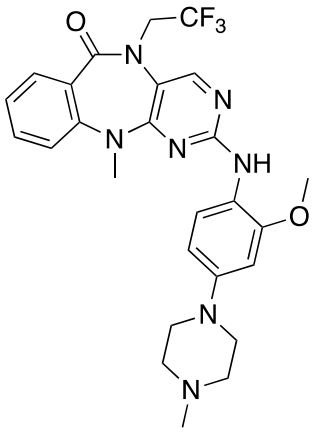
DCLK1-IN-1



Chemical Formula: $C_{26}H_{28}F_3N_7O_2$
Molecular Weight: 527.55

Category	Parameter	Description
Compound	Name	DCLK1-IN-1
	Citation	Nat Chem Biol. 2020 Jun;16(6):635-643. doi: 10.1038/s41589-020-0506-0. https://www.nature.com/articles/s41589-020-0506-0
	Chemical descriptors	O=C1N(CC(F)(F)F)C2=C(N=C(NC3=CC=C(N4CCN(C)CC4)C=C3OC)N=C2)N(C)C5=C1C=CC=C5
	Chemical name	2-((2-methoxy-4-(4-methylpiperazin-1-yl)phenyl)amino)-11-methyl-5-(2,2,2-trifluoroethyl)-5,11-dihydro-6H-benzo[e]pyrimido[5,4-b][1,4]diazepin-6-one
	Entries in chemical databases	n/a
	Availability	https://www.selleckchem.com/products/dclk1-in-1.html https://www.medchemexpress.com/dclk1-in-1.html
	Papers that use the compounds	https://pubmed.ncbi.nlm.nih.gov/?term=dclk1-in-1&sort=date
	Additional comments	Negative control DCLK1-NEG also available
In vitro profiling	Target (potency)	Dclk1: 57.2 nM
	Target (potency)	Dclk2: 103 nM
	Selectivity	No detected off targets across the kinome
	Potential reactivity	n/a
	SAR	See JMC paper, PMID 32530623
	Mechanism of inhibition	reversible
	Structure of target-probe complex	Patel and Lucet *et al*, unpublished
	Additional comments	
Cellular profiling	Validation of cellular target	NanoBRET, pulldown assay
	Validation of cellular specificity	KiNativ
	Additional comments	
Pharmacodynamics		n/a

Pharmacokinetics

DCLK1-IN-1 in male swiss albino mice

Parameter	Unit	IV	PO
Dose	mg kg^{-1}	2	10
T_{max}	hr	-	1.00
$^{a}C_0/C_{max}$	ng mL^{-1}	1199.15	1014.69
AUC_{last}	hr*ng mL^{-1}	1209.01	4879.61
AUC_{inf}	hr*ng mL^{-1}	1269.45	5506.28
$T_{1/2}$	hr	2.09	-
CL	ml min^{-1} kg^{-1}	26.26	-
V_{ss}	L kg^{-1}	3.27	-
F^{b}	%	-	81

Synthetic scheme