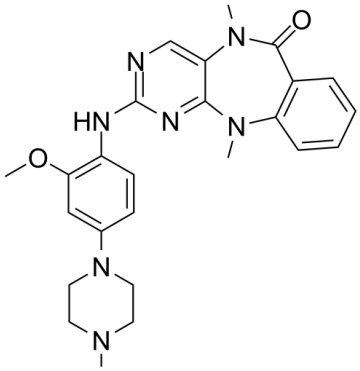
Data Sheet

Product Name:	ERK5-IN-1
Cat. No.:	CS-4938
CAS No.:	1234479-76-5
Molecular Formula:	C25H29N7O2
Molecular Weight:	459.54
Target:	ERK
Pathway:	MAPK/ERK Pathway; Stem Cell/Wnt
Solubility:	DMSO : ≥ 100 mg/mL (217.61 mM)



BIOLOGICAL ACTIVITY:

ERK5-IN-1 is a potent **ERK5** inhibitor with an **IC_{50}** of 87±7 nM. ERK5-IN-1 also inhibits **LRRK2**[G2019S] with an **IC_{50}** of 26 nM. IC50 & Target: IC50: 87±7 nM (ERK5), 26 nM (LRRK2[G2019S])[1] **In Vitro:** ERK5-IN-1 (Compound 5) exhibits a cellular EC_{50} for inhibiting epidermal growth factor (EGF) induced ERK5 autophosphorylation of 0.19±0.04 μM[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]Kinase activity is determined in an assay volume of 40 μL in kinase buffer (50 mM Tris-HCl, pH 7.5, 0.1 mM EGTA, 1 mM 2-mercaptoethanol) containing 200 ng of pure active ERK5 and the indicated amount of inhibitor. Reaction started by adding 10 mM magnesium acetate, and 50 μM [γ-^{32}P]-ATP (500 cpm/pmol) and 250 μM PIMtide (ARKKRRHPSGPPTA) as substrates. Assays are carried out for 20 min at 30°C, terminated by applying the reaction mixture onto p81 paper and the incorporated radioactivity measured[1].

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;70:758-767.

CAIndexNames:

6H-Pyrimido[4,5-b][1,4]benzodiazepin-6-one, 5,11-dihydro-2-[[2-methoxy-4-(4-methyl-1-piperazinyl)phenyl]amino]-5,11-dimethyl-

SMILES:

O=C1C2=C(C=CC=C2)N(C)C3=NC(NC4=C(OC)C=C(N5CCN(C)CC5)C=C4)=NC=C3N1C

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

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