# Data Sheet

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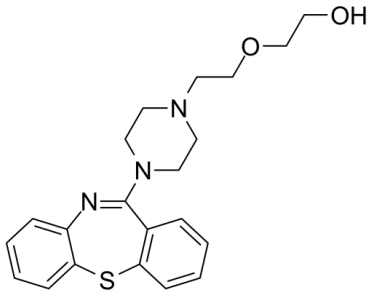
| **Product Name:** | Quetiapine |
| **Cat. No.:** | CS-1171 |
| **CAS No.:** | 111974-69-7 |
| **Molecular Formula:** | C21H25N3O2S |
| **Molecular Weight:** | 383.51 |
| **Target:** | 5-HT Receptor; Dopamine Receptor |
| **Pathway:** | GPCR/G Protein; Neuronal Signaling |
| **Solubility:** | H2O : < 0.1 mg/mL (insoluble) |




## BIOLOGICAL ACTIVITY:

Quetiapine is a **5-HT receptors** agonist with a **$pEC_{50}$** of 4.77 for human 5-HT1A receptor. Quetiapine is a **dopamine receptor** antagonist with a **$pIC_{50}$** of 6.33 for human D2 receptor. Quetiapine has moderate to high affinity for the human **D2**, **HT1A**, **5-HT2A**, **5-HT2C receptor** with **$pK_i$**s of 7.25, 5.74, 7.54, 5.55. Antidepressant and anxiolytic effects[1]. IC50 & Target: 5-HT Receptor[1]. **In Vitro:** Quetiapine (ICI204636) is indicated for the treatment of schizophrenia as well as for the treatment of acute manic episodes associated with bipolar I disorder. The antipsychotic effect of quetiapine is thought by some to be mediated through antagonist activity at dopamine and serotonin receptors. Specifically the D1 and D2 dopamine, the alpha 1 adrenoreceptor and alpha 2 adrenoreceptor, and 5-HT1A and 5-HT2 serotonin receptor subtypes are antagonized. Quetiapine (ICI204636) also has an antagonistic effect on the histamine H1 receptor.

## References:

[1]. Cross AJ, et al. 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.

## CAIndexNames:

Ethanol, 2-[2-(4-dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]-

## SMILES:

OCCOCCN(CC1)CCN1C2=NC3=CC=CC=C3SC4=C2C=CC=C4

**Caution: Product has not been fully validated for medical applications. For research use only.**

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