

Product Name	: Tofacitinib citrate
Synonyms	: Tasocitinib citrate; CP-690550 citrate; CP 690550 citrate; CP690550 citrate
Cat No.	: M14931
CAS Number	: 540737-29-9
Molecular Formula	: C ₂₂ H ₂₈ N ₆ O ₈
Formula Weight	: 504.49
Chemical Name	: 1-Piperidinepropanenitrile, 4-methyl-3-(methyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamino)-β-oxo-, (3R,4R)-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1)
Description	A potent, specific, orally active inhibitor of JAK3 with IC₅₀ of 1 nM in cell-free assays; displays 20- to 100-fold less potency for JAK2 and JAK1 (IC₅₀=20 nM and 112 nM, respectively), and shows no potent activity against 30 other kinases at >3 μM (CaMK1, ROCK2, Lck, MST2, etc.); effectively inhibits a murine mixed lymphocyte reaction (MLR) with IC₅₀ of 91 nM, significantly prolongs survival in a murine model of heart transplantation and in cynomolgus monkeys receiving kidney transplants. Rheumatoid Arthritis Approved
Pathway	: Angiogenesis
Target	: JAK
Receptor	: JAK1; JAK2; JAK3; Lck; ROCK2
Solubility	: DMSO: ≥ 122.5 mg/mL
SMILES	: <chem>C[C@@H]1CCN(C[C@@H]1N(C)C2=NC=NC3=C2C=CN3)C(=O)CC#N.C(C(=O)O)C(CC(=O)O)(C(=O)O)O</chem>
Storage	: (-20°C)
Stability	: ≥ 2 years
Reference	:

1. Changelian PS, et al. Science. 2003 Oct 31;302(5646):875-8. | 2. Jiang JK, et al. J Med Chem. 2008 Dec 25;51(24):8012-8. | 3. Kudlacz E, et al. Am J Transplant. 2004 Jan;4(1):51-7.