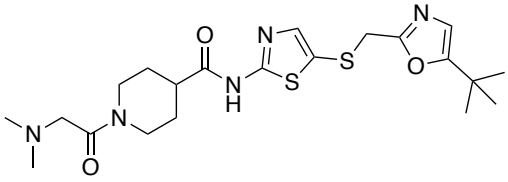
CDK16

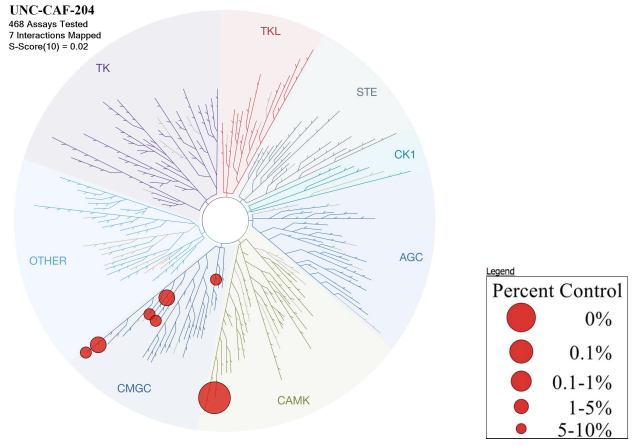


CAF-204

Chemical Name:
N-(5-(((5-(*tert*-butyl)oxazol-2-yl)methyl)thio)thiazol-2-yl)-1-(dimethylglycyl)piperidine-4-carboxamide
CHEBI:143123
Smile String:
O=C(NC1=NC=C(S1)SCC2=NC=C(O2)C(C)(C)C)C3CCN(CC3)C(CN(C)C)=O
Chemical Formula: $C_{21}H_{31}N_5O_3S_2$
Molecular Weight: 465.63
cLogP: 0.305
Source: SGC-UNC
Reference: N/A

Biochemical profiling

DiscoverX (403 wild-type human kinases)
S_{10} (1μM): 0.017 (7 kinases < 10% control)
CDK16 K_d = 20 nM



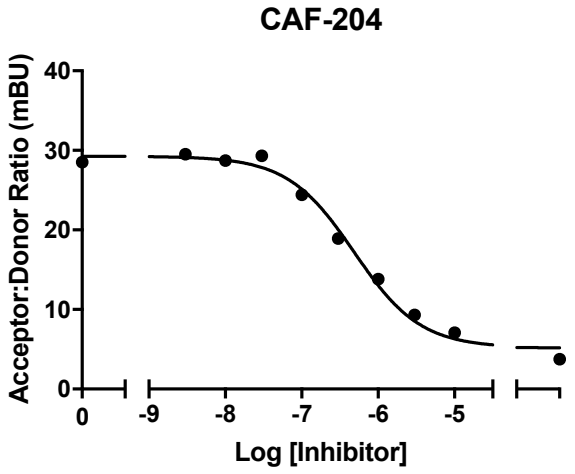
Kinase	% Control @ 1uM
SIK	0
PCTK1	2.7
CDK7	3
PCTK2	5.7
CDKL5	6.3
CDK4-cyclinD1	7.7
CDC2L5	8.2

a.Treespot of DiscoverX KINOMEscan data. b. List of kinases inhibited < 10% control

Cellular target engagement in HEK293 cells

CDK16-NLuc (C term)

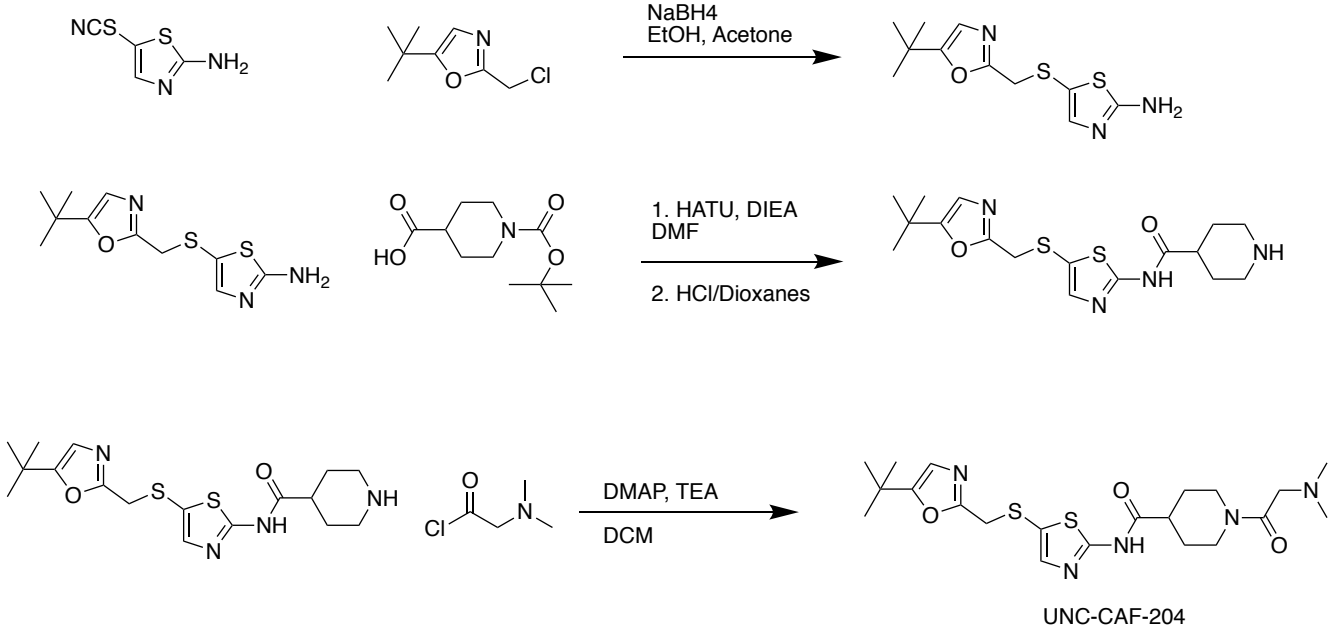
CDK16 IC_{50} = 480 nM



CDK16 IC_{50} = 484 nM

Cellular target engagement of CAF-204 with CDK16/Cyclin Y

Synthetic Route:



UNC-CAF-204