

Product Name: D 4476

Catalog No.: 2902

Batch No.: 2

CAS Number: 301836-43-1

IUPAC Name: 4-[4-(2,3-Dihydro-1,4-benzodioxin-6-yl)-5-(2-pyridinyl)-1H-imidazol-2-yl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{18}N_4O_3 \cdot \frac{3}{4}H_2O$

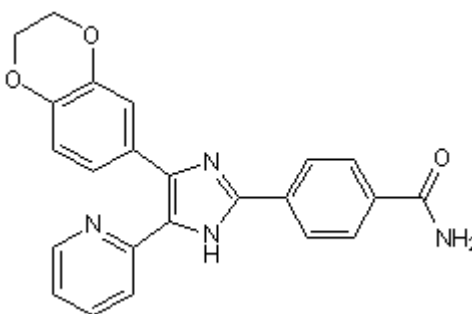
Batch Molecular Weight: 411.92

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.15$ (Dichloromethane:Methanol:NH₄OH [94:5:1])

HPLC: Shows 99.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.06	4.77	13.6
Found	67.38	4.56	13.74

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Description:

Selective inhibitor of casein kinase 1 (CK1) and TGF- β type-I receptor (ALK5) that displays > 20-fold selectivity over SAPK2/p38 and a much greater selectivity over all other protein kinases tested. Suppresses site-specific phosphorylation and nuclear exclusion of FOXO1a.

Physical and Chemical Properties:

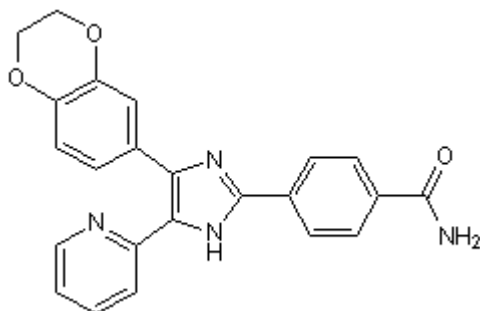
Batch Molecular Formula: C₂₃H₁₈N₄O₃· $\frac{3}{4}$ H₂O

Batch Molecular Weight: 411.92

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°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:

Callahan et al (2002) Identification of novel inhibitors of the transforming growth factor β 1 (TGF- β 1) type I receptor (ALK5). *J.Med.Chem.* **45** 999. PMID: 11855979.

Rena et al (2004) D4476, a cell-permeant inhibitor of CK1, suppresses the site-specific phosphorylation and nuclear exclusion of FOXO1a. *EMBO Rep.* **5** 60. PMID: 14710188.

Bain et al (2007) The selectivity of protein kinase inhibitors: a further update. *Biochem.J.* **408** 297. PMID: 17850214.

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