

**Product Name:** Ro 48-8071 fumarate

**Catalog No.:** 5389

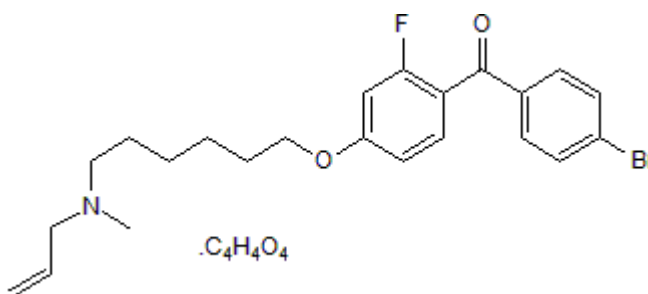
**Batch No.:** 1

CAS Number: 189197-69-1

IUPAC Name: (4-Bromophenyl)[2-fluoro-4-[[6-(methyl-2-propen-1-ylamino)hexyl]oxy]phenyl]methanone

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:**  $C_{23}H_{27}BrFNO_2 \cdot C_4H_4O_4$   
**Batch Molecular Weight:** 564.44  
**Physical Appearance:** Off White solid  
**Solubility:** water to 20 mM with gentle warming  
 DMSO to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.1% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	57.45	5.54	2.48
Found	57.6	5.47	2.62

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**Description:**

2,3-Oxidosqualene cyclase (OSC) inhibitor (IC<sub>50</sub> = 6.5 nM); blocks cholesterol synthesis in HepG2 cells. Reduces viability of breast cancer cell lines. Also inhibits Ebola virus (EBOV) cell entry (IC<sub>50</sub> = 1.74 μM).

**Physical and Chemical Properties:**

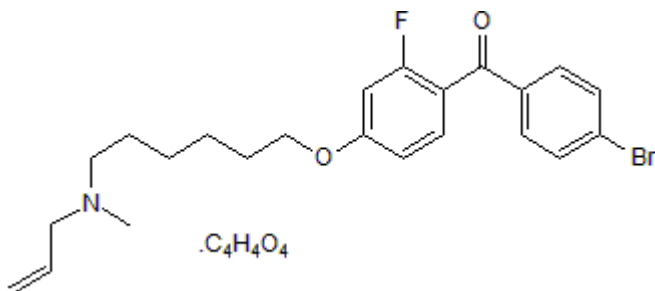
Batch Molecular Formula: C<sub>23</sub>H<sub>27</sub>BrFNO<sub>2</sub>.C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>

Batch Molecular Weight: 564.44

Physical Appearance: Off White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

water to 20 mM with gentle warming  
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:**

**Morand et al (1997)** Ro 48-8.071, a new 2,3-oxidosqualene:lanosterol cyclase inhibitor lowering plasma cholesterol in hamsters, squirrel monkeys, and minipigs: comparison to simvastatin. *J.Lipid.Res.* **38** 373. PMID: 9162756.

**Grinter et al (2011)** An inverse docking approach for identifying new potential anti-cancer targets. *J.Mol.Graph Model.* **29** 795. PMID: 21315634.

**Shoemaker et al (2013)** Multiple cationic amphiphiles induce a Niemann-Pick C phenotype and inhibit Ebola virus entry and infection. *PLoS One.* **8** e56265. PMID: 23441171.

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