Supplementary Information

Analyses on intracellular Fe^{3+} with a rhodamine probe: "turn-on" response, specific recognition and bioimaging

Zhao Cheng [a,*], Xiaojing Liu [b], Lei Zheng [a], Yue Xu [a], Hao He [a]

[a] *School of Pharmacy, Xi'an Medical University, Xi'an Shaanxi 710021, PR China.*

[b] *College of Chemistry & Materials Science, Northwest University, Xi'an Shaanxi 710127, PR China*

[*] *Corresponding author: Zhao Cheng, chengzhao@xiyi.edu.cn.*

Contents:

Synthesis of rhodamine B acyl chloride

Rhodamine B (1.59 g, 3.32 mmol) was dissolved in 15 mL 1,2-dichloroethane, then phosphorus oxychloride (1 mL, 10.7 mmol) was added dropwise to the rhodamine B solution with stirring. The reaction mixture was refluxed for 4 h. After the reaction, the mixture was concentrated *in vacuo* to eliminate the leftover 1,2-dichloroethane and unreacted phosphorus oxychloride, affording rhodamine B acyl chloride.

Table S1 Crystallographic data of **J3**.

Compound	**J3**
Molecular Formula	$C_{32}H_{33}N_5O_2$
Molecular Weight	519.63
Crystal system	Monoclinic
Space group	P2(1)/n
a/Å	12.828(4)
b/Å	16.694(5)
c/Å	13.040(4)
α/°	90
β/°	101.773(6)
γ/°	90
Z	4
V/Å^3	2733.9(13)
F(000)	1104
No. refs measured	13549
No.unique-refs(Rint)	4803 (0.0885)
$R_1[I>2\sigma(I)]$	0.0598
wR_2 (all data)	0.1586
Goodness of fit	0.943

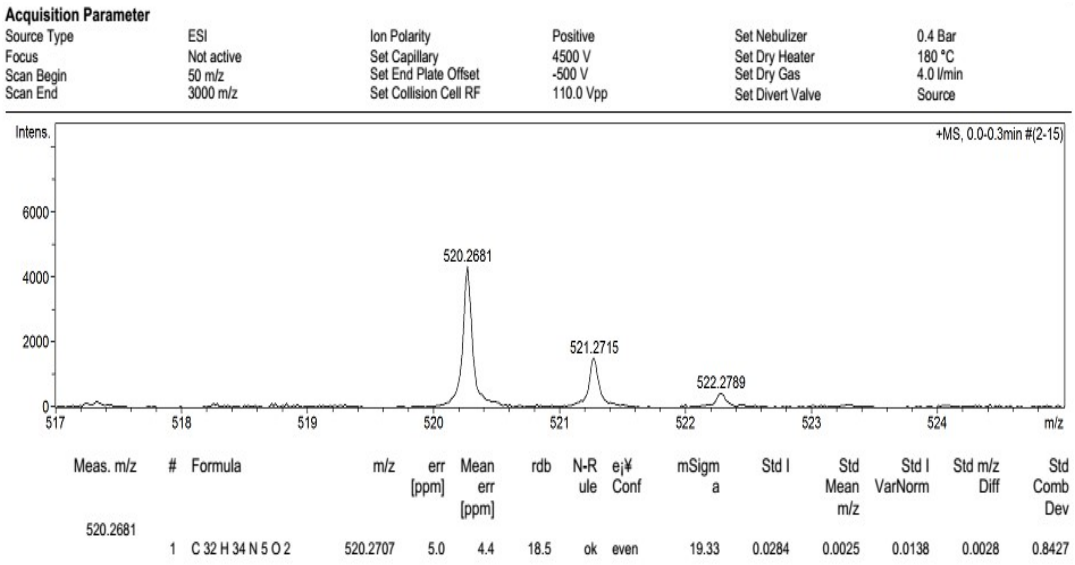

Fig. S1 ESI-MS of **J3**.

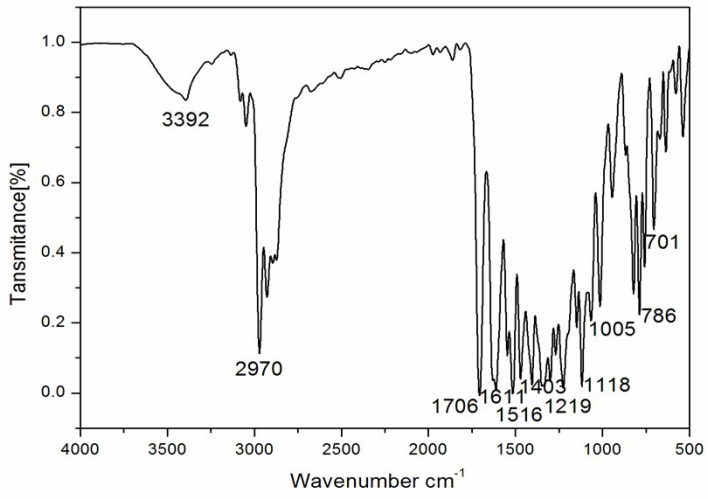

Fig. S2 IR of **J3**.

