Hello Bio, Inc.
304 Wall St., Princeton, NJ 08540 USA

T. 609-683-7500
F. 609-228-4994

customercare-usa@m2stage.hellobio.com

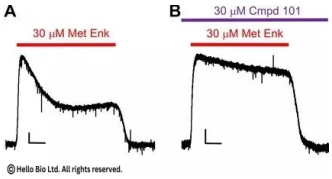
DATASHEET

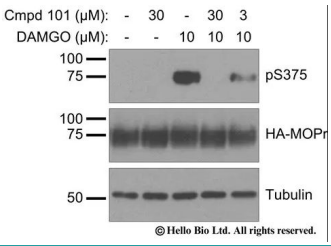
Cmpd101

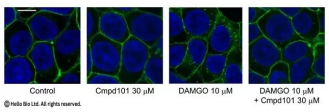
Product overview

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** *Your Cmpd101 – worked great!* **Dr Steven Gee, Pfizer Neuroscience, USA** *Your Cmpd101 behaved as expected.* **Verified customer, Monash University**
Description	Novel, potent and selective GRK2/GRK3 inhibitor

Images







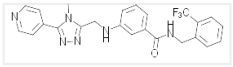
Biological Data

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). Shows no activity at GRK5 at concentrations up to 125 µM and shows little activity at a broad range of other kinases. Membrane permeable. Cmpd101 can be used to study roles of GRK2/3 in GPCR desensitization and other functions. Shown to potentiate phosphatidylinositol 4,5-bisphosphate (PIP2) depletion and slow agonist-induced desensitization of protease-activated receptor 2 (PAR2).

Solubility & Handling

Storage instructions	-20°C
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

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