Electronic supplementary information (ESI)

Ultra-sensitive Chemosensors for Fe(III) and Explosives Based on Highly Fluorescent Oligofluoranthene

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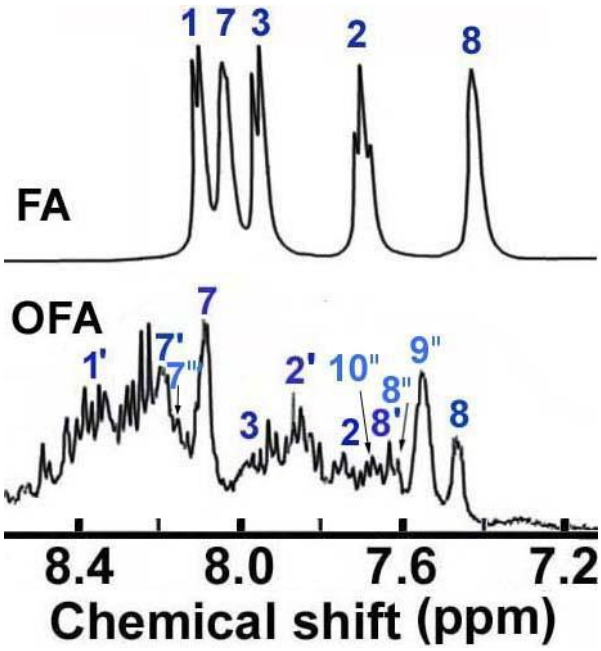


Fig. S1. 500 MHz ^{1}H-NMR spectra of FA monomer and OFA synthesized with a $FeCl_3$/FA molar ratio of 5:1.

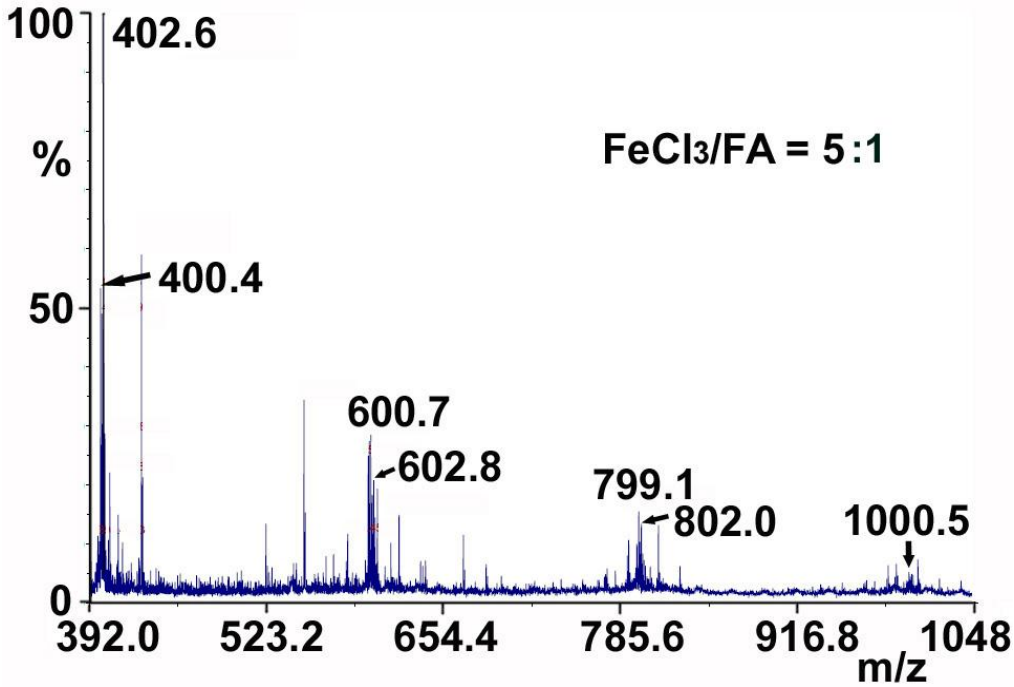


Fig. S2. MALDI-TOF mass spectrum of OFA synthesized with $FeCl_3$/FA molar ratio of 5:1.

