# **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:  $C_{26}H_{23}CIN_6$ FW: 455.0 **Purity:** ≥98% Supplied as: A solid -20°C Storage: 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<sub>50</sub> = 210 nM). It is also an antagonist of the Smoothened (Smo) receptor (IC<sub>50</sub> = 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<sub>29-152</sub>. It reduces the total number of lymphocytes, as well as the levels of CD4<sup>+</sup> T cells, CD8<sup>+</sup> 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.<sup>2</sup>

#### References

- 1. Weiler, S., Braendlin, N., Beerli, C., et al. Orally active 7-substituted (4-benzylphthalazin-1-yl)-2methylpiperazin-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).

WARNING
THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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