

## Product Data Sheet

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Product Name: NS2B/NS3-IN-3 dihydrochloride

Cat. No.: GC78930

### Chemical Properties

Cas. No.

Formula  $C_{19}H_{23}Cl_2N_3O_2$  M.Wt 396.31

Solubility  $H_2O$ : 10 mg/mL (25.23 mM; Need ultrasonic) Storage Store at  $-20^{\circ}C$ , away from moisture

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

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

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

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### Structure



### Background

NS2B/NS3-IN-3 dihydrochloride is an inhibitor of Flavivirus NS2B-NS3 protease, with an  $IC_{50}$  of 0.32  $\mu M$  against Zika virus NS2B-NS3 protease. NS2B/NS3-IN-3 dihydrochloride also exhibits inhibitory effects on dengue virus type 2 NS2B-NS3 protease and West Nile virus NS2B-NS3 protease. NS2B/NS3-IN-3 dihydrochloride inhibits the intracellular replication of Zika virus. NS2B/NS3-IN-3 dihydrochloride can be used in studies related to flavivirus infections [1].

In Vitro, NS2B/NS3-IN-3 (compound 66) dihydrochloride potently inhibits recombinant Zika virus NS2B-NS3 protease with an  $IC_{50}$  of 0.32  $\mu M$ ; it also inhibits recombinant dengue virus type 2 NS2B-NS3 protease with an  $IC_{50}$  of approximately 1-2  $\mu M$ , and exhibits a non-competitive inhibition mode<sup>[1]</sup>. NS2B/NS3-IN-3 (1-10  $\mu M$ ; 48 h) dihydrochloride exhibits dose-dependent antiviral activity

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against Zika virus (strain FLR) in human U87 glioma cells, with an EC<sub>68</sub> of 1  $\mu$ M, and shows no toxicity to U87 cells at a concentration of 10  $\mu$ M<sup>[1]</sup>.

### References:

[1]. Nie S, et al. Synthesis, structure-activity relationship and antiviral activity of indole-containing inhibitors of Flavivirus NS2B-NS3 protease. European journal of medicinal chemistry. 2021 Dec 05;225:113767.

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