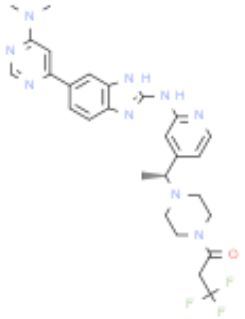
Product Data Sheet

Cas No.:	2409479-29-2	Cat. No:	PL03340
Product Name:	BAY-985		
Product synonym:	1-[4-[(1R)-1-[2-[[6-[6-(二甲氨基)嘧啶-4-基]-1H-苯并咪唑-2-基]氨基]吡啶-4-基]乙基]哌嗪-1-基]-3,3,3-三氟丙烷-1-酮		
Chemical name:	BAY-985		
MF:	C27H30F3N9O	FW:	553.5820
Purity:	≥99%	Batch No.:	-
Storage:			
Structural formula:			
λmax:	-	Formulation:	-
Solubility :			
SMILES :	FC(C([H])([H])C(N1C([H])([H])C([H])([H])N([C@]([H])(C([H])([H])[H])C2C([H])=C([H])N=C(C=2[H])N([H])C2=NC3C([H])=C([H])C(C4=C([H])C(=NC([H])=N4)N(C([H])([H])[H])C([H])([H])[H])=C([H])C=3N2[H])C([H])([H])C1([H])[H])=O)(F)F		
InChI Code:	-		
InChI Key:			
WARNING This product is not for human or veterinary use.			

Product Description

BAY-985 是一种高效的，有口服活性的、ATP 竞争性的，选择性 TBK1 和 IKKε 双重抑制剂，对 TBK1 (在低/高 ATP 实验中) 和 IKKε 的 IC_{50} 分别为 2/30 和 2 nM。BAY-985 具有抗肿瘤功效。

生物活性	BAY-985 is a highly potent, orally active and selective ATP-competitive dual inhibitor of TBK1 and IKKε with IC 50 s of 2/30 and 2 nM for TBK1 (low/high ATP) and IKKε, respectively. Antitumor efficacy.
IC50 & Target[1][2]	TBK1 2 nM (IC50, low ATP) TBK1 30 nM (IC
体外研究(In Vitro)	BAY-985 inhibits FLT3, RSK4, DRAK1, and ULK1 with IC50s of 123, 276, 311, and 7930 nM, respectively. BAY-985 inhibits the cellular phosphorylation of interferon regulatory factor 3 (IRF3) with an IC50 of 74 nM. BAY-985 is active in cellular mechanistic assay and shows anti-proliferative activity in a few cancer cell lines with IC50s of 900 and 7260 nM for SK-MEL2 (NRAS and TP53 mutated) and ACHN (CDKN2A mutated) cells, respectively. has not independently confirmed the accuracy of these methods. They are for reference only. <

体内研究(In Vivo)	BAY-985 (200 mg/kg; p.o.; b.i.d.; 111 days) results in weak antitumor efficacy. BAY-985 shows high clearance (CL b = 4.0 L/h/kg, ca. 95% hepatic extraction), large volume of distribution at steady state (V ss =2.9 L/kg) and a short terminal half-life (t 1/2 =0.79 h). has not independently confirmed the accuracy of these methods. They are for reference only.
包装储存	Powder -20°C 3 years；4°C 2 years
溶解度数据	In Vitro: DMSO : 50 mg/mL (90.32 mM; Need ultrasonic)配制储备液