

Product Name: Upadacitinib

Catalog No.: 7783

Batch No.: 2

CAS Number: 1310726-60-3

IUPAC Name: (3*S*,4*R*)-3-Ethyl-4-(3*H*-imidazo[1,2-*a*]pyrrolo[2,3-*e*]pyrazin-8-yl)-*N*-(2,2,2-trifluoroethyl)-1-pyrrolidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₉F₃N₆O.¼H₂O

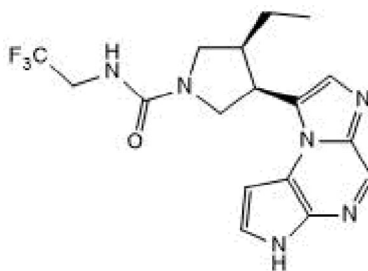
Batch Molecular Weight: 384.87

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol 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	53.05	5.11	21.84
Found	52.41	5.2	21.23

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Description:

Upadacitinib is a potent and selective JAK1 inhibitor (IC₅₀ = 47 nM). In a cellular assay, Upadacitinib shows selectivity for JAK1 over JAK2, JAK3 and TYK2 (IC₅₀ values are 0.014 μM, 0.593 μM, 1860 μM and 2715 μM). In vivo, Upadacitinib suppresses paw swelling and bone destruction in a rat model of arthritis.

Physical and Chemical Properties:

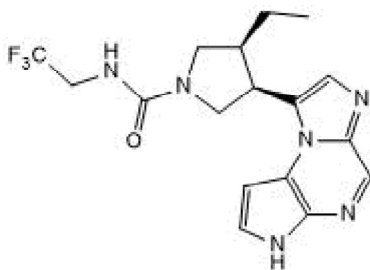
Batch Molecular Formula: C₁₇H₁₉F₃N₆O·¼H₂O

Batch Molecular Weight: 384.87

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Parmentier *et al* (2018) *In vitro* and *in vivo* characterization of the JAK1 selectivity of upadacitinib (ABT-494). BMC Rheumatol. 2 23. PMID: 30886973.

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