Regioselective Catalytic C-H Oxidation of Hydrocarbons in Aqueous Solution

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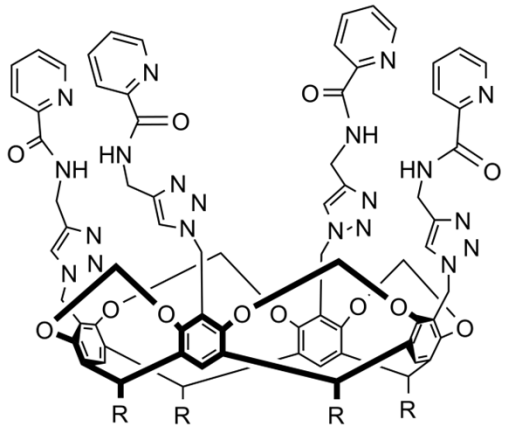
We aim to prepare new biomimetic catalysts that can *both* selectively bind substrate and activate it for reaction. This behavior is the hallmark of enzymatic catalysis: we seek to apply this to non-natural reactions such as hydrocarbon oxidation.

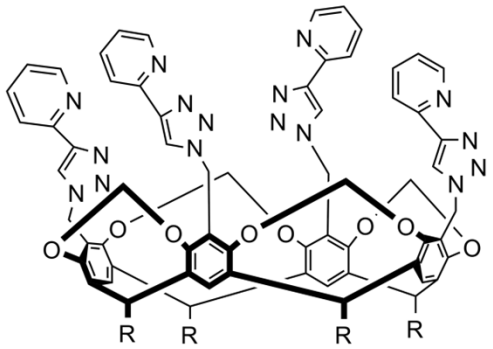
To achieve this, we have synthesized a series of water-soluble receptor molecules (cavitands) that can coordinate high oxidation state metal ions in aqueous solution while still retaining a defined cavity for molecular recognition. A sample of our targets is shown below. The properties of these molecules have been studied by techniques such as X-Ray crystallography and NMR spectroscopy.

We are in the process of testing their abilities as hydrocarbon oxidation catalysts in aqueous solution in the presence of bulk sacrificial oxidants such as hydrogen peroxide.

Sample metal-coordinating cavitands synthesized:

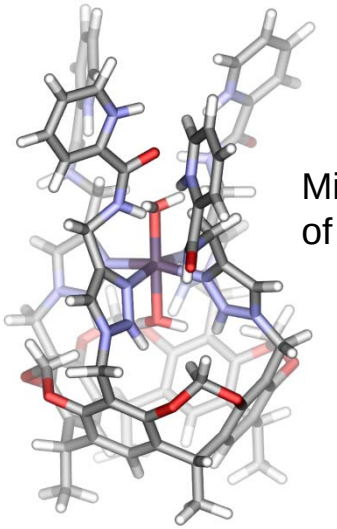


1



2

R = $(CH_2)_3OH$, $(CH_2)_3OSO_3^-$



Minimized representation of the **1**:Fe(II) complex