

Product data sheet



MedKoo Cat#: 318598 Name: Quetiapine hemifumarate CAS#: 111974-72-2 (hemifumarate) Chemical Formula: C ₂₁ H ₂₅ N ₃ O ₂ S*0.5C ₄ H ₄ O ₄ Exact Mass: TBD Molecular Weight: 441.5		
Product supplied as:	Powder	
Purity (by HPLC):	≥ 98%	
Shipping conditions	Ambient temperature	
Storage conditions:	Powder: -20°C > 4 years	
	In solvent: -80°C 3 months; -20°C 2 weeks.	

1. Product description:

Quetiapine hemifumarate is a synthetic salt that has been used as an antagonist for β -arrestin 2 mutant T205M recruitment.

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	22.08	50

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.2648 mL	11.3240 mL	22.6480 mL
5 mM	0.45 mL	2.26 mL	4.53 mL
10 mM	0.2265 mL	1.1324 mL	2.2648 mL
50 mM	0.05	0.23	0.45

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

- Bai O, Wei Z, Lu W, Bowen R, Keegan D, Li XM. Protective effects of atypical antipsychotic drugs on PC12 cells after serum withdrawal. *J Neurosci Res*. 2002 Jul 15;69(2):278-83. doi: 10.1002/jnr.10290. PMID: 12111809.

In vivo study

- Gahr M, Kölle MA, Freudenmann RW, Schönfeldt-Lecuona C. Aseptic gingivitis related to quetiapine hemifumarate. *Pharmacopsychiatry*. 2013 Jan;46(1):39-40. doi: 10.1055/s-0032-1321906. Epub 2012 Aug 22. PMID: 22915485.
- Cross AJ, Widzowski D, Maciag C, Zacco A, Hudzik T, Liu J, Nyberg S, Wood MW. Quetiapine and its metabolite norquetiapine: translation from in vitro pharmacology to in vivo efficacy in rodent models. *Br J Pharmacol*. 2016 Jan;173(1):155-66. doi: 10.1111/bph.13346. Epub 2015 Dec 1. PMID: 26436896; PMCID: PMC4813385.

7. Bioactivity

Biological target:

Quetiapine hemifumarate is a dopamine receptor antagonist with a pIC₅₀ of 6.33 for human D2 receptor. It has moderate to high affinity for the human D2, HT1A, 5-HT2A, 5-HT2C receptor with pK_is of 7.25, 5.74, 7.54, 5.55.

In vitro activity

Using PC12 cell cultures and the MTT assay for cell viability found that the atypical antipsychotics clozapine, quetiapine, and risperidone may exert a neuroprotective function after serum withdrawal through the modulation of SOD1 and p75NTR expression. They also found that 1) the atypical antipsychotics (clozapine, quetiapine, and risperidone) can protect PC12 cells from death after serum withdrawal and 2) these drugs up-regulated the SOD1 gene expression to more than 120% and also down-regulated p75NTR mRNA levels to less than 65% of their respective control values.

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Reference: J Neurosci Res. 2002 Jul 15;69(2):278-83. <https://pubmed.ncbi.nlm.nih.gov/12111809/>

In vivo activity

Quetiapine significantly reduced depressive-like behaviors induced by chronic mild stress in adult rats. MPO activity and IL-6 levels increased in the serum of animals submitted to CMS. Quetiapine significantly reduced MPO activity and IL-6 levels. These results corroborate other evidence, indicating that chronic stress is a relevant phenomenon in the etiology of depression and suggesting that quetiapine induces an antidepressant effect because it reduces oxidative and inflammatory mechanisms.

Reference: Naunyn Schmiedebergs Arch Pharmacol. 2023 Feb 3. <https://pubmed.ncbi.nlm.nih.gov/36735044/>

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.