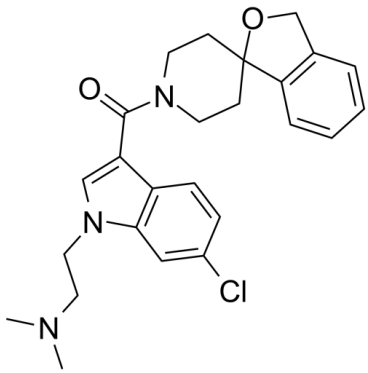
Data Sheet

Product Name:	RG7713
Cat. No.:	CS-7944
CAS No.:	920022-47-5
Molecular Formula:	$C_{25}H_{28}ClN_3O_2$
Molecular Weight:	437.96
Target:	Vasopressin Receptor
Pathway:	GPCR/G Protein
Solubility:	DMSO : 20 mg/mL (45.67 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

RG7713 (RO5028442) is a highly potent and selective **Brain-Penetrant Vasopressin 1a** (**V1a**) receptor antagonist with **K_i**s of 1 nM (**hV1a**) and 39 nM (**mV1a**). IC50 & Target: Ki: 1 nM (hV1a receptor), 39 nM (mV1a receptor)[1] **In Vitro:** RG7713 (RO5028442) (compound 8) has excellent binding in and functional affinity for hV1a, moderate mouse affinity, and excellent selectivity versus human V2 (hV2) and human oxytocin (hOT) receptors. RG7713 (RO5028442) shows high solubility. RG7713 (RO5028442) is found to be highly selective against a panel of 89 targets. Finally, RG7713 (RO5028442) is identified as a suitable compound for clinical studies[1].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: [1]CHO cells are stably transfected with expression plasmids encoding human V1a and grown in F-12 K, containing 10% fetal bovine serum, 1% penicillin-streptomycin, 1% glutamate, and 200 μg/mL geneticin at 37 °C in a 10% CO_2 incubator at 95% humidity. Cells are plated for 24 h at 50,000 cells/well in clear bottomed 96 well plates and are dye loaded for 60 min with 2 μM Fluo-4-AM in assay buffer. After cell washing, the plate is loaded on a fluorometric imaging plate reader, compound dilution series added to the cells, and agonist activity measured[1].

References:

[1]. Ratni H, et al. Discovery of highly selective brain-penetrant vasopressin 1a antagonists for the potential treatment of autism via a chemogenomic and scaffold hopping approach. J Med Chem. 2015 Mar 12;58(5):2275-89.

CAIndexNames:

Methanone, [6-chloro-1-[2-(dimethylamino)ethyl]-1H-indol-3-yl]spiro[isobenzofuran-1(3H),4'-piperidin]-1'-yl-

SMILES:

O=C(C1=CN(CCN(C)C)C2=C1C=CC(Cl)=C2)N3CCC4(C(C=CC=C5)=C5CO4)CC3

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

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