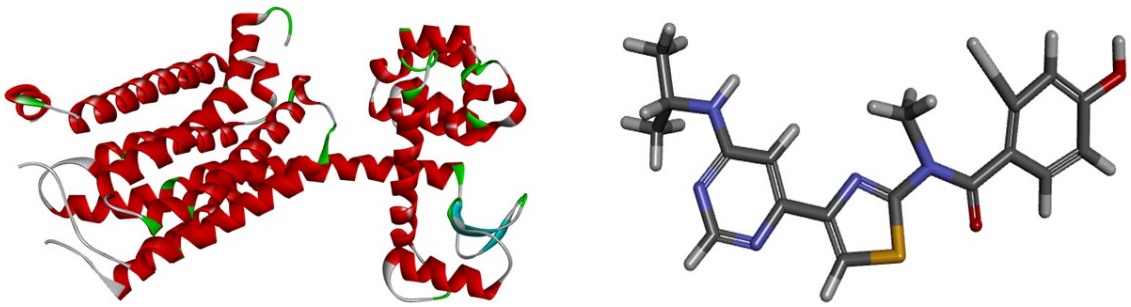

A B

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

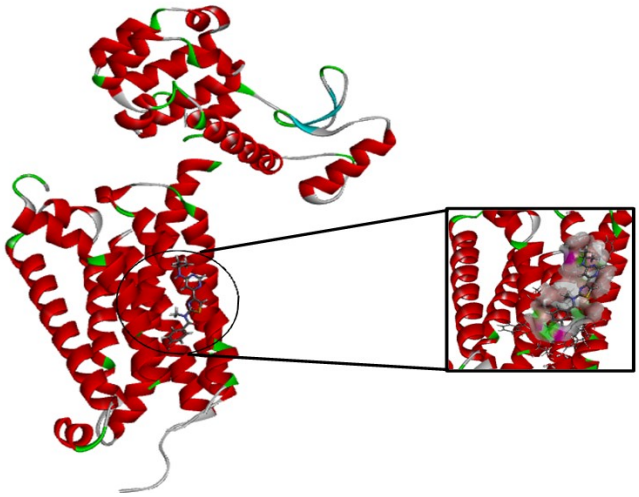

Fig S2: Protein-ligand in binding pocket

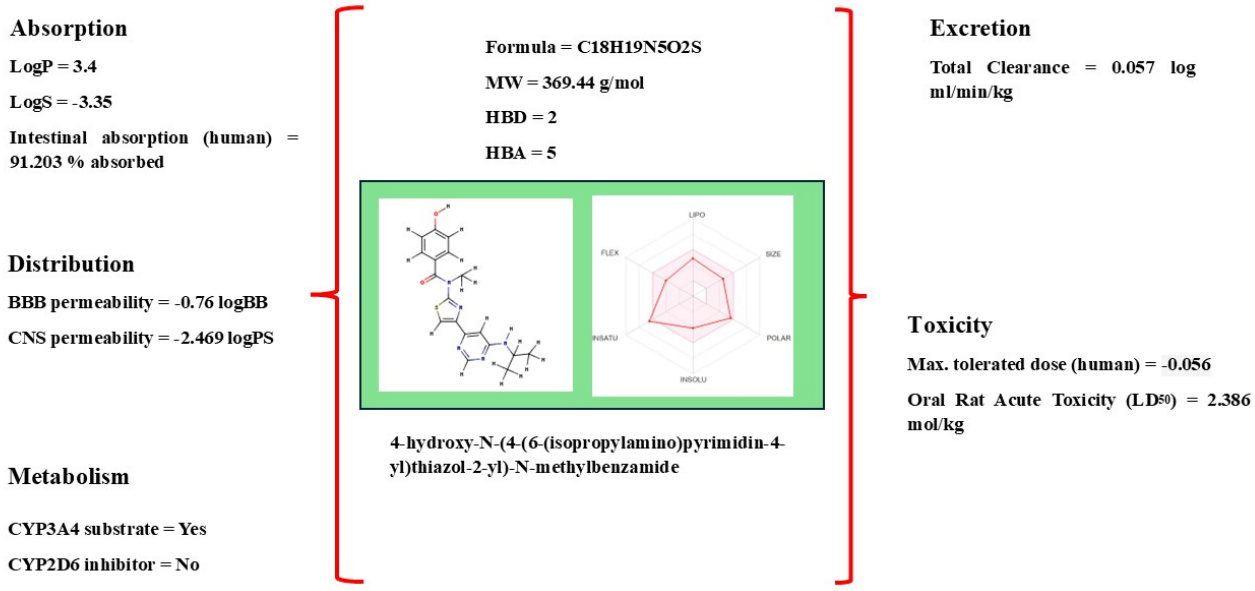

Fig. S3: Physicochemical analysis of RMGOH ligand

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	[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]
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