

Product Data Sheet

Vodobatinib

 Cat. No.:
 HY-137460

 CAS No.:
 1388803-90-4

 Molecular Formula:
 $C_{27}H_{20}ClN_3O_2$

Molecular Weight: 453.92 Target: Bcr-Abl

Pathway: Protein Tyrosine Kinase/RTK

Storage: Powder -20°C 3 years

 $\begin{array}{ccc} & 4^{\circ}\text{C} & 2 \text{ years} \\ \text{In solvent} & -80^{\circ}\text{C} & 6 \text{ months} \\ & -20^{\circ}\text{C} & 1 \text{ month} \end{array}$

SOLVENT & SOLUBILITY

In Vitro

DMSO: 125 mg/mL (275.38 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.2030 mL	11.0152 mL	22.0303 mL
	5 mM	0.4406 mL	2.2030 mL	4.4061 mL
	10 mM	0.2203 mL	1.1015 mL	2.2030 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: 2.08 mg/mL (4.58 mM); Suspended solution; Need ultrasonic
- 2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (4.58 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	Vodobatinib (K0706) is a potent, third generation and orally active Bcr-Abl1 tyrosine kinase inhibitor with an IC ₅₀ of 7 nM. Vodobatinib exhibits activity against most BCR-ABL1 point mutants, and has no activity against BCR-ABL1T315I. Vodobatinib can be used for chronic myeloid leukemia (CML) research ^{[1][2]} . Vodobatinib is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.
IC ₅₀ & Target	BCR-ABL1 7 nM (IC ₅₀)
In Vitro	In Ba/F3 cells expressing BCR-ABL1, BCR-ABL1 _{L248V} , BCR-ABL1 _{Y253H} , or BCR-ABL1 _{E255V} , Vodobatinib (K0706; 0-2000 nM) treatment shows potent inhibition of BCR-ABL1 tyrosine autophosphorylation ^[1] .

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

REFERENCES

[1]. Orlando Antelope, et al. BCR-ABL1 tyrosine kinase inhibitor K0706 exhibits preclinical activity in Philadelphia chromosome-positive leukemia. Exp Hematol. 2019 Sep;77:36-40.e2.

[2]. Phase 1 Trial of Vodobatinib, a Novel Oral BCR-ABL1 Tyrosine Kinase Inhibitor (TKI): Activity in CML Chronic Phase Patients Failing TKI Therapies Including Ponatinib. Session: 632: Chronic Myeloid Leukemia: Therapy: CML: New and Beyond.

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

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