Print Date: Sep 3rd 2020

Certificate of Analysis

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Product Name: **IMD 0354** **Catalog No.: 2611** **Batch No.: 1**

CAS Number: 978-62-1

IUPAC Name: *N*-[3,5-Bis(trifluoromethyl)phenyl]-5-chloro-2-hydroxybenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_8ClF_6NO_2$

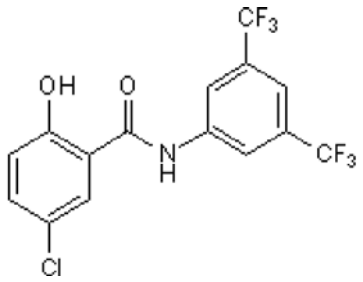
Batch Molecular Weight: 383.67

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Ethyl acetate:Hexane [9:1])

HPLC: Shows >99.78% purity

^{1}H NMR: Consistent with structure

^{13}C NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	46.96	2.1	3.65
Found	46.71	1.95	3.58

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

Inhibitor of IκB kinase-β (IKKβ) that blocks NF-κB nuclear translocation. Attenuates myocardial ischemia/reperfusion injury by decreasing expression of adhesion molecules ICAM-1 and P-selectin and inhibiting cytokine and chemokine production in cardiomyocytes. Induces G_0/G_1 cell cycle arrest and apoptosis in HMC-1 and breast cancer cells. Also antagonist at $P2X_1$, $P2X_4$ and $P2X_7$ receptors (IC_{50} values are 19, 156 and 175 nM respectively). Inhibits platelet aggregation induced by collegen in vitro.

Physical and Chemical Properties:

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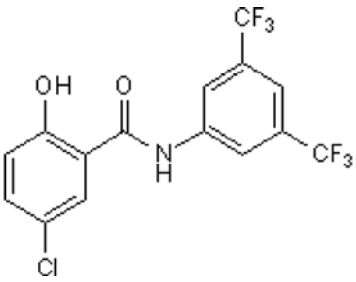
Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Tanaka *et al* (2006) A new IκB kinase β inhibitor prevents human breast cancer progression through negative regulation of cell cycle transition. Cancer Res. ***66*** 419. PMID: 16397257.

Tanaka *et al* (2005) A novel NF-κB inhibitor, IMD-0354, supresses neoplastic proliferation of human mast cells with constitutively activated c-*kit* receptors. Hematopoiesis ***105*** 2324.

Onai *et al* (2004) Inhibition of IκB phosphorylation in cardiomyocytes attenuates myocardial ischemia/reperfusion injury. Cardiovasc.Res. ***63*** 51. PMID: 15194461.