

## Certificate of Analysis

**Product Name:** Deguelin

**Catalog No.:** 1770

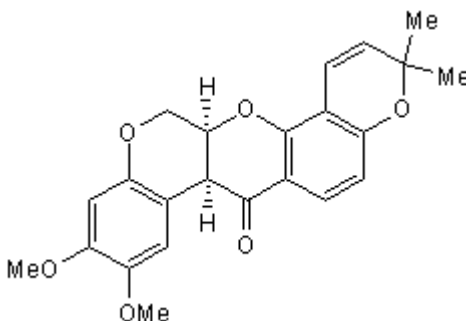
**Batch No.:** 2

CAS Number: 522-17-8

IUPAC Name: (7a*S*,13a*S*)-13,13a-Dihydro-9,10-dimethoxy-3,3-dimethyl-3*H*-bis[1]benzopyrano[3,4-*b*:6',5'-*e*]pyran-7(7a*H*)-one

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>22</sub>O<sub>6</sub>·¼H<sub>2</sub>O  
**Batch Molecular Weight:** 398.92  
**Physical Appearance:** Cream solid  
**Solubility:** ethanol to 50 mM  
DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.8 (Dichloromethane:Methanol [9:1])  
**HPLC:** Shows 97.1% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	69.25	5.68	
Found	69.56	5.63	

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**Description:**

Anticancer and antiviral agent; chemopreventive and pro-apoptotic. Inhibits phorbol ester-induced ornithine decarboxylase and NADH:ubiquinone oxidoreductase activities (IC<sub>50</sub> values are 11 and 6.9 nM respectively). Inhibits PI 3-kinase and reduces pAkt levels in pre-malignant and malignant human bronchial epithelial cells. Active in vivo.

**Physical and Chemical Properties:**

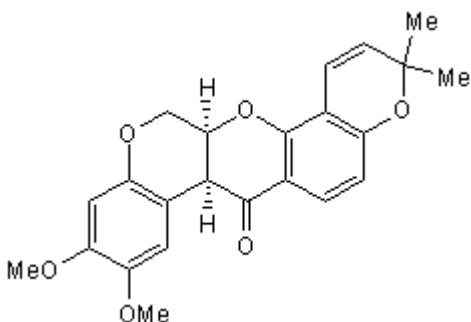
Batch Molecular Formula: C<sub>23</sub>H<sub>22</sub>O<sub>6</sub>·¼H<sub>2</sub>O

Batch Molecular Weight: 398.92

Physical Appearance: Cream solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

ethanol to 50 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:**

**Takatsuki et al** (1969) Antiviral and antitumor antibiotics. XX. Effects of rotenone, deguelin, and related compounds on animal and plant viruses. *Appl.Microbiol.* **18** 660. PMID: 4312925.

**Udeani et al** (1997) Cancer chemopreventive activity mediated by deguelin, a naturally occurring rotenoid. *Cancer Res.* **57** 3424. PMID: 9270008.

**Fang and Casida** (1998) Anticancer action of cube insecticide: correlation for rotenoid constituents between inhibition of NADH:ubiquinone oxidoreductase and induced ornithine decarboxylase activities. *Proc.Natl.Acad.Sci.U.S.A.* **95** 3380. PMID: 9520374.

**Chun et al** (2003) Effects of deguelin on the phosphatidylinositol 3-kinase/Akt pathway and apoptosis in premalignant human bronchial epithelial cells. *J.Natl.Cancer Inst.* **95** 291. PMID: 12591985.

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