Print Date: May 10th 2012

Certificate of Analysis

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Product Name: ML 130 **Catalog No.: 4354** **Batch No.: 1**

CAS Number: 799264-47-4

IUPAC Name: 1-[(4-Methylphenyl)sulfonyl]-1*H*-benzimidazol-2-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_{13}N_3O_2S$

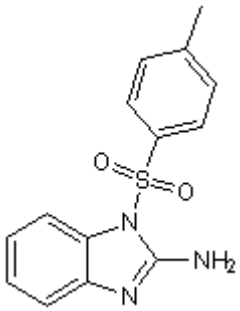
Batch Molecular Weight: 287.34

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 10 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.52	4.56	14.62
Found	58.52	4.58	14.61

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Description:

Potent and selective inhibitor of NOD1; displays 36-fold selectivity for NOD1 over NOD2 (IC_{50} values are 0.56 and >20 μM for NOD1 and NOD2 respectively). Inhibits NOD1-induced NF-κB activation in HEK293 cells with no cytotoxicity. Shown to alter subcellular targeting of NOD1; also thought to alter the conformation of NOD1 protein in vitro.

Physical and Chemical Properties:

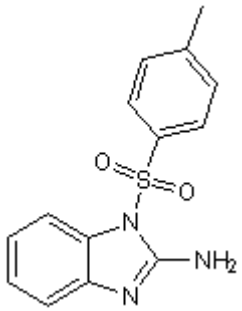
Batch Molecular Formula: $C_{14}H_{13}N_3O_2S$

Batch Molecular Weight: 287.34

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°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:

Correa *et al* (2011) Discovery and characterization of 2-aminobenzimidazole derivatives as selective NOD1 inhibitors. Chem.Biol. ***18*** 825. PMID: 21802003.

Khan *et al* (2011) Identification of inhibitors of NOD1-induced nuclear factor-κB activation. ACS Med.Chem.Lett. ***2*** 780. PMID: 22003428.