Mg(1) - O(4)b	2.0199(12)	O(1) - Mg(1) - O(3)c	98.65(5)	O(1) - C(1) - O(2)	121.36(15)
Mg(1) - O(3)c	2.0592(12)	O(1W) - Mg(1) - O(2W)	86.09(5)	O(3) - C(9) - O(4)	123.19(14)
O(1) - C(1)	1.244(2)	O(1W) - Mg(1) - O(3W)	87.88(6)		
O(2) - C(1)	1.259(2)	O(1W) - Mg(1) - O(4)b	172.35(5)	Symmetry transformations used to generate equivalent atoms:	
O(3) - C(9)	1.2523(19)	O(1W) - Mg(1) - O(3)c	91.22(5)	b = 1-x,1/2+y,1/2-z	
O(4) - C(9)	1.261(2)	O(2W) - Mg(1) - O(3W)	81.18(6)	c = 1-x,1-y,1-z	
		O(2W) - Mg(1) - O(4)b	87.31(5)		

Table S5 – Selected bond lengths (Å) and angles (°C) for **5**.

Mg(1) - O(1)	2.008(2)	O(1) - Mg(1) - O(1W)	89.65(9)	O(2W) - Mg(1) - O(3)b	173.64(9)
Mg(1) – O(1W)	2.154(2)	O(1) - Mg(1) - O(2W)	84.37(9)	O(3W) - Mg(1) - O(4)a	90.82(9)
Mg(1) – O(2W)	2.132(2)	O(1) - Mg(1) - O(3W)	168.39(9)	O(3W) - Mg(1) - O(3)b	95.25(9)
Mg(1) - O(3W)	2.093(3)	O(1) - Mg(1) - O(4)a	97.37(8)	O(4)a - Mg(1) - O(3)b	96.52(8)
Mg(1) – O(4)a	2.050(2)	O(1) - Mg(1) - O(3)b	92.01(8)	O(1) - C(1) - O(2)	120.4(2)
Mg(1) - O(3)b	2.006(2)	O(1W) - Mg(1) - O(2W)	87.43(8)	O(3) - C(9) - O(4)	123.3(2)
O(1) - C(1)	1.262(3)	O(1W) - Mg(1) - O(3W)	81.66(10)		
O(2) - C(1)	1.254(3)	O(1W) - Mg(1) - O(4)a	171.86(9)	Symmetry transformations used to generate equivalent atoms:	
O(3) - C(9)	1.275(3)	O(1W) - Mg(1) - O(3)b	87.31(8)	a = 1-x,y,1/2-z	
O(4) - C(9)	1.245(3)	O(2W) - Mg(1) - O(3W)	87.54(10)	b = 1-x,1-y,1-z	
		O(2W) - Mg(1) - O(4)a	89.15(8)		

Table S6 – List of the main hydrogen bonds found for compounds **1**-**5**.

	Sym. Op.	D–H···A	*d*(H···A) (Å)	*d*(D···A) (Å)	(DHA) (deg)
1	*x, y, z*	O_3–H_3···O_1	2.57(4)	3.022(2)	111(4)
	x, y, z	O_3–H_3···O_2	1.55(4)	2.460(3)	169(4)
	x, y, z	O_8–H_8···O_5	1.50(5)	2.457(3)	171(5)
	x, y, z	O_8–H_8···O_6	2.52(5)	3.012(3)	112(4)
2	*3/2-x, y, -1/2+z*	O_4–H_4···O_1	2.48(6)	3.126(6)	127(6)
	3/2-x, y, -1/2+z	O_4–H_4···O_2	1.55(6)	2.466	171(4)
	1-x, -y, 1/2+z	O_8–H_8···O_{13}	2.44(8)	3.034(6)	122(8)
	1-x, -y, 1/2+z	O_8–H_8···O_{14}	1.54(7)	2.464(6)	173(12)
	1-x, 1-y, -1/2+z	O_{12}–H_{12}···O_9	1.56(8)	2.452(6)	163(11)
	1-x, 1-y, -1/2+z	O_{12}–H_{12}···O_{10}	2.42(8)	3.084(7)	130(10)
	1-x, -y, 1/2+z	O_{16}–H_{16}···O_5	2.49(9)	3.089(6)	124(10)
	1-x, -y, 1/2+z	O_{16}–H_{16}···O_6	1.55(8)	2.462(6)	175(14)
3	*2-x, 1/2+y, 1/2-z*	O_{1w}–H_{1w}···O_1	1.92(3)	2.728(2)	176(3)
	1+x, y, z	O_{1w}–H_{2w}···O_3	1.87(3)	2.721(2)	175(3)
4	*x, 1/2-y, 1/2+z*	O_{1w}–H_{1w}···O_2	1.95(3)	2.7358(18)	170(2)
	x, 3/2-y, 1/2+z	O_{1w}–H_{2w}···O_{2w}	1.97(3)	2.8102(18)	168(2)
	2-x, 1-y, 1-z	O_{2w}–H_{3w}···O_{1w}	2.10(2)	2.8719(18)	166(2)
	2-x, 1-y, 1-z	O_{2w}–H_{4w}···O_1	2.39(3)	2.9304(17)	125(2)
	2-x, 1-y, 1-z	O_{2w}–H_{4w}···O_2	2.08(3)	2.8939(18)	177(2)
	1-x, 1-y, 1-z	O_{3w}–H_{5w}···O_4	2.07(3)	2.7170(19)	147(3)
	x, 1+y, z	O_{3w}–H_{6w}···O_2	1.98(3)	2.8134(19)	168(2)
5	*3/2-x, 1/2-y, 1-z*	O_{1w}–H_{1w}···O_{2w}	2.06(3)	2.822(3)	159(3)
	3/2-x, 1/2-y, 1-z	O_{1w}–H_{2w}···O_1	2.18(4)	2.859(3)	133(3)

3/2-x, 1/2-y, 1-z	O_{1w}–H_{2w}···O_2	2.20(4)	3.065(3)	164(4)
x, -y, -1/2+z	O_{2w}–H_{3w}···O_2	1.75(4)	2.715(3)	171(3)
x, 1-y, -1/2+z	O_{2w}–H_{4w}···O_{1w}	2.07(4)	2.822(3)	160(4)
x, 1+y, z	O_{3w}–H_{5w}···O_2	1.88(4)	2.802(3)	168(3)
1-x, y, 1/2-z	O_{3w}–H_{6w}···O_3	2.05(3)	2.726(3)	144(3)

