bio-techne
TOCRIS

Print Date: Apr 5th 2023

Certificate of Analysis

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Product Name: **SCIO 469 hydrochloride** **Catalog No.: 3528** **Batch No.: 1**

CAS Number: 2387505-88-4

IUPAC Name: 6-Chloro-5-[[(2*R*,5*S*)-4-[(4-fluorophenyl)methyl]-2,5-dimethyl-1-piperazinyl]carbonyl]-*N*,*N*,1-trimethyl-α-oxo-1*H*-Indole-3-acetamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{30}ClFN_4O_3.HCl.¾H_2O$

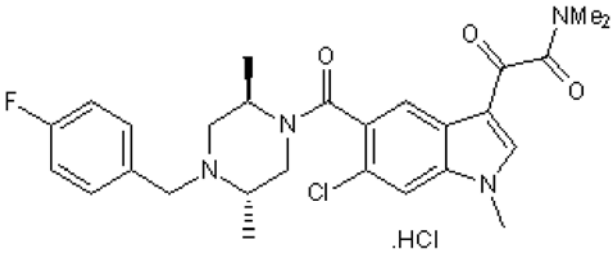
Batch Molecular Weight: 562.97

Physical Appearance: White solid

Solubility: water to 10 mM
DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Ethanol:Acetic acid)

HPLC: Shows 98.8% purity

Chiral HPLC: Shows 99.3% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +22.9 (Concentration = 1.04, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.6	5.82	9.95
Found	57.83	5.77	9.74

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Description:

SCIO 469 hydrochloride is a selective, ATP-competitive p38 inhibitor (IC_{50} = 9 nM for p38α in vitro). Displays approximately 10-fold selectivity for p38α over p38β and 2000-fold selectivity for p38α over 20 other kinases. Reduces p38α phosphorylation in multiple myeloma cells in vitro and in vivo; activity results in decreased tumor burden and angiogenesis in murine models of multiple myeloma. Also enhances bortezomib-induced cytotoxicity against multiple myeloma cells.

Physical and Chemical Properties:

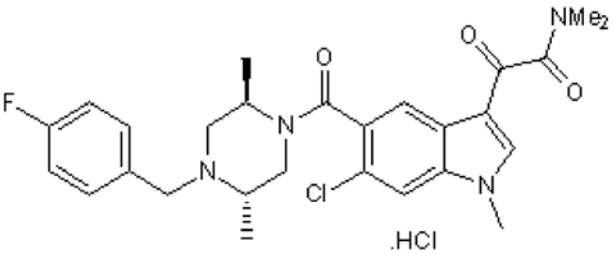
Batch Molecular Formula: $C_{27}H_{30}ClFN_4O_3.HCl.¾H_2O$

Batch Molecular Weight: 562.97

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 10 mM
DMSO 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°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:

Vanderkerken *et al* (2007) Inhibition of p38α mitogen-activated protein kinase prevents the development of osteolytic bone disease, reduces tumor burden, and increases survival in murine models of multiple myeloma. Cancer Res. ***67*** 4572. PMID: 17495322.

Giafis *et al* (2006) Role of the p38 mitogen-activated protein kinase pathway in the generation of arsenic trioxide-dependent cellular responses. Cancer Res. ***66*** 6763. PMID: 16818652.

Hideshima *et al* (2004) p38 MAPK inhibition enhances PS-341 (bortezomib)-induced cytotoxicity against multiple myeloma cells. Oncogene. ***23*** 8766. PMID: 15480425.