

Mechanism and Prediction of UGT Metabolism

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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 (epiglycosylation)
 - > Show specific active sites
 - > Refer to biological experiments

228 kJ mol⁻¹ (Observed)
243 kJ mol⁻¹ (Non-Observed)
320 kJ mol⁻¹

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

Tribuapentene

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