

Supplementary Information

An iron(III) complex-based supramolecular organic framework (SOF) as a theranostic platform via magnetic resonance imaging-guided chemotherapy

Pengpeng Hu,^a Hong Mo,^{*a} Saijie Song,^{*a} Jing Wu,^b Jihui Li,^c Jian Shen^{*ad}

^a National and Local Joint Engineering Research Center of Biomedical Functional Materials, Jiangsu Engineering Research Center for Biomedical Function Materials, School of Chemistry and Materials Science, Nanjing Normal University, Nanjing 210023, China

^b Nanjing Customs District Industrial Products Inspection Center, Nanjing 210019, China

^c Shenyang Institute of Industrial Technology, Shenyang 110000, China

^d Jiangsu Engineering Research Center of Interfacial Chemistry, Nanjing University, Nanjing, 210023, China

*Authors to whom all correspondence should be addressed

E-mail Address: 07198@njnu.edu.cn

or sjsong2014@sinano.ac.cn

or jianshen_nj@163.com

Tel: +86-25-83598031, Fax: +86-25-83716813

1. Crystallographic data for Fe(III)-SOF

Table S1 Crystallographic data for Fe(III)-SOF

	this work	previous work (ref. 1)
Moiety formula	$(C_{42}H_{30}N_6O_{12}Fe_2)(C_3H_7NO)_6$	$(C_{42}H_{30}N_6O_{12}Fe_2)(C_3H_7NO)_7(C_4H_{10}O)_{0.5}$
Crystal system	monoclinic	monoclinic
Space group	$C2/c$	$C2/c$
$a / \text{\AA}$	23.5899(9)	23.682(3)
$b / \text{\AA}$	23.4215(8)	23.465(3)
$c / \text{\AA}$	14.8124(6)	14.912 (2)
$\beta / ^\circ$	112.223(2)	112.501(2)
T / K	150	293
$V / \text{\AA}^3$	7576.1(5)	7656.0(18)
Z	4	4
$D_c / \text{g}\cdot\text{cm}^{-3}$	1.216	1.276
$F(000)$	2912	3092
μ / mm^{-1}	3.654	0.453
Reflections collected	39812	18224
Independent reflections	7773	6590
R_{int}	0.0619	0.0975
R_1	0.080	0.074
wR_2	0.218	0.127

2. Powder X-ray diffraction (XRD) patterns of Fe(III)-SOF

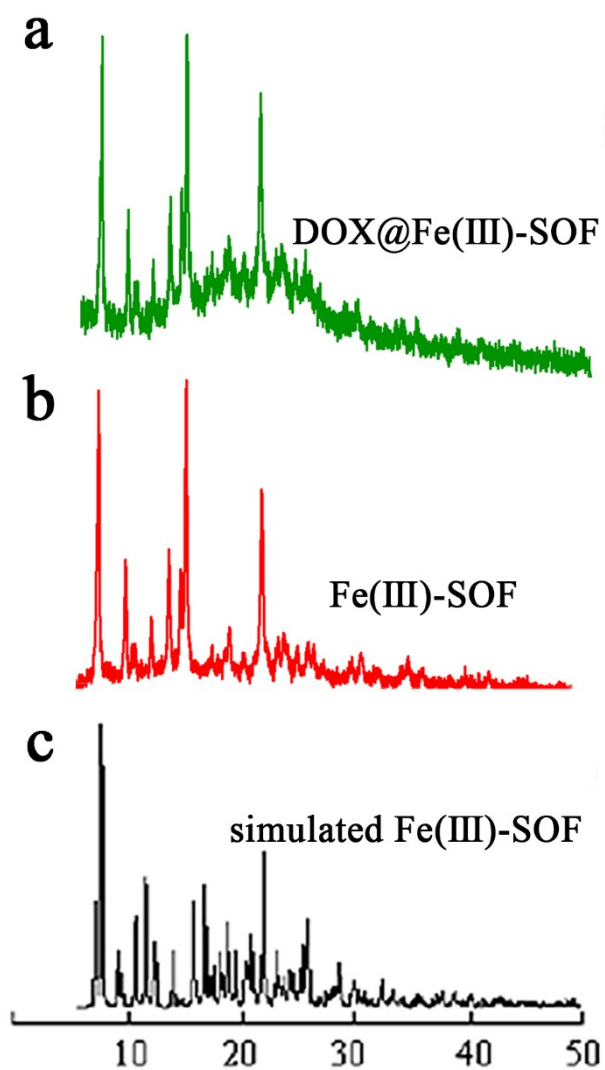


Fig. S1. Powder XRD patterns: (a) DOX@Fe(III)-SOF, (b) Fe(III)-SOF, (c) the pattern simulated from the single-crystal data.¹

