

Chromone Hydrazone-Based Fluorescent Chemosensor for Pb²⁺ Detection: Experimental and Theoretical Insights into a Turn-On Fluorescence Response

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The detection of Pb²⁺ ions is essential because of their extensive industrial applications and well-documented toxicity. In this study, a series of chromone hydrazone-based ligands, namely FCMSH, CFCMSH, and DCFCMSH, were synthesised under reflux conditions and characterised using CHNS elemental analysis, FTIR, NMR, and UV–Vis spectroscopy. The fluorescence properties of the ligands in the presence of Pb²⁺ ions were examined using a fluorescence spectrophotometer. Only DCFCMSH exhibited turn-on fluorescence, changing from silent quenching to a green glow upon Pb²⁺ ion coordination. The DCFCMSH sensor exhibited a binding constant of $1.17 \times 10^4 \text{ M}^{-1}$ and a limit of detection (LOD) of $2.4 \times 10^{-8} \text{ M}$, demonstrating its sensitivity toward Pb²⁺ ion detection. FTIR analysis of DCFCMSH revealed shifts in the C=O (1598 cm⁻¹) and C=N (1519 cm⁻¹) bands, suggesting coordination through carbonyl and imine sites, while the appearance of the $\nu(\text{SO}_2)$ band at 1050 cm⁻¹ confirmed sulphonyl-oxygen involvement. The disappearance of the N–H proton signal (10.67 ppm) in the ¹H NMR spectrum and the C=N signal shift (147.39 ppm) in the ¹³C NMR spectrum further supported Pb²⁺ ion coordination in DCFCMSH. DFT (B3LYP/6-311G(d,p)) calculations provided insights into the HOMO–LUMO transition responsible for fluorescence enhancement. Overall, coordination through ONO donor sites induces a chelation-enhanced fluorescence (CHEF) effect, and these findings represent an important step toward the development of chromone hydrazone-based as potential Pb²⁺ ion chemosensors in aqueous environments. Overall, the proposed coordination through ONO donor sites is associated with a chelation-enhanced fluorescence (CHEF) effect, and these findings highlight the potential of DCFCMSH as fluorescent chemosensors for Pb²⁺ ion detection.

Keywords: Chromone hydrazone-based, Pb²⁺ ion, turn-on fluorescence, HOMO–LUMO transition

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Heavy metal contamination of water sources has become a major global concern because of its severe impact on humans and the environment [1]. Among various toxic metals, lead (Pb²⁺) is one of the most persistent and hazardous pollutants, originating mainly from industrial processes, paints, and mining activities [2]. Chronic exposure to Pb²⁺ ions can cause neurological, cardiovascular, and renal disorders, especially in children and pregnant women [3]. Therefore, developing sensitive and selective methods for detecting Pb²⁺ ions is of paramount importance for environmental monitoring and public health protection.

Traditional analytical techniques such as atomic absorption spectroscopy (AAS), inductively coupled plasma mass spectrometry (ICP-MS), and voltammetric methods, offer high sensitivity and accuracy [4]. However, these approaches often require sophisticated instrumentation, costly reagents, and complex sample preparation. In contrast, fluorescent chemosensors have emerged as promising alternatives owing to their operational simplicity, low cost, rapid response, and potential for on-site detection through visible colour or fluorescence changes [5–8]. Chromone-based compounds have attracted increasing attention as versatile fluorescence scaffolds due to

their rigid aromatic framework, strong π - π^* conjugation and tunable photophysical properties [9, 10]. The presence of functional moieties such as hydrazide, hydrazone or thiosemicarbazone groups further enhances their metal-binding ability through coordination with nitrogen, oxygen, or sulfur donor atoms [11, 12]. These interactions often modulate fluorescence via mechanisms such as chelation-enhanced fluorescence (CHEF) or inhibition of photoinduced electron transfer (PET) [7].

Although various chromone derivatives have been reported for coordination applications and as fluorescent probes for metal ion sensing, studies on chromone-based sulfonylhydrazone analogues remain limited, particularly in the context of Pb²⁺ ion recognition. The influence of chlorine substitution on the Pb²⁺ sensing behaviour and electronic structure of chromone-based sulfonylhydrazone ligands has not been systematically investigated. Furthermore, the correlation between experimental spectroscopic observations and theoretical electronic structure analyses remains insufficiently explored. Therefore, in this study, the interaction of Pb²⁺ with three chromone hydrazone-based ligands with different substitution patterns (FCMSH, CFCMSH and DCFCMSH) was investigated to evaluate the effect of chlorine substitution on Pb²⁺ sensing performance. To further support the experimental findings, theoretical studies were conducted to gain deeper insight into the coordination mechanism and electronic transitions involved in Pb²⁺ induced fluorescence enhancement.

EXPERIMENTAL

Chemicals and Materials

All starting materials and solvents used in the synthesis and characterisation studies were purchased from Acros and Aldrich and used without further purification. 3-Formylchromone derivatives (FC), 6-Chloro-3-formylchromone (CFC), 6,8-dichloro-3-formylchromone (DCFC), *p*-toluenesulfonyl hydrazide (MSH), ethanol, DMSO, and DMSO-*d*₆ were used for ligand synthesis and characterisation. Lead(II) nitrate (Pb(NO₃)₂) was used as the Pb²⁺ source, and other metal nitrate salts were used for selectivity and sensitivity studies.

Characterisation Methods

All reagents and solvents used for the synthesis and spectroscopic measurements were purchased from Sigma-Aldrich. FTIR spectrum was obtained using Thermo Nicolet Nexus spectrometer from 4000-600 cm⁻¹ region with diamond as an Attenuated Total Reflectance (ATR) accessory. The UV-VIS measurements were performed in 200 to 800 nm region by using Cary 60 UV-Visible spectrophotometer. Fluorescence measurements were performed using dimethyl sulfoxide (DMSO) as the solvent. Elemental

analyses of C, H, and N were carried out using a CHNO-SEA 1112 Series Elemental Analyser. ¹H and ¹³C NMR spectra were recorded on a JEOL JNM-ECX500 NMR spectrometer using DMSO-*d*₆ and acetone-*d*₆ as the solvents.

Computational Methods

DFT and time-dependent density functional theory (TD-DFT) calculations for all ligand series and the Pb-DCFCMSH complex were performed using Gaussian 09 and visualised with GaussView 5.0 [13, 14]. The ligands and complexes were drawn using GaussView software. Geometrical optimisation and vibrational frequency calculations were performed without symmetry constraints (C1 point group). The basis set of Becke's three-parameter functional (B3LYP) and the 6-311G,d,p basis set were used for all ligands [15], while a hybrid basis set compliant with LANL2DZ was used to calculate the Pb metal atom [16, 17]. The solvent effects were considered in all calculations, employing dimethyl sulfoxide (DMSO) as the solvent in the IEFPCM model. Frequency calculations were performed on the fully optimised geometries, and no imaginary frequencies were found, confirming that the optimised structures were true minima [15].

Synthesis of Chromone Hydrazone-based Ligands: FCMSH, CFCMSH and DCFCMSH

Figure 1 presents the general synthetic pathway for the synthesis of chromone hydrazone-based ligands, following a modified literature procedure [18, 19]. An equimolar amount (1 mmol) of the corresponding 3-formylchromone derivative (FC, CFC or DCFC) was condensed with *p*-toluenesulfonyl hydrazide, MSH (1 mmol) in 30 mL of acidified ethanol (pH 4) under reflux at 110 °C. The synthesis duration was standardised by monitoring the progress of the reaction using thin-layer chromatography (TLC). After completion of the reaction, the resulting precipitate was filtered, washed with cold ethanol at room temperature, and dried in a desiccator. The crude products were subsequently recrystallised from ethanol to afford the corresponding ligands, FCMSH, CFCMSH, and DCFCMSH.

FCMSH: (Yield: 73%). FTIR (cm⁻¹): 3122 (N-H stretching), 1632 (C=O stretching), 1617 (C=N stretching), 1346 (S=O_{as} stretching), 1117 (S=O_s stretching). UV-vis: (DMSO): λ_{max} (nm): 305. ¹H NMR (500 MHz) δ 11.70 (s, 1H), 8.90 (d, *J* = 0.7 Hz, 1H), 8.23 (d, *J* = 0.7 Hz, 1H), 8.04 – 7.97 (m, 2H), 7.99 – 7.93 (m, 1H), 7.61 – 7.54 (m, 1H), 7.54 – 7.47 (m, 2H), 7.04 – 6.95 (m, 2H), 2.43 (s, 3H). ¹³C NMR (126 MHz) δ 20.83 (C-1), 117.98 (C-18), 119.59 (C-12), 123.29 (C-14), 126.44 (C-15), 128.62 (C-15), 128.62 (C-7), 130.49 (C-4), 130.49 (C-4), 133.29 (C-13), 134.64 (C-2), 136.63 (C-6), 145.28 (C-8), 147.26 (C-11), 162.12 (C-10), 191.68 (C-17). CHN elemental analysis: Calculated for C₁₇H₁₄N₂O₄S: C: 60.56%,

H: 4.50%, N: 7.70%. Found: C: 60.79%, H: 4.52%, N: 7.80%. EI-MS: *m/z* calculated: 342, found: 342.07.

CFCMSH: (Yield: 83%). FTIR (cm⁻¹): 3132 (N–H stretching), 1638 (C=O stretching), 1602 (C=N stretching), 1372 (S=O_{as} stretching), 1152 (S=O_s stretching), 813 (C–Cl stretching). UV–vis: (DMSO): λ_{max} (nm): 299. ¹H NMR (500 MHz) δ 11.55 (s, 1H), 8.62 (s, 1H), 7.95 (d, *J* = 2.6 Hz, 2H), 7.83 (ddd, *J* = 9.1, 2.8, 1.1 Hz, 1H), 7.76–7.70 (m, 3H), 7.39–7.35 (m, 2H), 2.33 (s, 3H). ¹³C NMR (126 MHz) δ 188.81(C-17), 155.79 (C-10), 155.76(C-8), 138.55 (C-11), 145.63 (C-8), 137.56 9 (C-6), 132.74(C-2), 129.17 (C-13), 128.72 (C-3), 127.99 (C-14), 127.96 (C-15), 126.02 (C-5), 123.05(C-14), 122.49 (C-12), 119.25(C-9), 40.87, 21.33(C-1). CHN elemental analysis: Calculated for C₁₇H₁₃ClN₂O₄S: C: 54.19%, H: 3.48%, N: 7.43%. Found: C: 54.27%, H: 3.29%, N: 8.30%. EI-MS: *m/z* calculated: 376, found: 376.03.

DCFCMSH: (Yield: 85%). FTIR (cm⁻¹): 3148 (N–H stretching), 1633 (C=O stretching), 1544 (C=N stretching), 1343 (S=O_{as} stretching), 1160 (S=O_s stretching), 814 (C–Cl stretching). UV–vis: (DMSO): λ_{max} (nm): 310. ¹H NMR (500 MHz) δ 10.68 (s, 1H), 8.96 (s, 1H), 8.23 (s, 1H), 7.95–7.92 (m, 2H), 7.76 (d, *J* = 2.6 Hz, 1H), 7.49–7.46 (m, 3H), 2.37 (s, 3H). ¹³C NMR (126 MHz) δ 187.38 (C-17), 151.61 (C-11), 147.61 (C-8), 145.81 (C-2), 136.66 (C-6), 133.09 (C-14), 132.88 (C-13), 131.12 (C-3), 128.83 (C-7), 128.69 (C-10), 128.61 (C-9), 124.67(C-12), 124.01 (C-16), 70.30 (C-18), 21.76 (C-1). CHN elemental analysis: Calculated for C₁₇H₁₂Cl₂N₂O₄S: C: 49.65%, H: 2.94%, N: 6.81%. Found: C: 49.91%, H: 2.75%, N: 7.66%. EI-MS: *m/z* calculated: 410, found: 410.28.

Fluorescence Measurement

The fluorescence emission spectra of the chromone hydrazone-based ligands in the absence and presence

of Pb²⁺ ions, were recorded using fluorescence spectrophotometer with excitation and emission slit widths of 5 nm. Stock solutions of the ligands and Pb²⁺ ions were prepared, and the effects of solvent, ligand concentration, ligand-to-Pb²⁺ molar ratio, pH, and response time were systematically investigated to establish the optimum fluorescence sensing conditions. Following optimisation, the ligand solution (1.0 × 10⁻³) was mixed with an equimolar Pb²⁺ ion solution (1:1 molar ratio), and the final volume was adjusted to 3 mL using DMSO. The samples were equilibrated for 5 min prior to analysis. For comparative fluorescence analysis, the excitation wavelength was set to 439 nm and the emission spectra were collected over the range of 400–700 nm. The interference study was further conducted by adding 1.0 eq of competing metal ions (Pb²⁺, Al³⁺, Co²⁺, Cu²⁺, Fe²⁺, Hg²⁺, Mn²⁺, Ni²⁺, and Zn²⁺) to the ligand solution in the presence of Pb²⁺.

RESULTS AND DISCUSSION

Structural Characterization of Chromone Hydrazone-Based Ligands

The synthesised chromone hydrazone-based ligands were obtained in good yields with high purity, as confirmed by elemental analysis and mass spectrometry. The ligand FCMSH was isolated as a white precipitate, whereas the chlorinated derivatives (CFCMSH and DCFCMSH) were isolated as yellow precipitates. These colour differences may be attributed to the electronic effects caused by the substitution patterns on the chromone ring, particularly the presence of halogen atoms [20, 21]. Additionally, the relatively high melting points suggest good thermal stability which is beneficial for their potential use in metal coordination and chemosensing studies.

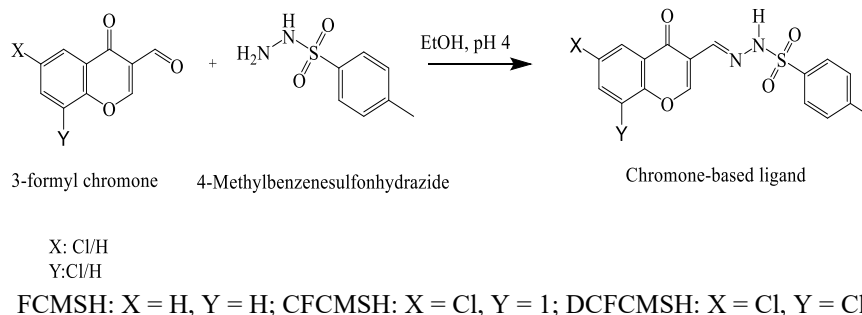


Figure 1. Chemical synthesis pathway for FCMSH, CFCMSH, DCFCMSH.

The elemental analysis of carbon, hydrogen, and nitrogen for all synthesised chromone hydrazone-based ligands showed good agreement with the calculated values, with deviations within ± 1.0 . This small variation range (± 1.0 %) indicates a high degree of homogeneity and suggests the presence of impurities in the bulky species [22]. Such consistency further validates the proposed molecular formulations and confirms the correct stoichiometry of the synthesised compounds. The accuracy of the CHNS analysis supports the successful synthesis of the target ligands and together with the mass spectrometry, FTIR, and NMR data, provides a robust foundation for structural confirmation. Moreover, the confirmed purity ensured the reliability of subsequent applications involving metal coordination and chemosensor development.

FTIR Spectroscopy

In summary, the FTIR spectra of the FCMSH, CFCMSH and DCFCMSH ligands exhibited almost similar patterns of absorption bands at 3122-3148 cm⁻¹, 1632-1638 cm⁻¹, 1592-1602 cm⁻¹, 1343-1372 cm⁻¹ and 1117-1160 cm⁻¹ which were assigned to $\nu(\text{N-H})$, $\nu(\text{C=O})$, $\nu(\text{C=N})$, $\nu(\text{S=O}_{\text{as}})$ and $\nu(\text{S=O}_{\text{s}})$, respectively [19, 23]. In addition, the vibration of $\nu(\text{C-Cl})$ from the aromatic chromone ring was observed at 813-814 cm⁻¹, confirming the structures of CFCMSH and DCFCMSH (Figure 1). The disappearance of the band of the primary amine (NH₂) in *p*-toluenesulfonyl hydrazide at 3200-3400 cm⁻¹ is accompanied by the appearance of a new band attributed to imine (C=N) at around 1602-1592 cm⁻¹. This indicates that condensation occurred between the NH₂ of *p*-toluenesulfonyl hydrazide and the carbonyl of 3-formyl chromone, confirming the successful formation of the targeted Schiff base compound [11].

UV-Vis Spectroscopy

The UV-Vis spectra displayed absorption bands at shorter wavelengths of 305, 299 and 310 nm for the FCMSH, CFCMSH, and DCFCMSH ligands, respectively. These transitions involve the excitation of electrons from the bonding π orbitals in the conjugated aromatic system of the 3-formylchromone and *p*-toluenesulfonyl hydrazide structures to antibonding π^* orbitals, corresponding to absorption bands at relatively higher energies [12]. However, no absorption bands could be clearly assigned to $n \rightarrow \pi^*$ transitions, which are typically associated with non-bonding electron transitions from functional groups

such as C=O, C=N, and S=O [24]. This phenomenon may be attributed to the overlapping contributions of intense $\pi \rightarrow \pi^*$ transitions with weaker $n \rightarrow \pi^*$ transitions, resulting in the latter being undetectable in the spectra [25, 26]. In addition, UV-Vis analysis demonstrated a bathochromic shift upon the introduction of two chloro substituents in DCFCMSH compared with FCMSH and CFCMSH. The presence of additional chloro substituents may enhance the conjugation with the chromone system, lowering the energy gap between the HOMO and LUMO, thereby resulting in a higher λ_{max} value (310 nm) [27].

NMR Spectroscopy (¹H and ¹³C NMR)

The detailed assignments of the significant ¹H and ¹³C resonances are summarised in Table 1 and 2, while the complete spectral data are provided in the Experimental section. According to Table 1, the ¹H-NMR spectra of FCMSH, CFCMSH, and DCFCMSH exhibited a multiplet range of δ 6.99-8.23 ppm corresponding to the aromatic protons (chromone and *p*-tolyl moieties), and a singlet at δ 8.62-8.96 ppm attributed to the azomethine proton ($-\text{CH=N}-$). Meanwhile a singlet peak occurred in the range of δ 10.67-11.70 ppm assigned to the NH group, and the methyl protons of the *p*-tolyl group appeared as a singlet at signal at δ 2.33-2.43 ppm [9, 25]. The ¹³C NMR spectra of the ligands showed signals between δ 117.98-162.12 ppm corresponding to aromatic carbons, an azomethine carbon ($-\text{CH=N}-$) at δ 145.28-147.61 ppm, a carbonyl carbon (C=O) at δ 187.38-191.68 ppm, and a methyl carbon at δ 20.83-21.76 ppm (Table 2) [12].

Fluorescence Properties

The photophysical behaviours of FCMSH, CFCMSH, and DCFCMSH were investigated via fluorescence studies. These studies were carried out through fluorescence-based screening of the ligands under UV light exposure, both visually and spectroscopically to evaluate their potential as fluorescent chemosensors, particularly for the detection of Pb²⁺. In this preliminary qualitative experiment, 1.0 eq of Pb²⁺ solution was added to each ligand solution. Figure 2 (inset:a) shows that no fluorescence emission was observed for the free ligands in the absence of Pb²⁺ ions. Upon the addition of Pb²⁺ (inset:b), only DCFCMSH exhibited noticeable green fluorescence under UV illumination, suggesting the formation of a new fluorescent species or enhanced conjugation due to metal coordination [28].

