

Certificate of Analysis

www.tocris.com

Product Name: ES 936

Catalog No.: 4022

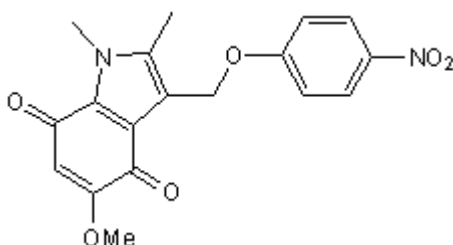
Batch No.: 1

CAS Number: 192820-78-3

IUPAC Name: 5-Methoxy-1,2-dimethyl-3-[(4-nitrophenoxy)methyl]-1*H*-indole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₆N₂O₆·¼H₂O
Batch Molecular Weight: 360.83
Physical Appearance: Orange solid
Solubility: DMSO to 20 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.36 (Dichloromethane:Ethyl acetate:Petrol [1:1:2])
HPLC: Shows 99.3% purity
¹H NMR: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.92	4.61	7.76
Found	60.03	4.66	7.89

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

Product Name: ES 936

Catalog No.: 4022

Batch No.: 1

CAS Number: 192820-78-3

IUPAC Name: 5-Methoxy-1,2-dimethyl-3-[(4-nitrophenoxy)methyl]-1*H*-indole

Description:

Mechanism-based inhibitor of NAD(P)H:quinone oxidoreductase (NQO1). Induces growth inhibition in human pancreatic carcinoma (MIA PaCa-2) and adenocarcinoma (BxPC-3) cell lines with IC₅₀ values of 108 and 365 nM respectively. Also inhibits TNF- α -induced E-selectin protein expression in human bone marrow endothelial cells. Exhibits no effects on other cellular reductases or levels of acid-soluble thiols.

Physical and Chemical Properties:

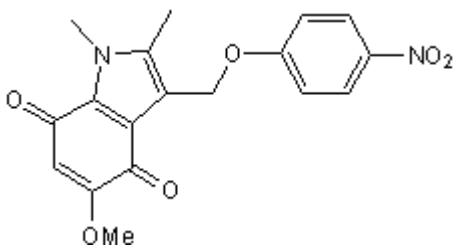
Batch Molecular Formula: C₁₈H₁₆N₂O₆. $\frac{1}{4}$ H₂O

Batch Molecular Weight: 360.83

Physical Appearance: Orange solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Dehn et al (2003) Biochemical, cytotoxic, and genotoxic effects of ES936, a mechanism-based inhibitor of NAD(P)H:quinone oxidoreductase 1, in cellular systems. *Mol.Pharmacol.* **64** 714. PMID: 12920209.

Dehn et al (2006) 5-Methoxy-1,2-dimethyl-3-[(4-nitrophenoxy)methyl]indole-4,7-dione, a mechanism-based inhibitor of NAD(P)H:quinone oxidoreductase 1, exhibits activity against human pancreatic cancer *in vitro* and *in vivo*. *Mol.Cancer Ther.* **5** 1702. PMID: 16891456.

Zhou et al (2010) NAD(P)H:quinone oxidoreductase 1-compromised human bone marrow endothelial cells exhibit decreased adhesion molecule expression and CD³⁴ hematopoietic cell adhesion. *J.Pharm.Exp.Ther.* **334** 260. PMID: 20378716.

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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.

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956