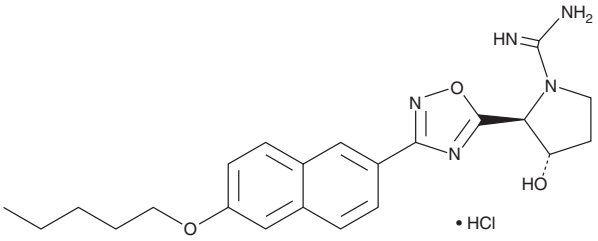
PRODUCT INFORMATION

SLC5111312 (hydrochloride)

Item No. 23288

CAS Registry No.:	1870811-01-0
Formal Name:	(2S,3S)-3-hydroxy-2-[3-[6-(pentyloxy)-2-naphthalenyl]-1,2,4-oxadiazol-5-yl]-1-pyrrolidinecarboximidamide, monohydrochloride
MF:	$C_{22}H_{27}N_5O_3$ • HCl
FW:	445.9
Purity:	≥98%
UV/Vis.:	λ_{max}: 237 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥2 years



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

Laboratory Procedures

SLC5111312 (hydrochloride) is supplied as a crystalline solid. A stock solution may be made by dissolving the SLC5111312 (hydrochloride) in the solvent of choice. SLC5111312 (hydrochloride) is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of SLC5111312 (hydrochloride) in these solvents is approximately 14, 3, and 2 mg/ml, respectively.

SLC5111312 (hydrochloride) is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, SLC5111312 (hydrochloride) should first be dissolved in ethanol and then diluted with the aqueous buffer of choice. SLC5111312 (hydrochloride) has a solubility of approximately 0.2 mg/ml in a 1:4 solution of ethanol:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

SLC5111312 is a dual inhibitor of sphingosine kinase 1 (SPHK1) and SPHK2 (K_is = 0.73 and 0.9 µM, respectively, using human recombinant kinases).[1] SLC5111312 binding is selective for Sphk2 over Sphk1 in mice (K_is = 1 and 20 µM, respectively) but not rat (K_is = 1.1 and 0.8 µM, respectively).[2] It decreases cell-associated sphingosine-1-phosphate (S1P) and increases sphingosine in U937 monocytic leukemia cells at concentrations of 0.1 and 0.3 µM. SLC5111312 (10 mg/kg) also decreases S1P *in vivo* in *Sphk1*$^{-/-}$ but not in *Sphk2*$^{-/-}$ mice and in rat, showing a functional selectivity for Sphk2 in mice.

References

1. Congdon, M.D., Kharel, Y., Brown, A.M., *et al.* Structure-activity relationship studies and molecular modeling of naphthalene-based sphingosine kinase 2 inhibitors. *ACS Med. Chem. Lett.* **7(3)**, 229-234 (2016).
2. Kharel, Y., Morris, E.A., Congdon, M.D., *et al.* Sphingosine kinase 2 inhibition and blood sphingosine 1-phosphate levels. *J. Pharmacol. Exp. Ther.* **355(1)**, 23-31 (2015).

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