

Certificate of Analysis

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Product Name: exo-IWR 1 Catalog No.: 3947 Batch No.: 1

CAS Number: 1127442-87-8

IUPAC Name: 4-[(3aR,4R,7S,7aS-rel)-1,3,3a,4,7,7a-Hexahydro-1,3-dioxo-4,7-methano-2*H*-isoindol-2-yl]-*N*-8-

quinolinylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{19}N_3O_3$. ¹/₄ H_2O

Batch Molecular Weight: 413.94

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.25$ (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 72.54 4.75 10.15 Found 72.73 4.65 10.17





Product Information

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quinolinylbenzamide

Description:

Negative control for endo-IWR 1 (Cat.No. 3532). 25-fold less active than endo-IWR 1; exhibits decreased activity against the Wnt/β-catenin pathway.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{25}H_{19}N_3O_3$. $\frac{1}{4}H_2O$

Batch Molecular Weight: 413.94 Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO 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:

Chen et al (2008) Small molecule-mediated disruption of Wnt-dependent signaling in tissue regeneration and cancer. Nature Chem.Biol. **5** 100.

Lu et al (2009) Structure-activity relationship studies of small-molecule inhibitors of Wnt response. Bioorg.Med.Chem.Lett. 19 3825. PMID: 19410457.

