# Data Sheet

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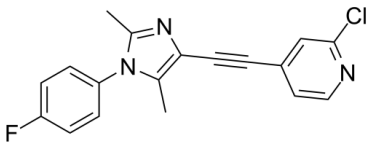
| **Product Name:** | Basimglurant |
| **Cat. No.:** | CS-3388 |
| **CAS No.:** | 802906-73-6 |
| **Molecular Formula:** | C18H13ClFN3 |
| **Molecular Weight:** | 325.77 |
| **Target:** | mGluR |
| **Pathway:** | GPCR/G Protein; Neuronal Signaling |
| **Solubility:** | DMSO : ≥ 33.33 mg/mL (102.31 mM); H2O : < 0.1 mg/mL (insoluble) |




## BIOLOGICAL ACTIVITY:

Basimglurant (RG7090) is a potent, selective and orally available **mGlu5** negative allosteric modulator with a $K_d$ of 1.1 nM. IC50 & Target: Kd: 1.1 nM (mGlu5)[1] **In Vitro:** [$^3$H]-basimglurant saturation analysis on recombinant human mGlu5 reveals monophasic saturation isotherms with $K_d$ of 1.1 nM. In competition binding experiments on human recombinant mGlu5, Basimglurant (RG7090) fully displaces [$^3$H]-MPEP with a $K_i$ of 35.6 nM and [$^3$H]-ABP688 with a $K_i$ of 1.4 nM. In HEK293 cells stably expressing human mGlu5, Basimglurant (RG7090) inhibits quisqualate induced $Ca^{2+}$ mobilization with an $IC_{50}$ of 7.0 nM and [$^3$H]-inositolphosphate accumulation with an $IC_{50}$ of 5.9 nM. Basimglurant (RG7090) shows similar potencies in radioligand binding and functional assay on human and rodent mGlu5 receptor orthologues[1]. **In Vivo:** Basimglurant (RG7090) is a potent, selective, and safe mGlu5 inhibitor with good oral bioavailability and long half-life supportive of once-daily administration, good brain penetration, and high in vivo potency. It has antidepressant properties which are corroborated by its functional magnetic imaging (fMRI) profile, as well as anxiolytic-like and antinociceptive features[1]. It is currently in phase II clinical studies for the treatment of depression and fragile X syndrome. In the Vogel conflict drinking test, Basimglurant dose dependently increases the drinking time. The total plasma exposure of efficacious doses of Basimglurant (RG7090) ranges from 5 ng/mL (0.03 mg/kg) to 37 ng/mL (0.3 mg/kg)[2].

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

**Animal Administration:** [1]Rats: For intravenous PK, Basimglurant (RG7090) is formulated in N-methyl-pyrollidone (NMP)/saline (30%/70%) as vehicle and administered at a volume of 2 mL/kg. For oral gavage (p.o.) the compound is administered as suspension using gelatine/saline (7.5%/0.62% in water) at an administration volume of 4 mL/kg[1].

Monkey: For intravenous PK, Basimglurant (RG7090) is formulated in cyclodextrin solution as vehicle and administered at a volume of 2 mL/kg. For oral gavage (p.o.), the compound is administered in capsule (2 mg in size-2 capsules, i.e. ~0.3 mg/kg) to fasted or fed monkeys in a cross-over design[1].

## References:

[1]. Lindemann L, et al. Pharmacology of basimglurant (RO4917523, RG7090), a unique metabotropic glutamate receptor 5 negative allosteric modulator in clinical development for depression. J Pharmacol Exp Ther. 2015 Apr;353(1):213-33.

[2]. Jaeschke G, et al. Metabotropic glutamate receptor 5 negative allosteric modulators: discovery of 2-chloro-4-[1-(4-fluorophenyl)-2,5-dimethyl-1H-imidazol-4-ylethynyl]pyridine (basimglurant, RO4917523), a promising novel medicine for psychiatric diseases.

## CAIndexNames:

Pyridine, 2-chloro-4-[2-[1-(4-fluorophenyl)-2,5-dimethyl-1H-imidazol-4-yl]ethynyl]-

## SMILES:

CC1=C(C#CC2=CC(Cl)=NC=C2)N=C(C)N1C3=CC=C(F)C=C3



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