3. Fourier transform infrared (FTIR) spectra

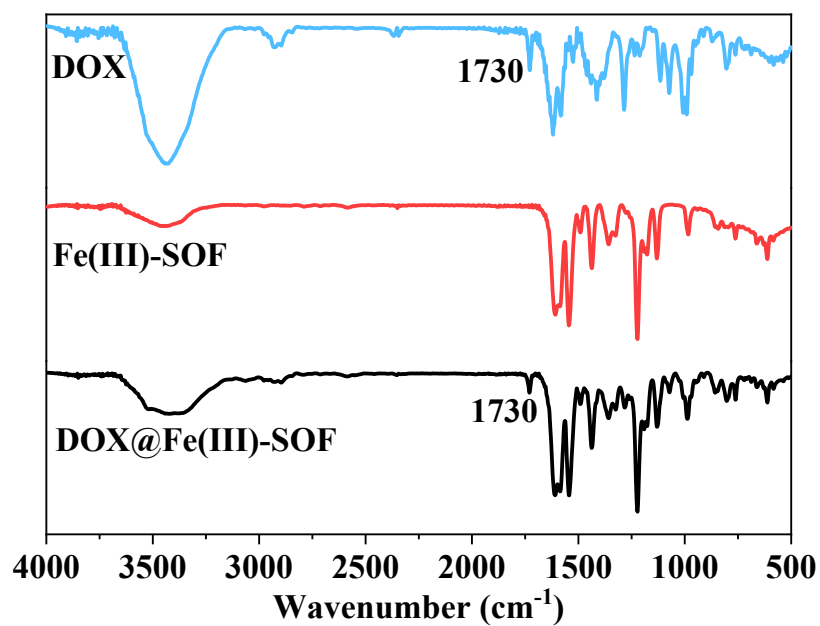


Fig. S2. FTIR spectra of DOX, Fe(III)-SOF and DOX@Fe(III)-SOF

4. Zeta potentials

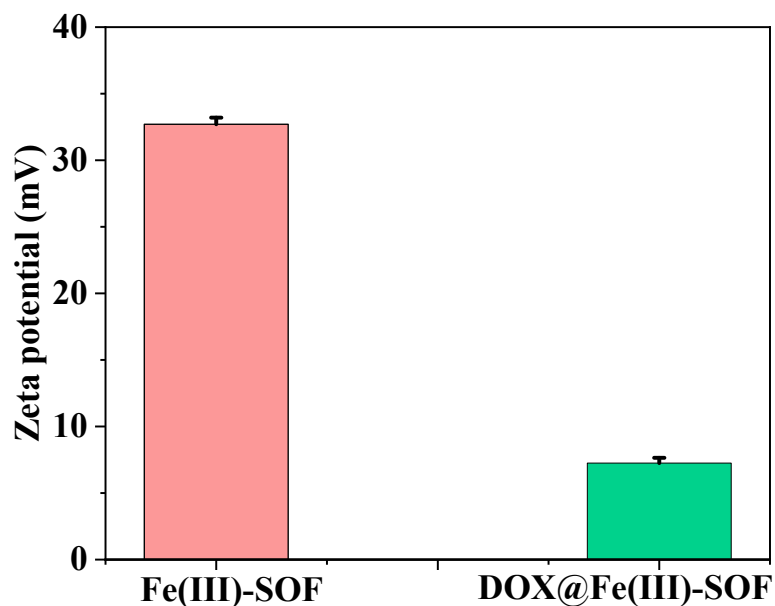


Fig. S3. The zeta potentials of Fe(III)-SOF and DOX@Fe(III)-SOF dispersed in water

