1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{33}\text{H}_{41}\text{ClN}_{6}\text{O}_{2} \)

Batch Molecular Weight: 589.17

Physical Appearance: White lyophilised solid

Storage: Store at -20°C

2. ANALYTICAL DATA

HPLC: Shows 96.0% purity

Mass Spectrum: Consistent with structure
Product Name: THIQ
Catalog No.: 3032
Batch No.: 4

CAS Number: 312637-48-2
IUPAC Name: \(N-[\{1R\}-1-\{4\text{-Chlorophenyl}\text{methyl}\}-2-\{4\text{-cyclohexyl}-4-(1H-1,2,4\text{-triazol}-1\text{-ylmethyl})-1\text{-piperidinyl}\}-2\text{-oxoethyl}]\)
\(-1,2,3,4\text{-tetrahydro-3-isoquinolinecarboxamide}\)

Description:
Potent and selective melanocortin 4 (MC4) receptor agonist (IC\(_{50}\) values are 1.2, 761 and 2067 nM for human MC4, MC3 and MC1 receptors respectively). Enhances intracavernosal pressure and stimulates erectile activity in rats ex copula following systemic administration.

Physical and Chemical Properties:
Batch Molecular Formula: C\(_{33}\)H\(_{41}\)ClN\(_8\)O\(_2\)
Batch Molecular Weight: 589.17
Physical Appearance: White lyophilised solid

Minimum Purity: >95%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:
This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:


Sebhat et al (2002) Design and pharmacology of \(N-[\{3R\}-1,2,3,4\text{-Tetrahydroisoquinolinium-3-ylcarbonyl}\]-\(1R\)-1-(4-chlorobenzyl)-2-\{4-cyclohexyl-4-(1H-1,2,4-triazol-1-methyl)piperidin-1-yl\}-2-oxoethylamine (1), a potent, selective melanocortin subtype-4 receptor agonist. J.Med.Chem. 45 4589. PMID: 12361385.

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