Supporting Information

Encapsulation of pharmaceutical ingredient linker in metal-organic framework: Combined experimental and theoretical insight into the drug delivery

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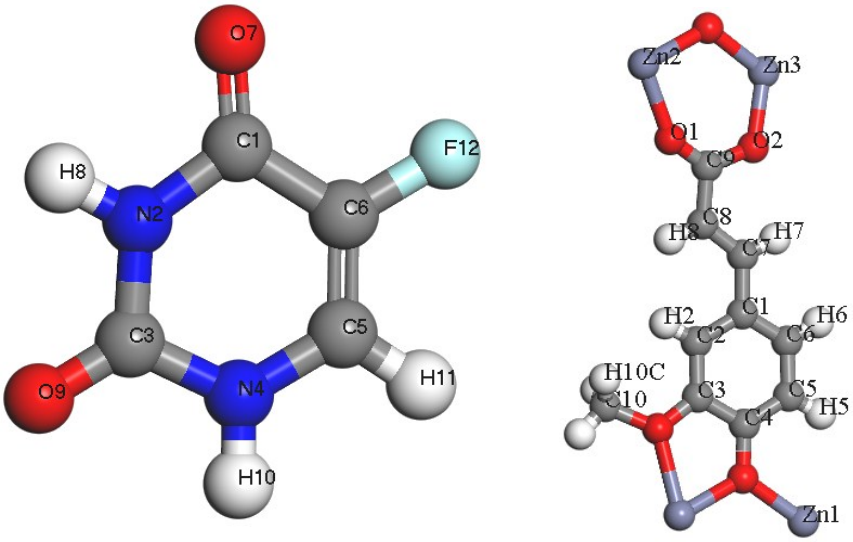

Fig. S1 (a)The atomic types used for 5-FU. (b)The atomic type used for **1** (Zn, purple; O, red; C, gray; H, white).

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Table S1 Lennard-Jones parameters and partial charges for studied **1**

Atom	σ/Å	(ε/kB)/K	Charge/e
MOF_Zn1	2.46	62.4	0.97025
MOF_Zn2	2.46	62.4	0.89325
MOF_Zn3	2.46	62.4	1.02125
MOF_O1	3.12	30.19	-0.528
MOF_O2	3.12	30.19	-0.545
MOF_C1	3.43	52.84	0.045
MOF_C2	3.43	52.84	-0.234
MOF_C3	3.43	52.84	0.271
MOF_C4	3.43	52.84	0.284
MOF_C5	3.43	52.84	-0.214
MOF_C6	3.43	52.84	-0.191
MOF_C7	3.43	52.84	-0.162
MOF_C8	3.43	52.84	-0.203
MOF_C9	3.43	52.84	0.415

MOF_C10	3.43	52.84	-0.266
MOF_H2	2.57	22.14	0.183
MOF_H5	2.57	22.14	0.222
MOF_H6	2.57	22.14	0.184
MOF_H7	2.57	22.14	0.228
MOF_H8	2.57	22.14	0.171
MOF_H10C	2.57	22.14	0.198

Table S2 Lennard-Jones parameters and partial charges for 5-FU

Atom	σ/Å	(ε/k_B)/K	Charge/e
C1	3.40	43.29	0.2600
N2	3.25	85.58	-0.5582
C3	3.40	43.29	0.4272
N4	3.25	85.58	-0.4713
C5	3.40	43.29	-0.1662
C6	3.40	43.29	0.1519
O7	3.40	105.71	-0.3133
H8	1.07	7.90	0.4706
O9	3.40	105.71	-0.3704
H10	1.07	7.90	0.4694
H11	2.51	7.55	0.2952
F12	3.12	30.71	-0.1948

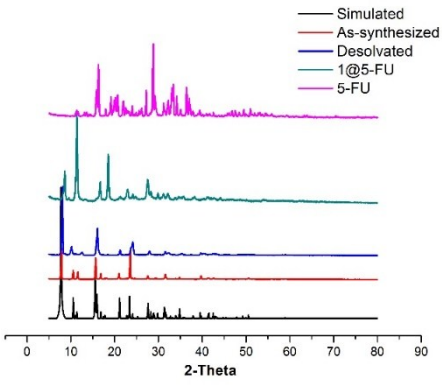

Fig. S2 the PXRD pattern of **1** and 5-FU at different condition.

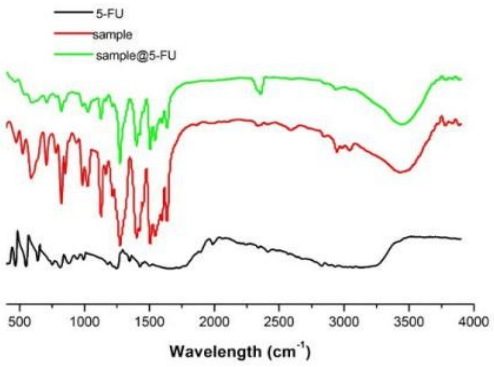

Fig. S3 IR spectra of 5-FU(black), **1**(red) and **1**@5-FU(green).

