

**Product Name:** JTC 801

**Catalog No.:** 2481

**Batch No.:** 4

CAS Number: 244218-51-7

IUPAC Name: *N*-(4-Amino-2-methyl-6-quinolinyl)-2-[(4-ethylphenoxy)methyl]benzamide hydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>26</sub>H<sub>25</sub>N<sub>3</sub>O<sub>2</sub>.HCl.1¼H<sub>2</sub>O

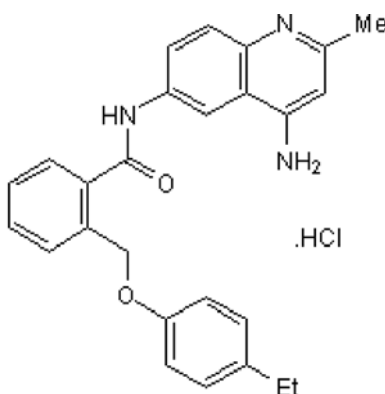
**Batch Molecular Weight:** 470.48

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 20 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 98.2% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	66.38	6.11	8.93
Found	66.2	6.08	8.8

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**Description:**

High affinity, selective NOP receptor antagonist ( $K_i = 8.2$  nM). Displays approximately 12.5-, 129- and 1055-fold selectivity over human  $\mu$ -,  $\kappa$ - and  $\delta$ -opioid receptors respectively. Exhibits anti-nociceptive effects in acute pain models in vivo. Orally active.

**Physical and Chemical Properties:**

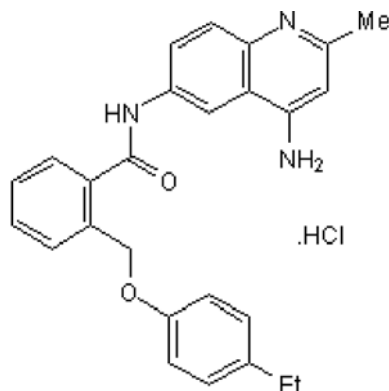
Batch Molecular Formula:  $C_{26}H_{25}N_3O_2 \cdot HCl \cdot 1\frac{1}{4}H_2O$

Batch Molecular Weight: 470.48

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 20 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:**

**Tamai *et al*** (2005) Anti-allodynic and anti-hyperalgesic effects of nociceptin receptor antagonist, JTC-801, in rats after spinal nerve injury and inflammation. *Eur.J.Pharmacol.* **510** 223. PMID: 15763246.

**Yamada *et al*** (2002) Pharmacological profiles of a novel opioid receptor-like1 (ORL1) receptor antagonist, JTC-801. *Br.J.Pharmacol.* **135** 323. PMID: 11815367.

**Shinkai *et al*** (2000) 4-Aminoquinolines: novel nociceptin antagonists with analgesic activity. *J.Med.Chem* **43** 4667. PMID: 11101358.

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