

**Product Name:** BMS 470539 dihydrochloride

**Catalog No.:** 4053

**Batch No.:** 1

CAS Number: 2341796-82-3

IUPAC Name: 1-[1-(3-Methyl-L-histidyl-O-methyl-D-tyrosyl)-4-phenyl-4-piperidiny]-1-butanone dihydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>32</sub>H<sub>41</sub>N<sub>5</sub>O<sub>4</sub>.2HCl.¼H<sub>2</sub>O

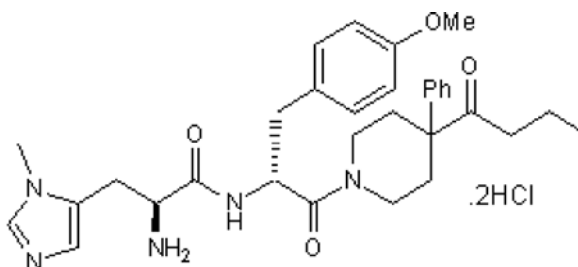
**Batch Molecular Weight:** 637.12

**Physical Appearance:** Beige solid

**Solubility:** water to 100 mM  
DMSO to 100 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.5 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.05])

**HPLC:** Shows 98.9% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	60.33	6.88	10.99
Found	60.21	6.87	10.95

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

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**Description:**

Potent, selective melanocortin MC<sub>1</sub> receptor agonist (IC<sub>50</sub> = 120 nM). Exhibits anti-inflammatory properties following ischemia-reperfusion in the vasculature. Inhibits leukocyte trafficking.

**Physical and Chemical Properties:**

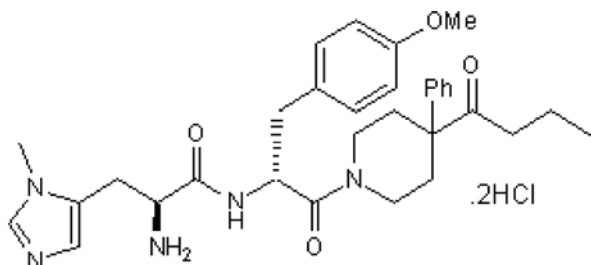
Batch Molecular Formula: C<sub>32</sub>H<sub>41</sub>N<sub>5</sub>O<sub>4</sub>.2HCl.¼H<sub>2</sub>O

Batch Molecular Weight: 637.12

Physical Appearance: Beige solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 100 mM

DMSO 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:**

**Leoni et al** (2010) The melanocortin MC<sub>1</sub> receptor agonist BMS-470539 inhibits leukocyte trafficking in the inflamed vasculature. *Br.J.Pharmacol.* **160** 171. PMID: 20331604.

**Kang** (2006) A selective small molecule agonist of the melanocortin-1 receptor inhibits lipopolysaccharide-induced cytokine accumulation and leukocyte infiltration in mice. *J.Leukoc.Biol.* **80** 897. PMID: 16888084.

**Herpin et al** (2003) Discovery of tyrosine-based potent and selective melanocortin-1 receptor small-molecule agonists with anti-inflammatory properties. *J.Med.Chem.* **46** 1123. PMID: 12646021.

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