Table S3 Impregnation parameters of drug loading experiments in title compound

Impregnation parameters	g 5-FU/g dehydrated **1**		
5-FU/ material weight ratio (in ethanol)	1:1	1day	0.196
		2 day	0.178
		3 day	0.205
	1:2	1 day	0.185
		2 day	0.183
		3 day	0.173
	1:3	1 day	0.181
		2 day	**0.388**
		3 day	0.201

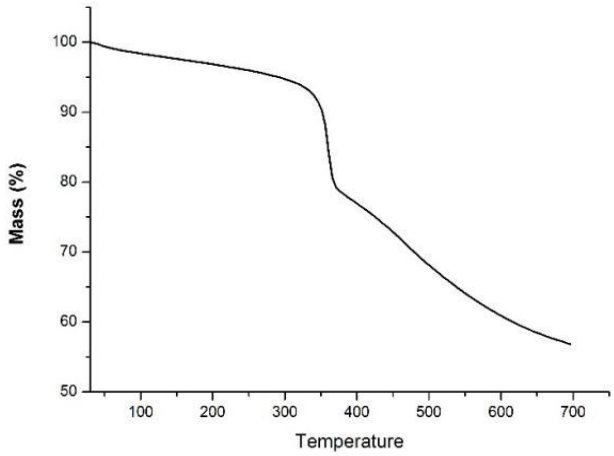

Fig. S4 The TGA curves of **1@5-FU**

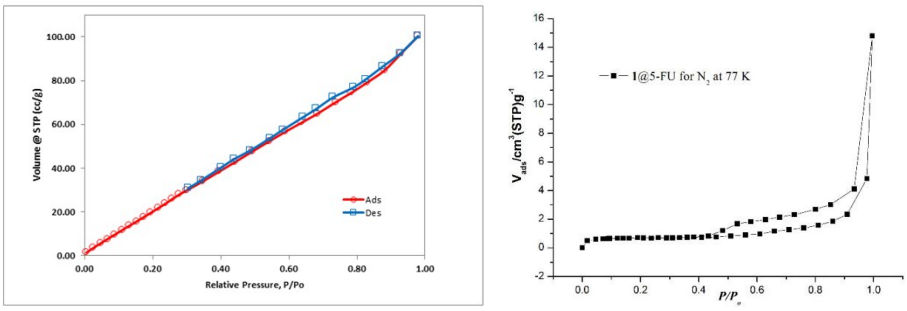

Fig. S5 view of the N_2 isotherms of **1** material (left) and 5-FU@**1** material (right). The data of the N_2 isotherms of **1** material was measured from the Ref 16.

In vitro degradation of 1

The degradation of **1** were investigated by suspending 20 mg of activated **1** in 100 mL PBS at 37 °C. These solutions were kept stirring for predetermined time intervals. During each time interval, 2 mL of solution was taken out, and 2 mL of fresh buffer was added. The concentration of released organic linker ferulic acid was quantified by UV-Vis spectrophotometer with the supernatant at 320 nm wavelength. The content of degraded H_2fer was calculated using as follows:

A=97.332C+0.4624

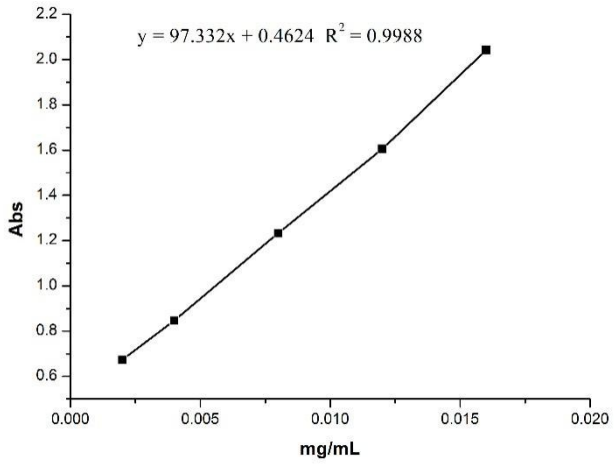

Fig. S6 Calibration plot of standard 5-FU in PBS obtained by UV-Vis spectrophotometer at 320 nm.

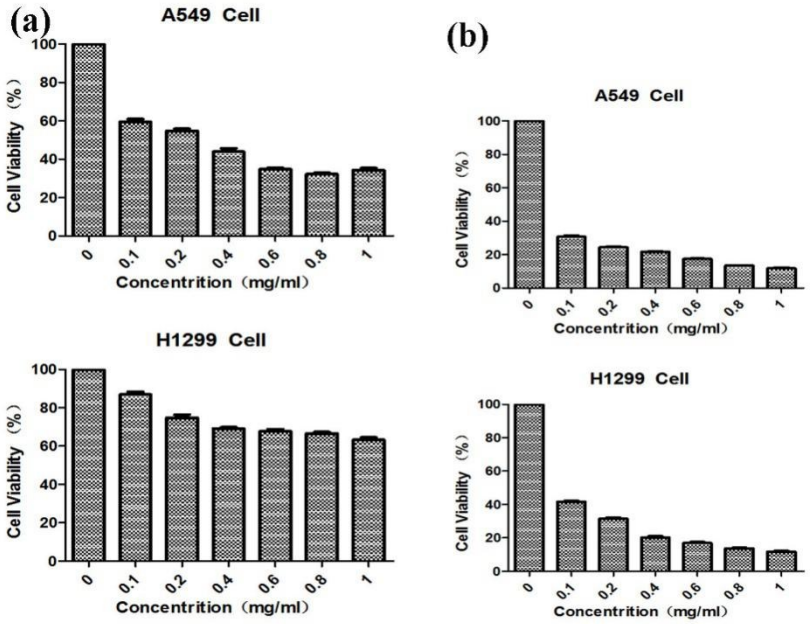

Fig.S7 In vitro viability of A549 and H1299 cells in the presence of **1** and **1**@5-FU.