

N- and S-Oxidation Model of the Flavin-containing Monooxygenases

Written by Peter Walton

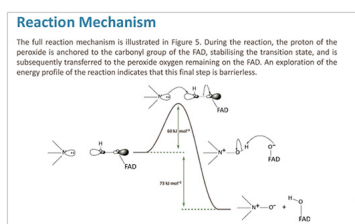
Wednesday, 03 July 2019 14:44 - Last Updated Wednesday, 03 July 2019 15:31

This poster was presented at the Eighth Joint Sheffield Conference on Chemoinformatics; 17-19 June 2019

Peter Walton, Mario Öeren, Peter Hunt, Matthew Segall

Existing computational models of drug metabolism are heavily focused on predicting oxidation by cytochrome P450 (CYP) enzymes, because of their importance in phase I drug metabolism, reactive metabolite formation, and drug-drug interactions. Due, in part, to the success of these models, new drug candidates are typically well-optimised with respect to CYP metabolism. However, novel metabolites are observed due to other, less-studied, enzyme families such as the flavin containing monooxygenases (FMOs) are found in multiple tissues, including the liver, and have five active isoforms (FMO 1-5). In common with CYPs, FMOs are responsible for phase I, oxidative metabolism and catalyse a variety of reaction types, including N- and S-oxidation, demethylation, desulphuration and Bayer-Villiger oxidation.

The objective of this study was to elucidate the reaction mechanism of FMO-mediated oxidation to inform the development of models to predict the metabolism of novel substrates.



You can download the poster as a [PDF](#)