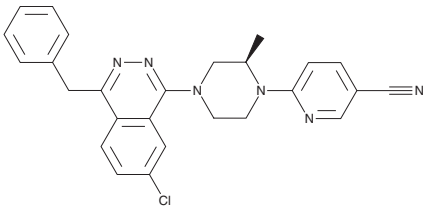
PRODUCT INFORMATION

S1PL-IN-31

Item No. 39826

CAS Registry No.:	1538574-95-6
Formal Name:	6-[(2R)-4-[7-chloro-4-(phenylmethyl)-1-phthalazinyl]-2-methyl-1-piperazinyl]-3-pyridinecarbonitrile
Synonyms:	Sphingosine-1-Phosphate Lyase Inhibitor 31, S1PL Inhibitor 31, S1P Lyase Inhibitor 31
MF:	$C_{26}H_{23}ClN_6$
FW:	455.0
Purity:	≥98%
Supplied as:	A solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

S1PL-IN-31 is supplied as a solid. A stock solution may be made by dissolving the S1PL-IN-31 in the solvent of choice, which should be purged with an inert gas. S1PL-IN-31 is soluble in acetonitrile and DMSO.

Description

S1PL-IN-31 is an inhibitor of sphingosine-1-phosphate (S1P) lyase (IC_{50} = 210 nM).[1] It is also an antagonist of the Smoothened (Smo) receptor (IC_{50} = 440 nM). *In vivo*, S1PL-IN-31 (2 mg/kg per day) prevents cervical and thoracic lymphocyte infiltration and neuromuscular weakness in a rat model of experimental autoimmune encephalomyelitis (EAE) induced by the myelin oligodendrocyte glycoprotein (MOG) peptide MOG_{29-152}. It reduces the total number of lymphocytes, as well as the levels of $CD4^+$ T cells, $CD8^+$ T cells, and B cells in rats. S1PL-IN-31 (100 mg/kg) increases S1P levels in the heart and lymph nodes of male and female rats and decreases heart rate in female rats when administered at doses of 3 and 10 mg/kg per day.[2]

References

1. Weiler, S., Braendlin, N., Beerli, C., *et al.* Orally active 7-substituted (4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl]nicotinonitriles as active-site inhibitors of sphingosine 1-phosphate lyase for the treatment of multiple sclerosis. *J. Med. Chem.* **57(12)**, 5074-5084 (2014).
2. Harris, C.M., Mittelstadt, S., Banfor, P., *et al.* Sphingosine-1-phosphate (S1P) lyase inhibition causes increased cardiac S1P levels and bradycardia in rats. *J. Pharmacol. Exp. Ther.* **359(1)**, 151-158 (2016).

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