

Product Name: Dabrafenib mesylate

Catalog No.: 7223

Batch No.: 1

CAS Number: 1195768-06-9

IUPAC Name: *N*-[3-[5-(2-Aminopyrimidin-4-yl)-2-*tert*-butyl-1,3-thiazol-4-yl]-2-fluorophenyl]-2,6-difluorobenzenesulfonamide methanesulfonate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₀F₃N₅O₂S₂.CH₃SO₃H

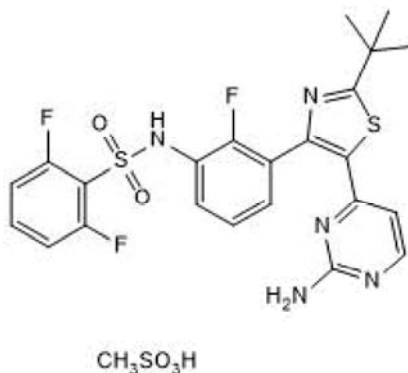
Batch Molecular Weight: 615.66

Physical Appearance: Off-white solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	46.82	3.93	11.38
Found	46.77	3.97	11.36

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

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Description:

Potent and selective Raf kinase inhibitor (IC₅₀ values are 0.8, 3.2 and 5.0 nM for B-Raf^{V600E}, wild-type B-Raf and c-Raf, respectively). Exhibits selectivity for B-Raf over a panel of 270 other kinases. Arrests cell cycle in the G₁ phase and inhibits growth of B-Raf^{V600E} mutant melanoma and colon cancer cells in vitro and in vivo. Orally bioavailable. Also inhibits NEK9 (IC₅₀ <10 nM) and CDK16. Identified as targeting human host proteins that interact with SARS-CoV-2.

Physical and Chemical Properties:

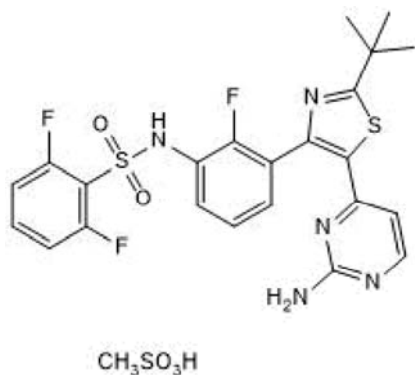
Batch Molecular Formula: C₂₃H₂₀F₃N₅O₂S₂.CH₃SO₃H

Batch Molecular Weight: 615.66

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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:

Gordon et al (2020) A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. *Nature*. PMID: 32353859.

Phadke et al (2018) Dabrafenib inhibits the growth of *BRAF-WT* cancers through CDK16 and NEK9 inhibition. *Mol.Oncol.* **12** 74. PMID: 29112787.

Rheault et al (2013) Discovery of Dabrafenib: a selective inhibitor of Raf kinases with antitumor activity against B.Raf-driven tumors. *ACS Med Chem Lett* **4** 358. PMID: 24900673.

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