



# METABOLISM & TRANSPORTER

The Metabolism & Transporter Module in GastroPlus® calculates Michaelis-Menten rates for gut and liver (or any PBPK tissue) metabolism and carrier-mediated transport (influx or efflux – again, for any tissue in a PBPK model) based on input values for  $V_{max}$  and  $K_m$ .



## What is the Metabolism and Transporter module?

The Metabolism and Transporter Module is an optional module that extends the capabilities of GastroPlus to include nonlinear pharmacokinetics into any compartment (gut, liver, and/or any PBPK tissue), along with metabolite tracking. Define multiple metabolic/transport pathways, with enzymes and transporters placed into the tissues or organs of your choice. Also, easily link the formation of different metabolites in a single simulation – no limit on the number of metabolites you want to track!

You can provide  $V_{max}$  and  $K_{m,max}$  values for each enzyme/transporter independently, or you can lump them into a single effective  $V_{max}$  and  $K_m$ , depending on your data. The distribution factors on the Physiology tab are automatically loaded for recognized gut enzymes and transporters, and provide the relative amounts of enzymes or transporters in the various ACAT™ gut model compartments. The  $V_{max}$  and  $K_m$  scale factors on the Pharmacokinetics tab are provided to allow fitting nonlinear kinetic models to your data.

The Metabolism and Transporter Module includes a Units Converter tool for easy transformation of a variety of your *in vitro* metabolism or transporter kinetic parameters into values and units that can be utilized by the GastroPlus PBPK model.



When linked with the upgraded ADMET Predictor® Module, predict nonlinear pharmacokinetics for CYP metabolism, and have the Enzyme Table automatically populated with the correct locations and units!



Enzyme and transporter expression levels across species and for pediatric subjects (Ontogony) - including UGTs, SULTs, and transporters in various tissues in PBPK models!

