

Certificate of Analysis

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Product Name: ZK 756326 dihydrochloride

Catalog No.: 2565

Batch No.: 2

CAS Number: 1780259-94-0

IUPAC Name: 2-[2-[4-[(3-phenoxyphenyl)methyl]-1-piperazinyl]ethoxy]ethanol dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₈N₂O₃·2HCl

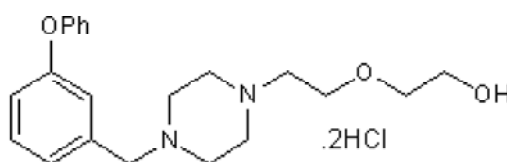
Batch Molecular Weight: 429.38

Physical Appearance: White solid

Solubility: water to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.37 (Chloroform:Methanol:Ammonia soln. [9:1:5])

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.74	7.04	6.52
Found	58.5	7.14	6.3

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

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Description:

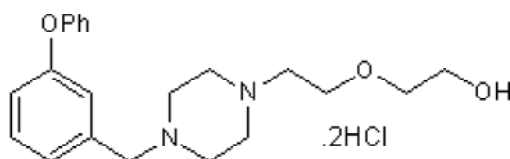
Selective, non-peptide CCR8 chemokine receptor agonist (IC₅₀ values are 1.8 and 2.6 μM for human and mouse receptors respectively). Displays no activity at CCR4, CXCR3, CXCR4 and CCR5 and shows > 28-fold selectivity over 26 other GPCRs (less selective at α_{2A} and 5-HT receptors). Induces chemotaxis and inhibits Env-mediated (HIV) cell-cell fusion.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₂₈N₂O₃.2HCl
 Batch Molecular Weight: 429.38
 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water 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:

Haskell *et al* (2006) Identification and characterization of a potent, selective nonpeptide agonist of the CC chemokine receptor CCR8. *Mol.Pharmacol.* **69** 309. PMID: 16221874.

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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
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