Certificate of Analysis

Product Name: **TCS 5861528** **Catalog No.: 3938** **Batch No.: 1**

CAS Number: 332117-28-9

IUPAC Name: 2-(1,3-Dimethyl-2,6-dioxo-1,2,3,6-tetrahydro-7*H*-purin-7-yl)-*N*-[4-(1-methylpropyl)phenyl]acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{23}N_5O_3$

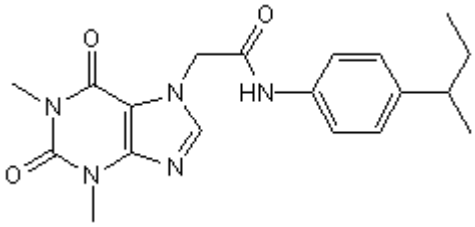
Batch Molecular Weight: 369.42

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 10 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.77	6.28	18.96
Found	61.52	6.13	18.9

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Description:

TRPA1 channel blocker that antagonizes AITC- and 4-HNE-evoked calcium influx (IC_{50} values are 14.3 and 18.7μM respectively). Attenuates diabetic hypersensitivity in an in vivo rat model.

Physical and Chemical Properties:

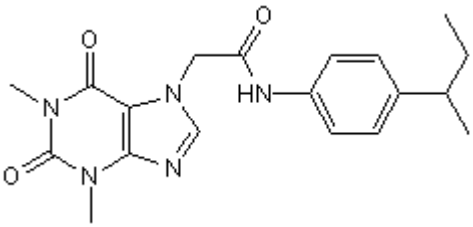
Batch Molecular Formula: $C_{19}H_{23}N_5O_3$

Batch Molecular Weight: 369.42

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 10 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:

Wei *et al* (2010) Roles of cutaneous versus spinal TRPA1 channels in mechanical hypersensitivity in the diabetic or mustard oil-treated non-diabetic rat. Neuropharmacology. ***58*** 578. PMID: 20004676.

Wei *et al* (2010) Spinal TRPA1 ion channels contribute to the cutaneous neurogenic inflammation in the rat. Neurosci.Letts. ***479*** 253.

Wei *et al* (2009) Attenuation of mechanical hypersensitivity by an antagonist of the TRPA1 ion channel in diabetic animals. Anesthesiology ***111*** 147. PMID: 19512877.

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