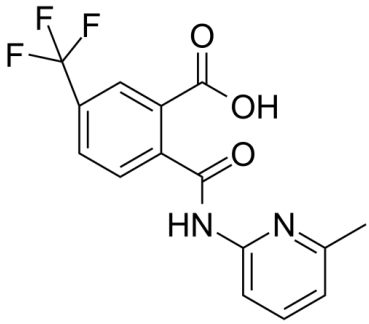
Data Sheet

Product Name:	AF38469
Cat. No.:	CS-4149
CAS No.:	1531634-31-7
Molecular Formula:	C15H11F3N2O3
Molecular Weight:	324.25
Target:	Neurotensin Receptor
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	DMSO : ≥ 43 mg/mL (132.61 mM)



BIOLOGICAL ACTIVITY:

AF38469 is a novel, selective, orally bioavailable **Sortilin** inhibitor with an **IC_{50}** value of 330 nM. IC50 & Target: IC50:330 nM (Sortilin)[1] **In Vitro:** AF38469 showed no inhibition or stimulation of >50% at 10 μM in a standard selectivity panel of ca. 70 targets run at CEREP. Importantly AF38469 showed no activity against the NTR1 receptor. In addition AF38469 showed no activity against a selected panel of targets known to bind acidic molecules (d-Opioid, GPR40, PPARd, EP1, Angiotensin AT1, Endothelin ETA & B, MMP-12). AF38469 will serve as an important tool to further delineate the biology of Sortilin, and to facilitate evaluation of the therapeutic potential of this protein[1].

PROTOCOL (Extracted from published papers and Only for reference)

Enzyme in vitro assay [1]: Compound affinity was determined by measuring the displacement of 3H-neurotensin binding to hSortilin in SPA format. Total volume of 40 μl in 50 mM HEPES pH 7.4 assay buffer containing 100 mM NaCl, 2.0 mM CaCl2, 0.1% BSA and 0.1% Tween-20. Compound pre-incubation for 30 min at RT with 150 nM of 6his-Sortilin before 5 nM [3H]-Neurotensin and Ni chelate imaging beads (Perkin Elmer) were added, after 6 h plate was read on a ViewLux with 360 s exposure time. Dose-response evaluation of compounds was performed with 10 concentrations of drugs (covering 3 decades). IC50 values were calculated by nonlinear regression using the sigmoid concentration-response (variable slope) using Xlfit 4 (IDBS, UK). All values reported are average of at least 4 determination.

References:

[1]. Schroder TJ, et al. The identification of AF38469: an orally bioavailable inhibitor of the VPS10P family sorting receptor Sortilin. Bioorg Med Chem Lett. 2014 Jan 1;24(1):177-80.

CAIndexNames:

Benzoic acid, 2-[[(6-methyl-2-pyridinyl)amino]carbonyl]-5-(trifluoromethyl)-

SMILES:

O=C(NC1=CC=CC(C)=N1)C2=CC=C(C(F)(F)F)C=C2C(O)=O

Caution: Product has not been fully validated for medical applications. For research use only.

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