Table S1. Vincristine Compound File (PK Sim 7.3.0.42)

Basic Physico-chemistry	
Is small molecule	Yes
Molecular Weight	824.96 g/mol
Effective Molecular Weight	824.96 g/mol
pKa value	5
Compound Type	Acid
Lipophilicity	2.82
Fraction Unbound	0.51 (Human)
Solubility	2.27
Solubility Reference pH	7.00
Solubility gain per charge	1000.00
Absorption	
Specific Intestinal Permeability	7.93×10^{-7}
Specific Organ Permeability	6.03×10^{-5}
Distribution	
Partition Coefficients	Schmitt
Cellular Permeabilities	PK-Sim Standard
Specific binding	
k_{off}	1.93×10^{-3} 1/s
K_D	0.05 µmol/L
Metabolism	
CYP3A4	
Process Type	In vitro metabolic rate in the presence of recombinant CYPs/enzymes - Michaelis-Menten
In vitro V_{max} / recombinant enzyme	0.90 pmol/min/pmol ~~rec.~~ enzyme
K_m	19.70 µmol/L
k_{cat}	0.90 1/min
CYP3A5	
Process Type	In vitro metabolic rate in the presence of recombinant CYPs/enzymes - Michaelis-Menten
In vitro V_{max} / recombinant enzyme	8.10 pmol/min/pmol ~~rec.~~ enzyme
K_m	14.30 µmol/L
k_{cat}	8.10 1/min
Transport and Excretion	
ABCB1	
Process Type	Specific active transport – Michaelis-Menten
Transporter concentration	1.00 µmol/L
V_{max}	416.10 pmol/mL/min
K_m	17.10 µmol/L
k_{cat}	0.42 1/min