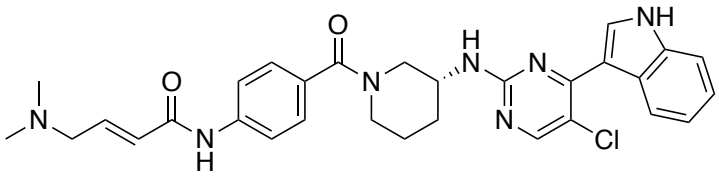
CDK13



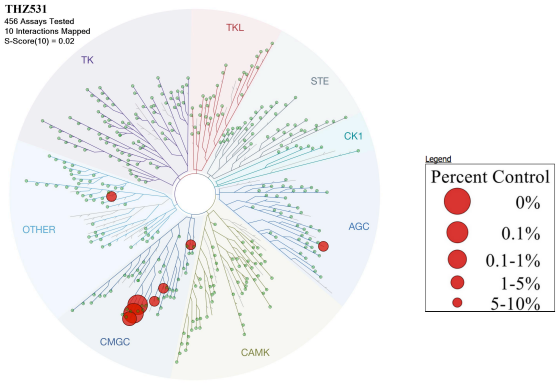
THZ531

Chemical Name:
(R,E)-N-(4-(3-((5-chloro-4-(1H-indol-3-yl)pyrimidin-2-yl)amino)piperidine-1-carbonyl)phenyl)-4-(dimethylamino)but-2-enamide
CHEBI:143122
Smile String:
ClC1=CN=C(N[C@H]2CN(C(C3=CC=C(NC(/C=C/CN(C)C)=O)C=C3)=O)CCC2)N=C1C4=CNC5=C4C=CC=C5
Chemical Formula: $C_{30}H_{32}ClN_7O_2$
Molecular Weight: 558.07
cLogP: 1.8925
Source: Selleck Chem, Med Chem Express
Reference:
Zhang, T.; *et al*. "Covalent targeting of remote cysteine residues to develop CDK12 and CDK13 inhibitors." *Nat Chem Biol*. **2016**, *12*, 876–84.

Biochemical profiling

Ambit/DiscoverX (456 kinases)
S_{10} (1μM): 0.023 (8 kinases < 10% control)

CDK13 IC_{50} (enzymatic assay) = 69 nM



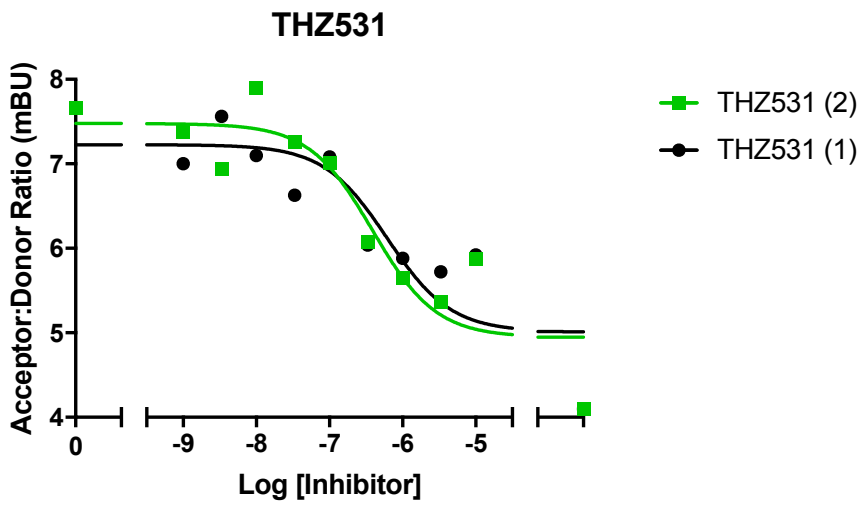
Kinase	% Control @ 1uM
JNK2	0.55
JNK1	0.95
CDK13	1
RSK2	2.8
GSK3A	5.7
DYRK1B	6.1
STK16	6.2
DYRK2	7.4

List of wild-type human kinases inhibited < 10% control in Ambit panel

Cellular target engagement in HEK293 cells

CDK13-NLuc (C term)

CDK13 IC_{50} = 260 nM
n=2



Cellular target engagement of THZ531 with CDK13/Cyclin K