

# Synthetic Modeling of Manganese Superoxide Dismutases

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Overproduction of superoxide, a reactive byproduct of oxygen metabolism, is associated with reperfusion injury, inflammatory diseases, and neurological disorders such as Parkinson's and Alzheimer's disease. Although several factors limit therapeutic application of natural superoxide dismutases (SODs), the design of synthetic, low-molecular-weight SOD mimics may result in useful pharmaceuticals. Using the pendant-arm macrocycle 1,4,7-triazacyclonane-1-acetate (TCMA), we synthesized a manganese (II) complex that models structural features of the active site in manganese superoxide dismutases. X-ray crystallography on  $[\text{MnTCMA}(\text{H}_2\text{O})]\text{PF}_6 \cdot \text{CH}_3\text{OH}$  reveals that manganese bonds to three nitrogen atoms and one oxygen atom of TCMA, as well as to a water molecule. Two more donor oxygen atoms to manganese from the pendant acetate of TCMA in a neighboring complex results in a polymeric chain in the solid-state with manganese atoms bridged by acetate groups. This structure and further details of our work are described.