

**Product Name:** Vemurafenib

**Catalog No.:** 7309

**Batch No.:** 1

CAS Number: 918504-65-1

IUPAC Name: *N*-[3-[[5-(4-Chlorophenyl)-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl]carbonyl]-2,4-difluorophenyl]-1-propanesulfonamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>18</sub>ClF<sub>2</sub>N<sub>3</sub>O<sub>3</sub>S.

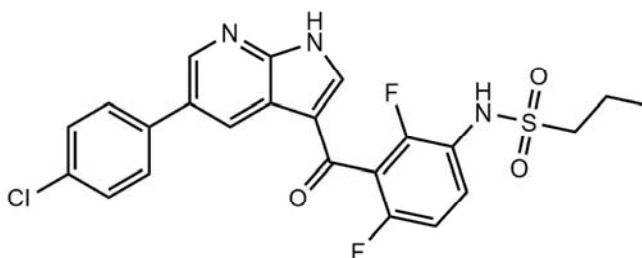
**Batch Molecular Weight:** 489.92

**Physical Appearance:** Off White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.9% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	56.39	3.7	8.58
Found	56.07	3.76	8.32

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**Description:**

Vemurafenib is a potent inhibitor of BRAF<sup>V600E</sup>, C-Raf and wild type B-Raf (IC<sub>50</sub> values are 13-31 nM, 6.7-48 nM and 100-160 nM, respectively). Vemurafenib also inhibits SRMS, ACK1 KHS1, FGR (IC<sub>50</sub> values are 18 nM, 19 nM, 51 nM and 63 nM, respectively). Vemurafenib shows antitumor activity and induces autophagy in BRAF-mutant thyroid cancer cells.

**Physical and Chemical Properties:**

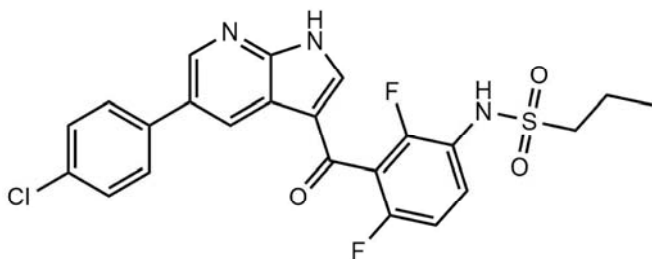
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Batch Molecular Weight: 489.92

Physical Appearance: Off 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:**

**Wang et al** (2017) Targeting autophagy sensitizes BRAF-mutant thyroid cancer to vemurafenib. *J.Clin.Endocrinol.Metab.* **102** 634. PMID: 27754804.

**Ibrahim et al** (2013) Chapter twenty-six - case history: vemurafenib, a potent, selective, and first-in-class inhibitor of mutant BRAF for the treatment of metastatic melanoma. *Annu.Rep.Med.Chem.* **48** 435.

**Davis and Schlessinger** (2012) The genesis of zelnoraf: targeting mutant B-Raf in melanoma. *J.Cell.Biol.* **199** 15. PMID: 23027900.

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