

Certificate of Analysis

Product Name: Metyrapone

CAS Number: 54-36-4

IUPAC Name: 2-Methyl-1,2-di-3-pyridinyl-1-propanone

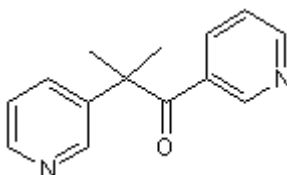
Catalog No.: 3292

Batch No.: 5

EC Number: 200-206-2

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₄N₂O
Batch Molecular Weight: 226.27
Physical Appearance: Off White solid
Solubility: water to 100 mM
DMSO to 100 mM
ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	74.31	6.24	12.38
Found	74.34	6.18	12.31

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

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Description:

Cytochrome P450 inhibitor. Blocks glucocorticoid synthesis via inhibition of steroid 11- β hydroxylase (CYP11B1) activity (IC_{50} = 7.83 μ M). Also inhibits CYP3A4 and cytochrome P450-mediated ω/ω -1 hydroxylase activity.

Physical and Chemical Properties:

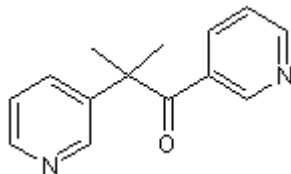
Batch Molecular Formula: C₁₄H₁₄N₂O

Batch Molecular Weight: 226.27

Physical Appearance: Off White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 100 mM
DMSO to 100 mM
ethanol 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:

Hays et al (1984) Structure-activity relationship study of the inhibition of adrenal cortical 11 β -hydroxylase by new metyrapone analogues. *J.Med.Chem.* **27** 15. PMID: 6606707.

Asakura and Shichi (1992) Cytochrome P450-mediated prostaglandin omega/omega-1 hydroxylase activities in porcine ciliary body epithelial cells. *Exp.Eye Res.* **55** 377. PMID: 1426070.

Park et al (2005) Structural and dynamic basis of broad substrate specificity, catalytic mechanism and inhibition of cytochrome P450 3A4. *J.Am.Chem.Soc.* **127** 13634. PMID: 16190729.

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