

Certificate of Analysis

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Product Name: Ebselen

Catalog No.: 5245

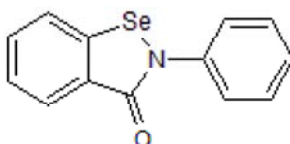
Batch No.: 1

CAS Number: 60940-34-3

IUPAC Name: 2-Phenyl-1,2-benzisoselenazol-3(2H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₉N₁O₁Se
Batch Molecular Weight: 274.18
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
ethanol to 10 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.95	3.31	5.11
Found	56.96	3.28	5.32

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

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CAS Number: 60940-34-3

IUPAC Name: 2-Phenyl-1,2-benzisoselenazol-3(2H)-one

Description:

Glutathione peroxidase mimic; peroxyxynitrite scavenger. Inhibits ferroptosis. Also inhibits lipoxygenase, cyclooxygenase, nitric oxide synthase, protein kinase C and H⁺/K⁺-ATPase activity. Inhibits the hepatic carcinogenic effects of aflatoxin B₁. Antioxidant and anti-inflammatory. Selectively inhibits G_q protein signaling and enhances differentiation of brown adipocytes. Inhibits SARS-CoV-2 M^{pro} in vitro (IC₅₀ = 0.67 μM in FRET assay)

Physical and Chemical Properties:

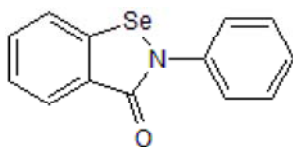
Batch Molecular Formula: C₁₃H₉NOSe

Batch Molecular Weight: 274.18

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Jin et al (2020) Structure of M^{pro} from SARS-CoV-2 and discovery of its inhibitors. *Nature*. **582** 289. PMID: 32272481.

Kuschak et al (2019) Cell-permeable high-affinity tracers for G_q proteins provide structural insights, reveal distinct binding kinetics, and identify small molecule inhibitors. *Br.J.Pharmacol.* **177** 1898. PMID: 31881095.

Xie et al (2016) Ferroptosis: process and function. *Cell Death Differ.* **23** 369. PMID: 26794443.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 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.

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