# **PRODUCT** INFORMATION



## Upadacitinib

Item No. 29706

CAS Registry No.:	1310726-60-3	0
Formal Name:	(3S,4R)-3-ethyl-4-(3H-imidazo[1,2-a]	
	pyrrolo[2,3-e]pyrazin-8-yl)-N-(2,2,2-	N
	trifluoroethyl)-1-pyrrolidinecarboxamide	F N
Synonym:	ABT-494	F H
MF:	$C_{17}H_{19}F_3N_6O$	F '' / \
FW:	380.4	Ń. N
Purity:	≥98%	
UV/Vis.:	λ <sub>max</sub> : 233, 337, 350 nm	
Supplied as:	A crystalline solid	N N
Storage:	-20°C	Ή
Stability:	≥4 years	

Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

#### Laboratory Procedures

Upadacitinib is supplied as a crystalline solid. A stock solution may be made by dissolving the upadacitinib in the solvent of choice, which should be purged with an inert gas. Upadacitinib is soluble in organic solvents such as DMSO and dimethyl formamide. The solubility of upadacitinib in these solvents is approximately 30 mg/ml.

Upadacitinib is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, upadacitinib should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Upadacitinib has a solubility of approximately 0.50 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

#### Description

Upadacitinib is a JAK1 inhibitor (IC<sub>50</sub> = 47 nM).<sup>1</sup> It is selective for JAK1 over JAK3 and tyrosine kinase 2 (Tyk2;  $IC_{50}$ s = 2,304 and 4,690 nM, respectively), as well as a panel of 83 additional kinases at 1  $\mu$ M, but does inhibit JAK2, Rho-associated kinase I (ROCK1), and ROCK2 (IC<sub>50</sub>s = 120, 920, and 430 nM, respectively). Upadacitinib decreases cytokine-induced STAT phosphorylation in a variety of human cells with IC<sub>50</sub> values ranging from 1.6 to 649 nM. It reduces M. tuberculosis-induced paw swelling and bone erosion in a rat model of arthritis when administered at doses of 1, 3, and 10 mg/kg twice per day for 17 days. Formulations containing upadacitinib have been used in the treatment of rheumatoid arthritis.

#### Reference

1. Parmentier, J.M., Voss, J., Graff, C., et al. In vitro and in vivo characterization of the JAK1 selectivity of upadacitinib (ABT-494). BMC Rheumatol. 2, 23 (2018).

WARNING THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

SAFETY DATA This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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