

Product Data Sheet

Product Name: XMD17-109

Cat. No.: GC12691

Chemical Properties

Cas. No. 1435488-37-1

SMILES CN1CCN(C2CCN(C(C3=CC(OCC)=C(NC4=NC=C5C(N(C6CCCC6)C(C=CC=C7)=C7C(N5C)=O)=N4)C=C3)=O)CC2)CC1

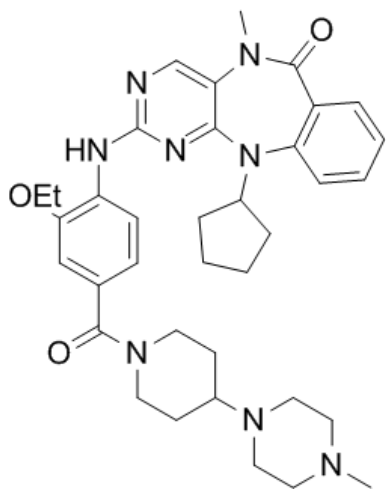
Formula $C_{36}H_{46}N_8O_3$ M.Wt 638.8

Solubility ≥ 31.95 mg/mL in DMSO, ≥ 86.6 mg/mL in EtOH Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

Caution: Product has not been fully validated for medical applications. For research use only.

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Cell experiment: HeLa cells are maintained in DMEM supplemented with 10% FBS, 2 mM L-glutamine, 50 U/mL penicillin G, and 50 µg/mL streptomycin. Before use HeLa cells are serum starved for 16 h in DMEM supplemented with 2 mM L-glutamine, 50 U/mL penicillin G, and 50 µg/mL streptomycin. HeLa cells are then incubated with ERK5-IN-1 at the indicated concentrations for 1 h prior to stimulation with 0.5mol/L sorbitol for 30 min. Cells are lysed in Triton lysis buffer (50 mM Tris-HCl, pH 7.5, 1 mM EGTA, 1 mM EDTA, 1 mM sodium orthovanadate, 50 mM sodium fluoride, 1 mM sodium pyrophosphate, 0.27mol/L sucrose, 1 µM microcystin-LR, 1% (v/v) Triton X-100, 0.1% (v/v) 2-mercaptoethanol) and 20 µg of protein loaded per well. Samples are run on 8% polyacrylamide gels using standard methods. Proteins are transferred onto nitrocellulose membranes and specific proteins detected by immunoblotting.

References:

- [1]. Deng X, et al. Structural determinants for ERK5 (MAPK7) and leucine rich repeat kinase 2 activities of benzo[e]pyrimido-[5,4-b]diazepine-6(11H)-ones. Eur J Med Chem. 2013;70:758-67.
- [2]. Elkins, Jonathan M., et al. X-ray Crystal Structure of ERK5 (MAPK7) in Complex with a Specific Inhibitor. Journal of Medicinal Chemistry (2013), 56(11), 4413-4421.
- [3]. Wilhelmsen K, et al. Extracellular signal-regulated kinase 5 promotes acute cellular and systemic inflammation. Sci Signal. 2015 Aug 25;8(391):ra86.

Background

XMD17-109 is a new inhibitor of ERK5, IC₅₀ value in HeLa cell is 0.09 ± 0.03 µM, and in vitro, Enzymatic IC₅₀ value is 0.162 ± 0.006 µM.

XMD17-109 is capable of inhibiting the ERK5 autophosphorylation in cells.[1]

Through intravenous injection and oral delivery of XMD17-109 in mice, the pharmacokinetic properties of this compound are as follows: the T_{1/2} (half time) is 8.2 h, the plasma clearance is 8.64 mL/min/Kg (data of intravenous injection), the AUC (area under the curve) of oral delivery is 15745 h*ng/mL and the oral bioavailability is 90%.

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1. Deng, X., et al., Structural determinants for ERK5 (MAPK7) and leucine rich repeat kinase 2 activities of benzo[e]pyrimido-[5,4-b]diazepine-6(11H)-ones. European Journal of Medicinal Chemistry, 2013. 70: p. 758-767.

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