

Table S5 ADMET descriptors of compounds generated using pkCSM

Compound	Adsorption		Distribution			Metabolism, CYP inhibitor				Excretion	Toxicity
	GIA <sup>a</sup>	BBB <sup>b</sup>	CNS <sup>c</sup>	1A2	2C19	2C9	2D6	3A4	CL <sup>d</sup>	Hepatotoxic effect	
C1	94.16	0.48	-1.35	+	+	+	-	-	0.19	-	
C2	94.06	0.26	-1.40	+	+	+	-	-	0.29	-	
C3	94.84	0.28	-1.43	+	+	+	-	-	0.23	-	
C4	95.12	0.30	-1.43	+	+	+	-	-	0.22	-	
C5	95.05	0.45	-1.48	+	+	+	-	-	0.36	-	
C6	92.50	0.44	-1.34	+	+	+	-	-	0.06	-	
C7	92.77	0.49	-1.34	+	+	+	-	-	0.05	-	
C8	93.52	0.29	-1.43	+	+	+	-	-	0.27	-	
C9	93.45	0.42	-1.47	+	+	+	-	-	0.42	-	
Nutlin-3a	93.57	-1.59	-1.72	-	-	-	-	+	0.25	-	
THIQ-PP	91.14	-0.92	-2.33	+	-	-	+	+	0.82	+	

<sup>a</sup>Gastrointestinal adsorption (%)

<sup>b</sup>Blood-brain barrier (Log BB)

<sup>c</sup>Central nervous system (Log PS)

<sup>d</sup>Total clearance (Log mL/min/kg)