FTIR

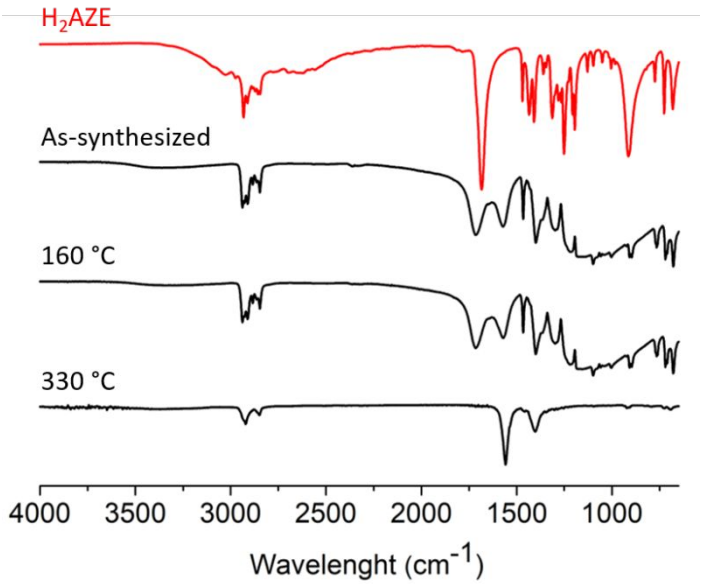

Figure S6 – FTIR (from the top to the bottom) for azelaic acid compared with as-synthesized, as-prepared and after thermal treatment at 160 °C and 330 °C for compound **1**.

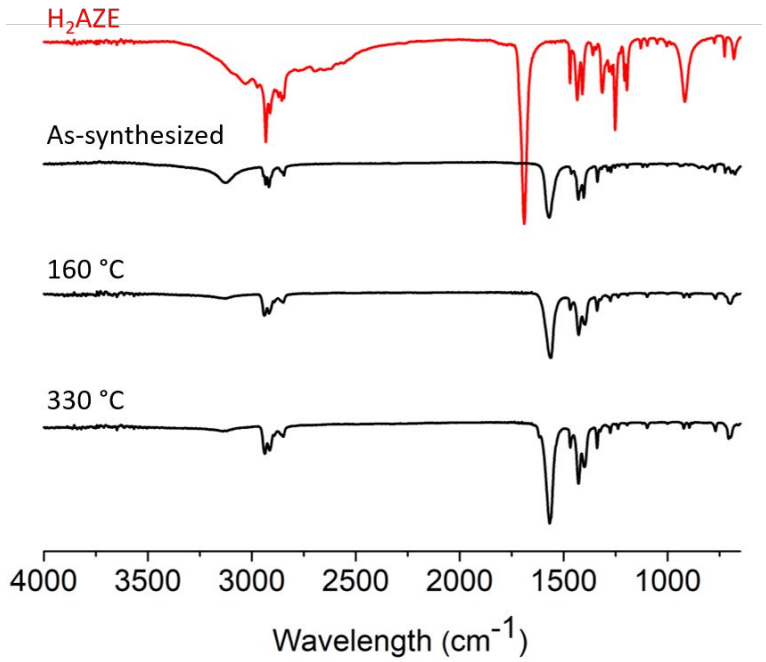

Figure S7 – FTIR (from the top to the bottom) for azelaic acid compared with as-synthesized, as-prepared and after thermal treatment at 160 °C and 330 °C for compound **3**.

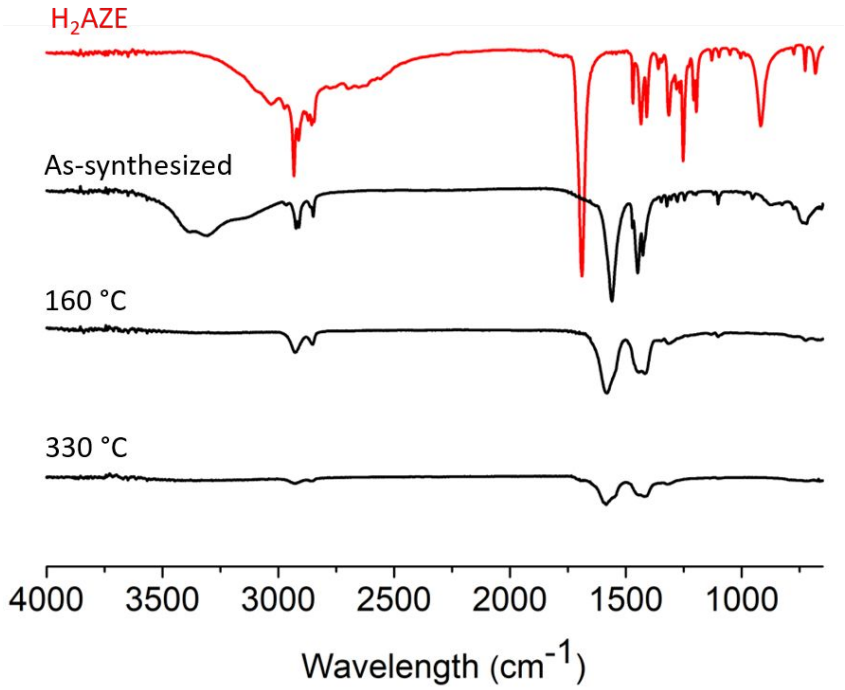

Figure S8 – FTIR (from the top to the bottom) for azelaic acid compared with as-synthesized, as-prepared and after thermal treatment at 160 °C and 330 °C for compound **4**.

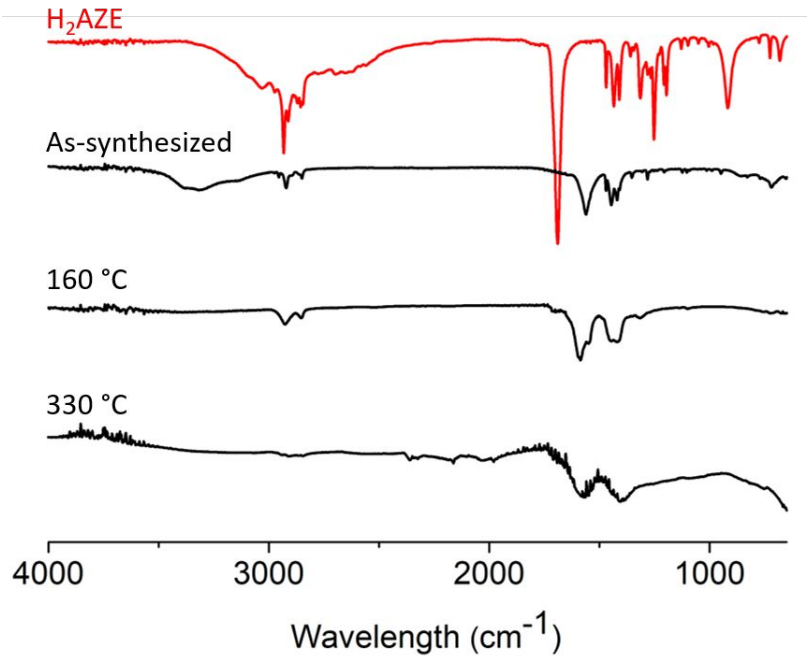

Figure S9 – FTIR (from the top to the bottom) for azelaic acid compared with as-synthesized, as-prepared and after thermal treatment at 160 °C and 330 °C for compound **5**.

Thermal Stability

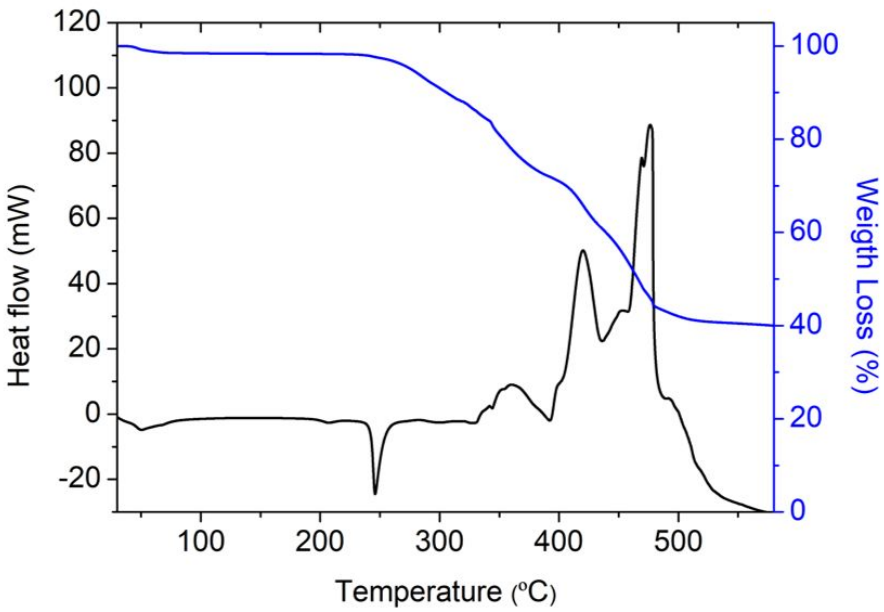

Figure S10 – DSC (black) and TGA (blue) of compound **1**

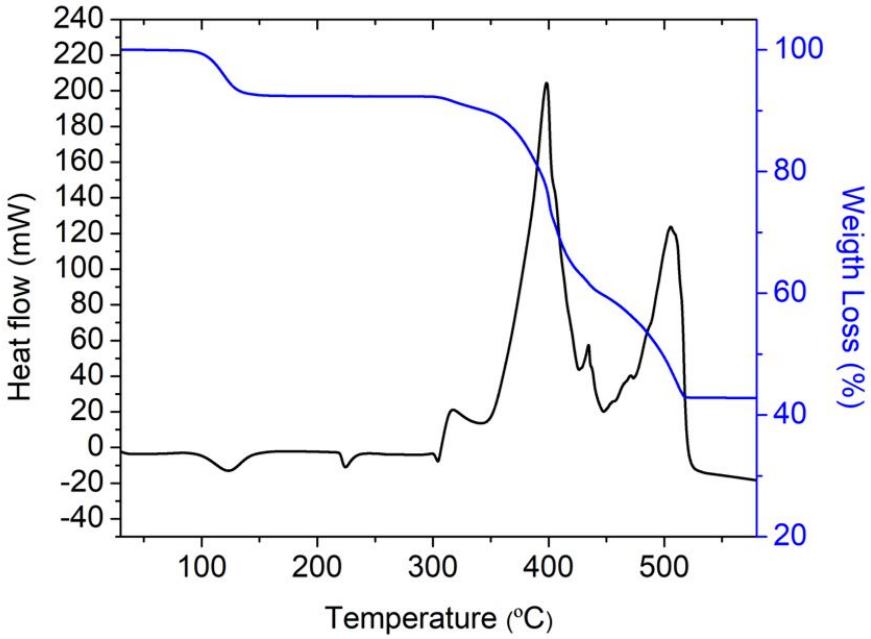

Figure S11 – DSC (black) and TGA (blue) of compound **3**.

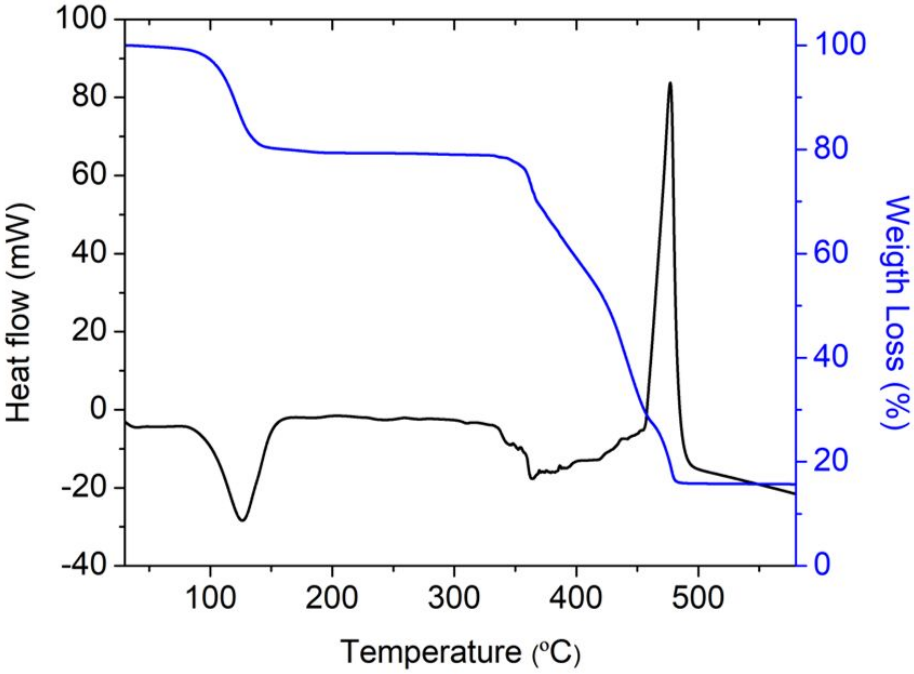

Figure S12 – DSC (black) and TGA (blue) of compound **4**.

