

Product Name: PACMA 31

Catalog No.: 5116

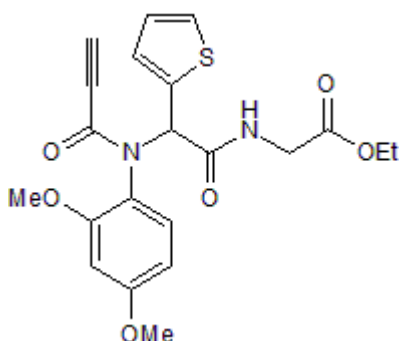
Batch No.: 1

CAS Number: 1401089-31-3

IUPAC Name: *N*-(2,4-Dimethoxyphenyl)-*N*-(1-oxo-2-propyn-1-yl)-2-(2-thienyl)glycylglycine ethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₂N₂O₆S
Batch Molecular Weight: 430.47
Physical Appearance: White crystalline solid
Solubility: DMSO to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.59	5.15	6.51
Found	58.68	5.24	6.42

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

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Description:

Irreversible protein disulfide isomerase (PDI) inhibitor; inhibits growth of ovarian cancer cells. Suppresses tumor growth in a mouse xenograph model of human ovarian cancer.

Physical and Chemical Properties:

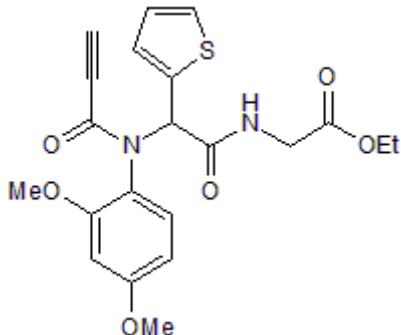
Batch Molecular Formula: C₂₁H₂₂N₂O₆S

Batch Molecular Weight: 430.47

Physical Appearance: White crystalline 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:

Xu et al (2012) Discovery of an orally active small-molecule irreversible inhibitor of protein disulfide isomerase for ovarian cancer treatment. *Proc.Natl.Acad.Sci.U.S.A.* **109** 16348. PMID: 22988091.

Ge et al (2013) Small molecule probe suitable for in situ profiling and inhibition of protein disulfide isomerase. *ACS.Chem.Biol.* **8** 2577. PMID: 24070012.

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