bio-techne
TOCRIS

Print Date: Jun 27th 2025

Certificate of Analysis

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Product Name: **BAY 390** **Catalog No.: 7978** **Batch No.: 1**

CAS Number: 2741956-55-6

IUPAC Name: (1*R*,2*R*)-2-[(4-Fluorophenyl)amino]-1-(trifluoromethyl)cyclohexanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{15}F_4NO$

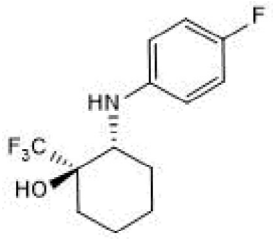
Batch Molecular Weight: 277.26

Physical Appearance: Yellow oil

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

BAY 390 is a potent and selective transient receptor potential ankyrin 1 (TRPA1) antagonist (IC_{50} values are 16, 63 and 82 nM for hTRPA1 FLIPR, rTRPA1 FLIPR and hTRPA1 Ephys, respectively). In vivo, BAY 390 exhibits efficacy in rat models of inflammatory and neuropathic pain. BAY 390 is orally bioavailable and brain penetrant. Suitable to use as an in vitro or in vivo probe to investigate the roles of TRPA1 in models of acute, inflammatory, and neuropathic pain.

Physical and Chemical Properties:

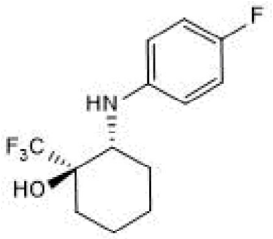
Batch Molecular Formula: $C_{13}H_{15}F_4NO$

Batch Molecular Weight: 277.26

Physical Appearance: Yellow oil

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

This product is supplied as a lyophilized oil and may be hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY 390 probe summary on the SGC website.

References:

Mesch *et al* (2023) Discovery of BAY-390, a selective CNS penetrant chemical probe as transient receptor potential ankyrin 1 (TRPA1) antagonist. J.Med.Chem. ***66*** 1583. PMID: 36622903.

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