

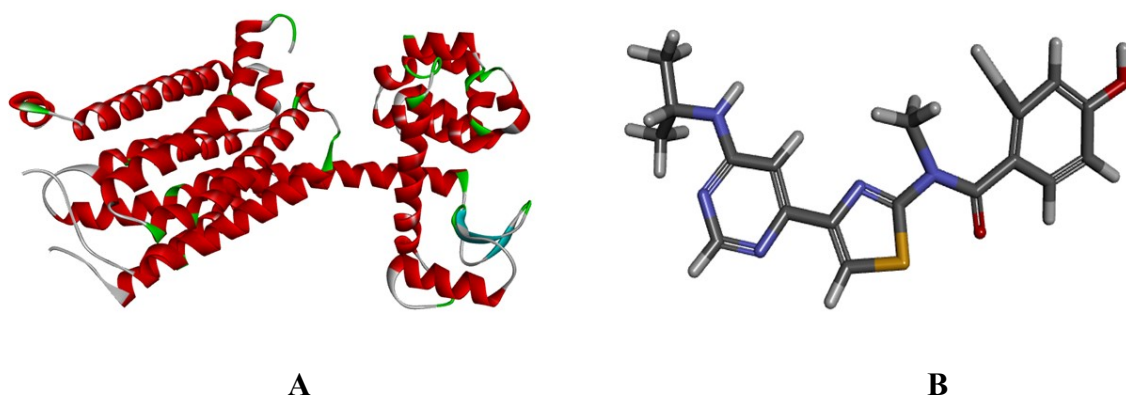


Fig S1: (A and B) Protein and ligand 3D structure

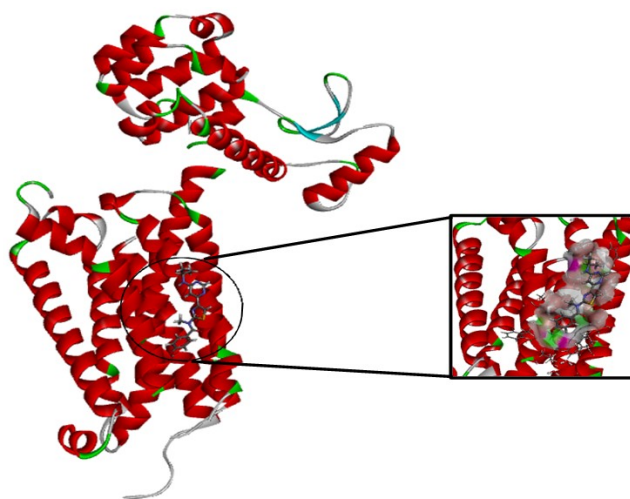


Fig S2: Protein-ligand in binding pocket

Absorption

LogP = 3.4

LogS = -3.35

Intestinal absorption (human) =
91.203 % absorbed

Distribution

BBB permeability = -0.76 logBB

CNS permeability = -2.469 logPS

Metabolism

CYP3A4 substrate = Yes

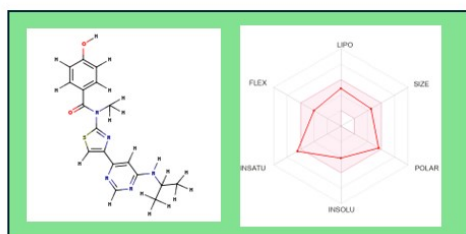
CYP2D6 inhibitor = No

Formula = C₁₈H₁₉NSO₂S

MW = 369.44 g/mol

HBD = 2

HBA = 5



4-hydroxy-N-(4-(6-(isopropylamino)pyrimidin-4-yl)thiazol-2-yl)-N-methylbenzamide

Excretion

Total Clearance = 0.057 log
ml/min/kg

Toxicity

Max. tolerated dose (human) = -0.056

Oral Rat Acute Toxicity (LD₅₀) = 2.386
mol/kg

Fig. S3: Physicochemical analysis of RMGOH ligand

Table S1: The pharmacokinetic and toxicity prediction of RMGOH ligand

Properties	Compounds	Ligand
	IUPAC Name	4-hydroxy-N-(4-(6-(isopropylamino)pyrimidin-4-yl)thiazol-2-yl)-N-methylbenzamide
	Smiles	<chem>[H]OC1=C([H])C([H])=C(C([H])=C1[H])C(=O)N(C1=NC(=C([H])S1)C1=C([H])C(=NC([H])=N1)N([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H]</chem>
Absorption	Water solubility	-3.351 log mol/L
	Caco2 permeability	1.255 log papp in 10 ⁻⁶ cm/s
	Intestinal absorption (human)	91.203 % absorbed
	Skin permeability	-2.812 log kp
	p-glycoprotein substrate	Yes
	p-glycoprotein inhibitor I	No
	p-glycoprotein inhibitor II	Yes
	BBB permeability	-0.76 logBB
Distribution	CNS permeability	-2.469 logPS
	VDss (Human)	0.289 log L/kg
	CYP3A4 substrate	Yes
Metabolism	CYP2D6 inhibitor	No
	Total Clearance	0.057 log ml/min/kg
Excretion	Max. tolerated dose (human)	-0.056
Toxicity	Oral Rat Acute Toxicity (LD ₅₀)	2.386 mol/kg