TOCRIS
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Print Date: Sep 7th 2020

Certificate of Analysis

www.tocris.com

Product Name: **FMF-04-159-2** **Catalog No.: 7158** **Batch No.: 1**

CAS Number: 2364489-81-4

IUPAC Name: *N*-[1-[[3-[[(2*E*)-4-(Dimethylamino)-1-oxo-2-buten-1-yl]amino]phenyl]sulfonyl]-4-piperidinyl]-4-[(2,4,6- trichlorobenzoyl) amino]-1*H*-pyrazole-3-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{30}Cl_3N_7O_5S.¼H_2O$

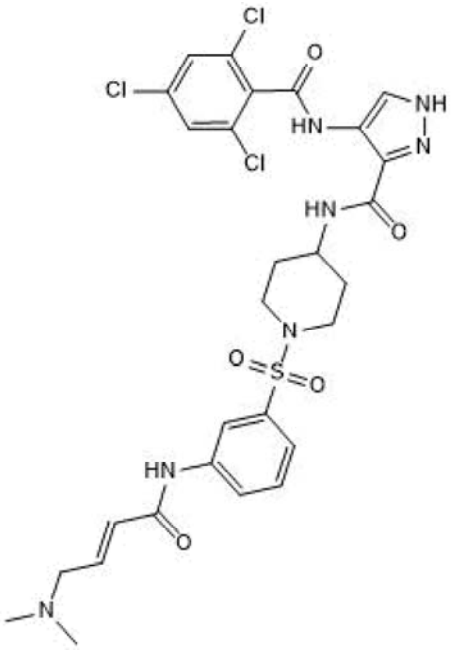
Batch Molecular Weight: 687.5

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.92	4.47	14.26
Found	48.83	4.28	13.85

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Description:

Potent inhibitor of CDK14 and CDK16 (IC_{50} = 40 nM for CDK14 in cellular BRET assay; IC_{50} values are 88 and 10 nM for CDK14 and CDK16 in kinase activity inhibition assay, respectively). Inhibits other TAIRE kinase family members at 1 µM (CDK17 and CDK18). Also binds CDK2 (IC_{50} = 256 nM). Displays covalent binding of CDK14, with binding sustained after washout. Causes cell cycle arrest at G_2/M in cancer cell lines. Reversible control FMF-04-159-R (Cat. No. 7159) also available.

Physical and Chemical Properties:

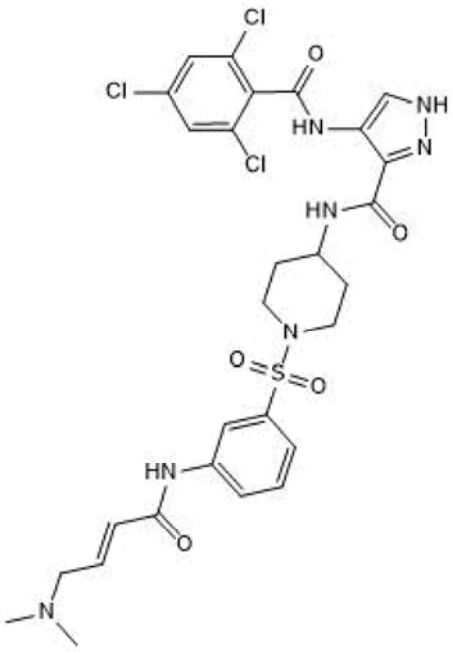
Batch Molecular Formula: $C_{28}H_{30}Cl_3N_7O_5S.¼H_2O$

Batch Molecular Weight: 687.5

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

Licensing Information:

Sold under license from Dana-Farber Cancer Institute.

References:

Ferguson *et al* (2019) Synthesis and structure activity relationships of a series of 4-amino-1*H*-pyrazoles as covalent inhibitors of CDK14 Bioorg.Med.Chem.Letts. ***29*** 1985. PMID: 31175010.

Ferguson *et al* (2019) Discovery of covalent CDK14 inhibitors with pan-TAIRE family specificity. Cell Chem.Biol. ***26*** 804. PMID: 30930164.