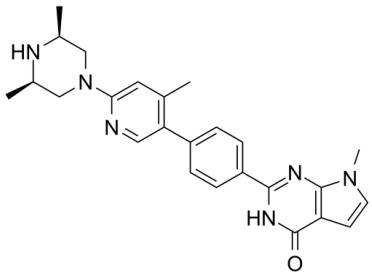
Data Sheet

Product Name:	AZ6102
Cat. No.:	CS-5610
CAS No.:	1645286-75-4
Molecular Formula:	C25H28N6O
Molecular Weight:	428.53
Target:	PARP
Pathway:	Cell Cycle/DNA Damage; Epigenetics
Solubility:	DMSO : ≥ 29 mg/mL (67.67 mM)



BIOLOGICAL ACTIVITY:

AZ6102 is a potent dual **TNKS1** and **TNKS2** inhibitor, with **IC_{50}**s of 3 nM and 1 nM, respectively, and alao has 100-fold selectivity against other PARP family enzymes, with **IC_{50}**s of 2.0 μM, 0.5 μM, and >3 μM, for PARP1, PARP2, and PARP6, respectively. IC50 & Target: IC50: 3 nM (TNKS1), 1 nM (TNKS2), 2.0 μM (PARP1), 0.5 μM (PARP2), >3 μM (PARP6)[1] **In Vitro:** AZ6102 is a potent dual TNKS1 and TNKS2 inhibitor, with IC_{50}s of 3 nM and 1 nM, respectively. AZ6102 alao has 100-fold selectivity against other PARP family enzymes, with IC_{50}s of 2.0 μM, 0.5 μM, and >3 μM, for PARP1, PARP2, and PARP6, respectively. AZ6102 shows Wnt pathway inhibition in DLD-1 cells[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]The assay is conducted using 0.11 μM of **tankyrase-1 protein** and 3 μM nicotinamide adenine dinucleotide (NAD^+, 2.12 μM ^3H-NAD^+ with a specific radioactivity of 1690 Ci/mol, 0.88 μM biotin- NAD^+), in pH 7.5 Tris buffer (60 mM Tris, 1 mM DTT, 0.01% (v/v) Tween-20®, 2.5 mM $MgCl_2$, 0.3 mg/mL BSA). For IC_{50} determination, 10 mM DMSO stock solution of a compound (**AZ6102**) **is sequentially diluted by two-fold in DMSO**, and aliquots of the diluted solutions are transferred to 384-well assay plates and mixed with Tankyrase-1 solution[1].

References:

[1]. Johannes JW, et al. Pyrimidinone nicotinamide mimetics as selective tankyrase and wnt pathway inhibitors suitable for in vivo pharmacology. ACS Med Chem Lett. 2015 Jan 13;6(3):254-9.

CAIndexNames:

4H-Pyrrolo[2,3-d]pyrimidin-4-one, 2-[4-[6-[(3R,5S)-3,5-dimethyl-1-piperazinyl]-4-methyl-3-pyridinyl]phenyl]-3,7-dihydro-7-methyl-,rel-

SMILES:

O=C1C2=C(N(C)C=C2)N=C(C3=CC=C(C4=C(C)C=C(N5C[C@@H](C)N[C@@H](C)C5)N=C4)C=C3)N1

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA