

Digitally Innovation in Bio Inorganic Chemistry of Lanthanides

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Abstract

Lanthanides occupy an important position in bioinorganic chemistry because of their distinctive electronic, magnetic, spectroscopic, and coordination properties. Recent advances in digital technologies are creating new opportunities for understanding the interaction of lanthanide ions with biological molecules and developing innovative applications in medicine, biotechnology, sensing, and materials science. This study explores the role of digital innovation in the bioinorganic chemistry of lanthanides, with particular emphasis on computational chemistry, artificial intelligence, machine learning, molecular modelling, and data-driven analysis. Computational methods can be used to investigate the coordination behaviour, electronic structures, thermodynamic properties, and interactions of lanthanide complexes with proteins, nucleic acids, and other biological ligands. Artificial intelligence and machine-learning approaches can assist in predicting molecular properties, identifying potential bioactive complexes, optimizing ligand structures, and analysing large chemical datasets. Digital spectroscopy and advanced imaging technologies further provide opportunities for studying lanthanide-based probes and their behaviour in biological environments. These innovations can accelerate the design of luminescent probes, contrast agents, therapeutic compounds, and responsive biosensors while reducing the time and resources required for experimental screening. Nevertheless, challenges related to the complexity of lanthanide coordination chemistry, limited high-quality datasets, computational accuracy, toxicity assessment, and experimental validation remain significant. The integration of digital tools with experimental bioinorganic chemistry therefore offers a promising approach for advancing lanthanide research. This study highlights how computational and data-driven methodologies can contribute to a deeper understanding and more efficient development of lanthanide-based biological applications.

Keywords: Lanthanides, Bioinorganic Chemistry, Digital Innovation, Artificial Intelligence, Machine Learning, Computational Chemistry, Molecular Modelling, Lanthanide Complexes, Biosensors, Luminescence.

