

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: C₂₆H₂₆N₂O₅·1/4H₂O

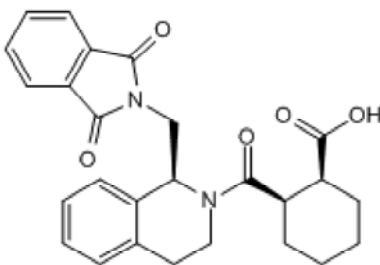
Batch Molecular Weight: 451

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.28 (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956

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

Description:

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:

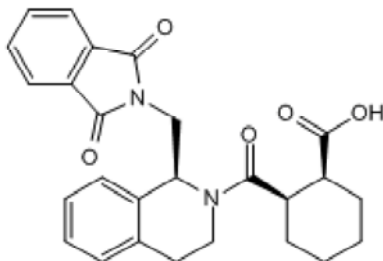
Batch Molecular Formula: $\text{C}_{26}\text{H}_{26}\text{N}_2\text{O}_5 \cdot \frac{1}{4}\text{H}_2\text{O}$

Batch Molecular Weight: 451

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at -20°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°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.

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956