

Product Name: ICG 001

Catalog No.: 4505

Batch No.: 3

CAS Number: 780757-88-2

IUPAC Name: (6*S*,9*aS*)-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: C₃₃H₃₂N₄O₄·1/4H₂O

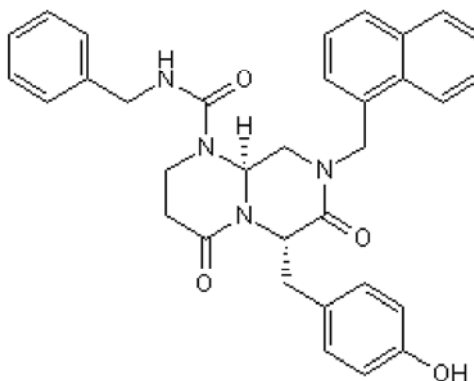
Batch Molecular Weight: 553.13

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +57.7 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	71.66	5.92	10.13
Found	71.52	6.02	10.02

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Description:

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:

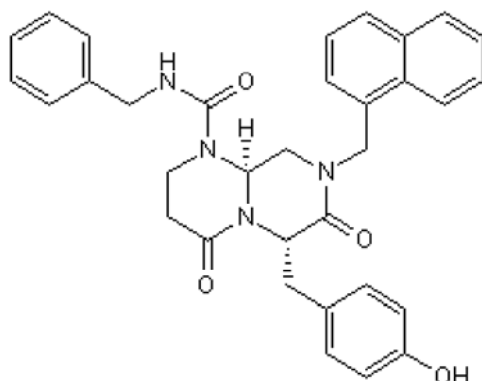
Batch Molecular Formula: C₃₃H₃₂N₄O₄·¼H₂O

Batch Molecular Weight: 553.13

Physical Appearance: 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.

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