

## Certificate of Analysis

**Product Name:** NGD 98-2 hydrochloride

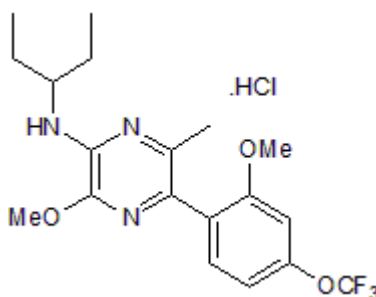
**Catalog No.:** 4315

**Batch No.:** 1

**IUPAC Name:** *N*-(1-Ethylpropyl)-3-methoxy-5-[2-methoxy-4-(trifluoromethoxy)phenyl]-6-methyl-2-pyrazinamine hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>19</sub> H <sub>24</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub> .HCl
<b>Batch Molecular Weight:</b>	435.87
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	DMSO to 100 mM water to 5 mM with gentle warming
<b>Storage:</b>	Desiccate at RT
<b>Batch Molecular Structure:</b>	



### 2. ANALYTICAL DATA

<b>TLC:</b>	R <sub>f</sub> = 0.38 (Dichloromethane:Methanol [9:1])
<b>HPLC:</b>	Shows >99.7% 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	52.36	5.78	9.64
Found	52.26	5.72	9.7

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

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**Description:**

High affinity antagonist of corticotropin-releasing factor receptor 1 (CRF<sub>1</sub>) (K<sub>i</sub> = 1 nM). Orally available and brain penetrant.

**Physical and Chemical Properties:**

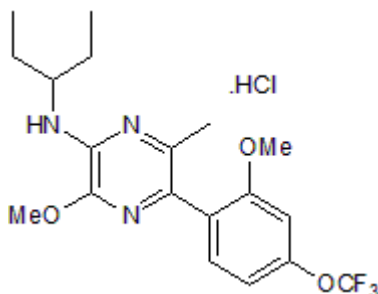
Batch Molecular Formula: C<sub>19</sub>H<sub>24</sub>F<sub>3</sub>N<sub>3</sub>O<sub>3</sub>.HCl

Batch Molecular Weight: 435.87

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

DMSO to 100 mM

water to 5 mM with gentle warming

**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:**

**Hodgetts et al** (2011) Discovery of *N*-(1-ethylpropyl)-[3-methoxy-5-(2-methoxy-4-trifluoromethoxyphenyl)-6-methyl-pyrazin-2-yl]amine 59 (NGD 98-2): an orally active corticotropin releasing factor-1 (CRF-1) receptor antagonist. *J.Med.Chem.* **54** 4187. PMID: 21618986.

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