

| Substrate | |
|-----------|--|
|-----------|--|

| | |
|--------------------------------|-----------------|
| Compound Name | Vancomycin |
| Version number | Not applicable |
| Compound Type | Small Molecule |
| Route | Infusion |
| Sub : Dose Units | Dose (mg) |
| Bolus Dose | 0.000 |
| Infusion Dose | 1000.000 |
| Infusion Duration (h) | 1.000 |
| Start Day | 1.000 |
| Start Time | 9h0m |
| Dosing Regimen | Single Dose |
| | |
| PhysChem and Blood Binding | |
| | |
| Mol Weight (g/mol) | 1449.254 |
| log P | -3.100 |
| Compound Type | Ampholyte |
| pKa 1 | 2.180 |
| pKa 2 | 8.890 |
| BP Input | User Input |
| B/P | 0.550 |
| Haematocrit | 45.000 |
| fu Input | User |
| fu | 0.450 |
| Reference Binding Component | HSA |
| Protein Reference Conc (g/L) | 45.000 |
| % Bound to Lipoprotein | 0.000 |
| % Bound to Lipoprotein (CV %) | 0.000 |
| | |
| Absorption | |
| | |
| | |
| Distribution | |
| | |
| Distribution Model | Full PBPK Model |
| Replacement Organ? | No |
| Organ Replaced | n/a |
| User-defined Additional Organ | No |
| Type | n/a |
| Vss mode | Predicted |
| Prediction Method | Method 1 |
| Concentration-dependent volume | No |
| log Po:w | -3.100 |
| fut switch | Predicted |
| fut value | 0.621 |

| | |
|--|-----------------|
| logDvo:w (pH=7.4) switch | Predicted |
| logDvo:w (pH=7.4) value | -11.530 |
| logP vo:w | Predicted |
| logP vo:w value | -4.806 |
| Compound Type | Ampholyte |
| pKa 1 | 2.180 |
| pKa 2 | 8.890 |
| B/P | 0.550 |
| Haematocrit | 45.000 |
| fu | 0.450 |
| Adipose Input Type | Predicted |
| Adipose Value | 0.086 |
| Bone Input Type | Predicted |
| Bone Value | 0.337 |
| Brain Input Type | Predicted |
| Brain Value | 0.609 |
| Gut Input Type | Predicted |
| Gut Value | 0.556 |
| Heart Input Type | Predicted |
| Heart Value | 0.587 |
| Kidney Input Type | Predicted |
| Kidney Value | 0.606 |
| Liver Input Type | Predicted |
| Liver Value | 0.584 |
| Lung Input Type | Predicted |
| Lung Value | 0.625 |
| Muscle Input Type | Predicted |
| Muscle Value | 0.585 |
| Skin Input Type | Predicted |
| Skin Value | 0.554 |
| Spleen Input Type | Predicted |
| Spleen Value | 0.610 |
| Pancreas Input Type | Predicted |
| Pancreas Value | 0.604 |
| Kp Scalar Value | 1.000 |
| | |
| Elimination | |
| | |
| Allometric Scaling | Not Used |
| | |
| Clearance Type | Enzyme Kinetics |
| FI Correction | Not used |
| PLR Correction | Not Used |
| In vitro metabolic system | Recombinant |
| | |
| Feed formed renal metabolite into kidney | No |
| | |

| | |
|---|------------------------|
| Use Allelic variants for Enzyme 1 | No |
| Enzyme | CYP2C9 |
| | |
| Use Allelic variants for Enzyme 2 | No |
| Enzyme | CYP1A2 |
| | |
| Ontogeny Profile | No Profile Used |
| Biliary CLint (Hep) ($\mu\text{L}/\text{min}/10^6$) | 0.180 |
| CV Biliary CLint (Hep) (%) | 30.000 |
| Ontogeny Profile | No Profile Used |
| Active Uptake into Hepatocyte | 1.000 |
| CL R (L/h) | 5.730 |