

Product Data Sheet

Product Name: SMS2-IN-1

Cat. No.: GC65364

Chemical Properties

Cas. No. 2098890-15-2

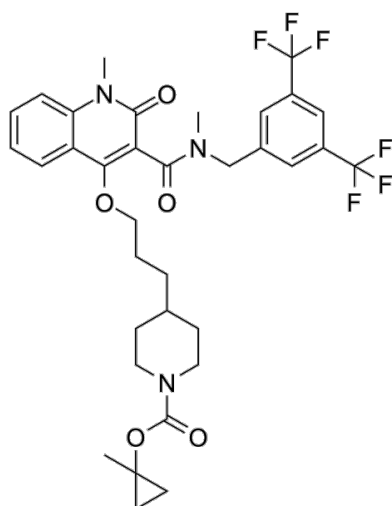
Formula $C_{34}H_{37}F_6N_3O_5$ M.Wt 681.67

Solubility DMSO : 27.78 mg/mL (40.75 mM; Storage Store at -20°C
Need ultrasonic)

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure



Protocol

Cell experiment [1]:

Cell lines NRK cells stably overexpressing Tspan4-mCherry

Caution: Product has not been fully validated for medical applications. For research use only.

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Cells were incubated with complete DMEM supplemented with 30 μ M SMS2-IN-1 Preparation Method 1 for 30min, respectively. Following the incubation, the cells were treated with 0.2pM TcdB3 for 4h before imaging.

Reaction Conditions 30 μ M; 30min

Applications SMS2-IN-1 blocked TcdB3-induced migracytosis.

References:

[1] Li D, Yang Q, Luo J, Xu Y, Li J, Tao L. Bacterial toxins induce non-canonical migracytosis to aggravate acute inflammation. Cell Discov. 2024;10(1):112.

Background

SMS2-IN-1 is a potent and highly selective inhibitor of sphingomyelin synthase 2 (SMS2), with an IC₅₀ value of 6.5nM for SMS2 and 1000nM for SMS1. SMS2-IN-1 binds to wild-type SMS2 with a K_d of 37nM, with S227 and H229 identified as key residues for binding^[1].

In vitro, pre-treatment with 30 μ M SMS2-IN-1 for 30min blocked TcdB3-induced migracytosis in NRK cells overexpressing Tspan4-mCherry^[2]. Treatment with 25 μ M SMS2-IN-1 for 16h significantly inhibited the formation of migrasome-like structures in NRK cells stably expressing Tspan4-GFP^[3].

References:

[1] Adachi R, et al. Discovery and characterization of selective human sphingomyelin synthase 2 inhibitors. Eur J Med Chem. 2017 Aug 18;136:283-293.

[2] Li D, Yang Q, Luo J, Xu Y, Li J, Tao L. Bacterial toxins induce non-canonical migracytosis to aggravate acute inflammation. Cell Discov. 2024;10(1):112.

[3] Wang D, Wang H, Wan W, et al. Engineered migrasomes provide a robust and thermally stable vaccination platform. Elife. 2025;13:RP97621.

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