

Certificate of Analysis

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Product Name: CMPD101

Catalog No.: 5642

Batch No.: 3

CAS Number: 865608-11-3

IUPAC Name: 3-[[[4-Methyl-5-(4-pyridinyl)-4H-1,2,4-triazol-3-yl]methyl]amino]-N-[[2-(trifluoromethyl)phenyl]methyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₁F₃N₆O.¼H₂O

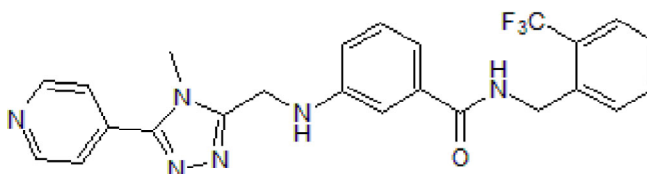
Batch Molecular Weight: 470.96

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.21	4.6	17.84
Found	60.47	4.69	17.59

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

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Description:

CMPD101 is a potent and selective GRK2/3 inhibitor (IC₅₀ values are 32 and 54 nM for GRK3 and GRK2, respectively). Exhibits selectivity for GRK2/3 over GRK1/5. Reduces DAMGO-induced desensitization and internalization of μ -opioid receptors.

Physical and Chemical Properties:

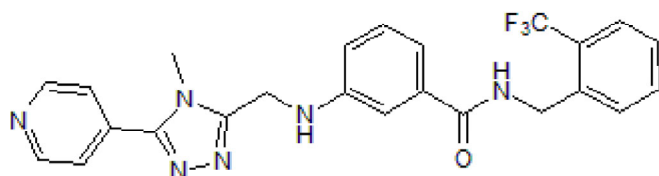
Batch Molecular Formula: C₂₄H₂₁F₃N₆O.¼H₂O

Batch Molecular Weight: 470.96

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Okawa *et al* (2017) Design, synthesis, and evaluation of the highly selective and potent G-protein-coupled receptor kinase 2 (GRK2) inhibitor for the potential treatment of heart failure. *J.Med.Chem.* **60** 6942. PMID: 28699740.

Lowe *et al* (2015) Role of G protein-coupled receptor kinases 2 and 3 in μ -opioid receptor desensitization and internalization. *Mol.Pharmacol.* **88** 347. PMID: 26013542.

Thal *et al* (2011) Molecular mechanism of selectivity among G protein-coupled receptor kinase 2 inhibitors. *Mol.Pharmacol.* **80** 294. PMID: 21596927.

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