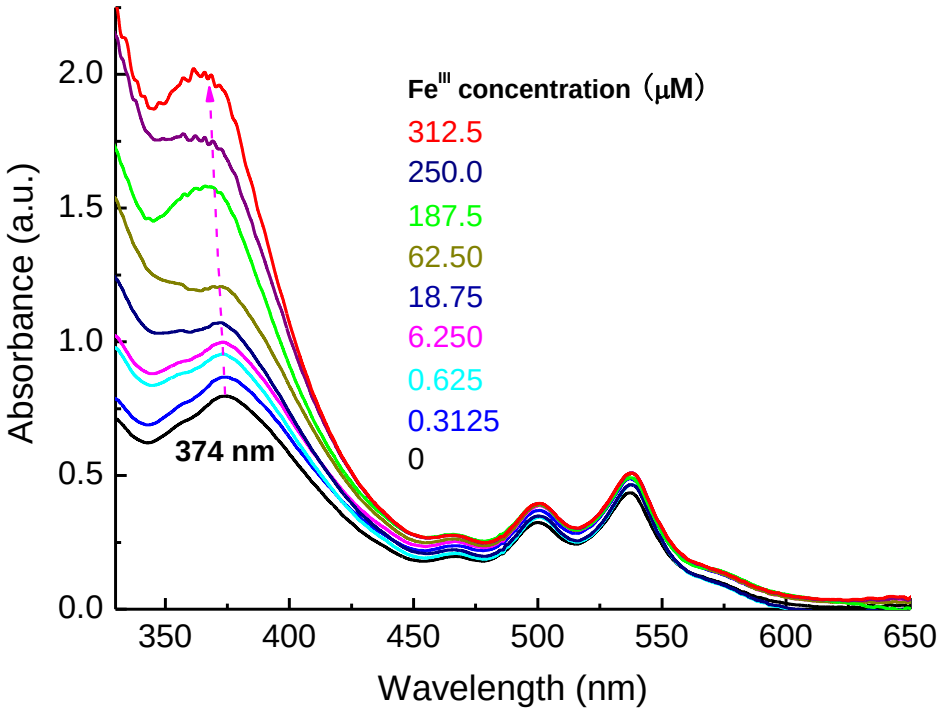


Fig. S3. UV-vis absorption spectra of OFA solution in NMP upon addition of Fe^{III} with different concentrations from 0 to 312.5 μM.

