

Certificate of Analysis

Product Name: NAD 299 hydrochloride

Catalog No.: 3282

Batch No.: 3

CAS Number: 184674-99-5

IUPAC Name: (3*R*)-3-(Dicyclobutylamino)-8-fluoro-3,4-dihydro-2*H*-1-benzopyran-5-carboxamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₃FN₂O₂·HCl·¼H₂O

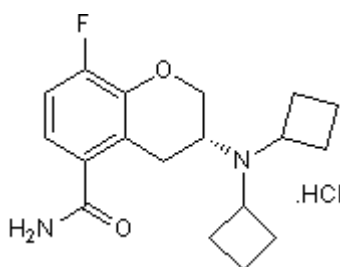
Batch Molecular Weight: 359.35

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 = 0.5 (Ethyl acetate:Methanol:Ammonia soln. [98:1:1])

HPLC: Shows 99.5% purity

Chiral HPLC: Shows >99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -62.4 (Concentration = 1, Solvent = Water)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.16	6.87	7.8
Found	60.24	7.17	7.57

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Description:

Selective, high affinity 5-HT_{1A} receptor antagonist ($K_i = 0.6$ nM in vitro). Enhances the action of selective 5-HT reuptake inhibitors and reverses citalopram-induced (Cat. No. 1427) inhibition of serotonergic cell firing.

Physical and Chemical Properties:

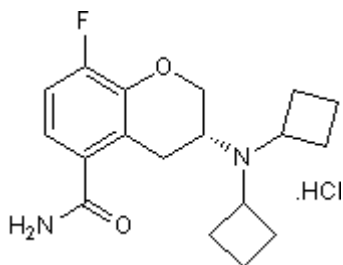
Batch Molecular Formula: C₁₈H₂₃FN₂O₂.HCl.¼H₂O

Batch Molecular Weight: 359.35

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:

Johansson et al (1997) The pharmacological characterization of a novel selective 5-hydroxytryptamine-_{1A} receptor antagonist, NAD-299. *J.Pharmacol.Exp.Ther.* **283** 216.

Larsson et al (1998) Differential regional antagonism of 8-OH-DPAT-induced decrease in serotonin synthesis by two 5-HT_{1A} receptor antagonists. *Eur.J.Pharmacol.* **346** 209. PMID: 9652362.

Arborelius et al (1999) The 5-HT_{1A} receptor antagonist robalzotan completely reverses citalopram-induced inhibition of serotonergic cell firing. *Eur.J.Pharmacol.* **382** 133. PMID: 10528148.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956