TOCRIS
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Print Date: Jan 24th 2023

Certificate of Analysis

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Product Name: **Metyrapone** **Catalog No.: 3292** **Batch No.: 9**

CAS Number: 54-36-4 EC Number: 200-206-2

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_{14}N_2O$.

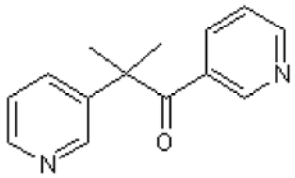
Batch Molecular Weight: 226.27

Physical Appearance: Pale orange solid

Solubility: water to 10 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	74.31	6.24	12.38
Found	73.8	6.2	12.29

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CAS Number: 54-36-4

EC Number: 200-206-2

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

Description:

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

Physical and Chemical Properties:

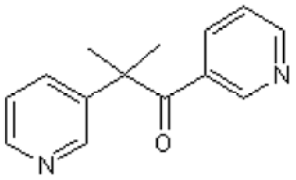
Batch Molecular Formula: $C_{14}H_{14}N_2O$.

Batch Molecular Weight: 226.27

Physical Appearance: Pale orange solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 10 mM
DMSO to 100 mM

Solutions in DMSO may appear slightly hazy.

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:

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.

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.

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