Scheme S1. Orbital Electron Distribution of Some Metal Ions

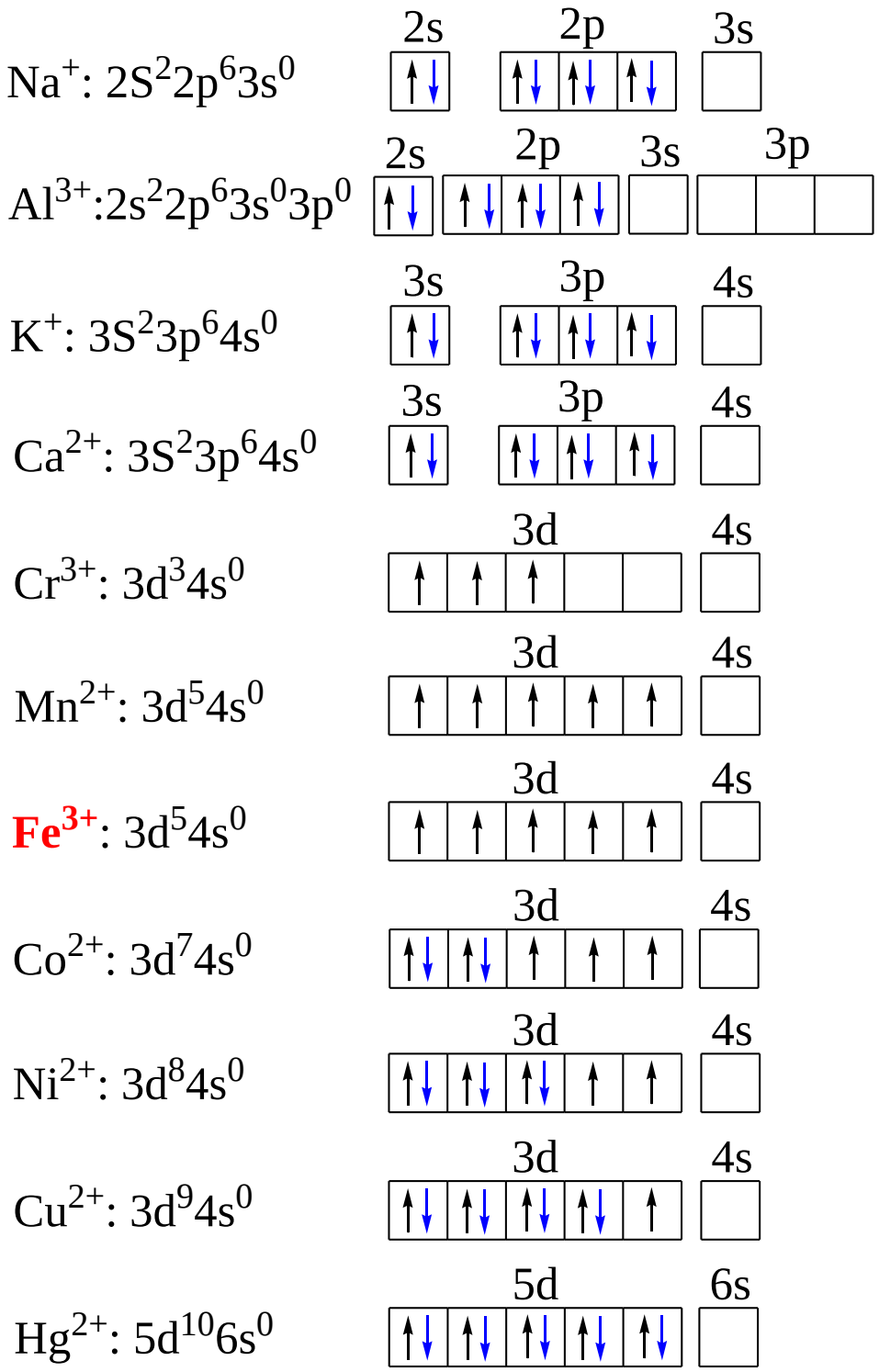


Table S1. Molecular structure of OFA Synthesized with An $FeCl_3$/FA Molar Ratio of 5:1 by MALDI-TOF Mass Spectrum

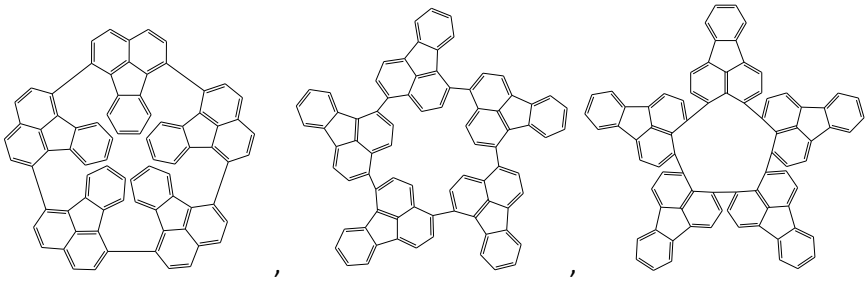
m/e	Formulae	Structure
1000.5	$C_{80}H_{40}$	

Table S2. **Standard Electrode Potentials (SEP) of Some Metal Ions**

Metal ions	Na^+/Na	Al^{3+}/Al	K^+/K	Ca^{2+}/Ca	Cr^{3+}/Cr^{2+}	Mn^{2+}/Mn	Fe^{3+}/Fe^{2+}	Co^{2+}/Co	Ni^{2+}/Ni	Cu^{2+}/Cu	Hg^{2+}/Hg^+
SEP (V)	-2.71	-1.66	-2.93	-2.87	-0.41	-1.17	+0.77	-0.29	-0.25	+0.34	+0.91

