**A highly selective fluorescent probe for nanomolar detection of ferric ions in the living cells and aqueous media**

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**Supplementary Information**

|  |  |
| --- | --- |
| **Benesi-Hildebrand equations** | **S2** |
| **Fig. S1.** 1H NMR spectrum of probe **3** | **S3** |
| **Fig S2.** 13C NMR spectrum of probe **3** | **S3** |
| **Fig. S3.** HR-Mass spectrum of probe **3** | **S4** |
| **Fig. S4.** Host guest relationship from Job’s plot obtained for the complexation of probe **3** with Fe3+ by (a) UV-visible absorption and (b) fluorescence spectroscopy | **S4** |
| **Fig S5.** Binding mode of Probe **3** with Fe3+ ions | **S5** |
| **Fig. S6.** HR-Mass spectrum of probe **3.Fe3+** complex | **S5** |
| **Fig S7.** Calibration curve | **S6** |
| **Table S1.** Crystal data, data collection, and structure refinement details for probe **3** and probe **3.Fe3+** complex | **S7** |
| **Table S2.** Selected bond lengths (Å) and bond angles (°) for probe **3** and probe **3.Fe3+** complex | **S7** |
| **Table S3.** Brief comparison of the results of various fluorescent sensing systems reported for Fe3+ detection. | **S8** |
| **References** | **S8** |

**Benesi-Hildebrand equations**

Where,

*A0* is the absorbance of probe **3** (λ = 326 nm)

*A* is the observed absorbance in the presence of the varying [Fe3+]

*Amax* is the maximum absorbance obtained at λ= 326 nm during the titration with [Fe3+]

*Ka* is the association constant (M-1)

[Fe3+] is the concentration of the Fe3+ ion added during titration studies.

Where,

*I0* is the fluorescence intensity of free probe **3**,

*I*, is the observed fluorescence intensity in the presence of the varying [Fe3+]

*Imax* is the maximum observed fluorescence intensity (λex = 326 nm, λem= 453 nm) up on titration with [Fe3+]

*Ka* is the association constant (M-1)

[Fe3+] is the concentration of the Fe3+ ion added during titration studies.



**Fig. S1.** 1H NMR spectrum of probe **3.**



**Fig. S2.** 13C NMR spectrum of probe **3.**



**Fig. S3.** HR-Mass spectrum of probe **3.**

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**Fig. S4.** Host guest relationship from Job’s plot obtained for the complexation of probe **3** with Fe3+ by (a) UV-visible absorption and (b) fluorescence spectroscopy.



**Fig. S5.** Binding mode of Probe **3** with Fe3+ ions.



**Fig. S6.** HR-Mass spectrum of probe **3.Fe3+** complex



**Fig. S7.** Calibration curve for determination of detection limit of detection for Fe3+. (λex = 326 nm, λem = 453 nm).

**Table S1.** Crystal data, data collection, and structure refinement details for probe **3** and probe **3.Fe3+** complex.

|  |  |  |
| --- | --- | --- |
| Crystal data | probe **3** | Probe **3.Fe3+** complex |
| Formula | C21H18N2O2 | C25H28FeN2O4·NO3·H2O |
| Formula mass (g/mol) | 330.37 | 556.37 |
| Crystal system | Orthorhombic | Orthorhombic |
| Space group | *P*212121 | *Pbca* |
| a, b, c (Å) | 6.2657 (3), 14.9103 (8), 18.0554 (9) | 10.7291 (7), 18.1450 (13), 26.5311 (18) |
| α, β, γ (°) | 90, 90, 90 | 90, 90, 90 |
| V (Å3); Z | 1686.80 (15); 4 | 5165.1 (6); 8 |
| Temperature (K) | 150 | 150 |
| Radiation type | CuKα (λ = 1.54178 Å) | MoKα (λ = 0.71073 Å) |
| μ(CuKα; Cu Kα), mm | 0.68 | 0.64 |
| Collected reflections | 6787 | 40733 |
| 2Θ range (°) | 2.5, 79.6 | 2.3, 28.2 |
| Unique reflections | 3370 | 6072 |
| Goodness-of-fit (GOF) on F2 | 1.052 | 1.058 |
| Rint | 0.0471 | 0.0615 |
| Rsigma | 0.0681 | 0.0447 |
| R1 [I≥2σ (I)] | 0.0556 | 0.0597 |
| wR2 | 0.159 | 0.152 |
| F(000) | 696 | 2328 |
| Crystal size (mm) | 0.4 × 0.07 × 0.06 | 0.33 × 0.29 × 0.12 |
| Crystal description | Needle, yellow | Plate, black |
| CCDC | CCDC 1985816 | CCDC 1985819 |

