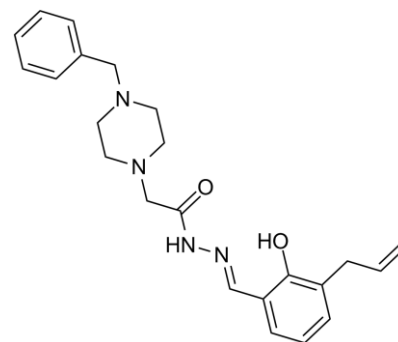


## Product Data Sheet

### Chemical Properties

<b>Product Name:</b>	PAC-1
<b>Cas No.:</b>	315183-21-2
<b>M.Wt:</b>	392.49
<b>Formula:</b>	C <sub>23</sub> H <sub>28</sub> N <sub>4</sub> O <sub>2</sub>



<b>Chemical Name:</b>	2-(4-benzylpiperazin-1-yl)-N'-[(Z)-(6-oxo-5-prop-2-enylcyclohexa-2,4-dien-1-ylidene)methyl]acetohydrazide
<b>Canonical SMILES:</b>	<chem>C=CCC1=CC=CC(=CNNC(=O)CN2CCN(CC2)CC3=CC=CC=C3)C1=O</chem>
<b>Solubility:</b>	Soluble in DMSO > 10 mM
<b>Storage:</b>	Store at -20°C
<b>General tips:</b>	For obtaining a higher solubility , please warm the tube at 37° C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20° C for several months.
<b>Shopping Condition:</b>	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request

### Biological Activity

<b>Targets :</b>	Caspase
<b>Pathways:</b>	Apoptosis >> Caspase

#### Description:

First procaspase-activating compound (PAC-1) is a small-molecule activator of procaspase-3 that directly catalyzes the maturation of procaspase-3 to the active caspase-3 by inducing the cleavage of procaspase-3 in a time-dependent manner. As a result of the direct and immediate activation of procaspase-3, PAC-1 potently induces apoptosis in cancer cell lines. The PAC-1 induced apoptosis has been observed to be proportional to the concentrations of procaspase-3 inside the cells of primary colon cancer isolates. Study results have demonstrated that PAC-1 is

able to induce cell death in both primary cancerous cells and adjacent normal tissues with 50% inhibition concentration IC50 values ranging from 0.003 to 1.41  $\mu\text{M}$  and 5.02 to 9.98  $\mu\text{M}$  respectively.

**Reference:**

Putt KS, Chen GW, Pearson JM, Sandhorst JS, Hoagland MS, Kwon JT, Hwang SK, Jin H, Churchwell MI, Cho MH, Doerge DR, Helferich WG, Hergenrother PJ. Small-molecule activation of procaspase-3 to caspase-3 as a personalized anticancer strategy. *Nat Chem Biol.* 2006 Oct;2(10):543-50. Epub 2006 Aug 27.

## Protocol

### Cell experiment:

Cell lines	Several cancer cell lines (leukemia, lymphoma, melanoma, neuroblastoma, breast cancer, lung cancer, adrenal cancer and renal cancer)
Preparation method	The solubility of this compound in DMSO is >10 mM. General tips for obtaining a higher concentration: Please warm the tube at 37 °C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20 °C for several months.
Reacting conditions	72 hrs
Applications	PAC-1 induces cell death in a procaspase-3-dependant manner. PAC-1 is most potent against the lung cancer cell line NCI-H226, with an IC50 value of 0.35 $\mu\text{M}$ .

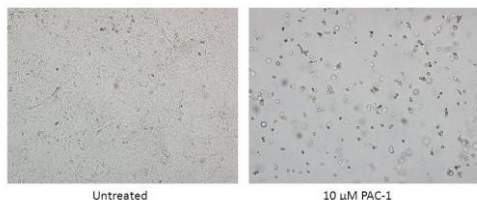
### Animal experiment [3]:

Animal models	Mice s.c. injected with NCI-H226 (lung cancer) cells
Dosage form	0, 50 or 100 mg/kg; p.o.; q.d., for 21 days
Applications	In mice s.c. injected with NCI-H226 (lung cancer) cells, PAC-1 significantly retarded tumor growth in a dose-dependent manner.
Other notes	Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

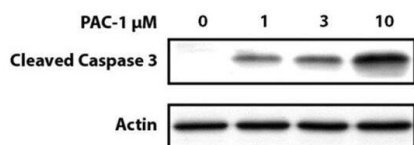
## Reference:

[1]. Putt KS, Chen GW, Pearson JM, Sandhorst JS, Hoagland MS, Kwon JT, Hwang SK, Jin H, Churchwell MI, Cho MH, Doerge DR, Helferich WG, Hergenrother PJ. Small-molecule activation of procaspase-3 to caspase-3 as a personalized anticancer strategy. *Nat Chem Biol.* 2006 Oct;2(10):543-50. Epub 2006 Aug 27.

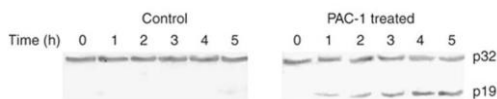
## Product Validation



HEY cells were treated with 10  $\mu$ M PAC-1 for 48 hrs



HEY cells were treated with 10  $\mu$ M PAC-1 for 48 hrs



Treatment of PAC-1 induces activation of cleaved caspase-3

## Caution

**FOR RESEARCH PURPOSES ONLY.**

**NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.**

*Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Short-term storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.*

**ApexBio Technology**

[www.apexbt.com](http://www.apexbt.com)

7505 Fannin street, Suite 410, Houston, TX 77054.

Tel: +1-832-696-8203 | Fax: +1-832-641-3177 | Email: [info@apexbt.com](mailto:info@apexbt.com)