

Product Name: AR-C 102222

Catalog No.: 3969

Batch No.: 1

CAS Number: 1781934-50-6

IUPAC Name: 5-[(4'-Amino-5',8'-difluorospiro[piperidine-4,2'(1'H)-quinaxolin]-1-yl)carbonyl]-2-pyridinecarbonitrile hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₆F₂N₆O.HCl.¼H₂O

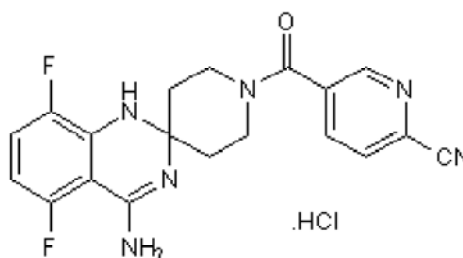
Batch Molecular Weight: 423.33

Physical Appearance: Pale yellow solid

Solubility: water to 25 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Chloroform:Methanol [9:1])

HPLC: Shows 98.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.91	4.17	19.85
Found	53.89	4.03	19.83

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

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Description:

Inducible nitric oxide synthase (iNOS) inhibitor; selective for iNOS over eNOS (IC₅₀ values are 0.037 and >100 μM for iNOS and eNOS respectively). Exhibits antinociceptive and anti-inflammatory activity in rodent pain models.

Physical and Chemical Properties:

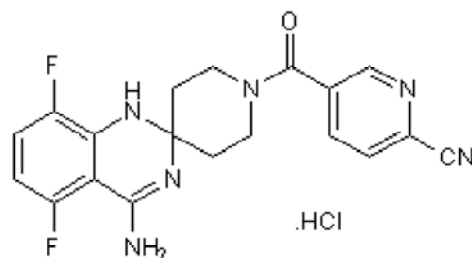
Batch Molecular Formula: C₁₉H₁₆F₂N₆O.HCl.½H₂O

Batch Molecular Weight: 423.33

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 25 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.

Licensing Information:

Sold with the permission of AstraZeneca UK Ltd.

References:

Bonnefous et al (2009) Discovery of inducible nitric oxide synthase (iNOS) inhibitor development candidate KD7332, Part 1: Identification of a novel, potent, and selective series of quinolinone iNOS dimerization inhibitors that are orally active in rodent pain models. *J.Med.Chem.* **52** 3047. PMID: 19374401.

LaBuda et al (2006) Antinociceptive activity of the selective iNOS inhibitor AR-C102222 in rodent models of inflammatory, neuropathic and postoperative pain. *Eur.J.Pain* **10** 505. PMID: 16125426.

Tinker et al (2003) 1,2-Dihydro-4-quinazolinamines: potent, highly selective inhibitors of inducible nitric oxide synthase which show antiinflammatory activity in vivo. *J.Med.Chem.* **46** 913. PMID: 12620067.

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