

Product Name: NBI 35965 hydrochloride

Catalog No.: 3100

Batch No.: 3

CAS Number: 1782228-59-4

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: C₂₁H₂₂Cl₂N₄.HCl.¾H₂O

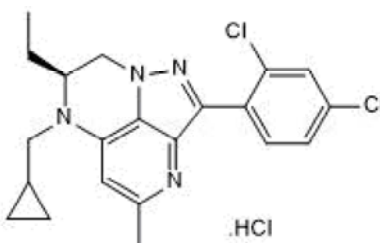
Batch Molecular Weight: 451.3

Physical Appearance: Off White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

Chiral HPLC: Shows >99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.89	5.47	12.41
Found	55.89	5.26	12.36

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Description:

Potent and selective corticotropin-releasing factor receptor 1 (CRF₁) antagonist (K_i values are 4 and > 10000 nM at CRF₁ and CRF₂ respectively). Inhibits cAMP accumulation and adrenocorticotrophic hormone (ACTH) production in vitro (pIC₅₀ 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:

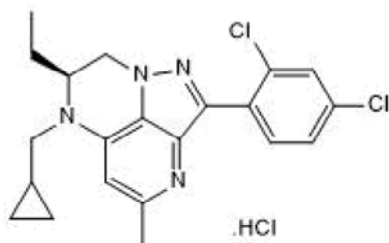
Batch Molecular Formula: C₂₁H₂₂Cl₂N₄.HCl.¼H₂O

Batch Molecular Weight: 451.3

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:

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

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

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.

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