Product Name: AC 5216
Catalog No.: 5281
Batch No.: 3
CAS Number: 226954-04-7
IUPAC Name: N-Ethyl-7,8-dihydro-7-methyl-8-oxo-2-phenyl-N-(phenylmethyl)-9H-purine-9-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{23}\text{H}_{23}\text{N}_{5}\text{O}_{2} \)
Batch Molecular Weight: 401.46
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 99.5% purity
\(^1\text{H NMR:}\) Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>68.81</td>
<td>5.77</td>
</tr>
<tr>
<td>Found</td>
<td>68.83</td>
<td>5.75</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: AC 5216
CAS Number: 226954-04-7
IUPAC Name: N-Ethyl-7,8-dihydro-7-methyl-8-oxo-2-phenyl-N-(phenylmethyl)-9H-purine-9-acetamide

Description:
Ligand of translocator protein (TSPO, peripheral benzodiazepine receptor). Exhibits high affinity for TSPO in rat whole brain ($K_i = 0.297$ nM), and high potency against human and rat glial TSPO ($IC_{50}$ values are 2.73 and 3.04 nM respectively). Displays no noticeable binding to a number of other receptors, transporters or ion channels. Also displays anxiolytic and antidepressant effects in rodent models, without inducing benzodiazepine-like adverse effects.

Physical and Chemical Properties:
Batch Molecular Formula: $C_{22}H_{12}N_2O_2$
Batch Molecular Weight: 401.46
Physical Appearance: White solid
Minimum Purity: >98%

References:

Storage: Store at +4°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.