

Product Data Sheet

Desmethyl Erlotinib

Cat. No.: HY-13256A CAS No.: 183321-86-0 Molecular Formula: $C_{21}H_{21}N_3O_4$ Molecular Weight: 379.41

Target: Drug Metabolite

Pathway: Metabolic Enzyme/Protease

Storage: Powder -20°C 3 years

4°C 2 years In solvent -80°C 6 months

t -80°C 6 months

-20°C 1 month

SOLVENT & SOLUBILITY

In Vitro

DMSO: 125 mg/mL (329.46 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.6357 mL	13.1784 mL	26.3567 mL
	5 mM	0.5271 mL	2.6357 mL	5.2713 mL
	10 mM	0.2636 mL	1.3178 mL	2.6357 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 (5.48 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE- β -CD in saline) Solubility: \geq 2.08 mg/mL (5.48 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (5.48 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	Desmethyl Erlotinib (OSI-420 free base) is an active metabolite of Erlotinib. Erlotinib is a potent EGFR tyrosin kinase inhibitor ^[1] . Desmethyl Erlotinib is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.
In Vivo	Desmethyl Erlotinib exhibits $t_{1/2}$ of 11.96±2.01 h in a pharmacokinetic study in Wistar rats ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Pharmacol Res. 2023 Mar 10;106724.
- Cell Rep. 2023 Mar 20;42(3):112275.
- Eur J Pharm Sci. 2019 May 15;133:145-159.

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REFERENCES

[1]. Thappali SR, et al. Simultaneous Determination of Celecoxib, Erlotinib, and its Metabolite Desmethyl-Erlotinib (OSI-420) in Rat Plasma by Liquid chromatography/Tandem Mass Spectrometry with Positive/Negative Ion-Switching Electrospray Ionisation. Sci Pharm. 2012 Jul-Sep;80(3):633-46.

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

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