bio-techne
TOCRIS

Print Date: Jul 24th 2024

Certificate of Analysis

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Product Name: **I-BET 762** **Catalog No.: 6521** **Batch No.: 1**

CAS Number: 1260907-17-2

IUPAC Name: (4*S*)-6-(4-Chlorophenyl)-*N*-ethyl-8-methoxy-1-methyl-4*H*-[1,2,4]triazolo[4,3-*a*][1,4]benzodiazepine-4-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{22}ClN_5O_2.¼H_2O$

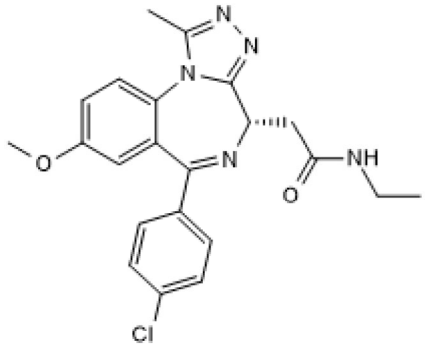
Batch Molecular Weight: 428.4

Physical Appearance: Beige solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +91.6 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.68	5.29	16.35
Found	61.8	5.29	16.13

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Description:

I-BET 762 is a potent and high affinity BET bromodomain inhibitor (IC_{50} = 32.5 - 42.5 nM; K_d = 50.5 - 61.3 nM). Inhibits myeloma cell proliferation. Attenuates transcription of oncogenic MYC and suppresses key inflammatory genes. Exhibits efficacy in a range of oncology and immunoinflammatory models. Displays antiproliferative effect in vitro and in vivo. Orally bioavailable.

Physical and Chemical Properties:

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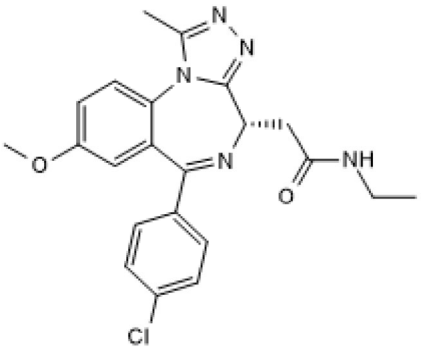
Minimum Purity: ≥98%

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. *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.

References:

Chaidos *et al* (2014) Potent antimyeloma activity of the novel bromodomain inhibitors I-BET151 and I-BET762. Blood ***123*** 697. PMID: 24335499.

Mirguet *et al* (2013) Discovery of epigenetic regulator I-BET762: lead optimization to afford a clinical candidate inhibitor of the BET bromodomains. J.Med.Chem. ***56*** 7501. PMID: 24015967.

Nicodeme *et al* (2010) Suppression of inflammation by a synthetic histone mimic. Nature ***468*** 1119. PMID: 21068722.