1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{38}H_{37}ClN_8O_7S.1\frac{1}{4}H_2O \)

Batch Molecular Weight: 807.79

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

![Molecular Structure]

2. ANALYTICAL DATA

HPLC: Shows 99% purity

\(^1\)H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

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

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-isoindol-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

Description:
dBET1 is a degrader (PROTAC®) comprising BET bromodomain antagonist (+)-JQ1 (Cat.No. 4499) conjugated to a cereblon E3 ubiquitin ligase ligand. Depletes BET bromodomains in cancer cell lines in vitro (EC₅₀ = 430 nM in breast cancer cells) and induces apoptosis. Delays tumor growth and downregulates MYC in mice bearing human AML xenografts. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license.

Physical and Chemical Properties:
Batch Molecular Formula: C₇₆H₆₂ClN₅O₁₁S.1¼H₂O
Batch Molecular Weight: 807.79
Physical Appearance: White solid
Minimum Purity: ≥98%

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: