

Certificate of Analysis

Print Date: Jan 14th 2016 www.tocris.com

Product Name: YC 1 Catalog No.: 4307 Batch No.: 1

CAS Number: 170632-47-0

IUPAC Name: 3-(5'-Hydroxymethyl-2'-furyl)-1-benzyl indazole

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{19}H_{16}N_2O_2$ **Batch Molecular Formula:** 304.34 **Batch Molecular Weight:** White solid **Physical Appearance:**

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

 $R_f = 0.2$ (Ethyl acetate:Petroleum ether [4:1]) TLC:

HPLC: Shows 99.5% purity ¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 74.98 9.2 5.3 Found 74.99 5.4 9.32

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Product Information

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IUPAC Name: 3-(5'-Hydroxymethyl-2'-furyl)-1-benzyl indazole

Description:

Nitric oxide-independent activator of soluble guanylyl cyclase (sGC). Significantly elevates cGMP levels and inhibits collagenstimulated aggregation of washed rabbit platelets (IC $_{50}$ = 14.6 μM); induces relaxation in denuded phenylephrine-contracted rabbit aortic rings (EC $_{50}$ = 1.9 μM). Also displays antiproliferative activity in vitro and in vivo by inducing G $_{1}$ cell cycle arrest in two human hepatocellular carcinoma (HCC) cell lines, and in HCC xenografts in athymic SCID mice. Exhibits low cytotoxicity in non-malignant cells.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₁₆N₂O₂ Batch Molecular Weight: 304.34 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Ko et al (1994) YC-1, a novel activator of platelet guanylate cyclase. Blood. 84 4226. PMID: 7527671.

Martin et al (2001) YC-1 activation of human soluble guanylyl cyclase has both heme-dependent and heme-independent components. Proc.Natl.Sci.U.S.A. 98 12938. PMID: 11687640.

Wang *et al* (2005) YC-1 [3-(5'-hydroxymethyl-2'-furyl)-1-benzyl indazole] exhibits a novel antiproliferative effect and arrests the cell cycle in G0-G1 in human hepatocellular carcinoma cells. J.Pharmacol.Exp.Ther. *312* 917. PMID: 15525795.

Teixeira *et al* (2006) Molecular mechanisms underlying rat mesenteric artery vasorelaxation induced by the nitric oxide-independent soluble guanylyl cyclase stimulators BAY 41-2272 [5-cyclopropyl-2-[1-(2-fluorobenzyl)-1*H*-pyrazolo[3,4-*b*]pyridin-3-yl]pyrimidin-4-ylamine] and YC-1 [3-(5'-hydroxymethyl-2'furyl)-1-benzyl indazole]. J.Pharmacol.Exp.Ther. **317** 258. PMID: 16352702.