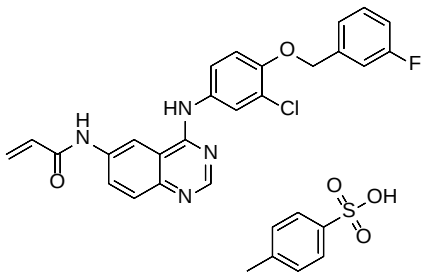
Product data sheet

MedKoo Cat#: 401070 Name: Allitinib tosylate CAS#: 1050500-29-2 (tosylate) Chemical Formula: $C_{31}H_{26}ClFN_4O_5S$ Molecular Weight: 621.08	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

Allitinib, also known as AST1306 and ALS 1306, is a potent, selective, irreversible ErbB2 and EGFR inhibitor. AST-1306 inhibits the enzymatic activities of wild-type epidermal growth factor receptor (EGFR) and ErbB2 as well as EGFR resistant mutant in both cell-free and cell-based systems. AST1306 was found to function as an irreversible inhibitor, most likely through covalent interaction with Cys797 and Cys805 in the catalytic domains of EGFR and ErbB2, respectively. In vivo, AST1306 potently suppressed tumor growth in ErbB2-overexpressing adenocarcinoma xenograft and FVB-2/N(neu) transgenic breast cancer mouse models, but weakly inhibited the growth of EGFR-overexpressing tumor xenografts.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	35.0	56.35
DMF	25.0	40.25
DMF:PBS (pH 7.2) (1:3)	0.25	0.40
Ethanol	1.0	1.61

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	1.61 mL	8.05 mL	16.10 mL
5 mM	0.32 mL	1.61 mL	3.22 mL
10 mM	0.16 mL	0.81 mL	1.61 mL
50 mM	0.03 mL	0.16 mL	0.32 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Xie H, Lin L, Tong L, Jiang Y, Zheng M, Chen Z, Jiang X, Zhang X, Ren X, Qu W, Yang Y, Wan H, Chen Y, Zuo J, Jiang H, Geng M, Ding J. 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. doi: 10.1371/journal.pone.0021487. Epub 2011 Jul 18. PMID: 21789172; PMCID: PMC3138742.

In vivo study

1. Xie H, Lin L, Tong L, Jiang Y, Zheng M, Chen Z, Jiang X, Zhang X, Ren X, Qu W, Yang Y, Wan H, Chen Y, Zuo J, Jiang H, Geng M, Ding J. 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. doi: 10.1371/journal.pone.0021487. Epub 2011 Jul 18. PMID: 21789172; PMCID: PMC3138742.

Product data sheet

7. Bioactivity

Biological target: Allitinib tosylate is an EGFR and ErbB2 inhibitor with IC50s of 0.5 and 3 nM, respectively.

In vitro activity

The antiproliferative effects of AST1306 were evaluated in a panel of human cancer cell lines with varying levels of EGFR and ErbB2 expression. As shown in Fig. 5A, AST1306 effectively suppressed the proliferation of human cancer cell lines; however, the IC50 values varied widely among them. The Calu-3 lung adenocarcinoma and BT474 breast cancer cell line, containing high levels of ErbB2, were more sensitive to AST1306, with IC50 values of 0.23 and 0.97 μmol/L, respectively. In contrast, cell lines with high levels of EGFR but lower levels of ErbB2 (MDA-MB-468, A549 and NCI-H23) or high levels of both ErbB2 and EGFR (SK-OV-3) were less sensitive to AST1306, with an IC50 values ranging from 6.2 to 7.5 μmol/L. The MCF-7 cell line, which expresses low levels of both EGFR and ErbB2, was the least sensitive to AST1306, with IC50 value of 16.0 μmol/L. These results indicate that AST1306 inhibits the proliferation of human cancer cell lines in vitro, and suggest that ErbB2 expression is associated with a consistently higher sensitivity to AST1306 across the various cell lines tested.

Reference: Reference: PLoS One. 2011;6(7):e21487. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3138742/

In vivo activity

The antitumor activity of AST1306 was measured in two different human ovarian cancer xenograft nude mice models (SK-OV-3 and HO-8910), and two different human lung cancer xenograft nude mice models (Calu-3 and A549). As shown in Fig. 6A, twice daily oral administration of AST1306 caused a dramatic suppression of tumor growth in SK-OV-3 and Calu-3 xenograft models. In SK-OV-3 models, tumors almost completely disappeared after treatment with AST1306 for 7 d. In contrast, AST1306 only slightly suppressed tumor growth in HO-8910 and A549 xenograft models (Fig. 6A). These results demonstrate that the antitumor efficacy of AST1306 is greater in ErbB2-overexpressing tumor models than in models expressing low levels of ErbB2.

Reference: PLoS One. 2011;6(7):e21487. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3138742/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.