Print Date: Jan 4th 2022

Certificate of Analysis

www.tocris.com

Product Name: **Defactinib** **Catalog No.: 7305** **Batch No.: 1**

CAS Number: 1073154-85-4

IUPAC Name: *N*-Methyl-4-[[4-[[[3-[methyl(methylsulfonyl)amino]-2-pyrazinyl]methyl]amino]-5-(trifluoromethyl)-2-pyrimidinyl]amino] benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{21}F_3N_8O_3S$

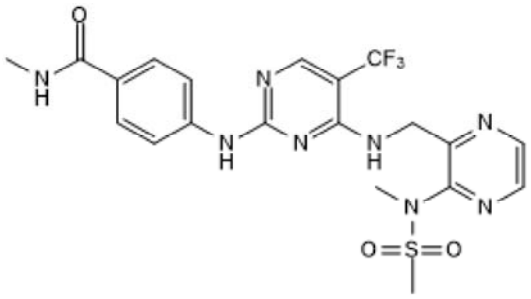
Batch Molecular Weight: 510.49

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.06	4.15	21.95
Found	47.04	4.22	21.99

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Product Information

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Description:

Defactinib is a potent and selective focal adhesion kinase (FAK) and proline rich tyrosine kinase 2 (Pyk2) inhibitor (IC_{50} = 0.6 nM at both). The compound shows >100-fold selectivity for FAK and Pyk2 over other kinases. Defactinib inhibits FAK phosphorylation in vivo (EC_{50} = 26 nM), and inhibits tumor growth. Defactinib also decreases the viability of thyroid cancer cells, showing greater selectivity for TT and K1 cells compared to FAK Inhibitor 14 (Cat. No. 3414) (IC_{50} values are 1.98 µM and 10.34 µM, respectively). Defactinib suppresses colony growth of Pnf cells when combined with Selumetinib (Cat. No. 6815). Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

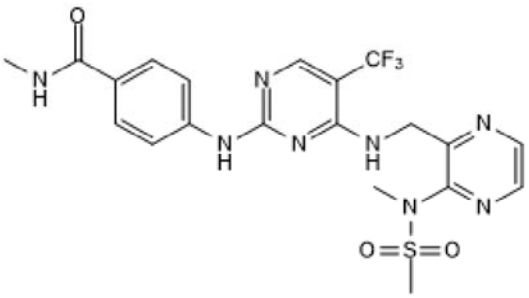
Batch Molecular Formula: $C_{20}H_{21}F_3N_8O_3S$

Batch Molecular Weight: 510.49

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the Defactinib (PF-04554878) probe summary on the SGC website.

References:

Errico *et al* (2021) Neurofibromin deficiency and extracellular matrix cooperate to increase transforming potential through FAK-dependent signaling. Cancers ***13***. PMID: 34066061.

Jones *et al* (2015) A phase I study of VS-6063, a second-generation focal adhesion kinase inhibitor, in patients with advanced solid tumors. Invest. New Drugs ***33*** 1100. PMID: 26334219.

O'Brien *et al* (2014) FAK inhibition with small molecule inhibitor Y15 decreases viability, clonogenicity, and cell attachment in thyroid cancer cell lines and synergizes with targeted therapeutics. Oncotarget. ***5*** 7945. PMID: 25277206.