Product Name: BAN ORL 24
Catalog No.: 3661
Batch No.: 3
CAS Number: 1401463-54-4
IUPAC Name: (2R)-1-(Phenylmethyl)-N-[3-(spiro[isobenzofuran-1(3H),4'-piperidin]-1-yl)propyl-2-pyrrolidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{27}H_{35}N_{3}O_{2}.2HCl.\frac{1}{2}H_{2}O
Batch Molecular Weight: 515.52
Physical Appearance: Off White solid
Solubility: water to 100 mM
DMSO to 100 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: R_f = 0.28 (Dichloromethane:Methanol [95:5])
HPLC: Shows >99.2% purity
Chiral HPLC: Shows >99.7% purity
^1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +10.8 (Concentration = 1, Solvent = Water)
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>62.91</td>
<td>7.43</td>
<td>8.15</td>
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<tr>
<td>Found</td>
<td>62.75</td>
<td>7.55</td>
<td>7.96</td>
</tr>
</tbody>
</table>

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

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Description:
Potent and selective NOP receptor antagonist (IC_{50} values are 0.27, 2500, 6700 and > 10000 nM for NOP, κ-, μ- and δ-receptors respectively). Inhibits nociceptin-induced stimulation of [³⁵S]-GTPγS binding and Ca^{2+} mobilization in CHO cells in vitro and antagonizes NOP agonist-induced reduction in locomotor activity in vivo. Brain penetrant.

Physical and Chemical Properties:
Batch Molecular Formula: C_{27}H_{33}N_{2}O_{2}·2HCl·½H_{2}O
Batch Molecular Weight: 515.52
Physical Appearance: Off White solid
Minimum Purity: >97%

Storage: Store at -20°C. This product is packaged under an inert atmosphere.

Solubility & Usage Info:
water to 100 mM
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: