TOCRIS
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Print Date: Sep 20th 2021

Certificate of Analysis

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Product Name: **BI-6901** **Catalog No.: 6141** **Batch No.: 1**

CAS Number: 2040401-92-9

IUPAC Name: *N*-[(1*R*)-3-(2-Cyano-1*H*-pyrrol-1-yl)-1-[(4-methyl-1-piperidinyl)carbonyl]propyl]-1*H*-indole-4-sulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{27}N_5O_3S$.

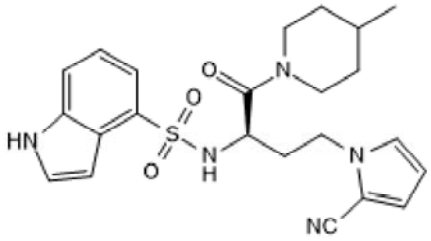
Batch Molecular Weight: 453.56

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

Chiral HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.91	6	15.44
Found	60.51	6.09	15.31

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Product Information

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Description:

BI-6901 is a potent and selective CCR10 antagonist (IC_{50} = 1 - 25 nM). BI-6901 inhibits CCL27-dependent chemotaxis of Ba/F3 cells (IC_{50} = 1 nM) and reduces inflammation in a DNFB-stimulated animal model of contact hypersensitivity.

Physical and Chemical Properties:

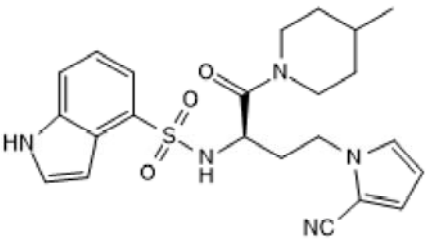
Batch Molecular Formula: $C_{23}H_{27}N_5O_3S$.

Batch Molecular Weight: 453.56

Physical Appearance: Pale yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

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:

Abeywardane *et al* (2016) N-Arylsulfonyl-a-amino carboxamides are potent and selective inhibitors of the chemokine receptor CCR10 that show efficacy in the murine DNFB model of contact hypersensitivity. Bioorg.Med.Chem.Lett. ***26*** 5277. PMID: 27692854.

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