

**Product Name:** NDT 9513727

**Catalog No.:** 3333

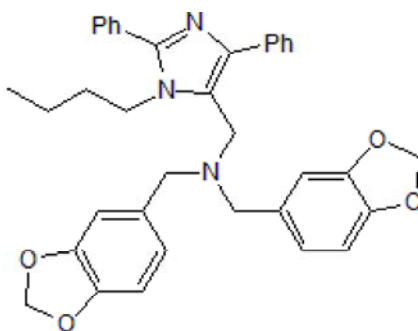
**Batch No.:** 2

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:** C<sub>36</sub>H<sub>35</sub>N<sub>3</sub>O<sub>4</sub>  
**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  
**<sup>1</sup>H 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

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**Description:**

Potent C5a receptor (C5aR) negative allosteric modulator (NAM) ( $IC_{50}$  = 11.6 nM); selective for human C5aR ( $IC_{50}$  values for rat and mouse C5aR are > 10  $\mu$ M). Exhibits inverse agonist pharmacokinetics. Blocks degranulation response in C5a-stimulated U937 cells ( $IC_{50}$  = 7.1 nM). Exhibits selectivity for primate and gerbil receptor over other species. Orally bioavailable.

**Physical and Chemical Properties:**

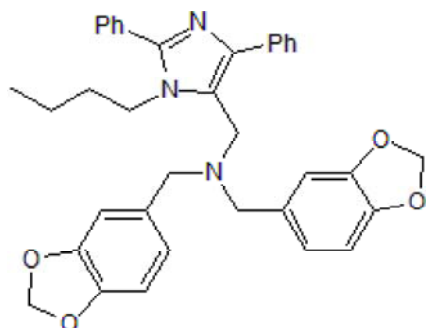
Batch Molecular Formula:  $C_{36}H_{35}N_3O_4$

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.

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