

**Product Name:** BIRT 377

**Catalog No.:** 4776

**Batch No.:** 1

CAS Number: 213211-10-0

IUPAC Name: (5*R*)-5-[(4-Bromophenyl)methyl]-3-(3,5-dichlorophenyl)-1,5-dimethyl-2,4-imidazolidinedione

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>18</sub>H<sub>15</sub>BrCl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>

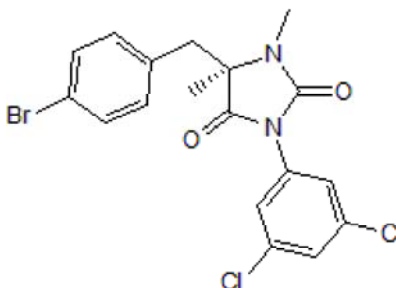
**Batch Molecular Weight:** 442.13

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.25 (Ethyl acetate:Petroleum ether [3:7])

**HPLC:** Shows 99.3% purity

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

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = +126.8 (Concentration = 1, Solvent = Ethanol)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	48.9	3.42	6.34
Found	49.16	3.43	6.31

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

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**Description:**

BIRT 377 is a potent negative allosteric modulator of LFA-1 (lymphocyte function-associated antigen-1) ( $K_d = 26$  nM). BIRT 377 binds to the I-domain of LFA-1. BIRT 377 reversibly inhibits LFA-1 mediated binding of SKW3 leukemia cells to ICAM-1. BIRT 377 inhibits superantigen (SEB)-induced IL-2 production from lymphocytes in vitro and attenuates the SEB-induced increase in IL-2 plasma levels in a mouse model in vivo. Orally available.

**Physical and Chemical Properties:**

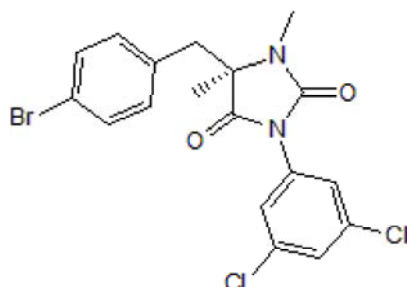
Batch Molecular Formula:  $C_{18}H_{15}BrCl_2N_2O_2$

Batch Molecular Weight: 442.13

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**References:**

**Wu et al** (2004) Second-generation lymphocyte function-associated antigen-1 inhibitors: 1*H*-imidazo[1,2- $\alpha$ ]imidazol-2-one derivatives. *J.Med.Chem.* **47** 5356. PMID: 15481974 .

**Last-Barney et al** (2001) Binding site elucidation of hydantoin-based antagonists of LFA-1 using multidisciplinary technologies: evidence for the allosteric inhibition of a protein–protein interaction. *J.Am.Chem.Soc.* **123** 5643. PMID: 11403595.

**Kelly et al** (1999) Cutting edge: a small molecule antagonist of LFA-1-mediated cell adhesion. *J.Immunol.* **163** 5173. PMID: 10553036.

**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 50 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.

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