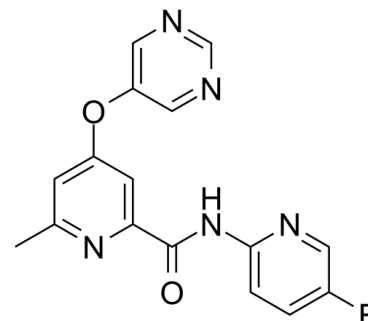


## Data Sheet

|                           |  |
|---------------------------|--|
| <b>Product Name:</b>      | Auglurant  |
| <b>Cat. No.:</b>          | CS-0009173   |
| <b>CAS No.:</b>           | 1396337-04-4   |
| <b>Molecular Formula:</b> | C <sub>16</sub> H <sub>12</sub> FN <sub>5</sub> O <sub>2</sub>                             |
| <b>Molecular Weight:</b>  | 325.30   |
| <b>Target:</b>            | mGluR  |
| <b>Pathway:</b>           | GPCR/G Protein; Neuronal Signaling   |
| <b>Solubility:</b>        | H <sub>2</sub> O : < 0.1 mg/mL (insoluble); DMSO : 22.73 mg/mL (69.87 mM; Need ultrasonic) |



### BIOLOGICAL ACTIVITY:

Auglurant (VU0424238) is a novel and selective **mGlu5** antagonist with an **IC<sub>50</sub>** value of 11 nM (rat) and an **IC<sub>50</sub>** value of 14 nM (human). Auglurant (VU0424238) has an acceptable CNS penetration<sup>[1]</sup>. **In Vitro:** Auglurant (VU0424238) with an **IC<sub>50</sub>** value of 14 nM in HEK293A cells. It also binding a known allosteric site with **K<sub>i</sub>** value of 4.4 nM in HEK293A cells. **In Vivo:** Auglurant (VU0424238) had a clearance of 19.3 mL/min/kg in rats and demonstrates 50% mGlu5 PET ligand occupancy at an oral dose of 0.8 mg/kg in rats. Plus, it also had a clearance of 15.5 mL/min/kg in cynomolgus monkeys and demonstrates 50% mGlu5 PET ligand occupancy at an oral dose of 0.06 mg/kg in baboons<sup>[1]</sup>.

### References:

[1]. Felts AS, et al. Discovery of N-(5-Fluoropyridin-2-yl)-6-methyl-4-(pyrimidin-5-yloxy)picolinamide (VU0424238): A Novel Negative Allosteric Modulator of Metabotropic Glutamate Receptor Subtype 5 Selected for Clinical Evaluation. *J Med Chem.* 2017 Jun 22;60(12):5072-5085.

### CAIndexNames:

2-Pyridinecarboxamide, N-(5-fluoro-2-pyridinyl)-6-methyl-4-(5-pyrimidinyl-oxo)-

### SMILES:

CC1=NC(C(NC2=CC=C(F)C=N2)=O)=CC(OC3=CN=CN=C3)=C1

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

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