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Metal Complexes Containing Bioactive Ligands

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Bioactive ligands are compounds with high selectivity and reactivity towards free radicals, cancer cell lines, bacteria, viruses, fungi, etc. Organometallic compounds, containing Cu, Fe, Zn, Pd, Sn, Ni, and Ru ions and bioactive ligands, also show prominent biological activities. Computational chemistry, in the first-line Density Functional Theory, is an inseparable tool in predicting their stability, synthetic reaction pathways, and assignment of spectra, as well as in the study of inter- and intramolecular interactions. Moreover, Molecular Docking and Molecular Dynamics are important for investigating the interactions of these compounds with important biomolecules, such as proteins, lipids, and DNA. Based on known biological activity, toxicity, and physicochemical properties, Quantitative Structure-Activity Studies (QSAR) can be applied for the prediction of the properties of theoretically developed or synthesized compounds.

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