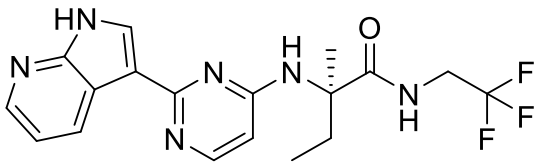
Product data sheet

MedKoo Cat#: 206134 Name: Decernotinib (VX-509) CAS#: 944842-54-0 Chemical Formula: $C_{18}H_{19}F_3N_6O$ Exact Mass: 392.15724 Molecular Weight: 392.38	
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:
Decernotinib, also known as VX-509 or VRT-831509 or adelatinib, is an oral, selective Janus kinase 3 (JAK3) inhibitor being developed by Vertex. VX-509 may represent a new approach to treating an underlying disease mechanism that triggers inflammation in a number of debilitating diseases, including RA. In immune-mediated diseases, JAK3 is an essential component of the immune signaling cascade. This cascade ultimately contributes to abnormal immune response that results in chronic inflammation and, in the case of RA, irreversible damage to cartilage and bones.

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	64.0	163.11

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.55 mL	12.74 mL	25.49 mL
5 mM	0.51 mL	2.55 mL	5.10 mL
10 mM	0.25 mL	1.27 mL	2.55 mL
50 mM	0.05 mL	0.25 mL	0.51 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. Mahajan S, Hogan JK, Shlyakhter D, Oh L, Salituro FG, Farmer L, Hoock TC. VX-509 (decernotinib) is a potent and selective janus kinase 3 inhibitor that attenuates inflammation in animal models of autoimmune disease. J Pharmacol Exp Ther. 2015 May;353(2):405-14. doi: 10.1124/jpet.114.221176. Epub 2015 Mar 11. PMID: 25762693.

In vivo study

1. Mahajan S, Hogan JK, Shlyakhter D, Oh L, Salituro FG, Farmer L, Hoock TC. VX-509 (decernotinib) is a potent and selective janus kinase 3 inhibitor that attenuates inflammation in animal models of autoimmune disease. J Pharmacol Exp Ther. 2015 May;353(2):405-14. doi: 10.1124/jpet.114.221176. Epub 2015 Mar 11. PMID: 25762693.
2. DeMars KM, Pacheco SC, Yang C, Siwarski DM, Candelario-Jalil E. Selective Inhibition of Janus Kinase 3 Has No Impact on Infarct Size or Neurobehavioral Outcomes in Permanent Ischemic Stroke in Mice. Front Neurol. 2017 Jul 25;8:363. doi: 10.3389/fneur.2017.00363. PMID: 28790974; PMCID: PMC5524742.

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7. Bioactivity

Biological target:

Decernotinib is a potent, orally active JAK3 inhibitor, with Kis of 2.5, 11, 13 and 11 nM for JAK3, JAK1, JAK2, and TYK2, respectively.

In vitro activity

The aim of this study was to evaluate the potency and selectivity of the investigational JAK3 inhibitor VX-509 (decernotinib) [(R)-2-((2-(1H-pyrrolo[2,3-b]pyridin-3-yl)pyrimidin-4-yl)amino)-2-methyl-N-(2,2,2-trifluoroethyl)butanamide] against JAK3 kinase activity and inhibition of JAK3-mediated signaling in vitro. hese results demonstrate that VX-509 potently inhibits JAK3 in enzyme assays (Ki = 2.5 nM + 0.7 nM) and cellular assays dependent on JAK3 activity (IC50 range, 50-170 nM), with limited or no measurable potency against other JAK isotypes or non-JAK kinases. These findings demonstrate that VX-509 is a selective and potent inhibitor of JAK3 in vitro.

Reference: J Pharmacol Exp Ther. 2015 May;353(2):405-14. https://pubmed.ncbi.nlm.nih.gov/25762693/

In vivo activity

VX-509 also showed activity in two animal models of aberrant immune function. VX-509 treatment resulted in dose-dependent reduction in ankle swelling and paw weight and improved paw histopathology scores in the rat collagen-induced arthritis model. In a mouse model of oxazolone-induced delayed-type hypersensitivity, VX-509 reduced the T cell-mediated inflammatory response in skin. The data support evaluation of VX-509 for treatment of patients with autoimmune and inflammatory diseases such as rheumatoid arthritis.

Reference: J Pharmacol Exp Ther. 2015 May;353(2):405-14. https://pubmed.ncbi.nlm.nih.gov/25762693/

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.