

Certificate of Analysis

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Product Name: GDC 0879

Catalog No.: 4453

Batch No.: 1

CAS Number: 905281-76-7

IUPAC Name: 2,3-Dihydro-5-[1-(2-hydroxyethyl)-3-(4-pyridinyl)-1*H*-pyrazol-4-yl]-1*H*-inden-1-one oxime

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₈N₄O₂·¼H₂O

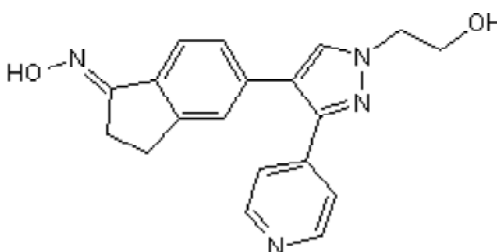
Batch Molecular Weight: 338.87

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	67.34	5.5	16.53
Found	67.41	5.43	16.71

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

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Description:

Potent and selective B-Raf inhibitor (IC_{50} = 0.13 nM against purified B-Raf^{V600E}). Activity reduces phospho-ERK (pERK) levels (IC_{50} = 63 nM in the Malme-3M cell line). Inhibits the Raf/MEK/ERK signaling pathway in V600E B-Raf mutant cell lines. Does not activate apoptotic pathways in A375 or Colo205 cell lines. Orally bioavailable.

Physical and Chemical Properties:

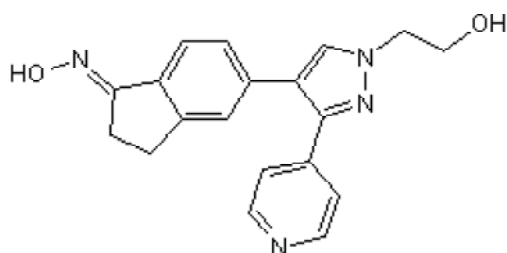
Batch Molecular Formula: C₁₉H₁₈N₄O₂· $\frac{1}{4}$ H₂O

Batch Molecular Weight: 338.87

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

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:

Hatzivassiliou et al (2010) RAF inhibitors prime wild-type RAF to activate the MAPK pathway and enhance growth. *Nature* **464** 431. PMID: 20130576.

Hoeflich et al (2009) Antitumor efficacy of the novel RAF inhibitor GDC-0879 is predicted by BRAF^{V600E} mutational status and sustained extracellular signal-regulated kinase/mitogen-activated protein kinase pathway suppression. *Cancer Res.* **69** 3042. PMID: 19276360.

Wong et al (2009) Pharmacodynamics of 2-[4-[(1E)-1-(hydroxyimino)-2,3-dihydro-1H-inden-5-yl]-3-(pyridine-4-yl)-1H-pyrazol-1-yl]ethan-1-ol (GDC-0879), a potent and selective B-Raf kinase inhibitor: understanding relationships between systemic conc J.Pharmacol.Exp.Ther. **329** 360. PMID: 19147858.

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