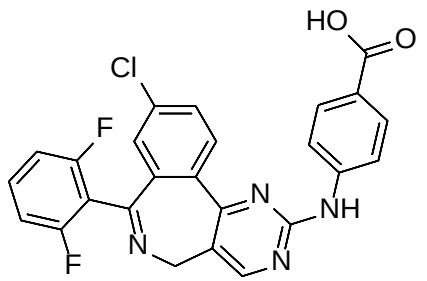
Product data sheet

MedKoo Cat#: 201930 Name: MLN8054 CAS: 869363-13-3 Chemical Formula: $C_{25}H_{15}ClF_2N_4O_2$ Exact Mass: 476.0852 Molecular Weight: 476.8678	
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:

MLN8054 is an aurora kinase inhibitor MLN8054, which is an orally bioavailable, highly selective small molecule inhibitor of the serine/threonine protein kinase Aurora A kinase with potential antineoplastic activity. Auora kinase inhibitor MLN8054 binds to and inhibits Aurora kinase A, resulting in disruption of the assembly of the mitotic spindle apparatus, disruption of chromosome segregration, and inhibition of cell proliferation. Aurora A localizes in mitosis to the spindle poles and to spindle microtubules and is thought to regulate spindle assembly. Aberrant expression of Aurora kinases occurs in a wide variety of cancers, including colon and breast cancers. Check for active clinical trials or closed clinical trials using this agent. (NCI Thesaurus).

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	57.92	121.45

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.10 mL	10.49 mL	20.97 mL
5 mM	0.42 mL	2.10 mL	4.19 mL
10 mM	0.21 mL	1.05 mL	2.10 mL
50 mM	0.04 mL	0.21 mL	0.42 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. Kaestner P, Stolz A, Bastians H. Determinants for the efficiency of anticancer drugs targeting either Aurora-A or Aurora-B kinases in human colon carcinoma cells. Mol Cancer Ther. 2009 Jul;8(7):2046-56. doi: 10.1158/1535-7163.MCT-09-0323. Epub 2009 Jul 7. PMID: 19584233.

2. LeRoy PJ, Hunter JJ, Hoar KM, Burke KE, Shinde V, Ruan J, Bowman D, Galvin K, Ecsedy JA. Localization of human TACC3 to mitotic spindles is mediated by phosphorylation on Ser558 by Aurora A: a novel pharmacodynamic method for measuring Aurora A activity. Cancer Res. 2007 Jun 1;67(11):5362-70. doi: 10.1158/0008-5472.CAN-07-0122. PMID: 17545617.

In vivo study

1. Moretti L, Niermann K, Schleicher S, Giacalone NJ, Varki V, Kim KW, Kopsombut P, Jung DK, Lu B. MLN8054, a small molecule inhibitor of aurora kinase a, sensitizes androgen-resistant prostate cancer to radiation. Int J Radiat Oncol Biol Phys. 2011 Jul 15;80(4):1189-97. doi: 10.1016/j.ijrobp.2011.01.060. Epub 2011 Apr 20. PMID: 21514073.

2. Manfredi MG, Ecsedy JA, Meetze KA, Balani SK, Burenkova O, Chen W, Galvin KM, Hoar KM, Huck JJ, LeRoy PJ, Ray ET, Sells TB, Stringer B, Stroud SG, Vos TJ, Weatherhead GS, Wysong DR, Zhang M, Bolen JB, Claiborne CF. Antitumor activity of

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MLN8054, an orally active small-molecule inhibitor of Aurora A kinase. Proc Natl Acad Sci U S A. 2007 Mar 6;104(10):4106-11. doi: 10.1073/pnas.0608798104. Epub 2007 Feb 23. PMID: 17360485; PMCID: PMC1820716.

7. Bioactivity

Biological target:

MLN8054 is a potent, selective and orally available aurora A kinase inhibitor with an IC_{50} of 4 nM.

In vitro activity

By using various isogenic knockout as well as inducible colon carcinoma cell lines, this study found that treatment with MLN8054 induces defects in mitotic spindle assembly, which causes a transient spindle checkpoint-dependent mitotic arrest. This cell cycle arrest is not maintained due to the activity of MLN8054 to override the spindle checkpoint. Subsequently, MLN8054-treated cells exit from mitosis and activate a p53-dependent postmitotic G(1) checkpoint, which subsequently induces p21 and Bax, leading to G(1) arrest followed by the induction of apoptosis.

Reference: Mol Cancer Ther. 2009 Jul;8(7):2046-56. https://pubmed.ncbi.nlm.nih.gov/19584233/

In vivo activity

In vivo, the addition of MLN8054 (30 mg/kg/day) to radiation in mouse prostate cancer xenografts (PC3 cells) significantly increased tumor growth delay and apoptosis (caspase-3 staining), with reduction in cell proliferation (Ki67 staining) and vascular density (von Willebrand factor staining).

Reference: Int J Radiat Oncol Biol Phys. 2011 Jul 15;80(4):1189-97. https://pubmed.ncbi.nlm.nih.gov/21514073/

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.