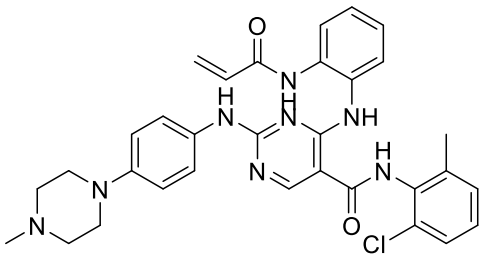
DGY-06-116



Chemical Formula: $C_{32}H_{33}ClN_8O_2$
Exact Mass: 596.24
Molecular Weight: 597.12

Category	Parameter	Description
Compound	Name	DGY-06-116
	Citation	J Med Chem. 2020 02 27; 63(4):1624-1641. https://pubs.acs.org/doi/10.1021/acs.jmedchem.9b01502
	Chemical descriptors	CN1CCN(CC1)C1=CC=C(NC2=NC(NC3=CC=CC=C3NC(=O)C=C)=C(C=N2)C(=O)NC2=C(C)C=CC=C2Cl)C=C1
	Chemical name	4-((2-acrylamidophenyl)amino)-N-(2-chloro-6-methylphenyl)-2-((4-(4-methylpiperazin-1-yl)phenyl)amino)pyrimidine-5-carboxamide
	Entries in chemical databases	PMID: 31935084
	Availability	N/A
	Papers that use the compounds	https://pubmed.ncbi.nlm.nih.gov/32509799/
In vitro profiling	Target (potency)	SRC: 3 nM; GAK: 4.87; ABL1: 0.98 nM; BLK: 7.56 nM; BTK: 8.44 nM; LCK: 4.33 nM; HCK: 4.04 nM; LYN A: 1.62 nM; YES1: 0.58 nM; FGFR1: 8340 nM.
	Target (potency)	
	Selectivity	Ambit at 1 uM
	Potential reactivity	N/A
	SAR	N/A
	Mechanism of inhibition	Competitive ATP inhibitor
	Structure of target-probe complex	PDB: 6E6E
Cellular profiling	Validation of cellular target	
	Validation of cellular specificity	
Pharmacodynamics		N/A
Pharmacokinetics		IP with 5 & 10 MPK

Synthetic scheme