Print Date: Aug 13th 2013

Certificate of Analysis

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Product Name: NPPB **Catalog No.: 0593** **Batch No.: 3**

CAS Number: 107254-86-4

IUPAC Name: 5-Nitro-2-(3-phenylpropylamino)benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{16}N_2O_4$

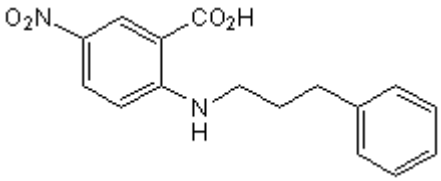
Batch Molecular Weight: 300.31

Physical Appearance: yellow solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.26 (Ethyl acetate:Acetic acid [9:1])

HPLC: Shows 99.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.99	5.37	9.33
Found	63.9	5.34	9.26

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IUPAC Name: 5-Nitro-2-(3-phenylpropylamino)benzoic acid

Description:

Inhibits calcium-sensitive chloride currents (10 µM). Putative GPR35 agonist.

Physical and Chemical Properties:

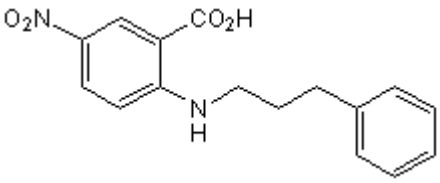
Batch Molecular Formula: $C_{16}H_{16}N_2O_4$

Batch Molecular Weight: 300.31

Physical Appearance: yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Wangemann *et al* (1986) Cl--channel blockers in the thick ascending limb of the loop of Henle. Structure-activity relationship. Pflugers Arch. ***407*** S128. PMID: 2434915.

Keeling *et al* (1991) Effects of NPPB (5-nitro-1-(3-phenylpropylamino)benzoic acid on chloride transport in intestinal tissues and the T_{84} cell line. Biochim.Biophys.Acta ***115*** 42. PMID: 1720331.

Kirkup *et al* (1996) Investigation of the effects of 5-nitro-2-(3-phenylpropylamino)-benzoic acid (NPPB) on membrane currents in rat portal vein. Br.J.Pharmacol. ***117*** 175. PMID: 8825360.

Taniguchi *et al* (2008) 5-nitro-2-(3-phenylpropylamino)benzoic acid is a GPR35 agonist Pharmacology ***82*** 245. PMID: 18818509.