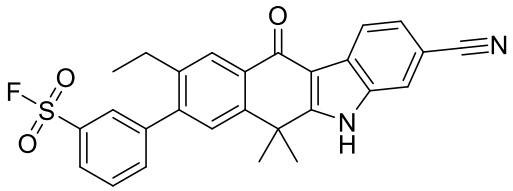
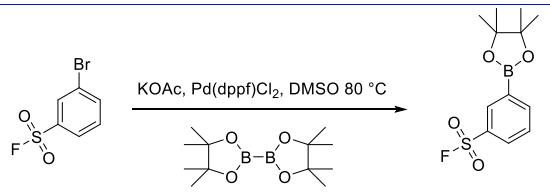
JH-XI-05-01



Chemical Formula: $C_{27}H_{21}FN_2O_3S$
Molecular Weight: 472.53

Category	Parameter	Description
Compound	Name	JH-XI-05-01
	Citation	*Cell Chemical Biology* ***2018****, 25(4), 460-470.e6. DOI:10.1016/j.chembiol.2018.01.013*
	Chemical descriptors	O=S(F)(C1=CC=CC(C2=C(CC)C=C3C(C(C4=C(N5)C=C(C=C4)C#N)=C5C(C)(C3=C2)C)=O)=C1)=O
	Chemical name	3-(3-cyano-9-ethyl-6,6-dimethyl-11-oxo-6,11-dihydro-5H-benzo[b]carbazol-8-yl)benzenesulfonyl fluoride
	Entries in chemical databases	**CID** 29478907
	Availability	None
In vitro profiling	Target (potency)	Enzyme IC50: SRPK1 = 35nM, SRPK2 = 98nM, ALK = 195nM, RET = 106nM, RET M918T = 346nM, LTK = 150nM
	Target (potency)	n/a
	Selectivity	
	Potential reactivity	
	SAR	
	Mechanism of inhibition	Tyrosine reactive
	Structure of target-probe complex	PDB: 3AOX
Cellular profiling	Validation of cellular target	MS-MS analysis confirmed covalent binding to TYR227. In addition, JH-XI-05-01 blocks phosphorylation of SR proteins..
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics		T1/2 = 0.75Hr; Tmax = 0.42Hr; Cmax = 0.07µM; AUC = 2484min*ng/mL; Cl = 1827 mL/min/kg; %F = 0.59



Synthetic scheme