

Certificate of Analysis

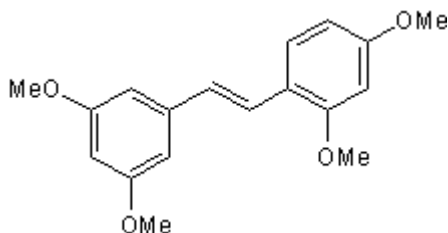
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Product Name: TMS
CAS Number: 24144-92-1
IUPAC Name: 1-[2,(3,5-Dimethoxyphenyl)ethenyl]-2,4-dimethoxybenzene

Catalog No.: 1509 **Batch No.:** 2

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₀O₄
Batch Molecular Weight: 300.35
Physical Appearance: White solid
Solubility: ethanol to 25 mM
DMSO to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Ethyl acetate:Petroleum ether [3:7])
HPLC: Shows >99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	71.98	6.71	
Found	72.02	6.86	

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

Product Information

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IUPAC Name: 1-[2,3,5-Dimethoxyphenyl]ethenyl]-2,4-dimethoxybenzene

Description:

Potent, selective and competitive inhibitor of cytochrome P450 1B1, an enzyme overexpressed in certain tumors ($IC_{50} = 6$ nM). 50- and 520-fold selective over P450 1A1 and 1A2 respectively. Inhibits cancer cell growth in vitro.

Physical and Chemical Properties:

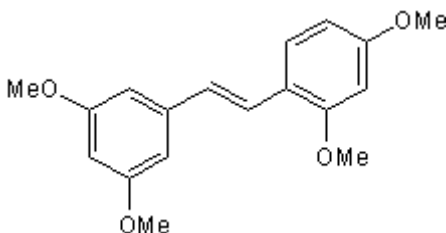
Batch Molecular Formula: $C_{18}H_{20}O_4$

Batch Molecular Weight: 300.35

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

ethanol to 25 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:

Chun et al (2001) A new selective and potent inhibitor of human cytochrome P450 1B1 and its application to antimutagenesis. *Cancer Res.* **61** 8164. PMID: 11719446.

Nam et al (2001) Resveratrol analog, 3,5,2',4'-tetramethoxy-trans-stilbene, potentiates the inhibition of cell growth and induces apoptosis in human cancer cells. *Arch.Pharm.Res.* **24** 441. PMID: 11693548.

Kim et al (2002) Design, synthesis, and discovery of novel *trans*-stilbene analogues as potent and selective human cytochrome P450 1B1 inhibitors. *J.Med.Chem.* **45** 160. PMID: 11754588.

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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