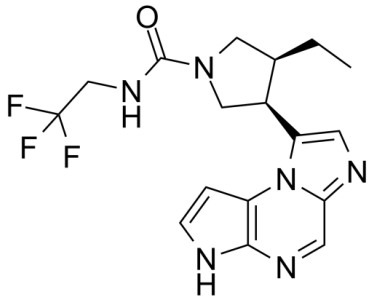
Data Sheet

Product Name:	Upadacitinib
Cat. No.:	CS-6150
CAS No.:	1310726-60-3
Molecular Formula:	$C_{17}H_{19}F_3N_6O$
Molecular Weight:	380.37
Target:	JAK
Pathway:	Epigenetics; JAK/STAT Signaling; Stem Cell/Wnt
Solubility:	DMSO : ≥ 22 mg/mL (57.84 mM); H2O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

Upadacitinib (ABT-494) is a potent, orally active and selective Janus kinase 1 (**JAK1**) inhibitor (**IC_{50}**=43 nM). Upadacitinib (ABT-494) displays approximately 74 fold selective for JAK1 over JAK2 (200 nM) in cellular assays dependent on specific, relevant cytokines. Upadacitinib (ABT-494) is used in development for the treatment of several autoimmune disorders[1][2]. IC50 & Target: IC50: 43 nM (JAK1), 200 nM (JAK2)[1] **In Vitro:** In biochemical assays, Upadacitinib is 74-fold more selective for JAK-1 than for JAK-2 (which is involved in erythropoiesis) and 58-fold more selective for JAK-1 than for JAK-3 (which is involved in immunosurveillance)[1]. The enhanced selectivity of Upadacitinib for JAK-1 over JAK-2 and JAK-3 may offer an improved benefit–risk profile in patients with RA range[2]. **In Vivo:** Upadacitinib (0.1-10 mg/kg; oral gavage; twice a day for 10 days) demonstrates efficacy in rat arthritis models[3].

References:

[1]. Nakayamada S, et al. Recent Progress in JAK Inhibitors for the Treatment of Rheumatoid Arthritis. BioDrugs. 2016 Oct;30(5):407-419.

[2]. J. Voss, et al. THU0127 Pharmacodynamics of A Novel JAK1 Selective Inhibitor in Rat Arthritis and Anemia Models and in Healthy Human Subjects. doi 10.1136/annrheumdis-2014-eular.3823.

[3]. Parmentier JM, et al. In vitro and in vivo characterization of the JAK1 selectivity of upadacitinib (ABT-494). BMC Rheumatol. 2018 Aug 28;2:23.

CAIndexNames:

1-Pyrrolidinecarboxamide, 3-ethyl-4-(3H-imidazo[1,2-a]pyrrolo[2,3-e]pyrazin-8-yl)-N-(2,2,2-trifluoroethyl)-, (3S,4R)-

SMILES:

O=C(N1C[C@@H](CC)[C@@H](C2=CN=C3C=NC(NC=C4)=C4N32)C1)NCC(F)(F)F

Caution: Product has not been fully validated for medical applications. For research use only.

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