

PRODUCT INFORMATION

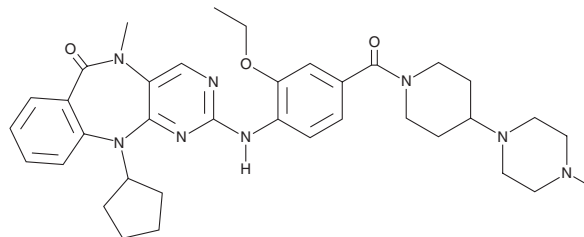


XMD17-109

Item No. 25448

CAS Registry No.: 1435488-37-1
Formal Name: 11-cyclopentyl-2-[[2-ethoxy-4-[[4-(4-methyl-1-piperazinyl)-1-piperidinyl]carbonyl]phenyl]amino]-5,11-dihydro-5-methyl-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one

Synonym: ERK5-IN-1
MF: C₃₆H₄₆N₈O₃
FW: 638.8
Purity: ≥98%
UV/Vis.: λ_{max}: 285, 312 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

XMD17-109 is supplied as a crystalline solid. A stock solution may be made by dissolving the XMD17-109 in the solvent of choice, which should be purged with an inert gas. XMD17-109 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of XMD17-109 in these solvents is approximately 1 mg/ml.

Description

XMD17-109 is a selective ERK5 inhibitor (IC₅₀ = 0.162 μM in an enzyme assay).¹ It is selective for ERK5 over a panel of more than 200 kinases, inhibiting only ERK5 with greater than 90% target occupancy at a concentration of 10 μM. XMD17-109 inhibits ERK5 phosphorylation (IC₅₀ = 0.09 μM in HeLa cells) and decreases AP-1 transcriptional activity (EC₅₀ = 4.2 μM).² It also inhibits human recombinant LRRK2[G2019S], which contains a mutation that has been linked to Parkinson's disease, with an IC₅₀ value of 0.339 μM in an enzyme assay.¹

References

- Deng, X., Elkins, J.M., Zhang, J., *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.* **70**, 758-767 (2013).
- Elkins, J.M., Wang, J., Deng, X., *et al.* X-ray crystal structure of ERK5 (MAPK7) in complex with a specific inhibitor. *J. Med. Chem.* **56(11)**, 4413-4421 (2013).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

WARRANTY AND LIMITATION OF REMEDY

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