TOCRIS
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Print Date: Aug 22nd 2022

Certificate of Analysis

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Product Name: **JNJ 55511118** **Catalog No.: 6278** **Batch No.: 1**

CAS Number: 2036081-86-2

IUPAC Name: 5-[2-Chloro-6-(trifluoromethoxy)phenyl]-1,3-dihydro-2*H*-benzimidazol-2-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_8ClF_3N_2O_2$

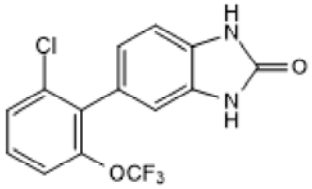
Batch Molecular Weight: 328.67

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.23 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.16	2.45	8.52
Found	51.03	2.31	8.34

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Product Information

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IUPAC Name: 5-[2-Chloro-6-(trifluoromethoxy)phenyl]-1,3-dihydro-2*H*-benzimidazol-2-one

Description:

JNJ 55511118 is a high affinity and selective negative modulator of AMPA receptors containing TARP-γ8 (K_i = 26 nM). Exhibits <50% binding against a panel of 52 receptors, ion channels and transporters (except $5HT_{2B}$ and melatonin receptors 78% and 57%, respectively). Also displays minimal activity against other TARP-less AMPARs and AMPARs coexpressed with other TARPs or CNIH2. It reduces alcohol self-administration in a mouse models of chronic drinking. Orally bioavailable and brain penetrant. Anticonvulsant.

Physical and Chemical Properties:

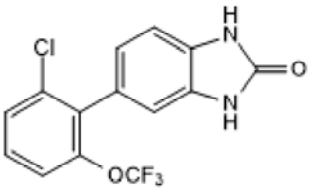
Batch Molecular Formula: $C_{14}H_8ClF_3N_2O_2$

Batch Molecular Weight: 328.67

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

USE WITH CARE; NOT FULLY TESTED - YOUR SUBLICENSE UNDER CERTAIN PATENT RIGHTS OF JANSSEN PHARMACEUTICA N.V. RESTRICTS USE TO INTERNAL RESEARCH ONLY - MAY NOT BE USED IN HUMANS - MAY NOT BE SOLD, TRANSFERRED, OR USED IN COMMERCIAL SERVICES.

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.

Licensing Information:

Sold with the permission of Janssen Pharmaceutica N.V.

References:

Hoffman (2021) Inhibition of AMPA receptors (AMPARs) containing transmembrane AMPAR regulatory protein γ-8 with JNJ-55511118 shows preclinical efficacy in reducing chronic repetitive alcohol self-administration. Alcohol Clin.Exp.Res. ***45*** 1424. PMID: 34086361.

Maher *et al* (2016) Discovery and Characterization of AMPA Receptor Modulators Selective for TARP-γ8. J.Pharmacol.Exp.Ther. ***357*** 394. PMID: 26989142.

Witkin *et al* (2016) A Comment on "Discovery and Characterization of AMPA Receptor Modulators Selective for TARP-γ8". J.Pharmacol.Exp.Ther. ***358*** 502. PMID: 27528544.