Product Data Sheet

Product Name: Nec-4
Cat. No.: GC33620

Chemical Properties

Cas. No.	1041644-43-2		
SMILES	C[C@@H](C1=C(C=CC=C1Cl)F)NC(C2=CC=C(N2C)C#N)=O		
Formula	$C_{15}H_{13}ClFN_3O$	M.Wt	305.73
Solubility	Soluble in DMSO	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	Nec-4		

Background

Nec-4, a tricyclic derivative, is a potent receptor interacting protein 1 (RIP1) inhibitor, with an IC50 of 2.6 μM, Ki of 0.46 μM.

Nec-4 (compound 9) is a slightly better competitor than 7 with a lower Ki value that is similar to R-3. Nec-4 is again a slightly better competitor than Rac-3 with Ki and IC50 values comparable to 7 (Nec-4: IC50=2.6±0.1 μM, Ki=0.46±0.05 μM; 7: IC50=10.7±1.8 μM, Ki=4.5±0.9 μM). Overall, all three compounds cross-compete with each other but Nec-4 is able to more effectively displace both 20 and 26 in comparison to the parent compounds Rac-3 and 7, respectively. This suggests that Nec-4 binding likely significantly overlaps with both the Nec-1 and the Nec-3 binding sites.

[1]. Maki JL, et al. Fluorescence polarization assay for inhibitors of the kinase domain of receptor interacting protein 1. Anal Biochem. 2012 Aug 15;427(2):164-74.

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