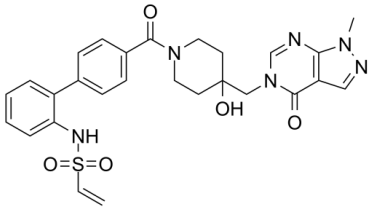
Data Sheet

Product Name:	FT827
Cat. No.:	CS-0039475
CAS No.:	1959537-86-0
Molecular Formula:	$C_{27}H_{28}N_6O_5S$
Molecular Weight:	548.61
Target:	Deubiquitinase
Pathway:	Cell Cycle/DNA Damage
Solubility:	DMSO : 125 mg/mL (227.85 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

FT827 is a selective and covalent **ubiquitin-specific protease 7 (USP7)** inhibitor (**K_i**=4.2 μM). FT827 binds to the USP7 catalytic domain ($USP7_{CD}$; residues 208-560) with an apparent **K_d** value of 7.8 μM[1]. IC50 & Target: Ki: 4.2 μM (USP7); Kd: 7.8 μM (USP7)[1]
In Vitro: FT827 features a vinylsulfonamide moiety that covalently modifies the catalytic Cys223 of USP7 and inhibits the enzyme with K_i and K_d of 4.2 and 7.8 μM, respectively. FT827 exclusively inhibit USP7 in a panel of 38 deubiquitinases (DUBs) from diverse families. FT827 inhibits USP7 probe reactivity with IC_{50}s of 0.1-2 μM, confirming 10 to 100-fold higher potency as compared to P22077 in crude cell extracts or with intact MCF7 breast cancer cells, followed by incubation with the ubiquitin active site suicide probe haemagglutinin (HA)-tagged ubiquitin bromoethyl (HA-UbC2Br)[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]To determine compound IC_{50}s, **FT827** is diluted in 100% DMSO in three-fold 12- point dilution series from 100 μM. 100 nL of 100-fold concentrated solutions are dispensed into black 384-well plate. 25 nM ubiquitin-rhodamine 110, along with recombinant USP7CD (3 nM), or USP7C-term (30-125 pM, depending on batch activity) are added and the plates incubated at room temperature for 1 h. The reaction is terminated by adding 2.5 μL citric acid to a final concentration of 10 mM prior to measuring fluorescence intensity on a Pherastar with a 485 nm excitation/520 nm emission optic module[1].

References:

[1]. Turnbull AP, et al. Molecular basis of USP7 inhibition by selective small-molecule inhibitors. Nature. 2017 Oct 26;550(7677):481-486.

CAIndexNames:

Ethenesulfonamide, N-[4'-[[4-[(1,4-dihydro-1-methyl-4-oxo-5H-pyrazolo[3,4-d]pyrimidin-5-yl)methyl]-4-hydroxy-1-piperidinyl]carbonyl][1,1'-biphenyl]-2-yl]-

SMILES:

C=CS(=O)(NC1=CC=CC=C1C2=CC=C(C(N3CCC(O)(CN(C=NC4=C5C=NN4C)C5=O)CC3)=O)C=C2)=O

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

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