

Product Name: NDT 9513727

Catalog No.: 3333

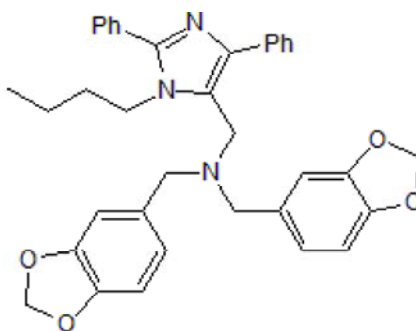
Batch No.: 2

CAS Number: 439571-48-9

IUPAC Name: *N,N*-Bis(1,3-benzodioxol-5-ylmethyl)-1-butyl-2,4-diphenyl-1*H*-Imidazole-5-methanamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₆H₃₅N₃O₄
Batch Molecular Weight: 573.68
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity
¹H NMR: consistent with structure
Mass Spectrum: consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	75.37	6.15	7.32
Found	75.4	6.16	7.39

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

Product Name: NDT 9513727

Catalog No.: 3333

2

CAS Number: 439571-48-9

IUPAC Name: *N,N*-Bis(1,3-benzodioxol-5-ylmethyl)-1-butyl-2,4-diphenyl-1*H*-Imidazole-5-methanamine

Description:

NDT 9513727 is a potent C5a receptor (C5aR) negative allosteric modulator (NAM) (IC₅₀ = 11.6 nM); selective for human C5aR (IC₅₀ values for rat and mouse C5aR are > 10 μM). Exhibits inverse agonist pharmacokinetics. Blocks degranulation response in C5a-stimulated U937 cells (IC₅₀ = 7.1 nM). Exhibits selectivity for primate and gerbil receptor over other species. Orally bioavailable.

Physical and Chemical Properties:

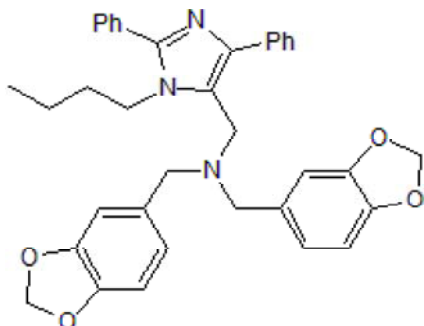
Batch Molecular Formula: C₃₆H₃₅N₃O₄

Batch Molecular Weight: 573.68

Physical Appearance: Off-white 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:

Robertson (2018) Structure of the complement C5a receptor bound to the extra-helical antagonist NDT9513727. *Nature* **553** (7686) 111. PMID: 29300009.

Brodbeck et al (2008) Identification and characterization of NDT 9513727 [N,N-bis(1,3-benzodioxol-5-ylmethyl)-1-butyl-2,4-diphenyl-1*H*-imidazole-5-methanamine], a novel, orally bioavailable C5a receptor inverse agonist. *J.Pharmacol.Exp.Ther.* **327** 898. PMID: 18753409.

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

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