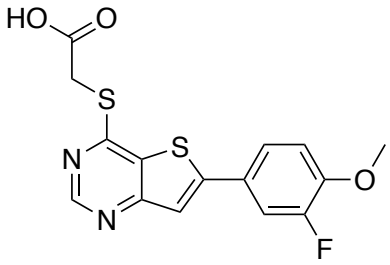
STK17B (DRAK2)

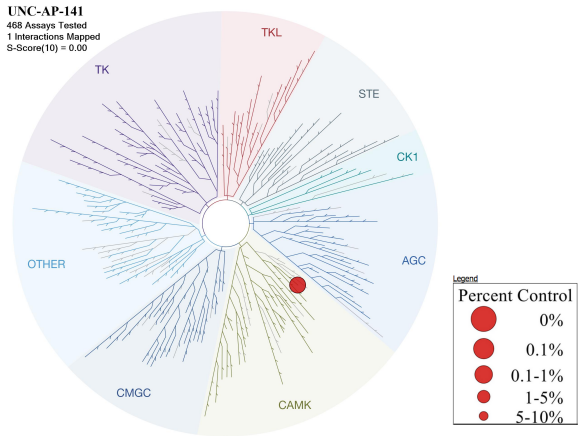


UNC-AP-141

Chemical Name:
2-((6-(3-fluoro-4-methoxyphenyl)thieno[3,2-*d*]pyrimidin-4-yl)thio)acetic acid
CHEBI: 143111
Smile String: OC(CSC1=C2C(C=C(C3=CC=C(SC)C=C3)S2)=NC=N1)=O
Chemical Formula: $C_{15}H_{11}FN_2O_3S_2$
Molecular Weight: 350.38
cLogP: 2.49
Solubility: 139 µM
MP: 209°C – 211°C
Source: SGC-UNC

Biochemical profiling

DiscoverX (403 wild type human kinases)
S_{10} (1µM): 0.002 (1 kinase < 10% control)
STK17B IC_{50} (Luceome) = 18 nM



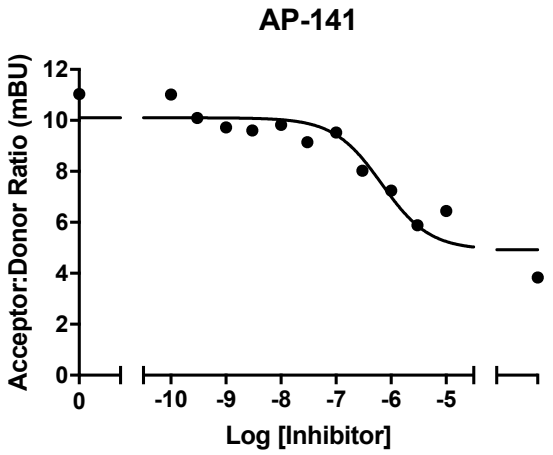
Kinase	% Control @ 1uM
DRAK2	4.2

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

Cellular target engagement in HEK293 cells

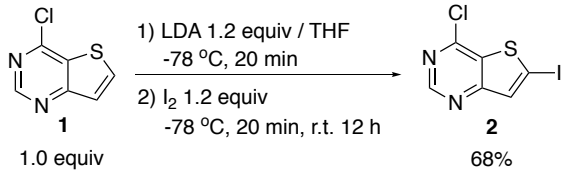
STK17B-NLuc (C term)

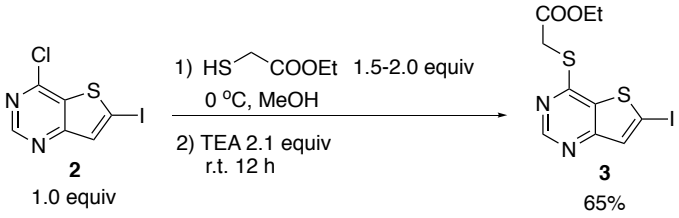
STK17B IC_{50} = 670 nM

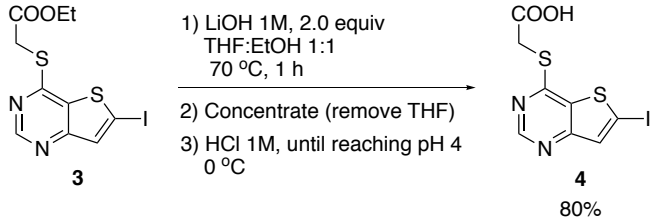


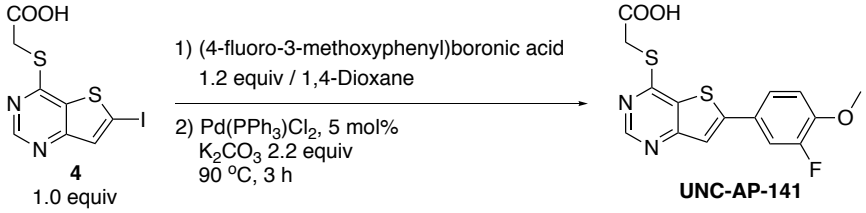
Cellular target engagement of AP-141 with a. STK17B and b. AURKB

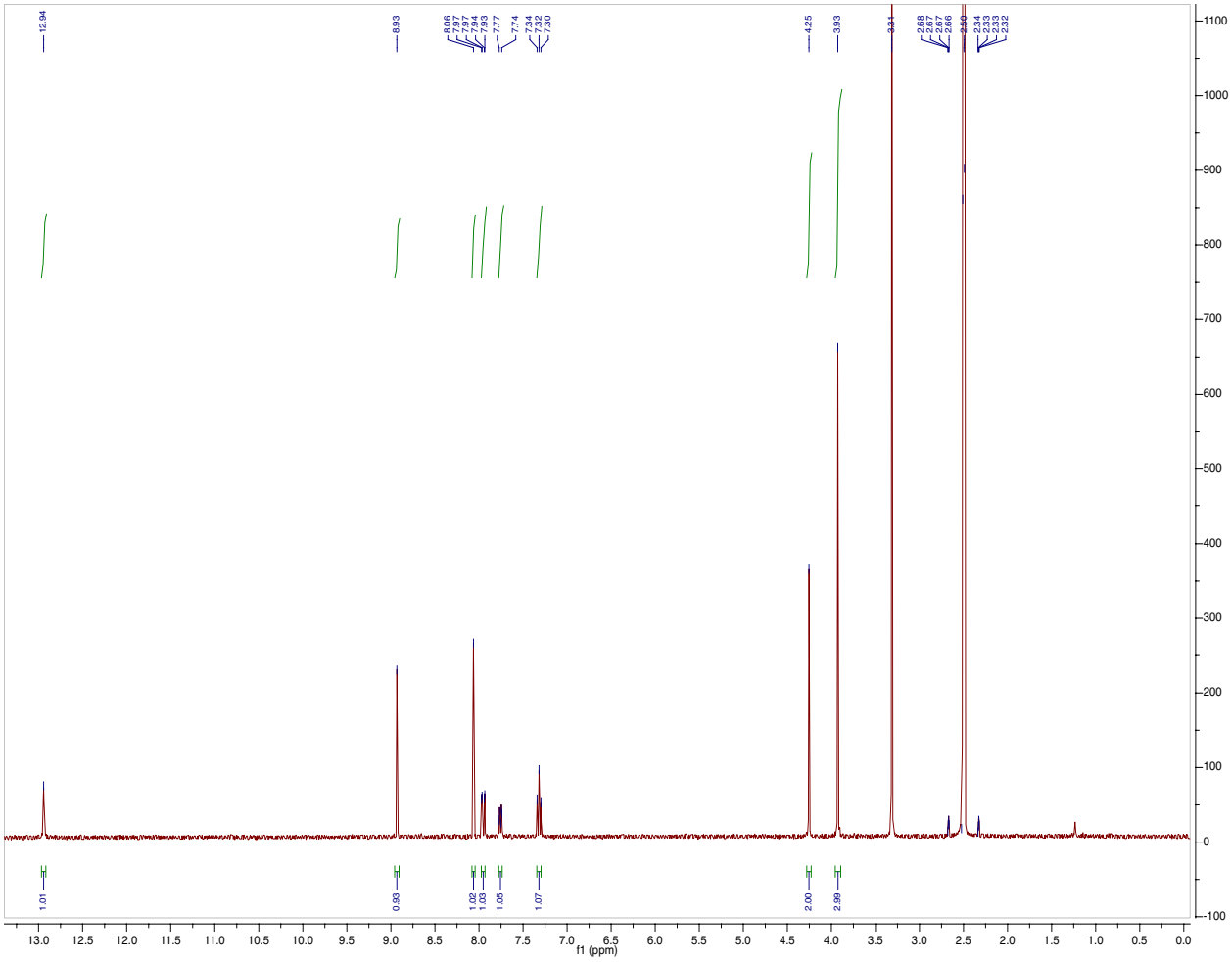
Synthetic Route:











Solvent: DMSO-d_6
Frequency: 400 MHz