MOLNOVA
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Datasheet (Version 1.0)

Product Name	:	BMS-986165
Synonyms	:	——
Cat No.	:	M21721
CAS Number	:	1609392-27-9
Molecular Formula	:	C20H19D3N8O3
Formula Weight	:	425.46
Chemical Name	:	——
Description	:	BMS-986165 is differentiated from previous JAK inhibitors due its unique ability to selectively bind to the pseudokinase (JH2) domain of TYK2 and inhibit its function through an allosteric mechanism.BMS-986165 maintains excellent potency in human and mouse whole blood (IC50s=13 and 100 nM, respectively) and shows no significant hERG inhibition in the flux assay (IC50>80 μM).
Pathway	:	Angiogenesis
Target	:	JAK
Receptor	:	——
Solubility	:	DMSO : 37.5 mg/mL (88.14 mM; Need ultrasonic)
SMILES	:	O=C(C1=NN=C(NC(C2CC2)=O)C=C1NC3=CC=CC(C4=NN(C)C=N4)=C3OC)NC([2H])([2H])[2H]
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	

1. Wrobleski ST, et al. Highly Selective Inhibition of Tyrosine Kinase 2 (TYK2) for the Treatment of Autoimmune Diseases: Discovery of the Allosteric Inhibitor BMS-986165. J Med Chem. 2019 Jul 18. 2. Catlett I, et al. SAT0226 A first-in-human, study of BMS-986165, a selective, potent, allosteric small molecule inhibitor of tyrosine kinase 2. Annals of the Rheumatic Diseases 2017;76:859.