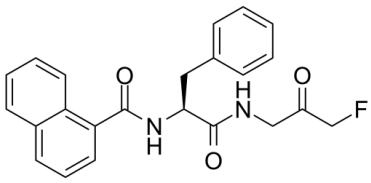
Data Sheet

Product Name:	FMK 9a
Cat. No.:	CS-6472
CAS No.:	1955550-51-2
Molecular Formula:	C23H21FN2O3
Molecular Weight:	392.42
Target:	Autophagy
Pathway:	Autophagy
Solubility:	DMSO : ≥ 150 mg/mL (382.24 mM)



BIOLOGICAL ACTIVITY:

FMK 9a is an **autophagin-1** inhibitor with **IC_{50}** values of 80 and 73 μM in FRET and LRA assay. IC50 & Target: IC50: 80 nM (autophagin-1, FRET assay); 73 nM (autophagin-1, LRA assay)[1] **In Vitro:** ATG4B or autophagin-1 is a cysteine protease that cleaves ATG8 family proteins. ATG4B plays essential roles in the autophagosome formation and the autophagy pathway. FMK 9a shows strong inhibition of ATG4B, with IC_{50} values of 80 and 73 nM in the TR-FRET and cellular-based LRA assays, respectively. LC−MS/MS study indicates that FMK 9a forms an irreversible covalent bond with the more reactive thiol group of Cys74 located at the catalytic site of ATG4B and thus inactivates ATG4B proteolytic activity[1]. **In Vivo:** FMK 9a shows moderate solubility (LYSA: 41 μg/mL) and high human and mouse liver microsome clearances of 13.9 and 70 mL/kg per minute[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]FMK 9a is dissolved in DMSO. 5 μL of serial-diluted FMK 9a (1% DMSO) in assay buffer is added into 5 μL of purified ATG4B (final 0.1 nM) in 384-well plate, and the solution is incubated at room temperature (rt) for 30 min. Then, 5 μL of His-GATE-16-GST (final 20 nM) is added into the wells, and the solution is incubated for another 30 min. 5 μL of detection solution (final 2 nM of Eu-anti-His and 20 nM of Ulight-anti-GST) is added, and the resulting mixture is incubated at rt for 40 min[1].

References:

[1]. Qiu Z, et al. Discovery of Fluoromethylketone-Based Peptidomimetics as Covalent ATG4B (Autophagin-1) Inhibitors. ACS Med Chem Lett. 2016 Jun 25;7(8):802-6.

CAIndexNames:

1-Naphthalenecarboxamide, N-[(1S)-2-[(3-fluoro-2-oxopropyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-

SMILES:

O=C(C1=C(C=CC=C2)C2=CC=C1)N[C@H](C(NCC(CF)=O)=O)CC3=CC=CC=C3

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

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