Table 1. Summary of significant ¹H NMR signal assignments for FCMSH, CFCMSH and DCFCMSH.

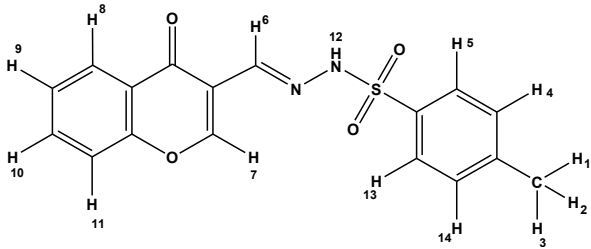
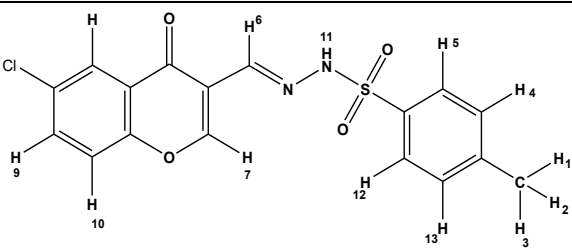
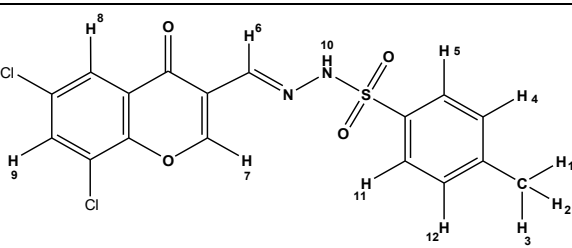
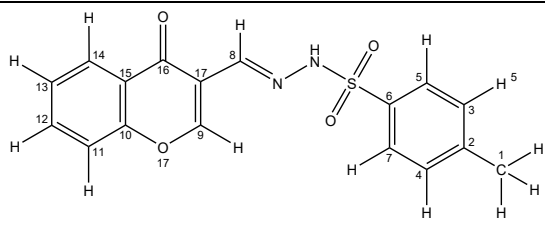
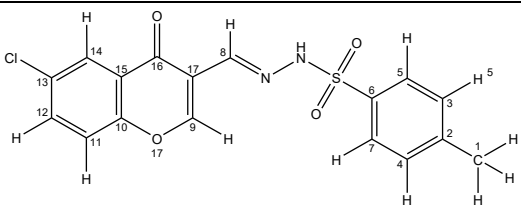
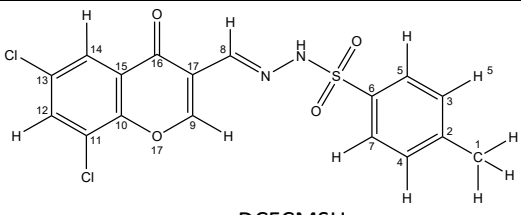
Chemical Structure	¹ H NMR Assignment	δ (ppm)
 FCMSH	N–H (H12) CH=N (H6) Aromatic H (H4–H14) CH ₃ (H1–H3)	11.70 8.90 6.99–8.23 2.43
 CFCMSH	N–H (H11) CH=N (H6) Aromatic H (H4–H13) CH ₃ (H1–H3)	11.55 8.62 7.37–7.95 2.33
 DCFCMSH	N–H (H12) CH=N (H6) Aromatic H (H4–H12) CH ₃ (H1–H3)	10.67 8.96 7.48–8.23 2.37

Table 2. Summary of significant ¹³C NMR signal assignments for FCMSH, CFCMSH and DCFCMSH.

Chemical Structure	¹³ C NMR Assignment	δ (ppm)
 FCMSH	(C=O) C(16) (C=N) C(8) Aromatic C (C2–C6, C9–15, C17) CH ₃ (C1)	191.68 147.28 117.98–162.12 21.33
 CFCMSH	(C=O) C(16) (C=N) C(8) Aromatic C (C2–C6, C9–15, C17) CH ₃ (C1)	188.81 145.63 119.25–155.79 21.33
 DCFCMSH	(C=O) C(16) (C=N) C(8) Aromatic C (C2–C6, C9–15, C17) CH ₃ (C1)	187.38 147.61 123.73–151.61 21.76

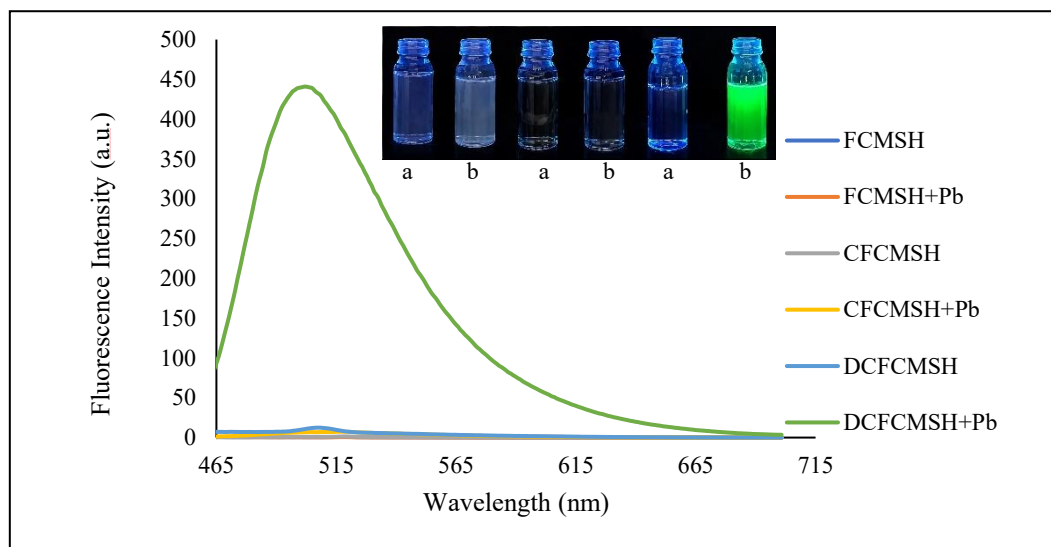


Figure 2. Fluorescence emission spectra of FCMSH, CFCMSH, and DCFMSH (1×10^{-3} M) in DMSO in the absence and presence of Pb²⁺ (1.0 eq) at 501 nm ($\lambda_{\text{ex}} = 439$ nm). Inset: photographs of ligands solution (a) before and (b) after Pb²⁺ addition under UV irradiation at 365 nm.

The fluorescence behaviour was further examined using fluorescence spectroscopy with an excitation wavelength of 439 nm (Figure 2). Interestingly, compound DCFMSH showed a strong emission peak at 501 nm upon the addition of Pb²⁺. In contrast, the other ligands showed no detectable emissions under the same conditions. No fluorescence emission from DCFMSH was observed in the absence of Pb²⁺ due to the quenching effect attributed to photoinduced electron transfer (PET) from the lone pair of electrons of nitrogen, oxygen, and sulfur atoms present in azomethine, sulfonyl, and carbonyl [7, 29]. Upon the addition of Pb²⁺ ions, the lone pairs on the donor atoms are involved in coordination with the metal ion, resulting in chelation-enhanced fluorescence (CHEF). This coordination inhibits both the excited-state intramolecular proton transfer (ESIPT) and photo-induced electron transfer processes (PET), thereby restoring fluorescence [30]. Consequently, a clear “off-on” fluorescence signal was observed, with strong green emissions at 501 nm for DCFMSH (Figure 2). This coordination-induced suppression of PET is consistent with literature-reported PET-based sensing mechanisms, in which analyte binding restores radiative decay processes [29]. These results indicate that the DCFMSH compound exhibits an ‘off-on’ fluorescence behaviour in the presence of Pb²⁺ ions, highlighting its potential as a chemosensor for Pb²⁺ ion detection.

A series of optimisation studies were carried out to determine the ideal experimental conditions for fluorescence sensing using the synthesised chromone-based ligands. Among the tested solvents, DMSO provided the highest fluorescence emission and was therefore selected as the working solvent. The optimal pH was found to be alkaline with pH 10, which offered

maximum emission intensity. Ligand concentration studies revealed that 1×10^{-3} M for DCFMSH in the presence of equimolar Pb²⁺ ion (1:1 molar ratio), yielded the most intense fluorescence signals. Time-dependent fluorescence measurements showed that DCFMSH responded rapidly within 5 minutes to reach a stable emission plateau. These optimised conditions were subsequently adopted for further selectivity studies.

The fluorescence selectivity of the ligands towards Pb²⁺ was subsequently evaluated in the presence of various metal ions including Cu²⁺, Fe²⁺, Mn²⁺, Co²⁺, Zn²⁺, Hg²⁺, and Ni²⁺ (Figure 3). These metal ions were selected due to their different electronic configurations, oxidation states, and coordination properties, which may influence their interactions with the donor atoms of the chromone hydrazone-based ligand. The goal was to identify the metal ion that yielded the highest fluorescence intensity with each ligand. The addition of Zn²⁺, Mn²⁺ and Pb²⁺ ions caused a significant bathochromic shift in the emission peak to 501 nm, with Pb²⁺ ion giving the highest response, with a substantial fluorescence enhancement of 440 a.u. Other metal ions did not induce a notable enhancement in the fluorescence of DCFMSH. This selective response to Pb²⁺ indicates the suitability of DCFMSH as a fluorescent probe for the detection of Pb²⁺.

