# **Certificate of Analysis**

# www.tocris.com

# Product Name: Squarunkin A hydrochloride

Catalog No.: 6364 Bat

Batch No.: 2

CAS Number: 2253744-55-5

IUPAC Name: Ethyl 4-((3,4-dioxo-2-((2-(4-(3-(trifluoromethyl)phenyl)piperazin-1-yl)ethyl)amino)cyclobut-1-en-1-yl)amino) piperidine-1-carboxylate hydrochloride

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance:

TOCR

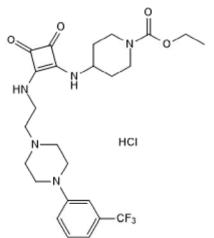
a biotechne

Solubility:

Storage:

**Batch Molecular Structure:** 

 $C_{25}H_{32}F_3N_5O_4.HCI.\frac{1}{2}H_2O$ 569.02 White solid DMSO to 50 mM Store at -20°C



## 2. ANALYTICAL DATA

HPLC:	Shows 99.7% purity			
<sup>1</sup> H NMR:	Consistent with structure			
Mass Spectrum:	Consistent with structure Carbon Hydrogen Nitrogen			
Microanalysis:				
	Theoretical 52.77 6.02	. 12.31		
	Found 52.72 6	12.29		

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

bio-techne.com	North America	China	Europe Middle East Africa	Rest of World
info@bio-techne.com techsupport@bio-techne.com	Tel: (800) 343 7475	info.cn@bio-techne.com Tel: +86 (21) 52380373	Tel: +44 (0)1235 529449	www.tocris.com/distributors Tel:+1 612 379 2956



2

# www.tocris.com

## Product Name: Squarunkin A hydrochloride

CAS Number: 2253744-55-5

IUPAC Name: Ethyl 4-((3,4-dioxo-2-((2-(4-(3-(trifluoromethyl)phenyl)piperazin-1-yl)ethyl)amino)cyclobut-1-en-1-yl)amino) piperidine-1-carboxylate hydrochloride

#### **Description:**

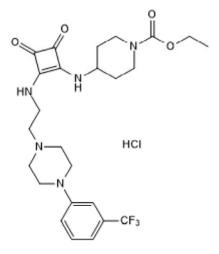
Squarunkin A hydrochloride is a potent inhibitor of UNC119 chaperone protein-cargo interaction ( $IC_{50} = 10$  nM for inhibition of UNC119A - myristoylated Src N-terminal peptide interaction). Disrupts activation of Src kinase in vitro.

## **Physical and Chemical Properties:**

Batch Molecular Formula:  $C_{25}H_{32}F_3N_5O_4$ .HCl.½ $H_2O$ Batch Molecular Weight: 569.02 Physical Appearance: White solid

#### Minimum Purity: ≥98%

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



Storage: Store at -20°C

## Solubility & Usage Info:

DMSO to 50 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).

Catalog No.: 6364

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:**

Mejuch et al (2017) Small-molecule inhibition of the UNC119-cargo interaction. Angew. Chem. Int. Ed. 56 6181. PMID: 28471079.

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