1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{24}\text{H}_{20}\text{F}_{3}\text{N}_{5}\text{O}_{0.5}\text{H}_{2}\text{O} \)

Batch Molecular Weight: 460.45

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99% purity

\(^1\text{H}\) 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>62.6</td>
<td>62.35</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.6</td>
<td>4.6</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>15.21</td>
<td>15.18</td>
</tr>
</tbody>
</table>
Product Name: GSK 2606414
CAS Number: 1337531-36-8
IUPAC Name: 1-[5-(4-Amino-7-methyl-7H-pyrrolo[2,3-d]pyrimidin-5-yl]-2,3-dihydro-1H-indol-1-yl]-2-[3-(trifluoromethyl)phenyl]ethanone

Description:
Potent and selective protein kinase R-like ER kinase (PERK) inhibitor (IC₅₀ = 0.4 nM). Exhibits >1000-fold selectivity for PERK over HR1 and PKR. Inhibits thapsigargin-induced PERK phosphorylation in lung carcinoma A549 cells. Attenuates subcutaneous pancreatic human tumor xenograft growth in mice. Orally bioavailable.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₉H₂₉F₃N₅O.½H₂O
Batch Molecular Weight: 460.45
Physical Appearance: Off White solid
Minimum Purity: >99%

Batch Molecular Structure:

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 for research purposes only under agreement from GlaxoSmithKline

References: