

Certificate of Analysis

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Product Name: PAC 1

Catalog No.: 2581

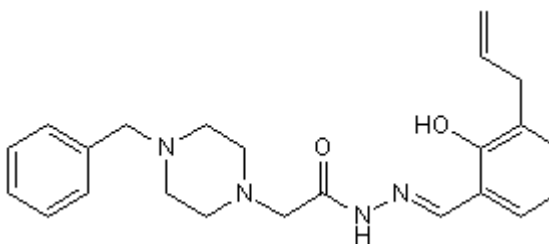
Batch No.: 1

CAS Number: 315183-21-2

IUPAC Name: 4-(Phenylmethyl)-1-piperazineacetic acid [[2-hydroxy-3-(2-propenyl)phenyl]methylene]hydrazide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₈N₄O₂
Batch Molecular Weight: 392.5
Physical Appearance: White solid
Solubility: 1eq. HCl to 75 mM
 DMSO to 100 mM
 ethanol to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >98.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.38	7.19	14.27
Found	70.09	7.25	14.18

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

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Description:

Procaspase-activating compound; activates procaspase-3 to produce caspase-3 ($EC_{50} = 0.22 \mu\text{M}$). Also activates procaspase-7 in a less efficient manner ($EC_{50} = 4.5 \mu\text{M}$). Pro-apoptotic; induces apoptosis in both cancerous and non-cancerous cells dependent on procaspase-3 concentration (IC_{50} values are 0.003 - 1.41 and 5.02 - 9.98 μM respectively).

Physical and Chemical Properties:

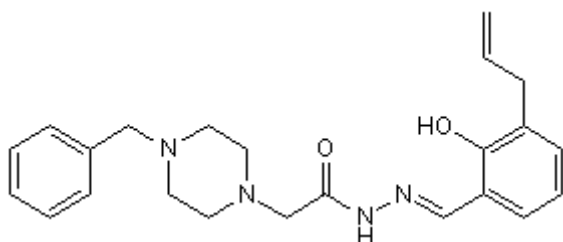
Batch Molecular Formula: $C_{23}H_{28}N_4O_2$

Batch Molecular Weight: 392.5

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Putt *et al* (2006) Small-molecule activation of procaspase-3 to caspase-3 as a personalized anticancer strategy. *Nat.Chem.Biol.* **2** 543. PMID: 16936720.

Peterson *et al* (2009) Procaspase-3 activation as an anti-cancer strategy: structure-activity relationship of procaspase-activating compound 1 (PAC-1) and its cellular co-localization with caspase-3. *J.Med.Chem.* **52** 5721. PMID: 19708658.

Storage: Store at +4°C

Solubility & Usage Info:

1eq. HCl to 75 mM
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.

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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