

Product Name: MRS 1334

Catalog No.: 1385

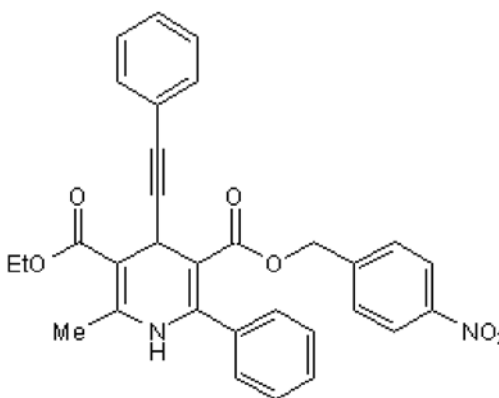
Batch No.: 2

CAS Number: 192053-05-7

IUPAC Name: 1,4-Dihydro-2-methyl-6-phenyl-4-(phenylethynyl)-3,5-pyridinedicarboxylic acid 3-ethyl-5-[(3-nitrophenyl)methyl] ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₁H₂₆N₂O₆
Batch Molecular Weight: 522.56
Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM
Storage: Desiccate at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.48 (Isohexane:Ethyl acetate [3:2])
Melting Point: Between 159 - 161°C
HPLC: Shows >98.2% purity
¹H NMR: Consistent with structure

| Microanalysis: | Carbon Hydrogen Nitrogen | | |
|----------------|--------------------------|-------|------|
| | Theoretical | Found | |
| | 71.25 | 71.5 | 5.01 |
| | | | 5.06 |
| | | | 5.36 |
| | | | 5.33 |

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

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Description:

Potent and highly selective antagonist for the human adenosine A₃ receptor. K_i values are 2.69 nM at hA₃, and > 100 μM at rat A₁ and rat A_{2A} receptors.

Physical and Chemical Properties:

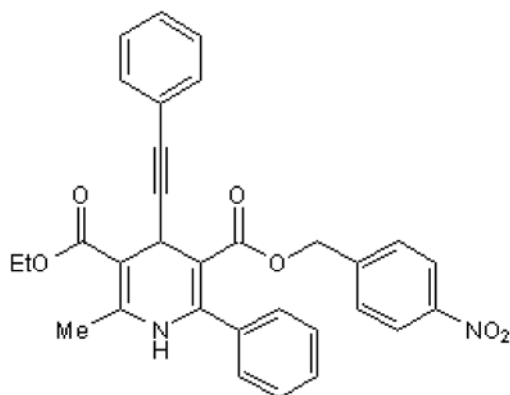
Batch Molecular Formula: C₃₁H₂₆N₂O₆

Batch Molecular Weight: 522.56

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

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.

Licensing Information:

Sold with the permission of the NIH, US Patent 60/029,855

References:

Corriden et al (2013) Adenosine-A₃ receptors in neutrophil microdomains promote the formation of bacteria-tethering cytonemes. *EMBO.Rep.* **14** 726. PMID: 23817552.

Baraldi and Borea (2000) New potent and selective human adenosine A₃ receptor antagonists. *TiPS* **21** 456. PMID: 11121831.

Li et al (1998) Structure-activity relationships and molecular modeling of 3,5-diacyl-2,4-dialkylpyridine derivatives as selective A₃ adenosine receptor antagonists. *J.Med.Chem.* **41** 3186. PMID: 9703464.

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