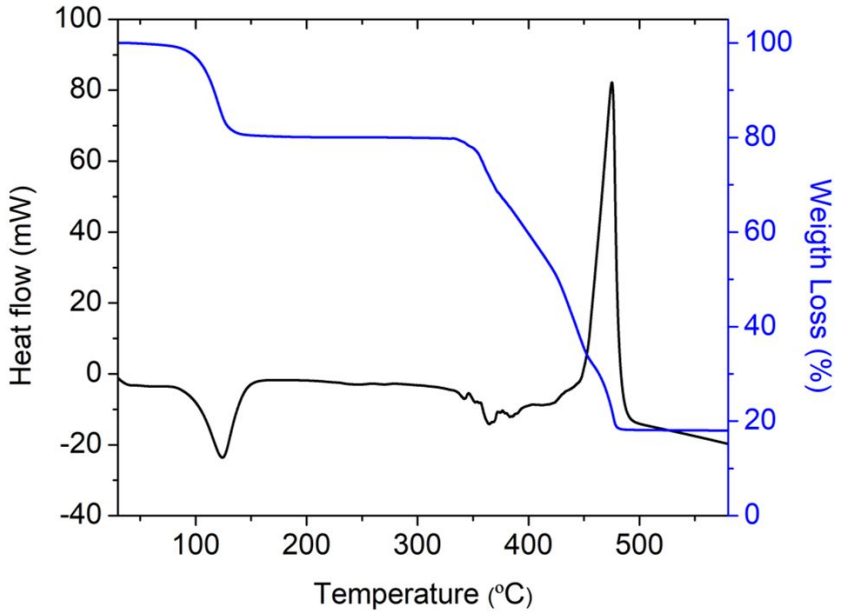

Figure S13 – DSC (black) and TGA (blue) of compound **5**.

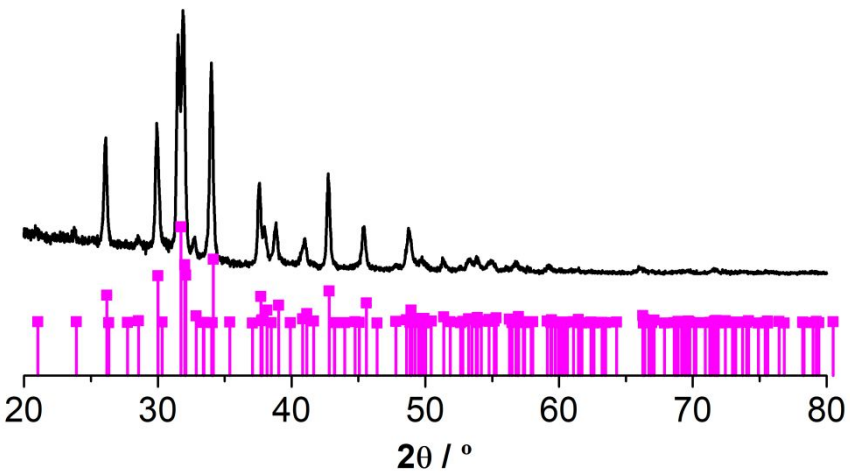

Figure S14 - Comparison between the experimental PXRD pattern of **1** obtained after TGA studies (*top*) and the powder pattern of K_2CO_3 (*bottom*) available at Crystallography Open Database with the code COD 9009645.

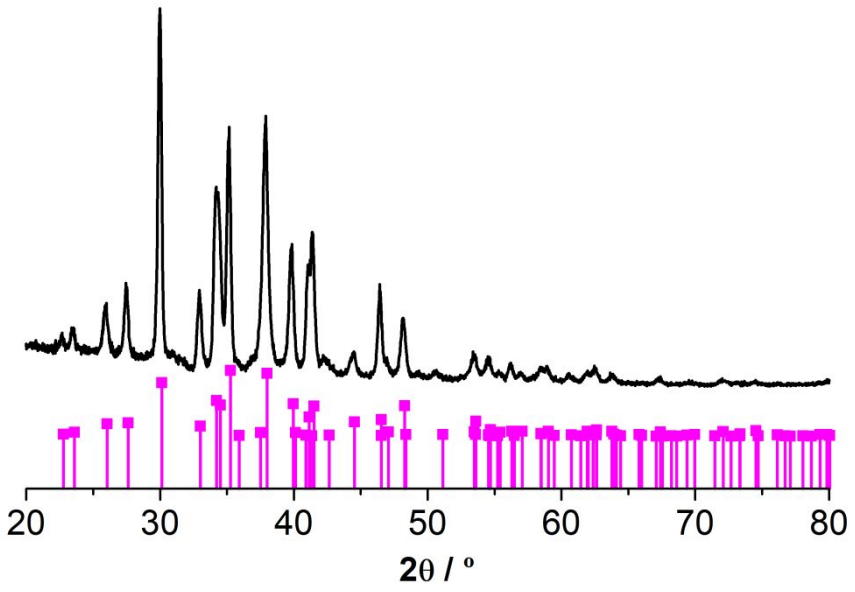

Figure S15 - Comparison between the experimental PXRD pattern of **3** obtained after TGA studies (*top*) and the powder pattern of Na_2CO_3 (*bottom*) available at Crystallography Open Database with the code COD 9009418.

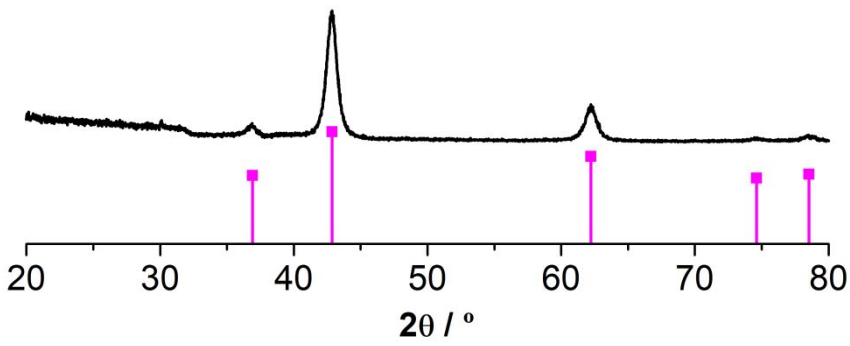

Figure S16 - Comparison between the experimental PXRD pattern of **4** obtained after TGA studies (*top*) and the powder pattern of MgO (*bottom*) available at Crystallography Open Database with the code COD 5000225.

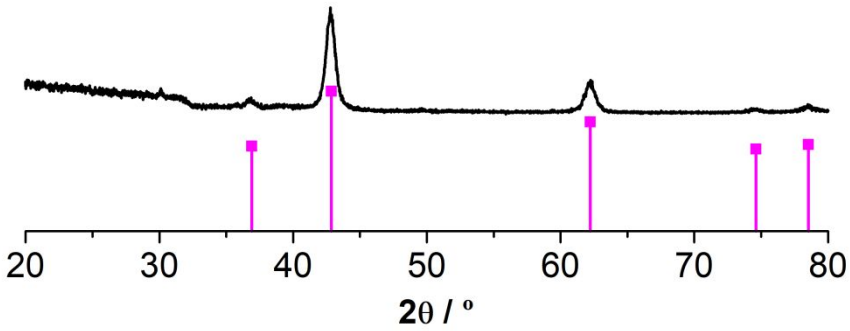

Figure S17 - Comparison between the experimental PXRD pattern of **5** obtained after TGA studies (*top*) and the powder pattern of MgO (*bottom*) available at Crystallography Open Database with the code COD 5000225.

