



Certificate of Analysis

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Product Name: Jervine Catalog No.: 4717 Batch No.: 1

EC Number: 207-417-9 CAS Number: 469-59-0

IUPAC Name: (2'R,3S,3'R,3'aS,6'S,6aS,6bS,7'aR,11aS,11bR)-2,3,3'a,4,4',5',6,6',6a,6b,7,7',7'a,8,11a,11b-hexadecahydro-3-

hydroxy-3',6',10,11b-tetramethyl-Spiro[9H-benzo[a]fluorene-9,2'(3'H)-furo[3,2-b]pyridin]-11(1H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{27}H_{39}NO_3.2H_2O$ **Batch Molecular Formula:**

461.63 **Batch Molecular Weight: Physical Appearance:** White solid

ethanol to 50 mM Solubility:

DMSO to 20 mM

Store at -20°C Storage:

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99% purity

¹H NMR: Consistent with structure **Mass Spectrum:** Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 70.25 9.39 3.03 Found 70.23 9.26 3.17

Europe Middle East Africa



Product Information

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Print Date: Jan 14th 2016

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hydroxy-3',6',10,11b-tetramethyl-Spiro[9H-benzo[a]fluorene-9,2'(3'H)-furo[3,2-b]pyridin]-11(1H)-one

Description:

Inhibitor of Hedgehog signaling ($IC_{50} = 500 - 700$ nM); binds directly to Smoothened (Smo). Inhibits the response of target tissues to Sonic hedgehog signaling, possibly via the sterol sensing domain of Patched. Teratogenic.

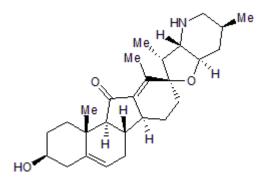
Physical and Chemical Properties:

Batch Molecular Formula: C₂₇H₃₉NO₃.2H₂O

Batch Molecular Weight: 461.63 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

ethanol to 50 mM DMSO to 20 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:

Cooper et al (1998) Teratogen-mediated inhibition of target tissue response to Shh signaling. Science 280 1603. PMID: 9616123.

ten Berge et al (2001) Prx1 and Prx2 are upstream regulators of sonic hedgehog and control cell proliferation during mandibular arch morphogenesis. Development 128 2929. PMID: 11532916.

Williams et al (2003) Identification of a small molecule inhibitor of the hedgehog signaling pathway: effects on basal cell carcinoma-like lesions. Proc.Natl.Acad.Sci.USA 100 4616. PMID: 12679522.