

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-2H-isoindol-2-yl]-N-8-quinolinylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₁₉N₃O₃·¼H₂O

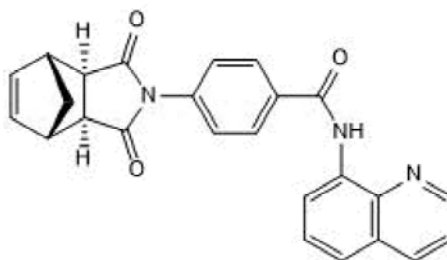
Batch Molecular Weight: 413.94

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

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

exo-IWR 1 is a negative control for endo-IWR 1 25-fold less active than endo-IWR 1; exhibits decreased activity against the Wnt/β-catenin pathway. Active Analog also available.

Physical and Chemical Properties:

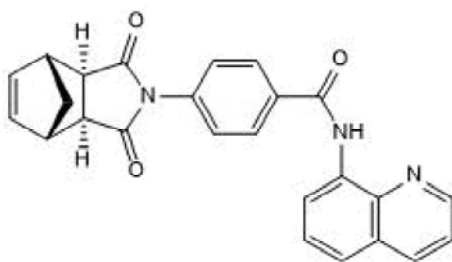
Batch Molecular Formula: C₂₅H₁₉N₃O₃·½H₂O

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:

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

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

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