

# Product data sheet



MedKoo Cat#: 471045 Name: Mavorixafor free base CAS: 558447-26-0 (free base) Chemical Formula: C <sub>21</sub> H <sub>27</sub> N <sub>5</sub> Exact Mass: 349.2266 Molecular Weight: 349.482	
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:

Mavorixafor, also known as AMD11070, AMD070, X4P-001, is an orally bioavailable and potent CXCR4 inhibitor. AMD11070 is an antagonist of SDF-1 $\alpha$  ligand binding (IC<sub>50</sub> = 12.5  $\pm$  1.3 nM), inhibits SDF-1 mediated calcium flux (IC<sub>50</sub> = 9.0  $\pm$  2.0 nM) and SDF-1 $\alpha$  mediated activation of the CXCR4 receptor as measured by a Eu-GTP binding assay (IC<sub>50</sub> = 39.8  $\pm$  2.5 nM) or a [(35S)]-GTP $\gamma$ S binding assay (IC<sub>50</sub> = 19.0  $\pm$  4.1 nM), and inhibits SDF-1 $\alpha$  stimulated chemotaxis (IC<sub>50</sub> = 19.0  $\pm$  4.0 nM). AMD11070 abrogates melanoma cell migration and is significantly more effective than AMD3100. AMD11070 represents a novel therapeutic strategy for both B-RAF wild-type and mutated melanomas.

## 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
TBD	TBD	TBD

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.86 mL	14.31 mL	28.61 mL
5 mM	0.57 mL	2.86 mL	5.72 mL
10 mM	0.29 mL	1.43 mL	2.86 mL
50 mM	0.06 mL	0.29 mL	0.57 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. Zmajkovicova K, Pawar S, Maier-Munsa S, Maierhofer B, Wiest I, Skerlj R, Taveras AG, Badarau A. Genotype-phenotype correlations in WHIM syndrome: a systematic characterization of CXCR4WHIM variants. *Genes Immun.* 2022 Sep;23(6):196-204. doi: 10.1038/s41435-022-00181-9. Epub 2022 Sep 12. PMID: 36089616; PMCID: PMC9519442.

2. Skerlj RT, Bridger GJ, Kaller A, McEachern EJ, Crawford JB, Zhou Y, Atsma B, Langille J, Nan S, Veale D, Wilson T, Harwig C, Hatse S, Princen K, De Clercq E, Schols D. Discovery of novel small molecule orally bioavailable C-X-C chemokine receptor 4 antagonists that are potent inhibitors of T-tropic (X4) HIV-1 replication. *J Med Chem.* 2010 Apr 22;53(8):3376-88. doi: 10.1021/jm100073m. PMID: 20297846.

### In vivo study

1. Uchida D, Kuribayashi N, Kinouchi M, Sawatani Y, Shimura M, Mori T, Hasegawa T, Miyamoto Y, Kawamata H. Effect of a novel orally bioavailable CXCR4 inhibitor, AMD070, on the metastasis of oral cancer cells. *Oncol Rep.* 2018 Jul;40(1):303-308. doi: 10.3892/or.2018.6400. Epub 2018 Apr 25. PMID: 29749473.

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2. Chow LN, Schreiner P, Ng BY, Lo B, Hughes MR, Scott RW, Gusti V, Lecour S, Simonson E, Manisali I, Barta I, McNagny KM, Crawford J, Webb M, Underhill TM. Impact of a CXCL12/CXCR4 Antagonist in Bleomycin (BLM) Induced Pulmonary Fibrosis and Carbon Tetrachloride (CCl4) Induced Hepatic Fibrosis in Mice. PLoS One. 2016 Mar 21;11(3):e0151765. doi: 10.1371/journal.pone.0151765. PMID: 26998906; PMCID: PMC4801399.

## 7. Bioactivity

### Biological target:

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Mavorixafor, also known as AMD11070, AMD070, X4P-001, is an orally bioavailable and potent CXCR4 inhibitor.

### In vitro activity

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As a result of lead optimization, this study identified (S)-N'-((1H-benzo[d]imidazol-2-yl)methyl)-N'-(5,6,7,8-tetrahydroquinolin-8-yl)butane-1,4-diamine (AMD070) 2 as a potent and selective antagonist of CXCR4 with an IC(50) value of 13 nM in a CXCR4 125I-SDF inhibition binding assay. Compound 2 inhibited the replication of T-tropic HIV-1 (NL4.3 strain) in MT-4 cells and PBMCs with an IC(50) of 2 and 26 nM, respectively, while remaining noncytotoxic to cells at concentrations exceeding 23 microM.

Reference: J Med Chem. 2010 Apr 22;53(8):3376-88. <https://pubmed.ncbi.nlm.nih.gov/20297846/>

### In vivo activity

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The current study evaluated AMD070, an orally bioavailable inhibitor of CXCL12/CXCR4 in alleviating BLM-induced pulmonary and CCl4-induced hepatic fibrosis in mice. Similar to other CXCR4 antagonists, treatment with AMD070 significantly increased leukocyte mobilization. However, in these two models of fibrosis, AMD070 had a negligible impact on extracellular matrix deposition.

Reference: PLoS One. 2016 Mar 21;11(3):e0151765. <https://pubmed.ncbi.nlm.nih.gov/26998906/>

*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.*