Supplementary Table 1. Drug-likeness and absorption, distribution, metabolism, excretion, and toxicity (ADMET) analysis results

Parameter	Panduratin A	5	6
Drug-likeness			
Molecular weight	406.210	460.130	460.130
H-bond acceptor	4	9	9
H-bond donor	2	3	3
LogP	7.246	3.318	3.303
TPSA	66.760	138.950	138.950
A (Absorption)			
Human intestinal absorption (HIA)	0.011	0.073	0.090
Caco-2 permeability (log cm/s)	–4.774	–5.307	–5.362
P-glycoprotein inhibitor	0.986	0.320	0.385
P-glycoprotein substrate	0.018	0.025	0.022
$F_{20\%}$	0.883	0.031	0.043
$F_{30\%}$	0.674	0.002	0.002
D (Distribution)			
Plasma protein binding (PPB) (%)	97.360	97.770	97.800
Blood-brain barrier penetration (BBB) (cm/s)	0.021	0.008	0.008
Volume distribution (l/kg)	1.584	0.594	0.655
Fraction unbound (Fu) (%)	4.645	1.635	1.634
M (Metabolism)			
CYP1A2 substrate	0.802	0.087	0.101
CYP1A2 inhibitor	0.817	0.041	0.041
CYP2C19 substrate	0.254	0.101	0.120
CYP2C19 inhibitor	0.968	0.044	0.048
CYP2C9 substrate	0.950	0.133	0.124
CYP2C9 inhibitor	0.945	0.495	0.635
CYP2D6 substrate	0.577	0.117	0.116
CYP2D6 inhibitor	0.931	0.020	0.039
CYP3A4 substrate	0.220	0.597	0.636
CYP3A4 inhibitor	0.840	0.099	0.127
E (Excretion)			
Half time ($t_{1/2}$)	0.061	0.711	0.779
Clearance (ml/min/kg)	12.251	0.630	0.666
T (Toxicity)			
Human hepatotoxicity (H-HT)	0.584	0.878	0.885
hERG blockers	0.272	0.014	0.008
Rat oral acute toxicity	0.092	0.822	0.768
Ames toxicity	0.041	0.033	0.018
Drug induced liver injury (DILI)	0.661	0.986	0.986
Carcinogencity	0.137	0.763	0.742

hERG – human ether-á-go-go-related gene, TPSA – topological polar surface area.