Deucravacitinib

Cat. No.: HY-117287

CAS No.: 1609392-27-9

Molecular Formula: $C_{20}H_{19}D_3N_8O_3$

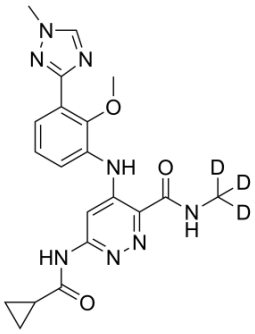
Molecular Weight: 425.46

Target: JAK; Interleukin Related; IFNAR

Pathway: Epigenetics; JAK/STAT Signaling; Stem Cell/Wnt; Immunology/Inflammation

Storage:

Powder	-20°C	3 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 37.5 mg/mL (88.14 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3504 mL	11.7520 mL	23.5040 mL
	5 mM	0.4701 mL	2.3504 mL	4.7008 mL
	10 mM	0.2350 mL	1.1752 mL	2.3504 mL

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

In Vivo

1. Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline
   Solubility: 3.83 mg/mL (9.00 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (4.89 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.89 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Deucravacitinib (BMS-986165) is a highly selective, orally bioavailable allosteric TYK2 inhibitor for the treatment of autoimmune diseases, which selectively binds to TYK2 pseudokinase (JH2) domain (IC_{50}=1.0 nM) and blocks receptor-mediated Tyk2 activation by stabilizing the regulatory JH2 domain. Deucravacitinib inhibits IL-12/23 and type I IFN pathways[1][2].

IC_{50} & Target				
	Tyk2 JH2	JAK1 JH2	IL-12	IL-23
	0.2 nM (IC_{50})	1 nM (IC_{50})		

In Vitro	Deucravacitinib (BMS-986165) is differentiated from previous JAK inhibitors due its unique ability to selectively bind to the pseudokinase (JH2) domain of TYK2 and inhibit its function through an allosteric mechanism[1]. Deucravacitinib maintains excellent potency in human and mouse whole blood (IC_{50}s=13 and 100 nM, respectively) and shows no significant hERG inhibition in the flux assay (IC_{50}>80 μM)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell Death Differ. 2021 Feb;28(2):748-763.
- iScience. 2021, 102498.
- Inflamm Bowel Dis. 2020 Dec 9;izaa318.
- Research Square Preprint. 2020 Nov.
- Patent. US20200345731A1.

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REFERENCES

[1]. Wrobleski ST, et al. Highly Selective Inhibition of Tyrosine Kinase 2 (TYK2) for the Treatment of Autoimmune Diseases: Discovery of the Allosteric Inhibitor BMS-986165. J Med Chem. 2019 Jul 18.

[2]. Catlett I, et al. SAT0226 A first-in-human, study of BMS-986165, a selective, potent, allosteric small molecule inhibitor of tyrosine kinase 2. Annals of the Rheumatic Diseases 2017;76:859.

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