

## **Product** Data Sheet

# 1-Ethynylnaphthalene

Cat. No.: HY-111430 CAS No.: 15727-65-8

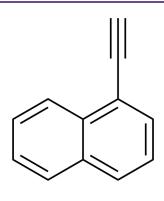
Molecular Formula: C<sub>12</sub>H<sub>8</sub> Molecular Weight: 152.19

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease Storage: Pure form -20°C 3 years

> 4°C 2 years In solvent -80°C 6 months

-20°C 1 month



## **SOLVENT & SOLUBILITY**

In Vitro DMSO : ≥ 125 mg/mL (821.34 mM)

\* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	6.5707 mL	32.8537 mL	65.7073 mL
	5 mM	1.3141 mL	6.5707 mL	13.1415 mL
	10 mM	0.6571 mL	3.2854 mL	6.5707 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 (13.67 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.08 mg/mL (13.67 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.08 mg/mL (13.67 mM); Clear solution

## **BIOLOGICAL ACTIVITY**

Description	1-Ethynylnaphthalene is a selective inhibitor of cytochrome P450 1B1. 1-Ethynylnaphthalene 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 <sub>50</sub> & Target	P450 1B1 <sup>[1]</sup>

### In Vitro

1-Ethynylnaphthalene, selective inhibitor of cytochrome P450 IB1, does not affect 2-hydroxylation but inhibits 4-hydroxylation by 38%. At higher concentrations, 1-Ethynylnaphthalene inhibits 2-hydroxylation of 2-Hydroxylation of estradiol ( $E_2$ ) by ~30% and 4-hydroxylation of  $E_2$  by up to  $80\%^{[1]}$ .

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

### **REFERENCES**

[1]. Liehr JG, et al. 4-Hydroxylation of estradiol by human uterine myometrium and myoma microsomes: implications for the mechanism of uterine tumorigenesis. Proc Natl Acad Sci U S A. 1995 Sep 26;92(20):9220-4.

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

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