

# Mechanism and Prediction of UGT Metabolism

Written by Mario Öeren

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## Presentation Overview

UGT metabolism – A short overview

Mechanistic studies – *Ab initio* – Semi empirical

QSAR models – Results from mechanistic studies – Steric and orientation descriptors

## Conclusions

**Mechanistic Studies - Validation**

- Simplification of the system
  - > Simplify the model
  - > Simplify the UGP-UG
- Identification of a transition state
  - > All atoms (SULFUR)
  - > Conformation for N and O glycosylation
- Validation of the transition state
  - > Experimental data ( $V_{max}$ )
  - >  $k_{cat}$
  - > Stereoselectivity (glycosylation)
  - > Show specific active sites
  - > Refer to biological experiments

228 kJ mol<sup>-1</sup> (Observed)  
243 kJ mol<sup>-1</sup> (Non-observed)  
320 kJ mol<sup>-1</sup>

C1=CC=C2C(=C1)N(C2)CCN(C)CCN(C)CC(F)(F)F  
Tiludoprone

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