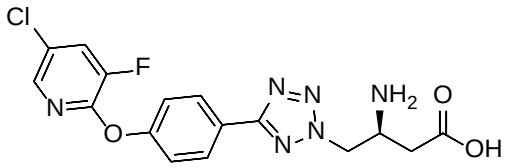
Product data sheet

MedKoo Cat#: 555854 Name: LYS-006 CAS: 1799681-85-8 Chemical Formula: $C_{16}H_{14}ClFN_6O_3$ Exact Mass: 392.08 Molecular Weight: 392.7754	
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:
LYS-006 is a Leukotriene A4 hydrolase (LTA4H) inhibitor for the treatment of Hidradenitis Suppurativa.

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	100.0	254.60

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.55 mL	12.73 mL	25.46 mL
5 mM	0.51 mL	2.55 mL	5.09 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. Markert C, Thoma G, Srinivas H, Bollbuck B, Lüönd RM, Miltz W, Wälchli R, Wolf R, Hinrichs J, Bergsdorf C, Azzaoui K, Penno CA, Klein K, Wack N, Jäger P, Hasler F, Beerli C, Loetscher P, Dawson J, Wieczorek G, Numao S, Littlewood-Evans A, Röhn TA. Discovery of LYS006, a Potent and Highly Selective Inhibitor of Leukotriene A4 Hydrolase. J Med Chem. 2021 Feb 25;64(4):1889-1903. doi: 10.1021/acs.jmedchem.0c01955. Epub 2021 Feb 16. PMID: 33592148.

In vivo study

1. Markert C, Thoma G, Srinivas H, Bollbuck B, Lüönd RM, Miltz W, Wälchli R, Wolf R, Hinrichs J, Bergsdorf C, Azzaoui K, Penno CA, Klein K, Wack N, Jäger P, Hasler F, Beerli C, Loetscher P, Dawson J, Wieczorek G, Numao S, Littlewood-Evans A, Röhn TA. Discovery of LYS006, a Potent and Highly Selective Inhibitor of Leukotriene A4 Hydrolase. J Med Chem. 2021 Feb 25;64(4):1889-1903. doi: 10.1021/acs.jmedchem.0c01955. Epub 2021 Feb 16. PMID: 33592148.

7. Bioactivity
Biological target:

LTA4H-IN-1 is a potent inhibitor of leukotriene A4 hydrolase (LTA4H).

In vitro activity

This study discloses the discovery and preclinical profile of LYS006, a highly potent and selective LTA4H inhibitor. A focused fragment screen identified hits that could be cocrystallized with LTA4H and inspired a fragment merging.

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Reference: J Med Chem. 2021 Feb 25;64(4):1889-1903. https://pubmed.ncbi.nlm.nih.gov/33592148/

In vivo activity

Further optimization led to chiral amino acids and ultimately to LYS006, a picomolar LTA4H inhibitor with exquisite whole blood potency and long-lasting pharmacodynamic effects. Due to its high selectivity and its ability to fully suppress LTB4 generation at low exposures in vivo, LYS006 has the potential for a best-in-class LTA4H inhibitor and is currently investigated in phase II clinical trials in inflammatory acne, hidradenitis suppurativa, ulcerative colitis, and NASH.

Reference: J Med Chem. 2021 Feb 25;64(4):1889-1903. https://pubmed.ncbi.nlm.nih.gov/33592148/