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Electronic Supplementary Information

Functionalization of MOF-5 with mono-substituent: the effect on the drug delivery behavior

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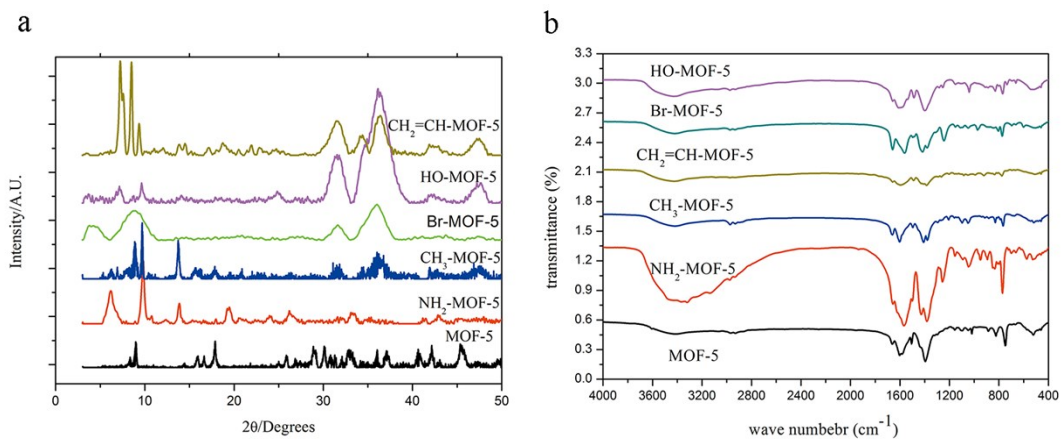


Fig. S1 PXRD patterns (a) and FTIR (b) spectra of MOF-5, NH₂-MOF-5, CH₃-MOF-5, Br-MOF-5, HO-MOF-5 and CH₂=CH-MOF-5.

