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DATASHEET

CGS 21680 hydrochloride

Product overview

Name	CGS 21680 hydrochloride
Cat No	HB2097
Species of origin	Synthetic
Biological action	Agonist
Purity	>98%
Description	Prototypic, selective A _{2A} receptor agonist

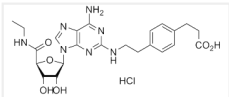
Biological Data

Biological description	Prototypic, selective A _{2A} receptor agonist that also shows some affinity at A ₁ and A ₃ receptors (K _i values are 25, 289 and 69 nM at A _{2A} , A ₁ and A ₃ , EC ₅₀ = 89 μM at A _{2B} receptors respectively). Can be used to distinguish A _{2A} - and A _{2B} - mediated effects. The crystal structure of hA _{2A} R thermostabilized in an active-like confirmation with CGS21680 has been described. Additionally shows hypotensive, anti-inflammatory and neuroprotective effects. Active <i>in vivo</i> .
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Solubility & Handling

Storage instructions	-20 °C (desiccate)
Solubility overview	Soluble in DMSO (100 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	4-[2-[[[6-Amino-9-(N-ethyl-β-D-ribofuranuronamidosyl)-9H-purin-2-yl]amino]ethyl]benzene propanoic acid hydrochloride
Molecular Weight	535.99
Chemical structure	
Molecular Formula	C ₂₃ H ₂₉ N ₇ O ₆ ·HCl
CAS Number	124431-80-7
PubChem identifier	44134621
SMILES	CCNC(=O)C1C(C(C(O1)N2C=NC3=C2N=C(N=C3N)NCCC4=CC=C(C=C4)CCC(=O)O)O)O.Cl
InChi	InChI=1S/C23H29N7O6.ClH/c1-2-25-21(35)18-16(33)17(34)22(36-18)30-11-27-15-19(24)28-23(29-20(15)30)26-10-9-13-5-3-12(4-6-13)7-8-14(31)32;/h3-6,11,16-18,22,33-34H,2,7-10H2,1H3,(H,25,35)(H,31,32)(H3,24,26,28,29);1H
InChiKey	QPHVMNOEKKJYJO-UHFFFAOYSA-N
MDL number	MFCD11045878
Appearance	White solid

References

Effects of CGS 21680, a selective A2A adenosine receptor agonist, on cardiac output and vascular resistance in acute heart failure in the anaesthetized rat

Nekooeian and Tabrizchi (1998) Br J Pharmacol. 123(8)

PubMedID [9605574](#)

The selective adenosine A2 receptor agonist, CGS 21680, is a potent depressant of cerebral cortical neuronal activity

Phillis JW (1990) Brain Res. 509(2)

PubMedID [2322828](#)

Molecular Determinants of CGS21680 Binding to the Human Adenosine A2A Receptor

Lebon et al (2015) Mol Pharmacol. 87(6)

PubMedID [25762024](#)
