

Certificate of Analysis

Product Name: SMANT hydrochloride

Catalog No.: 4662

Batch No.: 1

CAS Number: 1177600-74-6

IUPAC Name: *N*-(4-Bromophenyl)-3,5-dimethyl-1-piperidinepropanamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₂₃BrN₂O.HCl

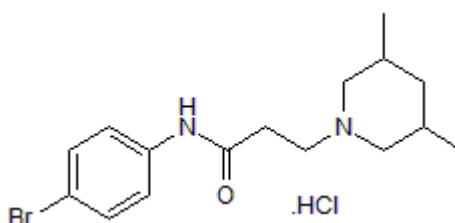
Batch Molecular Weight: 375.73

Physical Appearance: Off-white solid

Solubility: water to 20 mM
DMSO to 100 mM
ethanol to 20 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.15	6.44	7.46
Found	50.86	6.65	7.26

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

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Description:

Inhibitor of Smoothed (Smo) signaling via a unique mechanism. Inhibits Shh-induced accumulation of Smo::EGFP fusion protein in the primary cilium ($IC_{50} = 1.1 \mu M$). Inhibits both wild-type Smo and an oncogenic form (SmoM2) with similar efficacy.

Physical and Chemical Properties:

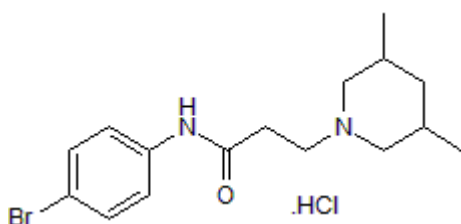
Batch Molecular Formula: $C_{16}H_{23}BrN_2O.HCl$

Batch Molecular Weight: 375.73

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Wang *et al* (2012) Selective identification of Hedgehog pathway antagonists by direct analysis of Smoothed ciliary translocation. ACS Chem.Biol. **7** 1040. PMID: 22554036.

Storage: Desiccate at RT

Solubility & Usage Info:

water to 20 mM
DMSO to 100 mM
ethanol to 20 mM

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. Our standard recommendations are:

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.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956