

## Certificate of Analysis

**Product Name:** Guggulsterone

**Catalog No.:** 2013

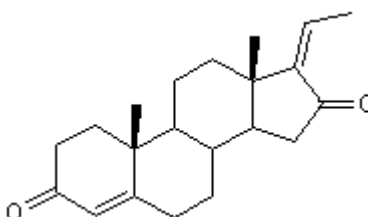
**Batch No.:** 1

CAS Number: 95975-55-6

IUPAC Name: Pregna-4,17(20)-diene-3,16-dione

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>21</sub>H<sub>28</sub>O<sub>2</sub>  
**Batch Molecular Weight:** 312.45  
**Physical Appearance:** White solid  
**Solubility:** ethanol to 10 mM with gentle warming  
**Storage:** Store at RT  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows >99.3% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	80.73	9.03	
Found	80.75	9.08	

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

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**Description:**

Broad spectrum steroid receptor ligand; binds with high affinity to mineralocorticoid receptors ( $K_i = 39$  nM) and lower affinity to progesterone, androgen and glucocorticoid receptors ( $K_i$  values are 201, 240 and 224 nM respectively). Functions primarily as an antagonist of these receptors, with the exception of the progesterone receptor where it displays partial agonist effects. Also exerts hypolipidemic activity, likely via antagonism of the receptor for bile acids (farnesoid X receptor; FXR).

**Physical and Chemical Properties:**

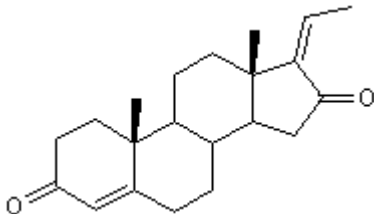
Batch Molecular Formula:  $C_{21}H_{28}O_2$

Batch Molecular Weight: 312.45

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Owsley and Chiang** (2003) Guggulsterone antagonizes farnesoid X receptor induction of bile salt export pump but activates pregnane X receptor to inhibit cholesterol 7 $\alpha$ -hydroxylase gene. *Biochem.Biophys.Res.Comm.* **304** 191.

**Burris et al** (2005) The hypolipidemic natural product guggulsterone is a promiscuous steroid receptor ligand. *Mol.Pharmacol.* **67** 948. PMID: 15602004.

**Meyer et al** (2005) Is antagonism of *E/Z*-guggulsterone at the farnesoid X receptor mediated by a noncanonical binding site? A molecular modeling study. *J.Med.Chem.* **48** 6948. PMID: 16250653.

**Storage:** Store at RT

**Solubility & Usage Info:**

ethanol to 10 mM with gentle warming

This compound is a mixture of (*Z*)- and (*E*)-Guggulsterone in a ratio of approximately 60:40.

**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.

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