

Product Name: Escitalopram oxalate

Catalog No.: 4796

Batch No.: 2

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: C₂₀H₂₁FN₂O.C₂H₂O₄

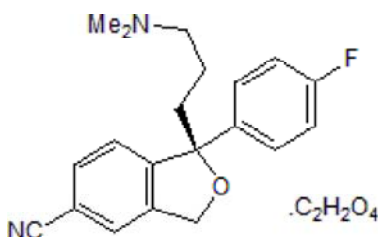
Batch Molecular Weight: 414.43

Physical Appearance: White solid

Solubility:
water to 50 mM
DMSO to 100 mM
ethanol to 10 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

Chiral HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +8.3 (Concentration = 2, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.76	5.59	6.76
Found	63.51	5.61	6.56

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

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Description:

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

Physical and Chemical Properties:

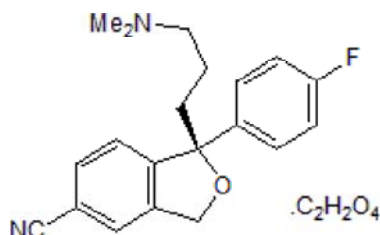
Batch Molecular Formula: $C_{20}H_{21}FN_2O \cdot C_2H_2O_4$

Batch Molecular Weight: 414.43

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Zhang *et al* (2010) Structure-activity relationships for a novel series of citalopram (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

ethanol to 10 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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