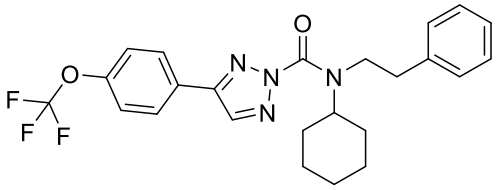
Product data sheet

MedKoo Cat#: 562277 Name: KLH45 CAS: 1632236-44-2 Chemical Formula: $C_{24}H_{25}F_3N_4O_2$ Exact Mass: 458.193 Molecular Weight: 458.4852	
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:
KLH45 is a selective inhibitor of DDHD2 (DDHD domain containing 2).

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	30.0	65.43
Ethanol	30.0	65.43

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.18 mL	10.91 mL	21.81 mL
5 mM	0.44 mL	2.18 mL	4.36 mL
10 mM	0.22 mL	1.09 mL	2.18 mL
50 mM	0.04 mL	0.22 mL	0.44 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. Inloes JM, Kiosses WB, Wang H, Walther TC, Farese RV Jr, Cravatt BF. Functional Contribution of the Spastic Paraplegia-Related Triglyceride Hydrolase DDHD2 to the Formation and Content of Lipid Droplets. Biochemistry. 2018 Feb 6;57(5):827-838. doi: 10.1021/acs.biochem.7b01028. Epub 2017 Dec 26. PMID: 29278326; PMCID: PMC5854151.

In vivo study

1. Inloes JM, Hsu KL, Dix MM, Viader A, Masuda K, Takei T, Wood MR, Cravatt BF. The hereditary spastic paraplegia-related enzyme DDHD2 is a principal brain triglyceride lipase. Proc Natl Acad Sci U S A. 2014 Oct 14;111(41):14924-9. doi: 10.1073/pnas.1413706111. Epub 2014 Sep 29. PMID: 25267624; PMCID: PMC4205627.

7. Bioactivity
Biological target:

KLH45 is a potent and selective DDHD2 inhibitor, with an IC_{50} of 1.3 nM.

In vitro activity

This study first confirmed inhibition of WT DDHD2 by treating transfected COS-7 cells with a concentration range of KLH45 (or KLH40) for 16 h, followed by ABPP with the DDHD2 probe HT-01 or the general serine hydrolase probe fluorophosphonate

rhodamine (FP-Rh). This experiment revealed that KLH45, but not KLH40, selectively blocked DDHD2 activity, with complete inhibition being observed with 2 μM KLH45 (Figure S5).

Reference: Biochemistry. 2018 Feb 6;57(5):827-838. https://pubmed.ncbi.nlm.nih.gov/29278326/

In vivo activity

In contrast, mice treated twice daily with KLH45 (20 $mg \cdot kg^{-1}$; administered every 12 h) for a total of 4 d exhibited significant elevations in several of the TAGs that accumulated in the brains of $DDHD2^{-/-}$ mice (Fig. 5*B* and *SI Appendix*, Fig. S13*B*).

Reference: Proc Natl Acad Sci U S A. 2014 Oct 14;111(41):14924-9. https://pubmed.ncbi.nlm.nih.gov/25267624/

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.