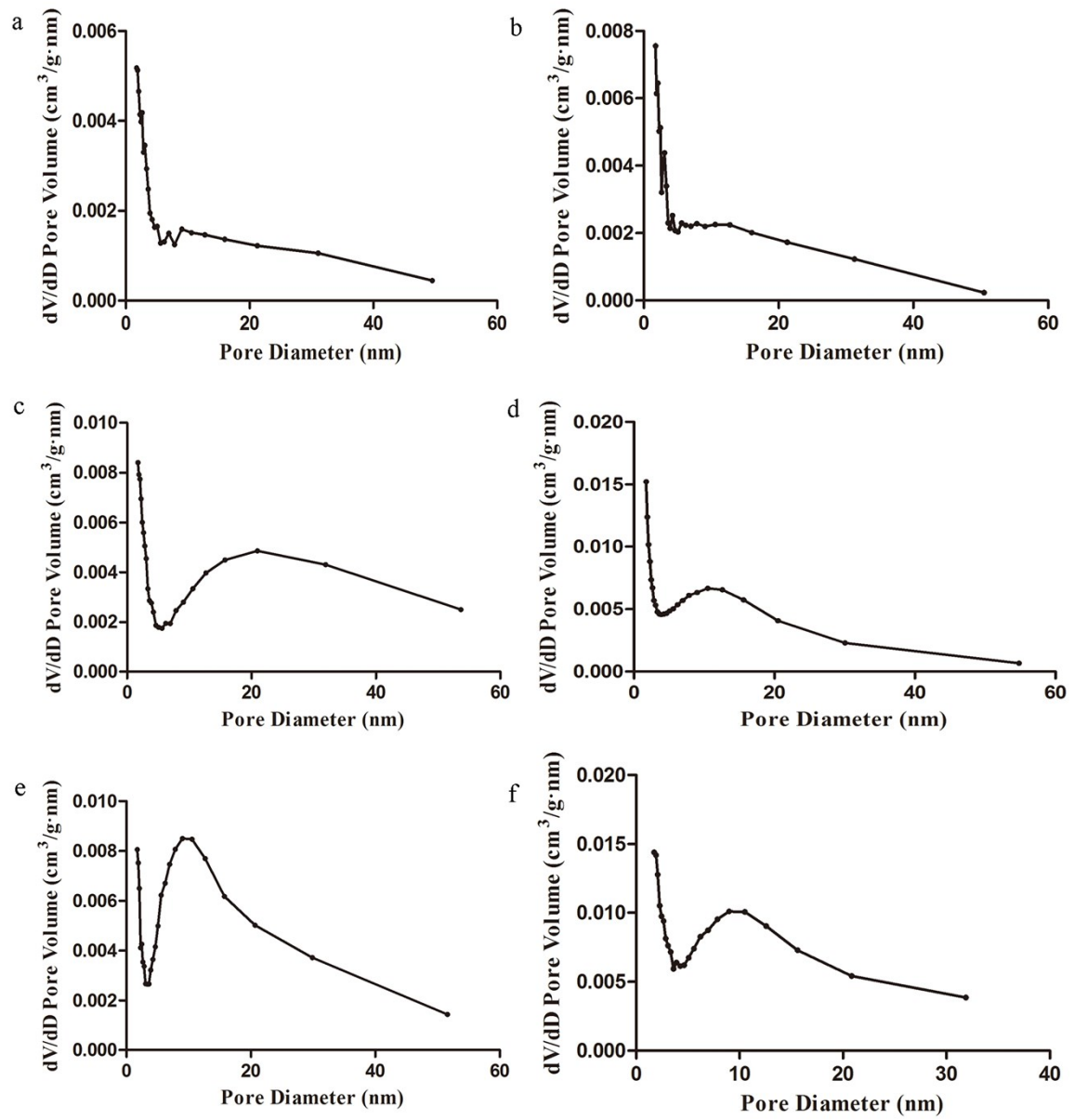


Fig. S2 Pore size distribution of MOFs calculated by the Horvath - Kawazoe model, MOF-5 (a), NH_2 -MOF-5 (b), CH_3 -MOF-5 (c), Br-MOF-5 (d), HO-MOF-5 (e) and $\text{CH}_2=\text{CH}$ -MOF-5 (f).

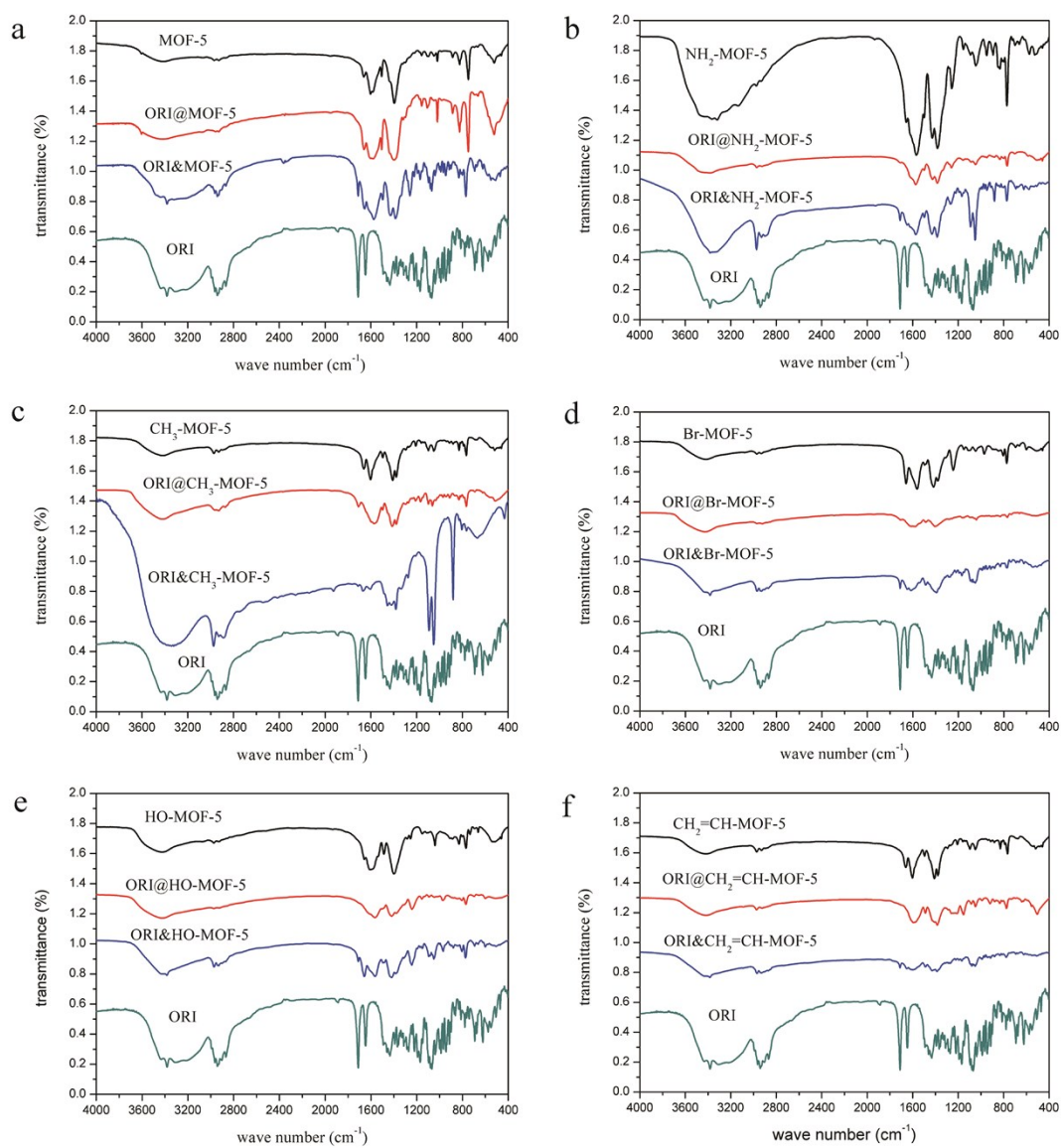


Fig. S3 FTIR spectra of ORI@MOF-5 (a), ORI@ NH_2 -MOF-5 (b), ORI@ CH_3 -MOF-5 (c), ORI@Br-MOF-5 (d), ORI@HO-MOF-5 (e) and ORI@ $\text{CH}_2=\text{CH}$ -MOF-5 (f).

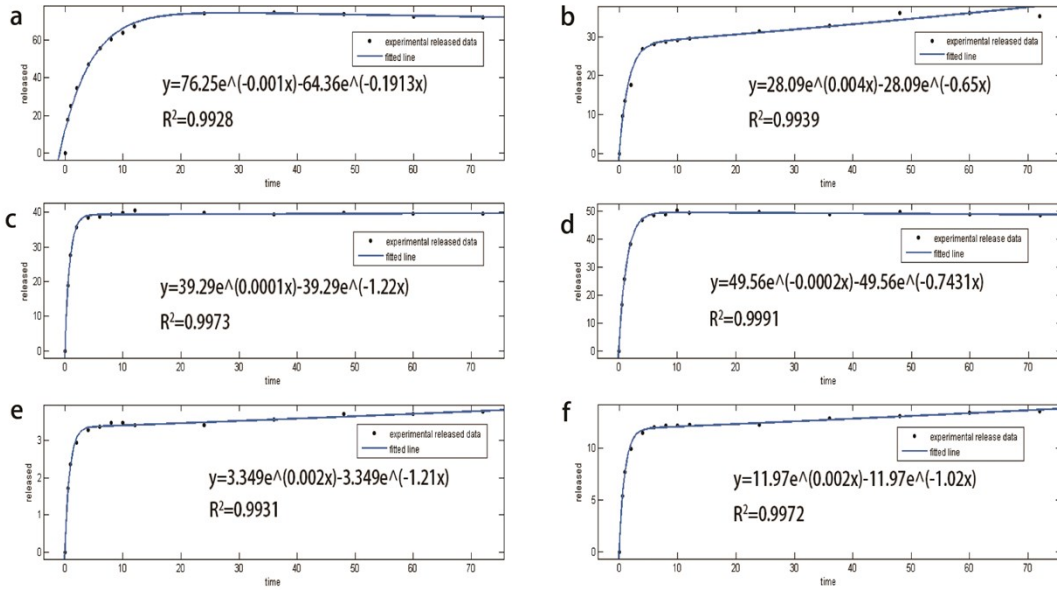


Fig. S4 The new distribution model simulation of ORI release curve.

