TOCRIS
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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **PU H71** **Catalog No.: 3104** **Batch No.: 2**

CAS Number: 873436-91-0

IUPAC Name: 6-Amino-8-[(6-iodo-1,3-benzodioxol-5-yl)thio]-*N*-(1-methylethyl)-9*H*-purine-9-propanamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{21}IN_6O_2S.¼H_2O$

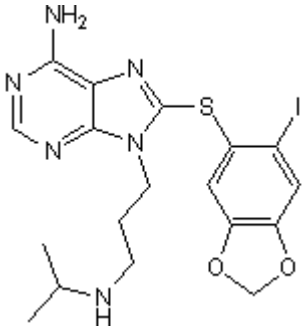
Batch Molecular Weight: 516.87

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
1eq. HCl to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.22 (DCM:7N NH3 in MeOH (30:1))

HPLC: Shows >98.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	41.83	4.19	16.26
Found	41.68	4.23	16.1

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Description:

Potent inhibitor of heat shock protein 90 (Hsp90) (IC_{50} = 51 nM in MDA-MB-468 cells). Also inhibits cell growth in a range of breast cancer cell lines (IC_{50} values are 17, 31, 65, 87 and 140 nM for SKBr3, MCF-7, MDA-MB-468, HCC-1806 and MDA-MB-231 cells respectively). Shown to inhibit cell proliferation and induce apoptosis in triple-negative breast cancer (TNBC) cells.

Physical and Chemical Properties:

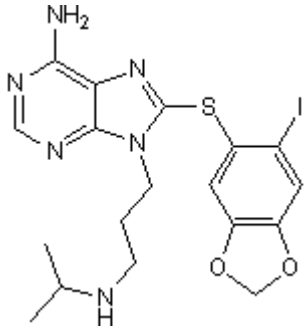
Batch Molecular Formula: $C_{18}H_{21}IN_6O_2S.¼H_2O$

Batch Molecular Weight: 516.87

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°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 100 mM
1eq. HCl 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:

He *et al* (2006) Identification of potent water soluble purine-scaffold inhibitors of the heat shock protein 90. J.Med.Chem. ***49*** 381. PMID: 16392823.

Chan *et al* (2008) Molecular imaging of the efficacy of heat shock protein 90 inhibitors in living subjects. Cancer Res. ***68*** 216. PMID: 18172314.

Caldas-Lopes *et al* (2009) Hsp90 inhibitor, PU-H71, a multimodal inhibitor of malignancy, induces complete responses in triple-negative breast cancer models. Proc.Natl.Acad.Sci.USA ***106*** 8368. PMID: 19416831.