

**Product Name:** CP 690550 citrate

**Catalog No.:** 4556

**Batch No.:** 1

CAS Number: 540737-29-9

IUPAC Name: (3*R*,4*R*)-4-Methyl-3-(methyl-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-ylamino)-β-oxo-1-piperidinepropanenitrile citrate

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>16</sub>H<sub>20</sub>N<sub>6</sub>O.C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>

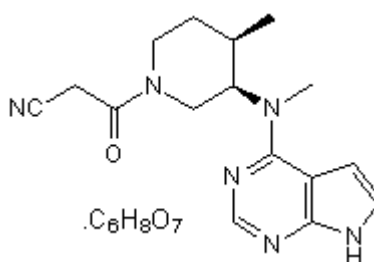
**Batch Molecular Weight:** 504.49

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.3% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = +40.8 (Concentration = 0.25, Solvent = Methanol)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	52.38	5.59	16.66
Found	52.59	5.19	16.7

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**Description:**

Potent JAK inhibitor (IC<sub>50</sub> values are 1, 20, and 112 nM for JAK3, JAK2 and JAK1 respectively). Orally active immunosuppressant; exhibits efficacy in rodent rheumatoid arthritis models.

**Physical and Chemical Properties:**

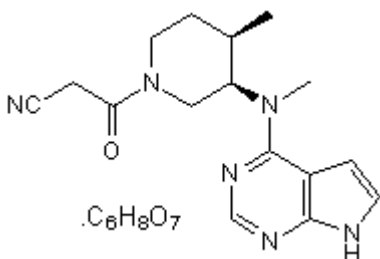
Batch Molecular Formula: C<sub>16</sub>H<sub>20</sub>N<sub>6</sub>O.C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>

Batch Molecular Weight: 504.49

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Jiang et al** (2008) Examining the chirality, conformation and selective kinase inhibition of 3-((3*R*,4*R*)-4-methyl-3-(methyl(7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino)piperidin-1-yl)-3-oxopropanenitrile (CP-690,550). *J.Med.Chem.* **51** 8012. PMID: 19053756.

**Flanagan et al** (2010) Discovery of CP-690,550: a potent and selective Janus kinase (JAK) inhibitor for the treatment of autoimmune diseases and organ transplant rejection. *J.Med.Chem.* **53** 8468. PMID: 21105711.

**Dowty et al** (2013) Preclinical to clinical translation of tofacitinib, a Janus kinase inhibitor, in rheumatoid arthritis. *J.Pharmacol.Exp.Ther.* **348** 165. PMID: 24218541.

**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.

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