

Product Name: AZD 5582 dihydrochloride

Catalog No.: 5141

Batch No.: 4

CAS Number: 1883545-51-4

IUPAC Name: 3,3'-[2,4-Hexadiyne-1,6-diylbis[oxy[(1*S*,2*R*)-2,3-dihydro-1*H*-indene-2,1-diyl]]]bis[*N*-methyl-*L*-alanyl-(2*S*)-2-cyclohexylglycyl-*L*-prolinamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₅₈H₇₈N₈O₈·2HCl·2³/₄H₂O

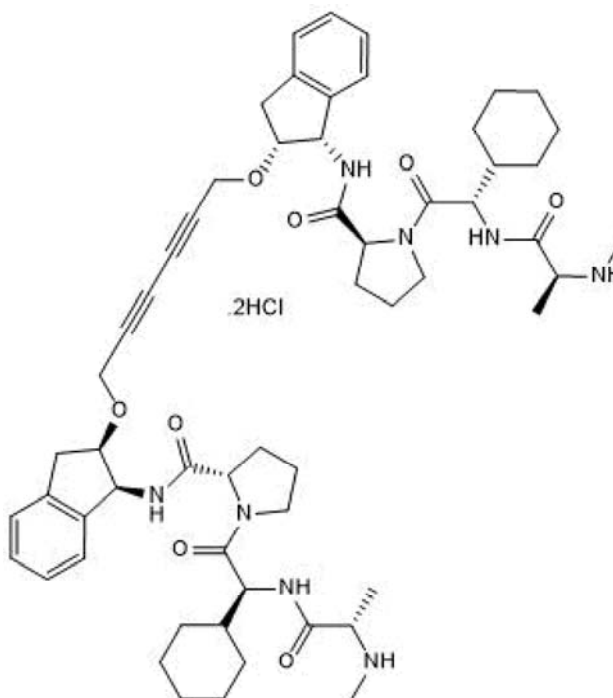
Batch Molecular Weight: 1137.75

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	61.23	7.57	9.85	6.23
Found	60.31	7.58	9.67	6.83

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Description:

Dimeric Smac mimetic; potent inhibitor of X-linked (XIAP) and cellular (cIAP) inhibitor of apoptosis protein (IC₅₀ values are 15, 15 and 21 nM for XIAP, cIAP1 and cIAP2 respectively). Binds to the BIR3 domain of XIAP to prevent interaction with caspase-9. Causes degradation of cIAP1 and cIAP2 and induces apoptosis in MDA-MB-231 breast cancer cells. Causes tumor regression in MDA-MB-231 xenograft-bearing mice.

Physical and Chemical Properties:

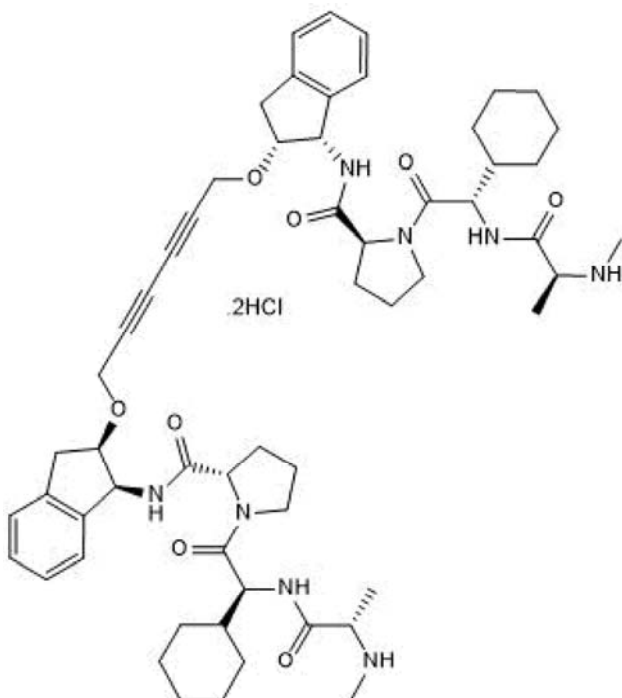
Batch Molecular Formula: C₅₈H₇₈N₈O₈·2HCl·2½H₂O

Batch Molecular Weight: 1137.75

Physical Appearance: White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



References:

Hennessy et al (2013) Discovery of a novel class of dimeric Smac mimetics as potent IAP antagonists resulting in a clinical candidate for the treatment of cancer (AZD5582). *J.Med.Chem.* **56** 9897. PMID: 24320998.

Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

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.

Licensing Information:

Sold with the permission of AstraZeneca UK Ltd

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