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DATASHEET

TCS OX2 29

Product overview

Name	TCS OX2 29
Cat No	HB3225
Biological action	Antagonist
Purity	>98%
Description	Potent and selective orexin OX ₂ antagonist

Biological Data

Biological description	Potent, selective orexin-2 receptor antagonist ($IC_{50} = 40$ nM) which displays >250-fold selectivity for OX2 over OX1 and over 50 other receptors, ion channels and transporters. Shows various biological effects. Active <i>in vivo</i> .
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Solubility & Handling

Storage instructions	+4°C
Solubility overview	Soluble in water (100 mM), and in DMSO (10 mM)
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	(2S)-1-(3,4-Dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)-3,3-dimethyl-2-[(4-pyridinylmethyl)amino]-1-butane hydrochloride
Molecular Weight	342.51
Chemical structure	The chemical structure shows a complex molecule with a central amine group. It features a quinolinic acid core substituted at position 2 with a dimethylaminomethyl group (-CH2-CH(NH2)2). This group is further substituted with a 4-pyridinylmethyl group (-CH2-pyridin-4-yl). The molecule also contains two hydrochloride (HCl) counterions, one associated with the amine and another with the carboxylic acid group.
Molecular Formula	C ₂₃ H ₃₁ N ₃ O ₃ ·2HCl
CAS Number	1610882-30-8
PubChem identifier	10408514
SMILES	CC(C)(C)[C@@H](C(=O)N1CCC2=CC(=C(C=C2C1)OC)OC)NCC3=CC=NC=C3
Source	Synthetic
InChi	InChI=1S/C23H31N3O3/c1-23(2,3)21(25-14-16-6-9-24-10-7-16)22(27)26-11-8-17-12-19(28-4)20(29-5)13-18(17)15-26/h6-7,9-10,12-13,21,25H,8,11,14-15H2,1-5H3/t21-/m1/s1
InChiKey	COFVZFLCAOUMJT-OAQYLSRUSA-N
Appearance	White solid

References

Central orexin (hypocretin) 2 receptor antagonism reduces ethanol self-administration, but not cue-conditioned ethanol-seeking, in ethanol-preferring rats.

Brown RM et al (2013) The international journal of neuropsychopharmacology 16

PubMedID

23601187

Intracerebroventricular injection of orexin-2 receptor antagonist promotes REM sleep.

Kummangal BA et al (2013) Behavioural brain research 237

PubMedID

22989413

Involvement of orexin-2 receptors in the ventral tegmental area and nucleus accumbens in the antinociception induced by the lateral hypothalamus stimulation in rats.

Azhdari-Zarmehri H et al (2013) Peptides 47

PubMedID

23891649
