Product Datasheet

TC-G 1006

Catalog No. **BP-02422** · CAS **1324003-64-6** · Form **free base** · Physical state **solid** · Color **White to off-white** · Version **1.0** · Revision **2026-09-11**

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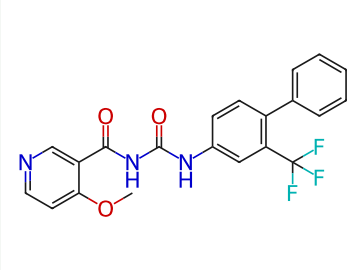
Target	Research area
LPL Receptor	**Inflammation/Immunology**

Molecular formula	**$C_{21}H_{16}F_3N_3O_3$**
Molecular weight	**415.3652**

STRUCTURE



DESCRIPTION

S1P1 agonist III is an orally active hS1P1 agonist with an EC50 value of 18 nM. S1P1 agonist III shows limited activity against hS1P3. S1P1 agonist III can be used in the research of multiple sclerosis .

BIOLOGICAL ACTIVITY

In Vitro

S1P1 agonist III (Compound 22) induces potent internalization of hS1P1 receptors in U2OS cells with an EC50 of 0.018 μM.

S1P1 agonist III shows minimal agonist activity at hS1P3 receptors in transfected CHO-K1 cells, with an EC50 greater than 25 μM.

S1P1 agonist III exhibits moderate permeability across LLC-PK1 porcine proximal tubule cells with no significant efflux, as shown by a Papp of 2.5 × 10-6 cm/s and an efflux ratio of 1.0.

S1P1 agonist III binds to 91.7% of rat plasma proteins under equilibrium conditions.

S1P1 agonist III is highly stable in rat liver microsomes, with an intrinsic clearance of less than 14 μL/min/mg microsomal protein.

In Vivo

S1P1 agonist III (Compound 22) (1-3 mg/kg; p.o.; single dose) produces statistically significant circulating blood lymphocyte reduction in female Lewis rats at 24 hours, with the 3 mg/kg dose causing an 88% reduction.

SOLUBILITY

Soluble in DMSO : 62.5 mg/mL

REFERENCES

[1].Harrington PE, et al. Optimization of a Potent, Orally Active S1P1 Agonist Containing a Quinolinone Core. ACS Med Chem Lett. 2011;3(1):74-78. Published 2011 Nov 23.

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