TOCRIS
a bio-techne brand

Print Date: Jan 15th 2016

Certificate of Analysis

www.tocris.com

Product Name: **SDZ NKT 343** **Catalog No.: 2394** **Batch No.: 1**

CAS Number: 180046-99-5

IUPAC Name: 1-[[(2-Nitrophenyl)amino]carbonyl]-L-prolyl-*N*-methyl-3-(2-naphthalenyl)-*N*-(phenylmethyl)-L-alaninamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{33}H_{33}N_5O_5 \cdot ¼H_2O$

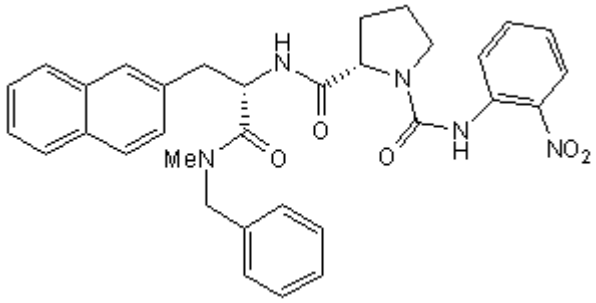
Batch Molecular Weight: 584.15

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.6 (Chloroform:Methanol [9:1])

Melting Point: Between 79 - 83°C

HPLC: Shows >98.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -59 (Concentration = 1, Solvent = methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.85	5.78	11.99
Found	67.73	5.83	11.64

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

Product Name: **SDZ NKT 343** **Catalog No.: 2394** **Batch No.: 1**

CAS Number: 180046-99-5

IUPAC Name: 1-[[(2-Nitrophenyl)amino]carbonyl]-L-prolyl-*N*-methyl-3-(2-naphthalenyl)-*N*-(phenylmethyl)-L-alaninamide

Description:

Highly selective human tachykinin NK_1 receptor antagonist (IC_{50} values are 0.62 and 451 nM for human and rat receptors respectively) that displays > 130-fold selectivity over human NK_2 and NK_3 receptors. Potently antagonizes SP-induced Ca^{2+} efflux in vitro and inhibits mechanical hyperalgesia in vivo.

Physical and Chemical Properties:

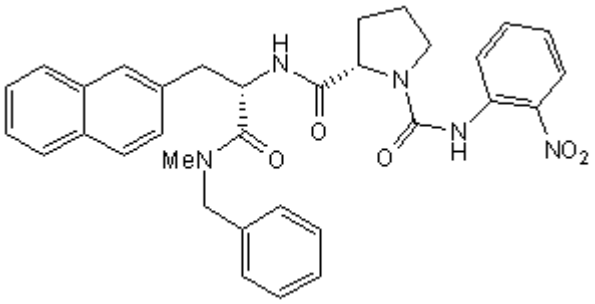
Batch Molecular Formula: $C_{33}H_{33}N_5O_5.¼H_2O$

Batch Molecular Weight: 584.15

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Walpole *et al* (1998) Comparative, general pharmacology of SDZ NKT 343, a novel, selective NK1 receptor antagonist. Br.J.Pharmacol. ***124*** 83. PMID: 9630347.

Walpole *et al* (1998) 2-Nitrophenylcarbamoyl-(*S*)-prolyl-(*S*)-3-(2-naphthyl)alanyl-*N*-benzyl-*N*-methylamide (SDZ NKT 343), a potent human NK_1 tachykinin receptor antagonist with good oral analgesic activity in chronic pain models. J.Med.Chem. ***41*** 3159. PMID: 9703462.

Campbell *et al* (1998) Selective neurokinin-1 receptor antagonists are anti-hyperalgesic in a model of neuropathic pain in the guinea-pig. Neuroscience. ***87*** 527. PMID: 9758219.