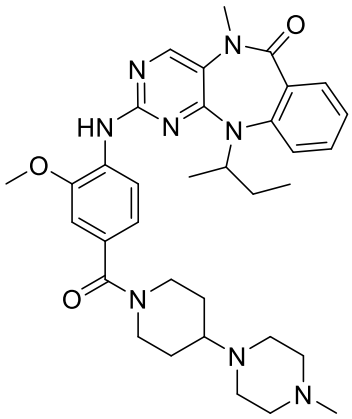
JWG-071



Chemical Formula: $C_{34}H_{44}N_8O_3$
Molecular Weight: 612.7790

Category	Parameter	Description
Compound	Name	BMK1/ERK5 inhibitor (JWG-071)
	Citation	*ACS Chem Biol,* **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)C 5=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	
In vitro 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 IC50 of 0.020 ± 0.003 µM.
	Validation of cellular specificity	
Pharmacodynamics		

Pharmacokinetics	No data
Synthetic scheme