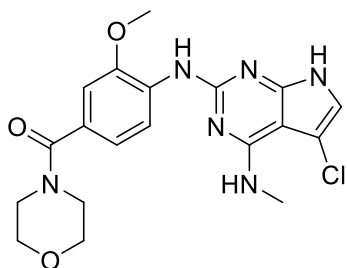


JH-II-127Chemical Formula: C₁₉H₂₁ClN₆O₃

Molecular Weight: 416.87

Category	Parameter	Description
Compound	Name	JH-II-127
	Citation	<i>ACS Med. Chem. Lett.</i> 2016 , 6, 584-589
	Chemical descriptors	C1C1=CNC2=NC(NC3=C(OC)C=C(C(N4CCOCC4)=O)C=C3)=NC(NC)=C21
	Chemical name	(4-((5-chloro-4-(methylamino)-7H-pyrrolo[2,3-d]pyrimidin-2-yl)amino)-3-methoxyphenyl)(morpholino)methanone
	Entries in chemical databases	CID 112499966
	Availability	Tocris https://www.tocris.com/products/jh-ii-127_6289
<i>In vitro</i> profiling	Target (potency)	LRRK2 (G2019S) (IC ₅₀ 2.2 nM in enzyme assay) LRRK2 wt (IC ₅₀ 6.6 nM in enzyme assay) LRRK2 (A2016T) (IC ₅₀ 47.7 nM in enzyme assay)
	Selectivity	S-Score(20) = 0.01
	Potential reactivity	Type 1
	SAR	
	Mechanism of inhibition	reversible
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	JH-II-127 dose-dependently inhibited phosphorylation of S910 & S935 in HEK293 cells transfected with LRRK2 wt and LRRK2 (G2019S) at a concentration of 0.3 μM
	Validation of cellular specificity	
Pharmacodynamics		
Pharmacokinetics (i.v. 2 mg/kg)		T1/2 = 0.66 h CL = 62.24 ml/min/Kg Vss=1.73 L/Kg

Synthetic scheme

