Certificate of Analysis

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Product Name: AEG 40730 dihydrochloride

Catalog No.: 5330 Batch No.: 1

CAS Number: 1883545-50-3

OCR

biotechr

IUPAC Name: 222, Trifluoro-N-[[(2S)-1-(N-methyl-L-analyl-L-threonyl)-2-pyrrolidinyl]methyl]-N-(2-phenylethyl)acetamide, diethyl ether with 2,4-hexadiyne-1.6-diol dihydrochloride

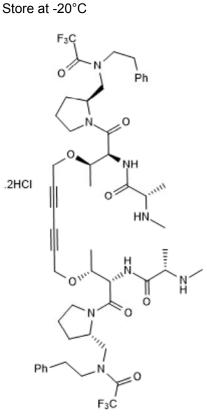
1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

C52H68F6N8O8.2HCI.H2O 1138.08 White solid water to 100 mM DMSO to 100 mM

Storage:

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC:

¹H NMR:

Mass Spectrum:

Microanalysis:

Shows 97.3% purity Consistent with structure Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 54.88 6.38 9.85 Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use Found 54.99 6.34 9.74

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Print Date: Jul 1st 2020

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Description:

IAP antagonist; binds to the BIR3 domain of cIAP1, cIAP2 and XIAP with nanomolar affinity. Reduces cIAP1, cIAP2 and XIAP protein levels in human breast cancer MDA-MB-231 cells. Induces apoptosis in combination with TNF, and potentiates TRAIL-mediated apoptosis in human colorectal carcinoma HCT 116 cells. Cell permeable.

Physical and Chemical Properties:

Batch Molecular Formula: C₅₂H₆₈F₆N₈O₈.2HCl.H₂O Batch Molecular Weight: 1138.08 Physical Appearance: White solid

Minimum Purity: ≥97%

Batch Molecular Structure:

F_3C Ph PhPh

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.

References:

Beug et al (2014) Smac mimetics and innate immune stimuli synergize to promote tumor death. Nat.Biotechnol. 32 182. PMID: 24463573.

Galbán et al (2009) Cytoprotective effects of IAPs revealed by a small molecule antagonist. Biochem, J. 417,765. PMID: 18851715. Bertrand et al (2008) cIAP1 and cIAP2 facilitate cancer cell survival by functioning as E3 ligases that promote RIP1 ubiquitination. Mol.

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