Certificate of Analysis

Product Name: **iBET-BD2** **Catalog No.: 7458** **Batch No.: 1**

CAS Number: 2474876-09-8

IUPAC Name: 4-(Acetylamino)-3-fluoro-*N*-(*trans*-4-hydroxycyclohexyl)-5-[(1*S*)-1-phenylethoxy]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{27}FN_2O_4.½H_2O$

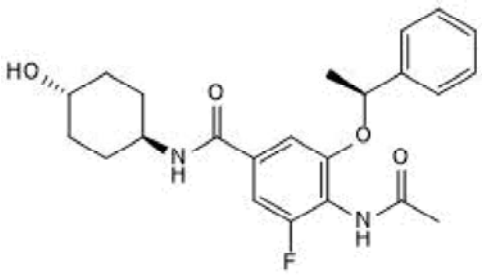
Batch Molecular Weight: 423.49

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

Chiral HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.23	6.66	6.62
Found	64.81	6.65	6.68

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Description:

iBET-BD2 is a potent and selective pan-BD2 inhibitor (IC_{50} values are 49, 98, 214 and 264 nM for BRD4BD2, BRD3BD2, BRDTBD2 and BRD2BD2, respectively). iBET-BD2 is selective for BD2 over BD1 (IC_{50} values are 10965, 36317, 70558, and >50119 µM for BRD2BD1, BRD3BD1, BRD4BD1, and BRDTBD1, respectively) in a time-resolved FRET (TR-FRET) assay. iBET-BD2 (1 µM) inhibits IFN-γ-induced protein expression of MHC class I in K562 cells. iBET-BD2 reduces the production of anti-KLH IgM antibodies in mice immunized with keyhole limpet hemocyanin (KLH). iBET-BD2 exhibits immunomodulatory activity. iBET-BD2 is orally bioavailable. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

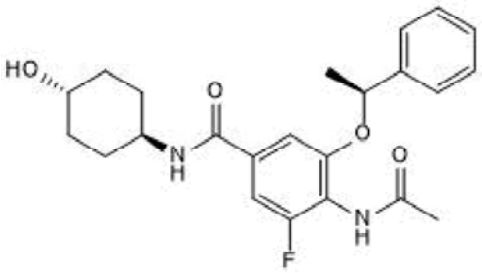
Batch Molecular Formula: $C_{23}H_{27}FN_2O_4.½H_2O$

Batch Molecular Weight: 423.49

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the iBET-BD2 probe summary on the SGC website.

References:

Gilan *et al* (2020) Selective targeting of BD1 and BD2 of the BET proteins in cancer and immunoinflammation. Science ***368*** 387. PMID: 32193360.

Preston *et al* (2020) Design and synthesis of a highly selective and *in vivo*-capable inhibitor of the second bromodomain of the bromodomain and extra terminal domain family of proteins. J.Med.Chem. ***63*** 9070. PMID: 32691591.