**Table S2.** Selected bond lengths (Å) and bond angles (°) for probe **3** and probe **3.Fe3+** complex.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Bond lengths (Å)** | | | **Bond Angles (**°**)** | | |
| **A-B** | Probe **3** | Probe **3·Fe3+**complex | **A-B-A** | Probe **3** | Probe **3·Fe3+**complex |
| O1-C1 | 1.344 (4) | 1.360 (3) | C7-N1-C8 | 119.5 (3) | 120.3 (15) |
| O2-C21 | 1.354 (4) | 1.380 (2) | C15-N2-C13 | 122.8 (3) | 112.0 (2) |
| N1-C7 | 1.283 (4) | 1.300 (2) | O1-C1-C2 | 118.4 (3) | 117.6 (11) |
| N1-C8 | 1.417 (4) | 1.437 (7) | O1-C1-C6 | 121.9 (3) | 126.0 (17) |
| N2-C15 | 1.289 (4) | 1.300 (2) | C2-C1-C6 | 119.7 (3) | 116.5 (18) |
| N2-C13 | 1.404 (4) | 1.310 (3) | N1-C7-C6 | 121.1 (3) | 127.4 (14) |
| C15-C16 | 1.398 (5) | 1.461 (18) | C9-C8-N1 | 120.8 (3) | 125.6 (11) |
| C6-C7 | 1.453 (5) | 1.487 (19) | C13-C8-N1 | 118.5 (3) | 114.2 (13) |
| C10-C14 | 1.505 (5) | 1.509 (12) | C12-C13-N2 | 126.3 (3) | 129.8 (16) |
| C8-C13 | 1.407 (5) | 1.410 (15) | N2-C13-C8 | 115.8 (3) | 111.6 (18) |
| C1-C6 | 1.409 (5) | 1.360 (3) | N2-C15-C16 | 120.8 (3) | 126.8 (16) |
| C16-C21 | 1.408 (5) | 1.410 (16) | O2-C21-C20 | 118.5 (3) | 116.8 (10) |
| O1-Fe1 | - | 1.893 (2) | O2-C21-C16 | 121.6 (3) | 125.4 (14) |
| O2-Fe1 | - | 1.892 (2) | O2-Fe1-N2 | - | 92.0 (6) |
| N1-Fe1 | - | 2.100 (2) | O1-Fe1-N2 | - | 164.4 (6) |
| N2-Fe1 | - | 2.090 (3) | O2-Fe1-N1 | - | 163.9 (4) |
| - | - | - | O1-Fe1-N1 | - | 92.6 (4) |
| - | - | - | N2-Fe1-N1 | - | 72.7 (7) |
| - | - | - | O2-Fe1-O1 | - | 103.06 (10) |

**Table S3.** Brief comparison of the results of various fluorescent sensing systems reported for Fe3+ detection.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sr. No. | Chemosensor | LoD, M | Samples | References |
| **1.** | Coumarin conjugate | 4.8 × 10−6 | Aqueous | [[[1]](#endnote-1)] |
| **2.** | Rhodamine and BODIPY conjugate | 3.91 × 10−7 | Adenocarcinoma cell line | [[[2]](#endnote-2)] |
| **3.** | Quinoline conjugated rhodamine | 40 × 10−9 | Zebrafish embryos | [[[3]](#endnote-3)] |
| **4.** | Triphenylamine-triazole based molecules | 1.2 × 10−7 | Semi-aqueous | [[[4]](#endnote-4)] |
| **5.** | Pyrophosphate functionalized gold nanoparticles | 5.6 × 10−6 | Aqueous | [[[5]](#endnote-5)] |
| **6.** | Probe **3** | 21.5 × 10−9 | Colorectal carcinoma cell line | **This study** |

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