

Product Name: W 54011

Catalog No.: 5455

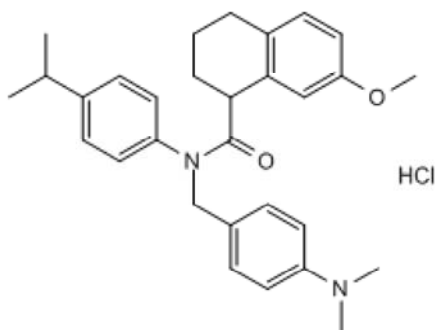
Batch No.: 1

CAS Number: 405098-33-1

IUPAC Name: *N*-[[4-(Dimethylamino)phenyl]methyl]-1,2,3,4-tetrahydro-7-methoxy-*N*-[4-(1-methylethyl)phenyl]-1-naphthalenecarboxamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₃₆N₂O₂.HCl.½H₂O
Batch Molecular Weight: 502.09
Physical Appearance: White solid
Solubility: DMSO to 50 mM
ethanol to 10 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.66 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 99% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	71.77	7.63	5.58
Found	71.66	7.94	5.43

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

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Description:

High affinity C5a receptor antagonist ($K_i = 2.2$ nM). Inhibits C5a-induced generation of reactive superoxide species, chemotaxis and intracellular Ca^{2+} mobilization in human neutrophils (IC_{50} values are 1.6, 2.7 and 3.1 nM, respectively).

Physical and Chemical Properties:

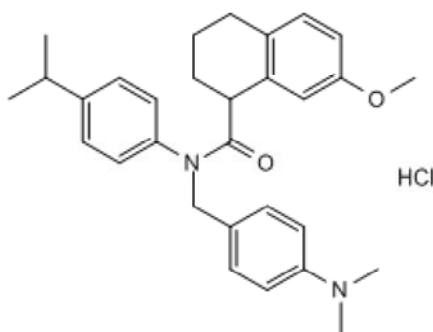
Batch Molecular Formula: $C_{30}H_{36}N_2O_2 \cdot HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 502.09

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

DMSO to 50 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 $45-60^{\circ}C$ 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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Cho et al (2014) Autocrine effects of tumor-derived complement. *Cell Rep.* **6** 1085. PMID: 24613353.

Monk et al (2007) Function, structure and therapeutic potential of complement C5a receptors. *Br.J.Pharmacol.* **152** 429. PMID: 17603557.

Sumichika et al (2002) Identification of a potent and orally active non-peptide C5a receptor antagonist. *J.Biol.Chem.* **277** 49403. PMID: 12384495 .

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