Reversibility Study

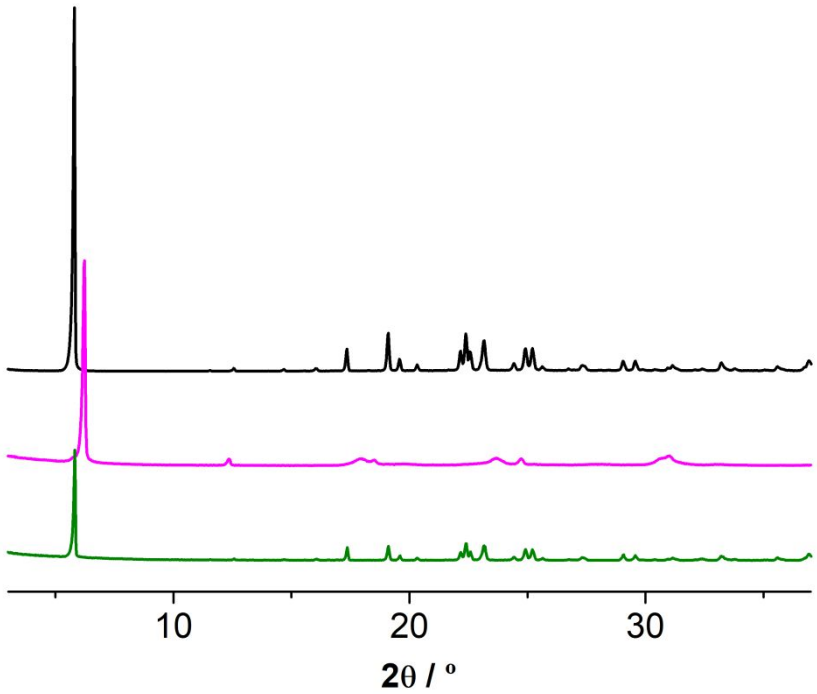

Figure S18 – PXRD patterns of the as-synthesized **3** (*top*), after treatment at 160 °C for 24h (*middle*) and after rehydration (*bottom*).

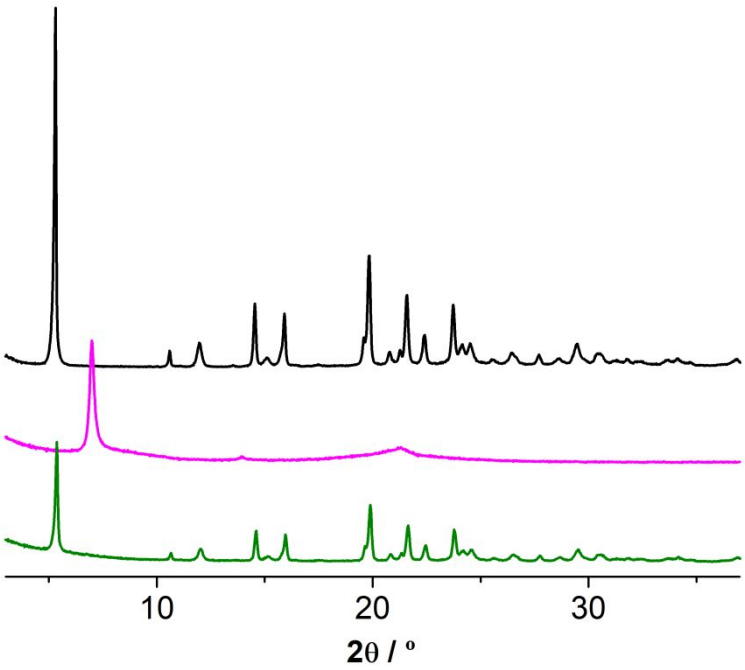

Figure S19 – PXRD patterns of the as-synthesized **4** (*top*), after treatment at 160 °C for 24h (*middle*) and after rehydration (*bottom*).

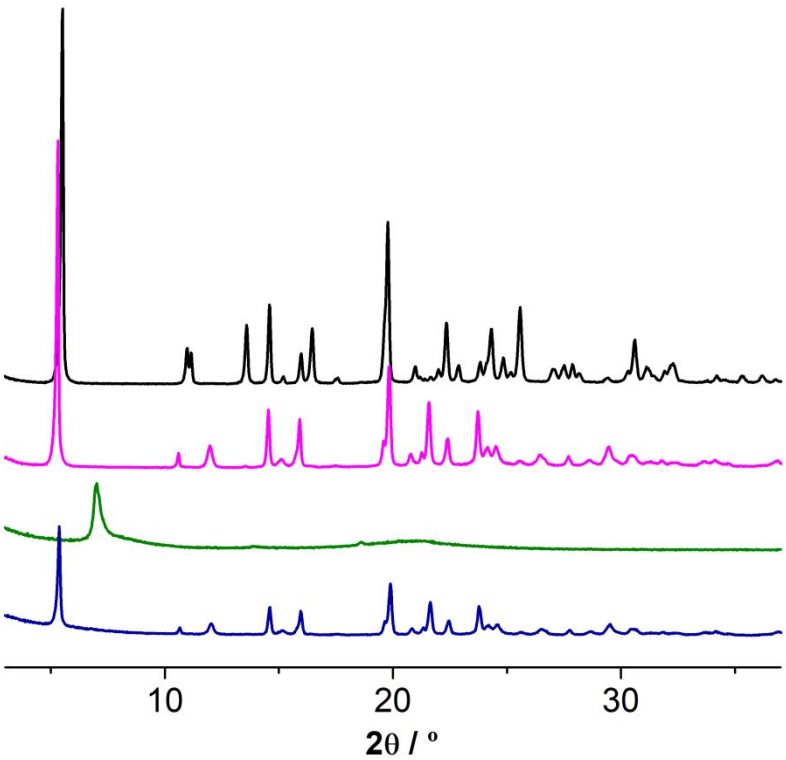

Figure S20 – PXRD patterns (from the top to bottom) of the as-synthesized **5** and **4**, after treatment of **5** at 160 °C for 24h and after rehydration.

