TOCRIS
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Print Date: Jun 27th 2019

Certificate of Analysis

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Product Name: **PF 543 hydrochloride** **Catalog No.: 5754** **Batch No.: 1**

CAS Number: 1706522-79-3

IUPAC Name: (2*R*)-1-[[(4-[[3-Methyl-5-[(phenylsulfonyl)methyl]phenoxy]methyl]phenyl]methyl]-2-pyrrolidinemethanol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{31}NO_4S.HCl$

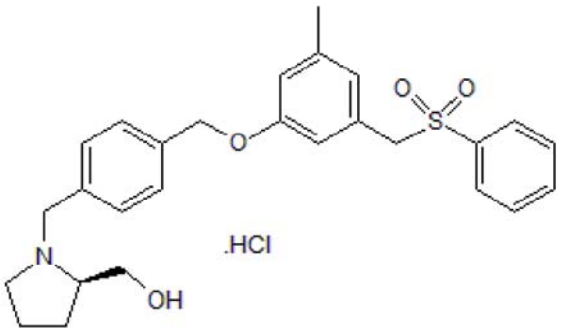
Batch Molecular Weight: 502.07

Physical Appearance: White solid

Solubility: water to 10 mM with gentle warming
DMSO to 100 mM
ethanol to 20 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.59	6.42	2.79
Found	64.57	6.37	2.86

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Description:

Potent and selective SphK1 inhibitor (IC_{50} = 2 nM; K_i = 3.6 nM). Exhibits >100-fold selectivity for Sphk1 over Sphk2. Also exhibits >5,000 fold selectivity over $S1P_{1-5}$ receptors and 48 protein and lipid kinases. Attenuates proliferation and induces necrosis in human colorectal cancer cells in vitro. Suppresses HCT-116 tumor xenograft growth in mice. Also reduces sickling, hemolysis and inflammation in a transgenic mouse model of sickle cell disease.

Physical and Chemical Properties:

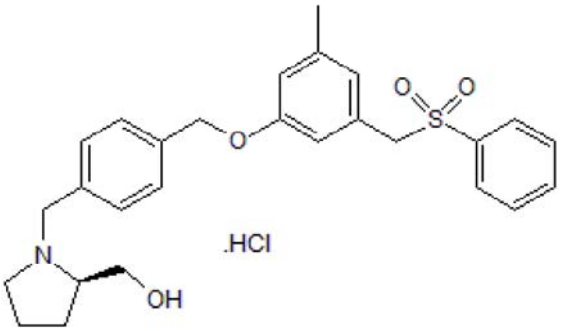
Batch Molecular Formula: $C_{27}H_{31}NO_4S.HCl$

Batch Molecular Weight: 502.07

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 10 mM with gentle warming
DMSO to 100 mM
ethanol to 20 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:

Schnute *et al* (2017) Discovery of a potent and selective sphingosine kinase 1 inhibitor through the molecular combination of chemotype-distinct screening hits J.Med.Chem. ***60*** 2562. PMID: 28231433.

Ju *et al* (2016) Targeting colorectal cancer cells by a novel sphingosine kinase 1 inhibitor PF-543. Biochem.Biophys.Res.Commun. ***470*** 728. PMID: 26775841.

Zhang *et al* (2014) Elevated sphingosine-1-phosphate promotes sickling and sickle cell disease progression. J.Clin.Invest. ***124*** 2750. PMID: 24837436 .

Schnute *et al* (2012) Modulation of cellular S1P levels with a novel, potent and specific inhibitor of sphingosine kinase-1. Biochem.J. ***444*** 79. PMID: 22397330.