

Product Name: FMF-04-159-2

Catalog No.: 7158

Batch No.: 1

CAS Number: 2364489-81-4

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₃₀Cl₃N₇O₅S.1/4H₂O

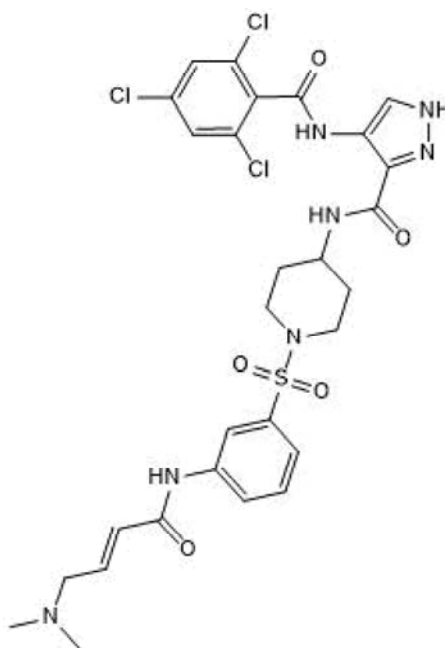
Batch Molecular Weight: 687.5

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

¹H 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

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

FMF-04-159-2 is a potent inhibitor of CDK14 and CDK16 (IC₅₀ = 40 nM for CDK14 in cellular BRET assay; IC₅₀ 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 (IC₅₀ = 256 nM). Displays covalent binding of CDK14, with binding sustained after washout. Causes cell cycle arrest at G₂/M in cancer cell lines. Reversible control FMF-04-159-R (Cat. No. 7159) also available.

Physical and Chemical Properties:

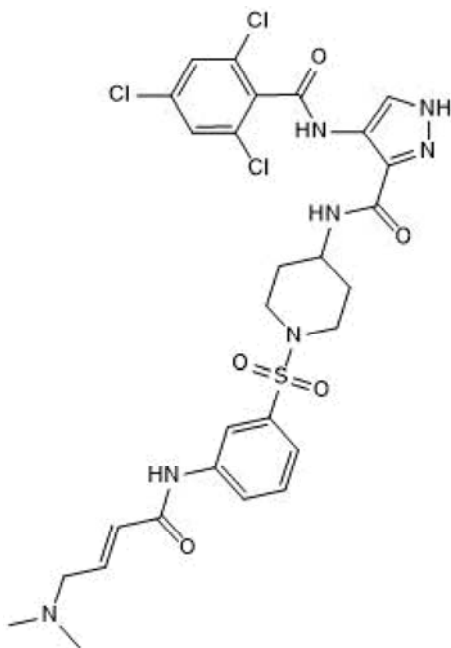
Batch Molecular Formula: C₂₈H₃₀Cl₃N₇O₅S·½H₂O

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.

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