

Certificate of Analysis

Print Date: Jul 16th 2025

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Product Name: ICI 182,780 Catalog No.: 1047 Batch No.: 23

CAS Number: 129453-61-8

IUPAC Name: $7\alpha,17\beta$ -[9-[(4,4,5,5,5-Pentafluoropentyl)sulfinyl]nonyl]estra-1,3,5(10)-triene-3,17-diol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{32}H_{47}F_5O_3S$.

Batch Molecular Weight: 606.78 **Physical Appearance:** White solid

Solubility: ethanol to 50 mM

DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 63.34 7.81 0
Found 63.43 7.85 0

Product Information

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Description:

ICI 182,780 is a high affinity estrogen receptor antagonist (IC $_{50}$ = 0.29 nM), devoid of any partial agonism both in vitro and in vivo. ICI 182,780 is a high affinity agonist at the membrane estrogen receptor GPER. ICI 182,780 inhibits MCF-7 human breast cancer cell growth in vitro and shows antitumor activity in mice models. ICI 182,780 penetrates the blood-brain-barrier and has neuronal functional effects in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{32}H_{47}F_5O_3S$. Batch Molecular Weight: 606.78

Physical Appearance: White solid

Batch Molecular Structure:

Minimum Purity: ≥99%

Storage: Store at RT

Solubility & Usage Info:

ethanol to 50 mM DMSO to 100 mM

When purchased as a 1mg unit, this product is supplied in lyophilized form. It may appear as a solid, gel or film and be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Alfinito et al (2008) ICI 182,780 penetrates brain and hypothalamic tissue and has functional effects in the brain after systemic dosing. Endocrinology 149 5219. PMID: 18599545.

Thomas et al (2005) Identity of an estrogen membrane receptor coupled to a G protein in human breast cancer cells. Endocrinology. **146** 624. PMID: 15539556.

Howell et al (2000) ICI 182,780 (Faslodex™): Development of a novel, "pure" antiestrogen. Cancer 89 817. PMID: 10951345.