bio-techne
TOCRIS

Print Date: Nov 27th 2024

Certificate of Analysis

www.tocris.com

Product Name: **PF 06651600 malonate** **Catalog No.: 6506** **Batch No.: 1**

CAS Number: 2140301-97-7

IUPAC Name: 1-[(2*S*,5*R*)-2-Methyl-5-(7*H*-pyrrolo[2,3-*d*]pyrimidin-4-ylamino)-1-piperidinyl]-2-propen-1-one malate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{19}N_5O.C_3H_4O_4$

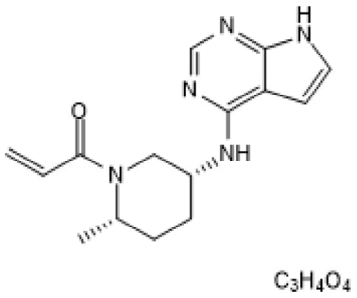
Batch Molecular Weight: 389.41

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM
ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.52	5.95	17.98
Found	55.54	6	17.78

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Description:

PF 06551600 malonate is a potent and selective JAK3 inhibitor (IC_{50} = 33.1 µM). Exhibits no significant activity against a panel of other kinases including JAK1, JAK2 and TYK2. Inhibits phosphorylation of STAT5, induced by IL-2, IL-4, IL-7 and IL-15. Suppresses Th1 and Th17 T-cell differentiation and function in vitro. Reduces paw swelling in a rat model of arthritis and reduces disease severity in a rat EAE model.

Physical and Chemical Properties:

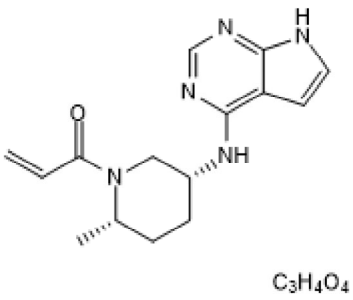
Batch Molecular Formula: $C_{15}H_{19}N_5O.C_3H_4O_4$

Batch Molecular Weight: 389.41

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



$C_3H_4O_4$

Storage: Store at +4°C

Solubility & Usage Info:

water to 100 mM
DMSO to 100 mM
ethanol to 50 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Thorarensen *et al* (2017) Design of a Janus Kinase 3 (JAK3) specific inhibitor 1-((2*S*,5*R*)-5-((7*H*-pyrrolo[2,3-d]pyrimidin-4-yl)amino)-2-methylpiperidin-1-yl)prop-2-en-1-one (PF-06651600) allowing for the interrogation of JAK3 signaling in humans. J.Med.Chem. ***60*** 1971. PMID: 28139931.

Telliez *et al* (2016) Discovery of a JAK3-selective inhibitor: functional differentiation of JAK3-selective inhibition over pan-JAK or JAK1-selective inhibition. ACS Chem.Biol. ***11*** 3442. PMID: 27791347.