

Supplementray Information

Table S1. ADME properties of the selected ligand molecules

Absorption properties					Distribution			Metabolism										Elimination	
Caco-2 Permeability higher than -5.15 Log unit or -4.70 or -4.80	Human intestinal absorption ≥30%: HIA+; <30%: HIA-	P-glycoprotein substrate	P-glycoprotein inhibitor	F (20% bioavaila- bility) ≥20%: F20+; <20%: F20-	PPB (plasma protein binding) Optimal up to 90%	VD (Volume Distributi- on) 0.04- 20L/kg	BBB (Blood Brain Barrier) BB ratio >=0.1: BBB+; BB ratio <0.1: BBB-	P450 CYP1A2 inhibitor	P450 CYP1A2 Substrate	P450 CYP3A4 inhibitor	P450 CYP3A4 substrate	P450 CYP2C9 inhibitor	P450 CYP2C9 substrate	P450 CYP2C19 inhibitor	P450 CYP2C19 substrate	P450 CYP2D6 inhibitor	P450 CYP2D6 substrate	T1/2 (Half-Life Time) Range: >8h: high; 3h< Cl < 8h: moderate; <3h: low	CL (Clearance rate) >15 mL/min/kg: high; 5mL/min/kg< Cl < 15mL/min/kg: moderate; <5 mL/min/kg: low
P-octylacetophenone -4.388 cm/s	0.897	-0.272	0.721	0.627	0.86893	0.593 L/kg	+++	0.954	0.534	-0.017	0.522	-0.329	0.59	0.789	-0.476	-0.47	-0.49	1.574 h	1.557 mL/min/kg
Oxalic acid, decyl 3,5- difluorophenyl ester -4.579 cm/s	0.633	-0.031	-0.387	-0.485	0.81743	-0.651 L/kg	+++	0.945	-0.448	-0.152	-0.398	-0.422	-0.406	0.54	-0.288	-0.427	-0.401	1.73 h	1.342 mL/min/kg
Oxalic acid, 3,5- difluorophenyl undecyl ester -4.634 cm/s	0.633	-0.031	-0.387	-0.485	0.82143	-0.503 L/kg	+++	0.945	-0.448	-0.152	-0.398	-0.422	-0.406	0.54	-0.288	-0.427	-0.401	1.791 h	1.342 mL/min/kg