# Data Sheet

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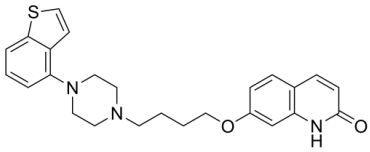
| **Product Name:** | Brexpiprazole |
| **Cat. No.:** | CS-2108 |
| **CAS No.:** | 913611-97-9 |
| **Molecular Formula:** | $C_{25}H_{27}N_3O_2S$ |
| **Molecular Weight:** | 433.57 |
| **Target:** | 5-HT Receptor; Adrenergic Receptor; Dopamine Receptor |
| **Pathway:** | GPCR/G Protein; Neuronal Signaling |
| **Solubility:** | DMSO : 25 mg/mL (ultrasonic;warming;heat to 80°C) |



## BIOLOGICAL ACTIVITY:

Brexpiprazole (OPC-34712), an atypical orally active antipsychotic drug, is a partial agonist of human **5-HT1A** and **dopamine $D_{2L}$ receptor** with **$K_i$**s of 0.12 nM and 0.3 nM, respectively. Brexpiprazole is also a **5-HT2A** receptor antagonist with a **$K_i$** of 0.47 nM. Brexpiprazole also shows potent antagonist activity at human noradrenergic $\alpha_{1B}$ ($K_i$=0.17 nM) and $\alpha_{2C}$ receptors ($K_i$=0.59 nM)[1][2]. IC50 & Target: Ki: 0.12 nM (5-HT1A), 0.3 nM (D2L), 0.47 nM (5-HT2A)[1] ***In Vitro:*** Brexpiprazole (0-1.0 μM, 4 days) potentiates NGF-induced neurite outgrowth in a dose-dependent manner in PC12 cells[1]. ***In Vivo:*** Brexpiprazole (0-0.1 mg/kg; p.o.; once) improves social recognition deficits in mice[2].

## PROTOCOL (Extracted from published papers and Only for reference)

**Cell Assay:** Brexpiprazole is dissolved in DMSO and stored, and then diluted with appropriate medium before use[1].[1]PC12 cells are cultured at 37°C, 5% $CO_2$ in Dulbecco's modified Eagle's medium (DMEM), supplemented with 5% heat-inactivated fetal bovine serum (FBS),10% heat-inactivated horse serum, and 1% penicillin-streptomycin. Medium is changed two to three times a week. PC12 cells are plated onto 24- well tissue culture plates coated with poly-D-lysine/laminin. Cells are plated at relatively low density ($0.25\times10^4$ cells/$cm^2$) in DMEM medium containing 0.5% FBS,1% penicillin-streptomyc in Medium containing a minimal level of serum (0.5% FBS) is used. In this study, 2.5 ng/mL of NGF is used to study the potentiating effects of Brexpiprazole on neurite outgrowth. Twenty-four hours after plating, the medium is replaced with DMEM medium containing 0.5% FBS and 1% penicillin-streptomycin with NGF (2.5 ng/mL), with or without Brexpiprazole (0.001,0.01,0.1 or 1 μM), WAY-100,635 (5-HT1A receptor antagonist;10 μM), raclopride (dopamine D2 receptor antagonist;10 μM), DOI (5-HT2A receptor agonist;0.1,1 or 10 μM), M100,907 (5-HT2A receptor antagonist; 0.1, 1 or 10 μM), xestospongin C (IP3 receptor antagonist; 1 μM), 2-APB (IP3 receptor antagonist;100 μM), fluoxetine (5-HT transporter inhibitor: 1 μM), or paroxetine (5-HT transporter inhibitor: 1 μM). Four days after incubation with NGF (2.5ng/mL) with or without specified drugs, morphometric analysis is performed on digitized images of live cells taken under phase-contrast illumination, with an inverted microscope linked to a camera. Images of three fields per well are taken, with an average of 100 cells per field. Differentiated cells are counted by visual examination of the field; only cells that had at least one neurite with a length equal to the cell body diameter are counted, and are then expressed as a percentage of the total cells in the field. Counting is performed in ablinded manner[1]. **Animal Administration:** Brexpiprazole is dissolved in 5% (w/v) gum Arabic[2].[2]Mice[2]
Male C57BL/6NCrSlc mice aged between 4 and 5 weeks old are selected as stranger mice, while animals between 8 and 10 weeks old are used for this study. All mice are housed in groups of five percage, in a room maintained at 23±2°C and 60±10% humidity, with a 12/12h light/dark cycle (lights on at 7:00 a.m.).The mice are given free access to food and water. Brexpiprazole is dissolved in 5% (w/v) gum Arabic and administered orally (p.o.), at 10 mL/kg, 1 h prior to sociability testing. The doses of antipsychotic drugs are selected based on doses that did not impact locomotion.

## References:

[1]. Ishima T, et al. Potentiation of neurite outgrowth by brexpiprazole, a novel serotonin-dopamine activity modulator: a role for serotonin 5-HT1A and 5-HT2A receptors. Eur Neuropsychopharmacol. 2015 Apr;25(4):505-11.

[2]. Yoshimi N, et al. Improvement of dizocilpine-induced social recognition deficits in mice by brexpiprazole, a novel serotonin-dopamine activity modulator. Eur Neuropsychopharmacol. 2015 Mar;25(3):356-64.

## CAIndexNames:

2(1H)-Quinolinone, 7-[4-(4-benzo[b]thien-4-yl-1-piperazinyl)butoxy]-

## SMILES:

O=C1NC2=C(C=CC(OCCCCN3CCN(C4=C(C=CS5)C5=CC=C4)CC3)=C2)C=C1



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