

Product Name: PHA 568487

Catalog No.: 3134

Batch No.: 4

CAS Number: 527680-57-5

IUPAC Name: *N*-(3*R*)-1-Azabicyclo[2.2.2]oct-3-yl-2,3-dihydro-1,4-benzodioxin-6-carboxamide fumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₂₀N₂O₃·C₄H₄O₄·H₂O

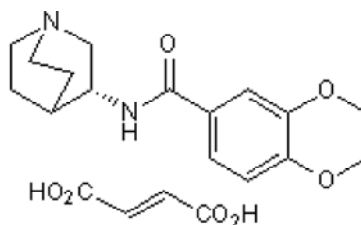
Batch Molecular Weight: 422.43

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.87	6.2	6.63
Found	56.88	6.2	6.52

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

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Description:

Agonist of the $\alpha 7$ nicotinic acetylcholine receptor (K_i values are 44 and 2800 for $\alpha 7$ and 5-HT₃ respectively, IC_{50} values are > 100 μ M for $\alpha 3\beta 4$ and $\alpha 1\beta 1\delta \gamma$ respectively, and % inhibition is < 1 and 5% for $\alpha 4\beta 2$ and hERG respectively). Orally active and brain penetrant.

Physical and Chemical Properties:

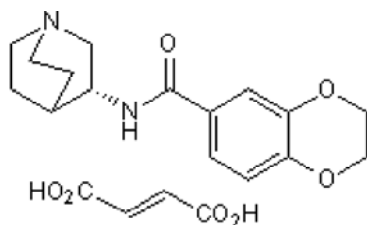
Batch Molecular Formula: C₁₆H₂₀N₂O₃·C₄H₄O₄·H₂O

Batch Molecular Weight: 422.43

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



References:

Walker et al (2006) Design, synthesis, structure-activity relationship, and in vivo activity of azabicyclic aryl amides as $\alpha 7$ nicotinic acetylcholine receptor agonists. *Bioorg.Med.Chem.* **14** 8219. PMID: 17011782.

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.

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