

Product Name: TC JL 37

Catalog No.: 6125

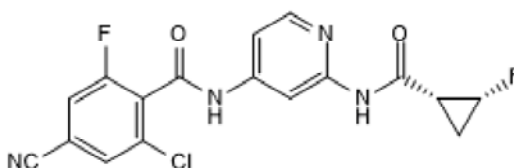
Batch No.: 1

CAS Number: 1258294-34-6

IUPAC Name: 2-Chloro-4-cyano-6-fluoro-N-[2-[[[(1R,2R)-2-fluorocyclopropyl]carbonyl]amino]-4-pyridinyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₁ClF₂N₄O₂
Batch Molecular Weight: 376.74
Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.19 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 99.1% purity
Chiral HPLC: Shows 98.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.2	2.94	14.87
Found	54.24	3.05	14.55

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Description:

Potent inhibitor of tyrosine kinase 2 (TYK2, $K_i = 1.6$ nM). Shows some selectivity for TYK2 over JAK1/2/3. Inhibits IFN γ production in vivo in mice. Orally bioavailable.

Physical and Chemical Properties:

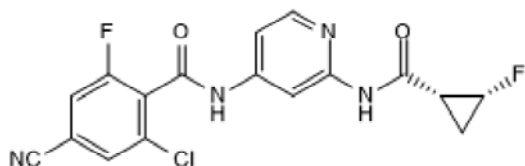
Batch Molecular Formula: C₁₇H₁₁ClF₂N₄O₂

Batch Molecular Weight: 376.74

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

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:

Liang *et al* (2013) Lead optimization of a 4-aminopyridine benzamide scaffold to identify potent, selective, and orally bioavailable TYK2 inhibitors. *J.Med.Chem.* **56** 4521. PMID: 23668484.

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