1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{22}\text{H}_{23}\text{N}_{5}\text{O}_{2}.3\text{H}_{2}\text{O} \)
Batch Molecular Weight: 443.5
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM, ethanol to 100 mM
Storage: Desiccate at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.19 \) (Dichloromethane:Methanol [9:1])
HPLC: Shows >99.6% purity
\( ^1\text{H} \) NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis: Carbon Hydrogen Nitrogen

<table>
<thead>
<tr>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>59.58</td>
<td>59.7</td>
</tr>
<tr>
<td>6.59</td>
<td>6.3</td>
</tr>
<tr>
<td>15.79</td>
<td>15.94</td>
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</tbody>
</table>
Description:
Potent inhibitor of the H3K27 histone demethylases JMJD3 (KDM6B) and UTX (KDM6A) (IC_{50} values are 28 and 53 nM respectively). Also inhibits KDM5B, KDM5C and KDM5A (IC_{50} values are 170, 550 and 6,800 nM respectively). Exhibits no activity against a panel of other histone demethylases (IC_{50} >20 μM), and displays no significant inhibitory activity against 100 protein kinases at a concentration of 30 μM. Ethyl ester derivative and Negative Control also available.

Physical and Chemical Properties:
Batch Molecular Formula: C_{22}H_{32}N_{6}O_{2}.3H_{2}O
Batch Molecular Weight: 443.5
Physical Appearance: Off-white solid
Minimum Purity: >99%

Storage: Desiccate at RT

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 GSK J1 probe summary on the SGC website.

References: