Certificate of Analysis

Product Name: **Alsterpaullone** **Catalog No.: 6400** **Batch No.: 1**

CAS Number: 237430-03-4

IUPAC Name: 7,12-Dihydro-9-nitroindolo[3,2-*d*][1]benzazepin-6(5*H*)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{11}N_3O_3.¼H_2O$

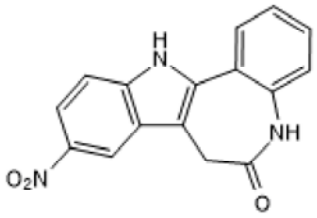
Batch Molecular Weight: 297.78

Physical Appearance: Yellow solid

Solubility: DMSO to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.54	3.89	14.11
Found	64.53	3.79	14.19

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Product Information

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Description:

Potent CDK1 and 2 inhibitor (IC_{50} values are 0.035 and 0.08 µM, respectively). Also inhibits GSK-3β and Lck (IC_{50} values are 0.11 and 0.47 µM, respectively). Induces apoptosis by activation of caspase-9; inhibits growth of cancer cell lines in vitro . Also glucocorticoid receptor inhibitor.

Physical and Chemical Properties:

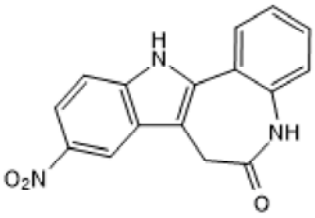
Batch Molecular Formula: $C_{16}H_{11}N_3O_3.¼H_2O$

Batch Molecular Weight: 297.78

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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 50 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:

Jiang *et al* (2017) A high-throughput chemical screen identifies novel inhibitors and enhancers of anti-inflammatory functions of the glucocorticoid receptor. Sci.Rep. ***7*** 6405. PMID: 28785063.

Bain *et al* (2003) The specificities of protein kinase inhibitors: an update. Biochem.J. ***371*** 199. PMID: 12534346.

Lahusen *et al* (2003) Alsterpaullone, a novel cyclin-dependent kinase inhibitor, induces apoptosis by activation of caspase-9 due to perturbation in mitochondrial membrane potential. Mol.Carcinog. ***36*** 183. PMID: 12669310.

Schulz *et al* (1999) Paullones, a series of cyclin-dependent kinase inhibitors: synthesis, evaluation of CDK1/cyclin B inhibition, and *in vitro* antitumor activity. J.Med.Chem. ***42*** 2909. PMID: 10425100.