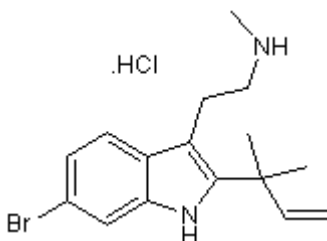


Certificate of Analysis

Product Name: Desformylflustrabromine hydrochloride **Catalog No.:** 3328 **Batch No.:** 3
CAS Number: 951322-11-5
IUPAC Name: 6-Bromo-2-(1,1-dimethyl-2-propenyl)-*N*-1*H*-indole-3-ethanamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₂₁BrN₂.HCl
Batch Molecular Weight: 357.72
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
 water to 10 mM with gentle warming
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.17 (Dichloromethane:Methanol:Aqueous ammonia. [7:3:0.1])
HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.72	6.2	7.83
Found	53.64	6.18	7.83

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

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Description:

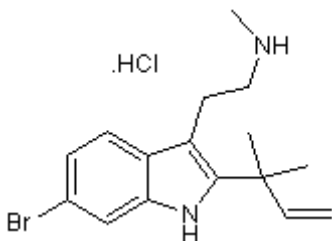
Positive allosteric modulator of nicotinic $\alpha 4\beta 2$ receptors; selectively increases the ionic current through $\alpha 4\beta 2$ in the presence of ACh. Displays 14.7-fold selectivity for $\alpha 4\beta 2$ over homomeric ($\alpha 7$) receptors. Moderately cytotoxic in HCT-116 cells. Also inhibits human muscle ($\alpha \beta \epsilon \delta$) and Torpedo ($\alpha \beta \gamma \delta$) nAChRs (IC_{50} values are 1.0 and 0.1 μM , respectively) by binding in the ion channel.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{16}H_{21}BrN_2.HCl$
 Batch Molecular Weight: 357.72
 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

- Sala et al** (2005) Potentiation of human $\alpha 4\beta 2$ neuronal nicotinic receptors by a *Flustra foliacea* metabolite. *Neurosci.Lett.* **373** 44.
Kim et al (2007) Synthesis of desformylflustrabromine and its evaluation as an $\alpha 4\beta 2$ and $\alpha 7$ nACh receptor modulator. *Bioorg.Med.Chem.Lett.* **17** 4855. PMID: 17604168.
Weltzin and Schulte (2010) Pharmacological characterization of the allosteric modulator desformylflustrabromine and its interaction with $\alpha 4\beta 2$ neuronal nicotinic acetylcholine receptor orthosteric ligands. *J.Pharm.Exp.Ther.* **334** 917.
Hamouda et al (2015) Desformylflustrabromine (dFBr) and [3H]dFBr-labeled binding sites in a nicotinic acetylcholine receptor. *Mol.Pharmacol.* **88** 1. PMID: 25870334.

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM
 water to 10 mM with gentle warming

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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