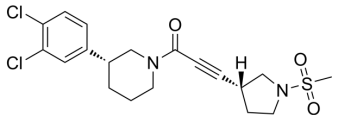
(R,R)-VVD-118313

Cat. No.:	HY-151385A
CAS No.:	2875046-31-2
Molecular Formula:	$C_{19}H_{22}Cl_2N_2O_3S$
Molecular Weight:	429.36
Target:	STAT; Interleukin Related; IFNAR; JAK
Pathway:	JAK/STAT Signaling; Stem Cell/Wnt; Immunology/Inflammation; Epigenetics; Protein Tyrosine Kinase/RTK
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (232.90 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3290 mL	11.6452 mL	23.2905 mL
	5 mM	0.4658 mL	2.3290 mL	4.6581 mL
	10 mM	0.2329 mL	1.1645 mL	2.3290 mL

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

BIOLOGICAL ACTIVITY

Description

(R,R)-VVD-118313 is the isomer of VVD-118313 (HY-151385). VVD-118313 is a selective JAK1 inhibitor and blocks JAK1-dependent trans-phosphorylation and cytokine signaling. VVD-118313 can be used for research of cancer[1]. (R,R)-VVD-118313 is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

JAK1

In Vitro

VVD-118313 (compound 5a; 0.01-10 μM; 3 h; primary human PBMCs) inhibits JAK1 by engagement of C817 and JAK2 by engagement of C838. VVD-118313 inhibits cysteine reactivity in a dose-dependent manner[1].

VVD-118313 (2 μM, 2h) blocks IFNα-simulated STAT1 and IL-6-stimulated STAT3 phosphorylation in WT- or C810A-JAK1-expressing 22Rv1 cells. VVD-118313 also blocks the constitutive phosphorylation of WT- and C810A-JAK1[1].

VVD-118313 (0.01-10 μM) selectively inhibits JAK1 signaling in primary human immune cells. VVD-118313 inhibits JAK1-dependent IFNα-pSTAT1, IL-6-pSTAT3, and IL-2-pSTAT5 pathways in human PBMCs in a dose-dependent manner[1].

VVD-118313 (0.1-0.4 μM; 24 h) inhibits T-cell activation induction. VVD-118313 inhibits the activation of human T cells co-stimulated with αCD3/αCD28 by a reduction in the proportion of $CD25^+$ T cells. VVD-118313 blocks the secretion of the Th1-

polarizing cytokine IFNγ and increases the production of IL-2[1].

VVD-118313 (0.1-0.5 μM; 2 h) inhibits on the production of pro-inflammatory cytokines and chemokines. VVD-118313 suppresses the induction of several pro-inflammatory chemokines, including CCL2/MCP-1, CXCL10/IP-10, and CCL4/MIP-1β [1].

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

Western Blot Analysis[1]

Cell Line:	22Rv1 cells
Concentration:	0.01, 0.1, and 1 μM
Incubation Time:	2 hours
Result:	Showed labeling of recombinant WT-JAK1 and C810A-JAK1, but not C817A-JAK1. Inhibited WT- and C810A-JAK1 phosphorylation with even greater potency than STAT1/STAT3 phosphorylation.

In Vivo

VVD-118313 (compound 5a; 25-50 mg/kg; i.h.; once) inhibits JAK1 signaling in TYK2 knockout mice[1].

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

REFERENCES

[1]. Kavanagh ME, et, al. Selective inhibitors of JAK1 targeting an isoform-restricted allosteric cysteine. Nat Chem Biol. 2022 Sep 12.

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