

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: Metergoline Catalog No.: 0590 Batch No.: 1

CAS Number: 17692-51-2 EC Number: 241-686-3

IUPAC Name: [(8β)-1,6-Dimethylergolin-8-yl)methyl]carbamic acid phenylmethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{29}N_3O_2$ Batch Molecular Weight: 403.52

Physical Appearance: Light yellow crystalline solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.7$ (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

Melting Point: At 148°C

¹H NMR: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 74.41 7.42 10.41 Found 74.07 7.35 10.42

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Product Information

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IUPAC Name: [(8β)-1,6-Dimethylergolin-8-yl)methyl]carbamic acid phenylmethyl ester

Description:

Antagonist at $5-HT_1/5-HT_2$ with activity at $5-HT_{1D}$. Has moderate affinity for $5-HT_6$ and high affinity for $5-HT_7$.

Physical and Chemical Properties:

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Physical Appearance: Light yellow crystalline solid

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

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.

References:

Aulakh *et al* (1992) Effects of various serotonin receptor subtype selective antagonists alone and on *m*-chlorophenylpiperazine-induced neuroendocrine changes in rats. J.Pharmacol.Exp.Ther. **263** 588. PMID: 1432690.

Bagdy et al (1992) Pharmacological characterization of serotonin receptor subtypes involved in vasopressin and plasma renin activity responses to serotonin agonists. Eur.J.Pharmacol. 210 285. PMID: 1535317.

Miller et al (1992) Agonist activity of sumatriptan and metergoline at the human 5-HT_{1D β} receptor in the action of sumatriptan. Eur.J.Pharmacol. **227** 99. PMID: 1330643.