

Certificate of Analysis

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Product Name: BYK 204165

Catalog No.: 3734

Batch No.: 1

CAS Number: 1104546-89-5

IUPAC Name: 4-[(1-Methyl-1*H*-pyrrol-2-yl)methylene]-1,3(2*H*,4*H*)-isoquinolinedione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₂N₂O₂·0.1H₂O

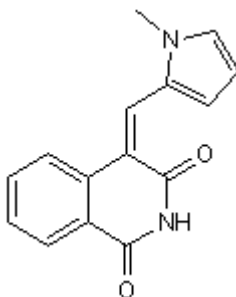
Batch Molecular Weight: 254.07

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Ethyl acetate:iso-Hexane [2:3])

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

	Carbon	Hydrogen	Nitrogen
Theoretical	70.91	4.84	11.03
Found	70.92	4.76	11.01

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

Product Information

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IUPAC Name: 4-[(1-Methyl-1H-pyrrol-2-yl)methylene]-1,3(2H,4H)-isoquinolinedione

Description:

Potent and selective poly(ADP-ribose) polymerase (PARP)-1 inhibitor (pIC₅₀ values are 5.38 and 7.35 for PARP-2 and PARP-1 respectively).

Physical and Chemical Properties:

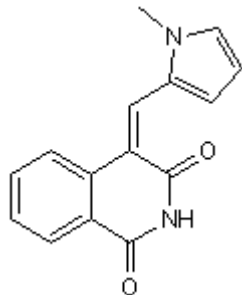
Batch Molecular Formula: C₁₅H₁₂N₂O₂·0.1H₂O

Batch Molecular Weight: 254.07

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at +4°C

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 45-60°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:

Eltze et al (2008) Imidazoquinolinone, imidazopyridine, and isoquinolindione derivatives as novel and potent inhibitors of the poly(ADP-ribose) polymerase (PARP): a comparison with standard PARP inhibitors. *Mol.Pharmacol.* **74** 1587. PMID: 18809672.

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