

PRODUCT INFORMATION

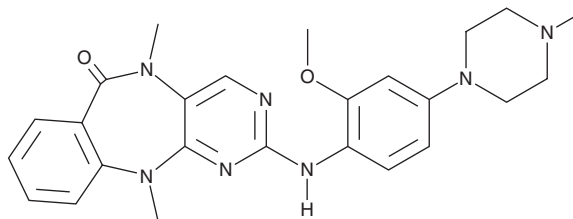


XMD8-85

Item No. 29662

CAS Registry No.: 1234479-76-5
Formal Name: 5,11-dihydro-2-[[2-methoxy-4-(4-methyl-1-piperazinyl)phenyl]amino]-5,11-dimethyl-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one

Synonym: ERK5-IN-1
MF: C₂₅H₂₉N₇O₂
FW: 459.5
Purity: ≥98%
UV/Vis.: λ_{max}: 291 nm
Supplied as: A 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

XMD8-85 is supplied as a solid. A stock solution may be made by dissolving the XMD8-85 in the solvent of choice, which should be purged with an inert gas. XMD8-85 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of XMD8-85 in these solvents is approximately 2, 15, and 10 mg/ml, respectively.

XMD8-85 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, XMD8-85 should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. XMD8-85 has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

XMD8-85 is an ERK5 inhibitor (IC₅₀ = 87 nM in an enzyme assay).¹ It is selective for ERK5 over tyrosine non-receptor kinase 2 (TNK2; IC₅₀ = 959 nM), but does inhibit the leucine-rich repeat kinase 2 (LRRK2) mutant LRRK2^{G2019S} (IC₅₀ = 26 nM), which has been found in patients with Parkinson's disease.^{1,2} XMD8-85 inhibits EGF-induced ERK5 autophosphorylation in HeLa cells (EC₅₀ = 0.19 μM).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).
- Groendyke, B.J., Powell, C.E., Feru, F., *et al.* Benzopyrimidodiazepinone inhibitors of TNK2. *Bioorg. Med. Chem. Lett.* **30**(4), 126948 (2020).

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.

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