

Product Name: PND 1186

Catalog No.: 6891

Batch No.: 1

CAS Number: 1061353-68-1

IUPAC Name: 2-[[2-[[2-Methoxy-4-(4-morpholinyl)phenyl]amino]-5-(trifluoromethyl)-4-pyridinyl]amino]-*N*-methylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₆F₃N₅O₃.H₂O

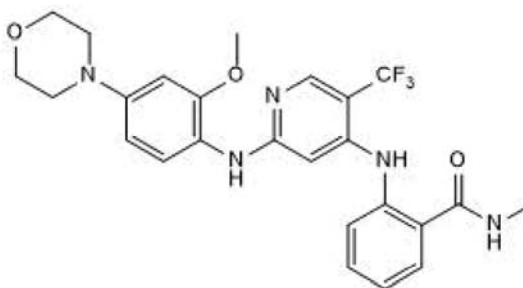
Batch Molecular Weight: 519.53

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.8	5.43	13.48
Found	57.84	5.07	13.24

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Description:

Potent FAK inhibitor (IC₅₀ values are 1.5 and 100 nM for recombinant FAK and FAK in breast carcinoma cells, respectively). Promotes caspase activation; triggering apoptosis. Inhibits 4T1 breast carcinoma subcutaneous tumor growth and breast carcinoma cell motility. Decreases spontaneous breast to lung metastasis in pre-clinical models. Orally bioavailable.

Physical and Chemical Properties:

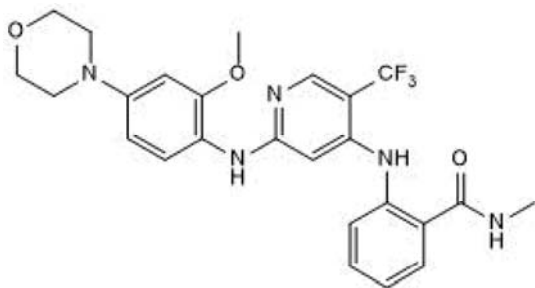
Batch Molecular Formula: C₂₅H₂₆F₃N₅O₃.H₂O

Batch Molecular Weight: 519.53

Physical Appearance: 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:

Jiang *et al* (2016) Targeting focal adhesion kinase renders pancreatic cancers responsive to checkpoint immunotherapy. *Nat.Med.* **22** 851. PMID: 27376576.

Tanjoni *et al* (2010) PND-1186 FAK inhibitor selectively promotes tumor cell apoptosis in three-dimensional environments. *Cancer Biol.Ther.* **9** 764. PMID: 20234191.

Walsh *et al* (2010) Oral delivery of PND-1186 FAK inhibitor decreases tumor growth and spontaneous breast to lung metastasis in pre-clinical models. *Cancer Biol.Ther.* **9** 778. PMID: 20234193.

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