

3-(1H-indol-5-yl)-5-(4-((4-methylpiperazin-1-yl)methyl)phenyl)-1H-pyrrolo[2,3-b]pyridine

CAS Registry No.: 1229582-33-5

Smiles String:

CN(CC1)CCN1CC2=CC=C(C3=CC(C(C4=CC=C(NC=C5)C5=C4)=CN6)=C6N=C3)C=C2

Molecular Weight: 421.54

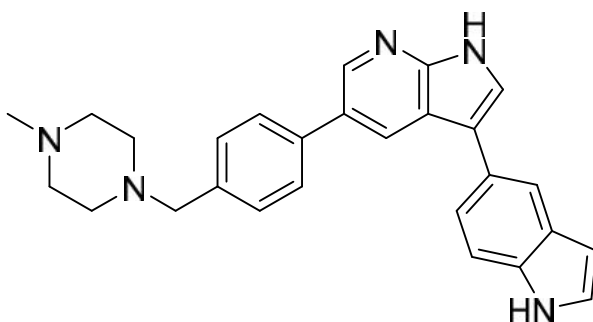
Molecular Formula: C₂₇H₂₇N₅

Lot Number: Refer to vial

¹H-NMR: Available on request

HPLC (Purity): > 95.0% @ 254 nm

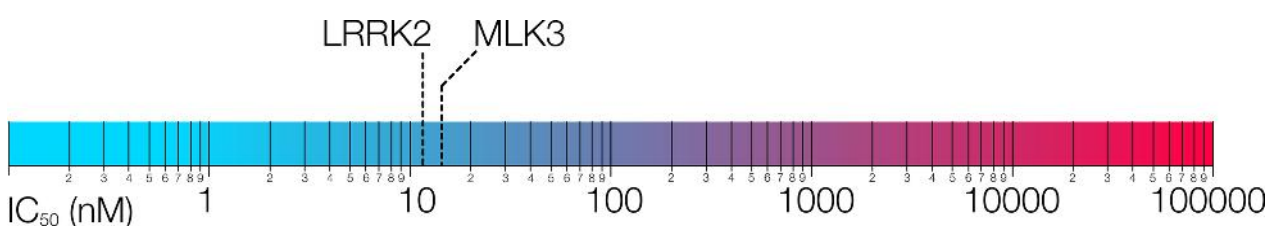
ES-MS: Available on request



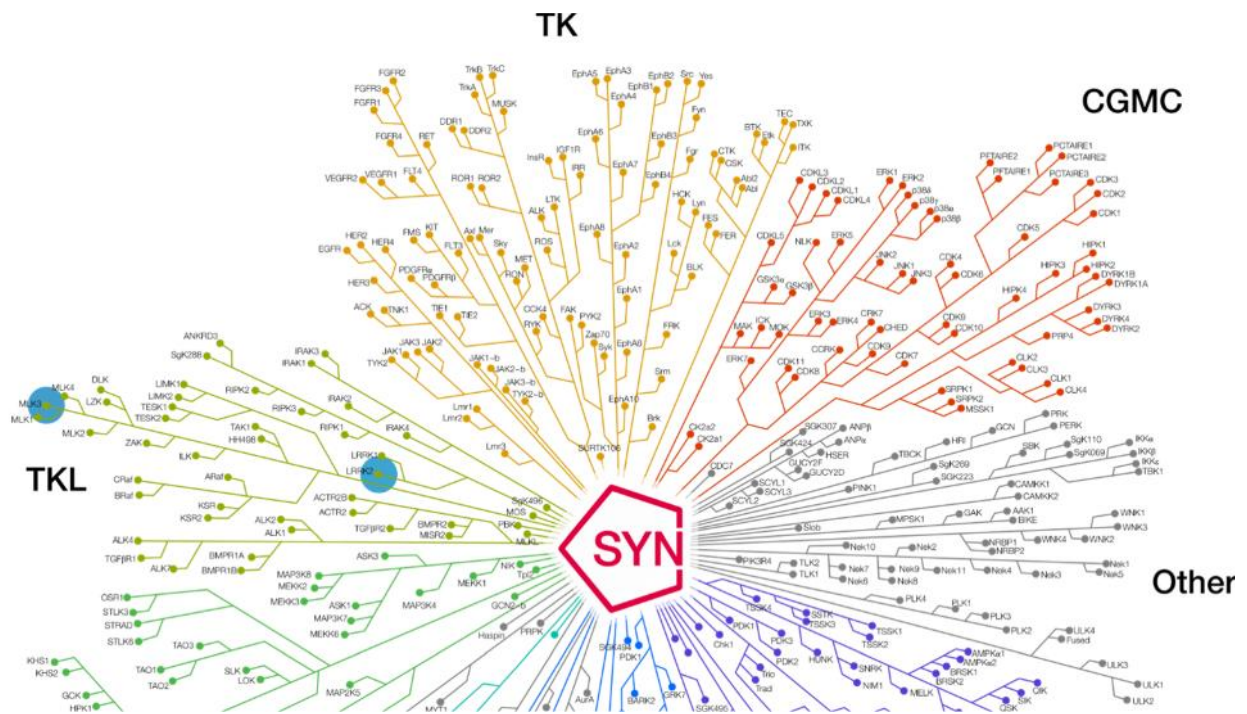
Description:

Inhibition of mixed lineage kinase 3 (MLK3) is a potential strategy for the treatment of Parkinson's disease and HIV-1 associated neuro-cognitive disorders (HAND), requiring an inhibitor that can achieve significant brain concentration levels. URMC-099 is an orally bioavailable MLK3 inhibitor with excellent brain exposure in mouse PK models and minimal interference with key human CYP450 enzymes or hERG channels. URMC-099 inhibits multiple kinase pathways, including MLK3 (14 nM) and LRRK2 (11 nM).

Biological Activity



Kinome Mapping



Shipping and Storage Temperature

Shipping:
Ambient

Storage:
3 Months at -4C (powder), >3 Years at -20C (powder), 1 Month at -4C (DMSO), >3 Months at -80C (DMSO)

Solubility

Water < 1 mg/mL, DMSO 80 mg/mL

Preparing Stock Solutions

Stock Solution (1ml DMSO)	1mM	10mM	20mM	50mM
Mass(mg)	0.422	4.215	8.431	21.077

References

1. Goodfellow VS, Loweth CJ, Ravula SB, Wiemann T, Nguyen T, Xu Y, Todd DE, Sheppard D, Pollack S, Poleskaya O, Marker DF, Dewhurst S, Gelbard HA. Discovery, synthesis, and characterization of an orally bioavailable, brain penetrant inhibitor of mixed lineage kinase 3. *J Med Chem*. 2013 Oct 24;56(20):8032-48. doi: 10.1021/jm401094t. Epub 2013 Oct 3. PubMed PMID: 24044867; PubMed Central PMCID: PMC4032177.

Ordering Information

To order more of this or any other SYNkinase compound, go to synkinase.com, Call us Toll Free (US Only) at 1- 877-854-6273 or email orders@synkinase.com.

Product Datasheet (Rev. 1.1)