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Print Date: Jan 13th 2016

# Certificate of Analysis

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**Product Name:** **Altanserin hydrochloride** **Catalog No.: 1809** **Batch No.: 3**

CAS Number: 1135280-78-2 EC Number: 278-422-1

IUPAC Name: 3-[2-[4-(4-Fluorobenzoyl)-1-piperidinyl]ethyl]-2,3-dihydro-2-thioxo-4(1*H*)-quinazolinone hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{22}H_{22}FN_3O_2S.HCl.1\frac{1}{2}H_2O$

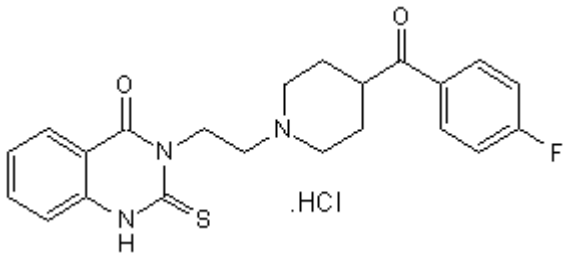
**Batch Molecular Weight:** 474.97

**Physical Appearance:** White solid

**Solubility:** DMSO to 20 mM with gentle warming

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.6 (Ethyl acetate)

**Melting Point:** Between 227 - 228°C

**HPLC:** Shows >98.6% purity

**$^1$H NMR:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 55.63 | 5.52 | 8.85 |
| Found | 55.8 | 5.32 | 8.83 |



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**Description:**

Potent and selective 5-$HT_{2A}$ receptor antagonist ($K_i$ values are 0.13, 4.55, 40, 62 and 1570 nM at 5-$HT_{2A}$, $\alpha_1$, 5-$HT_{2C}$, $D_2$ and 5-$HT_{1A}$ respectively). Centrally active following systemic administration in vivo.

**Physical and Chemical Properties:**

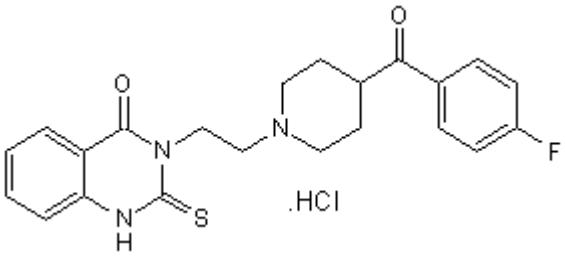
Batch Molecular Formula: $C_{22}H_{22}FN_3O_2S.HCl.1½H_2O$

Batch Molecular Weight: 474.97

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**

DMSO to 20 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.

**References:**

**Sietnick** (1985) Involvement of 5-$HT_2$ receptors in the LSD- and L-5-HTP-induced suppression of lordotic behavior in the female rat. J.Neural Transm. ***61*** 65. PMID: 3872342.

**Koenig** *et al* (1987) Stimulation of corticosterone and β-endorphin secretion in the rat by selective 5-HT receptor subtype activation. Eur.J.Pharmacol. ***137*** 1. PMID: 2956114.

**Kennett** *et al* (1994) Evidence that 5-$HT_{2C}$ receptor antagonists are anxiolytic in the rat Geller-Seifter model of anxiety. Psychopharmacology ***114*** 90. PMID: 7846211.

**Herth** *et al* (2009) Synthesis and in vitro affinities of various MDL 100907 derivatives as potential $^{18}$F-radioligands for 5-$HT_{2A}$ receptor imaging with PET. Bioorg.Med.Chem. ***17*** 2989. PMID: 19329329.