Current research in life and environmental sciences is dedicated to chemosensors able to detect metals of biological interest such as zinc and iron or other toxic and carcinogenic, as cadmium, mercury, chromium, lead. Recently, a new chemosensor strategy of “single chemosensor for multiple metals” has emerged. For this scope, many fluorescent sensors for Cd(II) and Zn(II) have been designed and synthesized, as ligand systems or in polymeric matrices [1–3]. The data presented in this article include experimental data on the of a pyridyl/phenolic/benzothiazole functionalized colorimetric receptor (BPAP) and its selectively recognise Fe(III) and Fe(II) ions with visible, naked eye colour changes and fluorometric selectivity towards Zn²⁺ and Cd²⁺ ions in aqueous medium.

This article is submitted as a companion paper to Caruso et al. (2018) [4].

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**Specifications Table**

| Subject area       | Chemistry, Materials Science |
|--------------------|------------------------------|
| More specific subject area | Electro-optic field sensors |
| Type of data       | Crystal data and structure refinement, NMR spectrum, tables and figure |
| How data was acquired | NMR recorded in DMSO using Bruker Spectrometers operating at 400 MHz. |
|                    | UV-Visible and fluorescence spectra recorded with JASCO spectrometers. |
|                    | Single crystals X-ray structural analysis performed on a BrukerNoniusKappaCCD diffractometer equipped with Oxford Cryostream apparatus. |
| Data format        | Raw data and their elaborations |
| Experimental factors | The data concerns structural information, UV/Vis calculation and some spectroscopic raw data |
| Experimental features | Elaboration of X-ray diffraction data and UV/Vis curves |
| Data source location | Naples, Italy |
| Data accessibility | Data is within this article |

**Value of the data**

- The data show some molecular structure of BPAP along a and c axes.
- The data report relevant structural data of BPAP and its zinc complex (lengths and angles).
- The data report Job's plot analysis for the binding Zn(II) and Cd(II) with ligand system.
- $^1$H NMR and $^{13}$C NMR of BPAP and BPAP metal complexes are reported.

1. Data

The data presented in this article are related to the research article entitled “A real-time tripodal colorimetric/fluorescence sensor for multiple target metal ions” [4]. Recently an impressive progress has been done toward the design and synthesis of novel sensitive ligands and fluorescent materials [5–8]. The data presented here include experimental data on the of a pyridyl/phenolic/benzothiazole functionalized colorimetric receptor (BPAP) and its selectively recognise Fe(III) and Fe(II) ions with visible, naked eye colour changes and fluorometric selectivity towards Zn$^{2+}$ and Cd$^{2+}$ ions in aqueous medium.

The following data are a necessary support for the identification of materials and properties of the ligand system and its complexes.

2. Experimental design, materials and methods

Structural analysis of single crystals of ligand and its Zinc complex has been performed on a BrukerNoniusKappaCCD diffractometer equipped with Oxford Cryostream apparatus (graphite monochromated MoK$_α$ radiation, $λ = 0.71073$ Å, CCD rotation images, thick slices, $φ$ and $ω$ scans to fill asymmetric unit). Semiempirical absorption corrections (SADABS [9]) were applied. Both the two structures were solved by direct methods (SIR97 program [10]) and anisotropically refined by the full matrix least-squares method on $F^2$ against all independent measured reflections using SHELXL-2016 [11] and WinGX software [12]. Crystal data and structure refinement details are reported in Table 1. Relevant bond lengths and angle are reported in Table 2. The figures were generated using ORTEP-3 [13] and Mercury CSD 3.9 [14] programs. Molecular structure of BPAP along a axis is shown in Fig. 1. Molecular structure of the complex Zn–BPAP along c axis is shown in Fig. 2.
### Table 1
Structural data and refinement details for BPAP and Zn-BPAP.

