1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  \(\text{C}_{30}\text{H}_{47}\text{N}_5\text{O}_2.3\text{H}_2\text{O}\)
Batch Molecular Weight:  523.24
Physical Appearance:  White solid
Solubility:  DMSO to 100 mM
              ethanol to 100 mM
              1eq. HCl to 100 mM
Storage:  Store at +4°C

2. ANALYTICAL DATA

TLC:  \(R_f = 0.3\) (Dichloromethane:Methanol:Ammonia soln. [90:9:1])
HPLC:  Shows 99.7% purity
\(^1\text{H NMR:}\)  Consistent with structure
Mass Spectrum:  Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
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<th>Found</th>
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<tbody>
<tr>
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<tr>
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Product Name: UNC 0638
Catalog No.: 4343  Batch No.: 1

CAS Number: 1255517-77-1
IUPAC Name: 2-Cyclohexyl-6-methoxy-N-[1-(1-methylethyl)-4-piperidinyl]-7-[3-(1-pyrrolidinyl)propoxy]-4-quinazolinamine

Description:
Selective inhibitor of G9a and GLP histone lysine methyltransferases (IC₅₀ values are < 15 nM and 19 nM for G9a and GLP respectively, and > 10000 nM for a range of other histone methyltransferases). Potently inhibits dimethylation of H3K9 in MCF-7 cells (IC₅₀ = 70 nM). Cell permeable.

Physical and Chemical Properties:
Batch Molecular Formula: CₓHᵧNₓOₜ½H₂O
Batch Molecular Weight: 523.24
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 100 mM
1eq. HCl 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.

References: