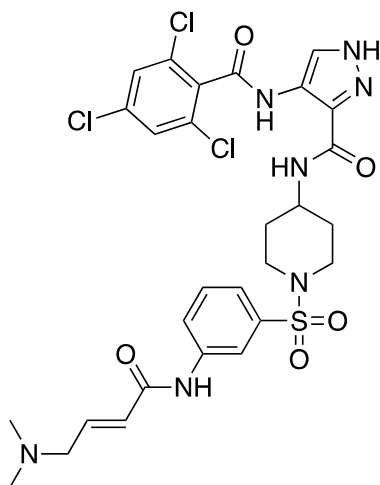
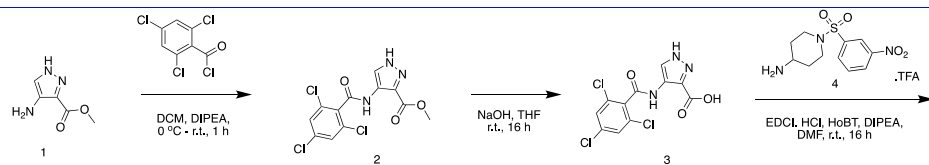


**FMF-04-159-2**



Chemical Formula: C<sub>28</sub>H<sub>30</sub>Cl<sub>3</sub>N<sub>7</sub>O<sub>5</sub>S  
Molecular Weight: 683.00

Category	Parameter	Description
Compound	Name	FMF-04-159-2
	Citation	Cell Chem Biol. 2019 (in press) <a href="https://doi.org/10.1016/j.chembiol.2019.02.015">https://doi.org/10.1016/j.chembiol.2019.02.015</a>
	Chemical descriptors	O=C(NC1CCN(S(C2=CC=CC(NC(/C=C/CN(C)C)=O)] =C2)(=O)=O)CC1)C3=NNC=C3NC(C4=C(Cl)C=C(Cl)C=C4Cl)=O
	Chemical name	(E)-N-(1-((3-(4-(dimethylamino)but-2-enamido)phenyl)sulfonyl)piperidin-4-yl)-4-(2,4,6-trichlorobenzamido)-1H-pyrazole-3-carboxamide
	Entries in chemical databases	N/A
	Availability	N/A
	Papers that use the compounds	N/A
	Additional comments	Negative control FMF-04-159-R also available
<i>In vitro</i> profiling	Target (potency)	88 nM (Lantha screen)
	Target (potency)	CDK16: 10 nM (Lantha screen), CDK2: 256 nM (NanoBRET)
	Selectivity	KiNativ at 1 μM (CDK14, CDK16, CDK17, CDK2 > 90%)
	Potential reactivity	acrylamide
	SAR	Described in accompanying BMCL publication ( <i>in press</i> )
	Mechanism of inhibition	Covalent binding to C218
	Structure of target-probe complex	Docking only
Cellular profiling	Validation of cellular target	NanoBRET (IC <sub>50</sub> = 38 nM), pulldown assay (500 nM)
	Validation of cellular specificity	Live cell KiNativ in HCT116
	Additional comments	
Pharmacodynamics		N/A
Pharmacokinetics		N/A



Synthetic scheme

