CDK11A

SNS-032

Chemical Name: N-[5-[[[5-(1,1-dimethylethyl)-2-oxazolyl]methyl]thio]-2-

thiazolyl]-4-piperidinecarboxamide

CHEBI: 91399

Smile String: CC(C)(C)C1=CN=C(CSC2=CN=C(NC(C3CCNCC3)=O)S2)O1

Chemical Formula: C₁₇H₂₄N₄O₂S₂

Molecular Weight: 380.53

cLogP: 0.554

Source: Selleck Chem, Med Chem Express

Reference:

Davis, M. I.; et al. "Comprehensive analysis of kinase inhibitor selectivity." Nat

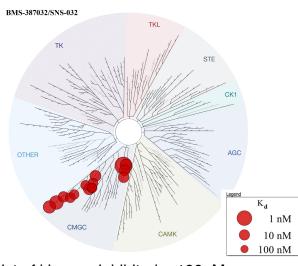
Biotechnol. 2011, 29, 1046-51.

Biochemical profiling

DiscoverX (403 wild-type human kinases)

16 kinases < 100nM

CDK11A $K_d = 48 \text{ nM}$



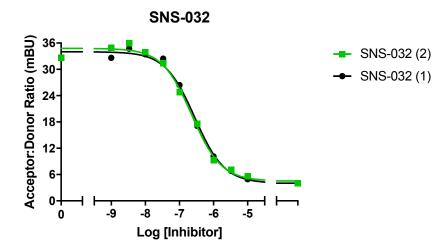
List of kinases inhibited < 100nM

Kinase	K _d (nM)
CDKL5	1.7
PCTK1	7.1
PCTK2	13
CDC2L5	23
GSK3A	28
CDK7	31
GSK3B	37
CDKL2	41
РСТК3	44
CDC2L2	48
CDK3	56
CDK4	66
CDK2	69
CDK4	69
CDK9	76
CDC2L1	98

Cellular target engagement in HEK293 cells

CDK11A-NLuc (C term)

CDK11A IC₅₀ = 280 nM



Cellular target engagement of SNS-032 with CDK11A / Cyclin K