Table S3. Comparison of the OFA Fluorescent Chemosensor with Other Ones for Sensing Fe^{III}

chemsensor	Fe^{3+} solvent	detection limit (M)	linear region (M)	association constant (M^{-1})
OFA[This work]	water	6.25×10^{-11}	6.25×10^{-11}–3.13×10^{-3}	2.09×10^{6}
AD-SRhB/β-CD-DNS supramolecular-complex[20]	water	1.0×10^{-6}	1.0×10^{-6}–5×10^{-5}	–
rhodamine-modified Fe_3O_4 nanoparticles[21]	water	3.6×10^{-8}	3.6×10^{-8} –7×10^{-7}	5.0×10^{6}
alexa fluor 488[22]	water	1.8×10^{-7}	2.0×10^{-7}–1.5×10^{-5}	2.7×10^{4}
meso-substituted boron-dipyrromethene derivative[23]	MOPS buffer	–	10^{-7}–10^{-4}	2.7×10^{4}
azotobactin δ[24]	buffer solution	8.95×10^{-9}	1.85×10^{-9}-1.7×10^{-6}	–
N,N-diethylsulfonate-1 -aminomethylnaphthalene[25]	buffer solution	2.0×10^{-6}	1.6×10^{-5}–6.3×10^{-5}	7.6×10^{4}
modified-rhodamine[26,27]	buffer solution	1.4×10^{-8}	6.0×10^{-8}–7.2×10^{-6}	6.43×10^{3}
PMBA-SBA[28]	ethanol/water(9:1)	1.98×10^{-6}	1.0×10^{-5}–4.0×10^{-5}	1.49×10^{4}
dipodal schiff base[29]	THF/H_2O (9:1)	5.0×10^{-6}	5.0×10^{-6}–8.0×10^{-5}	3.8×10^{4}
anthracene-based sensor with amide/β-amino alcohol[30]	CH_3CN/H_2O	1.0×10^{-6}	–	1.6×10^{3}
	CH_3CN	3.0×10^{-8}		
copolyacrylate of 4-amino-1,8-naphthalimide[29]	water	–	Two sections: 1.33×10^{-7}–6.67×10^{-7}; 6.67×10^{-7}–4.00×10^{-4}	9.12×10^{5}, 3.93×10^{4}
water-soluble polymer based on 1,8-naphthalimide[30]	water	–	1.3×10^{-7}–1.0×10^{-5}	3.63×10^{4}
poly(HQPEMA)[31]	DMF	5.0×10^{-5}	5.0×10^{-5}–7.5×10^{-4}	1.44×10^{4}

Table S4. Comparison of the OFA Fluorescent Chemosensor with Others Used for Sensing Picric Acid (PA)

chemosensors	PA solvent	detection limit (M)	linear region (M)	association constant (M^{-1})
OFA[This work]	water	1.0×10^{-12}	1.0×10^{-12}–5.0×10^{-4}	6.1×10^{4}
Am-functionalized 1-ethynylpentaphenylsilole [a35]	water	8.7×10^{-7}	8.7×10^{-7}–3.8×10^{-5}	8.0×10^{4}
polymetallole[a36]	toluene	1.0×10^{-5}	1.0×10^{-5}–1.0×10^{-4}	1.1×10^{4}
poly(trifluoropropylmethylsilane) [a37]	THF	2.6×10^{-5}	10^{-5}–10^{-4}	4.15×10^{4}
TPE-containing polytriazoles[a38]	THF/H_2O	2.5×10^{-7}	4.4×10^{-7}–2.2×10^{-4}	1.1×10^{5}
Eu^{3+}-TTA complex[39]	water	2.0×10^{-6}	4.0×10^{-5}– 4.0×10^{-6}	3.33×10^{3}
$Pt(PEt_3)_2(NO_3)$ triphenylamine and clip-type amide[40]	CH_2Cl_2/DMF	1.0×10^{-6}	1.0×10^{-6}–5.0×10^{-6}	4.81×10^{4}
phosphole oxide[a41]	THF/H_2O	1.0×10^{-5}	1.0×10^{-5}–4.0×10^{-5}	2.03×10^{4}

[a]: The linear range and detection limit are obtained from the corresponding Figs. in the references.