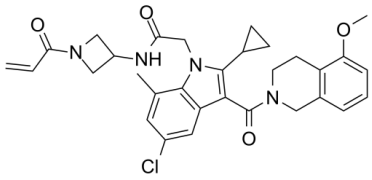
Data Sheet

Product Name:	K-Ras G12C-IN-4
Cat. No.:	CS-0105106
CAS No.:	2376328-55-9
Molecular Formula:	$C_{31}H_{33}ClN_4O_4$
Molecular Weight:	561.07
Target:	Ras
Pathway:	GPCR/G Protein
Solubility:	DMSO : 62.5 mg/mL (111.39 mM; ultrasonic and warming and heat to 60°C)



BIOLOGICAL ACTIVITY:

K-Ras G12C-IN-4, compound 1, is a potent Covalent Inhibitor of **$KRAS^{G12C}$**[1]. **In Vitro:** K-Ras G12C-IN-4 (4 hours) exhibits IC_{50} =0.219 μM for inhibition of MAPK signaling (p-ERK) in MIA PaCa-2 cells[1].

K-Ras G12C-IN-4 (72 hours) translates to a 0.067 μM IC_{50} for inhibition of cellular viability in a CellTiter-Glo experiment in MIA PaCa-2 cells[1].

References:

[1]. Shin Y, et al. Discovery of N-(1-Acryloylazetidin-3-yl)-2-(1H-indol-1-yl)acetamides as Covalent Inhibitors of KRASG12C. ACS Med Chem Lett. 2019 Aug 20;10(9):1302-1308.

CAIndexNames:

1H-Indole-1-acetamide, 5-chloro-2-cyclopropyl-3-[(3,4-dihydro-5-methoxy-2(1H)-isoquinolinyl)carbonyl]-7-methyl-N-[1-(1-oxo-2-propen-1-yl)-3-azetidinyl]-

SMILES:

O=C(NC1CN(C(C=C)=O)C1)CN2C(C3CC3)=C(C(N4CC5=C(C(OC)=CC=C5)CC4)=O)C6=C2C(C)=CC(Cl)=C6

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

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