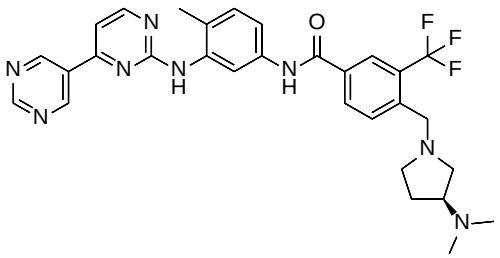
Product data sheet

MedKoo Cat#: 200316 Name: Bafetinib CAS#: 859212-16-1 Chemical Formula: $C_{30}H_{31}F_3N_8O$ Exact Mass: 576.2573 Molecular Weight: 576.61	
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:
Bafetinib, also known as INNO-406 and NS187, is an orally bioavailable 2-phenylaminopyrimidine derivative with potential antineoplastic activity. Bafetinib specifically binds to and inhibits the Bcr/Abl fusion protein tyrosine kinase, an abnormal enzyme produced by Philadelphia chromosomal translocation associated with chronic myeloid leukemia (CML). This agent also inhibits the Src-family member Lyn tyrosine kinase, upregulated in imatinib-resistant CML cells and in a variety of solid cancer cell types.

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	42.0	72.84

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	1.73 mL	8.67 mL	17.34 mL
5 mM	0.35 mL	1.73 mL	3.47 mL
10 mM	0.17 mL	0.87 mL	1.73 mL
50 mM	0.03 mL	0.17 mL	0.35 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. Grace MS, Lieu T, Darby B, Abogadie FC, Veldhuis N, Bunnett NW, McIntyre P. The tyrosine kinase inhibitor bafetinib inhibits PAR2-induced activation of TRPV4 channels in vitro and pain in vivo. Br J Pharmacol. 2014 Aug;171(16):3881-94. doi: 10.1111/bph.12750. PMID: 24779362; PMCID: PMC4128050.

In vivo study

1. Grace MS, Lieu T, Darby B, Abogadie FC, Veldhuis N, Bunnett NW, McIntyre P. The tyrosine kinase inhibitor bafetinib inhibits PAR2-induced activation of TRPV4 channels in vitro and pain in vivo. Br J Pharmacol. 2014 Aug;171(16):3881-94. doi: 10.1111/bph.12750. PMID: 24779362; PMCID: PMC4128050.

7. Bioactivity
Biological target: Bafetinib is a Lyn and Bcr-Abl tyrosine kinase inhibitor.

In vitro activity

Bafetinib (1–10 μM) concentration dependently inhibited PAR2-TRPV4 coupling. In TRPV4 HEKs, 10 μM bafetinib significantly inhibited the coupling response to SLIGRL (F340/F380 ratio 0.39 ± 0.04) and trypsin (0.52 ± 0.06) compared with vehicle control

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(0.66 ± 0.06 and 1.01 ± 0.11 respectively) ($P < 0.05$) (Figure 3). Conversely, bafetinib did not affect peak PAR2 or GSK1016790A responses ($P > 0.05$). Thus, bafetinib inhibits the signalling pathway leading to TRPV4 channel opening, downstream of PAR2 activation, most likely by blocking the activation of a tyrosine kinase.

Reference: Br J Pharmacol. 2014 Aug;171(16):3881-94. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4128050/

In vivo activity

To investigate whether tyrosine kinase activity mediates this hypersensitivity, C57BL/6 mice were treated with vehicle or bafetinib (10 mg·kg−1) by oral gavage 30 min prior to intraplantar injection of the PAR2 agonist SLIGRL into the left hind paw. von Frey mechanical pain threshold was subsequently measured at 0.5, 1, 2, 3 and 4 h after paw injection (for both the treated and non-treated paws). PAR2 activation caused marked mechanical hyperalgesia in the left paw of the vehicle-treated animals. Compared with vehicle controls, pretreatment of mice with bafetinib inhibited PAR2-induced mechanical hyperalgesia at all time points ($P < 0.05$) (Figure (Figure 7A). Unexpectedly, bafetinib also inhibited the GSK1016790A-mediated hyperalgesic response compared with controls ($P < 0.05$; Figure 6C).

Reference: Br J Pharmacol. 2014 Aug;171(16):3881-94. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4128050/