

Certificate of Analysis

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Product Name: PS 48

Catalog No.: 4087

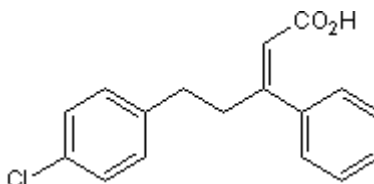
Batch No.: 2

CAS Number: 1180676-32-7

IUPAC Name: (2Z)-5-(4-Chlorophenyl)-3-phenyl-2-pentenoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₅ClO₂
Batch Molecular Weight: 286.75
Physical Appearance: White crystalline solid
Solubility: DMSO to 100 mM
 ethanol to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 99% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	71.2	5.27	
Found	71.3	5.28	

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

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Description:

Phosphoinositide-dependent protein kinase-1 (PDK1) activator ($K_d = 10.3 \mu\text{M}$). Binds exclusively to the PIF-binding pocket of PDK1, distinct from the ATP binding site.

Physical and Chemical Properties:

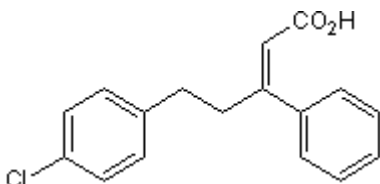
Batch Molecular Formula: $\text{C}_{17}\text{H}_{15}\text{ClO}_2$

Batch Molecular Weight: 286.75

Physical Appearance: White crystalline solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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

ethanol to 50 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:

Hindie et al (2009) Structure and allosteric effects of low-molecular-weight activators on the protein kinase PDK1. *Nat.Chem.Biol.* **5** 758. PMID: 19718043.

Stroba et al (2009) 3,5-diphenylpent-2-enoic acids as allosteric activators of the protein kinase PDK1: structure-activity relationships and thermodynamic characterization of binding as paradigms for PIF-binding pocket-targeting compounds. *J.Med.Chem.* **52** 4683. PMID: 19606904.

Williams (2010) Elastic network model of allosteric regulation in protein kinase PDK1. *BMC Struct.Biol.* **10** 11. PMID: 20500829.

Zhu et al (2010) Reprogramming of human primary somatic cells by OCT4 and chemical compounds. *Cell Stem Cell.* **7** 651. PMID: 21112560.

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