Print Date: Feb 10th 2020

Certificate of Analysis

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Product Name: **BC-LI-0186** **Catalog No.: 6791** **Batch No.: 1**

CAS Number: 695207-56-8

IUPAC Name: 4-[2,5-Dihydro-2,3-dimethyl-4-(1-methylethyl)-5-oxo-1*H*-pyrazol-1-yl]-*N*-(2-phenoxyethyl)benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{27}N_3O_4S$

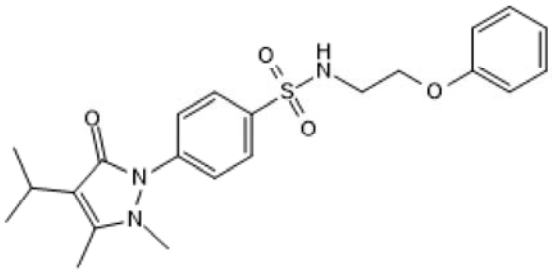
Batch Molecular Weight: 429.54

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.52	6.34	9.78
Found	61.3	6.36	9.87

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Description:

Potent and high affinity leucyl-tRNA synthase (TRS)/Ras-related GTP-binding protein D (RagD) interaction inhibitor (IC_{50} = 46.1 nM; K_d = 42.1 nM for binding to LRS). Inhibits mTOR complex 1 activity by blocking binding to LRS without affecting catalytic activity. Inhibits leucine-induced translocation of LRS to the lysosome.

Physical and Chemical Properties:

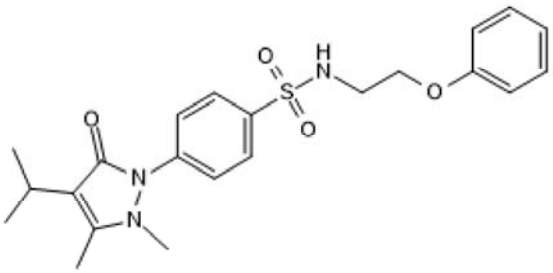
Batch Molecular Formula: $C_{22}H_{27}N_3O_4S$

Batch Molecular Weight: 429.54

Physical Appearance: White solid

Minimum Purity: ≥98%

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:

Lee *et al* (2018) Coordination of the leucine-sensing Rag GTPase cycle by leucyl-tRNA synthetase in the mTORC1 signaling pathway. Proc.Natl.Acad.Sci.USA. ***115*** E5279. PMID: 29784813.

Choi *et al* (2017) Leucine-induced localization of Leucyl-tRNA synthetase in lysosome membrane. Biochem.Biophys.Res.Commun. ***493*** 1129. PMID: 28882589.

Kim *et al* (2017) Control of leucine-dependent mTORC1 pathway through chemical intervention of leucyl-tRNA synthetase and RagD interaction. Nat.Commun. ***8*** 732. PMID: 28963468.