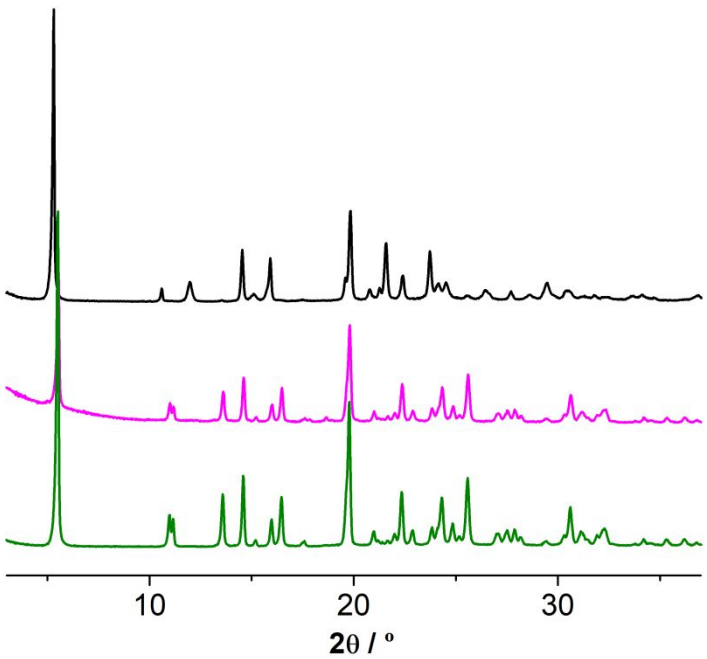

Figure S21 – PXRD patterns of the as-synthesized **4** (*top*), after grinding for 10 min with 30 µL of water (*middle*) and the as-synthesized **5** (*bottom*).

Solubility studies by quantitative ^{1}H NMR analysis

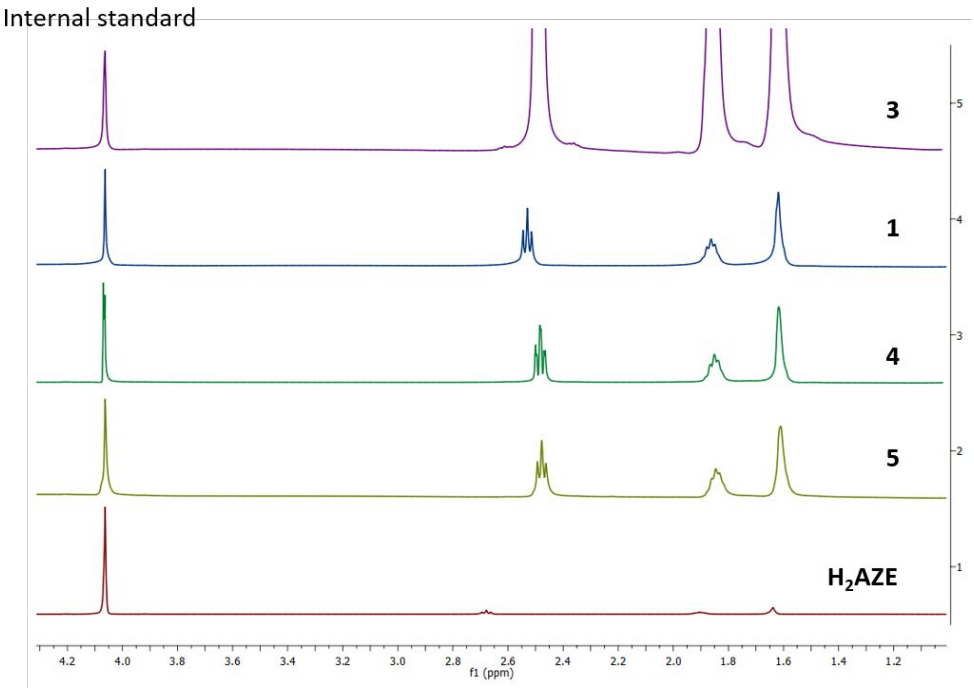

Figure S22 – ^{1}H NMR spectra of (from the bottom to top) Azelaic acid (H_2AZE), compound **5**, **4**, **1** and **3**.

Table S7 –BioMOFs **1**, **3**-**5** solubility in mol(H_2AZE).L^{-1} and in g(MOF).L^{-1}.

BioMOF	Solubility mol(H_2AZE).L^{-1}	Solubility g(MOF).L^{-1}
1	0.29(±2)	131(±8)
3	2.45(±11)	613(±27)
4	0.24(±2)	63(±6)
5	0.23(±2)	62(±5)

MM(**1**) = 452.62 g.mol^{-1}; MM(**3**) = 250.20 g.mol^{-1}; MM(**4** and **5**) = 264.56 g.mol^{-1}

Moisture stability Studies

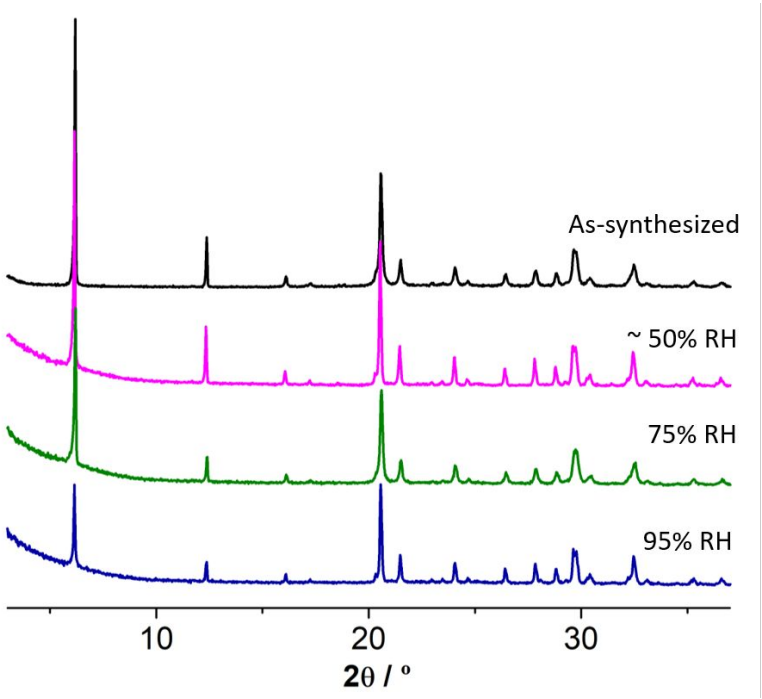

Figure S23 – PXRD patterns (from the top to the bottom) of the as-synthesized **1** and after shelf and moisture treatment for 3 months at ambient (~ 50%), 75 % and 95 % RH conditions.

