

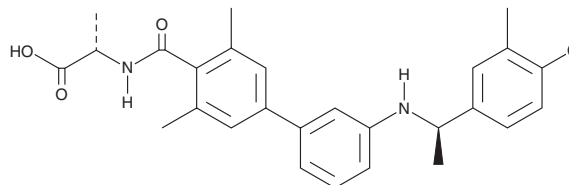
PRODUCT INFORMATION



NIBRO213

Item No. 21513

CAS Registry No.: 1233332-14-3
Formal Name: N-[[3'-[[[(1R)-1-(4-chloro-3-methylphenyl)ethyl]amino]-3,5-dimethyl[1,1'-biphenyl]-4-yl]carbonyl]-L-alanine
MF: C₂₇H₂₉ClN₂O₃
FW: 465.0
Purity: ≥98%
UV/Vis.: λ_{max}: 212, 249, 316 nm
Supplied as: A crystalline 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

NIBRO213 is supplied as a crystalline solid. A stock solution may be made by dissolving the NIBRO213 in the solvent of choice, which should be purged with an inert gas. NIBRO213 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of NIBRO213 in these solvents is approximately 25 mg/ml.

NIBRO213 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, NIBRO213 should first be dissolved in ethanol and then diluted with the aqueous buffer of choice. NIBRO213 has a solubility of approximately 0.15 mg/ml in a 1:5 solution of ethanol:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

NIBRO213 is an orally bioavailable, potent, and selective antagonist of sphingosine-1-phosphate receptor-1 (S1P₁) with IC₅₀ values of 2.5 and 2.0 nM for the hS1P₁ in a Ca²⁺ mobilization assay and GTPγS assay, respectively.¹ It is inactive at S1P₂, S1P₃, and S1P₄ receptors (IC₅₀s = >20, >10, and >10 μM, respectively in a Ca²⁺ mobilization assay). S1P₁ plays a key role in the immune system, regulating lymphocyte egress from lymphoid tissues into the circulation.² In rats, NIBRO213 (30 mg/kg) reduces peripheral blood lymphocytes by 75-85% for up to 24 hours.¹ In a mouse model of experimental autoimmune encephalitis (EAE), it significantly reduces disease severity up to 26 days, when administered at 30 mg/kg twice per day for three days, then 60 mg/kg twice per day. However, in a rat model of adjuvant-induced arthritis, chronic administration of 30 mg/kg induces pulmonary damage and chronic lung inflammation.³

References

1. Quancard, J., Bollbuck, B., Janser, P., *et al.* A potent and selective S1P₁ antagonist with efficacy in experimental autoimmune encephalomyelitis. *Chem. Biol.* **19(9)**, 1142-1151 (2012).
2. Huwiler, A., Kolter, T., Pfeilschifter, J., *et al.* Physiology and pathophysiology of sphingolipid metabolism and signaling. *Biochim. Biophys. Acta.* **1485(2-3)**, 63-99 (2000).
3. Bigaud, M., Dincer, Z., Bollbuck, B., *et al.* Pathophysiological consequences of a break in S1P1-dependent homeostasis of vascular permeability revealed by S1P1 competitive antagonism. *PLoS One* **11(12)**, e0168252 (2016).

WARNING

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

SAFETY DATA

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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