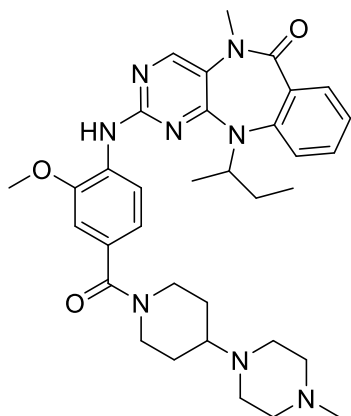


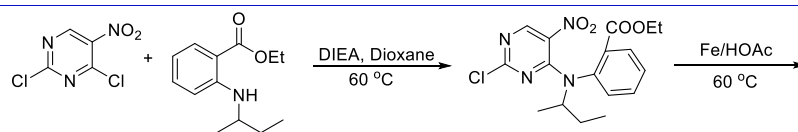
JWG-071Chemical Formula: C₃₄H₄₄N₈O₃

Molecular Weight: 612.7790

Category	Parameter	Description
Compound	Name	BMK1/ERK5 inhibitor (JWG-071)
	Citation	<i>ACS Chem Biol</i> , 2018 , 13(9), 2438-2448.
	Chemical descriptors	CN(C1=CN=C(NC2=C(OCC)C=C(N3CCC(O)CC3)C=C2)N=C1N(C)C4=C5C=CC=C4)C5=O
	Chemical name	2-((2-ethoxy-4-(4-hydroxypiperidin-1-yl)phenyl)amino)-5,11-dimethyl-5,11-dihydro-6H-benzo[e]pyrimido[5,4-b][1,4]diazepin-6-one
	Availability	
<i>In vitro</i> profiling	Target (potency)	ERK5 (88 nM)
	Target (potency)	LRRK2 (109 nM, Invitrogen Adapta) DCAMKL2 (223 nM, Invitrogen Z-lyte) PLK4 (328 nM, Invitrogen Lanthascreen)
	Selectivity	Equally potent against ERK5 and LRRK2. Selective over BRD4.
	Potential reactivity	None to our knowledge
	SAR	
	Mechanism of inhibition	ATP-competitive
	Structure of target-probe complex	
Cellular profiling	Validation of cellular target	Dose-dependently inhibited MAPK7 autophosphorylation induced by EGF in HeLa cells with IC ₅₀ of 0.020 ± 0.003 μM.
	Validation of cellular specificity	
Pharmacodynamics		

Pharmacokinetics

No data



Synthetic scheme

