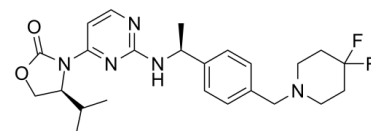


Data Sheet

Product Name:	Mutant IDH1-IN-2
Cat. No.:	CS-5119
CAS No.:	1429176-69-1
Molecular Formula:	C ₂₄ H ₃₁ F ₂ N ₅ O ₂
Molecular Weight:	459.53
Target:	Isocitrate Dehydrogenase (IDH)
Pathway:	Metabolic Enzyme/Protease
Solubility:	H ₂ O : < 0.1 mg/mL (insoluble); DMSO : 50 mg/mL (108.81 mM); Need ultrasonic)



BIOLOGICAL ACTIVITY:

Mutant IDH1-IN-2 is a inhibitor of mutant Isocitrate dehydrogenase (IDH) proteins, with IC₅₀ of in LS-MS biochemical assay, IC₅₀ of 16.6 nM in Fluorescence biochemical assay. Target: Mutant IDH1 Mutant IDH1-IN-2 has a neomorphic activity and in the treatment of diseases or disorders associated with such mutant IDH proteins including, but not limited to, cell-proliferation disorders, such as cancer. More bioactivity information in Patent WO 2013046136A1 (Example 224).

References:

[1]. Huangshu, et al. 3-Pyrimidin-4-yl-oxazolidin-2-ones as inhibitors of mutant IDH and their preparation

CAIndexNames:

2-Oxazolidinone, 3-[2-[[[(1S)-1-[4-[(4,4-difluoro-1-piperidinyl)methyl]phenyl]ethyl]amino]-4-pyrimidinyl]-4-(1-methylethyl)-, (4S)-

SMILES:

O=C1OC[C@H](C(C)C)N1C2=NC(N[C@H](C3=CC=C(CN4CCC(F)(F)CC4)C=C3)C)=NC=C2

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

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