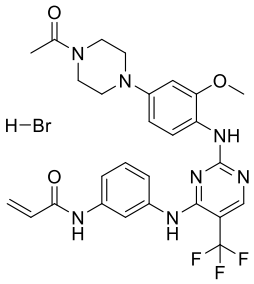
Product data sheet

MedKoo Cat#: 413217 Name: Rociletinib HBr CAS#: 1446700-26-0 (HBr) Chemical Formula: $C_{27}H_{29}BrF_3N_7O_3$ Molecular Weight: 636.47	
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:

Rociletinib HBr is the salt form of Rociletinib, also known as AVL-301 and CO-1686, an orally available small molecule, irreversible inhibitor of epidermal growth factor receptor (EGFR) with potential antineoplastic activity. Rociletinib binds to and inhibits mutant forms of EGFR, including T790M, thereby leading to cell death of resistant tumor cells. Rociletinib inhibits T790M, a secondary acquired resistance mutation, as well as other mutant EGFRs and may have therapeutic benefits in tumors with T790M-mediated resistance to other EGFR tyrosine kinase inhibitors.

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
To be determined	To be determined	To be determined

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	1.57 mL	7.86 mL	15.71 mL
5 mM	0.31 mL	1.57 mL	3.14 mL
10 mM	0.16 mL	0.79 mL	1.57 mL
50 mM	0.03 mL	0.16 mL	0.31 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. Walter AO, Sjin RT, Haringsma HJ, Ohashi K, Sun J, Lee K, Dubrovskiy A, Labenski M, Zhu Z, Wang Z, Sheets M, St Martin T, Karp R, van Kalken D, Chaturvedi P, Niu D, Nacht M, Petter RC, Westlin W, Lin K, Jaw-Tsai S, Raponi M, Van Dyke T, Etter J, Weaver Z, Pao W, Singh J, Simmons AD, Harding TC, Allen A. Discovery of a mutant-selective covalent inhibitor of EGFR that overcomes T790M-mediated resistance in NSCLC. Cancer Discov. 2013 Dec;3(12):1404-15. doi: 10.1158/2159-8290.CD-13-0314. Epub 2013 Sep 24. PMID: 24065731; PMCID: PMC4048995.

In vivo study

1. Sequist LV, Soria JC, Goldman JW, Wakelee HA, Gadgeel SM, Varga A, Papadimitrakopoulou V, Solomon BJ, Oxnard GR, Dziadziuszko R, Aisner DL, Doebele RC, Galasso C, Garon EB, Heist RS, Logan J, Neal JW, Mendenhall MA, Nichols S, Piotrowska Z, Wozniak AJ, Raponi M, Karlovich CA, Jaw-Tsai S, Isaacson J, Despain D, Matheny SL, Rolfe L, Allen AR, Camidge DR. Rociletinib in EGFR-mutated non-small-cell lung cancer. N Engl J Med. 2015 Apr 30;372(18):1700-9. doi: 10.1056/NEJMoa1413654. PMID: 25923550.
2. Walter AO, Sjin RT, Haringsma HJ, Ohashi K, Sun J, Lee K, Dubrovskiy A, Labenski M, Zhu Z, Wang Z, Sheets M, St Martin T, Karp R, van Kalken D, Chaturvedi P, Niu D, Nacht M, Petter RC, Westlin W, Lin K, Jaw-Tsai S, Raponi M, Van Dyke T, Etter J, Weaver Z, Pao W, Singh J, Simmons AD, Harding TC, Allen A. Discovery of a mutant-selective covalent inhibitor of EGFR that

overcomes T790M-mediated resistance in NSCLC. Cancer Discov. 2013 Dec;3(12):1404-15. doi: 10.1158/2159-8290.CD-13-0314. Epub 2013 Sep 24. PMID: 24065731; PMCID: PMC4048995.

7. Bioactivity

Biological target:

Rociletinib HBr specifically targets the mutant forms of EGFR including T790M. The Ki values for EGFRL858R/T790M and EGFR wild type are 21.5 nM and 303.3 nM, respectively.

In vitro activity

In on-small cell lung cancer cells with acquired resistance to rociletinib in vitro, there was no evidence of additional mutations or amplification of the EGFR gene, but resistant cells exhibited signs of epithelial-mesenchymal transition and demonstrated increased sensitivity to AKT inhibitors.

Reference: Cancer Discov. 2013 Dec;3(12):1404-15. https://pubmed.ncbi.nlm.nih.gov/24065731/

In vivo activity

Oral administration of rociletinib as single agent induces tumor regression in EGFR-mutated non-small cell lung cancer tumor xenograft and transgenic models. Rociletinib potentially offers potent inhibition of mutant EGFR while avoiding the on-target toxicity observed with inhibiting the wild type EGFR.

Reference: Cancer Discov. 2013 Dec;3(12):1404-15. https://pubmed.ncbi.nlm.nih.gov/24065731/

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.