|                      | BPAP                | Zn-BPAP               |
|----------------------|---------------------|-----------------------|
| **CCDC number**      | 1582069             | 1582070               |
| **Empirical formula**| C23H22N4O2S         | C23H22Cl2N4O2Szn      |
| **Formula weight**   | 418.50              | 554.77                |
| **Temperature (K)**  | 298(2)              | 173(2)                |
| **Wavelength (Å)**   | 0.71073             | 0.71073               |
| **Crystal system (Å)**| Triclinic           | Monoclinic            |
| **Space group**      | P -1                | P2₁/c                 |
| **a (Å)**            | 7.2950(15)          | 18.542(5)             |
| **b (Å)**            | 16.3670(18)         | 14.650(3)             |
| **c (Å)**            | 18.592(2)           | 17.217(2)             |
| **α (°)**            | 77.506(8)           | 90.                   |
| **β (°)**            | 87.794(11)          | 92.373(13)            |
| **γ (°)**            | 85.826(11)          | 90.                   |
| **Volume (Å³)**      | 2160.9(6)           | 4672.8(17)            |
| **Z4**               | 8                   |                       |
| **Dcalc (Mg/m³)**    | 1.286               | 1.577                 |
| **F(000)**           | 880                 | 2272                  |
| **Crystal size (mm)**| 0.480 × 0.150 × 0.020 | 0.200 × 0.060 × 0.040 |
| **θ range (°)**      | 2.333 to 25.996     | 2.602 to 27.022       |
| **Reflections collected / unique** | 19,458 / 8234 [R(int) = 0.0671] | 39,344 / 10,013 [R(int) = 0.1524] |
| **Refl. method**     | Full-matrix least-squares on F² | Full-matrix least-squares on F² |
| **Data / restraints / parameters** | 8234 / 0 / 556 | 10,013 / 0 / 609 |
| **Goodness-of-fit on F²** | 1.034              | 1.079                 |
| **Final R indices [I > 2σ(I)]** | R1 = 0.0628, wR2 = 0.1340 | R1 = 0.0787, wR2 = 0.1561 |
| **R indices (all data)** | R1 = 0.1416, wR2 = 0.1695 | R1 = 0.1891, wR2 = 0.2013 |
| **Largest diff. peak and hole (eÅ⁻³)** | 0.448 and −0.283     | 0.800 and −0.878       |

### Table 2
Selected bond lengths (Å) and angles (°).

|                      | **BPAP**             | **Zn-BPAP**            |
|----------------------|----------------------|------------------------|
| **Molecule A**       |                      |                        |
| C9-O1                | 1.219(4)             | 1.212(4)               |
| C9-N2                | 1.357(8)             | 1.357(5)               |
| S1-C8                | 1.746(3)             | 1.742(4)               |
| S1-C6                | 1.734(4)             | 1.730(4)               |
| Zn1-N2               | 2.207(6)             | 2.213(6)               |
| Zn1-N3               | 2.182(6)             | 2.165(6)               |
| Zn1-N4               | 2.157(6)             | 2.140(6)               |
| Zn1-Cl1              | 2.250(3)             | 2.289(2)               |
| Zn1-Cl2              | 2.288(3)             | 2.282(2)               |
| **Molecule B**       |                      |                        |
| C8-N2-C9             | 1.262(3)             | 1.260(3)               |
| N2-C9-C10            | 1.158(3)             | 1.153(3)               |
| O1-C9-N2             | 1.22(4)              | 1.12(4)                |
All crystal data were deposited at Cambridge Crystallographic Data Centre with assigned number CCDC 1582069 (BPAP) and 1582070 (Zn-BPAP). These data can be obtained free of charge from www.ccdc.cam.ac.uk/data_request/cif.

NMR spectra were recorded in DMSO using a Bruker Spectrometer operating at 400 MHz. For BPAP, both $^1$H and $^{13}$C NMR are reported in Figs. 3 and 4. In Fig. 5, $^1$H NMR spectrum of Zn-BPAP is shown.
Job’s plot measurement of Zn$^{2+}$ and Cd$^{2+}$ (Fig. 6) has been performed on 500μM solutions of Zn (II) chloride (or Cd(II) chloride) in bidistilled water (pH 6.25) and 500μM of BPAP in ethanol. Volumes of 3.00, 2.75, 2.50, 2.00, 1.50, 1.00, 0.50, 0.25 and 0 mL of the solution of ligand were taken and transferred to vials and volumes of 0, 0.25, 0.50, 1.00, 1.50, 2.00, 2.50, 2.75, 3.00 mL of metal ion added, each vial having a total volume of 3.0 mL. Fluorescence spectra were recorded at room temperature after shaking each vial for a few seconds.
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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.06.096.
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