Title: **Theoretical study of the relative stability of pyrrolidine enamines and their nitro derivatives in α, β, γ and δ positions.**

Student: Pol Sanz Berman

Date: July 2020

Supervisor/s: Dra. Anna Maria Costa Arnau
Departament de Química Inorgànica i Orgànica
Dr. Jaume Vilarrasa i Llorens
Departament de Química Inorgànica i Orgànica

The chemistry of enamines has gained importance in recent years due to the increased popularity of asymmetric organocatalysis using chiral secondary amines. The main goal of this dissertation is to gain insight, from a theoretical point of view, of the position of the equilibrium involved in the catalytic cycle of nitro-Michael reactions between the product enamine, containing a nitro group, and the starting aldehyde enamine.

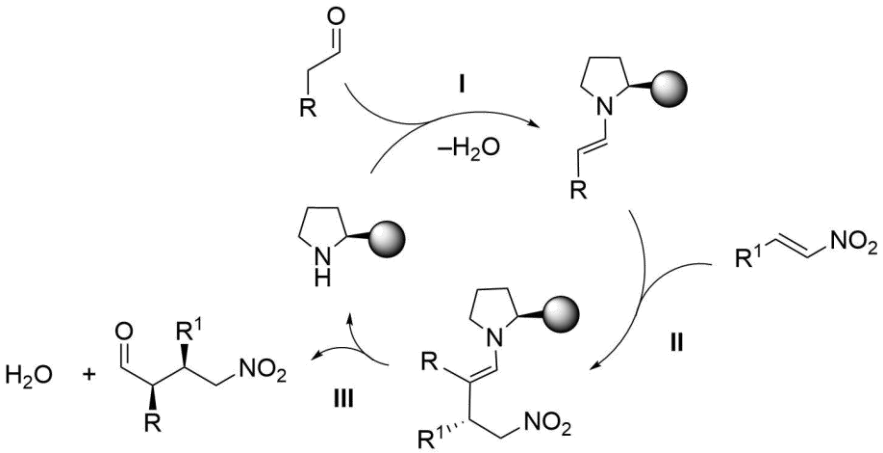

Figure 1. Catalytic cycle of a nitro-Michael reaction.

To do so, the energies of the species involved in the equilibria shown below were calculated, at different levels of theory. The calculations were performed with the Gaussian computational chemistry package and some scripts in Bash command language and in Python programming language were written to assist in the automatization of the process.

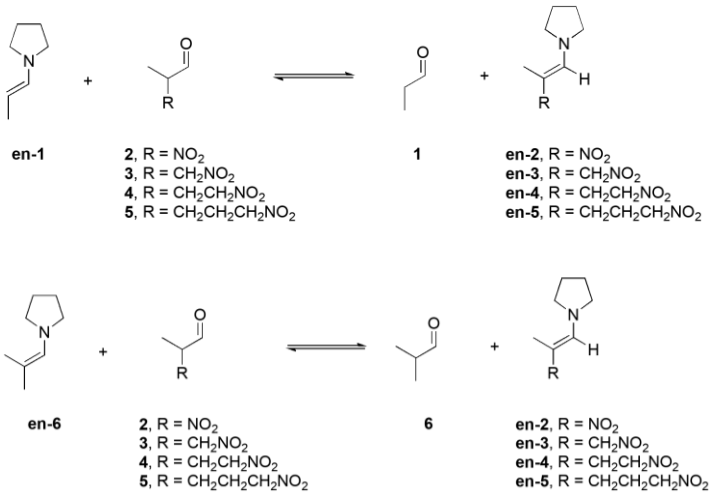

Figure 2. Summary image of all the reactions from this paper.

Keywords: organocatalysis, ab initio calculations, enamines, nitroalkenes, Python, Bash, scripting, cheminformatics.