

NDT 9513727

## Chemical Properties

CAS No. : 439571-48-9

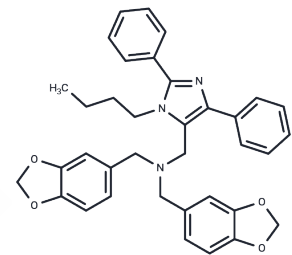
Formula: C<sub>36</sub>H<sub>35</sub>N<sub>3</sub>O<sub>4</sub>

Molecular Weight: 573.68

Storage: Store at low temperature, Keep away from direct sunlight

Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



## Biological Description

Description	NDT 9513727 is a potent, selective, and competitive C5aR1 inverse agonist used in the study of inflammatory and immune disorders.
Targets(IC50)	Complement System
In vitro	NDT 9513727 inhibited C5a-stimulated responses, including guanosine 5'-3-O-(thio) triphosphate binding, Ca <sup>2+</sup> mobilization, oxidative burst, degranulation, cell surface CD11b expression and chemotaxis in various cell types with IC <sub>50</sub> s from 1.1 to 9.2 nM, respectively[1].
In vivo	NDT 9513727 (3-30 mg/kg) effectively inhibited C5a-induced neutropenia in vivo in both gerbils and cynomolgus macaques[1].

## Solubility Information

Solubility	Ethanol: 30 mg/mL (52.29 mM), Sonication is recommended. DMSO: 80 mg/mL (139.45 mM), Sonication is recommended. ( $< 1$ mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 3.3 mg/mL (5.75 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

### Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.7431 mL	8.7157 mL	17.4313 mL
5 mM	0.3486 mL	1.7431 mL	3.4863 mL
10 mM	0.1743 mL	0.8716 mL	1.7431 mL
50 mM	0.0349 mL	0.1743 mL	0.3486 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

### Reference

Robbin M Brodbeck, et al. Identification and characterization of NDT 9513727 [N,N-bis(1,3-benzodioxol-5-ylmethyl)-1-butyl-2,4-diphenyl-1H-imidazole-5-methanamine], a novel, orally bioavailable C5a receptor inverse agonist. *J Pharmacol Exp Ther.* 2008 Dec;327(3):898-909.

Brodbeck RM, Cortright DN, Kieltyka AP, Yu J, Baltazar CO, Buck ME, Meade R, Maynard GD, Thurkauf A, Chien DS, Hutchison AJ, Krause JE. Identification and characterization of NDT 9513727 [N,N-bis(1,3-benzodioxol-5-ylmethyl)-1-butyl-2,4-diphenyl-1H-imidazole-5-methanamine], a novel, orally bioavailable C5a receptor inverse agonist. *J Pharmacol Exp Ther.* 2008 Dec;327(3):898-909. doi: 10.1124/jpet.108.141572. Epub 2008 Aug 27. PubMed PMID: 18753409.

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