

Product Name: **THIQ**

Catalog No.: **3032**

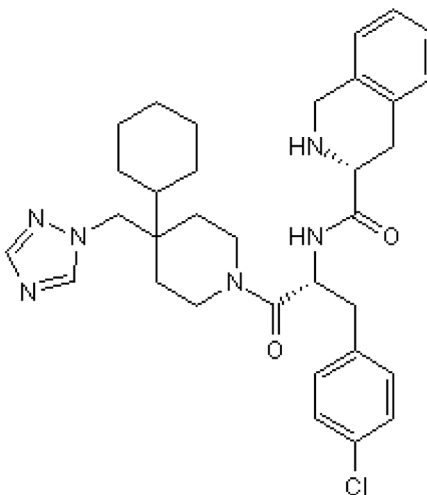
Batch No.: **4**

CAS Number: 312637-48-2

IUPAC Name: *N*-[(1*R*)-1-[4-Chlorophenyl)methyl]-2-[4-cyclohexyl-4-(1*H*-1,2,4-triazol-1-ylmethyl)-1-piperidinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-3-isoquinolinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₃₃ H ₄₁ ClN ₆ O ₂
Batch Molecular Weight:	589.17
Physical Appearance:	White lyophilised solid
Solubility:	DMSO to 10 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 95.1% purity
Mass Spectrum:	Consistent with structure

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

Product Name: THIQ

Catalog No.: 3032

4

CAS Number: 312637-48-2

IUPAC Name: N-[(1R)-1-[4-(4-Chlorophenyl)methyl]-2-[4-cyclohexyl-4-(1H-1,2,4-triazol-1-ylmethyl)-1-piperidinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-3-isoquinolinecarboxamide

Description:

THIQ is a potent and selective melanocortin 4 (MC₄) receptor agonist (IC₅₀ 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:

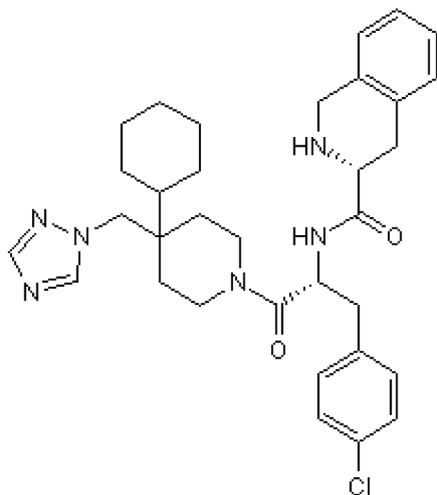
Batch Molecular Formula: C₃₃H₄₁ClN₆O₂

Batch Molecular Weight: 589.17

Physical Appearance: White lyophilised solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 10 mM

This product is supplied in lyophilized form. It may appear as a solid, gel or film and 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Mutulis et al (2004) New substituted piperazines as ligands for melanocortin receptors. Correlation to the X-ray structure of "THIQ". J.Med.Chem. **47** 4613. PMID: 15317471.

Martin et al (2002) Activation of melanocortin MC₄ receptors increases erectile activity in rats ex copula. Eur.J.Pharmacol. **454** 71. PMID: 12409007.

Sebhat et al (2002) Design and pharmacology of N-[(3R)-1,2,3,4-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 melanocorti J.Med.Chem. **45** 4589. PMID: 12361385.

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