# PRODUCT INFORMATION



## NDT 9513727

Item No. 24448

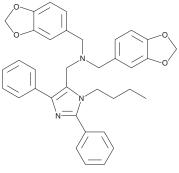
CAS Registry No.: 439571-48-9

Formal Name: N,N-bis(1,3-benzodioxol-5-ylmethyl)-1-butyl-

2,4-diphenyl-1H-imidazole-5-methanamine

MF:  $C_{36}H_{35}N_3O_4$ 

573.7 FW: **Purity:** 98% Supplied as: A solid Storage: -20°C Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

#### **Laboratory Procedures**

NDT 9513727 is supplied as a solid. A stock solution may be made by dissolving the NDT 9513727 in the solvent of choice. NDT 9513727 is soluble in organic solvents such as ethanol and DMSO, which should be purged with an inert gas, at a concentration of 100 mM.

### Description

NDT 9513727 is a competitive antagonist of the C5a receptor (C5aR;  $IC_{50}$  = 11.6 nM for human recombinant receptors) that has inverse agonist activity in a GTP $\gamma$ [35S] assay.<sup>1,2</sup> It is selective for human recombinant over rat and mouse recombinant C5aRs ( $IC_{50} = >10 \mu M$  for both) but does have activity at macaque and gerbil receptors ( $IC_{50}s = 7.3$  and 6.4 nM, respectively). NDT 9513727 inhibits degranulation in U937 cells stimulated with C5a ( $IC_{50} = 7.1$  nM). It also prevents neutropenia induced by human recombinant C5a in gerbils (ED $_{50}$  = 2.2 mg/kg) and in cynomolgus macaques when administered at doses of 5 and 25 mg/kg.<sup>2</sup>

#### References

- 1. Robertson, N., Rappas, M., Dore, A.S., et al. Structure of the complement C5a receptor bound to the extra-helical antagonist NDT9513727. Nature 553(7686), 111-114 (2018).
- 2. Broadbeck, R.M., Cortright, D., Kieltyka, A.P., 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. 327(3), 898-909 (2008).

WARNING
THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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