

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: SB 297006 Catalog No.: 4213 Batch No.: 1

CAS Number: 58816-69-6

IUPAC Name: N-Benzoyl-4-nitroaniline ethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{18}N_2O_5$ Batch Molecular Weight:342.35Physical Appearance:White solid

Solubility: DMSO to 100 mM

ethanol to 20 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.4$ (Ethyl acetate:Petroleum ether [2:3])

HPLC: Shows >99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = -73.3$ (Concentration = 1.02, Solvent = Ethanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 63.15 5.3 8.18 Found 63.25 5.32 8.19



Product Information

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Description:

Potent and selective CCR3 antagonist (IC_{50} = 39 nM). Displays 250-fold selectivity for CCR3 over other chemokine receptors, including CXCR1, CXCR2, CCR1 and CCR7 (IC50 >27 µM). Inhibits calcium mobilization induced by MCP-4, eotaxin-2 and eotaxin in RBL-2H3 cells transfected with CCR3 (IC50 values are 80, 90 and 210 nM respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₈N₂O₅ Batch Molecular Weight: 342.35 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM ethanol to 20 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:

Yoshimoto and Hansch (1976) Quantitative structure-activity relationships of D- and L-N-actyl-alpha-aminoamide ligands binding to chymotrypsin. On the problem of combined treatment of stereoisomers. J.Org.Chem. 41 2269. PMID: 932854.

White et al (2000) Identification of a potent, selective non-peptide CC chemokine receptor-3 antagonist that inhibits eotaxin-, eotaxin-2-, and monocyte chemotactic protein-4-induced eosinophil migration. J.Biol.Chem. 275 36626. PMID: 10969084.

Tel: +44 (0)1235 529449