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IUPAC Name:

Print Date: Sep 25th 2023

Certificate of Analysis

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Batch No.: 3

Catalog No.: 6451

Product Name: Pexacerfont

459856-18-9 CAS Number:

8-(6-Methoxy-2-methyl-3-pyridinyl)-2,7-dimethyl-N-[(1R)-1-methylpropyl]pyrazolo[1,5-a]-1,3,5-triazin-4-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

 $C_{18}H_{24}N_6O$. 340.43 Off White solid DMSO to 100 mM ethanol to 100 mM Store at -20°C

Storage: **Batch Molecular Structure:**

NH

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: **Optical Rotation: Microanalysis:**

Shows 99.7% purity Consistent with structure Consistent with structure $[\alpha]_D$ = -28.6 (Concentration = 0.5, Solvent = Chloroform) Carbon Hydrogen Nitrogen Theoretical 63.51 7.11 24.69 Found 63.55 24.92 7.27

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

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8-(6-Methoxy-2-methyl-3-pyridinyl)-2,7-dimethyl-N-[(1R)-1-methylpropyl]pyrazolo[1,5-a]-1,3,5-triazin-4-amine

Description:

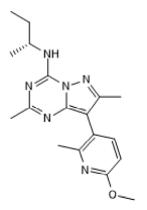
Pexacerfont is a potent and selective corticotropin-releasing factor 1 receptor (CRF₁) antagonist (IC₅₀ = 6.1 nM). Displays >150 fold selectivity for CRF₁ over CRF_{2b}. Inhibits CRF-mediated adrenocorticotropic hormone (ACTH) release from pituitary cell culture (IC₅₀ = 129 nM). Displays anxiolytic effects in rat behavioral paradigms.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{18}H_{24}N_6O$. Batch Molecular Weight: 340.43 Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Gilligan *et al* (2009) Synthesis and structure-activity relationships of 8-(pyrid-3-yl)pyrazolo[1,5-a]-1,3,5-triazines: potent, orally bioavailable corticotropin releasing factor receptor-1 (CRF₁) antagonists. J.Med.Chem. **52** 3084. PMID: 19361209.

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Storage: Store at -20°C

Solubility & Usage Info: DMSO to 100 mM

ethanol 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 $45-60^{\circ}C$ water bath).

Catalog No.: 6451

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.