

Product Name: A01

Catalog No.: 5397

Batch No.: 1

CAS Number: 1007647-73-5

IUPAC Name: [4-[4-Chloro-3-(trifluoromethyl)phenyl]sulfonyl]-1-piperazinyl][4-(5-methyl-1H-pyrazol-1-yl)phenyl]methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₀ClF₃N₄O₃S

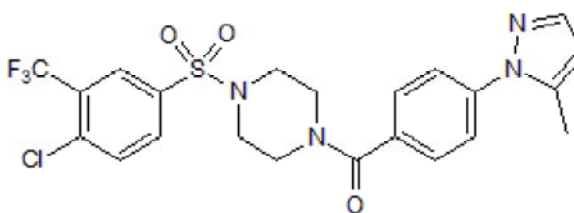
Batch Molecular Weight: 512.93

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.51	3.93	10.92
Found	51.31	3.9	10.87

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

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Description:

High affinity Smurf1 E3 ubiquitin ligase inhibitor ($K_d = 3.7$ nM). Attenuates Smurf1-mediated Smad 1/5 degradation and enhances BMP signaling. Potentiates BMP-2-induced osteoblastic activity in C2C12 myoblasts and MC3T3-E1 osteoblast precursor cells.

Physical and Chemical Properties:

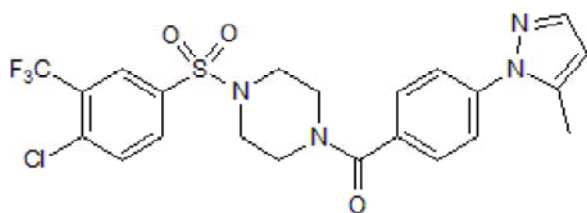
Batch Molecular Formula: $C_{22}H_{20}ClF_3N_4O_3S$

Batch Molecular Weight: 512.93

Physical Appearance: Off White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

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:

Cao et al (2014) Selective small molecule compounds increase BMP-2 responsiveness by inhibiting Smurf1-mediated Smad1/5 degradation. *Sci.Rep.* **4** 4965. PMID: 24828823.

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