Print Date: Nov 14th 2022

Certificate of Analysis

www.tocris.com

Product Name: **Ozanimod** **Catalog No.: 7663** **Batch No.: 1**

CAS Number: 1306760-87-1

IUPAC Name: 5-[3-[(1*S*)-2,3-Dihydro-1-[(2-hydroxyethyl)amino]-1*H*-inden-4-yl]-1,2,4-oxadiazol-5-yl]-2-(1-methylethoxy)benzonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{24}N_4O_3$.

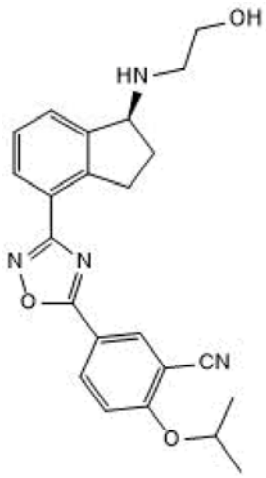
Batch Molecular Weight: 404.46

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -28 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.3	5.98	13.85
Found	68.28	6.05	13.85

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Description:

Ozanimod is a potent and selective sphingosine-1-phosphate receptor 1 ($S1P_1$) and 5 ($S1P_5$) agonist (EC_{50} values are 0.41 and 11 nM, respectively, in a [^{35}S]-GTPγS assay). Ozanimod exhibits 27-fold selectivity over $S1P_5$, and >10,000-fold selectivity over $S1P_{2-4}$. In vitro, Ozanimod induces sustained $S1P_1$ receptor internalization and degradation in $S1P_1$ receptor-HEK293T cells. In vivo, Ozanimod reduces inflammation and disease parameters in rat models of autoimmune disease. Ozanimod reduces chronic inflammation and alleviates kidney pathology in a murine model of systemic lupus erythematosus. Ozanimod is orally bioavailable. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

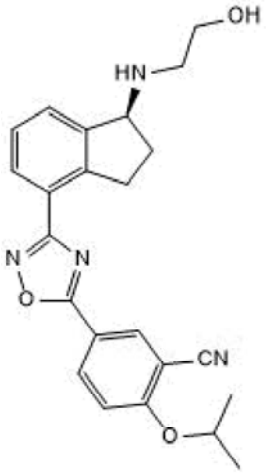
Batch Molecular Formula: $C_{23}H_{24}N_4O_3$.

Batch Molecular Weight: 404.46

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Selkirk *et al* (2021) Deconstructing the pharmacological contribution of sphingosine-1 phosphate receptors to mouse models of multiple sclerosis using the species selectivity of ozanimod, a dual modulator of human sphingosine 1-phosphate receptor subtypes 1 and 5. J.Pharmacol.Exp.Ther. ***379*** 379. PMID: 34535564.

R Taylor Meadows *et al* (2018) Ozanimod (RPC1063), a selective S1PR1 and S1PR5 modulator, reduces chronic inflammation and alleviates kidney pathology in murine systemic lupus erythematosus. PLoS One ***13*** e0193236. PMID: 29608575.

Scott *et al* (2016) Ozanimod (RPC1063) is a potent sphingosine-1-phosphate receptor-1 (S1P1) and receptor-5 (S1P5) agonist with autoimmune diseasemodifying activity. Br.J.Pharmacol. ***173*** 1778. PMID: 26990079.