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### Reactive metabolites prediction: What can molecular orbitals tell us?

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The ability to predict the formation of reactive metabolites during the metabolism of a drug would allow speeding up the drug discovery process by identifying potentially toxic compounds at an early stage. Most of the detoxification of xenobiotics takes place in the liver, where, among others, Cytochrome P450 (CYPs) enzymes oxidize drugs to make them more water soluble and easier to excrete. However, the metabolites produced by this oxidation may be highly reactive and could cause toxicity by covalently binding to macromolecules in the body. Using Density Functional Theory, we modeled the active site of CYPs and a set of small substrates in order to better understand the reactivity of CYPs. Based on our findings, we have developed a fast yet efficient model to predict CYP aromatic oxidation metabolites. Herein we present our progress in the study of aromatic oxidation, olefin epoxidation and aliphatic hydroxylation and the use of Fukui coefficients in the prediction of their metabolism.

#### Biography

Anna Tomberg is currently pursuing PhD in Prof. Nicolas Moitessier's research group at McGill University, Canada. Her interest in computational chemistry and molecular modeling started when she was working as a Research Assistant in Prof. Christopher Barrett's group.

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