

Product Name: ML 339

Catalog No.: 5943

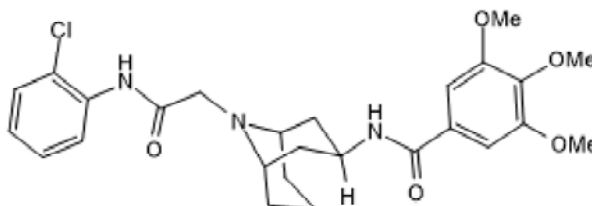
Batch No.: 1

CAS Number: 2080300-49-6

IUPAC Name: *N*-[(1*R*,3*S*,5*S*)-9-(2-((2-Chlorophenyl)amino)-2-exoethyl)-9-azabicyclo[3.3.1]nonan-3-yl)-3,4,5-trimethoxybenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₃₂ClN₃O₅
Batch Molecular Weight: 502
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 20 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.13 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.21	6.43	8.37
Found	61.88	6.64	8.53

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

Product Name: ML 339

Catalog No.: 5943

Batch No.: 1

CAS Number: 2080300-49-6

IUPAC Name: *N*-[(1*R*,3*S*,5*S*)-9-(2-((2-Chlorophenyl)amino)-2-exoethyl)-9-azabicyclo[3.3.1]nonan-3-yl)-3,4,5-trimethoxybenzamide

Description:

Potent and selective hCXCR6 antagonist (IC₅₀ = 140 nM); 100-fold less active at the murine CXCR6 receptor (IC₅₀ = 18 μM). Exhibits selectivity over CXCR5, CXCR4, CCR6 and APJ receptors (IC₅₀ >79 μM).

Physical and Chemical Properties:

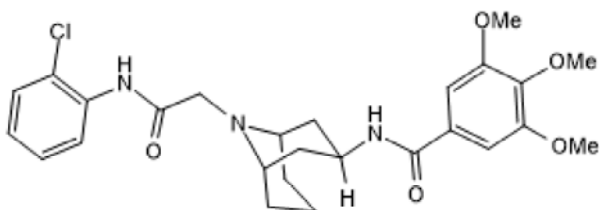
Batch Molecular Formula: C₂₆H₃₂ClN₃O₅

Batch Molecular Weight: 502

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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:

Hershberger et al (2012) Probing the CXCR6/CXCL16 Axis: targeting prevention of prostate cancer metastasis. Probe Reports from the NIH Molecular Libraries Program. PMID: 24049849.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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