

**Product Name:** CYM 5520

**Catalog No.:** 5418

**Batch No.:** 1

CAS Number: 1449747-00-5

IUPAC Name: 1-[2-[2,5-Dimethyl-1-(phenylmethyl)-1*H*-pyrrol-3-yl]-2-oxoethyl]-1,6-dihydro-6-oxo-3-pyridinecarbonitrile

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>·¼H<sub>2</sub>O

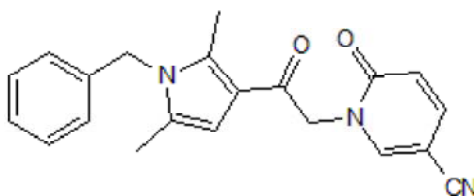
**Batch Molecular Weight:** 349.89

**Physical Appearance:** Beige solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.48 (Dichloromethane:Methanol [98:2])

**HPLC:** Shows 99.5% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	72.09	5.62	12.01
Found	72.05	5.45	11.99

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

**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel: +1 612 379 2956

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**Description:**

Selective S1P<sub>2</sub> allosteric agonist (EC<sub>50</sub> = 0.48 μM). Selective for S1P<sub>2</sub> receptors over a panel of 29 other receptors and transporters.

**Physical and Chemical Properties:**

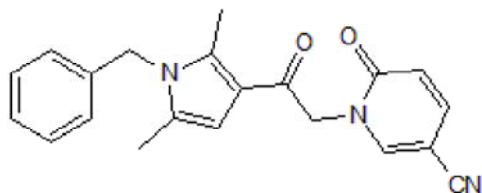
Batch Molecular Formula: C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>·½H<sub>2</sub>O

Batch Molecular Weight: 349.89

Physical Appearance: Beige solid

**Minimum Purity:** ≥99%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

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:**

Satsu *et al* (2013) A sphingosine 1-phosphate receptor 2 selective allosteric agonist. *Bioorg.Med.Chem.* **21** 5373. PMID: 23849205.

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Tel:+1 612 379 2956