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Print Date: Jan 15th 2016

Certificate of Analysis

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Product Name: **TC-S 7006** **Catalog No.: 5240** **Batch No.: 1**

CAS Number: 871307-18-5

IUPAC Name: 4-[(3-Chloro-4-fluorophenyl)amino]-6-[(3-pyridinylmethyl)amino]-1,7-naphthyridine-3-carbonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{14}ClFN_6.H_2O$

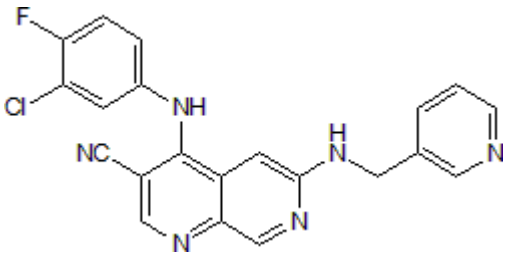
Batch Molecular Weight: 422.85

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Chloroform:Methanol [9:1])

HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.65	3.81	19.87
Found	59.71	3.96	19.64

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IUPAC Name: 4-[(3-Chloro-4-fluorophenyl)amino]-6-[(3-pyridinylmethyl)amino]-1,7-naphthyridine-3-carbonitrile

Description:

Potent and selective Tpl2 (Cot; MAP3K8) inhibitor (IC_{50} = 50 nM). Selective for Tpl2 over MEK, p38, Src, MK2, PKC and EGFR. Inhibits LPS-induced TNF-α secretion from monocytes and attenuates acute myeloid leukemia (AML) cell proliferation in vitro. Also reduces cytolytic activity of human $CD8^+$ cytotoxic T lymphocytes. Cell permeable.

Physical and Chemical Properties:

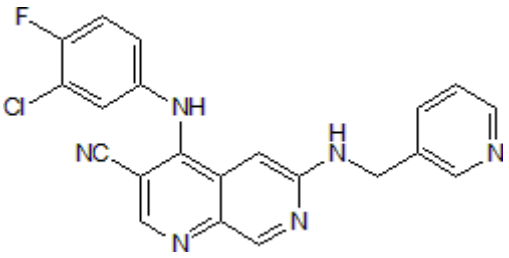
Batch Molecular Formula: $C_{21}H_{14}ClFN_6.H_2O$

Batch Molecular Weight: 422.85

Physical Appearance: Yellow solid

Minimum Purity: >99%

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:

Gavrin *et al* (2005) Inhibition of Tpl2 kinase and TNF-α production with 1,7-naphthyridine-3-carbonitriles: synthesis and structure-activity relationships. Bioorg.Med.Chem.Lett. ***15*** 5288. PMID: 16165349.

Wang *et al* (2010) Inhibition of Cot1/Tlp2 oncogene in AML cells reduces ERK5 activation and up-regulates $p27^{Kip1}$ concomitant with enhancement of differentiation and cell cycle arrest induced by silibinin and 1,25-dihydroxyvitamin D_3. Cell Cycle ***9*** 4542. PMID: 21084834.

Chowdhury *et al* (2014) Pharmacological inhibition of TPL2/MAP3K8 blocks human cytotoxic T lymphocyte effector functions. PLoS ONE ***9*** e92187. PMID: 24642963.