

**Product Name:** ML 334

**Catalog No.:** 5625

**Batch No.:** 1

CAS Number: 1432500-66-7

IUPAC Name: (1*S*,2*R*)-2-[[[(1*S*)-1-[(1,3-Dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl]-3,4-dihydro-2(1*H*)-isoquinolinyl]carbonyl]cyclohexanecarboxylic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>26</sub>H<sub>26</sub>N<sub>2</sub>O<sub>5</sub>·1/4H<sub>2</sub>O

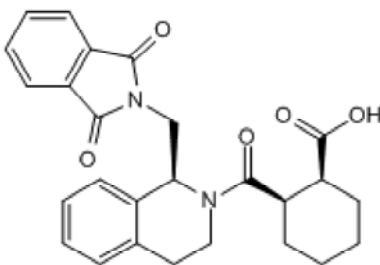
**Batch Molecular Weight:** 451

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.28 (Ethyl acetate:Petroleum ether [1:1])

**HPLC:** Shows 99.6% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = -120 (Concentration = 1, Solvent = Methanol)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	69.24	5.92	6.21
Found	69.22	5.96	6.2

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

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**Description:**

ML 334 is an Nrf2 activator; inhibits Nrf2/Keap1 interaction ( $K_d = 1 \mu\text{M}$ ). Promotes Nrf2 nuclear translocation and induces antioxidant response element (ARE) activity in vitro. Cell permeable.

**Physical and Chemical Properties:**

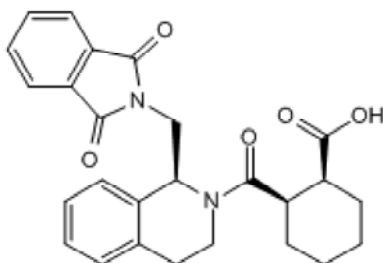
Batch Molecular Formula:  $\text{C}_{26}\text{H}_{26}\text{N}_2\text{O}_5 \cdot \frac{1}{4}\text{H}_2\text{O}$

Batch Molecular Weight: 451

Physical Appearance: White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Store at  $-20^\circ\text{C}$

**CAUTION** - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

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  $45\text{-}60^\circ\text{C}$  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  $-20^\circ\text{C}$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Rosini et al** (2014) Oxidative stress in Alzheimer's disease: are we connecting the dots? *J.Med.Chem.* **57** 2821. PMID: 24131448.

**Hu et al** (2013) Discovery of a small-molecule inhibitor and cellular probe of Keap1-Nrf2 protein-protein interaction. *Bioorg.Med.Chem.Lett.* **23** 3039. PMID: 23562243.

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