

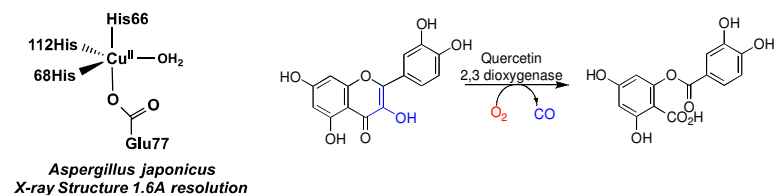
# Development, Synthesis and Characterization of Biomimetic Model Complexes

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## Introduction

**Metalloenzymes** are proteins that catalyze a specific reaction and contain metals that are tightly bound at the active site. Hemoglobin is a common metalloprotein that transfers  $O_2$  in the blood. A subclass of metalloenzymes are dioxygenases. **Dioxygenases** transfer both oxygen atoms of  $O_2$  into substrate. They have the ability to cleave and degrade aromatic compounds and play an important role in many biological functions, such as mammalian metabolism.<sup>1</sup> A specific dioxygenase, **Quercetin 2,3 Dioxygenase (QDO)**, is unique in that it is the only known dioxygenase that is copper dependent. The copper center is bound to 3 histidines, 1 glutamate, and the antioxidant quercetin.<sup>2</sup> QDO is found in bacteria, where they use the enzyme to degrade aromatic compounds. Aromatic compounds are one of the most prevalent and persistent pollutants in the environment. A synthetic model that mimics the active site of QDO, could be used for possible bioremediation purposes.

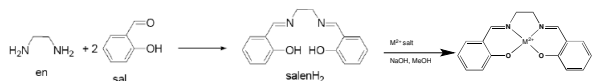


## Research Goals

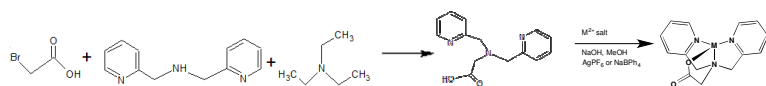
- Synthesize ligands that mimic the 3-His-1-Carboxylate coordination
- Synthesize and characterize metal complexes
- Study reactivity of metal complexes and substrates

## Synthesis

Synthesis of Ligands  
SalenH<sub>2</sub><sup>4</sup>:



*N,N*-bis(2-pyridylmethyl)glycine)(BPG)<sup>3</sup>:



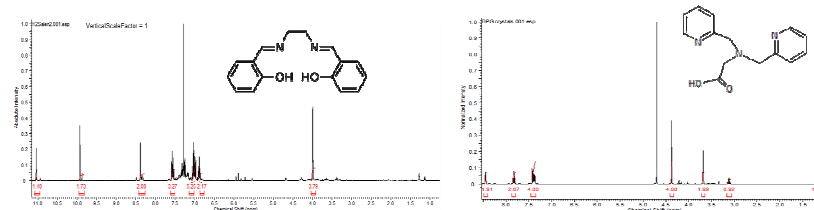
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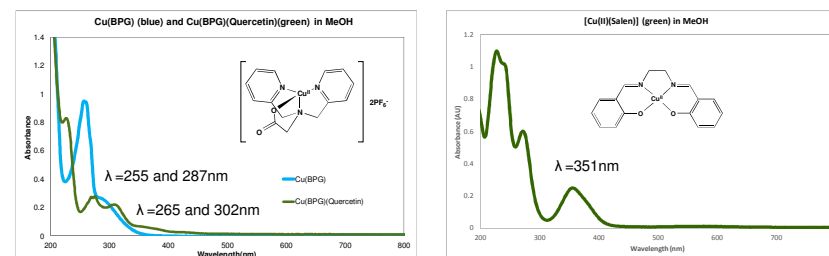
## Characterization

Characterization of Ligands

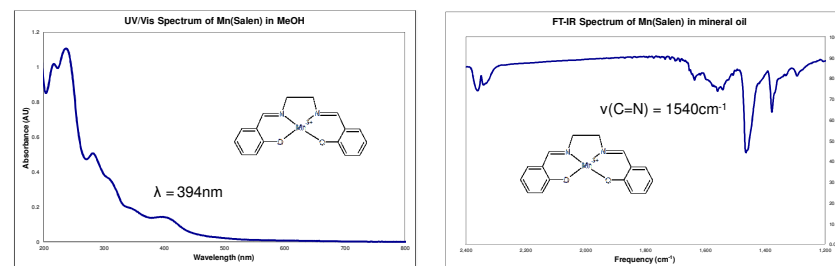
SalenH<sub>2</sub> and BPG were characterized by <sup>1</sup>H NMR. <sup>1</sup>H NMR is used elucidate the structure of compound by measuring the number and chemical shift of protons.



## UV-Visible Spectra of Copper Complexes



## UV-Visible and IR Spectra of Manganese Complex



## Future Work

- Synthesize and characterize Fe<sup>2+</sup>(BPG) complex to model the active site of quercetin dioxygenase.
- Study reactivity of Fe<sup>2+</sup>(BPG) and substrates.

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