Certificate of Analysis

Product Name: **(-)-Xestospongin C** **Catalog No.: 1280** **Batch No.: 5**

CAS Number: 88903-69-9

IUPAC Name: (1*R*,4a*R*,11*R*,12a*S*,13*S*,16a*S*,23*R*,24a*S*)-Eicosahydro-5*H*,17*H*-1,23:11,13-diethano-2*H*,14*H*-[1,11]dioxacycloeicosino[2,3-*b*:12,13-*b*']dipyridine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{50}N_2O_2$

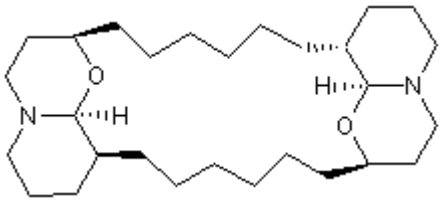
Batch Molecular Weight: 446.71

Physical Appearance: Clear lyophilised film

Solubility: DMSO to 2 mM
ethanol to 2 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Chloroform:Methanol:Water [85:15:2])

Mass Spectrum: Consistent with structure

Product Name: **(-)-Xestospongin C** **Catalog No.: 1280** **Batch No.: 5**

CAS Number: 88903-69-9

IUPAC Name: (1*R*,4a*R*,11*R*,12a*S*,13*S*,16a*S*,23*R*,24a*S*)-Eicosahydro-5*H*,17*H*-1,23:11,13-diethano-2*H*,14*H*-[1,11] dioxacycloeicosino[2,3-*b*:12,13-*b*']dipyridine

Description:

Highly potent, reversible and cell-permeable inhibitor of IP_3-mediated Ca^{2+} release (IC_{50} = 358 nM). Does not interact with the IP_3 binding site and exhibits high selectivity over ryanodine receptors.

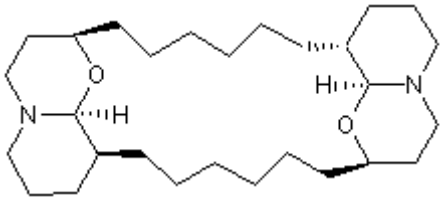
Physical and Chemical Properties:

Batch Molecular Formula: $C_{28}H_{50}N_2O_2$

Batch Molecular Weight: 446.71

Physical Appearance: Clear lyophilised film

Batch Molecular Structure:



Storage: Desiccate at -20°C. This product is packaged under an inert atmosphere.

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 2 mM
ethanol to 2 mM

CAUTION - 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°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:

Gafni *et al* (1997) Xestospongins: potent membrane permeable blockers of the inositol 1,4,5-trisphosphate receptor. Neuron ***19*** 723. PMID: 9331361.

Wilcox *et al* (1998) New developments in the molecular pharmacology of the *myo*-inositol 1,4,5-trisphosphate receptor. TiPS ***19*** 467. PMID: 9850611.

Ozaki *et al* (2002) Inhibitory mechanism of xestospongin-C on contraction and ion channels in the intestinal smooth muscle. Br.J.Pharmacol. ***137*** 1207. PMID: 12466229.

Dadsetan *et al* (2008) Store-operated Ca^{2+} influx causes Ca^{2+} release from the intracellular Ca^{2+} channels that is required for T cell activation. J.Biol.Chem. ***283*** 12512. PMID: 18316371.