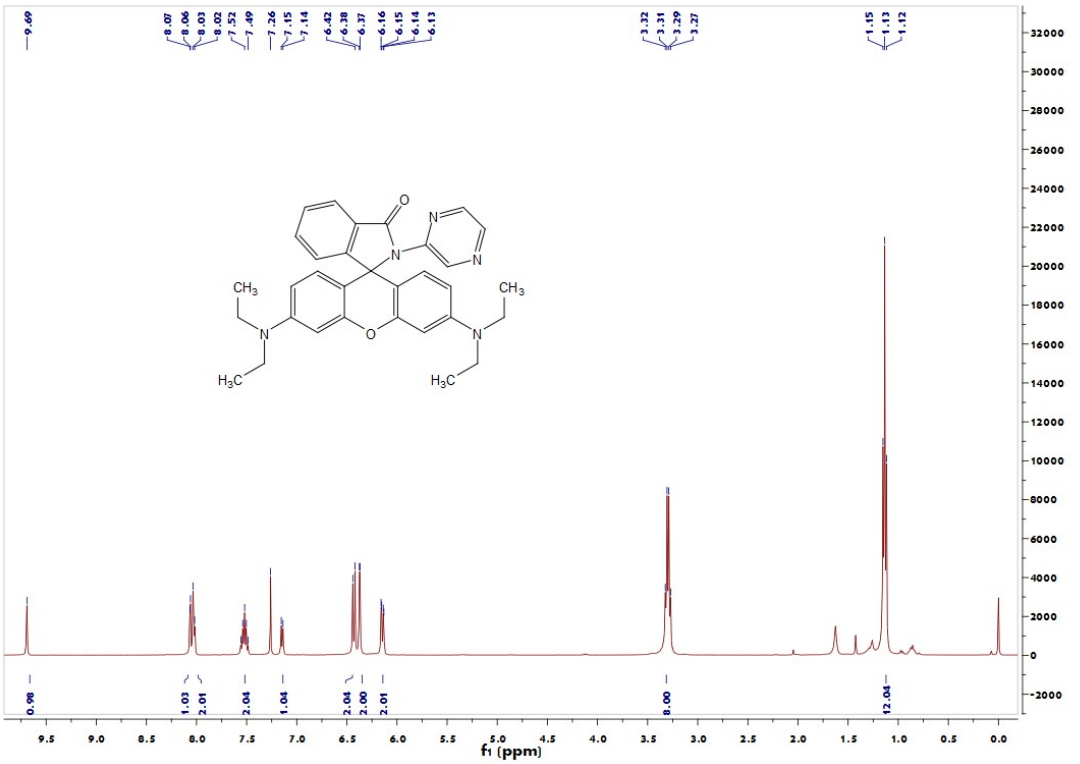

Fig. S3 ^{1}H NMR of **J3**.

