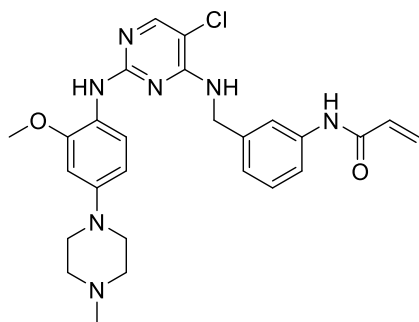
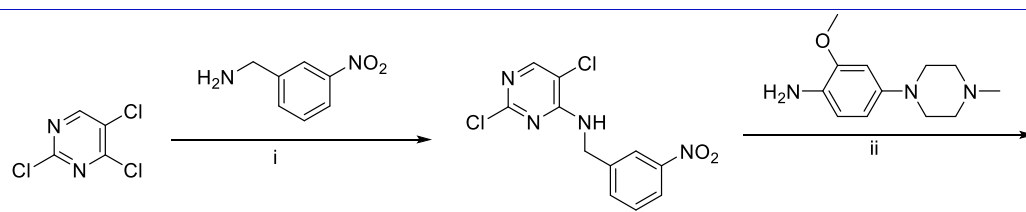


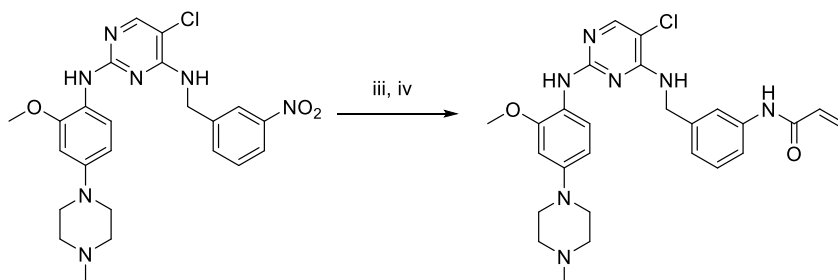
**TL6-144**Chemical Formula: C<sub>26</sub>H<sub>30</sub>ClN<sub>7</sub>O<sub>2</sub>

Molecular Weight: 508.02

Category	Parameter	Description
Compound	Name	TL6-144
	Citation	<i>J. Med. Chem.</i> , 2015, 58 (16), pp 6589–6606. <a href="https://www.ncbi.nlm.nih.gov/pubmed/28927786">https://www.ncbi.nlm.nih.gov/pubmed/28927786</a>
	Chemical descriptors	C1C=C(NCC2=CC=CC(NC(C=C)=O)=C2)N=C(NC3=CC=C(N4CCN(C)CC4)C=C3O)N=C1
	Chemical name	N-(3-((5-chloro-2-((2-methoxy-4-(4-methylpiperazin-1-yl)phenyl)amino)pyrimidin-4-yl)amino)methyl)phenyl)prop-2-enamide
	Entries in chemical databases	CAS# 1805787-93-2; PubChem CID# 92042864
	Availability	MedChemExpress <a href="https://www.medchemexpress.com/JAK3-IN-1.html">https://www.medchemexpress.com/JAK3-IN-1.html</a>
<i>In vitro</i> profiling	Primary target (potency)	<b>JAK3</b> (IC <sub>50</sub> of 4.8 nM)
	Other target (potency)	<b>TTK</b> (IC <sub>50</sub> of 49 nM)
	Selectivity	<b>JAK1</b> (IC <sub>50</sub> of 896 nM), <b>JAK2</b> (IC <sub>50</sub> of 1050 nM), <b>TYK2</b> (IC <sub>50</sub> of >10000 nM)
	Potential reactivity	
	SAR	See above reference paper.
	Mechanism of inhibition	Covalent inhibitor
	Structure of target-probe complex	PDB 4Z16
Additional comments	You can delete this line if you don't have anything	
Cellular profiling	Validation of cellular target	Ba/F3 cellular assay: <b>TEL-JAK3</b> (IC <sub>50</sub> of 69 nM)
	Validation of cellular specificity	Ba/F3 cellular assayS: <b>TEL-JAK1</b> (IC <sub>50</sub> of 3124 nM), <b>TEL-JAK2</b> (IC <sub>50</sub> of 3194 nM), <b>TEL-TYK2 (E957D)</b> (IC <sub>50</sub> of 2266 nM), <b>TEL-ABL</b> (IC <sub>50</sub> of 3047 nM)
Pharmacodynamics		
Pharmacokinetics		



Synthetic scheme



(i) DIEA, 1,4-dioxane, RT; (ii) TFA, 2-BuOH, 100 °C; (iii) Raney nickel, H<sub>2</sub>, MeOH; (iv) acryloyl chloride, satd NaHCO<sub>3</sub>, THF, 0 °C to RT.

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