Print Date: Apr 3rd 2013

Certificate of Analysis

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Product Name: TPCA-1 **Catalog No.: 2559** **Batch No.: 5**

CAS Number: 507475-17-4

IUPAC Name: 2-[(Aminocarbonyl)amino]-5-(4-fluorophenyl)-3-thiophenecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_{10}FN_3O_2S$

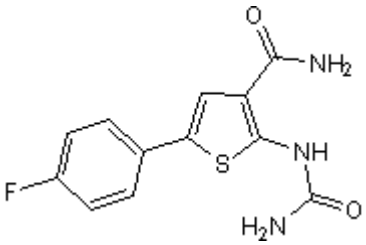
Batch Molecular Weight: 279.29

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 10 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.16 (Ethyl acetate:Methanol [9:1])

HPLC: Shows 97.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.61	3.61	15.05
Found	51.59	3.72	14.95

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Description:

Potent, selective inhibitor of IκB kinase (IKK) β (IC_{50} = 17.9 nM) that displays > 22-fold selectivity over IKKα and > 550-fold selectivity over other kinases and enzymes. Inhibits production of pro-inflammatory cytokines in vitro and in vivo and inhibits NF-κB nuclear localization. Reduces the severity and onset of collagen-induced arthritis; anti-inflammatory.

Physical and Chemical Properties:

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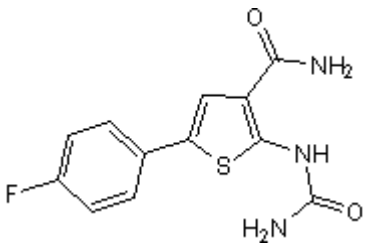
Batch Molecular Weight: 279.29

Physical Appearance: Off-white solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Desiccate at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 10 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:

Podolin *et al* (2005) Attenuation of murine collagen-induced arthritis by a novel, potent, selective small molecule inhibitor of IκB kinase 2, TPCA-1 (2-[aminocarbonyl)amino]-5-(4-fluorophenyl)-3-thiophenecarboxamide), occurs via reduction of proinflammatory cytokines and antigen-induced T cell proliferation. J.Pharmacol.Exp.Ther. ***312*** 373. PMID: 15316093.

Birrell *et al* (2005) IK-B kinase-2 inhibitor blocks inflammation in human airway smooth muscle and a rat model of asthma. Am.J.Respir.Crit.Care Med. ***172*** 962. PMID: 16002568.

Birrell *et al* (2006) IκB kinase-2-independent and-dependent inflammation in airway disease models: relevance of IKK-2 inhibition to the clinic. Mol.Pharmacol. ***69*** 1791. PMID: 16517756.