

Superoxide dismutase (SOD) enzymes are a major defense against superoxide, which is a potent reactive oxygen species. SOD mimics have potential clinical relevance as treatments for neurodegenerative diseases. The Green group at TCU synthesized tetra-aza macrocycle copper complexes since they serve as promising SOD mimics. The redox potential of these complexes is a critical factor in their antioxidant activity, as it determines their ability to bind and transfer electrons. However, the vast number of possible tetra-aza macrocycles presents a challenge for experimental synthesis and testing. To address this, we perform computational simulations to predict the redox potential of un-synthesized tetra-aza macrocycles, helping to identify the most promising candidates for further study. This work, in combination with other predictive models for properties such as pKa, solubility, permeability, and metal binding, accurate redox potential simulations can help focus experimental efforts on the most viable SOD mimics, accelerating the development of effective treatments.