

*Title:* **Analysis of the active site in mononuclear manganese enzymes and identification of biomimetic coordination compounds.**

*Student:* Joan Caldentey Gutiérrez

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*Supervisor/s:* Dr. Silvia Gómez Coca

*Departament de Química Inorgànica i Orgànica. Secció de Química Inorgànica.*

Nowadays, remarkably few biological reactions are known to be catalyzed by manganese mononuclear enzyme. Despite many other metal ions in the cell form more stable protein complexes, manganese has exhibited the ability to perform a wide range of catalytic functions, resulting essential in many biological processes. Here, five manganese mononuclear enzyme families are deeply structurally studied: lipoxygenases (LOX), homoprotocatechuate 2,3-dioxygenases, oxalate decarboxylases (OxDC), oxalate oxidases (OxO) and superoxide dismutases (SOD). The obtained information of the active site is employed in the identification of new possible biomimetic coordination compounds, based on the key role elements of the first coordination sphere and their geometrical patterns and behavior analysis.

**Keywords:** manganese, mononuclear coordination compounds, biocatalysts, biomimetic compounds, metalloenzymes, structural databases, structural correlations