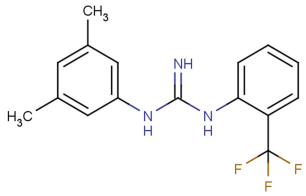
Data Sheet (Cat.No.T14004)

TargetMol
A DRUG SCREENING EXPERT

1A-116

Chemical Properties



CAS No.:	1430208-73-3
Formula:	C16H16F3N3
Molecular Weight:	307.31
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	1A-116 is a specific inhibitor of Rac1 .
Targets(IC_{50})	Rac1: None
In vitro	1A-116 shows lesser effect on MCF7::pcDNA.3 cells than on MCF7::C1199 cells. 1A-116 treatment decreases phospho-PAK1 levels in a time-dependent manner. The presence of 1A-116 reverts the PAK1 phosphorylation induced by 4-hydroxytamoxifen (Tam). The presence of 1A-116 also effectively reverts Rac1-PAK1-mediated estrogen receptor (ER) phosphorylation at Ser305[1]. 1A-116 shows a significant increase in antiproliferative activity on F3II cells, showing an IC50 value of 4 μM. A-116 also dramatically impairs Rac1 activation at low micromolar range (1 μM)[2].
In vivo	Daily treatment of mice with compound 1A-116 at 3mg/kg body weight/day reduces about 60% the formation of total metastatic lung colonies. A significant antitumor activity is obtained for macronodules (more than 1 mm in diameter) by treatment with 1A-116 in this highly aggressive breast cancer model. The treatment with 1A-116 reduces the total lung weight compare to the control group, leading to a total weight similar to the average pulmonary weight of Balb/c mice[2].

Solubility Information

Solubility	DMSO: 100 mg/mL (325.40 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.254 mL	16.27 mL	32.54 mL
5 mM	0.651 mL	3.254 mL	6.508 mL
10 mM	0.325 mL	1.627 mL	3.254 mL
50 mM	0.065 mL	0.325 mL	0.651 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Gonzalez N, et al. Pharmacological inhibition of Rac1-PAK1 axis restores tamoxifen sensitivity in human resistant breast cancer cells. Cell Signal. 2017 Jan;30:154-161.

2. Cardama GA, et al. Preclinical development of novel Rac1-GEF signaling inhibitors using a rational design approach in highly aggressive breast cancer cell lines. Anticancer Agents Med Chem. 2014;14(6):840-51.

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