

Product Name: PD 123319 ditrifluoroacetate

Catalog No.: 1361

Batch No.: 3

CAS Number: 136676-91-0

IUPAC Name: 1-[[4-(Dimethylamino)-3-methylphenyl]methyl]-5-(diphenylacetyl)-4,5,6,7-tetrahydro-1*H*-imidazo[4,5-*c*]pyridine-6-carboxylic acid ditrifluoroacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₁H₃₂N₄O₃·2CF₃CO₂H·1³/₄H₂O

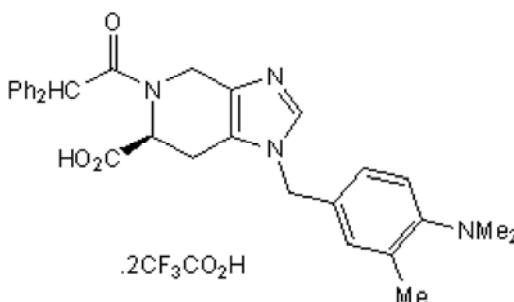
Batch Molecular Weight: 768.19

Physical Appearance: Off-white solid

Solubility: water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +6 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.72	4.92	7.29
Found	54.5	4.61	7.06

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

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Description:

Potent, selective, non-peptide angiotensin AT₂ receptor antagonist. IC₅₀ values are 34 and 210 nM in rat adrenal tissue and brain respectively.

Physical and Chemical Properties:

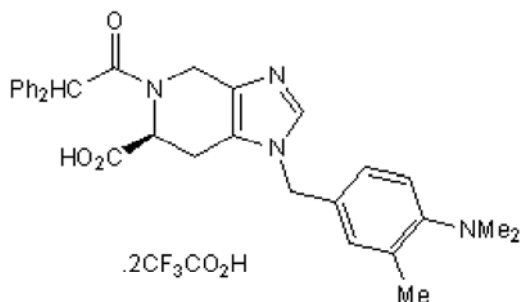
Batch Molecular Formula: C₃₁H₃₂N₄O₃.2CF₃CO₂H.1¼H₂O

Batch Molecular Weight: 768.19

Physical Appearance: Off-white solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

CAUTION - This product is hygroscopic and we recommend that it is desiccated upon arrival. Solutions should be made up as soon as the vial is opened.

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:

Tamura et al (2000) Induction of angiotensin II subtype 2 receptor-mediated blood pressure regulation in synthetic diet-fed rats. *J.Hypertens.* **18** 1239. PMID: 10994755.

Boulay et al (1992) Modulation of angiotensin II binding affinity by allosteric interaction of polyvinyl sulfate with an intracellular domain of the DuP-753-sensitive angiotensin II receptor of bovine adrenal glomerulosa. *Mol.Pharmacol.* **41** 809. PMID: 1569928.

Blankley et al (1991) Synthesis and structure-activity relationships of a novel series of non-peptide angiotensin II receptor binding inhibitors specific for the AT₂ subtype. *J.Med.Chem.* **34** 3248. PMID: 1956044.

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