

Certificate of Analysis

Product Name: kb NB 142-70

Catalog No.: 3962

Batch No.: 2

CAS Number: 1233533-04-4

IUPAC Name: 9-Hydroxy-3,4-dihydro-2*H*-[1]-benzothio[2,3-*f*][1,4]thiazepin-5-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₁H₉NO₂S₂·H₂O

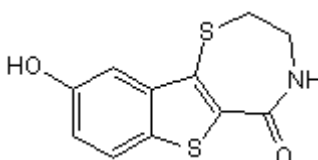
Batch Molecular Weight: 269.34

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.23 (Dichloromethane:Methanol [95:5])

HPLC: Shows >98% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.05	4.12	5.2
Found	48.86	3.96	5.31

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

Product Name: kb NB 142-70

Catalog No.: 3962

Batch No.: 2

CAS Number: 1233533-04-4

IUPAC Name: 9-Hydroxy-3,4-dihydro-2H-[1]-benzothio[2,3-f][1,4]thiazepin-5-one

Description:

Selective protein kinase D (PKD) inhibitor (IC₅₀ values are 28.3, 58.7 and 53.2 nM for PKD1, 2 and 3 respectively). More potent analog of CID 755673 (Cat. No. 3327) with 7-fold greater inhibition. Inhibits prostate cancer cell migration and invasion and reduces wound healing in vitro; displays prominent cytotoxic and anti-proliferative effects.

Physical and Chemical Properties:

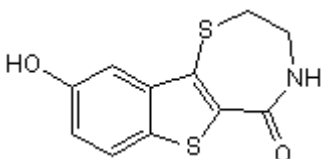
Batch Molecular Formula: C₁₁H₉NO₂S₂·H₂O

Batch Molecular Weight: 269.34

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

LaValle et al (2010) Novel protein kinase D inhibitors cause potent arrest in cancer cell growth and motility. *BMC Chemical Biology* **10** 5. PMID: 20444281.

Bravo-Altamirano et al (2011) Synthesis and structure-activity relationships of benzothienothiazepinone inhibitors of protein kinase D. *ACS Med.Chem.Lett.* **2** 154. PMID: 21617763.

Ni et al (2013) PKD1 mediates negative feedback of PI3K/Akt activation in response to G protein-coupled receptors. *PLoS One* **8** e73149. PMID: 24039875.

Storage: Store at RT

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.

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956