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PHARMA CHEMISTS, CAN YOU COLLABORATE WITH OUR BIOINORGANIC HYBRID SYSTEMS USING AI?

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Recently, author has published new bioinorganic hybrid materials composed of Schiff base complexes and laccase (A metalloprotein to reduce molecular oxygen to water). In recent conference, he was presented molecular design and preliminary data of new Cu(II/I) or Mn(III/II) Schiff base complexes having redox active (anthraquinone) ligands and photochromic (azobenzene) ligands by means of electrochemical and computational methods (DFT calculations and docking simulation of protein-ligand employed in drug chemistry commonly). Thus, not only experimental methods but also computational methods may be useful to develop such bioinorganic materials. Furthermore, to decrease empirical trial-and-error using high-cost biomolecules as well as to realize sophisticated molecular design beyond the computational method or crystal structure database, he would like to employ AI (machine learning) for searching and prediction in bioinorganic studies.

Note: