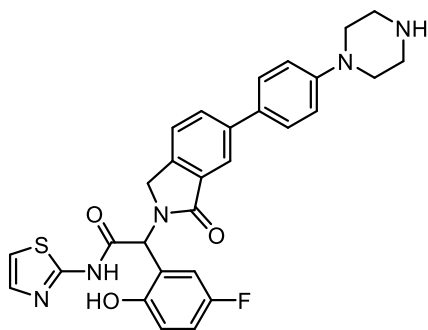


JBJ-04-125-02

 Chemical Formula: C₂₉H₂₆FN₅O₃S

Molecular Weight: 543.62

Category	Parameter	Description
Compound	Name	JBJ-04-125-02
	Citation	<i>Cancer Discov.</i> 2019 , 9, 926-943 https://doi.org/10.1158/2159-8290.CD-18-0903
	Chemical descriptors	O=C(NC1=NC=CS1)C(N2C(C=C(C3=CC=C(N4CCNCC4)C=C3)C=C5)=C5C2)=O)C6=CC(F)=CC=C6O
	Chemical name	2-(5-fluoro-2-hydroxyphenyl)-2-(1-oxo-6-(4-(piperazin-1-yl)phenyl)isoindolin-2-yl)-N-(thiazol-2-yl)acetamide
	Entries in chemical databases	N/A
	Availability	https://www.medchemexpress.com/rac-jbj-04-125-02.html
	Papers that use the compounds	https://pubmed.ncbi.nlm.nih.gov/?term=jbj-04-125-02&sort=date
	Additional comments	
<i>In vitro</i> profiling	Target (potency)	EGFR T790M/L858R (IC ₅₀ = 0.26 nM)
	Target (potency)	N/A
	Selectivity	KINOMEscan at 10 μM (ErbB family and their mutants)
	Potential reactivity	N/A
	SAR	To be published
	Mechanism of inhibition	Allosteric EGFR inhibition
	Structure of target-probe complex	PDB 6DUK
	Additional comments	Relative papers
Cellular profiling	Validation of cellular target	Use EGFR-dependent Ba/F3 cells/pull down assay
	Validation of cellular specificity	N/A
	Additional comments	
Pharmacodynamics	Available in the paper	
Pharmacokinetics	Half life 2.99 hr (IV), C _{max} 609 ng/mL (PO) Oral bioavailability 3%	

Synthetic scheme

