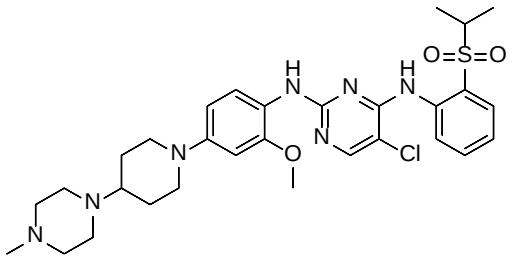
Product data sheet

MedKoo Cat#: 202045 Name: TAE684 CAS#: 761439-42-3 Chemical Formula: $C_{30}H_{40}ClN_7O_3S$ Exact Mass: 613.2602 Molecular Weight: 614.20	
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:
TAE684, also known as NVP-TAE684, is a highly potent and selective small-molecule ALK inhibitor, which blocked the growth of ALCL-derived and ALK-dependent cell lines with IC(50) values between 2 and 10 nM . TAE684 is also a potent inhibitor of LRRK2 kinase activity (IC(50) of 7.8nM against wild-type LRRK2, 6.1nM against the G2019S mutant).

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	6.90	11.23
DMF	20.0	32.56
DMF:PBS (pH 7.2) (1:1)	0.50	0.81

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	1.63 mL	8.14 mL	16.28 mL
5 mM	0.33 mL	1.63 mL	3.26 mL
10 mM	0.16 mL	0.81 mL	1.63 mL
50 mM	0.03 mL	0.16 mL	0.33 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. Galkin AV, Melnick JS, Kim S, Hood TL, Li N, Li L, Xia G, Steensma R, Chopiuk G, Jiang J, Wan Y, Ding P, Liu Y, Sun F, Schultz PG, Gray NS, Warmuth M. Identification of NVP-TAE684, a potent, selective, and efficacious inhibitor of NPM-ALK. Proc Natl Acad Sci U S A. 2007 Jan 2;104(1):270-5. doi: 10.1073/pnas.0609412103. Epub 2006 Dec 21. Proc Natl Acad Sci U S A. 2007 Feb 6;104(6):2025. PMID: 17185414; PMCID: PMC1765448.

In vivo study

1. Galkin AV, Melnick JS, Kim S, Hood TL, Li N, Li L, Xia G, Steensma R, Chopiuk G, Jiang J, Wan Y, Ding P, Liu Y, Sun F, Schultz PG, Gray NS, Warmuth M. Identification of NVP-TAE684, a potent, selective, and efficacious inhibitor of NPM-ALK. Proc Natl Acad Sci U S A. 2007 Jan 2;104(1):270-5. doi: 10.1073/pnas.0609412103. Epub 2006 Dec 21. Proc Natl Acad Sci U S A. 2007 Feb 6;104(6):2025. PMID: 17185414; PMCID: PMC1765448.

7. Bioactivity
Biological target: NVP-TAE 684 (TAE 684) is an ALK inhibitor which blocks the growth of ALCL-derived and ALK-dependent cell lines with IC50 values between 2 and 10 nM.

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In vitro activity

As shown in Fig. 4 C and D, TAE684 induced G1 phase arrest in a time-dependent manner. After 72 h of treatment with TAE684 (25 nM), 72% of Karpas-299 cells were arrested in G1 phase compared with 26% of cells in G1 phase in DMSO-treated controls. The number of cells in S phase was reduced from 60% to 14% (Fig. 4 C and D). Collectively, these data suggest that TAE684 inhibits the growth of ALCL (anaplastic large-cell lymphomas) cells by both inhibiting the progression of cell cycle and induction of apoptosis.

Reference: Proc Natl Acad Sci U S A. 2007 Feb 6;104(6):2025. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1765448/

In vivo activity

TAE684 was administered at 1, 3, and 10 mg/kg once daily by oral gavage to mice starting 72 h after Karpas-299 i.v. injection. After 2 weeks of treatment, a 100-fold reduction in bioluminescence signal was observed in the 3- and 10-mg/kg treatment groups. Although the compound was not efficacious at 1 mg/kg, after 4 weeks of treatment with TAE684 at 3 and 10 mg/kg, there was a significant (P = 0.005) delay in lymphoma development and 100- to 1,000-fold reduction in luminescence signal (Fig. 5 B–D).

Reference: Proc Natl Acad Sci U S A. 2007 Feb 6;104(6):2025. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC1765448/