

The Influence of OAT1 Density and Functionality on Indoxyl Sulfate Transport in the Human Proximal Tubule: An Integrated Computational and In Vitro Study

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Table S1: Conservation of mass calculation

Time Point	Toxin in Blood	OAT bound Toxin	OAT1 Unbound	Toxin in Dialysate	Total Toxin	Total OAT1
Start	1.51×10^{14}	0.00×10^0	3.68×10^{14}	0×10^0	1.51×10^{14}	3.68×10^{14}
Steady State	1.22×10^{14}	2.87×10^{13}	3.39×10^{14}	2.16×10^{11}	1.51×10^{14}	3.68×10^{14}

Table S2. All settings for COPASI parameter fitting models.

COPASI Parameter Fitting Settings for Guessing Fitted Values for the Parameter Fitting Model				
	Parameter	Initial Guess	Lower Limit	Upper Limit
Case 1	$k_{f_{\text{Uptake}}}$ [s ⁻¹ .μM ⁻¹] IS binding to transporter	1×10^{-4}	5×10^{-7}	1×10^{-3}
	$k_{f_{\text{dissociation}}}$ [s ⁻¹] IS dissociation from transporter	1×10^{-3}	5×10^{-5}	1×10^{-3}
	[OAT1] [molecules.μm ⁻²] Density of transporter	5×10^6	7×10^5	2×10^7
Case 3	$k_{f_{\text{dissociation}}}$ [s ⁻¹] IS dissociation from transporter	4.18×10^{-4}	4×10^{-4}	1×10^{-3}
	K_M	1×10^2	1×10^0	1×10^3
	V_{Max} [s ⁻¹]	1×10^{-1}	1×10^{-5}	1×10^1
Case 3	$k_{f_{\text{dissociation}}}$ [s ⁻¹] IS dissociation from transporter	1.69×10^{-4}	1.69×10^{-5}	1.69×10^{-3}
	K_M	1×10^0	1×10^{-3}	1×10^3
	V_{Max} [s ⁻¹]	1×10^0	1×10^{-6}	1×10^2