Product Name: dBET1
Catalog No.: 6327
Batch No.: 1

CAS Number: 1799711-21-9

IUPAC Name: (6S)-4-(4-Chlorophenyl)-N-[4-[[2-[[2-(2,6-dioxo-3-piperidinyl)-2,3-dihydro-1,3-dioxo-1H-isooindol-4-yl]oxy]acetyl]amino]butyl]-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: C₃₈H₃₇ClN₈O₇S·1½H₂O
   Batch Molecular Weight: 807.79
   Physical Appearance: White solid
   Solubility: DMSO to 100 mM
   Storage: Store at -20°C
   Batch Molecular Structure:

2. ANALYTICAL DATA

   HPLC: Shows 99% purity
   ¹H NMR: Consistent with structure
   Mass Spectrum: Consistent with structure
   Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>56.5</td>
<td>4.93</td>
<td>13.87</td>
</tr>
<tr>
<td>Found</td>
<td>56.34</td>
<td>4.82</td>
<td>13.78</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: dBET1
Catalog No.: 6327
Batch No.: 1

Product Information
www.tocris.com

Description:
PROTAC comprising BET antagonist (+)-JQ1 (Cat.No. 4499) conjugated to a cereblon E3 ubiquitin ligase ligand. Depletes BET bromodomains in cancer cell lines in vitro (EC_{50} = 430 nM in breast cancer cells) and induces apoptosis. Delays tumor growth and downregulates MYC in mice bearing human AML xenografts.

Physical and Chemical Properties:
Batch Molecular Formula: C_{38}H_{37}ClN_{12}O_{12}S.1½H_{2}O
Batch Molecular Weight: 807.79
Physical Appearance: White solid
Minimum Purity: >98%

Solubility & Usage Info:
DMSO to 100 mM

Storage: Store at -20°C

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: