

Certificate of Analysis

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Product Name: CL 82198 hydrochloride

Catalog No.: 2632

Batch No.: 2

CAS Number: 1188890-36-9

IUPAC Name: *N*-[4-(4-Morpholinyl)butyl]-2-benzofurancarboxamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₃₃N₂O₃.HCl

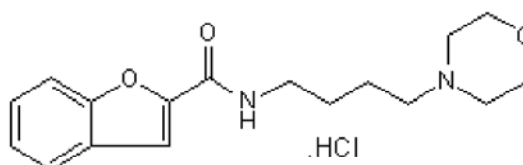
Batch Molecular Weight: 338.83

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 75 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 60.26 | 7.14 | 8.27 |
| Found | 60.05 | 6.84 | 8.28 |

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

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Batch No.: 2

CAS Number: 1188890-36-9

IUPAC Name: N-[4-(4-Morpholinyl)butyl]-2-benzofurancarboxamide hydrochloride

Description:

Selective inhibitor of MMP-13 (89% inhibition at 10 µg/mL) that displays no activity at MMP-1, MMP-9 or TACE. Inhibits in vitro invasion by the human pituitary adenoma cell line HP75. Rescues paclitaxel induced axon degradation and reduces associated neurotoxicity in zebrafish.

Physical and Chemical Properties:

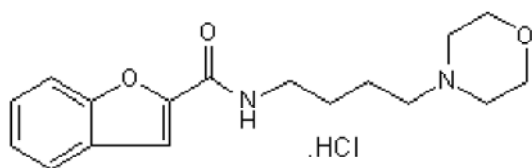
Batch Molecular Formula: C₁₇H₃₃N₂O₃.HCl

Batch Molecular Weight: 338.83

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM

DMSO to 75 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.

References:

Lisse et al (2016) Paclitaxel-induced epithelial damage and ectopic MMP-13 expression promotes neurotoxicity in zebrafish. *Proc Natl Acad Sci U S A* **113** E2189. PMID: 27035978.

Borg et al (2003) IL1 alpha, IL6 and MMP13 are required for invasion by the human pituitary cell line HP75. *Endocrine Abstr.* **5** 122.

Chen et al (2000) Structure-based design of a novel, potent, and selective inhibitor for MMP-13 utilizing NMR spectroscopy and computer-aided molecular design. *J.Am.Chem.Soc.* **122** 9648.

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