Certificate of Analysis

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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

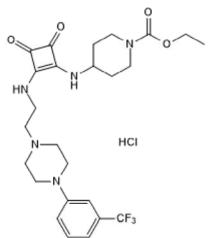
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Solubility:

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			
¹ 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

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Description:

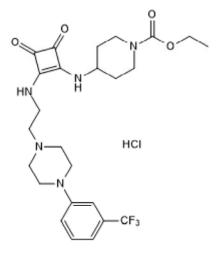
Squarunkin A hydrochloride is a potent inhibitor of UNC119 chaperone protein-cargo interaction ($IC_{50} = 10$ nM for inhibition of UNC119A - myristoylated Src N-terminal peptide interaction). Disrupts activation of Src kinase in vitro.

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.

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