Título: COMPUTATIONAL UNDERSTANDING OF HETEROCYCLISATION REACTIONS AND SYNTHESIS OF FLUORINATED ISOQUINOLINES

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Resumen: The present thesis deals with three different topics that have in common the formation of carbo- and heterocycles. The whole work is organized as a synergy of experimental and computational studies to provide a deep understanding of the systems of interest.The first chapter contains an introduction about computational chemistry with a particular focus on DFT and its application. The second chapter regards asymmetric catalysis and includes two works made in collaboration with the group of Prof. Palomo at the Universidad del País Vasco. Bifunctional catalysts are employed to afford good levels of stereoselectivity in the ¿-functionalization of challenging substrates, as substituted dienolates and trienolates, with olefins. Computational studies were performed mainly to rationalize the role of the catalyst. The third chapter in collaboration with the group of Prof. E. Occhiato at the Universitá degli Studi di Firenze presents two examples of gold catalysis applied to the [3,3]-rearrangement/Nazarov reaction of propargylic esters and the tandem Claisen Rearrangement/Hydroarylation reaction of propargyl vinyl ethers. The mechanism of the reactions were studied computationally, as well as the effect of particular features in the substrates or in the catalysts. The last two chapters concern the synthesis of

fluorinated isoquinolines and computational studies on particular issues encountered experimentally. The strategy employed is a two step reaction that includes a Rh-catalyzed CH activation of oximes with difluoroalkenes and an electrocyclisation.