

**Product Name:** NBI 35965 hydrochloride

**Catalog No.:** 3100

**Batch No.:** 1

**CAS Number:** 603151-83-3

**IUPAC Name:** (7S)-6-(Cyclopropylmethyl)-2-(2,4-dichlorophenyl)-7-ethyl-7,8-dihydro-4-methyl-6H-1,3,6,8a-tetraazaacenaphthylene hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{21}H_{22}Cl_2N_4 \cdot HCl \cdot 1\frac{1}{4}H_2O$

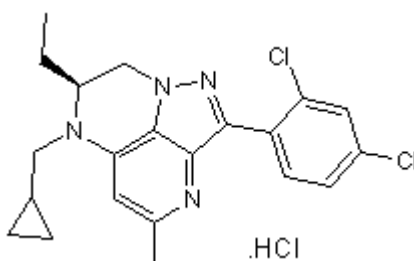
**Batch Molecular Weight:** 460.31

**Physical Appearance:** Off-white solid

**Solubility:** water to 100 mM  
DMSO to 100 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.4$  (Chloroform:Methanol [95:5])

**HPLC:** Shows 99% purity

**Chiral HPLC:** Shows 100% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	54.8	5.58	12.17
Found	54.69	5.29	11.99

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**Description:**

Potent and selective corticotropin-releasing factor receptor 1 (CRF<sub>1</sub>) antagonist (K<sub>i</sub> values are 4 and > 10000 nM at CRF<sub>1</sub> and CRF<sub>2</sub> respectively). Inhibits cAMP accumulation and adrenocorticotrophic hormone (ACTH) production in vitro (pIC<sub>50</sub> values are 7.1 and 6.9 respectively) and attenuates CRF and ACTH production in vivo. Orally active and brain penetrant with anxiolytic activity.

**Physical and Chemical Properties:**

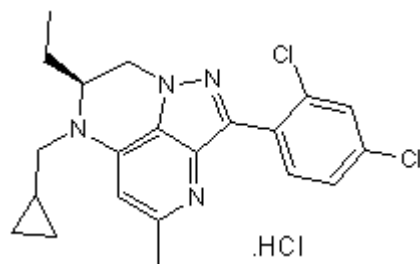
Batch Molecular Formula: C<sub>21</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>4</sub>.HCl.1 ¼H<sub>2</sub>O

Batch Molecular Weight: 460.31

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 100 mM  
DMSO to 100 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:**

**Million et al** (2003) A novel water-soluble selective CRF1 receptor antagonist, NBI 35965, blunts stress-induced visceral hyperalgesia and colonic motor function in rats. *Brain Res.* **985** 32. PMID: 12957366.

**Hoare et al** (2003) Mechanism of corticotropin-releasing factor type I receptor regulation by non-peptide antagonists. *Mol.Pharmacol.* **63** 751. PMID: 12606786.

**Gross et al** (2005) Design and synthesis of tricyclic corticotropin-releasing factor-1 antagonists. *J.Med.Chem.* **48** 5780. PMID: 16134945.

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