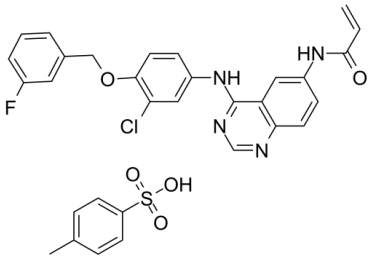
Data Sheet

Product Name:	Allitinib tosylate
Cat. No.:	CS-1209
CAS No.:	1050500-29-2
Molecular Formula:	C31H26ClFN4O5S
Molecular Weight:	621.08
Target:	EGFR
Pathway:	JAK/STAT Signaling; Protein Tyrosine Kinase/RTK
Solubility:	DMSO : 50 mg/mL (80.50 mM; Need ultrasonic); H2O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

Allitinib tosylate (AST-1306 (TsOH)) is an orally active and irreversible **EGFR** and **ErbB2** inhibitor with **IC_{50}s** of 0.5 and 3 nM, respectively. Allitinib tosylate also inhibits **ErbB4** with an IC_{50} of 0.8 nM. Allitinib tosylate is an anilino-quinazoline compound and has anti-cancer activity[1] **In Vitro:** AST1306 tosylate (AST-1306 (TsOH); 0.19-6.25 μM; 72 hours) induces a significant, concentration-dependent inhibition of the growth of HIH3T3-EGFR T790M/L858R cells[1].

AST1306 tosylate inhibits the activation of tyrosine kinases and downstream signaling pathways in A549 cells, Calu-3 cells and SK-OV-3 cells. AST1306 tosylate dose-dependently and markedly inhibits EGF-induced EGFR phosphorylation in A549 cells[1].

AST1306 tosylate (0.1, 0.5, 1.0, 5.0 μM) can dramatically inhibit the growth of both tumor cells on soft agar, and SK-OV-3 cells exhibited much more sensitivity than that of A549 cells[1].

AST1306 tosylate (0.001-1.0 μM; 4 hours) is more than 3000-fold selective for ErbB family kinases over other kinase families[1].

AST1306 tosylate potently inhibits the EGFR T790M/L858R double mutant, exhibiting an IC_{50} value of 12±2 nmol/L[1].

In Vivo: AST1306 tosylate (AST-1306 (TsOH); p.o.; 25-100 mg/kg; twice daily; for 28 days) causes a dramatic suppression of tumor growth in SK-OV-3 and Calu-3 xenograft models[1].

References:

[1]. Xie H, Lin L, Tong L et al. AST1306, a novel irreversible inhibitor of the epidermal growth factor receptor 1 and 2, exhibits antitumor activity both in vitro and in vivo. PLoS One. 2011;6(7):e21487.

CAIndexNames:

2-Propenamide, N-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-6-quinazolinyl]-, 4-methylbenzenesulfonate (1:1)

SMILES:

FC1=CC=CC(COC2=C(Cl)C=C(NC3=NC=NC4=C3C=C(NC(C=C)=O)C=C4)C=C2)=C1.O=S(C5=CC=C(C)C=C5)(O)=O

Caution: Product has not been fully validated for medical applications. For research use only.

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