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# DATASHEET

Cmpd101

## Product overview

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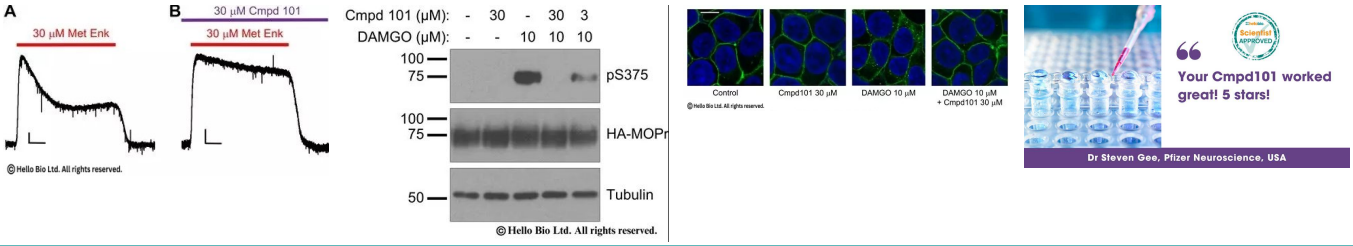
| **Name** | Cmpd101 |
| **Cat No** | HB2840 |
| **Alternative names** | Compound 101; Takeda compound 101 |
| **Biological action** | Inhibitor |
| **Purity** | >98% |
| **Customer comments** | *We would recommend Cmpd 101 from Hello Bio – it performs exactly as expected in assays looking at MOPr desensitisation, phosphorylation and internalisation.* **Dr Chris Bailey, University of Bath, UK and author on Mol Pharmacol paper, PubMed ID 26013542**<br><br>*Your Cmpd101 – worked great!* **Dr Steven Gee, Pfizer Neuroscience, USA**<br><br>*Your Cmpd101 behaved as expected.* **Verified customer, Monash University** |
| **Description** | Novel, potent and selective GRK2/GRK3 inhibitor |

## Images




## Biological Data

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| **Biological description** | Cmpd101 (Compound 101) is a novel, potent and selective G-protein coupled receptor kinase 2 and 3 (GRK2/GRK3) inhibitor ($IC_{50}$ values are 35 and 32 nM at GRK2 and GRK3 respectively).<br><br>Shows no activity at GRK5 at concentrations up to 125 µM and shows little activity at a broad range of other kinases.<br><br>Membrane permeable.<br><br>Cmpd101 can be used to study roles of GRK2/3 in GPCR desensitization and other functions.<br><br>Shown to potentiate phosphatidylinositol 4,5-bisphosphate (PIP2) depletion and slow agonist-induced desensitization of protease-activated receptor 2 (PAR2). |

## Solubility & Handling

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| **Storage instructions** | -20°C |

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| **Solubility overview** | Soluble in DMSO (100mM) |
| **Handling** | Hydroscopic solid, contact with air may cause material to become sticky. Product performance should not be affected but we recommend storing the material in a sealed jar. |
| **Important** | This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use. |

## Chemical Data

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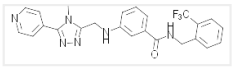
| **Chemical name** | 3-[(4-methyl-5-pyridin-4-yl-1,2,4-triazol-3-yl)methylamino]-N-[[2-(trifluoromethyl)phenyl]methyl]benzamide hydrochloride |
| **Molecular Weight** | 502.92 |
| **Chemical structure** |  |
| **Molecular Formula** | $C_{24}H_{21}N_6OF_3.HCl$ |
| **CAS Number** | 865608-11-3 |
| **PubChem identifier** | 11677079 |
| **SMILES** | CN1C(=NN=C1C2=CC=NC=C2)CNC3=CC=CC(=C3)C(=O)NCC4=CC=CC=C4C(F)(F)F |
| **Source** | Synthetic |
| **InChi** | InChI=1S/C24H21F3N6O/c1-33-21(31-32-22(33)16-9-11-28-12-10-16)15-29-19-7-4-6-17(13-19)23(34)30-14-18-5-2-3-8-20(18)24(25,26)27/h2-13,29H,14-15H2,1H3,(H,30,34) |
| **InChiKey** | WFOVEDJTASPCIR-UHFFFAOYSA-N |
| **Appearance** | Yellow solid |

## References


**Molecular mechanism of selectivity among G protein-coupled receptor kinase 2 inhibitors.**

Thal et al (2011) Mol Pharmacol 80
**PubMedID** 21596927

**Role of G Protein-Coupled Receptor Kinases 2 and 3 in μ-Opioid Receptor Desensitization and Internalization.**

Lowe et al (2015) Mol Pharmacol 88(2)
**PubMedID** 26013542

**Contributions of protein kinases and β-arrestin to termination of protease-activated receptor 2 signaling.**

Jung et al (2016) J Gen Physiol 147(3)
**PubMedID** 26927499

**Distinct cortical and striatal actions of a β-arrestin-biased D2 receptor ligand reveal unique antipsychotic-like properties.**

Urs et al (2016) Proc Natl Acad Sci U S A 113(50)
**PubMedID** 27911814

**Agonist-selective recruitment of engineered protein probes and of GRK2 by opioid receptors in living cells**

Stoeber et al (2019) bioRxiv https://doi.org/10.1101/866780