

**Product Name:** (±)-ML 209

**Catalog No.:** 5987

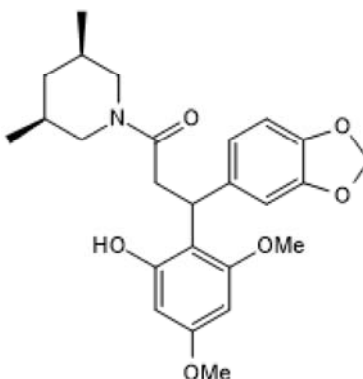
**Batch No.:** 1

CAS Number: 1334526-14-5

IUPAC Name: 3-(1,3-Benzodioxol-5-yl)-1-(cis-3,5-dimethyl-1-piperidinyl)-3-(2-hydroxy-4,6-dimethoxyphenyl)-1-propanone

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>25</sub>H<sub>31</sub>NO<sub>6</sub>  
**Batch Molecular Weight:** 441.52  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.6 (15% EtOAc in DCM)  
**HPLC:** Shows >99.4% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	68.01	7.08	3.17
Found	68.03	7.14	3.05

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**Description:**

ROR $\gamma$ t inverse agonist (IC<sub>50</sub> = 460 nM). Suppresses Th<sub>17</sub> cell differentiation and IL17A expression in vitro. Does not suppress transcription of ROR $\alpha$ . Minimal activity displayed on ER $\alpha$ , LXR $\alpha$  and thyroid hormone receptors (IC<sub>50</sub> values >4.4  $\mu$ M).

**Physical and Chemical Properties:**

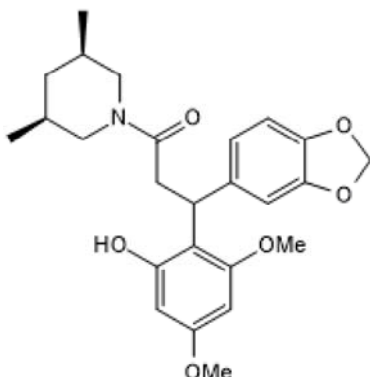
Batch Molecular Formula: C<sub>25</sub>H<sub>31</sub>NO<sub>6</sub>

Batch Molecular Weight: 441.52

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

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:**

**Huang *et al*** (2015) DDX5 and its associated lncRNA Rmrp modulate TH17 cell effector functions. *Nature* **528** 517. PMID: 26675721.

**Kojetin *et al*** (2014) REV-ERB and ROR nuclear receptors as drug targets. *Nat.Rev.Drug Discov.* **13** 197. PMID: 24577401.

**Wang *et al*** (2014) Discovery of novel *N*-(5-(arylcarbonyl)thiazol-2-yl)amides and *N*-(5-(arylcarbonyl)thiophen-2-yl)amides as potent ROR $\gamma$ t inhibitors. *Bioorg.Med.Chem.* **22** 692. PMID: 24388993.

**Huang *et al*** (2010) Identification of Potent and Selective ROR $\gamma$  Antagonists. *Probe Reports from the NIH Molecular Libraries Program.* PMID: 23658948.

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