Table S1 The fitting results of ORI@MOFs in the zero order, first order, Higuchi and Riter-Peppas model.

MOFs	pH	Model	Equation	R ²
MOF-5	5.5	zero order equation	$Mt = 0.6331t + 44.242$	0.3931
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0146t - 0.6777$	0.4884
		Higuchi equation	$Mt/M_{\infty} = 8.9591t^{1/2} - 1.4634$	0.6392
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.2281\ln t - 1.0566$	0.8431
	7.4	zero order equation	$Mt = 0.6812t + 38.965$	0.4562
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0147t - 0.5624$	0.5576
		Higuchi equation	$Mt/M_{\infty} = 9.4012t^{1/2} - 1.311$	0.7021
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.2749\ln t - 1.262$	0.8648
NH ₂ -MOF-5	5.5	zero order equation	$Mt = 0.315t + 18.966$	0.4820
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0042t - 0.217$	0.5322
		Higuchi equation	$Mt/M_{\infty} = 21.008t^{1/2} - 1.6755$	0.7096
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.2396\ln t + 2.7074$	0.8596
	7.4	zero order equation	$Mt = 0.2718t + 19.5$	0.3955
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0035t - 0.2245$	0.4301
		Higuchi equation	$Mt/M_{\infty} = 20.79t^{1/2} - 1.5495$	0.6307
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.2203\ln t + 2.7442$	0.8160
CH ₃ -MOF-5	5.5	zero order equation	$Mt = 0.2036t + 30.002$	0.1810
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0028t - 0.3726$	0.1976
		Higuchi equation	$Mt/M_{\infty} = 14.375t^{1/2} - 1.2566$	0.3694
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.106\ln t + 3.3485$	0.5892
	7.4	zero order equation	$Mt = 0.2555t + 29.047$	0.2345
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0036t - 0.3613$	0.2556
		Higuchi equation	$Mt/M_{\infty} = 0.0235t^{1/2} + 0.166$	0.5950
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.1567\ln t + 3.2213$	0.6537
Br-MOF-5	5.5	zero order equation	$Mt = 0.3009t + 34.578$	0.2182
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0045t - 0.4568$	0.2344
		Higuchi equation	$Mt/M_{\infty} = 11.498t^{1/2} - 1.0276$	0.4286
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.1682\ln t + 3.3619$	0.6267
	7.4	zero order equation	$Mt = 0.3274t + 37.948$	0.2112
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0051t - 0.522$	0.2234
		Higuchi equation	$Mt/M_{\infty} = 10.332t^{1/2} - 0.9569$	0.4231
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.1712\ln t + 3.4454$	0.6278
HO-MOF-5	5.5	zero order equation	$Mt = 0.023t + 2.5558$	0.2853
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0002t - 0.026$	0.2884
		Higuchi equation	$Mt/M_{\infty} = 183.59t^{1/2} - 1.8995$	0.4895
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.1229\ln t + 0.8853$	0.7505
	7.4	zero order equation	$Mt = 0.0166t + 2.5879$	0.1636
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0002t - 0.0263$	0.1644
		Higuchi equation	$Mt/M_{\infty} = 163.14t^{1/2} - 1.1223$	0.3511
		Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.1046\ln t + 0.8946$	0.5710
CH ₂ =CH-MOF-5	5.5	zero order equation	$Mt = 0.0894t + 8.7941$	0.3194
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.001t - 0.093$	0.3320
		Higuchi equation	$Mt/M_{\infty} = 52.214t^{1/2} - 1.8884$	0.5330
	7.4	Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.1458\ln t + 2.0822$	0.7665
		zero order equation	$Mt = 0.0655t + 8.013$	0.2213
		first order equation	$\ln(1-Mt/M_{\infty}) = -0.0007t - 0.0843$	0.2258

Higuchi equation	$Mt/M_{\infty} = 53.189t^{1/2} - 1.3187$	0.4285
Ritger-Peppas equation	$\ln(Mt/M_{\infty}) = 0.139\ln t + 1.9691$	0.6476
