

Certificate of Analysis

Print Date: Jan 15th 2016

www.tocris.com

Product Name: SB 452533 Catalog No.: 3265 Batch No.: 1

CAS Number: 459429-39-1

IUPAC Name: N-(2-Bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₂BrN₃O

Batch Molecular Weight: 376.29

Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM

ethanol to 10 mM with gentle warming

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.3$ (Ethyl acetate:Petroleum ether [9:1])

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.45 5.89 11.17 Found 57.42 5.86 11.11



Product Information

Print Date: Jan 15th 2016

www.tocris.com

Product Name: SB 452533 Catalog No.: 3265 Batch No.: 1

CAS Number: 459429-39-1

IUPAC Name: N-(2-Bromophenyl)-N'-[2-[ethyl(3-methylphenyl)amino]ethyl]-urea

Description:

Potent TRPV1 antagonist against capsaicin (pK_b = 7.7), noxious heat and acid-mediated (pIC₅₀ = 7.0) receptor activation (pK_i = 6.22 at the recombinant hTRPV1 receptor). Exhibits analgesic properties.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₂₂BrN₃O Batch Molecular Weight: 376.29 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with gentle warming

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:

Rami et al (2004) Discovery of small molecule antagonists of TRPV1. Bioorg.Med.Chem.Lett. 14 3631. PMID: 15203132.

Weil et al (2005) Conservation of functional and pharmacological properties in the distantly related temperature sensors TRPV1 and TRPM8. Mol.Pharmacol. 68 518. PMID: 15911692.

Bianchi *et al* (2007) [3H]A-778317 [1-((*R*)-5-tert-Butyl-indan-1-yl)-3-isoquinolin-5-ylurea]: a novel, stereoselective, high-affinity antagonist is a useful radioligand for the human transient receptor potential vanilloid-1 (TRPV1) receptor. J.Pharmacol.Exp.Ther. *323* 285. PMID: 17660385.