

Certificate of Analysis

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Product Name: DOI hydrochloride

Catalog No.: 2643

Batch No.: 4

CAS Number: 42203-78-1

IUPAC Name: 4-Iodo-2,5-dimethoxy- α -methylbenzeneethanamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₁H₁₆INO₂.HCl

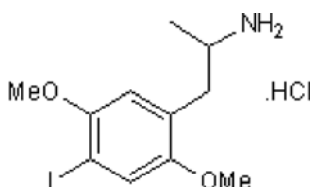
Batch Molecular Weight: 357.62

Physical Appearance: Off White solid

Solubility: water to 50 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.29 (3% MeOH, 0.1% NH₄OH in DCM)

HPLC: Shows 99.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

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

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CAS Number: 42203-78-1

IUPAC Name: 4-Iodo-2,5-dimethoxy- α -methylbenzeneethanamine hydrochloride

Description:

DOI hydrochloride is a brain penetrant, mixed 5-HT_{2A}/5-HT_{2C} receptor agonist (K_i values are 0.7, 2.4 and 20 nM for 5-HT_{2A}, 5-HT_{2C} and 5-HT_{2B} receptors respectively). Reduces rapid eye movement (REM) and slow wave sleep and increases waking in the rat. Hallucinogenic agent. Acts via 5-HT_{2A} receptors to inhibit the inflammatory effects of tumor necrosis factor (TNF)- α .

Physical and Chemical Properties:

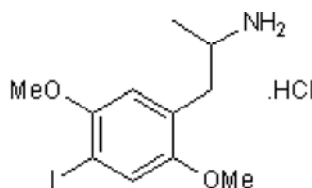
Batch Molecular Formula: C₁₁H₁₆INO₂.HCl

Batch Molecular Weight: 357.62

Physical Appearance: Off White solid

Minimum Purity: \geq 98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

water to 50 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.

Other Information:

INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 1 Home Office controlled substance and customers in the UK are required to hold the relevant licence or be exempt from restrictions in order to purchase and possess this material.

References:

Yu *et al* (2008) Serotonin 5-hydroxytryptamine_{2A} receptor activation suppresses tumor necrosis factor- α -induced inflammation with extraordinary potency. *J.Pharmacol.Exp.Ther.* **327** 316. PMID: 18708586.

Monti and Jantos (2006) Effects of serotonin 5-HT_{2A/2C} receptor agonist DOI and of the selective 5-HT_{2A} or 5-HT_{2C} receptor antagonists EMD 281014 and SB-243213 respectively, on sleep and waking in the rat. *Eur.J.Pharmacol.* **553** 163. PMID: 17059817.

Nelson *et al* (1999) Comparisons of hallucinogenic phenylisopropylamine binding affinities at cloned human 5-HT_{2A}, 5-HT_{2B} and 5-HT_{2C} receptors. *Naunyn-Schmied.Arch.Pharmacol.* **359** 1.

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