An ongoing theme in our research group involves the development of biomimetic transition metal complexes that serve to activate small molecules, promote reactions similar to those of metalloenzymes, and provide new synthetic routes to novel ligands. In one instance, we have developed models of iron-containing bleomycin that rely on robust tetradentate aminopyridine macrocyclic (PyMAC) ligands. These simple systems serve as rigid scaffolds that are suitable for coordination of transition metal ions and their success as structural and functional models has led to the design and study of more elaborate ligand architectures. Our group has developed novel PyMACs containing functionalized pendant arms that can provide an additional donor atom as well as modulate the spin state of the metal center. A second area of focus involves the template synthesis of a wide range of imidoylamidines promoted by a urease model complex containing Ni(II) supported by tert-butyl-dipicolylamine (tBuDPA). Structures of the model complex with a bound imidoylamidine reveal that the tertiary amine donor atom of tBuDPA behaves in a similar fashion to pendant arm donor atoms in PyMAC ligands and its degree of coordination dictates the metal's spin state. Novel iron(II) and copper(II) complexes supported by our modified PyMAC ligands as well as examples of our structurally characterized nickel(II) imidoylamide and imidoylamidine complexes will be presented.

Keywords: inorganic chemistry, biomimicry, small molecule crystallography