Synthesis and structure of three new alkaline earth metal-organic frameworks with high thermal stability as catalyst for Knoevenagel condensation

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Table S1 Selected bond distances (Å) and angles (°) for **Mg-HBDC**

Bond length (Å)			
Mg1-O11	2.012(3)	Mg2-O2^{iii}	2.067(3)
Mg1-O1	2.005(3)	Mg2-O3^{iv}	2.096(3)
Mg1-O14^{i}	2.016(3)	Mg2-O31	2.117(3)
Mg1-O4^{ii}	2.113(3)	Mg2-O41	2.069(3)
Mg1-O21	2.116(3)	Mg2-O13	2.041(3)
Mg1-O3	2.229(3)	Mg2-O12^{v}	2.067(2)
Bond angles (º)			
O1-Mg1-O11	100.72(11)	O13-Mg2-O41	87.10(11)
O1-Mg1-O21	85.35(11)	O13-Mg2-O31	170.98(11)
O11-Mg1-O21	84.95(11)	O41-Mg2-O31	86.60(10)
(i) -1/2+x, y, 3/2-z; (ii) 1/2-x, 1-y, 1/2+z; (iii) 1-x, -1/2+y, 3/2-z; (iv) 1-x, 1-y, 1-z; (v) 1/2+x, y, 3/2-z			

Table S2 Selected bond distances (Å) and angles (°) for **Ca-HBDC**

Bond length (Å)		Bond angles (°)	
Ca1-O1	2.373(17)	O2-Ca1-O3	85.60(6)
Ca1-O3^{i}	2.3737(17)	O3^{i}-Ca1-O2	85.29(6)
Ca1-O2	2.2938(15)	O3^{i}-Ca1-O3	29.90(9)
Ca1-O1^{ii}	2.3287(15)	O1^{iii}-Ca-O2	88.16(6)
Ca1-O1^{iii}	2.3287(15)	O2^{i}-Ca1-O2	166.77(9)

(i) 1-x, y, 3/2-z; (ii) 1-x, 2-y, 1-z; (iii) x, 2-y, 1/2+z

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Table S3 Selected bond distances (Å) and angles (°) for **Sr-HBDC**

Bond length (Å)			
Sr1-O6	2.489(6)	Sr1-O3^{ii}	2.518(5)
Sr1-O1	2.491(5)	Sr1-O3^{iii}	2.662(5)
Sr1-O2^{i}	2.554(5)	Sr1-O4^{iii}	2.725(5)
Sr1-O1^{i}	2.742(5)	Sr1-O4^{iv}	2.596(5)
Bond angles (º)			
O1-Sr1-O1^{i}	164.181(18)	O6-Sr1-O4^{iii}	146.94(19)
O1-Sr1-O2^{i}	145.57(17)	O3^{ii}-Sr1-O1	89.03(16)
O6-Sr1-O3^{ii}	93.4(2)	O3^{ii}-Sr1-O6	93.4(2)
O6-Sr1-O1^{i}	84.81(18)	O2^{i}-Sr1-O4^{iii}	82.1(2)
(i) 1-y, x-1-y, z-1/3; (ii) 2-y, x-y, z-1/3; (iii) x, y-1, z; (iv) 1+y-x, 1-x, 1/3+z			

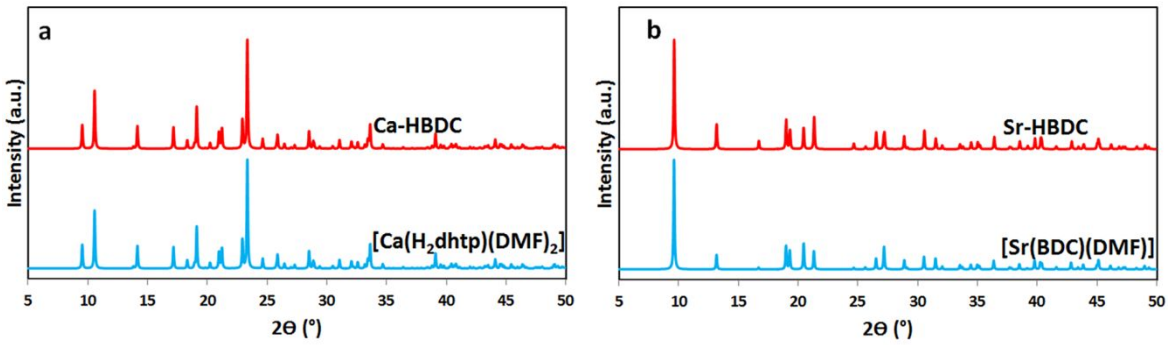

Figure S1 comparison of simulated patterns of **Ca-HBDC** and **Sr-HBDC** with their corresponding isostructural MOFs

