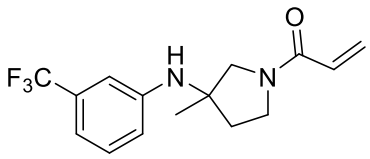
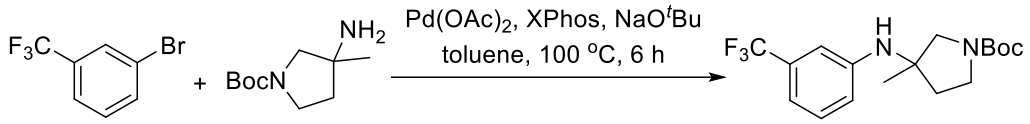
MYF-01-037

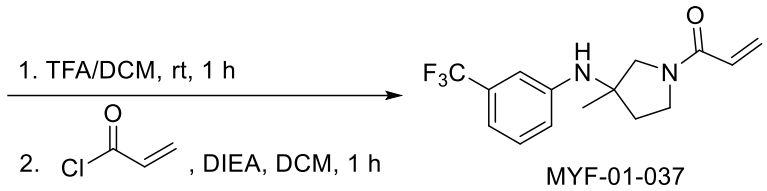


Chemical Formula: $C_{15}H_{17}F_3N_2O$
Molecular Weight: 298.30921

Category	Parameter	Description
Compound	Name	MYF-01-037
	Citation	Kurppa, K.J., Liu, Y., To, C., Zhang, T., Fan, M., Vajdi, A., Knelson, E.H., Xie, Y., Lim, K., Cejas, P., et al. (2020). Treatment-Induced Tumor Dormancy through YAP-Mediated Transcriptional Reprogramming of the Apoptotic Pathway. Cancer Cell 37, 104-122.e112.
	Chemical descriptors	O=C(C=C)N(C1)CCC1(C)NC2=CC(C(F)(F)F)=CC=C2
	Chemical name	1-(3-methyl-3-((3-(trifluoromethyl)phenyl)amino)pyrrolidin-1-yl)prop-2-en-1-one
	Entries in chemical databases	N/A
	Availability	N/A
	Additional comments	Negative control MYF-01-104 also available
In vitro profiling	Target (potency)	Gel-Based TEAD2 palmitoylation inhibition assay (IC_{50} > 50uM)
	Target (potency)	TEAD mCherry reporter assay on PC-9 cells (IC_{50} ~ 5uM)
	Selectivity	Chemoproteomics data available, R value = 2.5 (Chouchani lab)
	Potential reactivity	acrylamide
	SAR	In progress, not published yet
	Mechanism of inhibition	Covalent binding to conserved Cys on TEAD palmitate pocket (for example C380 on TEAD2)
	Structure of target-probe complex	Docking only
	Additional comments	
Cellular profiling	Validation of cellular target	Pull down by dethiobiotin probe MYF-01-108
	Validation of cellular specificity	Chemoproteomics data available, R value = 2.5 (Chouchani lab)
	Additional comments	
Pharmacodynamics		N/A
Pharmacokinetics		N/A



Synthetic scheme



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