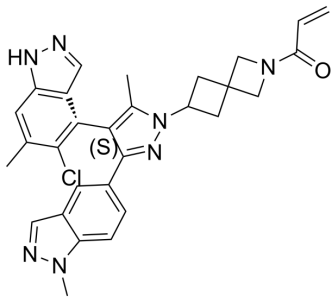
(S)-JDQ-443

Cat. No.:	HY-139612A
CAS No.:	2653994-10-4
Molecular Formula:	$C_{29}H_{28}ClN_7O$
Molecular Weight:	526.03
Target:	Ras; PERK
Pathway:	GPCR/G Protein; Cell Cycle/DNA Damage
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (190.10 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9010 mL	9.5052 mL	19.0103 mL
	5 mM	0.3802 mL	1.9010 mL	3.8021 mL
	10 mM	0.1901 mL	0.9505 mL	1.9010 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

(S)-JDQ-443 is an isomer of JDQ-443 (HY-139612). JDQ-443 is an orally active, potent, selective, and covalent KRAS G12C inhibitor (extracted from patent WO2021120890A1). JDQ-443 shows antitumor activity[1][2].

In Vitro

JDQ-443 promotes dose-dependent reductions of phosphorylated ERK (pERK) levels and the proliferation of the KRASG12C-mutated cell lines NCI-H358 and NCI-H2122, with IC_{50} values of 0.018 and 0.063 μM, respectively[2].

JDQ443 covalently and selectively binds and inhibits GDP-bound KRASG12C with low reversible binding affinity to the RAS switch II pocket, and also inhibits proliferation of KRASG12C-mutated and KRAS G12C/H95, G12C/R68S, and G12C/Y96 double-mutant cell lines[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

JDQ443 (10-100 mg/kg, Orally, daily for 14 days) shows antitumor activity and inhibits the growth of tumor in a dose-dependent manner in KRAS G12C-mutated CDX models[2].

JDQ443 (Orally, 100 mg/kg, daily (JDQ443) + 7.5 mg/kg, twice daily (TNO155), for 36 days) shows greater cell growth inhibition or cell killing compared with single-agent JDQ443 when combined with TNO155[2].

JDQ443 generates categorical antitumor responses in PDX models of NSCLC and colorectal tumors that are improved by

combination treatment with other agents[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. LIU BO, et al. PYRAZOLYL DERIVATIVES USEFUL AS ANTI-CANCER AGENTS. Patent WO2021120890A1.

[2]. Weiss A, Lorthiois E, Barys L, et al. Discovery, Preclinical Characterization, and Early Clinical Activity of JDQ443, a Structurally Novel, Potent and Selective, Covalent Oral Inhibitor of KRASG12C. Cancer Discov. 2022;candisc.0158.2022.

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