Certificate of Analysis

Product Name: **Ro 60-0175 fumarate** **Catalog No.: 1854** **Batch No.: 2**

CAS Number: 169675-09-6

IUPAC Name: (α*S*)-6-Chloro-5-fluoro-α-methyl-1*H*-indole-1-ethanamine fumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{11}H_{12}ClFN_2.C_4H_4O_4$

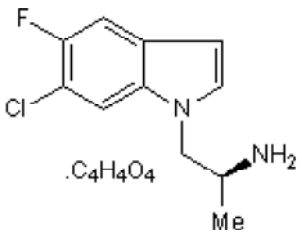
Batch Molecular Weight: 342.75

Physical Appearance: White solid

Solubility: water to 5 mM
DMSO to 20 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +31 (Concentration = 0.25, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.5	4.7	8.17
Found	52.48	4.63	8.23

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IUPAC Name: (α*S*)-6-Chloro-5-fluoro-α-methyl-1*H*-indole-1-ethanamine fumarate

Description:

Ro 60-0175 fumarate is a potent, selective 5-HT_2 receptor agonist; shows selectivity for the 5-HT_{2C} subtype (pK_i values are 9, 7.5, 5.4, 5.2 and 5.6 for human 5-HT_{2C}, $_{2A}$, $_{1A}$, $_6$ and $_7$ receptors respectively). Centrally active following oral or systemic administration in vivo.

Physical and Chemical Properties:

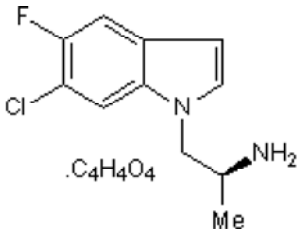
Batch Molecular Formula: $C_{11}H_{12}ClFN_2.C_4H_4O_4$

Batch Molecular Weight: 342.75

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 5 mM
DMSO to 20 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.

References:

Jensen *et al* (2013) Design, synthesis, and pharmacological characterization of N- and O-substituted 5,6,7,8-tetrahydro-4H-isoxazolo [4,5-d]azepin-3-ol analogues: novel 5-HT2A/5-HT2C receptor agonists with pro-cognitive J.Med.Chem. ***56*** 1211. PMID: 23301527.

Damjanoska *et al* (2003) Neuroendocrine evidence that (*S*)-2-(chloro-5-fluoro-indol-l-yl)-1-methylethylamine fumarate (Ro 60-0175) is not a selective 5-hydroxytryptamine$_{2C}$ receptor agonist. J.Pharmacol.Exp.Ther. ***304*** 1209. PMID: 12604698.

Kennett *et al* (2000) Effects of Ro 60 0175, a 5-HT_{2C} receptor agonist, in three animal models of anxiety. Eur.J.Pharmacol. ***387*** 197. PMID: 10650160.