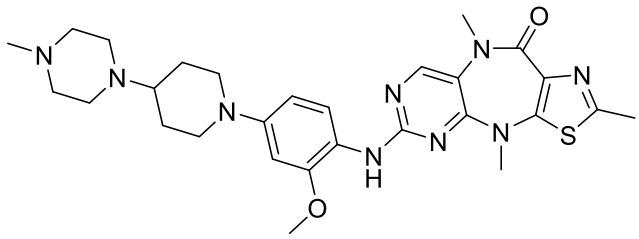
BJG-03-025



Chemical Formula: $C_{28}H_{37}N_9O_2S$
Molecular Weight: 563.73

Category	Parameter	Description
Compound	Name	BJG-03-025
	Citation	*ACS Med. Chem. Lett*. **2021**, *12*, 30−38
	Chemical descriptors	COC1=C(NC2=NC=C3N(C)C(=O)C4=C(SC(C)=N4)N(C)C3=N2)C=CC(=C1)N1CCC(CC1)N1CCN(C)CC1
	Chemical name	6-((2-methoxy-4-(4-(4-methylpiperazin-1-yl)piperidin-1-yl)phenyl)amino)-2,4,9-trimethyl-4,9-dihydro-10H-pyrimido[5,4-b]thiazolo[5,4-e][1,4]diazepin-10-one
	Entries in chemical databases	CAS No.: 2553213-90-2
	Availability	Synthesis on demand
In vitro profiling	Target (potency)	FAK IC_{50} 20nM. ThermoFisher Z'LYTE biochemical assay
	Target (potency)	IC_{50} 3.6uM. Viability of MDA-MB-231 cells in ultra-low adherent 3D-spheroid suspensions.
	Selectivity	KinomeScan - "complete" selectivity for FAK at a screening concentration of 1 μM, with an S(35) score of 0.01. 100−300-fold selective for FAK.
	Potential reactivity	None
	SAR	Yes, see publication
	Mechanism of inhibition	Reversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		Mouse $T_{1/2}$ = 5.3 h CL = 18 ml/min/Kg Vss=4.1 L/Kg F= 18%

Synthetic scheme