## ALW-II-49-7

H .N H<sub>2</sub>N  $CF_3$ || 0 н 0

 $\begin{array}{c} Chemical \ Formula: \ C_{21}H_{17}F_3N_4O_2\\ Molecular \ Weight: \ 414.39 \end{array}$ 

Category	Parameter	Description
Compound	Name	ALW-II-49-7
	Citation	ACS Chem. Biol., 2015, 10 (12), pp 2687–2696
	Chemical descriptors	CC1=CC=C(C=C1NC1=CN=CC(=C1)C(N)=O)C(=O)NC1=CC=CC(=C1)C(F)(F)F
	Chemical name	5-[(2-methyl-5-{[3-(trifluoromethyl)phenyl]carbamoyl}phenyl)amino]pyridine-3- carboxamide
	Entries in chemical databases	CAS# 1135219-23-6
	Availability	
	Papers that use the compounds	Bioorganic & Medicinal Chemistry Letters (2009), 19(15), 4467-4470
<i>In vitr</i> o profiling	Primary target (potency)	DDR2 (IC <sub>50</sub> of 18.6 nM), DDR1 (IC <sub>50</sub> of 12.4 nM)
	Other Target (potency)	<b>RAF1</b> (IC <sub>50</sub> of 22 nM), <b>LYN</b> (IC <sub>50</sub> of 257 nM)
	Selectivity	KinomeScan S-Score(5)=0.05. See reference paper for detail.
	Potential reactivity	
	SAR	
	Mechanism of inhibition Structure of target- probe complex	Туре II
Cellular profiling	Validation of cellular target Validation of cellular specificity	Antiproliferative activity against DDR2-mutated lung cancer cell lines: NCI-H2286 (GI <sub>50</sub> of 36 $\mu$ M), HCC-366 (GI <sub>50</sub> of 11 $\mu$ M),
Pharmacodynamics		
Pharmacokinetics		
Synthetic scheme	$H_2N$	$ \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \end{array} \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \end{array} \\ \begin{array}{c} \\ \end{array} \\ $