

Product Name: B 973B

Catalog No.: 6764

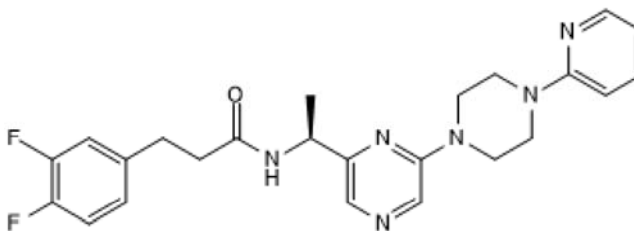
Batch No.: 1

CAS Number: 2244989-34-0

IUPAC Name: 3,4-Difluoro-N-[(1S)-1-[6-[4-(2-pyridinyl)-1-piperazinyl]-2-pyrazinyl]ethyl]benzenepropanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₆F₂N₆O
Batch Molecular Weight: 452.5
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
 ethanol to 50 mM
 1eq. HCl to 20 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.9% purity
Chiral HPLC: Shows 99.9% purity
¹H NMR: Consistent with structure
 Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.7	5.79	18.57
Found	63.69	5.76	18.48

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

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Description:

Positive allosteric modulator of $\alpha 7$ nAChRs (EC_{50} ~0.3 μ M); active enantiomer. Increases potency of acetylcholine (EC_{50} values are 0.007 mM and 0.3 mM in the presence and absence of B 937B, respectively). Potentiates peak acetylcholine-induced currents 6-fold relative to maximal acetylcholine, and slows channel desensitization, resulting in a 6900-fold increase in charge transfer. Decreases paw edema in vivo. Analgesic.

Physical and Chemical Properties:

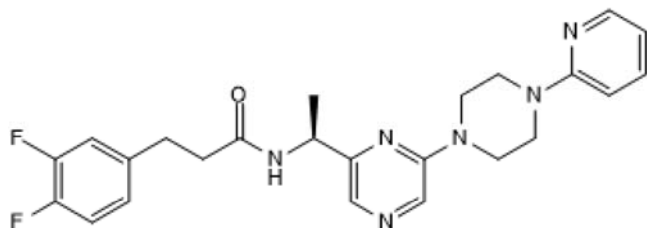
Batch Molecular Formula: $C_{24}H_{26}F_2N_6O$

Batch Molecular Weight: 452.5

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Quadri et al (2019) Macroscopic and microscopic activation of $\alpha 7$ nicotinic acetylcholine receptors by the structurally unrelated allosteric agonist-positive allosteric modulators (ago-PAMs) B-973B and GAT107. *Mol.Pharmacol.* **95** 43. PMID: 30348894.

Garai et al (2018) B-973, a novel $\alpha 7$ nAChR Ago-PAM: racemic and asymmetric synthesis, electrophysiological studies, and *in vivo* evaluation. *ACS Med.Chem.Lett.* **9** 1144. PMID: 30429960.

Post-Munson et al (2017) B-973, a novel piperazine positive allosteric modulator of the $\alpha 7$ nicotinic acetylcholine receptor. *Eur.J.Pharmacol.* **15** 799. PMID: 28132910.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 50 mM

1eq. HCl to 20 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.

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