5. The chemical and thermal stability of Fe(III)-SOF

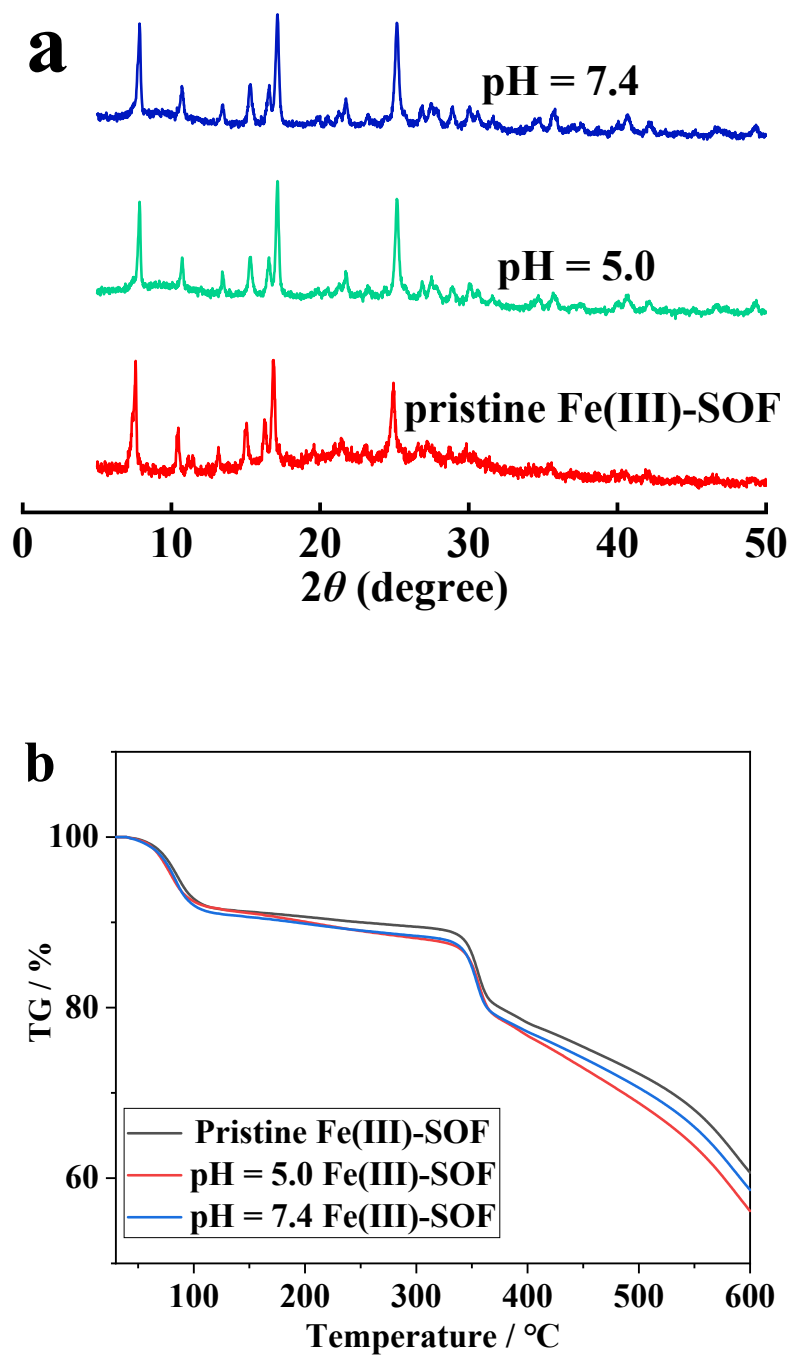


Fig. S4. (a) The powder XRD patterns and (b) the thermogravimetric analysis (TGA) of Fe(III)-SOF soaked in PBS (pH=7.4, 5.0) for 24 h

6. The UV-vis spectra and the standard curve of DOX for the loading content

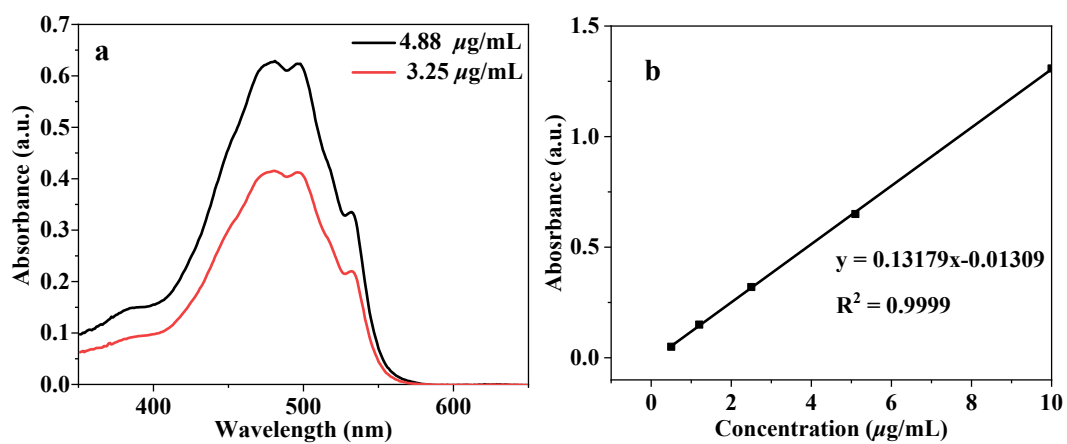


Fig. S5. (a) The UV-vis spectra of DOX, (b) the standard curve of DOX

References

- 1 H. Mo, D. Guo, C. Y. Duan, Y. T. Li and Q. J. Meng, *J. Chem. Soc., Dalton Trans.*, 2002, 3422–3424.