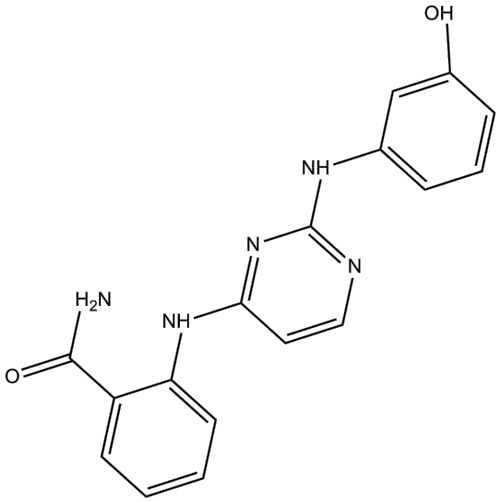
Product Data Sheet

Product Name: DB07268
Cat. No.: GC14114

Chemical Properties

Cas. No.	929007-72-7		
Chemical Name	2-[[2-(3-hydroxyanilino)pyrimidin-4-yl]amino]benzamide		
SMILES	C1=CC=C(C(=C1)C(=O)N)NC2=NC(=NC=C2)NC3=CC(=CC=C3)O		
Formula	$C_{17}H_{15}N_5O_2$	M.Wt	321.33
Solubility	≥ 15.2 mg/mL in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		

Structure



Background

IC50: 9 nM for JNK1

DB07268 is a JNK1 inhibitor. The c-Jun N-terminal kinases (JNKs) are members of the mitogen-activated protein kinase family. Three JNK isoforms (JNK1, 2 and 3) have been identified. There is

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growing evidences indicating that activation of the JNK activity is involved in a number of human disease settings. Therefore, considerable efforts have been directed toward the identification of JNK inhibitors suitable for clinical development.

In vitro: The selectivity data of DB07268 against a panel of kinases has been tested. Results showed that DB07268 had some degree of selectivity over quite a few kinases with the exceptions of PLK, CHK1, and CK2. Although d DB07268 showed submicromolar potency against these three kinases, it still appeared to exhibit at least 70- to 90-fold greater potency against JNK1 than PLK, CHK1, and CK2 [1].

In vivo: Several analogs of DB07268 were profiled in vivo. These compounds had a range of exposure in rats and mice. Some had excellent brain penetration despite having poor rat pharmacokinetics, while others had a more balanced profile. Unfortunately, the most potent analog exhibited poor rat pk demonstrated by a short half-life, low oral absorption and poor brain penetration. One DB07268 analog likely exhibited modest rat pk with low clearance and decent oral absorption. This analog also showed modest brain penetration [1].

Clinical trial: So far, no clinical study has been reported.

References:
[1] Liu M,Wang S,Clampit JE,Gum RJ,Haasch DL,Rondinone CM,Trevillyan JM,Abad-Zapatero C,Fry EH,Sham HL,Liu G. Discovery of a new class of 4-anilinopyrimidines as potent c-Jun N-terminal kinase inhibitors: Synthesis and SAR studies. Bioorg Med Chem Lett.2007 Feb 1;17(3):668-72. Epub 2006 Nov 2.
[2] Romain Nol, Youseung Shin, Xinyi Song, Yuanjun He, Marcel Koenig, Weimin Chen, Yuan Yuan Ling, Li Lin, Claudia H. Ruiz, Phil LoGrasso, Michael D. Cameron, Derek R. Duckett, Theodore M. Kamenecka. Synthesis and SAR of 4-(pyrazol-3-yl)-pyridines as novel c-Jun N-terminal kinase inhibitors.Bioorg Med Chem Lett. 2011 May 1; 21(9): 2732–2735.

Caution: Product has not been fully validated for medical applications. For research use only.
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