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# DATASHEET

Deschloroclozapine dihydrochloride (DCZ) (water soluble)

## Product overview

| | |
|---|---|
| **Name** | Deschloroclozapine dihydrochloride (DCZ) (water soluble) |
| **Cat No** | HB9126 |
| **Alternative names** | DCZ |
| **Biological action** | Agonist |
| **Purity** | >99% |
| **Description** | Potent, selective and metabolically stable hM3Dq and hM4Di muscarinic DREADD actuator. Water soluble. |

## Images


## Biological Data

**Biological description**

**Overview**

Deschloroclozapine (DCZ) is reported to be a potent, selective and highly brain-penetrable muscarinic hM3Dq and hM4Di DREADD actuator with minimal off-target actions ($K_i$ = 6.3 and 4.2 nM at hM3Dq and hM4Di respectively) and ($EC_{50}$ values are 0.13 and 0.081 nM at hM3Dq and hM4Di respectively in a BRET-based assay.

It represents a potent, selective, metabolically stable and fast acting DREADD agonist with utility in both mice and non-human primates for a variety of applications.

It shows 100-fold improved affinity and greater agonist potency for hM3Dq and hM4Di compared to Clozapine n-Oxide (CNO) or DREADD agonist 21 (C21) with reduced off-target binding compared with clozapine in vitro.It has lower affinity at $D_1$, $D_2$ and 5-$HT_{2A}$ and 5-$HT_{2C}$ receptors compared with clozapine.

PET studies demonstrate the compound is rapidly brain penetrable, is apparently selective and doses for DREADD occupancy are 20-fold and 60-fold lower than CNO or DREADD agonist 21 (C21) respectively.

**Uses and applications**

Systemic delivery of low doses of DCZ (1 or 3 µg/kg) were shown to enhance neuronal activity via hM3Dq in mice and monkeys within minutes.

Intramuscular doses of 100 µg/kg reversibly induced spatial working memory deficits in hM4Di expressing monkeys.

Deschloroclozapine freebase also available.

## Solubility & Handling

**Storage instructions** -20°C
**Solubility overview** Soluble in water (100 mM). Always store solutions at -20°C.
**Handling**

Storage of solid

- Store at -20°C.
- Please note that the compound is a hydroscopic solid and 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.

Storage of solutions

- Make up solutions and use immediately.
- If storage of solutions is required, you should aliquot out the solution into tightly sealed vials and store at -20°C and store these for up to one month.
- Allow the product to equilibrate to RT for at least one hour before opening and using.

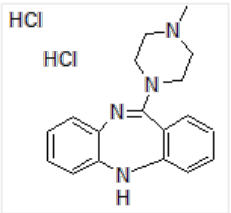
Storage of solutions at room temperature

- We recommend only keeping solutions at room temperature (25°C) for a few days as our studies have shown that after 96 hours the purity of the compound in solution drops to ~97% and will continue to drop over time.

**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** 6-(4-methylpiperazin-1-yl)-11H-benzo[b][1,4]benzodiazepine dihydrochloride
**Molecular Weight** 365.3
**Chemical structure**




**Molecular Formula** $C_{18}H_{20}N_4.2HCl$
**CAS Number** 1977-07-7 (free base)
**SMILES** Cl.Cl.CN1CCN(CC1)C2=Nc4ccccc4Nc3ccccc23
**Source** Synthetic
**InChi** InChI=1S/C18H20N4.2ClH/c1-21-10-12-22(13-11-21)18-14-6-2-3-7-15(14)19-16-8-4-5-9-17(16)20-18;;/h2-9,19H,10-13H2,1H3;2*1H
**InChiKey** ZMDCCOPUWCVMFM-UHFFFAOYSA-N
**Appearance** Yellow solid

## References


**Deschloroclozapine, a potent and selective chemogenetic actuator enables rapid neuronal and behavioral modulations in mice and monkeys**

Nagai et al (2020) Nature Neuroscience 1157-1167
**PubMedID** 32632286

**Binding of 5H-dibenzo[b,e][1,4]diazepine and chiral 5H-dibenzo[a,d]cycloheptene analogues of clozapine to dopamine and serotonin receptors.**

Phillips et al (1994) J Med Chem 37(17)
**PubMedID** 8064797