

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: BMS 753 Catalog No.: 3505 Batch No.: 1

CAS Number: 215307-86-1

IUPAC Name: 4-[[(2,3-Dihydro-1,1,3,3-tetramethyl-2-oxo-1*H*-inden-5-yl)carbonyl]amino]benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{21}NO_4$

Batch Molecular Weight: 351.4

Physical Appearance: Off-white solid **Solubility:** DMSO to 100 mM

ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:

HO₂C

2. ANALYTICAL DATA

TLC: $R_f = 0.2$ (Chloroform:Methanol [10:1])

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 71.78 6.02 3.99 Found 71.64 6.17 3.98



Product Information

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IUPAC Name: 4-[[(2,3-Dihydro-1,1,3,3-tetramethyl-2-oxo-1H-inden-5-yl)carbonyl]amino]benzoic acid

Description:

RAR α -selective agonist (K_i = 2 nM).

Physical and Chemical Properties:

Batch Molecular Formula: C21H21NO4 Batch Molecular Weight: 351.4 Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

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°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:

Taneja et al (1996) Cell-type and promoter-context dependent retinoic acid receptor (RAR) redundancies for RARB2 and Hoxa-1 activation in F9 and P19 cells can be artefactually generated by gene knockouts. Proc.Natl.Acad.Sci.USA 93 6197.

Dilworth et al (1999) Ligand-dependent activation of transcription in vitro by retinoid acid receptor α/retinoid X receptor α heterodimers that mimics transactivation by retinoids in vivo. Proc.Natl.Acad.Sci.USA 96 1995.

Gehin et al (1999) Structural basis for engineering of retinoic acid receptor isotype-selective agonists and antagonists. Chem. Biol. 6 519. PMID: 10421757.

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