EAI001

Cat. No.: HY-100214

CAS No.: 892772-75-7

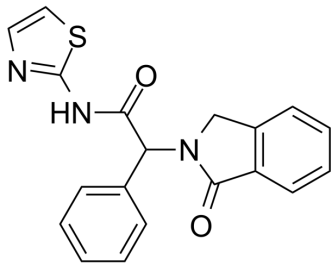
Molecular Formula: $C_{19}H_{15}N_3O_2S$

Molecular Weight: 349.41

Target: EGFR

Pathway: JAK/STAT Signaling; Protein Tyrosine Kinase/RTK

Storage: 4°C, sealed storage, away from moisture and light
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (286.20 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.8620 mL	14.3098 mL	28.6197 mL
	5 mM	0.5724 mL	2.8620 mL	5.7239 mL
	10 mM	0.2862 mL	1.4310 mL	2.8620 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 (7.15 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.15 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

EAI001 is a potent, selective mutant epidermal growth factor receptor (EGFR) allosteric inhibitor with an IC_{50} value of 24 nM for $EGFR^{L858R/T790M}$. EAI001 can be used for research of cancer[1][2].

In Vitro

EAI001 (50 μM) binds to EGFR T790M/C797S/V948R that lies deep inside the EGFR towards the ATP binding site and C-helix. EAI001 showed inhibitory activity due to hydrophobic interaction with amino acid Ile759, Leu747, Leu788, Leu777 and Met766[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Maity S, et, al. Advances in targeting EGFR allosteric site as anti-NSCLC therapy to overcome the drug resistance. Pharmacol Rep. 2020 Aug;72(4):799-813.

[2]. Tinivella A, et, al. Investigating the selectivity of allosteric inhibitors for mutant t790m egfr over wild type using molecular dynamics and binding free energy calculations. 2018 Dec 4;3(12):16556-62.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA