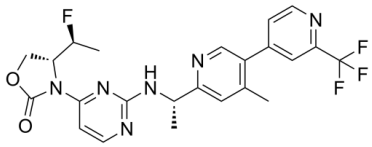
Data Sheet

Product Name:	IDH-305
Cat. No.:	CS-8084
CAS No.:	1628805-46-8
Molecular Formula:	$C_{23}H_{22}F_4N_6O_2$
Molecular Weight:	490.45
Target:	Isocitrate Dehydrogenase (IDH)
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 150 mg/mL (305.84 mM)



BIOLOGICAL ACTIVITY:

IDH-305 is an orally available, mutant-selective and brain-penetrant **IDH1** inhibitor that targets IDH1 (R132) mutation. IDH-305 exhibits greater than 200 fold selectivity for mutant IDH1 isoforms vs. WT (**IC_{50}**= 27 nM ($IDH1^{R132H}$), 28 nM ($IDH1^{R132C}$), 6.14 μM ($IDH1^{WT}$))[1][2]. IC50 & Target: IC50: 27 nM ($IDH1^{R132H}$), 28 nM ($IDH1^{R132C}$), 6.14 μM ($IDH1^{WT}$)[1] ***In Vitro:*** IDH-305 inhibits HCT116-$IDH1^{R132H+/-}$ cells with an IC_{50} of 24 nM[1]. ***In Vivo:*** IDH-305 (30-300 mg/kg; p.o.; twice daily for 21 days) inhibits 2-HG production and 2-HG-dependent tumor growth of an IDH1 mutant PDX melanoma model[1].

References:

[1]. Cho YS, et al. Discovery and Evaluation of Clinical Candidate IDH305, a Brain Penetrant Mutant IDH1 Inhibitor. ACS Med Chem Lett. 2017 Sep 18;8(10):1116-1121.

[2]. Courtney D DiNardo, et al. A Phase I Study of IDH305 in Patients with Advanced Malignancies Including Relapsed/Refractory AML and MDS That Harbor IDH1R132 Mutations. Blood, 128(22), 1073.

CAIndexNames:

2-Oxazolidinone, 4-[(1S)-1-fluoroethyl]-3-[2-[[(1S)-1-[4-methyl-2'-(trifluoromethyl)[3,4'-bipyridin]-6-yl]ethyl]amino]-4-pyrimidinyl]-, (4R)-

SMILES:

O=C1OC[C@H]([C@@H](F)C)N1C2=NC(N[C@H](C3=CC(C)=C(C4=CC(C(F)(F)F)=NC=C4)C=N3)C)=NC=C2

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

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