

Product Name: dBET6

Catalog No.: 6945

Batch No.: 1

CAS Number: 1950634-92-0

IUPAC Name: (6S)-4-(4-Chlorophenyl)-N-[8-[[2-[[2-(2,6-dioxo-3-piperidiny)-2,3-dihydro-1,3-dioxo-1H-isoindol-4-yl]oxy]acetyl]amino]octyl]-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine-6-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₂H₄₅ClN₈O₇S·½H₂O

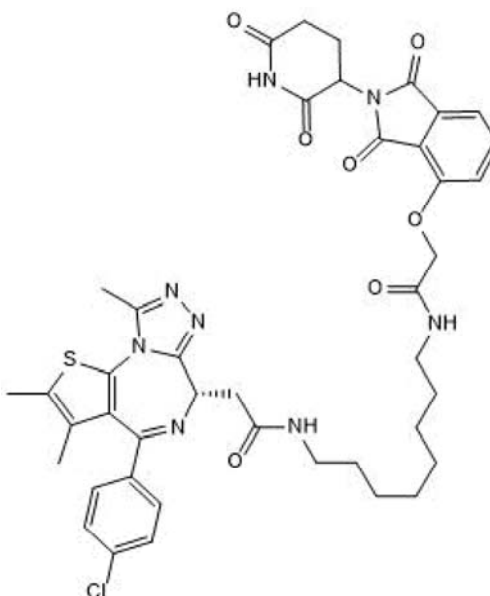
Batch Molecular Weight: 850.39

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 59.32 | 5.45 | 13.18 |
| Found | 58.9 | 5.46 | 13.06 |

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

dBET6 is a potent and selective Degradator (PROTAC®) of BET bromodomains (IC₅₀ = ~10 nM). dBET6 comprises BET antagonist (+)-JQ1 (Cat.No. 4499) conjugated to a cereblon E3 ubiquitin ligase ligand. Exhibits antitumor activity against T cell acute lymphoblastic leukemia (T-ALL) lines through BRD4 degradation. Induces apoptosis. Reduces leukemic burden in a mouse model of T-ALL. Cell permeable. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:

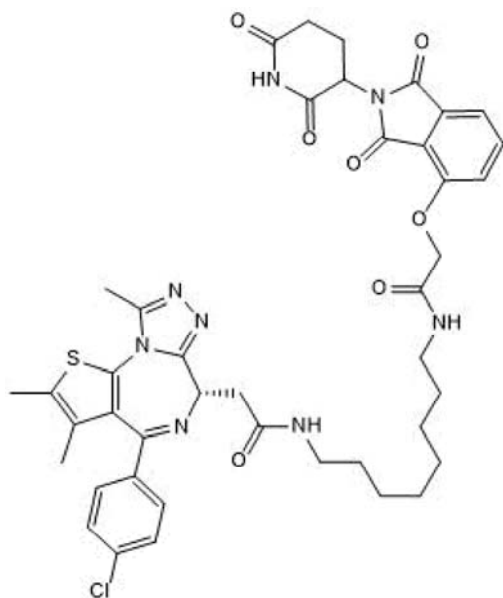
Batch Molecular Formula: C₄₂H₄₅ClN₈O₇S.½H₂O

Batch Molecular Weight: 850.39

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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 under license from Dana-Farber Cancer Institute

References:

Nowak et al (2018) Plasticity in binding confers selectivity in ligand-induced protein degradation. *Nat.Chem.Biol.* **14** 706. PMID: 29892083.

Verstovsek et al (2017) Targeting cistrome and dysregulated transcriptome of post-MPN sAML. *Oncotarget* **8** 93301. PMID: 29212143.

Winter et al (2017) BET Bromodomain proteins function as master transcription elongation factors independent of CDK9 recruitment. *Mol. Cell* **67** 5. PMID: 28673542.

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