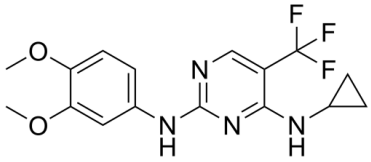
Data Sheet

Product Name:	SBP-7455
Cat. No.:	CS-0141672
CAS No.:	1884222-74-5
Molecular Formula:	$C_{16}H_{17}F_3N_4O_2$
Molecular Weight:	354.33
Target:	Autophagy; ULK
Pathway:	Autophagy
Solubility:	DMSO : 125 mg/mL (352.78 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

SBP-7455 is a potent, high affinity and orally active dual **ULK1/ULK2** autophagy inhibitor with **IC_{50}**s of 13 nM and 476 nM in the ADP-Glo assays, respectively. SBP-7455 potently inhibits **ULK1/2** enzymatic activity and can be used for triple-negative breast cancer (TNBC) research[1]. ***In Vitro:*** SBP-7455 (compound 26; 72 h) treatment inhibits cell growth with an IC_{50} of 0.3 μM for MDA-MB-468 cells. SBP-7455 inhibits starvation-induced autophagic flux in TNBC cells that are dependent on autophagy for survival[1]. ***In Vivo:*** A single dose of SBP-7455 (compound 26) (30 mg/kg) is orally administered to mice. The T_{max} for SBP-7455 is approximately 1 h, the C_{max} is 990 nM and the $T_{1/2}$ is 1.7 h. The plasma concentration of SBP-7455 remains above the ULK1 IC_{50} for almost 4 h after oral dosing[1].

The mice are dosed with SBP-7455 (compound 26) (10 mg/kg) by oral gavage, and liver samples were collected after 2 h. The results reveals robust inhibition of pATG13 (Ser318), as well as downregulation of total ATG13 and ULK1 levels by SBP-7455[1].

References:

[1]. Huiyu Ren, et al. Design, Synthesis, and Characterization of an Orally Active Dual-Specific ULK1/2 Autophagy Inhibitor that Synergizes with the PARP Inhibitor Olaparib for the Treatment of Triple-Negative Breast Cancer. J Med Chem. 2020 Dec 10;63(23):14609-14625

CAIndexNames:

2,4-Pyrimidinediamine, N4-cyclopropyl-N2-(3,4-dimethoxyphenyl)-5-(trifluoromethyl)-

SMILES:

FC(C1=CN=C(NC2=CC=C(OC)C(OC)=C2)N=C1NC3CC3)(F)F

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