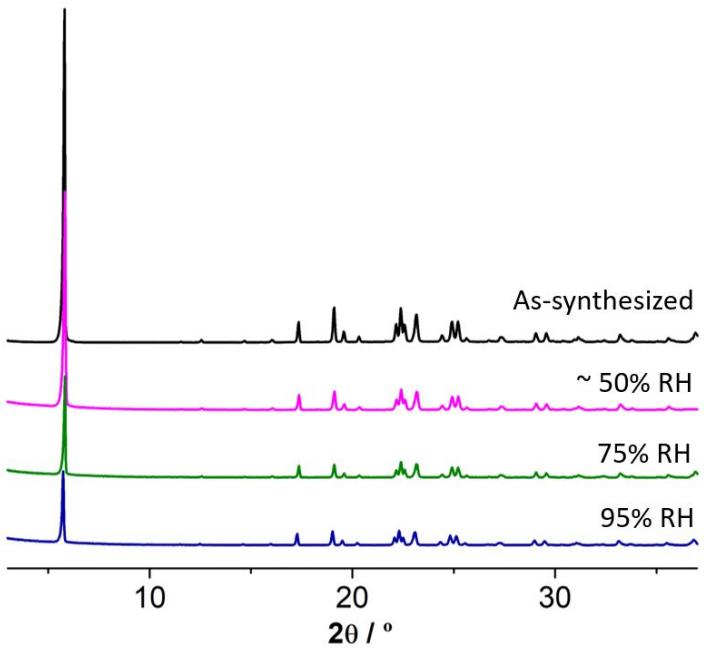

Figure S24 – PXRD patterns (from the top to the bottom) of the as-synthesized **3**, after shelf and moisture treatment for 3 months at ambient (~ 50%) and 75 % RH conditions and after 1 day at 95 % RH conditions, as it liquifies after that.

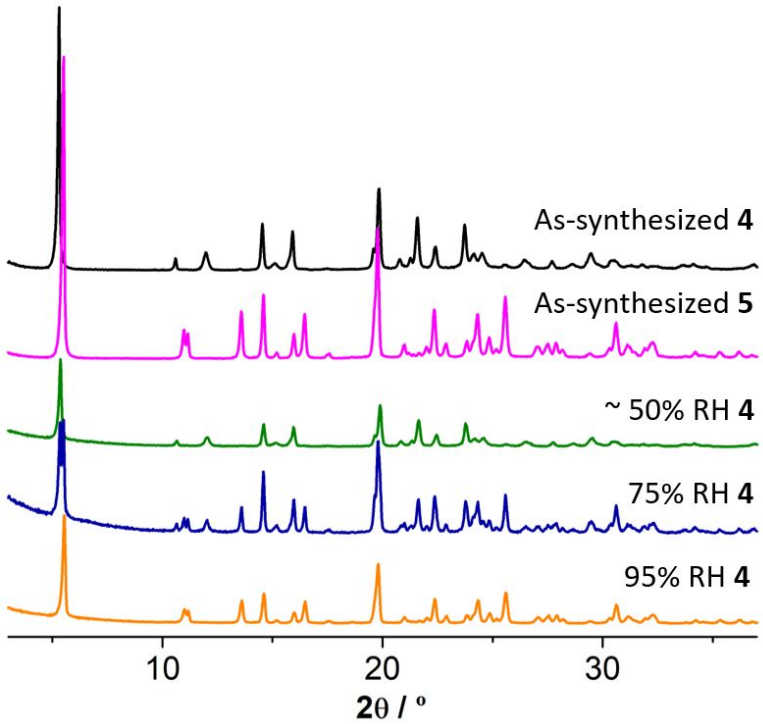

Figure S25 – PXRD patterns (from the top to the bottom) of the as-synthesized **4** and **5** and after shelf and moisture treatment of **4** for 3 months at ambient (~ 50%), 75 % and 95 % RH conditions.

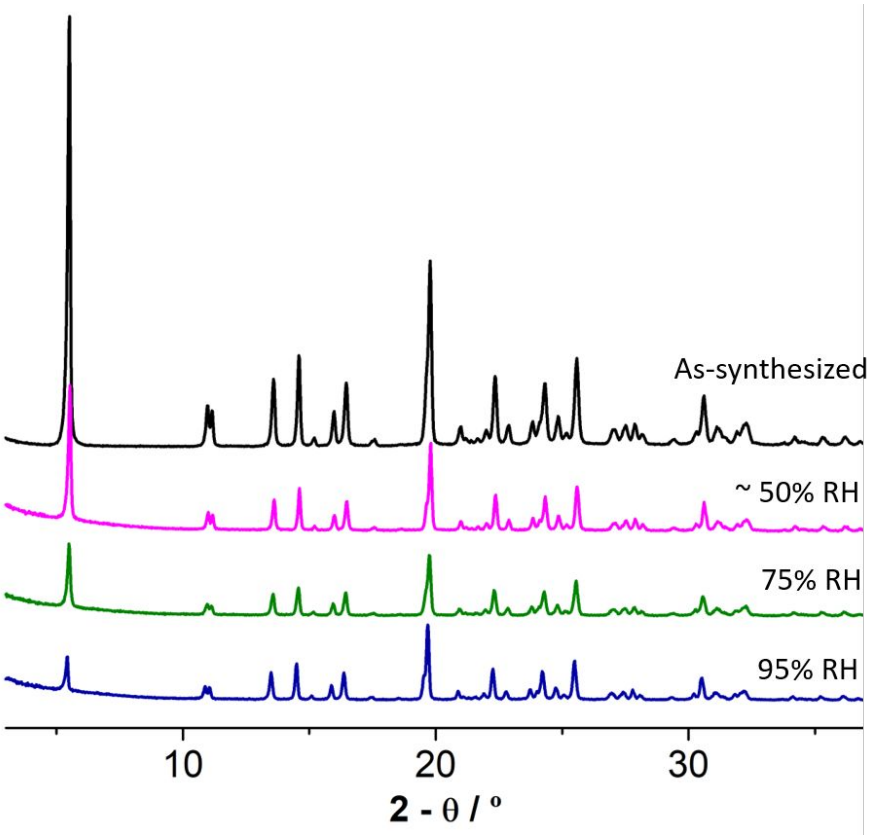

Figure S26 – PXRD patterns (from the top to the bottom) of the as-synthesized **5** and after shelf and moisture treatment for 3 months at ambient (~ 50%), 75 % and 95 % RH conditions.

