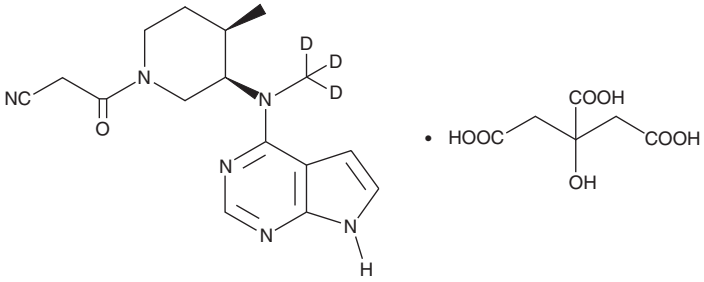
PRODUCT INFORMATION

Tofacitinib-d_3 (citrate)

Item No. 25046

Formal Name:	(3R,4R)-4-methyl-3-(methyl-d_3-7H-pyrrolo[2,3-d]pyrimidin-4R-ylamino)-β-oxo-1-piperidinepropanenitrile, 2-hydroxy-1,2,3-propanetricarboxylate
Synonym:	CP 690,550-d_3
MF:	$C_{16}H_{17}D_3N_6O \bullet C_6H_8O_7$
FW:	507.5
Chemical Purity:	≥98% (Tofacitinib)
Deuterium Incorporation:	≥99% deuterated forms (d_1-d_3); ≤1% d_0
Supplied as:	A solid
Storage:	-20°C
Stability:	≥4 years



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

Laboratory Procedures

Tofacitinib-d_3 (citrate) is intended for use as an internal standard for the quantification of tofacitinib (Item No. 11598) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated *versus* unlabeled).

Tofacitinib-d_3 (citrate) is supplied as a solid. A stock solution may be made by dissolving the tofacitinib-d_3 (citrate) in the solvent of choice, which should be purged with an inert gas. Tofacitinib-d_3 (citrate) is soluble in the organic solvent DMSO at a concentration of approximately 5 mg/ml.

Description

Tofacitinib is a potent, cell-permeable inhibitor of all JAK isoforms (IC_{50}s = 6.1, 12, and 8 nM for JAK1, JAK2, and JAK3, respectively).[1] It is selective for JAK1-3 over ROCK-2 and Lck (IC_{50}s = 3,400 and 3,870 nM, respectively) as well as 28 additional kinases in enzyme assays (IC_{50}s = >10,000 nM). It inhibits IL-2-mediated phosphorylation of JAK3 and STAT5 when used at a concentration of 30 ng/ml.[2] Tofacitinib prevents rejection and prolongs survival in murine and cynomolgus monkey models of heterotopic heart and kidney transplantation, respectively. Formulations containing tofacitinib have been used in the prevention of organ allograft rejection as well as in the treatment of the inflammatory or autoimmune components of a host of diseases, including rheumatoid arthritis and ulcerative colitis.[2-5]

References

1. Haan, C., Rolvering, C., Raulf, F., *et al. Chem. Biol.* **18(3)**, 314-323 (2011).
2. Changelian, P.S., Flanagan, M.E., Ball, D.J., *et al. Science* **302(5646)**, 875-878 (2003).
3. Flanagan, M.E., Blumenkopf, T.A., Brissette, W.H., *et al. J. Med. Chem.* **53(24)**, 8468-8484 (2010).
4. Cutolo, M. *Ther. Adv. Musculoskelet. Dis.* **5(1)**, 3-11 (2013).
5. Sandborn, W.J., Ghosh, S., Panes, J., *et al. N. Engl. J. Med.* **367(7)**, 616-624 (2012).

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