

Product Name: PF 04449913 maleate

Catalog No.: 6538

Batch No.: 1

CAS Number: 2030410-25-2

IUPAC Name: 1-((2*R*,4*R*)-2-(1*H*-Benzimidazol-2-yl)-1-methylpiperidin-4-yl)-3-(4-cyanophenyl)urea maleate salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₂N₆O.C₄H₄O₄.¼H₂O

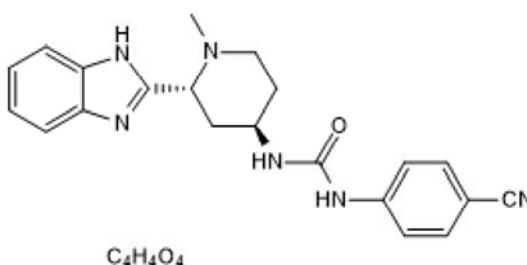
Batch Molecular Weight: 495.01

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.66	5.4	16.98
Found	60.64	5.34	17.1

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

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Description:

Potent Smo antagonist (IC₅₀ = 5 nM). Attenuates the leukemia-initiation potential of AML cells in a serial transplantation mouse model. Also eliminates self-propagation capacity of AML cells.

Physical and Chemical Properties:

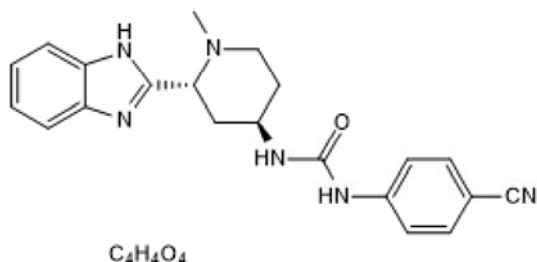
Batch Molecular Formula: C₂₁H₂₂N₆O.C₄H₄O₄.½H₂O

Batch Molecular Weight: 495.01

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Fukushima *et al* (2016) Small-molecule Hedgehog inhibitor attenuates the leukemia-initiation potential of acute myeloid leukemia cells. *Cancer Sci.* **107** 1422. PMID: 27461445.

Giordani *et al* (2016) The human Smoothened inhibitor PF-04449913 induces exit from quiescence and loss of multipotent Drosophila hematopoietic progenitor cells. *Oncotarget* **7** 55313. PMID: 27486815.

Munchhof *et al* (2011) Discovery of PF-04449913, a potent and orally bioavailable inhibitor of smoothened. *ACS Med.Chem.Lett.* **3** 106. PMID: 24900436.

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