



Certificate of Analysis

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Product Name: ISO 1 Catalog No.: 4288 Batch No.: 1

CAS Number: 478336-92-4

IUPAC Name: 4,5-Dihydro-3-(4-hydroxyphenyl)-5-isoxazoleacetic acid methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_{13}NO_4$ Batch Molecular Weight: 235.24 Physical Appearance: White solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

MeO_oC OH

2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen
Theoretical 61.27 5.57 5.95
Found 61.16 5.49 6.02



Product Information

Print Date: Feb 6th 2014

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CAS Number: 478336-92-4

IUPAC Name: 4,5-Dihydro-3-(4-hydroxyphenyl)-5-isoxazoleacetic acid methyl ester

Description:

Macrophage migration inhibitory factor (MIF) inhibitor (IC $_{50}$ = 7 μ M); inhibits MIF tautomerase activity in vitro and in vivo. Protective against mouse models of streptozotocin-induced diabetes mellitus; blocks anti-inflammatory response following LPS exposure and increases survival. Inhibits airway remodeling in a mouse model of chronic asthma. Cell permeable; orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₂H₁₃NO₄ Batch Molecular Weight: 235.24 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

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:

Lubetsky *et al* (2002) The tautomerase active site of macrophage migration inhibitory factor is a potential target for discovery of novel anti-inflammatory agents. J.Biol.Chem. **277** 24976. PMID: 11997397.

Al-Abed *et al* (2005) ISO-1 binding to the tautomerase active site of MIF inhibits its pro-inflammatory activity and increases survival in severe sepsis. J.Biol.Chem. *280* 36541. PMID: 16115897.

Cvetkovic *et al* (2005) Critical role of macrophage migration inhibitory factor activity in experimental autoimmune diabetes. Endocrinology *146* 2942. PMID: 15790730.

Chen et al (2010) ISO-1, a macrophage migration inhibitory factor antagonist, inhibits airway remodeling in a murine model of chronic asthma. Mol.Med. 16 400. PMID: 20485865.

