

Product Name: Squarunkin A hydrochloride

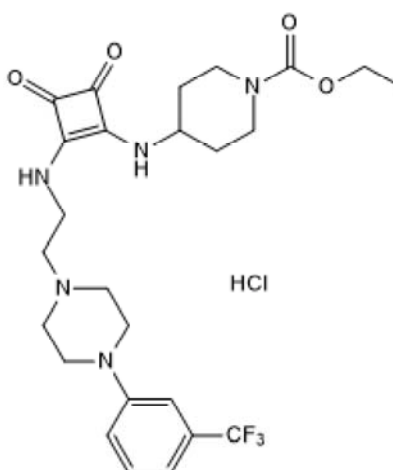
Catalog No.: 6364

Batch No.: 2

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: C₂₅H₃₂F₃N₅O₄.HCl.½H₂O
Batch Molecular Weight: 569.02
Physical Appearance: White solid
Solubility: DMSO to 50 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.77	6.02	12.31
Found	52.72	6	12.29

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Description:

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:

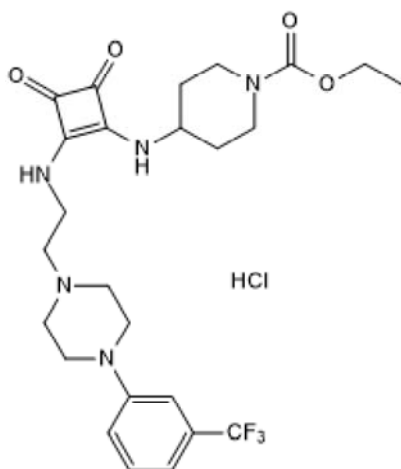
Batch Molecular Formula: $C_{25}H_{32}F_3N_5O_4 \cdot HCl \cdot \frac{1}{2}H_2O$

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°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:

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

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