MOLECULAR DYNAMICS STUDY ON THE CYTOCHROME P450 MEDIATED C-H HYDROXYLATION OF NON-AROMATIC *N*-HETEROCYCLES

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The P450-mediated C-H hydroxylation has great potential in the late-stage synthesis of nitrogen containing pharmaceutical compounds.[1] However, strong nitrogen haem interactions can obstruct C-H hydroxylation.[2] Intriguingly, we found a starting activity for the conversion of (*S*)-2-methylpyrrolidine **1** to (*S*)-2-pyrrolidinemethanol **2** using CYP151A2 from *Mycobacterium* sp HE5 (MorA). Long-scale molecular dynamics (MD) simulations were used to study the dynamical behaviour of **1** in MorA in comparison to an *in silico* generated design and non-active CYP116B46 from *Tepidiphilus thermophilus* (TT)[3] to obtain insights into this promising activity.

[1] Urlacher et al., Trends Biotechnol, 37(8):882-897, 2019.
[2] Zhang et al., Front Chem, 5(1):1-10, 2017.
[3] Tavanti et al., Biochem Biophys Res Commun, 501(4):846-850, 2018.