Estradiol 3-sulfamate

Cat. No.: HY-U00112

CAS No.: 172377-52-5

Molecular Formula: $C_{18}H_{25}NO_4S$

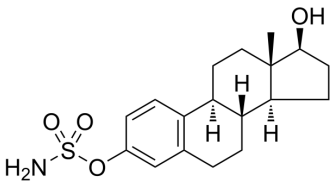
Molecular Weight: 351.46

Target: Steroid Sulfatase

Pathway: 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 : 62.5 mg/mL (177.83 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.8453 mL	14.2264 mL	28.4527 mL
5 mM	0.5691 mL	2.8453 mL	5.6905 mL
10 mM	0.2845 mL	1.4226 mL	2.8453 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 (5.92 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.92 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.92 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Estradiol 3-sulfamate (BLE 00084; E2MATE; ES-J 995) is a potent, long-acting, and orally active steroid sulfatase inhibitor; inhibits estrone sulfatase with an IC_{50} of 251 nM and a K_i of 133 nM.

IC_{50} & Target

IC50: 251 nM (estrone sulfatase)[1]

Ki: 133 nM (estrone sulfatase)[1]

In Vitro	Introduction of a fluoro, chloro, or bromo moiety at the C-2 position of EMATE and Estradiol 3-sulfamate and that of a fluoro moiety at the C-4 position of the parent sulfamates markedly increase the estrone sulfatase inhibitory activity[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Estradiol 3-sulfamate is readily transformed and absorbed in the gut into its oxidative metabolite, EMATE, and both compounds have already been shown to be potent, long-acting, and orally active STS inhibitors[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Numazawa M, et al. Inhibition of estrone sulfatase by aromatase inhibitor-based estrogen 3-sulfamates. Steroids. 2006 May;71(5):371-9.

[2]. Pohl O, et al. Synergistic effects of E2MATE and norethindrone acetate on steroid sulfatase inhibition: a randomized phase I proof-of-principle clinical study in women of reproductive age. Reprod Sci. 2014 Oct;21(10):1256-65.

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