

Certificate of Analysis

Print Date: Jan 14th 2016

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Product Name: UPF 1069 Catalog No.: 3736 Batch No.: 2

CAS Number: 1048371-03-4

IUPAC Name: 5-(2-Oxo-2-phenylethoxy)-3,4-dihydroisoquinolin-1(2H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{13}NO_3$. ½ H_2O

Batch Molecular Weight: 288.3 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.18$ (Dichloromethane:Methanol [19:1])

HPLC: Shows 99.5% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 70.82 4.89 4.86 Found 71.21 4.66 4.97



Product Information

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1048371-03-4 CAS Number:

IUPAC Name: 5-(2-Oxo-2-phenylethoxy)-3,4-dihydroisoquinolin-1(2H)-one

Description:

Selective poly(ADP-ribose) polymerase (PARP) 2 inhibitor (IC₅₀ values are 0.3 and 8.0 µM for PARP-2 and PARP-1 respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₁₃NO₃.½H₂O

Batch Molecular Weight: 288.3 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

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:

Pellicciari et al (2008) On the way to selective PARP-2 inhibitors. Design, synthesis and preliminary evaluation of a series of isoguinolinone derivatives. Chem. Med. Chem 3 914.

Moroni et al (2009) Selective PARP-2 inhibitors increase apoptosis in hippocampal slices but protect cortical cells in models of postischaemic brain damage. Br.J.Pharmacol. 157 854. PMID: 19422384.