

Product Name: BI 3231

Catalog No.: 8039

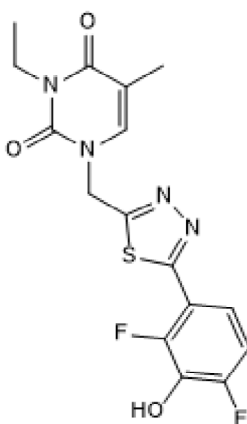
Batch No.: 1

CAS Number: 2894848-07-6

IUPAC Name: 1-[[5-(2,4-Difluoro-3-hydroxyphenyl)-1,3,4-thiadiazol-2-yl]methyl]-3-ethyl-5-methyl-2,4(1*H*,3*H*)pyrimidinedione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₄F₂N₄O₃S.
Batch Molecular Weight: 380.37
Physical Appearance: Off White solid
Solubility: DMSO to 10 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.0% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.52	3.71	14.73
Found	50.53	3.72	14.3

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

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Description:

BI 3231 is a potent and selective hydroxysteroid 17β dehydrogenase 13 (HSD17B13) inhibitor (IC₅₀ values are 1 nM and 13 nM at hHSD17B13 and mHSD17B13 respectively; K_i = 0.7 nM). Reduces palmitic acid-induced toxicity in hepatocytes. Suitable for use in vivo and in vitro.

Physical and Chemical Properties:

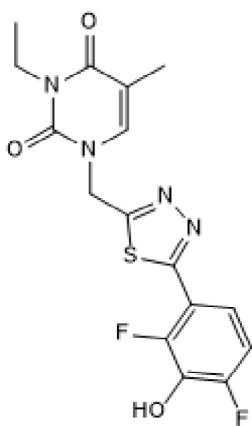
Batch Molecular Formula: C₁₆H₁₄F₂N₄O₃S.

Batch Molecular Weight: 380.37

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 10 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BI 3231 probe summary on the SGC website.

References:

Thamm *et al* (2023) Discovery of a novel potent and selective HSD17B13 inhibitor, BI-3231, a well-characterized chemical probe available for open science. *J.Med.Chem.* **66** 2832. PMID: 36727857.

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