Antibacterial and Antibiofilm Activity

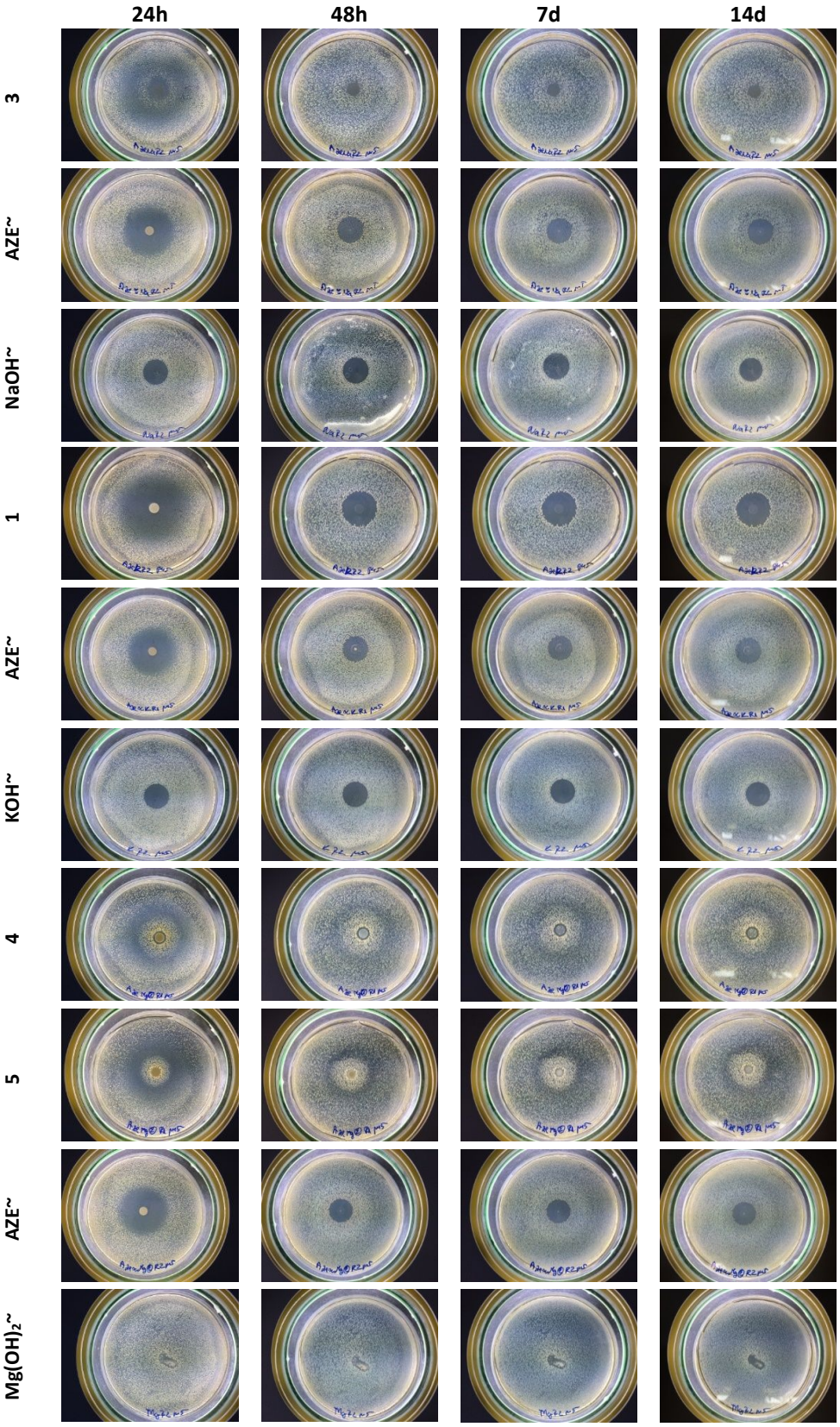

Figure S27 - Halo inhibition zone experiments for the pelletized compounds **1** and **3**-**5** prepared in this work in contact with *S.aureus* cultures in agar plates (pH 5) at 37 °C for 14 days.

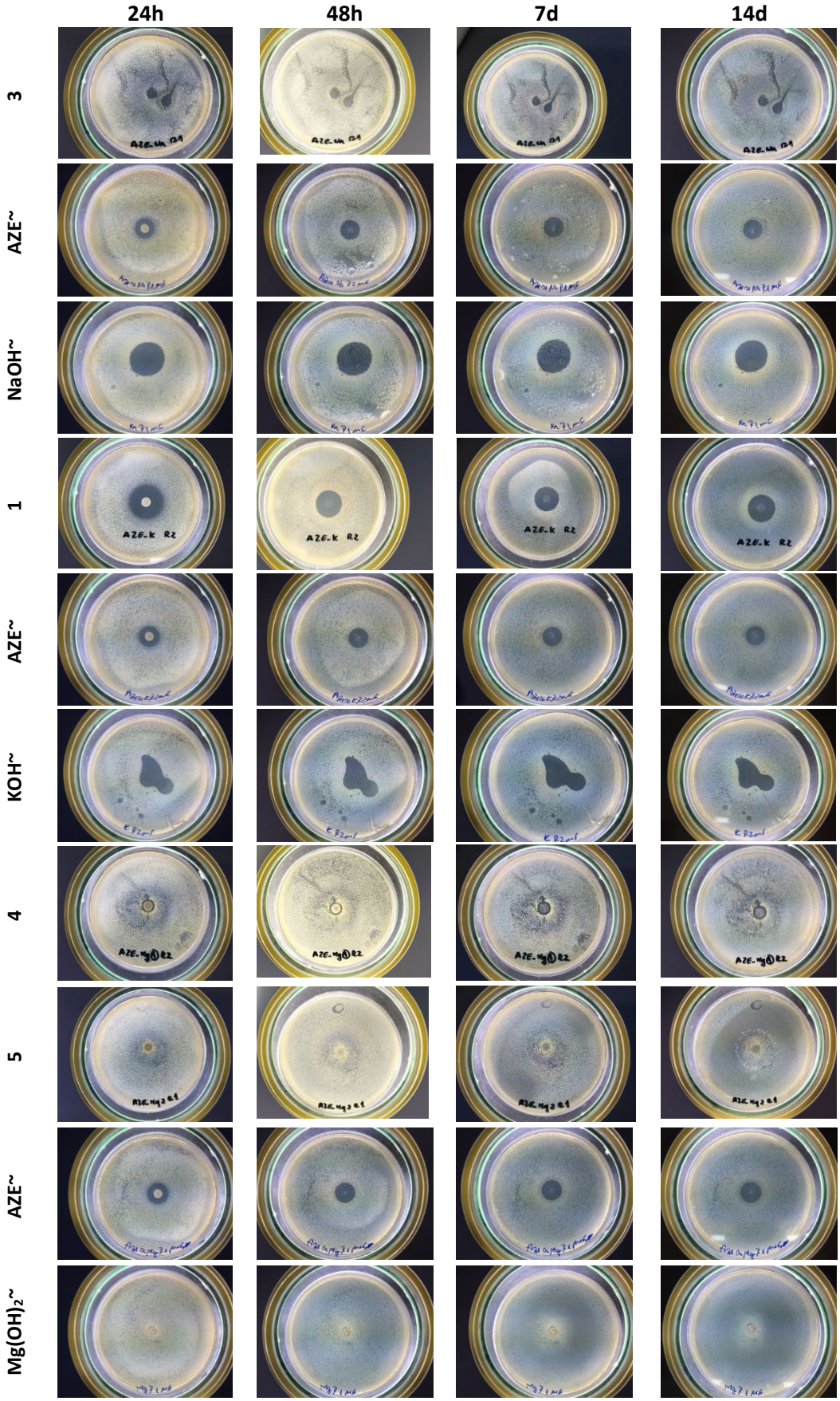

Figure S28 - Halo inhibition zone experiments for pelletized compounds **1** and **3**-**5** prepared in this work in contact with *S.aureus* cultures in agar plates (pH 6.5) at 37 °C for 14 days.