1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{25}H_{24}F_{4}N_{4}O_{5} \cdot \frac{1}{2}H_{2}O \)
Batch Molecular Weight: 545.49
Physical Appearance: White solid
Solubility: DMSO to 100 mM, ethanol to 100 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.57 \) (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.9% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: \([\alpha]_D = +43.6\) (Concentration = 0.74, Solvent = Methanol)
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>55.05</td>
<td>4.62</td>
<td>10.27</td>
</tr>
<tr>
<td>Found</td>
<td>55</td>
<td>4.66</td>
<td>10.22</td>
</tr>
</tbody>
</table>
Description:
Potent and selective p300/CREB-binding protein (CBP) HAT domain inhibitor (IC\textsubscript{50} values are 2.6 and 9.8 nM for the CBP-bromodomain HAT-C/H3 (BHC) and p300-BHC domains, respectively). Displays > 1000-fold selectivity over closely related HATs. Suppresses proliferation in several hematological malignancies and AR\textsuperscript{+} prostate cancer cell lines in vitro. Inhibits tumor growth in a castration-resistant prostate cancer xenograft model. Orally bioavailable. To request the negative control for A 485, please fill out the A 486 request form on the SGC website. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:
Batch Molecular Formula: C\textsubscript{28}H\textsubscript{24}F\textsubscript{4}N\textsubscript{3}O\textsubscript{5}·\textfrac{1}{2}H\textsubscript{2}O
Batch Molecular Weight: 545.49
Physical Appearance: White solid
Minimum Purity: >98%

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. 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:
This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the A-485 probe summary on the SGC website.

References: