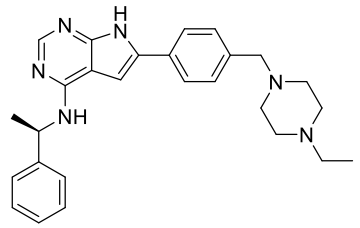
Product data sheet

MedKoo Cat#: 200100 Name: AEE-788 CAS#: 497839-62-0 Chemical Formula: $C_{27}H_{32}N_6$ Exact Mass: 440.26885 Molecular Weight: 440.58	
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:

AEE-788 is an orally bioavailable multiple-receptor tyrosine kinase inhibitor. AEE788 inhibits phosphorylation of the tyrosine kinases of epidermal growth factor receptor (EGFR), human epidermal growth factor receptor 2 (HER2), and vascular endothelial growth factor receptor 2 (VEGF2), resulting in receptor inhibition, the inhibition of cellular proliferation, and induction of tumor cell and tumor-associated endothelial cell apoptosis. 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	51.77	117.50
DMSO:PBS (pH 7.2) (1:3)	0.25	0.57
DMF	25.0	56.74
Ethanol	5.0	11.35

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.27 mL	11.35 mL	22.70 mL
5 mM	0.45 mL	2.27 mL	4.54 mL
10 mM	0.23 mL	1.13 mL	2.27 mL
50 mM	0.05 mL	0.23 mL	0.45 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. Barbarroja N, Torres LA, Rodriguez-Ariza A, Valverde-Estepa A, Lopez-Sanchez LM, Ruiz-Limon P, Perez-Sanchez C, Carretero RM, Velasco F, López-Pedrera C. AEE788 is a vascular endothelial growth factor receptor tyrosine kinase inhibitor with antiproliferative and proapoptotic effects in acute myeloid leukemia. Exp Hematol. 2010 Aug;38(8):641-52. doi: 10.1016/j.exphem.2010.03.017. Epub 2010 Apr 7. PMID: 20380868.
2. Venkatesan P, Das S, Krishnan MM, Chakraborty C, Chaudhury K, Mandal M. Effect of AEE788 and/or Celecoxib on colon cancer cell morphology using advanced microscopic techniques. Micron. 2010 Apr;41(3):247-56. doi: 10.1016/j.micron.2009.10.008. Epub 2009 Nov 10. PMID: 19945288.

In vivo study

Product data sheet

1. Meco D, Servidei T, Zannoni GF, Martinelli E, Prisco MG, de Waure C, Riccardi R. Dual Inhibitor AEE788 Reduces Tumor Growth in Preclinical Models of Medulloblastoma. Transl Oncol. 2010 Oct 1;3(5):326-35. doi: 10.1593/tlo.10163. PMID: 20885895; PMCID: PMC2935636.
2. Deng M, Huang H, Jin H, Dirsch O, Dahmen U. The anti-proliferative side effects of AEE788, a tyrosine kinase inhibitor blocking both EGF- and VEGF-receptor, are liver-size-dependent after partial hepatectomy in rats. Invest New Drugs. 2011 Aug;29(4):593-606. doi: 10.1007/s10637-010-9394-6. Epub 2010 Feb 12. PMID: 20148349.

7. Bioactivity

Biological target:

AEE788 is an inhibitor of the EGFR and ErbB2 with IC50 values of 2 and 6 nM, respectively.

In vitro activity

This study analyzed the ability of AEE788 to induce apoptosis using Annexin-V and propidium iodide by flow cytometric analysis. THP-1, MOLM-13, and MV4-11 cell lines were treated in vitro with different concentrations of AEE788 for 48 hours. AEE788 induced apoptosis of the AML cells in a dose-dependent manner (Fig. 1A). An apoptosis response of 50% was induced at a concentration of 10 μM for MOLM-13 and MV4-11, and of 15 μM for THP-1 cells.

Reference: Exp Hematol. 2010 Aug;38(8):641-52. https://pubmed.ncbi.nlm.nih.gov/20380868/

In vivo activity

This study compared the antitumor activity of AEE788 against Daoy, $Daoy^{Pt}$, $Daoy^{HER2}$, and $Daoy^{V}$ xenografts. AEE788 caused a statistically significant reduction in tumor volume of Daoy and $Daoy^{Pt}$ xenografts, with a TVI of 51% and 45%, respectively (Figure 4, *A* and *B*). $Daoy^{V}$ xenografts behaved as Daoy (data not shown). On the $Daoy^{HER2}$ xenografts, AEE788 induced a more pronounced tumor inhibition (TVI = 72%; Figure 4*C*). All the mice survived until the end of the 4-week treatment period, with a less than 15% body weight loss at worst, which was partially recovered by the end of the experiment (Figure 4, *D–F*).

Reference: Transl Oncol. 2010 Oct; 3(5): 326–335. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2935636/

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.