bio-techne
TOCRIS

Print Date: Apr 28th 2023

Certificate of Analysis

www.tocris.com

Product Name: **ICG 001** **Catalog No.: 4505** **Batch No.: 4**

CAS Number: 780757-88-2

IUPAC Name: (6*S*,9a*S*)-Hexahydro-6-[(4-hydroxyphenyl)methyl]-8-(1-naphthalenylmethyl)-4,7-dioxo-*N*-(phenylmethyl)-2*H*-pyrazino[1,2-*a*]pyrimidine-1(6*H*)-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{33}H_{32}N_4O_4.¼H_2O$

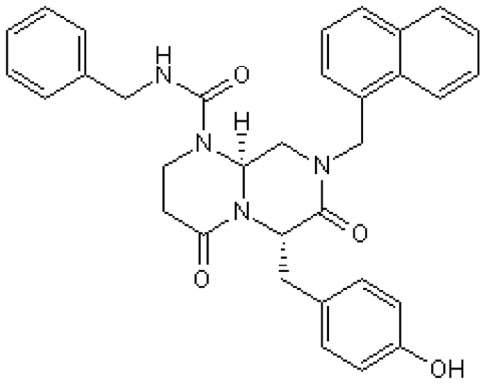
Batch Molecular Weight: 553.13

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +62 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	71.66	5.92	10.13
Found	70.9	5.92	9.98

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Name: ICG 001 **Catalog No.: 4505** 4

CAS Number: 780757-88-2

IUPAC Name: (6*S*,9a*S*)-Hexahydro-6-[(4-hydroxyphenyl)methyl]-8-(1-naphthalenylmethyl)-4,7-dioxo-*N*-(phenylmethyl)-2*H*-pyrazino[1,2-*a*]pyrimidine-1(6*H*)-carboxamide

Description:

ICG 001 is an inhibitor of TCF/β-catenin-mediated transcription. Selectively inhibits β-catenin/CBP interaction; displays no effect on β-catenin/p300 interaction. Exhibits growth inhibitory effects in colon carcinoma cell lines (SW480 and HCT-116 cells); also displays efficacy in Min mouse and nude mouse SW620 xenograft models.

Physical and Chemical Properties:

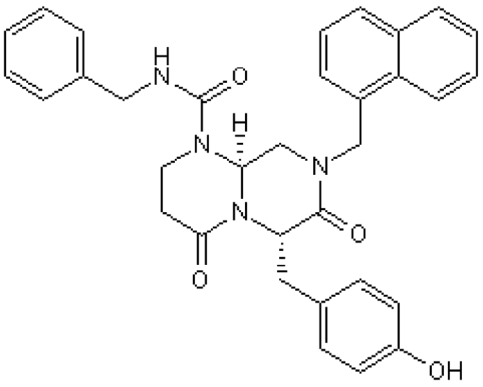
Batch Molecular Formula: $C_{33}H_{32}N_4O_4.¼H_2O$

Batch Molecular Weight: 553.13

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

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:

Zhou *et al* (2012) Interactions between β-catenin and transforming growth factor-β signaling pathways mediate epithelial-mesenchymal transition and are dependent on the transcriptional co-activator cAMP-respo J.Biol.Chem. ***287*** 7026. PMID: 22241478.

De Sousa *et al* (2011) Targeting wnt signaling in colon cancer stem cells. Clin.Cancer Res. ***17*** 647. PMID: 21159886.

Emami *et al* (2004) A small molecule inhibitor of β-catenin/CREB-binding protein transcription. Proc.Natl.Acad.Sci.USA ***101*** 12682. PMID: 15314234.