

Product Name: AF-DX 116

Catalog No.: 1105

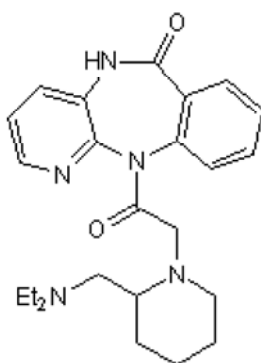
Batch No.: 4

CAS Number: 102394-31-0

IUPAC Name: 11-[[2-[(Diethylamino)methyl]-1-piperidinyl]acetyl]-5,11-dihydro-6H-pyrido[2,3-b][1,4]benzodiazepin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₃₁N₅O₂
Batch Molecular Weight: 421.54
Physical Appearance: White solid
Solubility: DMSO to 25 mM with gentle warming
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.51 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])
HPLC: Shows 99.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.38	7.41	16.61
Found	68.01	7.66	16.72

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

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Description:

Selective M₂ muscarinic receptor antagonist. K_i values are 64, 417, 786, 211 and 5130 nM for human recombinant M₂, M₁, M₃, M₄ and M₅ muscarinic receptors, respectively.

Physical and Chemical Properties:

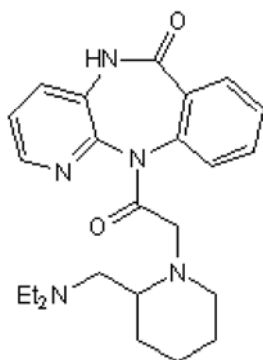
Batch Molecular Formula: C₂₄H₃₁N₅O₂

Batch Molecular Weight: 421.54

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 25 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.

Licensing Information:

Sold with the permission of Boehringer Ingelheim GmbH

References:

Mansfield et al (2005) Muscarinic receptor subtypes in human bladder detrusor and mucosa, studied by radioligand binding and quantitative competitive RT-PCR: changes in ageing. *Br.J.Pharmacol.* **114** 1089. PMID: 15723094.

Eglen et al (1996) Muscarinic receptor subtypes and smooth muscle function. *Pharmacol.Rev.* **48** 531. PMID: 8981565.

Billard et al (1995) Identification of the primary muscarinic autoreceptor subtype in rat striatum as M₂ through a correlation of *in vivo* microdialysis and *in vitro* receptor binding data. *J.Pharmacol.Exp.Ther.* **273** 273. PMID: 7714776.

Hammer et al (1986) Binding profile of a novel cardioselective muscarinic receptor antagonist, AF-DX 116, to membranes of peripheral tissues and brain in the rat. *Life Sci.* **38** 1653. PMID: 3754610.

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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