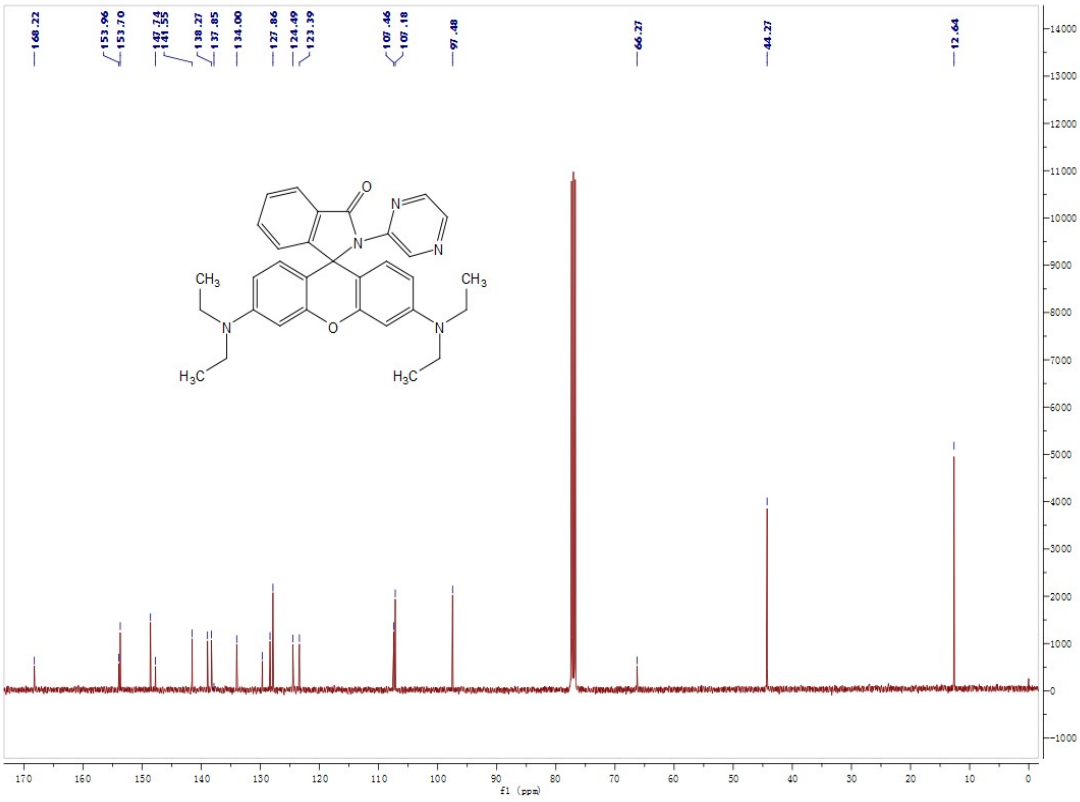

Fig. S4 ^{13}C NMR of **J3**.

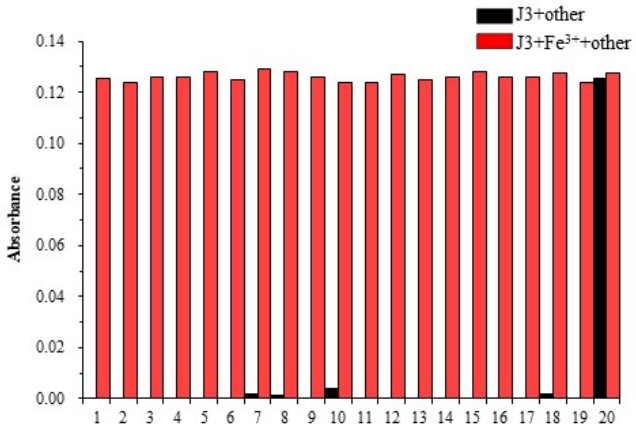

Fig. S5 UV-vis absorption selectivity and competition of **J3** towards Fe^{3+} in Fe^{3+}-competing ions coexisting systems.

*Black bars: absorbance of **J3** and competing ions at 523 nm.

Red bars: subsequent addition of 10 μmol L^{-1} Fe^{3+} to the black bars-represented solutions.

Metal ions (from left to right) : 1: K^{+}, 2: Ca^{2+}, 3: Mg^{2+}, 4: Ba^{2+}, 5: Mn^{2+}, 6: Cu^{2+}, 7: Zn^{2+}, 8: Cr^{3+}, 9: Hg^{2+}, 10: Ag^{+}, 11: Cd^{2+}, 12: Ni^{2+}, 13: Li^{+}, 14: NH_4^{+}, 15: Al^{3+}, 16: Sn^{2+}, 17: Co^{2+}, 18: Pb^{2+}, 19: Fe^{2+} and 20: Fe^{3+}.

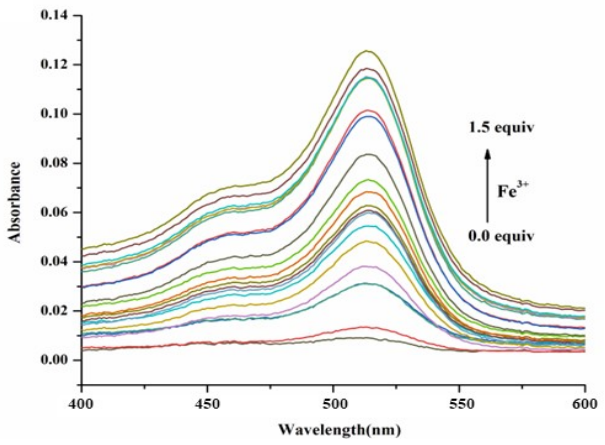

Fig. S6 UV-vis absorption titration of **J3** by Fe^{3+}.