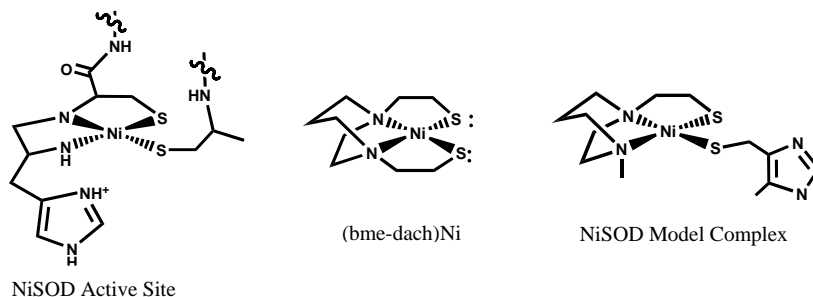


Synthetic Analogs for the Nickel-Containing Superoxide Dismutase Active Site Using N_2S_2 Ligands

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A recent protein structure of the nickel-containing superoxide dismutase, NiSOD, illustrates that the active site is comprised of a Ni^{II} coordinated to two N atoms and two S atoms from a peptide backbone in a square planar coordination environment.¹ The compound, (bme-dach)Ni, has structural features similar to the active site of the NiSOD enzyme. Small molecule models of enzyme active sites which mimic the structure frequently show similar reactivity which gives insight into the mechanism catalyzed by the enzyme. The reactivity of the $N_2S_2Ni^{II}$ square planar coordination complexes have been demonstrated to nicely mimic the active site of other enzymes which contain Ni^{II} in a N_2S_2 coordination such as Acetyl-coA synthase.² Analogs of these compounds are being developed to explore chemistry related to the active site of the NiSOD enzyme. The study of SOD's are of particular interest because they catalyze the dismutation of superoxide to peroxide and molecular oxygen. The synthesis of these analogs and their characterization by UV-Vis spectroscopy, ESI-MS, and cyclic voltammetry is underway. Electrochemical studies and KO_2 assays will be used to study the SOD activity of these biomimetic chelating ligands. The reactivity between a linear chain with an N_2S_2 binding site vs. N_2S_2 coordination environment comprised of a N_2S tridentate and a monodentate SR donor site will be compared.



¹Barondeau, D., Kassmann, C., Bruns, C., Tainer, J., Getzoff, E.; *Biochemistry*. **2004**, 43(25); 8038-8047.

²Golden, M. L., Rampersad, M.V., Reibenspies, J. H., Darensbourg, M.Y.; *Chem. Commun.* **2003**, 1824.