Product Data Sheet

BMS-707035

Cat. No.: HY-13269

CAS No.: 729607-74-3

Molecular Formula: $C_{17}H_{19}FN_4O_5S$ Molecular Weight: 410.42

Target: HIV; HIV Integrase

Pathway: Anti-infection; Metabolic Enzyme/Protease

Storage: Powder -20°C 3 years

4°C 2 years

In solvent -80°C 2 years

-20°C 1 year

SOLVENT & SOLUBILITY

In Vitro

DMSO: 50 mg/mL (121.83 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.4365 mL	12.1826 mL	24.3653 mL
	5 mM	0.4873 mL	2.4365 mL	4.8731 mL
	10 mM	0.2437 mL	1.2183 mL	2.4365 mL

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

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (6.09 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (6.09 mM); Clear solution

BIOLOGICAL ACTIVITY

DescriptionBMS-707035 is a potent orally active HIV-1 integrase strand transfer inhibitor (INSTI). BMS-707035 has enzyme inhibitory with an IC₅₀ value of 3 nM. BMS-707035 also has weak CYP inhibiton and antiviral activity. BMS-707035 can be used for the

research of human immunodeficiency virus-1 (HIV-1) $^{[1]}$.

In Vitro BMS-707035 has antiviral activity with EC₅₀ values of 2 nM and 17 nM in the presence of 10% FBS and 15 mg/mL human

serum albumin, $respectively^{[1]}$.

BMS-707035 has high plasma protein binding and not overtly cytotoxicy to several cell lines, with CC₅₀ value of \geq 45 μ M^[1].

BMS-707035 has a relatively weak CYP inhibiton with IC $_{50}$ value of ${\ge}40~\mu\text{M}^{[1]}.$

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

BMS-707035 has a low clearance effect in the rat, dog and monkey with moderate to long elimination half-lives in all species [1].

Pharmacokinetic Parameters of BMS-707035 in rat, dog and monkey (IV) $^{[1]}$.

	Rat	Monkey	Dog
IV dose (mg/kg)	0.87	1	1
CL (ml/min/kg)	9.7	6.8	2.0
T _{1/2} (h)	4.0	6.5	6.0
V _{ss} (L/kg)	0.86	0.87	0.45
PO dose (mg/kg)	4.4	5	5.2
C _{max} (μM)	4.51	6.12	72.8
t _{max} (h)	0.25	0.25	0.25
AUC (μM*h)	19.1	19.2	162
F (%)	86	56	129

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CUSTOMER VALIDATION

• Int J Antimicrob Agents. 2019 Dec;54(6):814-819.

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REFERENCES

[1]. B Narasimhulu Naidu, et al. The discovery and preclinical evaluation of BMS-707035, a potent HIV-1 integrase strand transfer inhibitor. Bioorg Med Chem Lett. 2018 Jul 1;28(12):2124-2130.

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

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA