TOCRIS
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Print Date: Jan 14th 2016

Certificate of Analysis

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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: $C_{22}H_{14}F_3NO_3$

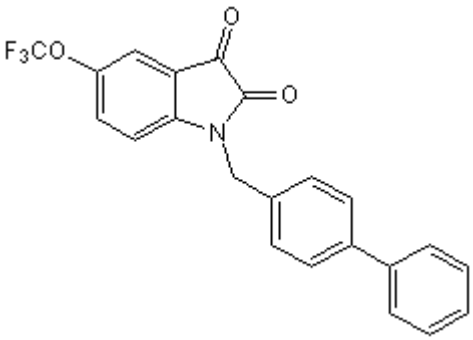
Batch Molecular Weight: 397.35

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_f = 0.55 (Ethyl acetate:Petroleum ether [3:7])

HPLC: Shows 98.4% purity

^{1}H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.5	3.55	3.53
Found	66.49	3.36	3.56

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Description:

Selective positive allosteric modulator of M_5 (EC_{50} values are 2.7 µM for human M_5, and >30 µM for M_1, M_2, M_3 and M_4 receptors).

Physical and Chemical Properties:

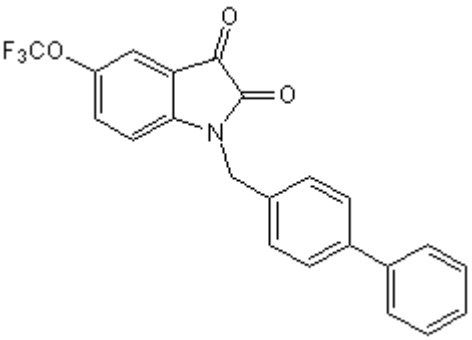
Batch Molecular Formula: $C_{22}H_{14}F_3NO_3$

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_q mAChR M_1, M_3, M_5 positive allosteric modulator (PAM) lead. Part I: development of the first highly selective M_5 PAM. Bioorg.Med.Chem.Lett. ***20*** 558. PMID: 20004578.

Bridges *et al* (2010) Heterobiaryl and heterobiaryl ether derived M_5 positive allosteric modulators. Bioorg.Med.Chem.Lett. ***20*** 5617. PMID: 20801651.

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