

Product Data Sheet

Product Name: Estradiol 3-sulfamate

Cat. No.: GC36010

Chemical Properties

Cas. No. 172377-52-5

SMILES C[C@@]1([C@H]2O)[C@](CC2)([H])[C@@](CCC3=C4C=CC(=C(C=C3)C(=O)N)C=C4)[C@]4([H])CC1

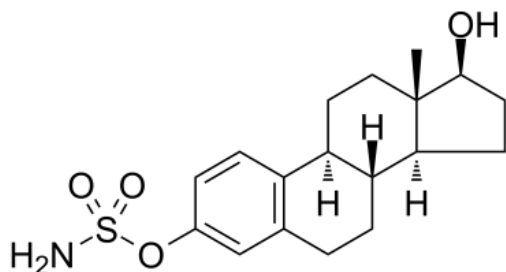
Formula $C_{18}H_{25}NO_4S$ M.Wt 351.46

Solubility DMSO: 62.5 mg/mL (177.83 mM) Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



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

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Background

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 IC₅₀ of 251 nM and a K_i of 133 nM. IC₅₀: 251 nM (estrone sulfatase)[1]K_i: 133 nM (estrone sulfatase)[1]

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].

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].

[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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