



Certificate of Analysis

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Product Name: PD 123319 ditrifluoroacetate Catalog No.: 1361 Batch No.: 3

CAS Number: 130663-39-7

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: $C_{31}H_{32}N_4O_3.2CF_3CO_2H.1^{3}H_2O$

Batch Molecular Weight: 768.19

Physical Appearance: Off-white solid

Solubility: water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

$$\begin{array}{c} O \\ Ph_2HC \\ HO_2C \\ \\ .2CF_3CO_2H \\ \end{array}$$

2. ANALYTICAL DATA

HPLC: Shows >99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.72 4.92 7.29 Found 54.5 4.61 7.06



Product Information

Print Date: Apr 15th 2015 **WWW.tocris.com**

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Description:

Potent, selective, non-peptide angiotensin AT_2 receptor antagonist. IC_{50} values are 34 and 210 nM in rat adrenal tissue and brain respectively.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{31}H_{32}N_4O_3.2CF_3CO_2H.1\%H_2O$

Batch Molecular Weight: 768.19 Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:

$$\begin{array}{c|c} \mathsf{Ph_2HC} & \mathsf{N} & \mathsf{N} \\ \mathsf{HO_2C} & \mathsf{N} & \mathsf{N} \\ \mathsf{.2CF_3CO_2H} & \mathsf{Me} \end{array}$$

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:

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.

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.

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.

