TOCRIS
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Print Date: Jan 15th 2016

# Certificate of Analysis

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**Product Name:** **T 98475** **Catalog No.: 2519** **Batch No.: 1**

CAS Number: 199119-18-1

IUPAC Name: 7-[(2,6-Difluorophenyl)methyl]-4,7-dihydro-2-[4-[(2-methyl-1-oxopropyl)amino]phenyl]-3-[[methyl(phenylmethyl) amino]methyl]-4-oxo-thieno[2,3-*b*]pyridine-5-carboxylic acid 1-methylethyl ester

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{37}H_{37}F_2N_3O_4S.1¾H_2O$

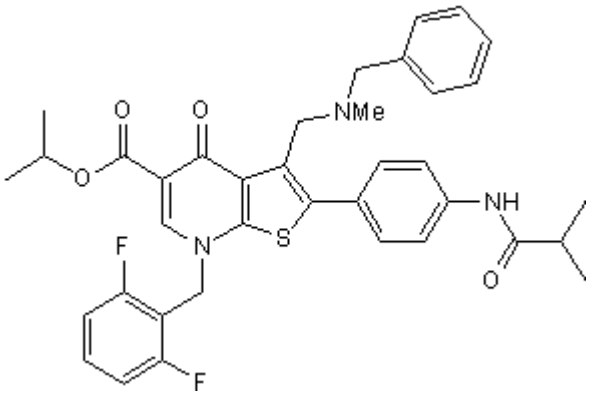
**Batch Molecular Weight:** 689.29

**Physical Appearance:** White solid

**Solubility:** DMSO to 50 mM

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**HPLC:** Shows >98% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 64.47 | 5.92 | 6.1 |
| Found | 64.46 | 5.47 | 6.11 |



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**Description:**

Potent, orally active and non-peptide gonadotropin-releasing hormone (GnRH, LHRH) receptor antagonist ($IC_{50}$ values are 0.2, 4.0 and 60 nM for human, monkey and rat GnRH receptors respectively). Inhibits LH release in vitro ($IC_{50}$ = 100 nM) and reduces plasma LH concentration in castrated male cynomolgus monkeys.

**Physical and Chemical Properties:**

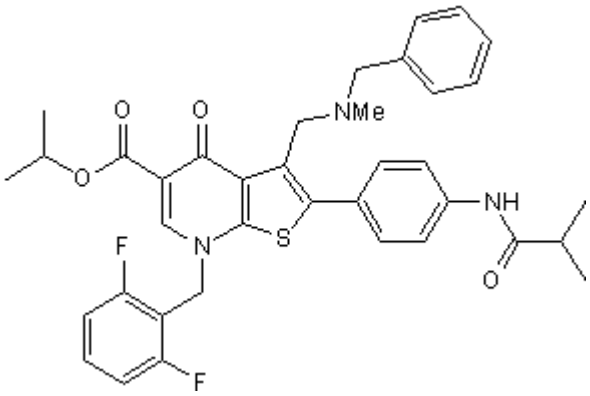
Batch Molecular Formula: $C_{37}H_{37}F_2N_3O_4S.1¾H_2O$

Batch Molecular Weight: 689.29

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**

DMSO to 50 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:**

**Cho** *et al* (1998) Discovery of a novel, potent, and orally active nonpeptide antagonist of the human luteinizing hormone-releasing hormone (LHRH) receptor. J.Med.Chem. ***41*** 4190. PMID: 9784092.

**Sasaki** *et al* (2003) Discovery of a thieno[2,3-*d*]pyrimidine-2,4-dione bearing a *p*-methoxyureidophenyl moiety at the 6-position: a highly potent and orally bioavailable non-peptide antagonist for the human luteinizing hormone-releasing hormone receptor. J.Med.Chem. ***46*** 113. PMID: 12502365.

**Imada** *et al* (2006) Design, synthesis, and structure-activity relationships of thieno[2,3-*b*]pyridin-4-one derivatives as a novel class of potent, orally active, non-peptide luteinizing hormone-releasing hormone receptor antagonists. J.Med.Chem. ***49*** 3809. PMID: 16789738.