Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B

Supporting information

Template role of caffeine in its one-step encapsulation in MOF NH_2-MIL-88B(Fe)

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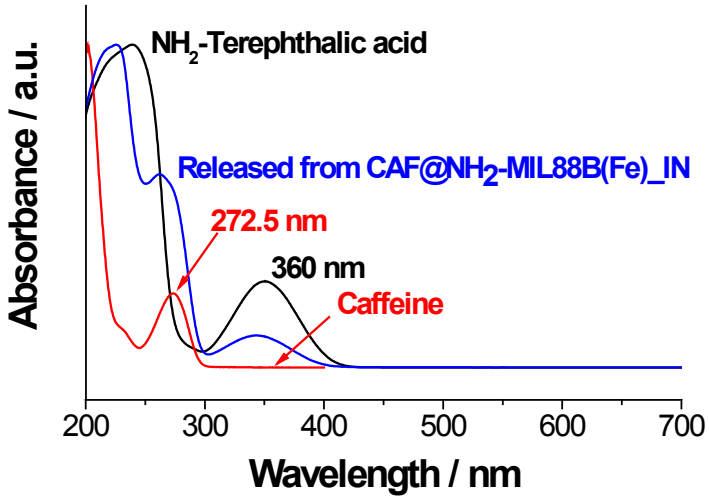

Figure S1. UV-VIS in water for caffeine, 2-aminoterephthalic acid and the liquid extract from CAF@NH_2-MIL-88B(Fe) at the end of the drug release experiment at 80 ºC.

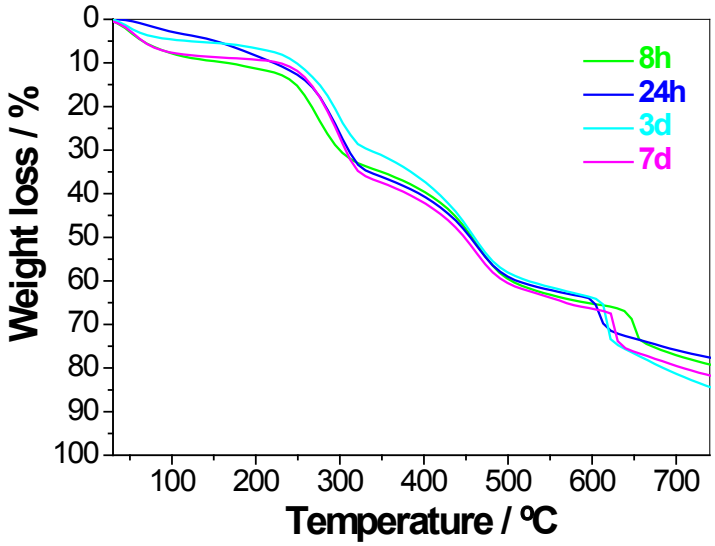

Figure S2. TGA curves of CAF@NH_2-MIL-88B(Fe)_EX after caffeine encapsulation during 8 h, 24 h, 3 days and 7 days.

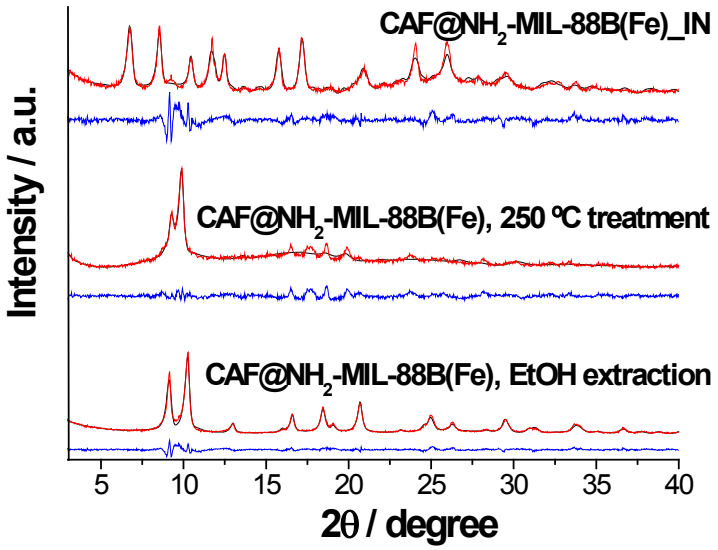

Figure S3. Experimental (red line) and simulated (black line) X-ray diffraction patterns after structure resolution of CAF@NH_2-MIL-88B(Fe)_IN, NH_2-MIL-88B(Fe) obtained by ethanol extraction of CAF@NH_2-MIL-88B(Fe)_IN and NH_2-MIL-88B obtained by treatment at 250 ºC of CAF@NH_2-MIL-88B(Fe)_IN.

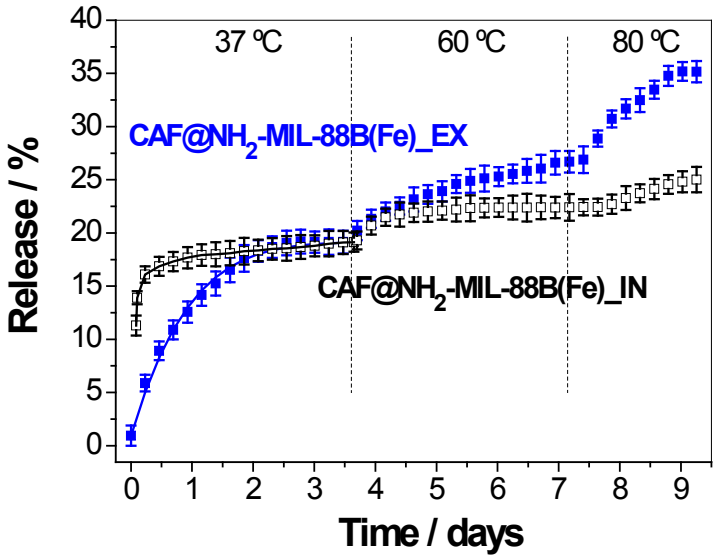

Figure S4. Caffeine release experiments in water at 37, 60 and 80 ºC determined by UV-VIS absorption from CAF@NH_2-MIL-88B(Fe)_IN and CAF@NH_2-MIL-88B(Fe)_EX. The release was related to the sum of the total amount of dry solid, excluding remaining solvent, i.e. TGA weight loss below 150 ºC, and including encapsulated caffeine.

The continuous lines in Figures S4, 6 and 7 were obtained applying the following equation:

$$X_A = \left\{1 - [k_1(n-1)t + k_2]^{\frac{1}{(1-n)}}\right\} X_{Ao}$$

where X_A and X_{Ao} are the amount released in a given time and the total amount released (both in g caffeine per (g caffeine + g dry solid)), t the time (days), and k_1 ($days^{-1}$), k_2 and n constants. The regression factors (R^2) were above 0.9, while the k_1, k_2 and n values are shown in Table S1.

Table S1. Parameter values according to equation (1); (w) and (PBS) refer to release experiments carried out at 37 ºC in water and PBS media.

CAF@NH_2-MIL-88B(Fe)_IN	k_1 (d^{-1})	k_2	n	R^2
Caffeine	0.9 (w)	1.1 (w)	3.6 (w)	0.991 (w)
	2.0 (PBS)	1.0 (PBS)	0.9 (PBS)	0.992 (PBS)
2-NH_2-BDC	0.3 (w)	1.1 (w)	3.7 (w)	0.990 (w)
	1.7 (PBS)	1.0 (PBS)	1.2 (PBS)	0.993 (PBS)
CAF@NH_2-MIL-88B(Fe)_EX	k_1 (d^{-1})	k_2	n	R^2
Caffeine	5633 (w)	18173 (w)	9.6 (w)	0.974 (w)
NH_2-MIL-88B(Fe)	k_1 (d^{-1})	k_2	n	R^2
2- NH_2-BDC	297 (PBS)	1.7 (PBS)	2.5 (PBS)	0.991 (PBS)