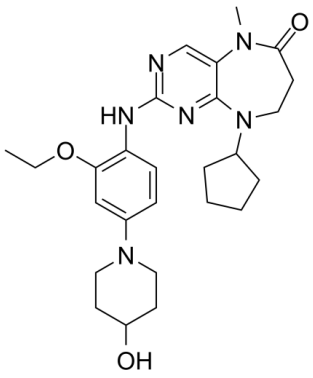
Data Sheet

Product Name:	Mps1-IN-2
Cat. No.:	CS-2027
CAS No.:	1228817-38-6
Molecular Formula:	C26H36N6O3
Molecular Weight:	480.60
Target:	Mps1; Polo-like Kinase (PLK)
Pathway:	Cell Cycle/DNA Damage; Cytoskeleton
Solubility:	DMSO : 14.3 mg/mL (29.75 mM; Need ultrasonic and warming)



BIOLOGICAL ACTIVITY:

Mps1-IN-2 is a potent, selective and ATP-competitive dual **Mps1/Plk1** inhibitor, with an **IC_{50}** and a **K_d** of 145 nM and 12 nM for Mps1 and a **K_d** of 61 nM for Plk1. IC50 & Target: IC50: 145 nM (Mps1)[1]
Kd: 12 nM (Mps1)[1] **In Vitro:** Mps1-IN-2 is a potent, selective and ATP-competitive Mps1 kinase inhibitor, with an IC_{50} and a K_d of 145 nM and 12 nM. Mps1-IN-2 also shows high affinity for PLK1 and GAK with K_ds of 61 and 140 nM, respectively, but shows little or no inhibition on other 352 member kinases. Mps1-IN-2 can induces bypass of a checkpoint-mediated mitotic arrest in U2OS cells[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]The kinase binding assay is used to assess compound binding to **TTK** by monitoring displacement of a fluorescently labeled, ATP site-directed kinase inhibitor (Kinase Tracer 236) from the kinase active site. Each 15 µL assay contains 5 nM TTK, **variable amounts of test compound (Mps1-IN-2)**, 30 nM Kinase Tracer 236, 2 nM Eu-anti-GST Antibody, and 1% DMSO (residual from compound dilution) in Kinase Buffer A (50 mM HEPES pH 7.5, 10 mM $MgCl_2$, 1 mM EGTA, 0.01% Brij-35). Binding assays are initiated by addition of 5 µL of test compound (from 2-fold dilution series) to 5 µL of a kinase/antibody mixture, followed by addition of 5 µL of antibody. Assay plates are read using using standard Eu-based TR-FRET settings with excitation at 340 nm and emission monitored at 615 nm (donor) and 665 nm (acceptor). Emission intensities are measured over a 200 µs window following a 100 µs post-excitation delay[1].

References:

[1]. Kwiatkowski N, et al. Small-molecule kinase inhibitors provide insight into Mps1 cell cycle function. Nat Chem Biol. 2010 May;6(5):359-68.

CAIndexNames:

6H-Pyrimido[4,5-b][1,4]diazepin-6-one, 9-cyclopentyl-2-[[2-ethoxy-4-(4-hydroxy-1-piperidinyl)phenyl]amino]-5,7,8,9-tetrahydro-5-methyl-

SMILES:

CN(C1=CN=C(NC2=C(OCC)C=C(N3CCC(O)CC3)C=C2)N=C1N(C4CCCC4)CC5)C5=O

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