A sensitivity study was performed to investigate the interference of other metal ions on the fluorescence behaviour of the DCFMSH. Figure 4 shows the addition of interfering metal ions such as Al³⁺, Hg²⁺, Mn²⁺ and Zn²⁺ decreased the fluorescence intensity, but a significant fluorescence signal of the DCFMSH–Pb²⁺ system remained observable. The presence of

Co^{2+} reduced the fluorescence signal to approximately one-sixth of that observed for the Pb^{2+} system, while Cu^{2+} and Fe^{3+} completely quenched the fluorescence intensity and Ni^{2+} caused substantial fluorescence quenching.

The great drop in the fluorescence intensity particularly Cu^{2+} , Fe^{2+} , Co^{2+} and Ni^{2+} is consistent

with previous reports, which attribute such behavior to the strong coordination ability and paramagnetic nature of these transition-metal ions [31]. Although the DCFCMSH sensor exhibited a preferential response toward Pb^{2+} , its selectivity may be further improved through ligand modification or appropriate sample pretreatment using selective masking agents in future studies.

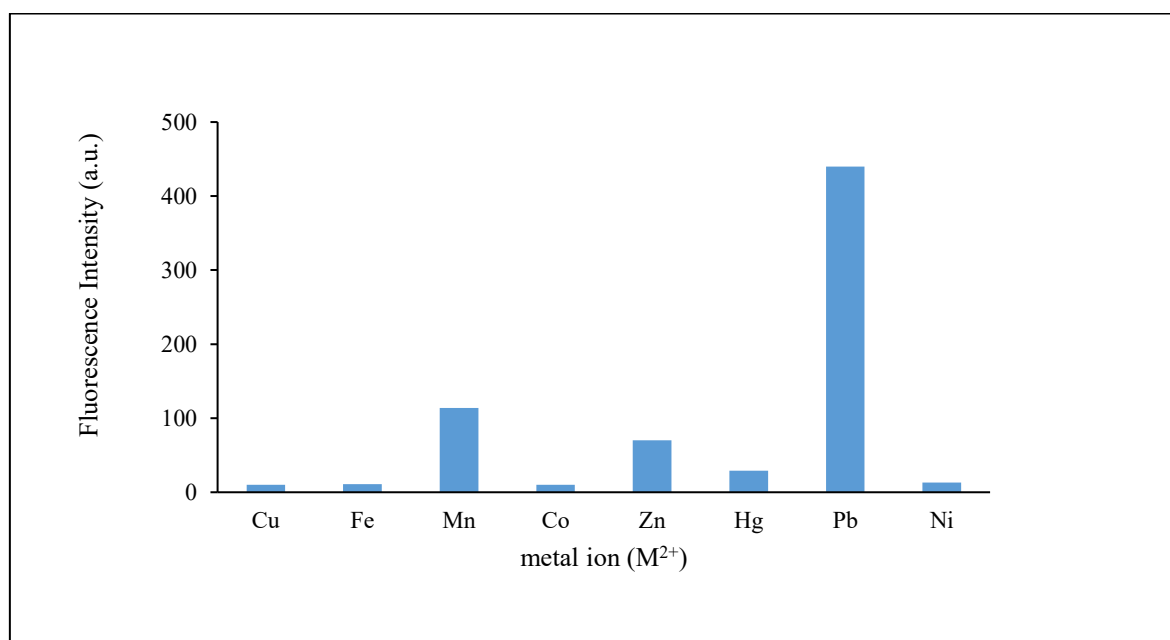


Figure 3. Selectivity study of DCFCMSH (1×10^{-3} M) towards various metal ions (1.0 eq) in DMSO based on fluorescence intensity at 501 nm ($\lambda_{\text{ex}} = 439$ nm).

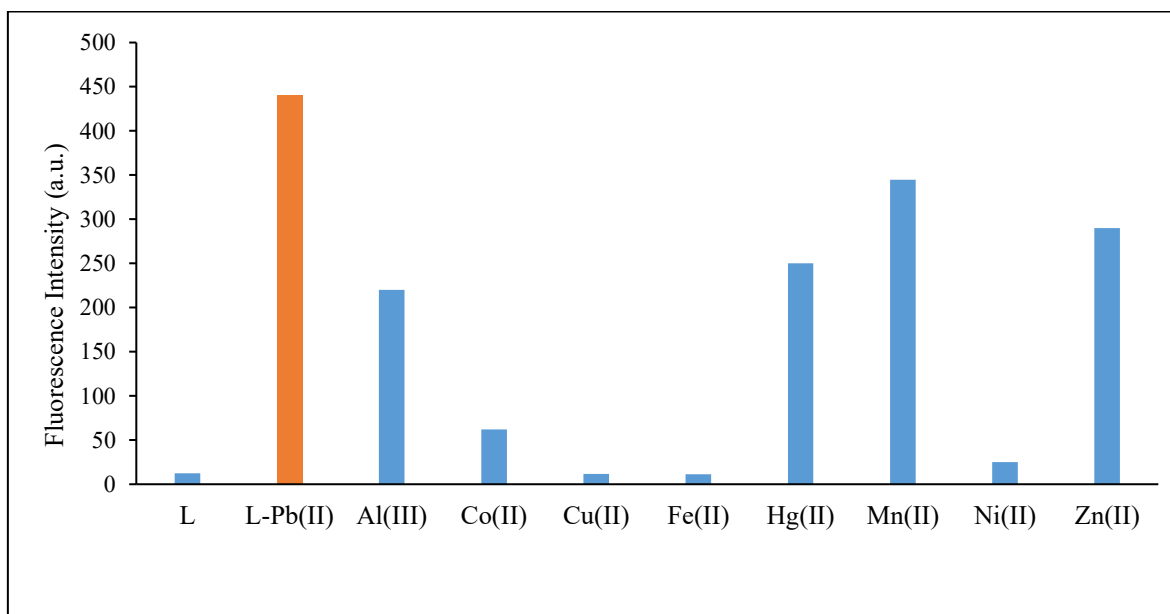


Figure 4. Fluorescence emission spectra of DCFCMSH (L) (1.0×10^{-3} M) in DMSO upon addition of Pb^{2+} (1.0 equiv.) in the presence of competing metal ions (1.0 eq) at 501 nm ($\lambda_{\text{ex}} = 439$ nm).

Binding Study

To elucidate the interaction between DCFCMSH and Pb^{2+} , binding studies were performed by characterising the ligand in the absence and presence of Pb^{2+} ions using complementary spectroscopic techniques. Changes in the electronic and structural properties of the ligand upon coordination with metal ions are commonly monitored using UV–Vis, FTIR and NMR spectroscopy, which provide valuable information on complex formation and the possible coordination sites. In addition, Job's plot was employed to support the proposed complex composition and binding stoichiometry of the complexes. The combined experimental results provide a basis for proposing the coordination mode of the Pb–DCFCMSH complex.

Figure 5 presents the UV-Visible absorption analysis of the interaction between Pb^{2+} ions and DCFCMSH, using DMSO as a solvent. The addition of Pb^{2+} ions causes a reduction in the absorbance intensity at 310 nm, accompanied by the appearance of a new absorption band at 439 nm. The newly formed band is likely attributed to a bathochromic (red) shift of the intraligand $n\text{--}\pi$ transition upon complexation. This spectral change suggests that the coordination of Pb^{2+} modifies the electronic structure of the ligand through ligand-to-metal interactions, consistent with previous reports [28, 32]. These results indicate that DCFCMSH coordinates with Pb^{2+} ions, demonstrating the selective sensing behaviour of the Schiff base ligand towards Pb^{2+} .

Figure 6 shows that upon the addition of Pb^{2+} , the bands for $\nu(\text{C}=\text{O})$ and $\nu(\text{C}=\text{N})$ shifted to lower frequencies at 1598 cm^{-1} and 1519 cm^{-1} , respectively, suggesting the coordination of Pb^{2+} to the carbonyl oxygen of the chromone moiety and azomethine nitrogen [18]. The disappearance of the $\nu(\text{N}\text{--}\text{H})$ band indicates deprotonation of the amine nitrogen during metal chelation. A weakening and shift of the

asymmetric and symmetric $\text{S}=\text{O}$ stretching bands of the sulfonyl group were observed at 1303 cm^{-1} and 1154 cm^{-1} , respectively, accompanied by the appearance of a new band at 1050 cm^{-1} , suggesting the coordination of the sulfonyl oxygen atom to Pb^{2+} [33]. The absorption band observed at 1380 cm^{-1} was attributed to the asymmetric stretching vibration of nitrate ions, which likely originated from the $\text{Pb}(\text{NO}_3)_2$ salt used as the Pb^{2+} source [34]. New bands in the IR spectra were assigned to $\nu(\text{M}\text{--}\text{O})$ and $\nu(\text{M}\text{--}\text{N})$ at 603 cm^{-1} and 473 cm^{-1} , respectively, providing coordination information between metal chelation toward carbonyl oxygen and azomethine nitrogen [12].

^1H NMR spectral assignments in Table 3 show that, upon the addition of Pb^{2+} ions, the $\text{N}\text{--}\text{H}(10)$ proton signal disappeared, which is attributed to rapid proton exchange or strong coordination between the Pb^{2+} ion and the nitrogen atom bearing the $\text{N}\text{--}\text{H}(10)$ proton. This interaction caused significant broadening and eventual loss of the NH signal in the spectrum. This such behaviour reflects notable changes in the chemical environment and molecular dynamics induced by the Pb^{2+} ion coordination. The downfield shift of the $\text{CH}=\text{N}$ proton resonance from 8.96 to 9.00 ppm indicates deshielding due to the coordination of Pb^{2+} to the azomethine nitrogen. This coordination reduces the electron density around the $\text{CH}(6)=\text{N}$ proton, causing the signal to appear at a higher chemical shift (downfield) [19]. Furthermore, the coordination process likely involves both the carbonyl oxygen and the azomethine nitrogen atoms of DCFCMSH interacting with Pb^{2+} ions. This is supported by FTIR data, where the stretching frequencies of the $\nu(\text{C}=\text{O})$ and $\nu(\text{C}=\text{N})$ bands shift to lower wavenumbers at 1598 cm^{-1} and 1519 cm^{-1} , respectively, consistent with the coordination of Pb^{2+} ions to these functional groups. These combined spectroscopic results confirm the formation of the Pb–DCFCMSH complex [28, 31].

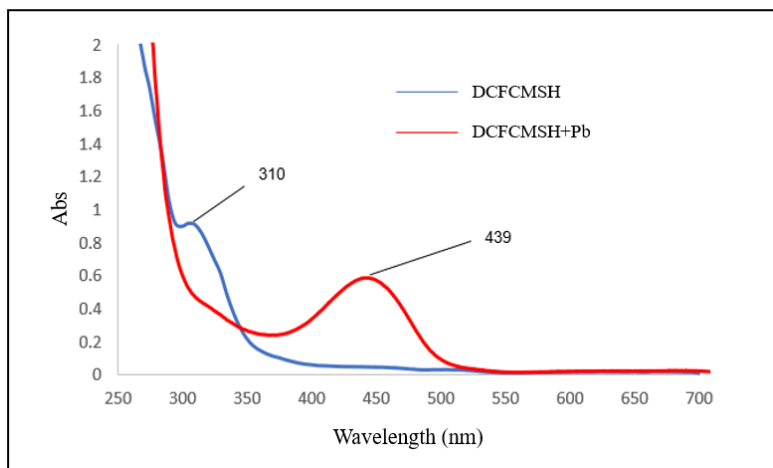


Figure 5. UV–Vis absorption spectra of DCFCMSH ($1.0 \times 10^{-3}\text{ M}$) in DMSO upon addition of Pb^{2+} (1.0 equiv.).

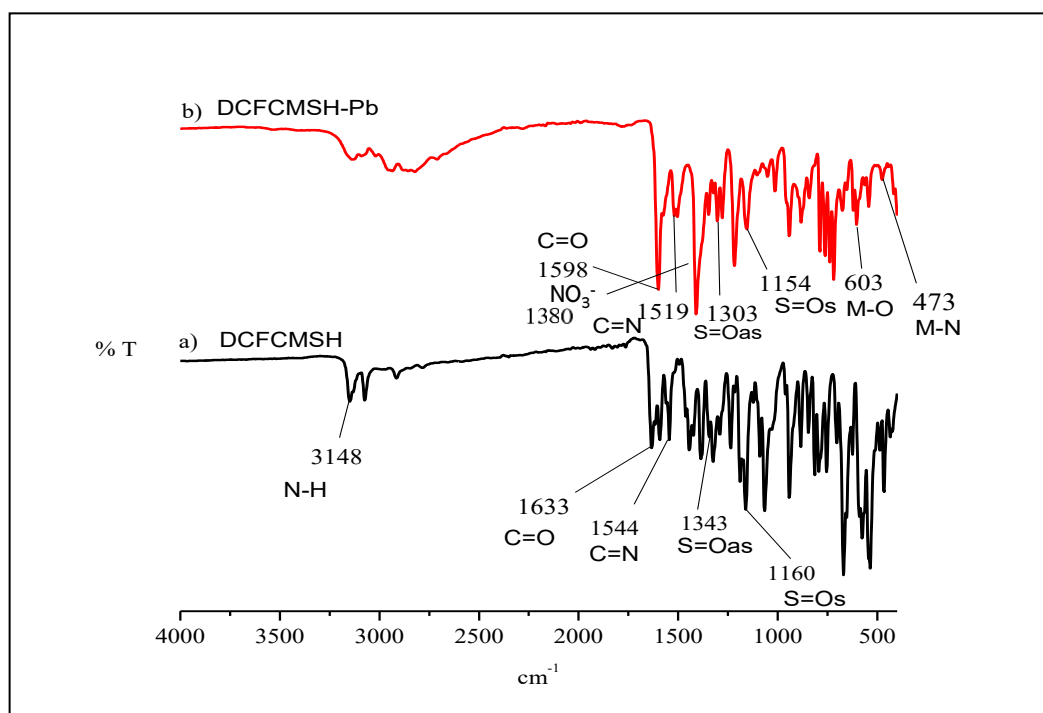


Figure 6. FTIR spectra of DCFCMSH and upon the addition of Pb²⁺.

Table 3. ¹H NMR spectral assignments for DCFCMSH in the absence and presence of Pb²⁺ ion

Compound	N-H(10) (δ)	H(6)-C=N (δ)	H (aromatic) (δ)
DCFCMSH	10.67	8.96	7.48 - 8.23
DCFCMSH+Pb	-	9.00	7.50 - 8.25

Table 4. ¹³C NMR spectral assignments for DCFCMSH in the absence and presence of Pb²⁺ ion.

Compound	C(16) (C=O)	C(8) (C=N)	C (aromatic)	C(1) (methyl)
DCFCMSH	187.38	147.61	123.73-151.61	21.76
DCFCMSH+Pb	190.15	147.39	122.83-156.03	20.84

Table 4 shows the ¹³C NMR spectral assignments of DCFCMSH in the presence of Pb²⁺ ions. Upon the addition of Pb²⁺, the signals assigned to the carbonyl (C=O) and azomethine (C=N) carbons shifted to 190.15 ppm and 147.39 ppm, respectively, indicating changes in the electronic environment at these sites due to metal binding [19, 28]. The aromatic signals shifted slightly to 122.83-156.03 ppm in the presence of Pb²⁺, whereas the methyl carbon signal shifted to 20.84 ppm. These ¹³C NMR chemical shift changes suggest the coordination of Pb²⁺ through the carbon oxygen of the chromone moiety and azomethine nitrogen atom of the ligand. This

observation confirms the formation of the Pb–DCFCMSH complex, consistent with the results obtained from electronic absorption spectroscopy, FTIR, and ¹H NMR analyses.

Job's Plot

Fluorescence titration of DCFCMSH with Pb²⁺ ions was carried out by gradually increasing the concentration of Pb²⁺ ions from 0.2 to 2.0 equivalents while maintaining a constant ligand concentration (Figure 7a). Job's plot analysis (Figure 7b) was carried out by varying the molar fractions of DCFCMSH and Pb²⁺ while maintaining a constant total concentration

of DCFCMSH and Pb^{2+} . The analysis reached the maximum value at a molar fraction of 0.5 for $[\text{DCFCMSH}]/([\text{DCFCMSH}]+[\text{Pb}^{2+}])$, indicating that the binding ratio between DCFCMSH and Pb^{2+} ion is 1:1 complexation stoichiometry [28, 34]. This was

found to be consistent with the saturation behaviour in the fluorescence titration experiments when reaching between 1.0-2.0 molar equivalence, confirming that the coordination ratio of DCFCMSH to Pb^{2+} ions is 1:1.

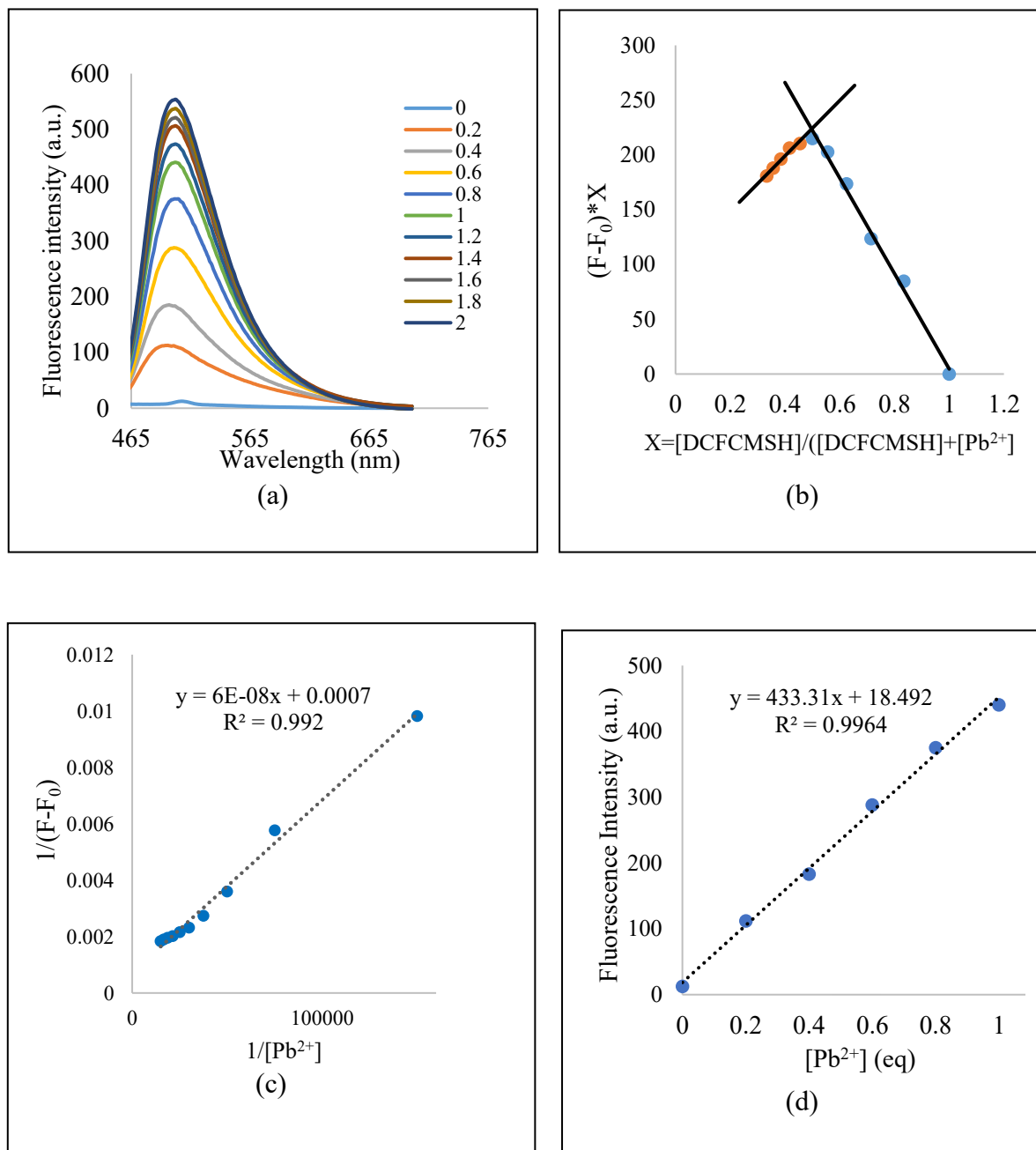


Figure 7: (a) Effect of Pb^{2+} ion concentration (0-2.0 eq) on the fluorescence spectra of DCFCMSH (1.0×10^{-3} M) in DMSO at 501 nm ($\lambda_{\text{ex}} = 439$ nm). (b) Job's plot of the interaction between DCFCMSH and Pb^{2+} . (c) The Benesi-Hildebrand plot of $1/(F - F_0)$ versus $1/[\text{Pb}^{2+}]$. (d) Linear calibration plot for LOD calculation of DCFCMSH and in the presence of Pb^{2+}

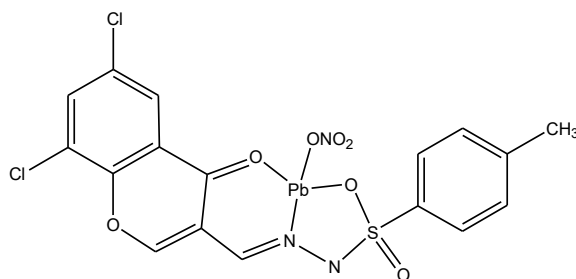


Figure 8. Proposed binding mode of Pb–DCFCMSH complex.

Based on this result, the binding constant of Pb²⁺ with DCFCMSH was determined using the Benesi–Hildebrand equation (eq. 1) for a 1:1 binding model [36], where F_0 , F , and F_{max} represent the fluorescence intensities of the free ligand (DCFCMSH), DCFCMSH in the presence of Pb²⁺, and the maximum fluorescence intensity at saturation, respectively. The plot of $1/(F-F_0)$ versus $1/[Pb^{2+}]$ in Figure 7c resulted a good linear relationship with $y = 6 \times 10^{-8}x + 0.0007$ ($R^2 = 0.992$). Subsequently, the association constant (K_a) was calculated from the slope and intercept to be $1.17 \times 10^4 \text{ M}^{-1}$, indicating a moderate binding affinity of DCFCMSH towards Pb²⁺ ions.

$$\left(\frac{1}{F_{max}-F_0}\right) = \frac{1}{K_a(F-F_0)}\left(\frac{1}{[Pb^{2+}]}\right) + \left(\frac{1}{F-F_0}\right) \quad \text{eq. 1}$$

Based on the Job's plot results and the alignment of data from FTIR, ¹H and ¹³C NMR, the probable binding mode of DCFCMSH and Pb²⁺ is proposed as shown in Figure 8. DCFCMSH acts as a tridentate ligand and is coordinated to the Pb²⁺ ion through the carbonyl oxygen, azomethine nitrogen, and sulfonyl oxygen. The binding mode of metal complexation with one molecule of ligand has also been reported [26, 37]. In addition, the appearance of a new FTIR band at approximately 1380 cm⁻¹, suggests the incorporation of a nitrate group into the complex. Based on these findings, a Pb–DCFCMSH complex containing a coordinated nitrate ion was included. Nevertheless, this structural assignment should be regarded as tentative, as definitive confirmation of the coordination environment requires further characterisation using single-crystal X-ray diffraction and high-resolution mass spectrometry (HRMS).

Table 5. Comparison of the sensing performance of previously reported fluorescent chemosensors for Pb²⁺.

Probe	Binding (L:M)	medium	LOD (M)	Response	Reference
QMC	1:2	CH ₃ CN/HEPES buffer	1.3×10^{-5}	turn on	[32]
curcumin derivative	2:1	CH ₃ CN/H ₂ O	5×10^{-7}	turn on	[41]
triazole bis-Schiff base	1:2	CH ₃ OH–tris buffer	3.1×10^{-7}	turn on	[28]
quinoline-based-Schiff base	1:1	CH ₃ OH–H ₂ O	9.9×10^{-7}	turn off	[35]
half-salamo-based	1:2	DMF / H ₂ O	3.80×10^{-7}	turn on	[39]
rhodamine 6G	1:1	HEPES buffer	2.7×10^{-9}	turn on	[40]

Limit of Detection (LOD)

A linear calibration plot (Figure 7d) was constructed based on the fluorescence titration data to obtain the correlation coefficient (R^2) for the calculation of the limit of detection (LOD). The LOD was calculated using $3 \times \sigma_{\text{blank}}/k$, where σ_{blank} is the standard deviation of the blank and k is the slope of the calibration curve [36]. The data showed a 1:1 binding ratio and the LOD was determined to be 2.4×10^{-8} M (4.97 $\mu\text{g/L}$), which is below the limit of lead in drinking water (10 $\mu\text{g/L}$) by the World Health Organization (WHO) [38]. This shows that the sensor has great potential for detecting Pb²⁺. The sensing performance of the DCFCMSH was compared with that of previously reported Pb²⁺ chemosensors (Table 5). The detection limit of DCFCMSH is comparable to those reported in the literature, demonstrating its potential as a sensitive fluorescent chemosensor for Pb²⁺ detection.

Frontier Molecular Orbital Analysis

Figure 9 shows the optimised structures of FCMSH, CFMSH and DCFCMSH using DFT-B3LYP/6-311G(d,p) basis set level calculation to explore the electronic properties through frontier molecular orbital (FMO) analysis. The HOMO of all three ligands was mainly distributed over the chromone–hydrazone π -conjugated framework, whereas the LUMO exhibited a more extensive delocalisation towards the *p*-toluenesulfonyl moiety (Figure 10). Chlorine substitution did not significantly alter the spatial characteristics of the frontier molecular orbitals, as evidenced by the similar orbital distributions across all three ligands. However,

additional orbital density was observed around the chlorine-substituted positions in the LUMO of CFCMSH and became more noticeable in DCFCMSH, indicating a progressive contribution of the chlorine substituents to the electron-accepting orbital. Consequently, the HOMO–LUMO energy gap decreased progressively from 4.453 for FCMSH to 4.288 eV for DCFCMSH, indicating that chlorine substitution gradually stabilises the electronic properties of the ligands and facilitates electronic excitation. Accordingly, both the HOMO and LUMO energies decrease with increasing chlorine substitution, with the HOMO energy decreasing from -6.562 to -6.677 eV and the LUMO energy decreasing from -2.109 to -2.389 eV. This trend is consistent with the electron-withdrawing inductive effect of the chlorine substituents, which stabilises the frontier molecular orbitals and reduces the HOMO–LUMO energy gap, thereby facilitating electronic transitions [12, 26].

Although chlorine substitution gradually reduced the HOMO–LUMO energy gap among the free ligands, the reduction was relatively small, suggesting that chlorine substitution alone is insufficient to account for the significant fluorescence enhancement observed experimentally. Therefore, the electronic structure of the Pb–DCFCMSH complex was further investigated to evaluate the influence of metal coordination on the frontier molecular orbitals. To gain further insight into the electronic properties of the sensing mechanism, the optimised Pb–DCFCMSH was subjected to DFT calculations. The optimised structure was constructed based on the experimentally proposed coordination environment in Figure 8.

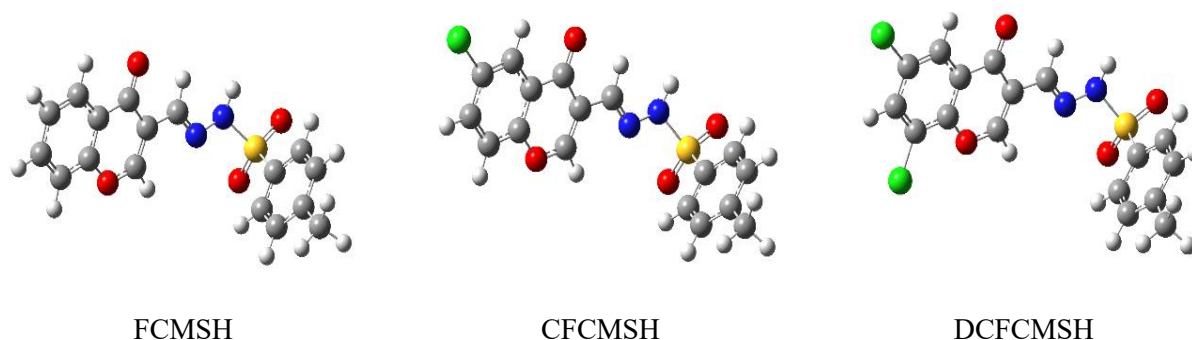


Figure 9. Optimised structure of FCMSH, CFMSH and DCFCMSH using DFT-B3LYP/6-311G(d,p).

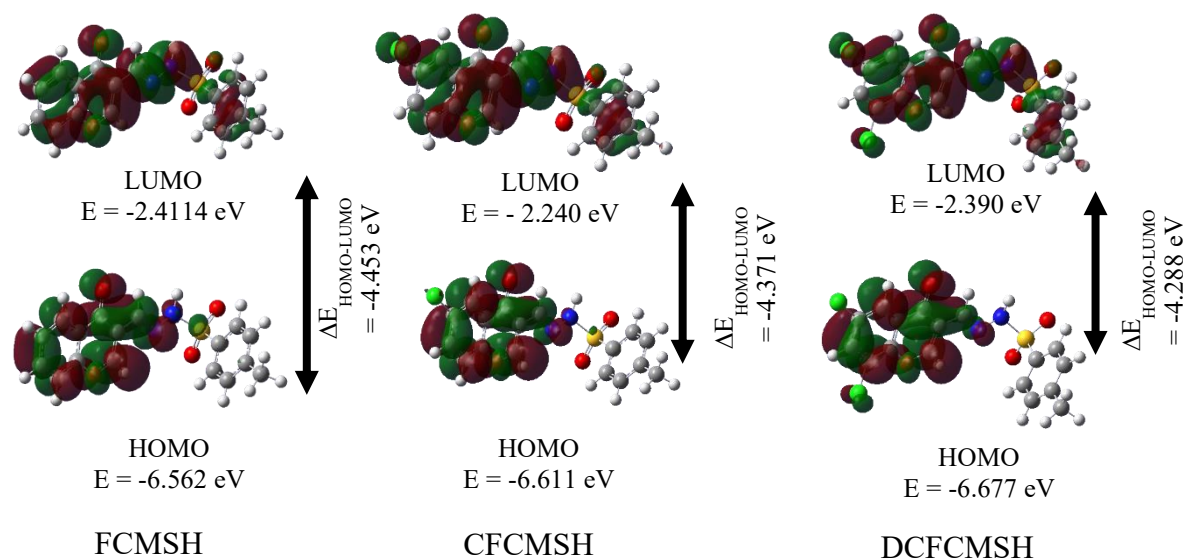


Figure 10. Frontier molecular orbital (HOMO and LUMO) distributions and energy gaps (ΔE) of the synthesised chromone hydrazone-based ligands

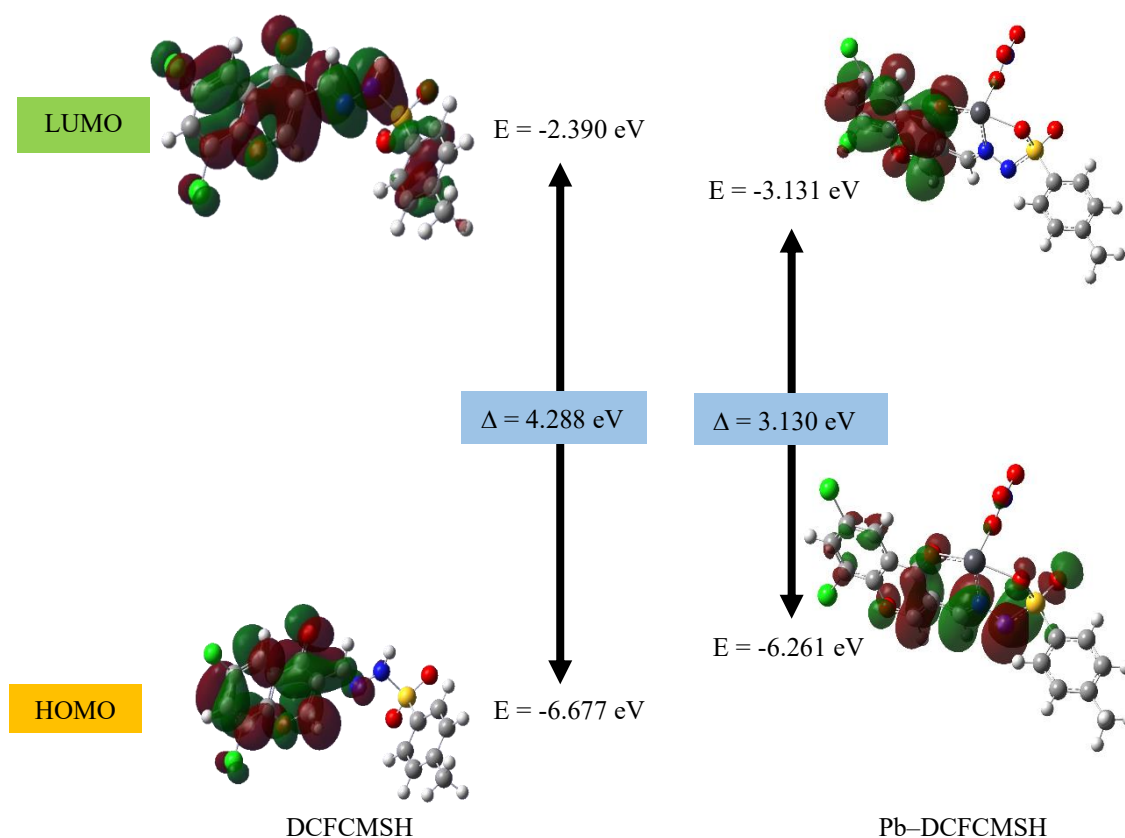


Figure 11: Frontier molecular orbital (HOMO and LUMO) distributions and energy gaps (ΔE) of DCFCMSH and Pb-DCFCMSH complex

In the Pb–DCFCMSH, both the HOMO and LUMO exhibited noticeable orbital redistribution (Figure 11). The HOMO was partially localised over the γ -pyrone ring, imine linkage and sulfonyl group, whereas the LUMO was predominantly confined to the chromone moiety. This redistribution suggests that Pb(II) coordination modifies the electron distribution within the π -conjugated framework, resulting in a different electronic environment compared to that of the free ligand. Orbital redistribution is accompanied by significant changes in the frontier orbital energies. Upon complexation, the HOMO energy increased by 0.417 eV from –6.678 to –6.261 eV, whereas the LUMO energy decreased by 0.741 eV from –2.390 to –3.131 eV. The substantially greater stabilisation of the LUMO compared to the relatively small increase in the HOMO energy indicates that complex formation preferentially influences the electron-accepting orbital, consistent with previous reports describing preferential LUMO stabilisation upon metal coordination [28, 30, 39]. Consequently, the HOMO–LUMO energy gap decreased markedly from 4.288 to 3.130 eV, indicating that electronic excitation requires lower energy after complex formation [39]. This is consistent with the experimentally observed bathochromic shift in the UV–Vis spectrum (Figure 5), where the absorption band at 310 nm was replaced by a new band at 439 nm following Pb(II) complexation. The reduced HOMO–LUMO energy gap also supports the experimentally observed fluorescence turn-on response of the Pb–DCFCMSH complex.

CONCLUSION

Three chromone hydrazone-based ligands (FCMSH, CFCMSH and DCFCMSH) were successfully synthesised and characterised. The results demonstrate that, only DCFCMSH exhibited a selective fluorescence enhancement towards Pb²⁺ ions. Moreover, the findings highlight the formation of a 1:1 Pb²⁺–DCFCMSH complex through spectroscopic analyses, Job’s plot, and Benesi–Hildebrand analysis. The LOD (2.4×10^{-8} M) was well below the maximum permissible concentration of Pb²⁺. Furthermore, DFT calculations supported the experimental findings by revealing the influence of chlorine substitution on the electronic properties of ligands. Overall, the combined experimental and theoretical findings demonstrate the potential of DCFCMSH as a fluorescent chemosensor for Pb²⁺ detection. Thus, future studies should focus on validating the sensing performance of DCFCMSH in real samples and evaluating its practical applicability.

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REFERENCES

1. Pourret, O., Bollinger, J. -C. and Hursthouse, A. (2021) Heavy metal: A misused term? *Acta Geochimica*, **40**(3), 466–471.
2. Sankhla, M. S. (2019) Contaminant of heavy metals in groundwater and its toxic effects on human health and environment. *International Journal of Environmental Sciences and Natural Resources*, **18**(5).
3. Kumar, A., Kumar, A., Cabral-Pinto, M. M. S., Chaturvedi, A. K., Shabnam, A. A., Subrahmanyam, G., Mondal, R., Gupta, D. K., Malyan, S. K., Kumar, S. S., Khan, S. A., and Yadav, K. K. (2020) Lead toxicity: health hazards, influence on food chain, and sustainable remediation approaches. *International Journal of Environmental Research and Public Health*, **17**(7), 2179.
4. Carter, K. P., Young, A. M. and Palmer, A. E. (2014) Fluorescent sensors for measuring metal ions in living systems. *Chemical Reviews*, **114**(8), 4564–4601.
5. Lian, J., Xu, Q., Wang, Y. and Meng, F. (2020) Recent developments in fluorescent materials for heavy metal ions analysis from the perspective of forensic chemistry. *Frontiers in Chemistry*, **8**, 593291.
6. Niu, G., Zhang, R., Shi, X., Park, H., Xie, S., Kwok, R. T. K., Lam, J. W. Y. and Tang, B. Z. (2020) AIE luminogens as fluorescent bioprobes. *TrAC Trends in Analytical Chemistry*, **123**, 115769.
7. Nootem, J., Daengngern, R., Sattayanon, C., Wattanathana, W., Wannapaiboon, S., Rashatasakhon, P. and Chansaenpak, K. (2021) The synergy of CHEF and ICT toward fluorescence ‘turn-on’ probes based on push-pull benzothiazoles for selective detection of Cu²⁺ in acetonitrile/water mixture. *Journal of Photochemistry and Photobiology A: Chemistry*, **415**, 113318.
8. Wu, D., Hu, Y., Cheng, H. and Ye, X. (2023) Detection Techniques for Lead Ions in Water: A Review. *Molecules*, **28**(8), 3601.
9. Abdelrhman, E. M., El-Shetary, B. A., Shebl, M. and Adly, O. M. I. (2021) Coordinating behavior of hydrazone ligand bearing chromone moiety towards Cu(II) ions: Synthesis, spectral, density functional theory (DFT) calculations, antitumor, and docking studies. *Applied Organometallic Chemistry*, **35**(5), 1–22.
10. Bhalla, P., Tomer, N., Bhagat, P. and Malhotra, R. (2022) Chromone functionalized pyridine

- 161 Nur Aziani Hermanto, Yusnita Juahir, Wan Mohd Hilmei W Mohd Arifin, Noorshida Mohd Ali, Mohamad Syahrizal Ahmad, Faridah Lisa Supian, Uwaisulqarni M. Osman and Nurul Husna As Saedah Bain

chemosensor for cupric ions detection. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **264**, 120279.
11. Kumar, S., Arora, A., Maikhuri, V. K., Chaudhary, A., Kumar, R., Parmar, V. S., Singh, B. K. and Mathur, D. (2024) Advances in chromone-based copper(II) Schiff base complexes: Synthesis, characterization, and versatile applications in pharmacology and biomimetic catalysis. *RSC Advances*, **14**, 17102–17139.
12. Gaber, M., El-Baradie, K., El-Wakiel, N. and Hafez, S. (2020) Synthesis and characterization studies of 3-formyl chromone Schiff base complexes and their application as antitumor, antioxidant and antimicrobial. *Applied Organometallic Chemistry*, **34**(2).
13. Frisch, M. G., Trucks, G. Schlegel, H., Scuseria, G., Robb, M., Cheeseman, J., Scalmani, G., Barone, V., Petersson, G. and Nakatsuji, H. (2009) Gaussian 09, Revision A. 02, Gaussian, Inc. Wallingford, CT.
14. Nielsen, A. and Holder, A. (2009) Gauss view 5.0, user's reference, GAUSSIAN Inc., Pittsburgh.
15. Alsaeedi, M. S. (2003) A theoretical study on the electronic structures and phosphorescence properties of light-emitting electrochemical cell champions reported in early 2022. *Polyhedron*, **242**, 116490.
16. Parr, R. and Yang, W. (1989) Density-functional theory of atoms and molecules. *Oxford Univ. Press, ed: Oxford*.
17. Lee, C., Yang, W. and Parr, R. G. (1988) Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Physical Review B*, **37**, 785.
18. Hermanto, N. A., Juahir, Y., Mustafar, S., Sharif, A. M., Osman, U. M. and Ulianas, A. (2024) Green fluorescence property of chromone-based hydrazone towards Zn^{2+} ion. *Journal of Science and Mathematics Letters*, **12**(2), 161–169.
19. Arifin, W. M. H., Juahir, Y., Ali, N. M., Bakar, N. A., Ahmad, M. S., Supian, F. L. and Osman, U. M. (2018) Synthesis and characterization of chromone-based ligand and its fluorescence property towards Zn^{2+} . *IOP Conference Series: Materials Science and Engineering*, **440**, 012015.
20. Ma, C., Zhang, X., Yang, Y., Ma, Z., Yang, L., Wu, Y., Liu, H., Jia, X. and Wei, Y. (2016) Halogen effect on mechanofluorochromic properties of alkyl phenothiazinyl phenylacrylonitrile derivatives. *Dyes and Pigments*, **129**, 141–148.
21. Rode, M., Gupta, R. C., Karale, B. K. and Rindhe, S. S. (2008) Synthesis and characterization of some substituted chromones as an anti-infective and antioxidant agents. *Journal of Heterocyclic Chemistry*, **45**(6), 1597–1602.
22. Kandioller, W., Theiner, J., Keppler, B. K. and Kowol, C. R. (2022) Elemental analysis: An important purity control but prone to manipulations. *Inorganic Chemistry Frontiers*, **9**(3), 412–416.
23. Tomer, N., Goel, A., Ghule, V. D. and Malhotra, R. (2021) A chromone based Schiff base: An efficient colorimetric sensor for specific detection of Cu (II) ion in real water samples. *Journal of Molecular Structure*, **1227**, 129549.
24. Pratiwi, R. A. and Nandiyanto, A. B. D. (2022) How to read and interpret UV-VIS spectrophotometric results in determining the structure of chemical compounds. *Indonesian Journal of Educational Research and Technology*, **2**(1), 1–20.
25. AlObaid, A. A., Suleiman, M., Jama, C., Zarrouk, A. and Warad, I. (2021) Synthesis, physico-chemical, optical, thermal and TD-DFT of (E)-N'-((9-ethyl-9H-carbazol-3-yl)-methylene)-4-methyl-benzene-sulfonohydrazide (ECMMBSH): Naked eye and colorimetric Cu^{2+} ion chemosensor. *Journal of King Saud University - Science*, **33**(8), 101633.
26. Karmakar, M. and Chattopadhyay, S. (2020) Synthesis, structure and nitroaromatic sensing ability of a trinuclear zinc complex with a reduced Schiff base ligand: Assessment of the ability of the ligand to sense zinc ion. *Polyhedron*, **187**, 114639.
27. Miar, M., Shiroudi, A., Pourshamsian, K., Oliaey, A. R. and Hatamjafari, F. (2021) Theoretical investigations on the HOMO–LUMO gap and global reactivity descriptor studies, natural bond orbital, and nucleus-independent chemical shifts analyses of 3-phenylbenzo[d]thiazole-2(3H)-imine and its *para*-substituted derivatives: Solvent and substituent effects. *Journal of Chemical Research*, **45**(1–2), 147–158.
28. Rout, K., Manna, A. K., Sahu, M., Mondal, J., Singh, S. K. and Patra, G. K. (2019) Triazole-based novel bis Schiff base colorimetric and fluorescent turn-on dual chemosensor for Cu^{2+} and Pb^{2+} : Application to living cell imaging and molecular logic gates. *RSC Advances*, **9**(44), 25919–25931.

- 162 Nur Aziani Hermanto, Yusnita Juahir, Wan Mohd Hilmei W Mohd Arifin, Noorshida Mohd Ali, Mohamad Syahrizal Ahmad, Faridah Lisa Supian, Uwaisulqarni M. Osman and Nurul Husna As Saedah Bain
29. Niu, H., Liu, J., O'Connor, H. M., Gunnlaugsson, T., James, T. D. and Zhang, H. (2023) Photoinduced electron transfer (PeT) based fluorescent probes for cellular imaging and disease therapy. *Chemical Society Reviews*, **52**(7), 2322–2357.
30. Goshisht, M. K., Patra, G. K. and Tripathi, N. (2022) Fluorescent Schiff base sensors as a versatile tool for metal ion detection: Strategies, mechanistic insights, and applications. *Materials Advances*, **3**(6), 2612–2669.
31. Kowser, Z., Rayhan, U., Akther, T., Redshaw, C. and Yamato, T. (2021) A brief review on novel pyrene based fluorometric and colorimetric chemosensors for the detection of Cu^{2+} . *Materials Chemistry Frontiers*, **5**(5), 2173–2200.
32. Velmurugan, K., Vickram, R., Jipsa, C. V., Karthick, R., Prabakaran, G., Suresh, S., Prabhu, J., Velraj, G., Tang, L. and Nandhakumar, R. (2021) Quinoline based reversible fluorescent probe for Pb^{2+} ; applications in milk, bioimaging and inhibit molecular logic gate. *Food Chemistry*, **348**, 129098.
33. Juahir, Y., Puvaneswary, S., Ali, H. M., Robinson, W. T. and Thong, K. L. (2009) Synthesis, structural characterization and antibacterial activity of 2,6-diacetylpyridine bis(benzenesulfonohydrazide) Schiff bases and their copper(II) complexes. *Polyhedron*, **28**(14), 3050–3054.
34. Gatehouse, B. M., Livingstone, S. E. and Nyholm, R. S. (1958) Infrared spectra of some nitrate and other oxy-anion co-ordination complexes. *Journal of Inorganic and Nuclear Chemistry*, **8**(1–2), 75–78.
35. Sharma, V., Dutta, S., Sahu, D., Pandey, A., Kumar, D., Das, S. and Patra, G. K. (2025) Chromone Hydrazone-Based Fluorescent Chemosensor for Pb^{2+} Detection: Experimental and Theoretical Insights into a Turn-On Fluorescence Response
- A new quinoline-based fluorescent-colorimetric chemosensor for sensitive and selective “on–off” detection of Pb^{2+} ions. *RSC Advances*, **15**(6), 4236–4249.
36. Fufa, T. O., Ma, H., Ayub, A. R., Nabat, K. Y., Khan, Y. and Li, H. (2025) Zinc(II) ion detection and fluorescence emission properties of a diaminomaleonitrile-derived unsymmetrical Schiff base ligand. *RSC Advances*, **15**(30), 24192–24201.
37. Dong, Y., Fan, R., Chen, W., Wang, P. and Yang, Y. (2017) A simple quinolone Schiff-base containing CHEF based fluorescence ‘turn-on’ chemosensor for distinguishing Zn^{2+} and Hg^{2+} with high sensitivity, selectivity and reversibility. *Dalton Trans.*, **46**, 6769–6775.
38. World Health Organization (2022) Guidelines for drinking-water quality: Fourth edition incorporating the first and second addenda. *World Health Organization*.
39. Wang, L., Pan, Y. -Q., Wang, J. -F., Zhang, Y. and Ding, Y. -J. (2020) A highly selective and sensitive half-salamo-based fluorescent chemosensor for sequential detection of $\text{Pb}(\text{II})$ ion and Cys. *Journal of Photochemistry and Photobiology A: Chemistry*, **400**, 112719.
40. Wan, J., Zhang, K., Li, C., Li, Y. and Niu, S. (2017) A novel fluorescent chemosensor based on a rhodamine 6G derivative for the detection of Pb^{2+} ion. *Sensors and Actuators B: Chemical*, **246**, 696–702.
41. Sadia, M., Khan, J., Khan, R., Ali Shah, S. W., Zada, A., Zahoor, M., Ullah, R. and Ali, E. A. (2025) Trace level detection of Pb^{2+} ion using organic ligand as fluorescent-on probes in aqueous media. *Heliyon*, **11**(1), e41125.