Print Date: Jan 3rd 2020

Certificate of Analysis

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Product Name: **TAK 21d** **Catalog No.: 5209** **Batch No.: 1**

CAS Number: 1143578-94-2

IUPAC Name: 4-[4-(3,4-Difluorophenyl)-2-pyrimidinyl]-*N*-3-pyridazinyl-1-piperazinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{17}F_2N_7O.¼H_2O$

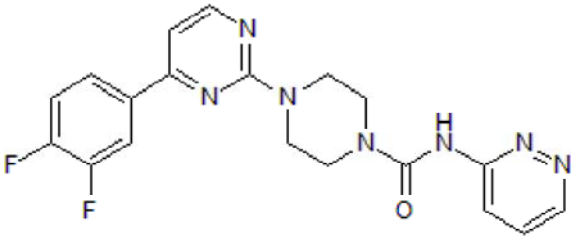
Batch Molecular Weight: 401.88

Physical Appearance: Off White solid

Solubility: DMSO to 10 mM
1eq. HCl to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.0% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.78	4.39	24.4
Found	56.78	4.26	24.45

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Information

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IUPAC Name: 4-[4-(3,4-Difluorophenyl)-2-pyrimidinyl]-*N*-3-pyridazinyl-1-piperazinecarboxamide

Description:

Potent FAAH inhibitor; (IC_{50} values are 0.28 and 0.72 nM, at rat and human FAAH respectively). Displays analgesic effects in vivo models of neuropathic and inflammatory pain. Brain penetrant.

Physical and Chemical Properties:

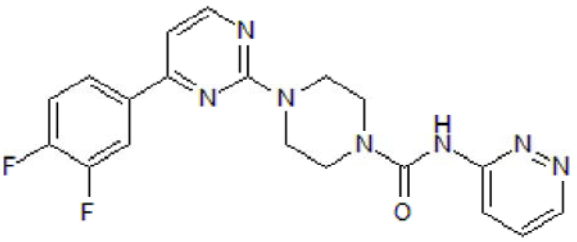
Batch Molecular Formula: $C_{19}H_{17}F_2N_7O.¼H_2O$

Batch Molecular Weight: 401.88

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 10 mM
1eq. HCl to 20 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.

References:

Kono *et al* (2014) Design, synthesis, and biological evaluation of a series of piperazine ureas as fatty acid amide hydrolase inhibitors. Bioorg.Med.Chem. ***22*** 1468. PMID: 24440478.

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956