

Certificate of Analysis

Print Date: Sep 5th 2019

www.tocris.com

Product Name: Bicalutamide Catalog No.: 3389 Batch No.: 1

CAS Number: 90357-06-5

IUPAC Name: N-[4-Cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{14}F_4N_2O_4S$

Batch Molecular Weight: 430.37

Physical Appearance: White solid

Solubility: DMSO to 100 mM

ethanol to 10 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point: Between 191 - 193°C

HPLC: Shows 99.9% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 50.23 3.28 6.51 Found 50.15 3.21 6.42

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



Product Information

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Description:

Orally active non-steroidal androgen receptor antagonist (IC_{50} = 190 nM). Displays peripheral selectivity and does not effect serum levels of LH and testosterone. Exhibits potent anticancer activity in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₄F₄N₂O₄S

Batch Molecular Weight: 430.37 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM ethanol to 10 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 for research purposes only under agreement from AstraZeneca

References:

Furr and Tucker (1996) The preclinical development of bicalutamide: pharmacodynamics and mechanism of action. Urology 47 13. PMID: 8560673.

Tucker *et al* (1988) Nonsteroidal antiandrogens. Synthesis and structure-activity relationships of 3-substituted derivatives of 2-hydroxypropionanilides. J.Med.Chem. *31* 954. PMID: 3361581.

Furr et al (1987) ICI 176,334: a novel non-steroidal, peripherally selective antiandrogen. J.Endocrinol. 113 R7. PMID: 3625091.