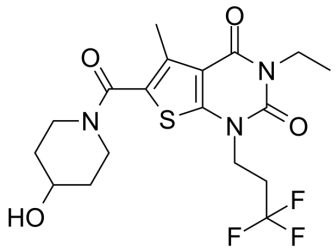
BAY-545

Cat. No.:	HY-111767
CAS No.:	1699717-32-2
Molecular Formula:	$C_{18}H_{22}F_3N_3O_4S$
Molecular Weight:	433.45
Target:	Adenosine Receptor
Pathway:	GPCR/G Protein
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 150 mg/mL (346.06 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3071 mL	11.5354 mL	23.0707 mL
	5 mM	0.4614 mL	2.3071 mL	4.6141 mL
	10 mM	0.2307 mL	1.1535 mL	2.3071 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (5.77 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.77 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.77 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-545 is a potent and selective A_{2B} adenosine receptor antagonist, with an IC_{50} of 59 nM. BAY-545 also exhibits IC_{50}s of 66, 400, 280 nM for human, mouse, rat A_{2B} adenosine receptor in cells, respectively, and a K_i of 97 nM for human A_{2B} adenosine receptor, with more selectivity over A_1, A_{2A}, and A_3 adenosine receptor[1].

IC_{50} & Target

IC50: 59 nM (A_{2B} adenosine receptor), 66 nM (Human A_{2B} adenosine receptor), 400 nM (Mouse A_{2B} adenosine receptor), 280 nM (Rat A_{2B} adenosine receptor), 1300 nM (Human A_1 adenosine receptor), 820 nM (Human A_{2A} adenosine receptor), 470 nM

	(Mouse A_{2A} adenosine receptor) and 750 nM (Rat A_{2A} adenosine receptor)[1] Ki: 97 nM (A_{2B} adenosine receptor)[1]
In Vitro	BAY-545 is selective at A_{2B} adenosine receptor over A_1, A_{2A}, and A_3 adenosine receptor, with IC_{50}s of 1300 nM (Human A_1 adenosine receptor), 820 nM (Human A_{2A} adenosine receptor), 470 nM (Mouse A_{2A} adenosine receptor) and 750 nM (Rat A_{2A} adenosine receptor)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Härter M, et al. Novel non-xanthine antagonist of the A2B adenosine receptor: From HTS hit to lead structure. Eur J Med Chem. 2019 Feb 1;163:763-778.

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