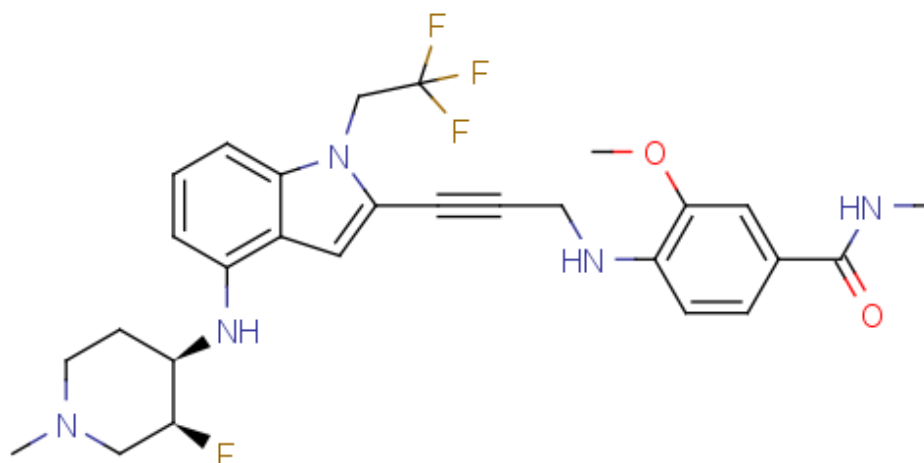


Name: Rezatapopt cat#: EX-A8780

Chemical Structure:



Absolute stereochemistry shown

Chemical Name	Benzamide, 4-[[3-[4-[[[(3S,4R)-3-fluoro-1-methyl-4-piperidyl]amino]-1-(2,2,2-trifluoroethyl)-1H-indol-2-yl]-2-propyn-1-yl]amino]-3-methoxy-N-methyl-
Canonical SMILES	<chem>O=C(NC)C1=CC=C(NCC#CC2=CC=CC3=CC=CC3N2CC(F)(F)F)NC4CCN(C)CC4F)C(OC)=C1</chem>
Isomeric SMILES	<chem>N(C1=C2C(N(CC(F)(F)F)C(C#CCNC3=C(OC)C=C(C(NC)=O)C=C3)=C2)=CC=C1)[C@H]4[C@@H](F)CN(C)CC4</chem> InChI
InChI	InChI=1S/C28H31F4N5O2/c1-33-27(38)18-9-10-24(26(14-18)39-3)34-12-5-6-19-15-20-22(35-23-11-13-36(2)16-21(23)29)7-4-8-25(20)37(19)17-28(30,31)32/h4,7-10,14-15,21,23,34-35H,11-13,16-17H2,1-3H3,(H,33,38)/t21-,23+/m0/s1
InChI Key	NKRKBSQLUPEVCZ-JTHBVZDNSA-N

Molecular Weight	545.5717	Storage	3 years -20°C powder
Formula	C ₂₈ H ₃₁ F ₄ N ₅ O ₂		6 months -80°C in solvent Away from moisture
CAS No.	2636846-41-6	Synonyms	PC-14586

Solubility (25°C) *	In vitro	DMSO	Soluble in DMSO
		Ethanol	N/A
		Water	N/A
	In vivo (should be freshly prepared each time)		

* <1 mg/ml means slightly soluble or insoluble.

* Please note that Selleck tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.

Preparing Stock Solutions:

Concentration \ Mass / Volume	Mass	1 mg	5 mg	10 mg
	Volume			
1 mM		1.8329 mL	9.1647 mL	18.3295 mL
5 mM		0.3666 mL	1.8329 mL	3.6659 mL
10 mM		0.1833 mL	0.9165 mL	1.8329 mL

DMSO : *The above data is based on the product molecular weight 545.57.

Biological Activities:

Description	Rezatapopt is an antineoplastic agent, used to inhibit solid tumor with p53 mutation ^[1] .
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References	[1]. Li Sujing, et al. Heteroarylalkyne compounds for targeting mutant of p53 and their preparation. World Intellectual Property Organization, WO2023016434 A1. 2023-02-16.
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