Supplementary Material: Cubitt et al., Prediction of human drug clearance by multiple metabolic pathways – integration of hepatic and intestinal microsomal and cytosolic data, DMD #36566

Different in vitro conditions used to study sulphation

<table>
<thead>
<tr>
<th>Concentration of Human Cytosolic Protein (mg/ml)</th>
<th>Concentration of PAPS (µM)</th>
<th>Buffer Type</th>
<th>Buffer pH</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.002-0.012</td>
<td>22</td>
<td>50mM phosphate</td>
<td>7.4</td>
<td>(Schrag et al., 2004)</td>
</tr>
<tr>
<td>0.004</td>
<td>0.4</td>
<td>33mM Tris</td>
<td>7.4</td>
<td>(Pacifici et al., 1997b)</td>
</tr>
<tr>
<td>0.02-0.1</td>
<td>1</td>
<td>10mM phosphate</td>
<td>7.4</td>
<td>(Tamura et al., 2001)</td>
</tr>
<tr>
<td>0.2</td>
<td>5</td>
<td>50mM Tris-HCl</td>
<td>7.4</td>
<td>(Honma et al., 2002)</td>
</tr>
<tr>
<td>0.2</td>
<td>20</td>
<td>Phosphate</td>
<td>6.2</td>
<td>(Chen et al., 2003)</td>
</tr>
<tr>
<td>0.5-2</td>
<td>3.1-50</td>
<td>0.2M glycine NaOH, 7mM DTT</td>
<td>9.5</td>
<td>(Pacifici et al., 1997a)</td>
</tr>
</tbody>
</table>
References for in vitro sulfation studies:


Sources of UGT recombinant data:


Sources of SULT specificity (and recombinant) data

**Quercetin**


**Raloxifene**


**Salbutamol**


**Troglitazone**

Honma et al. (2002) Phenol sulfotransferase, ST1A3, as the main enzyme catalyzing sulfation of troglitazone in human liver. *Drug Metab Dispos* **30**:944-949.
Sources of Clinical Data

**Quercetin**


Walle et al. (2001) Carbon dioxide is the major metabolite of quercetin in humans. *J Nutr* 131:2648-2652


**Raloxifene**


**Salbutamol**


**Troglitazone**

Izumi et al. (1996) Prediction of the human pharmacokinetics of troglitazone, a new and extensively metabolized antidiabetic agent, after oral administration, with an animal scale-up approach. *J Pharmacol Exp Ther* 277:1630-1641


