

Product Data Sheet

Product Name: SJB2-043 analog (trifluoroacetate salt)

Cat. No.: GC92010

Chemical Properties

Cas. No.

Chemical Name (R)-2-(2-chloro-6-fluoro-3-((1-methylpyrrolidin-3-yl)oxy)phenyl)naphtho[2,3-d]oxazole-4,9-dione, trifluoroacetate salt

SMILES O=C1C2=C(C(C3=C1C=CC=C3)=O)N=C(C4=C(F)C=CC(O[C@H]5CN(C)CC5)=C4Cl)O2.FC(F)(C(O)=O)F

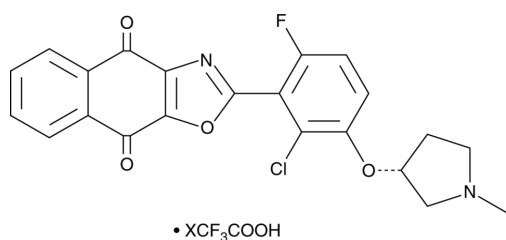
Formula $C_{22}H_{16}ClFN_2O_4 \cdot XCF_3COOH$ M.Wt 426.8

Solubility Acetonitrile: Slightly soluble: 0.1-1 mg/ml, DMSO: Sparingly soluble: 1-10 mg/ml Storage $-20^{\circ}C$

General tips For obtaining a higher solubility, please warm the tube at $37^{\circ}C$ and shake it in the ultrasonic bath for a while. Stock solution can be stored below $-20^{\circ}C$ 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



Background

SJB2-043 analog is an inhibitor of OTUB1 and ubiquitin-specific protease 8 (USP8; $IC_{50}s = 0.17$ and 0.28 nM, respectively) and a derivative of the USP1/UAF1 complex and SARS-CoV-2 PL^{Pro} inhibitor SJB2-043.¹ It is selective for OTUB1 and USP8 over USP1, USP2, USP7, USP36, and ataxin-3 ($IC_{50}s = 1,370, 3,800, >10,000, 8,400,$ and $>10,000$ nM, respectively). SJB2-043 analog reduces viability in H1975, EBC-1, NCI H1703, H23, and A549 non-small cell lung cancer (NSCLC) cells ($IC_{50}s = 118, 172, 145, 431,$ and $1,004$ nM, respectively). *In vivo*, SJB2-043 analog (5 mg/kg twice

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

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daily) decreases tumor volume in an H1975 mouse xenograft model.

References:

[1]. Tan, L., Shan, H., Han, C., et al. Discovery of potent OTUB1/USP8 dual inhibitors targeting proteostasis in non-small-cell lung cancer. *J. Med. Chem.* 65(20)13645-13659(2022).

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