Product Data Sheet

Product Name: AD57 (hydrochloride)
Cat. No.: GC16362

Chemical Properties

Cas. No.	2320261-72-9		
Chemical Name	N-[4-[4-amino-1-(1-methylethyl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]phenyl]-N'-[3-(trifluoromethyl)phenyl]-urea, monohydrochloride		
SMILES	CC(C)N1C2=NC=NC(N)=C2C(C3=CC=C(NC(NC4=CC(C(F)(F)F)=CC=C4)=O)C=C3)=N1.Cl		
Formula	$C_{22}H_{20}F_3N_7O$ • HCl	M.Wt	491.9
Solubility	≤5mg/ml in ethanol;10mg/ml in DMSO;14mg/ml in dimethyl formamide	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	AD57 (hydrochloride)		

Background

IC50: 2 nM: blocks the receptor tyrosine kinase RET in Drosophila.

AD57, as a polypharmacological cancer therapeutic, is designed to regulate multiple targets related to cancer. AD57 effectively suppresses tyrosine kinase RET, weakens the activity of numerous other kinases, and interferes with kinases downstream of RET, including Raf, Src, and S6K, providing further efficacy in preventing signaling leading to invasion, proliferation, and metabolism related to cancer. Tyrosine kinase RET is probably sufficient to initiate a series of transformation events including medullary thyroid carcinoma, multiple endocrine neoplasias type 2A (MEN2A) and 2B (MEN2B).

In vitro: AD57 was demonstrated to be able to inhibit tyrosine kinase RET. But the efficacy of AD57 did not correlate solely with the blockade of RET, suggesting that the targeting of additional kinases is necessary for its biological efficacy. AD57 potently

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dampened the pathway-related human kinases B-Raf, mTOR, S6K, and Src [1].

In vivo: Male nu nu mice, injected subcutaneously with MEN2A cell lines, were administered AD57 (20 mg/kg) by oral gavage (per os) once daily, five times a week. AD57 inhibited the activity of relevant target kinases at 1 μM compared with the vehicle-treated nude mice transplanted with MEN2A cells [1].

Reference:
[1]. Dar, A., Das, T., Shokat, K., & Cagan, R. Chemical genetic discovery of targets and anti-targets for cancer polypharmacology. Nature. 2012; 486(7401): 80-84.

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