

**Product Name:** Sumaniole maleate

**Catalog No.:** 2773

**Batch No.:** 2

CAS Number: 179386-44-8

IUPAC Name: (R)-5,6-Dihydro-5-(methylamino)-4H-imidazo[4,5,1-j]quinolin-2(1H)-one (2Z)-2-butenedioate

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>11</sub>H<sub>13</sub>N<sub>3</sub>O.C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>.

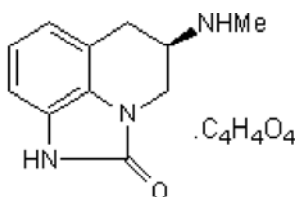
**Batch Molecular Weight:** 319.31

**Physical Appearance:** Off-white solid

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

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 98.3% purity

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

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = -26.2 (Concentration = 1, Solvent = Water)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	56.42	5.37	13.16
Found	56.36	5.28	13.05

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**Description:**

Sumanirole maleate is a high affinity D<sub>2</sub> receptor agonist (EC<sub>50</sub> values are between 17 and 75 nM in cell-based assays). Originally reported to exhibit >200-fold selectivity for the D<sub>2</sub> receptor versus other dopamine receptor subtypes (K<sub>i</sub> values are 9.0, 1940, >2190 and >7140 for D<sub>2</sub>, D<sub>3</sub>, D<sub>4</sub> and D<sub>1</sub> receptors respectively). More recently reported to be around 32-fold selective for D<sub>2</sub> over D<sub>3</sub> receptors (K<sub>i</sub> values are 17.1 and 546 nM respectively). Exhibits antiParkinsonian activity.

**Physical and Chemical Properties:**

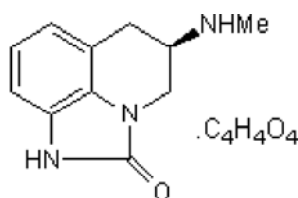
Batch Molecular Formula: C<sub>11</sub>H<sub>13</sub>N<sub>3</sub>O.C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>.

Batch Molecular Weight: 319.31

Physical Appearance: Off-white solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**References:**

**Zou et al** (2016) Novel analogues of (R)-5-(methylamino)-5,6-dihydro-4H-imidazo[4,5,1-ij]quinolin-2(1H)-one (Sumanirole) provide clues to DA D<sub>2</sub>/D<sub>3</sub> receptor agonist selectivity. *J.Med.Chem.* **59** 2973. PMID: 27035329.

**McCall et al** (2005) Sumanirole, a highly DA D<sub>2</sub>-selective receptor agonist: in vitro and in vivo pharmacological characterization and efficacy in animal models of Parkinson's disease. *J.Pharmacol.Exp.Ther.* **314** 1248. PMID: 15980060.

**Stephenson et al** (2005) The effects of a selective DA D<sub>2</sub> receptor agonist on behavioral and pathological outcome in 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine-treated squirrel monkeys. *J.Pharmacol.Exp.Ther.* **314** 1257. PMID: 15980058.

**Storage:** Store at -20°C

**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.

**Licensing Information:**

Sold for research purposes under agreement from Pfizer Inc.

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