

Product Name: ISOX DUAL

Catalog No.: 5806

Batch No.: 2

CAS Number: 1962928-22-8

IUPAC Name: [3-[4-[2-[5-(Dimethyl-1,2-oxazol-4-yl)-1-[2-(morpholin-4-yl)ethyl]-1*H*-1,3-benzodiazol-2-yl]ethyl]phenoxy]propyl]dimethylamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₁H₄₁N₅O₃·1/4H₂O

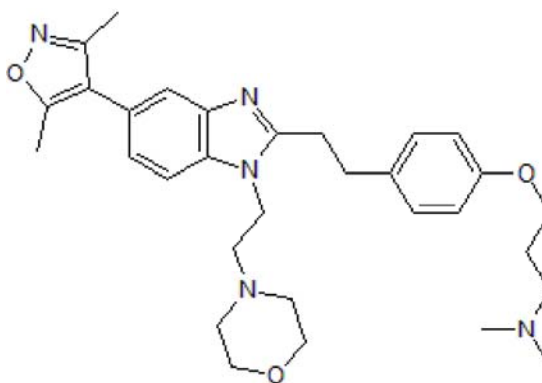
Batch Molecular Weight: 536.19

Physical Appearance: White solid

Solubility: 1eq. HCl to 100 mM
DMSO to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.69 (Dichloromethane:Methanol [9:1] with 0.5% NH₄OH)

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.44	7.8	13.06
Found	69.32	7.85	12.74

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Description:

Dual CBP/p300 and BRD4 bromodomain inhibitor (IC₅₀ values are 0.65 and 1.5 μM for CBP and BRD4 respectively). Downregulates IL-6, IL-1β and IFN-β in macrophages.

Physical and Chemical Properties:

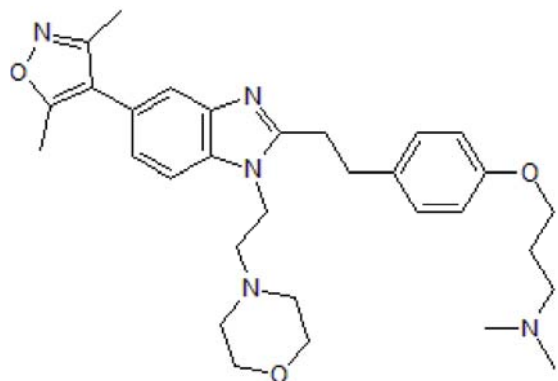
Batch Molecular Formula: C₃₁H₄₁N₅O₃·¼H₂O

Batch Molecular Weight: 536.19

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

1eq. HCl to 100 mM
DMSO to 50 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.

Other Information:

INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 1 Home Office controlled substance and customers in the UK are required to hold the relevant licence or be exempt from restrictions in order to purchase and possess this material.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Chekler (2015) Transcriptional profiling of a selective CREB binding protein bromodomain inhibitor highlights therapeutic opportunities. *Chem.Biol.* **22** 1588. PMID: 26670081.

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