



Certificate of Analysis

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Product Name: CB 839 Catalog No.: 7591 Batch No.: 1

CAS Number: 1439399-58-2

IUPAC Name: N-[5-[4-[6-[[2-[3-(Trifluoromethoxy)phenyl]acetyl]amino]-3-pyridazinyl]butyl]-1,3,4-thiadiazol-2-yl]-2-

pyridineacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{24}F_3N_7O_3S$.

Batch Molecular Weight: 571.58 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.64 4.23 17.15 Found 54.49 4.19 17.11



Product Information

Print Date: Jan 24th 2022

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Description:

CB 839 is a potent non-competitive glutaminase (GLS1) inhibitor (IC $_{50}$ = 24 nM for recombinant human GAC). The compound exhibits selectivity for GLS1 over GLS2. CB 839 displays antiproliferative activity in a triple-negative breast cancer cell line (GI $_{50}$ values are 19 and 55 nM against MDA-MB-231 and HCC1806, respectively); it reduces glutamine consumption and glutamate production rates in HCC1806 cells. CB 839 displays significant antitumor activity as a single agent in a patient-derived TNBC xenografts model. CB 839 inhibits the growth of basal-like HER2 cell line JIMT-1 xenografts in mice, both as a single agent and in combination with Pacl... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₆H₂₄F₃N₇O₃S.

Batch Molecular Weight: 571.58 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°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.

References:

Zhou et al (2019) Estrogen inhibits autophagy and promotes growth of endometrial cancer by promoting glutamine metabolism. Cell Commun.Signal. **17** 99. PMID: 31429768.

Biancur *et al* (2017) Compensatory metabolic networks in pancreatic cancers upon perturbation of glutamine metabolism. Nat.Commun. *8* 15965. PMID: 28671190.

Momcilovic *et al* (2017) Targeted inhibition of EGFR and glutaminase induces metabolic crisis in EGFR mutant lung cancer. Cell Rep. **18** 601. PMID: 28099841.

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