



Certificate of Analysis

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Product Name: SNC 80 Catalog No.: 0764 Batch No.: 21

CAS Number: 156727-74-1

 $(+) - 4 - [(\alpha R) - \alpha - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 1 - piperazinyl) - 3 - methoxybenzyl] - N, N - diethylbenzamide - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethyl - 2 - dimethylbenzyl - ((2S, 5R) - 4 - Allyl - 2, 5 - dimethylbenzyl - ((2S, 5R) - 4 - Allyl - 2,$ **IUPAC Name:**

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{28}H_{39}N_3O_2$ **Batch Molecular Formula: Batch Molecular Weight:** 449.64

Physical Appearance: Off White solid

1eq. HCl to 100 mM with gentle warming Solubility:

DMSO to 20 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

 $R_f = 0.5$ (Dichloromethane:Methanol [9:1]) TLC:

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

 $[\alpha]_D$ = +23 (Concentration = 1, Solvent = Methanol) **Optical Rotation:**

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 74.8 8.74 9.35 Found 74.47 8.74 9.31

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



Product Information

Print Date: Mar 18th 2019

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Product Name: SNC 80 Catalog No.: 0764 Batch No.: 21

CAS Number: 156727-74-1

IUPAC Name: (+)-4- $[(\alpha R)$ - α -((2S,5R)-4-Allyl-2,5-dimethyl-1-piperazinyl)-3-methoxybenzyl]-N,N-diethylbenzamide

Description:

A highly selective and potent non-peptide δ -opioid agonist, 2000-fold selective over μ-opioid receptors.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₈H₃₉N₃O₂ Batch Molecular Weight: 449.64 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

1eq. HCl to 100 mM with gentle warming DMSO 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:

Knapp et al (1996) Structure-activity relationships for SNC80 and related compounds at cloned human delta and mu opioid receptors. J.Pharmacol.Exp.Ther. 277 1284. PMID: 8667189.

Bilsky et al (1995) SNC 80, a selective, nonpeptidic and systemically active opioid δ agonist. J.Pharmacol.Exp.Ther. 273 359. PMID: 7714789.

Calderon et al (1994) Probes for narcotic receptor mediated phenomena. 19. Synthesis of $(+)-4-[(\alpha R)-\alpha-((2S,5R)-4-allyl-2,5-dimethyl-1-allyl-2,5-dimethyl$ piperazinyl)-3-methoxybenzyl]-N,N-diethylbenzamide (SNC80): a highly selective nonpeptide σ opioid receptor agonist. J.Med.Chem. 37 2125. PMID: 8035418.