Product Name: Desformylfluorobromine hydrochloride
Catalog No.: 3328
Batch No.: 3

CAS Number: 951322-11-5
IUPAC Name: 6-Bromo-2-(1,1-dimethyl-2-propenyl)-N-1H-indole-3-ethanamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{16}\text{H}_{21}\text{BrN}_{2}\cdot\text{HCl} \)
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

2. ANALYTICAL DATA

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

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
<td>53.72</td>
<td>53.64</td>
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<tr>
<td>Hydrogen</td>
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<td>6.18</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>7.83</td>
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</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: Desformylflustrabromine hydrochloride

CAS Number: 951322-11-5
IUPAC Name: 6-Bromo-2-(1,1-dimethyl-2-propenyl)-N-1H-indole-3-ethanamine hydrochloride

Description:
Positive allosteric modulator of nicotinic α4β2 receptors; selectively increases the ionic current through α4β2 in the presence of ACh. Displays 14.7-fold selectivity for α4β2 over homomeric (α7) receptors. Moderately cytotoxic in HCT-116 cells. Also inhibits human muscle (αβεδ) and Torpedo (αβγδ) nAChRs (IC50 values are 1.0 and 0.1 μM, respectively) by binding in the ion channel.

Physical and Chemical Properties:
- Batch Molecular Formula: C19H21BrN2.HCl
- Batch Molecular Weight: 357.72
- Physical Appearance: Off White solid
- Minimum Purity: >98%

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).

References:
Weltzin and Schulte (2010) Pharmacological characterization of the allosteric modulator desformylflustrabromine and its interaction with α4β2 neuronal nicotinic acetylcholine receptor orthosteric ligands. J.Pharm.Exp.Ther. 334 917.