Synthetic Model Studies for Quercetin 2,3-Dioxygenase

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Quercetin 2,3-dioxygenase (2,3-QD) is an metalloenzyme found in *Aspergillus Japonicus.* A mononuclear copper center resides at the active site and is bonded to three histidine nitrogens and partially to one carboxylate oxygen. 2,3-QD is responsible for the degradation of rutin and quercetin. In this process, the cleavage of the *O*-heteroaromatic ring of flavonols is effected yielding the corresponding depside (phenolic carboxylic acid ester) and carbon monoxide. Oxygen is required for this reaction, however, very little is know about the mechanism. The development of small molecule mimics for this protein could be useful in bioremediation of aromatic and heteroaromatic waste products, as well as plant based stain removal. Such molecules would also be helpful in shedding light on the mechanism of this unusual reaction. Herein we describe the synthesis and characterization of a small molecule mimic for 2,3-QD (CuL^1Cl) and the kinetics for oxygenation of 3-hydroxyflavonol (a quercetin mimic) in the presence of dioxygen and catalytic amounts of CuL^1Cl and show that this compound is effective at substrate degradation. Deletion of the Glu73 ligand in 2,3-QD results in loss of activity for the enzyme. In accordance with this observation, removal of the carboxylate group in the mimic also leads to loss of reactivity.