

Certificate of Analysis

Print Date: Jul 20th 2016

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Product Name: CID 755673 Catalog No.: 3327 Batch No.: 3

CAS Number: 521937-07-5

IUPAC Name: 2,3,4,5-Tetrahydro-7-hydroxy-1*H*-benzofuro[2,3-*c*]azepin-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_{11}NO_3$ Batch Molecular Weight: 217.22

Physical Appearance: Off White solid **Solubility:** DMSO to 100 mM

ethanol to 5 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

Microanalysis:

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 66.35 5.1 6.45 Found 66.52 5.06 6.32



Product Information

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IUPAC Name: 2,3,4,5-Tetrahydro-7-hydroxy-1*H*-benzofuro[2,3-*c*]azepin-1-one

Description:

Selective protein kinase D (PKD) inhibitor (IC $_{50}$ values are 0.182, 0.280, 0.227, >10, 15.3, 20.3, 40.5 and >50 μ M at PKD1, PKD2, PKD3, PKC, CAK, PLK1, CAMKII α and Akt respectively). Blocks PKD-mediated protein transport and inhibits prostate cancer cell proliferation, migration and invasion in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₂H₁₁NO₃ Batch Molecular Weight: 217.22 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 5 mM with gentle warming

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:

Sharlow *et al* (2008) Potent and selective disruption of protein kinase D functionality by benzoxoloazepinolone. J.Biol.Chem. **283** 33516. PMID: 18829454.