



Certificate of Analysis

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Product Name: Bay 11-7821 Catalog No.: 1744 Batch No.: 1

CAS Number: 19542-67-7

IUPAC Name: (2E)-3-[(4-Methylphenyl)sulfonyl]-2-propenenitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{10}H_9NO_2S$ Batch Molecular Weight:207.25Physical Appearance:White solid

Solubility: ethanol to 25 mM

DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: R_f = 0.3 (Dichloromethane:Petroleum ether [1:1])

Melting Point:

HPLC:

Shows >99.8% purity

TH NMR:

Consistent with structure

Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.96 4.38 6.76 Found 57.89 4.33 6.91

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Product Information

Print Date: Feb 19th 2020

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IUPAC Name: (2E)-3-[(4-Methylphenyl)sulfonyl]-2-propenenitrile

Description:

E2 ubiquitin (Ub) conjugating enzyme inhibitor. Inhibits the conjugation of Ub to a range of E2 enzymes. Inhibits E2 enzyme mediated IkB α phosphorylation and indirectly decreases NF-kb activity. Also reversibly activates MAPK signaling. Induces apoptosis of leukemic T cell and B-cell lymphoma cell lines. Also inhibits activation of NLRP3 inflammasome. Binds and inhibits gasdermin D (GSDMD) pore formation. Pyroptosis inhibitor.

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:

ethanol to 25 mM 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:

Pandeya *et al* (2019) Gasdermin D (GSDMD) as a new target for the treatment of infection. Medchemcomm *10* 660. PMID: 31191857. **Strickson** *et al* (2013) The anti-inflammatory drug BAY 11-7082 suppresses the MyD88-dependent signalling network by targeting the ubiquitin system. Biochem.J. *451* 427. PMID: 23441730.

Juliana et al (2010) Anti-inflammatory compounds parthenolide and Bay 11-7082 are direct inhibitors of the inflammasome. J.Biol.Chem. **285** 9792. PMID: 20093358.

Mori et al (2002) Bay 11-7082 inhibits transcription factor NF-κB and induces apoptosis of HTLV-l-infected T-cell lines and primary adult T-cell leukemia cells. Blood **100** 1828. PMID: 12176906.

Pierce *et al* (1997) Novel inhibitors of cytokine-induced IκBα phosphorylation and endothelial cell adhesion molecule expression show anti-inflammatory effects *in vivo*. J.Biol.Chem. **272** 21096. PMID: 9261113.