Table 4: Pharmacokinetic assessment of Quercetin

S.No.	Property	Model Name	Predicted Value	Unit
1.	Absorption	Water solubility	-2.925	Numeric (log mol/L)
2.	Absorption	Caco2 permeability	-0.229	Numeric (log Papp in 10-6 cm/s)
3.	Absorption	Intestinal absorption (human)	96.902	Numeric (% Absorbed)
4.	Absorption	Skin Permeability	-2.735	Numeric (log Kp)
5.	Absorption	P-glycoprotein substrate	Yes	Categorical (Yes/ No)
6.	Absorption	P-glycoprotein I inhibitor	No	Categorical (Yes/ No)
7.	Absorption	P-glycoprotein II inhibitor	No	Categorical (Yes/ No)
8.	Distribution	VDss (human)	1.559	Numeric (log L/kg)
9.	Distribution	Fraction unbound (human)	0.206	Numeric (Fu)
10.	Distribution	BBB permeability	-1.098	Numeric (log BB)
11.	Distribution	CNS permeability	-3.065	Numeric (log PS)
12.	Metabolism	CYP2D6 substrate	No	Categorical (Yes/ No)
13.	Metabolism	CYP3A4 substrate	No	Categorical (Yes/ No)
14.	Metabolism	CYP1A2 inhibitior	Yes	Categorical (Yes/ No)
15.	Metabolism	CYP2C19 inhibitior	No	Categorical (Yes/ No)
16.	Metabolism	CYP2C9 inhibitior	No	Categorical (Yes/ No)
17.	Metabolism	CYP2D6 inhibitior	No	Categorical (Yes/ No)

18.	Metabolism	CYP3A4 inhibitior	No	Categorical (Yes/ No)
19.	Excretion	Total Clearance	0.407	Numeric (log ml/ min/kg)
20.	Excretion	Renal OCT2 substrate	No	Categorical (Yes/ No)
21.	Toxicity	AMES toxicity	No	Categorical (Yes/ No)
22.	Toxicity	Max. tolerated dose (human)	0.499	Numeric (log mg/ kg/day)
23.	Toxicity	hERG I inhibitor	No	Categorical (Yes/ No)
24.	Toxicity	hERG II inhibitor	No	Categorical (Yes/ No)
25.	Toxicity	Oral Rat Acute Toxicity (LD50)	2.471	Numeric (mol/kg)
26.	Toxicity	Oral Rat Chronic Toxicity (LOAEL)	2.612	Numeric (log mg/ kg_bw/day)
27.	Toxicity	Hepatotoxicity	No	Categorical (Yes/ No)
28.	Toxicity	Skin Sensitisation	No	Categorical (Yes/ No)
29.	Toxicity	T.Pyriformis toxicity	0.288	Numeric (log ug/ L)
30.	Toxicity	Minnow toxicity	3.721	Numeric (log mM)0