

Product Data Sheet

Product Name: ML188
Cat. No.: GC39497

Chemical Properties

Cas. No. 1417700-13-0

SMILES O=C(NC(C)(C)C)[C@@H](C1=CN=CC=C1)N(C(C=C2)=CC=C2C(C)(C)C)C(C3=CC=C(O3)=O

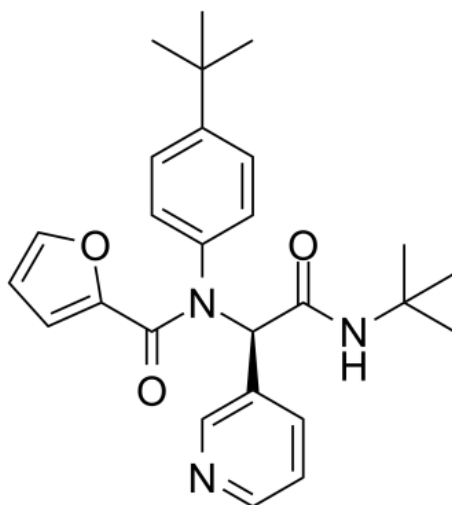
Formula $C_{26}H_{31}N_3O_3$ M.Wt 433.54

Solubility DMSO: 250 mg/mL (576.65 mM) Storage Store at -20°C

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

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

Structure



Background

ML188, a first in class probe, is a selective non-covalent SARS-CoV 3CLpro inhibitor with an IC₅₀ of 1.5 μM. Antiviral activity[1].

[1]. Jacobs J, et al. Discovery, synthesis, and structure-based optimization of a series of N-(tert-butyl)-2-(N-arylamido)-2-(pyridin-3-yl) acetamides (ML188) as potent noncovalent small molecule inhibitors of the severe acute respiratory syndrome coronavirus (SARS-CoV) 3CL protease. J Med

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

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Chem. 2013 Jan 24;56(2):534-46.

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