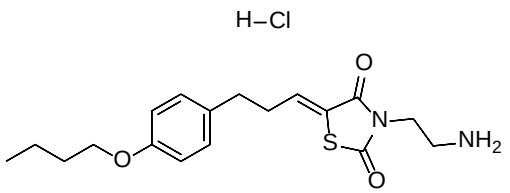
Product data sheet

MedKoo Cat#: 558222 Name: K145 HCl salt CAS#: 1449240-68-9 (HCl) Chemical Formula: $C_{18}H_{24}N_2O_3S$ Exact Mass: 348.1508 Molecular Weight: 348.46	
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:
K145 is a selective sphingosine kinase-2 (SphK2) inhibitor and anticancer agent. K145 inhibited the activity of SphK2 in a dose-dependent manner with an IC50 of 4.30Â±0.06 ÂµM. K145 also exhibited inhibitory effects on the growth of U937 cells as well as apoptotic effects in U937 cells. K145 exhibits comparable in vivo anti-tumor activity to tamibarotene, while concomitantly exhibiting less toxicity in this U937 xenograft cancer model.

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
Water	126.70	363.60
DMSO	30.0	86.09
DMSO:PBS (pH 7.2) (1:1)	0.50	1.43
DMF	10.0	28.70

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.87 mL	14.35 mL	28.70 mL
5 mM	0.57 mL	2.87 mL	5.74 mL
10 mM	0.29 mL	1.43 mL	2.87 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. Shi Y, Qiao J, Mu B, Zuo B, Yuan J. 3-(2-amino-ethyl)-5-[3-(4-butoxyl-phenyl)-propylidene]-thiazolidine-2,4-dione (K145) ameliorated dexamethasone induced hepatic gluconeogenesis through activation of Akt/FoxO1 pathway. Biochem Biophys Res Commun. 2017 Nov 4;493(1):286-290. doi: 10.1016/j.bbrc.2017.09.029. Epub 2017 Sep 11. PMID: 28911865.
2. Liu K, Guo TL, Hait NC, Allegood J, Parikh HI, Xu W, Kellogg GE, Grant S, Spiegel S, Zhang S. Biological characterization of 3-(2-amino-ethyl)-5-[3-(4-butoxyl-phenyl)-propylidene]-thiazolidine-2,4-dione (K145) as a selective sphingosine kinase-2 inhibitor and anticancer agent. PLoS One. 2013;8(2):e56471. doi: 10.1371/journal.pone.0056471. Epub 2013 Feb 20. PMID: 23437140; PMCID: PMC3577900.

In vivo study

1. Shi Y, Qiao J, Mu B, Zuo B, Yuan J. 3-(2-amino-ethyl)-5-[3-(4-butoxyl-phenyl)-propylidene]-thiazolidine-2,4-dione (K145) ameliorated dexamethasone induced hepatic gluconeogenesis through activation of Akt/FoxO1 pathway. Biochem Biophys Res Commun. 2017 Nov 4;493(1):286-290. doi: 10.1016/j.bbrc.2017.09.029. Epub 2017 Sep 11. PMID: 28911865.

Product data sheet

2. Liu K, Guo TL, Hait NC, Allegood J, Parikh HI, Xu W, Kellogg GE, Grant S, Spiegel S, Zhang S. Biological characterization of 3-(2-amino-ethyl)-5-[3-(4-butoxyl-phenyl)-propylidene]-thiazolidine-2,4-dione (K145) as a selective sphingosine kinase-2 inhibitor and anticancer agent. PLoS One. 2013;8(2):e56471. doi: 10.1371/journal.pone.0056471. Epub 2013 Feb 20. PMID: 23437140; PMCID: PMC3577900.

7. Bioactivity

Biological target: K145 hydrochloride is a SphK2 inhibitor with an IC50 of 4.3 μM.

In vitro activity

The anti-proliferative and apoptotic effects of K145 in U937 cells were evaluated. As shown in Figure 6A, K 145 significantly inhibited the growth of U937 cells cultured in the presence of 10% serum in a concentration-dependent manner. K145 also significantly induced apoptosis in U937 cells under these experimental conditions (Figure 6B). Notably, K145 induced mainly late apoptosis with a very small percentage of necrotic cells after 24 h treatment in the presence of 10% serum.

Reference: PLoS One. 2013;8(2):e56471. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3577900/

In vivo activity

The anticancer activity of K145 to inhibit the tumor growth of U937 cells was examined in nude mice (BALB/c-nu) by oral administration. As shown in Figure 10A, tumor weights of K145-treated mice were significantly less than that in vehicle-treated mice and K145 exhibited antitumor activity (TGI for K145 was 51.25%). Visual examination of the tumor samples also confirmed the significant inhibition of U937 tumor growth by K145 (Figure 10B-C). Collectively, the results of in vivo studies with K145 by oral administration demonstrated that K145 is orally available to inhibit the growth of U937 tumors at 50 mg/kg dose.

Reference: PLoS One. 2013;8(2):e56471. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3577900/