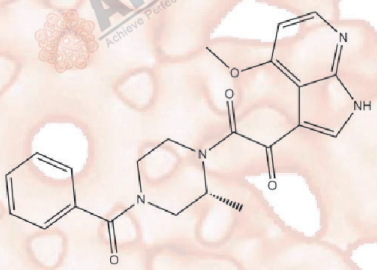
Product Name: BMS-378806
Revision Date: 10/27/2023

Product Data Sheet

BMS-378806



Cat. No.:	B1533
CAS No.:	357263-13-9
Formula:	C22H22N4O4
M.Wt:	406.43
Synonyms:	
Target:	Microbiology & Virology
Pathway:	gp120/CD4
Storage:	Store at -20°C

Solvent & Solubility

In Vitro

insoluble in H2O; insoluble in EtOH; ⩾20.2 mg/mL in DMSO

Preparing Stock Solutions

Mass / Solvent / Concentration	1mg	5mg	10mg
1 mM	2.4604 mL	12.3022 mL	24.6045 mL
5 mM	0.4921 mL	2.4604 mL	4.9209 mL
10 mM	0.2460 mL	1.2302 mL	2.4604 mL

Please refer to the solubility information to select the appropriate solvent.

Biological Activity

Shortsummary	Gp120/CD4 inhibitor
IC_{50} & Target	0.85 nM-26.5 nM(EC50) (CD4-gp120 interactions)

In Vitro

Cell Viability Assay

Cell Line:	MT-2 cells
Preparation method:	The solubility of this compound in DMSO is >10 mM. General tips for obtaining a higher concentration: Please warm the tube at 37°C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.
Reacting conditions:	0-3 mM for 6 days; or 0.8, 1.6, and 3.2 μM

	Applications:	BMS-378806 showed HIV-1 inhibitory activity and cytotoxicity in MT-2 cells with EC50 value of 2.68 nM [1]. Moreover, BMS-378806 inhibited the interaction between viral gp120 and cellular CD4 receptors and showed direct binding affinity to gp120 [2].
In Vivo	**Animal experiment**	
	Animal models:	Rats, monkeys and dogs model.
	Dosage form:	i.v. 1 and 5 mg/kg and p.o. 5 and 25 mg/kg for 0.17, 0.5, 1, 1.5 and 2 h
	Applications:	BMS-378806 showed species-dependent oral bioavailability which was 19%–24% in rats and monkeys and 77% in dogs [3].
	Other notes:	Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

Product Citations

1. Pancera M, Lai YT, et al. "Crystal structures of trimeric HIV envelope with entry inhibitors BMS-378806 and BMS-626529." Nat Chem Biol. 2017 Oct;13(10):1115-1122.PMID:28825711

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References

1. Wang, T., Zhang, Z., Wallace, O. B., Deshpande, M., Fang, H., Yang, Z., Zadjura, L. M., Tweedie, D. L., Huang, S., Zhao, F., Ranadive, S., Robinson, B. S., Gong, Y. F., Ricarrdi, K., Spicer, T. P., Deminie, C., Rose, R., Wang, H. G., Blair, W. S., Shi, P. Y., Lin, P. F., Colonno, R. J. and Meanwell, N. A. (2003) Discovery of 4-benzoyl-1-[(4-methoxy-1H- pyrrolo[2,3-b]pyridin-3-yl)oxoacetyl]-2-(R)-methylpiperazine (BMS-378806): a novel HIV-1 attachment inhibitor that interferes with CD4-gp120 interactions. J Med Chem. 46, 4236-4239

2. Guo, Q., Ho, H. T., Dicker, I., Fan, L., Zhou, N., Friborg, J., Wang, T., McAuliffe, B. V., Wang, H. G., Rose, R. E., Fang, H., Scarnati, H. T., Langley, D. R., Meanwell, N. A., Abraham, R., Colonno, R. J. and Lin, P. F. (2003) Biochemical and genetic characterizations of a novel human immunodeficiency virus type 1 inhibitor that blocks gp120-CD4 interactions. J Virol. 77, 10528-10536

3. Yang, Z., Zadjura, L., D'Arienzo, C., Marino, A., Santone, K., Klunk, L., Greene, D., Lin, P. F., Colonno, R., Wang, T., Meanwell, N. and Hansel, S. (2005) Preclinical pharmacokinetics of a novel HIV-1 attachment inhibitor BMS-378806 and prediction of its human pharmacokinetics. Biopharm Drug Dispos. 26, 387-402

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most APExBIO products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt

of the product, follow the storage recommendations on the product data sheet.

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