Title: **Redox activity of metalloporphyrins with metal ions of the first transition.**

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In this project, a computational study about metalloporphyrins was performed. We have analysed porphyrin complexes containing metals from the first transition series, such as manganese, iron, cobalt and nickel, in the centre of the ring and estimated the redox potential between +2 and +3 oxidation states. Nevertheless, these transition metals are commonly bound to two extra ligands in the axial positions, and different groups were considered to obtain models with biological significance. As example, our iron models can be compared with these cytochromes.

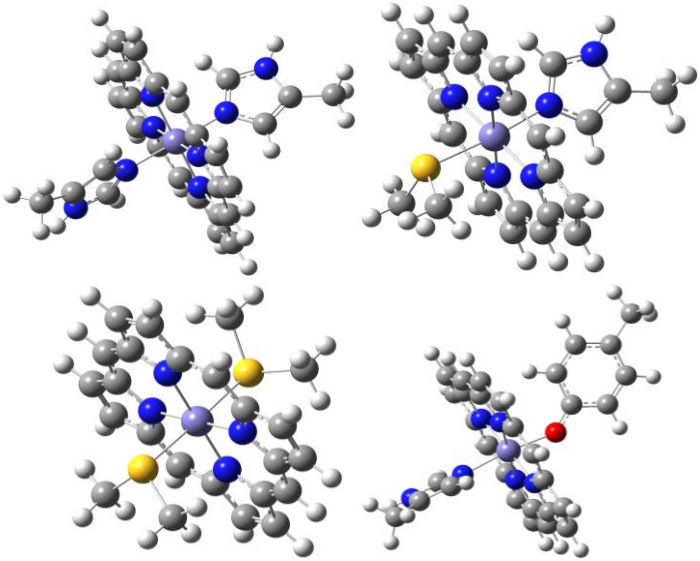

Figure 1. Iron Porphyrins with the different axial ligands studied.

To evaluate the influence of the solvent in the reduction/oxidation process, we have carried out our calculations in three solvents with very different polarities such as water, acetonitrile, and dichloromethane.

Keywords: Metalloporphyrins, reduction potential, computational studies, first transition series.