

**Product Name:** VU 0365114

**Catalog No.:** 4404

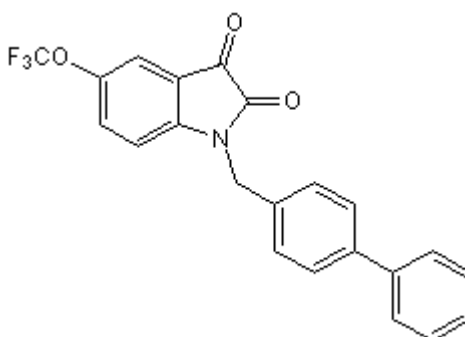
**Batch No.:** 1

**CAS Number:** 1208222-39-2

**IUPAC Name:** 1-[(1,1'-Biphenyl)-4-ylmethyl]-5-(trifluoromethoxy)-1*H*-indole-2,3-dione

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>22</sub>H<sub>14</sub>F<sub>3</sub>NO<sub>3</sub>  
**Batch Molecular Weight:** 397.35  
**Physical Appearance:** Orange solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 10 mM  
**Storage:** Store at RT  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.55 (Ethyl acetate:Petroleum ether [3:7])  
**HPLC:** Shows 98.4% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	66.5	3.55	3.53
Found	66.49	3.36	3.56

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

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**Description:**

Selective positive allosteric modulator of M<sub>5</sub> (EC<sub>50</sub> values are 2.7 μM for human M<sub>5</sub>, and >30 μM for M<sub>1</sub>, M<sub>2</sub>, M<sub>3</sub> and M<sub>4</sub> receptors).

**Physical and Chemical Properties:**

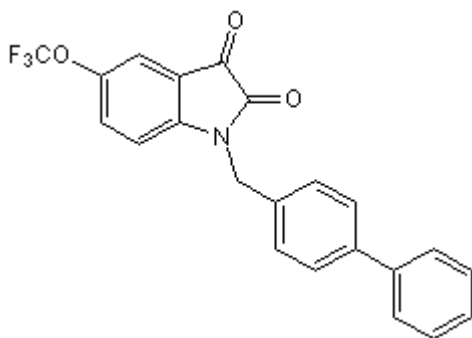
Batch Molecular Formula: C<sub>22</sub>H<sub>14</sub>F<sub>3</sub>NO<sub>3</sub>

Batch Molecular Weight: 397.35

Physical Appearance: Orange solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at RT

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 10 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:**

**Bridges et al** (2010) Chemical lead optimization of a pan G<sub>q</sub> mAChR M<sub>1</sub>, M<sub>3</sub>, M<sub>5</sub> positive allosteric modulator (PAM) lead. Part I: development of the first highly selective M<sub>5</sub> PAM. *Bioorg.Med.Chem.Lett.* **20** 558. PMID: 20004578.

**Bridges et al** (2010) Heterobiaryl and heterobiaryl ether derived M<sub>5</sub> positive allosteric modulators. *Bioorg.Med.Chem.Lett.* **20** 5617. PMID: 20801651.

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