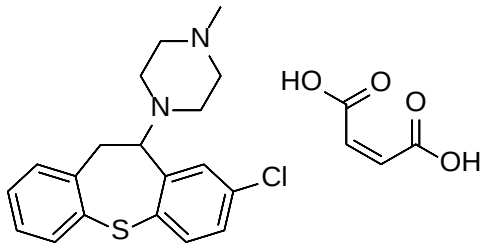
Product data sheet

MedKoo Cat#: 574828 Name: Octoclothepin maleate salt CAS: 4789-68-8 Chemical Formula: $C_{23}H_{25}ClN_2O_4S$ Exact Mass: 460.1224 Molecular Weight: 460.973	
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:
Octoclothepin maleate salt is a D2 dopamine receptor antagonist and 5-HT2 serotonin receptor antagonist.

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
TBD	TBD	TBD

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.17 mL	10.85 mL	21.69 mL
5 mM	0.43 mL	2.17 mL	4.34 mL
10 mM	0.22 mL	1.09 mL	2.17 mL
50 mM	0.04 mL	0.22 mL	0.43 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. Nisa S, Blokpoel MC, Robertson BD, Tyndall JD, Lun S, Bishai WR, O'Toole R. Targeting the chromosome partitioning protein ParA in tuberculosis drug discovery. J Antimicrob Chemother. 2010 Nov;65(11):2347-58. doi: 10.1093/jac/dkq311. Epub 2010 Sep 1. PMID: 20810423; PMCID: PMC2980951.

In vivo study

1. Metysová J, Metys J, Dlabac A, Kazdová E, Valchár M. Pharmacological properties of a potent neuroleptic drug octoclothepin. Acta Biol Med Ger. 1980;39(6):723-40. PMID: 6893891.

7. Bioactivity
Biological target:

Octoclothepin maleate salt is a D2 dopamine receptor antagonist and 5-HT2 serotonin receptor antagonist.

In vitro activity

Two compounds identified from library screening, phenoxybenzamine and octoclothepin, also inhibited the in vitro ATPase activity of ParA from M. tuberculosis. Structural in silico analyses predict that phenoxybenzamine and octoclothepin undergo interactions compatible with the active site of ParA. Octoclothepin exhibited significant bacteriostatic activity towards M. tuberculosis.

Reference: J Antimicrob Chemother. 2010 Nov;65(11):2347-58. https://pubmed.ncbi.nlm.nih.gov/20810423/

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In vivo activity

Octoclothepin possesses high cataleptogenic and anti-apomorphine activities in rats; it is able to exert full protection against apomorphine-induced emesis in dogs after the dose of 0.1 mg kg-1 s.c. Octoclothepin reduces some actions and toxicity of d,l-amphetamine and phenmetrazine in rodents. In the rat corpus striatum, octoclothepin in doses of 0.5 and d1.5 mg kg-1 s.c. reduces the DA level and raises the HVA and DOPAC levels significantly.

Reference: Acta Biol Med Ger. 1980;39(6):723-40. https://pubmed.ncbi.nlm.nih.gov/6893891/