Product Name: 8-(3-Chlorostyryl)caffeine
Catalog No.: 3306
Batch No.: 1
CAS Number: 147700-11-6
IUPAC Name: (E)-8-[2-(3-Chlorophenyl)ethenyl]-3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: \( \text{C}_{16}\text{H}_{15}\text{ClN}_{4}\text{O}_{2} \)
   Batch Molecular Weight: 330.77
   Physical Appearance: Pale yellow solid
   Solubility: DMSO to 25 mM
   Storage: Store at -20°C
   Batch Molecular Structure:

![Chemical Structure]

2. ANALYTICAL DATA

   HPLC: Shows >99.9% purity
   \(^1^H\) NMR: Consistent with structure
   Mass Spectrum: Consistent with structure
   Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
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<tr>
<td>Hydrogen</td>
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<td>Nitrogen</td>
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<td>16.81</td>
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</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: 8-(3-Chlorostyrlyl)caffeine
Catalog No.: 3306
Batch No.: 1

CAS Number: 147700-11-6
IUPAC Name: (E)-8-[2-(3-Chlorophenyl)ethenyl]-3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione

Description:
Selective adenosine A₂A receptor antagonist and monoamine oxidase B (MAO-B) inhibitor (Kᵢ values are 54 and 28200 nM at rat A₂A and A₁ receptors respectively and Kᵢ ~ 100 nM at MAO-B). Potently protects against quinolinic acid-induced (Cat. No. 0225) neuronal damage and is neuroprotective in the MPTP model of Parkinson's disease.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₈H₁₅ClN₅O₂
Batch Molecular Weight: 330.77
Physical Appearance: Pale yellow solid
Minimum Purity: >99%

Storage: Store at -20°C
CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:
DMSO to 25 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: