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Specialization: Inorganic/Analytical Chemistry

Title of the Proposed Research Development of Metal-Enhanced Squaramide-Based Chemosensors for Selective Anion Detection in Aqueous Media

Background and Rationale Anion sensing has gained significant attention due to its applications in environmental and biological systems. Fluoride, in particular, is widely studied due to its beneficial effects on dental health at low concentrations and its toxicity at elevated levels. Developing highly selective and sensitive chemosensors for fluoride detection is crucial for monitoring its levels in water sources and biological systems.

Previous studies have demonstrated the effectiveness of squaramide-based receptors in anion recognition due to their strong hydrogen-bonding ability (Kaur et al., 2017; Sharma et al., 2015). Additionally, incorporating metal centers into sensor frameworks has been shown to enhance selectivity and sensitivity (Liu et al., 2013; Sun et al., 2015). Building upon this, the proposed research aims to develop metal-enhanced squaramide-based chemosensors with improved detection capabilities in aqueous environments.

Objectives of the Research- To synthesize squaramide-based ligands modified with chromophoric or fluorophoric units.
- To incorporate transition metals (e.g., Zn^{2+}, Cu^{2+}, Fe^{3+}) to form coordination complexes that improve sensor performance.
- To evaluate the selectivity and sensitivity of the synthesized chemosensors toward fluoride and other biologically relevant anions.
- To explore the sensors' response in aqueous or mixed solvent systems.

Methodology- Ligand Design and Synthesis: Develop derivatives of squaramide with electron-withdrawing groups and chromophores.
- Complex Formation: Introduce metal ions to form hybrid organic-inorganic chemosensors.
- Characterization: FT-IR, NMR, Mass Spectrometry, UV-Vis, Fluorescence Spectroscopy, and single-crystal XRD (if possible).
- Sensing Studies: Titration experiments with various anions; determine detection limit (LOD), binding constant (Ka), and selectivity.
- Solvent Studies: Optimize conditions for performance in aqueous systems using surfactants or micelles if needed.

Expected Outcomes- Development of highly selective, sensitive fluoride chemosensors that work under near-physiological conditions.

- Insight into structure–activity relationships between metal coordination, electronic behavior, and sensing capability.
- Potential application in environmental monitoring and bioanalytical sensing.

Significance of the Research This research will contribute to the field of supramolecular chemistry and sensor development, with real-world applications in environmental safety, public health, and clinical diagnostics. Enhancing sensor performance through metal coordination is a promising strategy for achieving reliable detection under practical conditions.

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