

**Product Name:** THIQ

**Catalog No.:** 3032

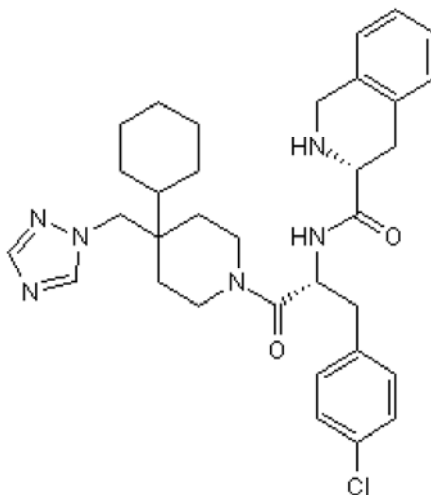
**Batch No.:** 4

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

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



## 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 95.1% purity
<b>Mass Spectrum:</b>	Consistent with structure

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

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**Description:**

Potent and selective melanocortin 4 (MC<sub>4</sub>) receptor agonist (IC<sub>50</sub> values are 1.2, 761 and 2067 nM for human MC<sub>4</sub>, MC<sub>3</sub> and MC<sub>1</sub> receptors respectively). Enhances intracavernosal pressure and stimulates erectile activity in rats ex copula following systemic administration.

**Physical and Chemical Properties:**

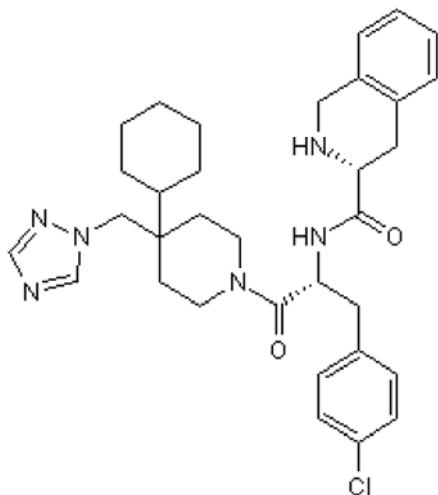
Batch Molecular Formula: C<sub>33</sub>H<sub>41</sub>ClN<sub>6</sub>O<sub>2</sub>

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 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:**

**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 MC<sub>4</sub> receptors increases erectile activity in rats ex copula. *Eur.J.Pharmacol.* **454** 71. PMID: 12409007.

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

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