# **Certificate of Analysis**

Print Date: Apr 8th 2024

#### Product Name: ICI 182,780

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: Batch Molecular Weight: Physical Appearance:** Solubility:

**Batch Molecular Structure:** 

 $C_{32}H_{47}F_5O_3S$ 606.77 White solid ethanol to 50 mM DMSO to 100 mM Store at RT



2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR:

Mass Spectrum:

**Microanalysis:** 

Shows 99.7% purity Consistent with structure Consistent with structure

Carbon Hydrogen Nitrogen Theoretical 63.34 7.81

Found 63.76 7.66

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Catalog No.: 1047 Batch No.: 22

Storage:

**biotechne**<sup>®</sup> **TOCRIS** 

# biotechne<sup>®</sup> TOCRIS

# **Product Information**

### www.tocris.com

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#### Product Name: ICI 182,780

CAS Number: 129453-61-8

IUPAC Name:

7α,17β-[9-[(4,4,5,5,5-Pentafluoropentyl)sulfinyl]nonyl]estra-1,3,5(10)-triene-3,17-diol

#### **Description:**

ICI 182,780 is a high affinity estrogen receptor antagonist (IC<sub>50</sub> = 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<sub>32</sub>H<sub>47</sub>F<sub>5</sub>O<sub>3</sub>S Batch Molecular Weight: 606.77 Physical Appearance: White solid

#### Minimum Purity: ≥99%

#### **Batch Molecular Structure:**



#### 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.

Catalog No.: 1047

#### 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.

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