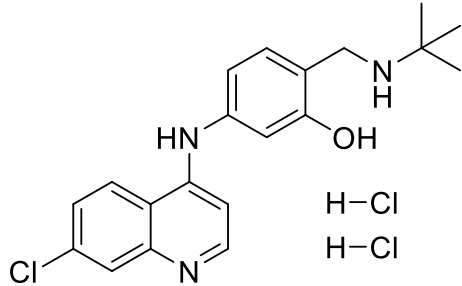


Product data sheet



MedKoo Cat#: 530320 Name: GSK369796 Dihydrochloride CAS: 1010411-21-8 (HCl) Chemical Formula: C ₂₀ H ₂₄ Cl ₃ N ₃ O Molecular Weight: 428.782	
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:

GSK369796, also known as N-tert-butylisoquine, is an anti-malaria drug candidate. GSK369796 was rationally designed based on chemical, toxicological, pharmacokinetic, and pharmacodynamic considerations and was selected based on excellent activity against Plasmodium falciparum in vitro and rodent malaria parasites in vivo.

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	100.0	233.22
Water	50.0	116.61

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.33 mL	11.66 mL	23.32 mL
5 mM	0.47 mL	2.33 mL	4.66 mL
10 mM	0.23 mL	1.17 mL	2.33 mL
50 mM	0.05 mL	0.23 mL	0.47 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. O'Neill PM, Shone AE, Stanford D, Nixon G, Asadollahy E, Park BK, Maggs JL, Roberts P, Stocks PA, Biagini G, Bray PG, Davies J, Berry N, Hall C, Rimmer K, Winstanley PA, Hindley S, Bambal RB, Davis CB, Bates M, Gresham SL, Brigandi RA, Gomez-de-Las-Heras FM, Gargallo DV, Parapini S, Vivas L, Lander H, Taramelli D, Ward SA. Synthesis, antimalarial activity, and preclinical pharmacology of a novel series of 4'-fluoro and 4'-chloro analogues of amodiaquine. Identification of a suitable "back-up" compound for N-tert-butyl isoquine. J Med Chem. 2009 Apr 9;52(7):1828-44. doi: 10.1021/jm8012757. PMID: 19284751.

In vivo study

1. O'Neill PM, Shone AE, Stanford D, Nixon G, Asadollahy E, Park BK, Maggs JL, Roberts P, Stocks PA, Biagini G, Bray PG, Davies J, Berry N, Hall C, Rimmer K, Winstanley PA, Hindley S, Bambal RB, Davis CB, Bates M, Gresham SL, Brigandi RA, Gomez-de-Las-Heras FM, Gargallo DV, Parapini S, Vivas L, Lander H, Taramelli D, Ward SA. Synthesis, antimalarial activity, and preclinical pharmacology of a novel series of 4'-fluoro and 4'-chloro analogues of amodiaquine. Identification of a suitable "back-up" compound for N-tert-butyl isoquine. J Med Chem. 2009 Apr 9;52(7):1828-44. doi: 10.1021/jm8012757. PMID: 19284751.

7. Bioactivity

Biological target:

Product data sheet



GSK369796 Dihydrochloride is an affordable and effective antimalarial and inhibits hERG potassium ion channel repolarization with an IC_{50} of 7.5 μ M.

In vitro activity

It is also clear that N-tert-butyl analogue 2k (GSK369796 Dihydrochloride) is potent against chloroquine resistant strains, though it is not quite as active as amodiaquine against both chloroquine-sensitive and resistant parasites. On the basis of the activity presented in Table 4, 2k was selected alongside its direct 4-chloro analogue for further studies in the mouse model of malaria.

Reference: J Med Chem. 2009 Apr 9;52(7):1828-44. <https://pubmed.ncbi.nlm.nih.gov/19284751/>

In vivo activity

The therapeutic efficacy of 2k (GSK369796 Dihydrochloride), 3k, and selected 4-aminoquinolines was evaluated in a standard "4-day test" in CD1 mice infected intravenously with the murine pathogen P berghei ANKA at GSK, Tres Cantos, Spain (Table 5). Isoquine (1d) showed in vivo therapeutic efficacy against Plasmodium berghei ANKA with ED50 and ED90 in the same range as that of amodiaquine. Analogue 2k was also potent in this in vivo assay with an ED50 value of 5.3 mg/kg, whereas chloro analogue 3k was less potent with an ED50 of 13.4 mg/kg.

Reference: J Med Chem. 2009 Apr 9;52(7):1828-44. <https://pubmed.ncbi.nlm.nih.gov/19284751/>

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.