

**Product Name:** Escitalopram oxalate

**Catalog No.:** 4796

**Batch No.:** 3

CAS Number: 219861-08-2

IUPAC Name: (+)-(S)-1-[3-(Dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile oxalate

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>20</sub>H<sub>21</sub>FN<sub>2</sub>O.C<sub>2</sub>H<sub>2</sub>O<sub>4</sub>

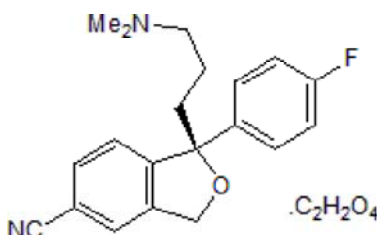
**Batch Molecular Weight:** 414.43

**Physical Appearance:** White solid

**Solubility:** water to 50 mM  
DMSO to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 100% purity

**Chiral HPLC:** Shows 99.8% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = +12 (Concentration = 2, Solvent = Methanol)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	63.76	5.59	6.76
Found	63.77	5.61	6.72

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

Escitalopram oxalate is a selective 5-HT reuptake inhibitor ( $K_i$  values are 0.89, 8150, and 10500 nM for serotonin, noradrenalin, and dopamine transporters respectively). Escitalopram oxalate is an S-enantiomer and eutomer of citalopram (Cat. No. 1427).

**Physical and Chemical Properties:**

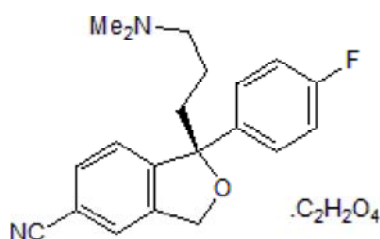
Batch Molecular Formula:  $C_{20}H_{21}FN_2O \cdot C_2H_2O_4$

Batch Molecular Weight: 414.43

Physical Appearance: White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**References:**

Zhang *et al* (2010) Structure-activity relationships for a novel series of cital. (1-(3-(dimethylamino)propyl)-1-(4-fluorophenyl)-1,3-dihydroisobenzofuran-5-carbonitrile) analogues at monoamine transporters. *J.Med.Chem.* **53** 6112. PMID: 20672825.

**Storage:** Store at +4°C

**Solubility & Usage Info:**

water to 50 mM

DMSO to 100 mM

**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. Our standard recommendations are:

**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.

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