

Product Name: AL 8697

Catalog No.: 4753

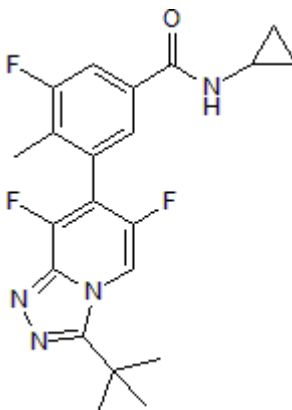
Batch No.: 2

CAS Number: 1057394-06-5

IUPAC Name: *N*-Cyclopropyl-3-[3-(1,1-dimethylethyl)-6,8-difluoro-1,2,4-triazolo[4,3-*a*]pyridin-7-yl]-5-fluoro-4-methylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₁F₃N₄O
Batch Molecular Weight: 402.41
Physical Appearance: White solid
Solubility: DMSO to 100 mM
ethanol to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.56 (Dichloromethane:Methanol [95:5])
HPLC: Shows 99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.68	5.26	13.92
Found	62.62	5.15	13.97

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

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Description:

Potent and selective p38 α inhibitor (IC₅₀ = 6 nM). Exhibits 14-fold greater inhibition of p38 α compared to p38 β ; also displays 300-fold selectivity for p38 α compared to a panel of 91 kinases. Exhibits anti-inflammatory properties.

Physical and Chemical Properties:

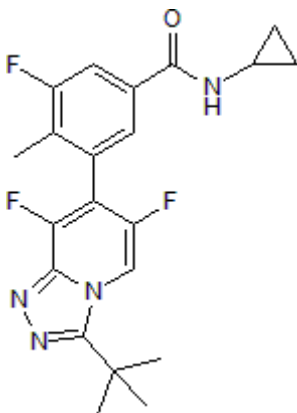
Batch Molecular Formula: C₂₁H₂₁F₃N₄O

Batch Molecular Weight: 402.41

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Balagué *et al* (2012) Profiling of dihydroorotate dehydrogenase, p38 and JAK inhibitors in the rat adjuvant-induced arthritis model: a translational study. *Br.J.Pharmacol.* **166** 1320. PMID: 22229697.

Aiguadé *et al* (2012) Novel triazolopyridylbenzamides as potent and selective p38 α inhibitors. *Bioorg.Med.Chem.Lett.* **22** 3431. PMID: 22521646.

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