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

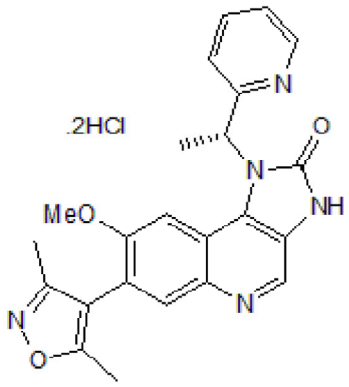
Batch Molecular Weight: 506.39

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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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. Used in protocol to differentiate fibroblasts directly into neurons (see below). For more information about how I-B... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

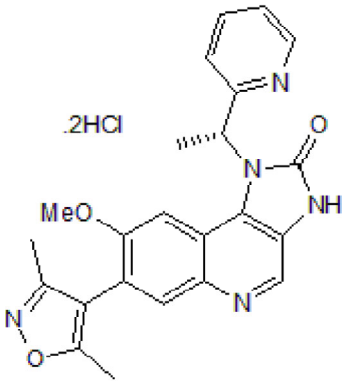
Batch Molecular Formula: $C_{23}H_{21}N_5O_3.2HCl.H_2O$

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. *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:

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.