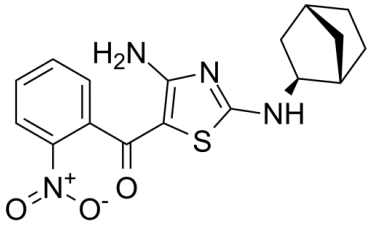
Data Sheet

Product Name:	MC180295
Cat. No.:	CS-0081067
CAS No.:	2237942-08-2
Molecular Formula:	C17H18N4O3S
Molecular Weight:	358.41
Target:	CDK
Pathway:	Cell Cycle/DNA Damage
Solubility:	DMSO : 100 mg/mL (279.01 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

MC180295 ((rel)-MC180295) is a potent and selective **CDK9-Cyclin T1** inhibitor, with an **IC_{50}** of 5 nM, at least 22-fold more selective for CDK9 over other CDKs. MC180295 also inhibits GSK-3α and GSK-3β. MC180295 ((rel)-MC180295) has potent anti-tumor effect[1]. IC50 & Target: IC50: 5 nM (CDK9-Cyclin T1), 138 nM (CDK1-Cyclin B), 233 nM (CDK2-Cyclin A), 367 nM (CDK2-Cyclin E), 399 nM (CDK3-Cyclin E), 112 nM (CDK4-Cyclin D), 159 nM (CDK5-P35), 186 nM (CDK5-P25), 712 nM (CDK6-Cyclin D3), 555 nM (CDK7-CycH/MAT1)[1] **In Vitro:** MC180295 is a potent and selective CDK9-Cyclin T1 inhibitor, with an IC_{50} of 5 nM, at least 22-fold more selective for CDK9 over other CDKs, such as CDK1-Cyclin B (IC_{50}, 138 nM), CDK2-Cyclin A (IC_{50}, 233 nM), CDK2-Cyclin E (IC_{50}, 367 nM), CDK3-Cyclin E (IC_{50}, 399 nM), CDK4-Cyclin D (IC_{50}, 112 nM), CDK5-P35 (IC_{50}, 159 nM), CDK5-P25 (IC_{50}, 186 nM), CDK6-Cyclin D3 (IC_{50}, 712 nM), and CDK7-CycH/MAT1 (IC_{50}, 555 nM). MC180295 also inhibits GSK-3α and GSK-3β[1].
MC180295 (500 nM) reactivates epigenetically silenced genes by targeting CDK9 without affecting DNA methylation[1].
MC180295 (0.1 μM) inhibits the proliferation in cancer cells[1]. **In Vivo:** MC180295 (20 mg/kg, i.p., qod) inhibits significant anti-tumor activity in mice bearing SW48 cells, shows no inhibitory activity against human T cell growth in vivo[1].

References:

[1]. Zhang H, et al. Targeting CDK9 Reactivates Epigenetically Silenced Genes in Cancer. Cell. 2018 Nov 15;175(5):1244-1258.e26.

CAIndexNames:

Methanone, [4-amino-2-[(1R,2R,4S)-bicyclo[2.2.1]hept-2-ylamino]-5-thiazolyl](2-nitrophenyl)-, rel-

SMILES:

NC1=C(C(C2=CC=CC=C2[N+]([O-])=O)=O)SC(N[C@@H]3[C@H](C4)CC[C@H]4C3)=N1

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