# TOCRIS a biotechne brand

### Print Date: Jan 4th 2022

## **Certificate of Analysis**

## www.tocris.com

## Product Name: VCP 171

Catalog No.: 6261

Batch No.: 1

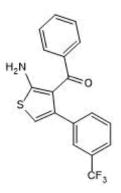
CAS Number: IUPAC Name: 1018830-99-3

ne: [2-Amino-4-[3-(trifluoromethyl)phenyl]-3-thienyl]phenylmethanone

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C<sub>18</sub>H<sub>12</sub>F<sub>3</sub>NOS. 347.35 Pale yellow solid DMSO to 100 mM ethanol to 100 mM Store at -20°C

## Storage: Batch Molecular Structure:



## 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis:

Shows 99.8% purity							
Consistent with structure							
Consistent with structure							
Carbon Hydrogen Nitrogen							
Theoretica	l 62.24	3.48	4.03				
Found	61.86	3.24	3.98				

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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## **Product Information**

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## Product Name: VCP 171

CAS Number: 1018830-99-3 IUPAC Name: [2-Amino-4-[3-(trifluoromethyl)pl

[2-Amino-4-[3-(trifluoromethyl)phenyl]-3-thienyl]phenylmethanone

### Description:

VCP 171 is an adenosine  $A_1$  receptor positive allosteric modulator (PAM) (pK<sub>B</sub> = 5.65, binding cooperativity with NECA 0.68). In absence of orthosteric agonist, VCP171 behaves as an allosteric partial agonist, inhibiting cAMP activity. Inhibits AMPA receptor-mediated evoked excitatory postsynaptic current (eEPSC) amplitude in lamina I and II neurons in a rat partial nerve-injury model of neuropathic pain.

#### **Physical and Chemical Properties:**

Batch Molecular Formula:  $C_{18}H_{12}F_3NOS$ . Batch Molecular Weight: 347.35 Physical Appearance: Pale yellow solid

#### Minimum Purity: ≥98%

#### **Batch Molecular Structure:**

H<sub>2</sub>N S CF<sub>3</sub>

### **References:**

**Christopoulos** *et al* (2016) Role of the second extracellular loop of the adenosine A<sub>1</sub> receptor on allosteric modulator binding, signaling, and cooperativity. Mol.Pharmacol. **90** 715. PMID: 27683013.

**Imlach** *et al* (2015) A positive allosteric modulator of the adenosine A<sub>1</sub> receptor selectively inhibits primary afferent synaptic transmission in a neuropathic pain model. Mol.Pharmacol. **88** 460. PMID: 26104547.

**Aurelio** *et al* (2008) 5-Substituted 2-aminothiophenes as A<sub>1</sub> adenosine receptor allosteric enhancers. Bioorg.Med.Chem. **16** 1319. PMID: 17980606.

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#### Storage: Store at -20°C

#### Solubility & Usage Info: DMSO to 100 mM

ethanol to 100 mM

#### **Stability and Solubility Advice:**

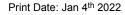
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a  $45-60^{\circ}C$  water bath).

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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.



Batch No.: 1