

Product Name: (R)-(+)-Bay K 8644

Catalog No.: 1545

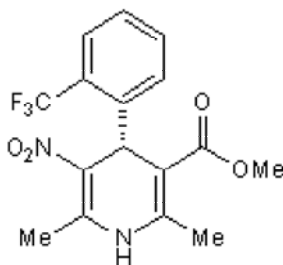
Batch No.: 4

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: C₁₆H₁₅F₃N₂O₄
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 >99.9% purity
¹H NMR: Consistent with structure
 Mass Spectrum: Consistent with structure
 Optical Rotation: [α]_D = +51.4 (Concentration = 0.416, Solvent = 1,4-dioxane)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.94	4.24	7.86
Found	53.97	4.27	7.79

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Description:

L-type Ca²⁺-channel blocker with negative inotropic and vasodilatory effects in vivo. Enantiomer showing opposite effects to the racemate (±)-Bay K 8644 and (S)-(-)- enantiomer. Also TMEM176B inhibitor. Induces IL-1β 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:

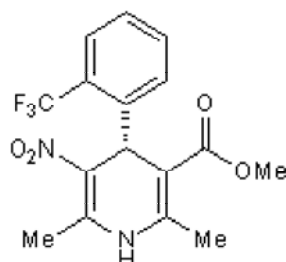
Batch Molecular Formula: C₁₆H₁₅F₃N₂O₄

Batch Molecular Weight: 356.3

Physical Appearance: Yellow solid

Minimum Purity: >97%

Batch Molecular Structure:



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. 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:

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 guinea-pig papillary muscles. *Naunyn Schmiedebergs Arch.Pharmacol*. **341** 232. PMID: 1692975.

O'Neill and Bolger (1988) Enantiomer selectivity and the development of tolerance to the behavioral effects of the calcium channel activator BAY K 8644. *Brain Res.Bull*. **21** 865. PMID: 2465070.

Franckowiak et al (1985) The optical isomers of the 1,4-dihydropyridine BAY K 8644 show opposite effects on Ca channels. *Eur.J.Pharmacol*. **114** 223. PMID: 2412855.

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