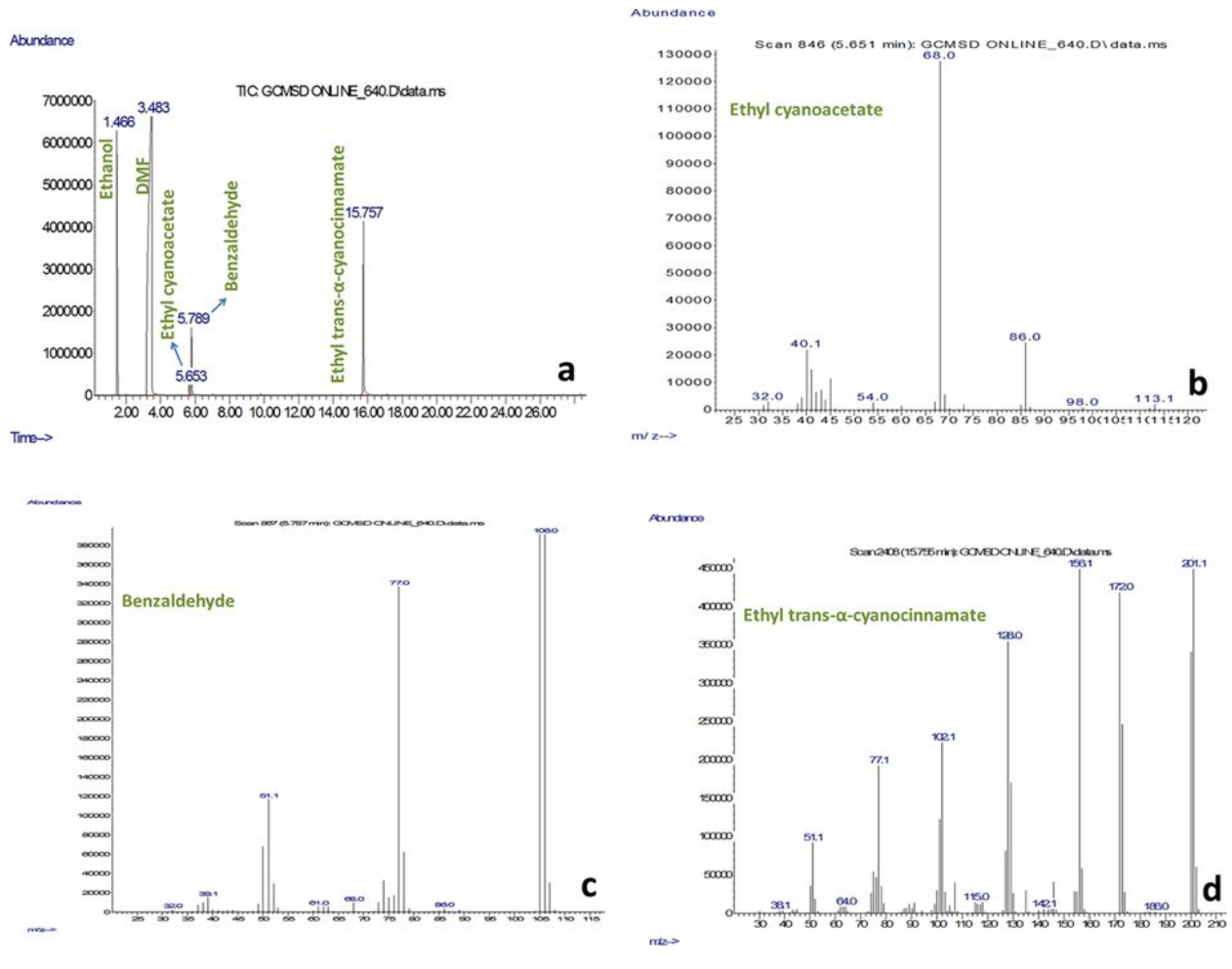

Figure S2 GC-Ms for the Knoevenagel condensation of benzaldehyde and ethyl cyanoacetate using **Mg-HBDC** catalyst (Table 2, entry 7)