Certificate of Analysis

Product Name: **I-BET 151 dihydrochloride** **Catalog No.: 4650** **Batch No.: 6**

CAS Number: 1883545-47-8

IUPAC Name: 7-(3,5-Dimethyl-4-isoxazolyl)-1,3-dihydroxy-8-methoxy-1-[(1*R*)-1-(2-pyridinyl)ethyl]-2*H*-imidazo[4,5-*c*]quinolin-2-one dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{21}N_5O_3.2HCl.H_2O$

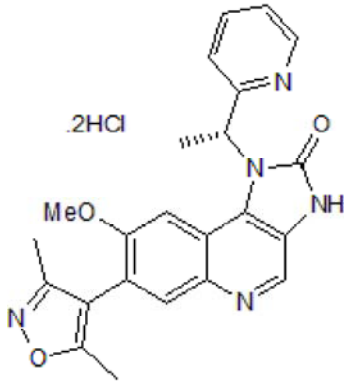
Batch Molecular Weight: 506.39

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM
water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.21 (Dichloromethane:Methanol [9:1] 7N NH3)

HPLC: Shows 99.0% purity

Chiral HPLC: Shows >99% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +41.8 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.55	4.98	13.83
Found	54.93	5.36	13.83

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Product Information

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Description:

I-BET 151 dihydrochloride is a BET bromodomain inhibitor; blocks recruitment of BET to chromatin. Induces apoptosis and G_0/G_1 cell cycle arrest in MLL-fusion leukemic cell lines in vitro (IC_{50} values are 15, 26, 120 and 192 nM for NOMO1, MV4;11, MOLM13 and RS4;11 cell lines respectively); reduces BCL2 expression in NOMO1 cells. Improves survival in two rodent models of MLL-fusion leukemia in vivo. Enhances differentiation of human iPSC into megakaryocytes. Also enhances fibroblast reprogramming to hiPSCs at low concentration. For more information about how I-BET 151 dihydrochloride may be used, see our protocol: Transdifferentiating Fibrob... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

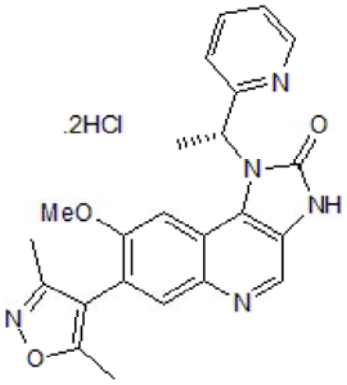
Batch Molecular Formula: $C_{23}H_{21}N_5O_3.2HCl.H_2O$

Batch Molecular Weight: 506.39

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 100 mM
water 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:

Sold for research purposes under agreement from GlaxoSmithKline

References:

Shao *et al* (2016) Reprogramming by de-bookmarking the somatic transcriptional program through targeting of BET bromodomains. Cell Rep. ***16*** 3138. PMID: 27653680 .

Feng *et al* (2014) Scalable generation of universal platelets from human induced pluripotent stem cells. Stem Cell Reports ***3*** 817. PMID: 25418726.

Dawson *et al* (2011) Inhibition of BET recruitment to chromatin as an effective treatment for MLL-fusion leukaemia. Nature ***478*** 529. PMID: 21964340.

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