Print Date: Nov 26th 2019

Certificate of Analysis

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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-1*H*-purine-2,6-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{15}ClN_4O_2$

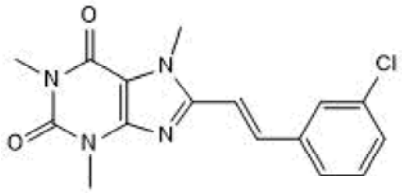
Batch Molecular Weight: 330.77

Physical Appearance: Pale yellow solid

Solubility: DMSO to 25 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.1	4.57	16.94
Found	57.91	4.52	16.81

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Product Information

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Description:

Selective adenosine A_{2A} receptor antagonist and monoamine oxidase B (MAO-B) inhibitor (K_i values are 54 and 28200 nM at rat A_{2A} and A_1 receptors respectively and K_i ~ 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:

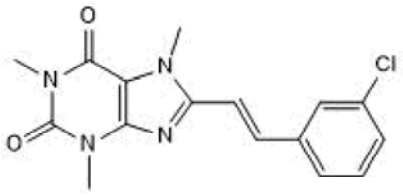
Batch Molecular Formula: $C_{16}H_{15}ClN_4O_2$

Batch Molecular Weight: 330.77

Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



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:

Vlok *et al* (2006) Inhibition of monoamine oxidase B by analogues of the adenosine A2A receptor antagonist (*E*)-8-(3-chlorostyryl) caffeine (CSC). Bioorg.Med.Chem. ***14*** 3512. PMID: 16442801.

Behan and Stone (2002) Enhanced neuronal damage by co-administration of quinolinic acid and free radicals, and protection by adenosine A_{2A} receptor antagonists. Br.J.Pharmacol. ***135*** 1435. PMID: 11906956.

Chen *et al* (2002) 8-(3-Chlorostyryl)caffeine may attenuate MPTP neurotoxicity through dual actions on monoamine oxidase inhibition and A_{2A} receptor antagonism. J.Biol.Chem. ***277*** 36040. PMID: 12130655.