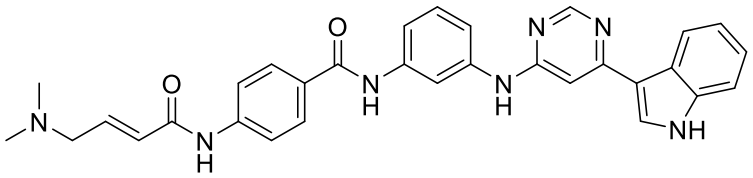
THZ-P1-2



Chemical Formula: $C_{31}H_{29}N_7O_2$
Molecular Weight: 531.6200

Category	Parameter	Description
Compound	Name	THZ-P1-2
	Citation	*Cell Chem. Bio*. **2020**, *27*, 525–537 https://doi.org/10.1016/j.chembiol.2020.02.003
	Chemical descriptors	CN(C/C=C/C(NC1=CC=C(C(NC2=CC=CC(NC3=CC(C4=CNC5=CC=CC=C45)=NC=N3)=C2)=O)C=C1)=O)C
	Chemical name	(E)-N-(3-((6-(1H-indol-3-yl)pyrimidin-4-yl)amino)phenyl)-4-(4-(dimethylamino)but-2-enamido)benzamide
	Entries in chemical databases	N/A
	Availability	N/A
	Papers that use the compounds	N/A
	Additional comments	Negative control THZ-P1-2-R is also available
In vitro profiling	Target (potency)	PI5P4K2A: 0.95 µM (ADP Glo)
	Target (potency)	PI5P4K2B: 5.9 µM (Transcreener)
	Target (potency)	PI5P4K2C: 4.8 nM (K_D; Invitrogen)
	Selectivity	Ambit KINOMEscan at 1 µM (S-Score (35) = 0.04)
	Potential reactivity	Cysteine reactive
	SAR	Described in *ACS Med. Chem. Lett.* **2020**, *11*, 346−352 https://doi.org/10.1021/acsmedchemlett.9b00402
	Mechanism of inhibition	Irreversible
	Structure of target-probe complex	PDB-ID: 6OSP
	Additional comments	N/A
Cellular profiling	Validation of cellular target	Isothermal CETSA; cellular pulldown with dtb-labeled probe
	Validation of cellular specificity	Cellular pulldown with dtb-labeled probe to check for potential off-targets
	Additional comments	N/A
Pharmacodynamics		N/A
Pharmacokinetics		N/A

Synthetic scheme