

Certificate of Analysis

Print Date: Nov 12th 2019

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Product Name: DY 268 Catalog No.: 5656 Batch No.: 1

CAS Number: 1609564-75-1

IUPAC Name: 1-[(3-Methoxyphenyl)methyl]-N-[4-methyl-3-(4-morpholinylsulfonyl)phenyl]-3-(4-methylphenyl)-1H-pyrazole-4-

carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₃₂N₄O₅S

Batch Molecular Weight: 560.66

Physical Appearance: White solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.5$ (Dichloromethane:Ethyl acetate [4:1])

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 64.27 5.75 9.99 Found 64.45 5.64 10

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



Product Information

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Description:

Potent FXR antagonist ($IC_{50} = 7.5$ nM). Exhibits no detectable cytotoxicity in cell-based assays.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{30}H_{32}N_4O_5S$

Batch Molecular Weight: 560.66 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

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.

Other Information:

INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 1 Home Office controlled substance and customers in the UK are required to hold the relevent licence or be exempt from restrictions in order to purchase and posess this material.

Licensing Information:

Sold under license from the Beckman Research Institute of the City of Hope.

References:

Yu et al (2014) Identification of trisubstituted-pyrazol carboxamide analogs as novel and potent antagonists of farnesoid X receptor. Bioorg.Med.Chem. 22 2919. PMID: 24775917.

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