

# Certificate of Analysis

**Product Name:** ML 298 hydrochloride

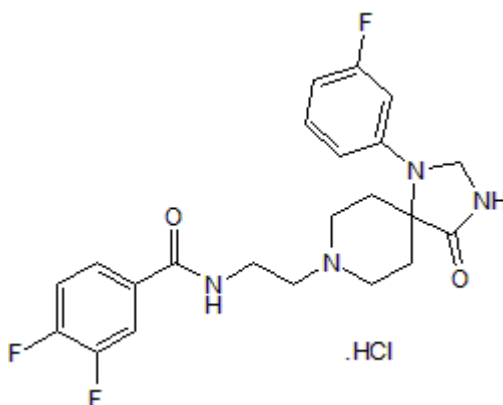
**Catalog No.:** 4895

**Batch No.:** 1

**IUPAC Name:** 3,4-Difluoro-N-[2-[1-(3-fluorophenyl)-4-oxo-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]benzamide hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>22</sub> H <sub>23</sub> F <sub>3</sub> N <sub>4</sub> O <sub>2</sub> .HCl.¼H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	473.4
<b>Physical Appearance:</b>	Off-white solid
<b>Solubility:</b>	DMSO to 25 mM
<b>Storage:</b>	Desiccate at RT
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>TLC:</b>	R <sub>f</sub> = 0.3 (Dichloromethane:Methanol [95:5])
<b>HPLC:</b>	Shows >99% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	55.82	5.22	11.83
Found	55.86	5.15	11.62

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

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**Description:**

Selective inhibitor of phospholipase D2 (PLD2) (IC<sub>50</sub> values are 355 and >20,000 nM for PLD2 and PLD1, respectively). Decreases invasive migration in U87-MG glioblastoma cells, without affecting cell viability.

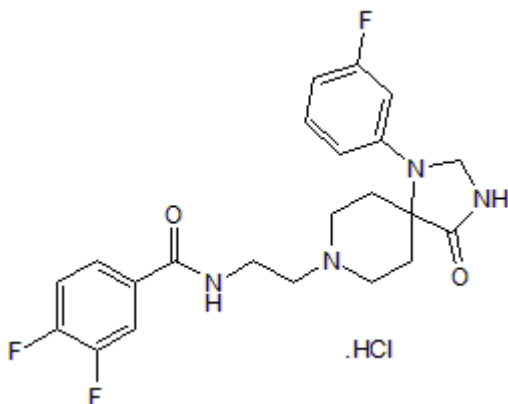
**Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>22</sub>H<sub>23</sub>F<sub>3</sub>N<sub>4</sub>O<sub>2</sub>.HCl.¼H<sub>2</sub>O

Batch Molecular Weight: 473.4

Physical Appearance: Off-white solid

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

DMSO to 25 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:**

**O'Reilly et al** (2013) Development of dual PLD1/2 and PLD2 selective inhibitors from a common 1,3,8-triazaspiro[4.5]decane core: discovery of ML298 and ML299 that decrease invasive migration in U87-MG glioblastoma cells. *J.Med.Chem.* **56** 2695. PMID: 23445448.

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