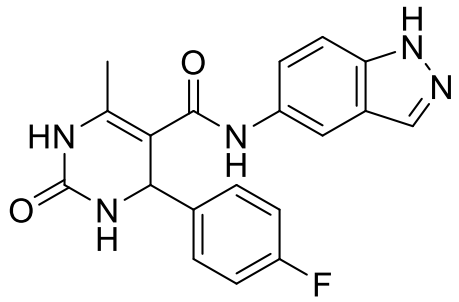
Product data sheet

MedKoo Cat#: 522708 Name: GSK180736A CAS: 817194-38-0 Chemical Formula: $C_{19}H_{16}FN_5O_2$ Exact Mass: 365.1288 Molecular Weight: 365.3684	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
GSK180736A is potent and selective inhibitor of GRK2 with an IC50 of 0.77 μM25 and >100-fold selectivity over other GRKs. It is a weak inhibitor of PKA with an IC50 of 30 μM, but highly potent against ROCK1 (IC50 = 100 nM).

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	57.67	157.83
Ethanol	3.0	8.21

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.74 mL	13.69 mL	27.37 mL
5 mM	0.55 mL	2.74 mL	5.47 mL
10 mM	0.27 mL	1.37 mL	2.74 mL
50 mM	0.05 mL	0.27 mL	0.55 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Bouley R, Waldschmidt HV, Cato MC, Cannavo A, Song J, Cheung JY, Yao XQ, Koch WJ, Larsen SD, Tesmer JJG. Structural Determinants Influencing the Potency and Selectivity of Indazole-Paroxetine Hybrid G Protein-Coupled Receptor Kinase 2 Inhibitors. Mol Pharmacol. 2017 Dec;92(6):707-717. doi: 10.1124/mol.117.110130. Epub 2017 Oct 25. PMID: 29070696; PMCID: PMC5691592.
2. Waldschmidt HV, Homan KT, Cruz-Rodríguez O, Cato MC, Waninger-Saroni J, Larimore KM, Cannavo A, Song J, Cheung JY, Kirchhoff PD, Koch WJ, Tesmer JJ, Larsen SD. Structure-Based Design, Synthesis, and Biological Evaluation of Highly Selective and Potent G Protein-Coupled Receptor Kinase 2 Inhibitors. J Med Chem. 2016 Apr 28;59(8):3793-807. doi: 10.1021/acs.jmedchem.5b02000. Epub 2016 Apr 13. PMID: 27050625; PMCID: PMC4890168.

In vivo study

1. Bouley RA, Weinberg ZY, Waldschmidt HV, Yen YC, Larsen SD, Puthenveedu MA, Tesmer JJG. A New Paroxetine-Based GRK2 Inhibitor Reduces Internalization of the μ-Opioid Receptor. Mol Pharmacol. 2020 Jun;97(6):392-401. doi: 10.1124/mol.119.118661. Epub 2020 Mar 31. PMID: 32234810; PMCID: PMC7237867.

7. Bioactivity
Biological target:

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GSK180736A is potent Rho-associated coiled-coil kinase 1 (ROCK1) inhibitor with an IC50 of 100 nM. GSK180736A is also a selective and ATP-competitive G protein-coupled receptor kinase 2 (GRK2) inhibitor with an IC50 of 0.77 μM.

In vitro activity

GSK180736A, developed as a Rho-associated coiled-coil kinase 1 (ROCK1) inhibitor, was identified as an inhibitor of GRK2 and co-crystallized in the active site.

Reference: J Med Chem. 2016 Apr 28;59(8):3793-807. https://pubmed.ncbi.nlm.nih.gov/27050625/

In vivo activity

A new inhibitor, CCG258747, which is based on paroxetine, demonstrates increased potency against the GRK2 subfamily and favorable pharmacokinetic parameters in mice.

Reference: Mol Pharmacol. 2020 Jun;97(6):392-401. https://pubmed.ncbi.nlm.nih.gov/32234810/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.