

Certificate of Analysis

Print Date: Sep 12th 2024

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Product Name: (R)-(+)-Bay K 8644 Catalog No.: 1545 Batch No.: 5

CAS Number: 98791-67-4

IUPAC Name: (4R)-1,4-Dihydro-2,6-dimethyl-5-nitro-4-[2-trifluoromethyl)phenyl]-3-pyridinecarboxylic acid methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{15}F_3N_2O_4$.

Batch Molecular Weight: 356.3

Physical Appearance: Yellow solid

Solubility: ethanol to 100 mM

DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.9% purity
Chiral HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = +44.9$ (Concentration = 0.4, Solvent = 1,4-dioxane)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 53.94 4.24 7.86 Found 54.48 4.26 7.97

Product Information

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Description:

(R)-(+)-Bay K 8644 is a L-type Ca²+-channel blocker with negative inotropic and vasodilatatory effects in vivo. Enantiomer showing opposite effects to the racemate (±)-Bay K 8644 (Cat. No. 1544) and (S)-(-)- enantiomer (Cat. No. 1546). Also TMEM176B inhibitor. Induces IL-1 β secretion and caspase-1 activation in bone marrow-derived dendritic cells in vitro and increases survival of tumor-bearing mice, both alone and in combination with immune checkpoint blockers. Racemate and (S)-(-)-Enantiomer also available.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₆H₁₅F₃N₂O₄.

Batch Molecular Weight: 356.3 Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:

$$\begin{array}{c|c} F_3 C & & \\ \hline O_2 N & & \\ \hline Me & & \\ Me & & \\ \end{array}$$

Storage: Store at +4°C

Solubility & Usage Info:

ethanol 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Segovia et al (2019) Targeting TMEM176B enhances antitumor immunity and augments the efficacy of immune checkpoint blockers by unleashing inflammasome activation. Cancer Cell. 35 767. PMID: 31085177.

Shi et al (2008) Induction of pluripotent stem cells from mouse embryonic fibroblasts by Oct4 and Klf4 with small-molecule compounds. Cell Stem Cell. **3** 568. PMID: 18983970.

Ravens and Schopper (1990) Opposite cardiac actions of the enantiomers of Bay K 8644 at different membrane potentials in guineapig papillary muscles. Naunyn Schmiedebergs Arch.Pharmacol. **341** 232. PMID: 1692975.

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