

**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:** C<sub>21</sub>H<sub>22</sub>N<sub>6</sub>O.C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>.1/4H<sub>2</sub>O

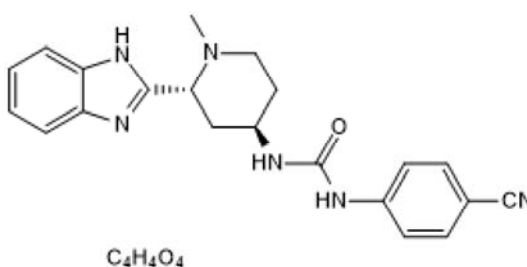
**Batch Molecular Weight:** 495.01

**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

**<sup>1</sup>H 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

**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

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**Description:**

Potent Smo antagonist (IC<sub>50</sub> = 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:**

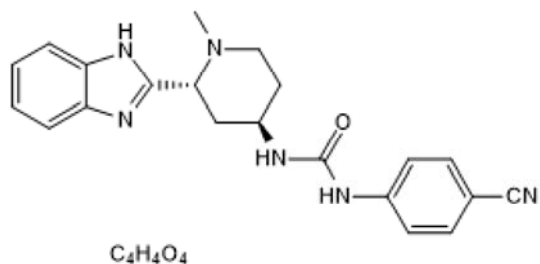
Batch Molecular Formula: C<sub>21</sub>H<sub>22</sub>N<sub>6</sub>O.C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>.¼H<sub>2</sub>O

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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