

Product Name: P1

Catalog No.: 5127

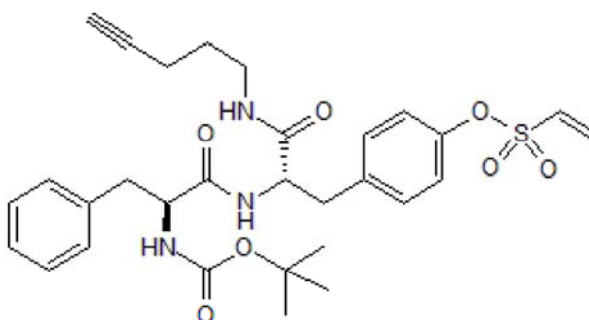
Batch No.: 1

CAS Number: 1461648-55-4

IUPAC Name: *N*-[(1,1-Dimethylethoxy)carbonyl]-*L*-phenylalanyl-*O*-(ethenylsulfonyl)-*N*-4-pentyn-1-yl-*L*-tyrosinamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₃₇N₃O₇S
Batch Molecular Weight: 583.7
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.23 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 98.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.73	6.39	7.2
Found	62.04	6.5	7.1

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

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Description:

Protein disulfide isomerase (PDI) inhibitor ($IC_{50} = 1.7 \mu M$). Inhibits proliferation of numerous cancer cell lines. Cell permeable.

Physical and Chemical Properties:

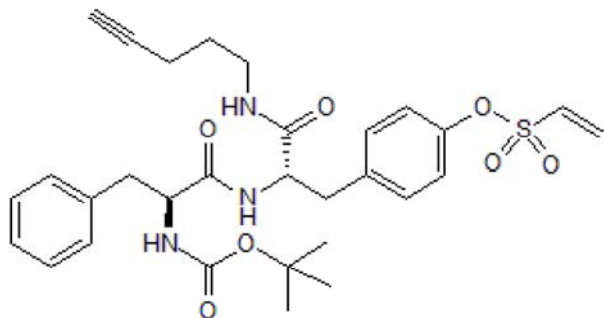
Batch Molecular Formula: $C_{30}H_{37}N_3O_7S$

Batch Molecular Weight: 583.7

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

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

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a $45-60^{\circ}C$ 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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

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.

Xu et al (2013) Protein disulfide isomerase interacts with tau protein and inhibits its fibrillization. PLoS One **8** e76657. PMID: 24098548.

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