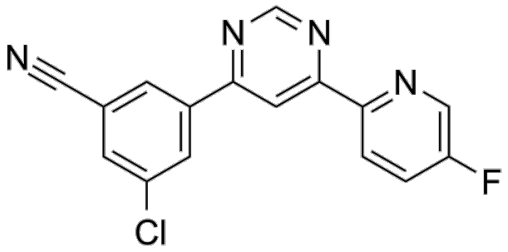
# Product Data Sheet

Product Name: HTL14242
Cat. No.: GC63008

## Chemical Properties

| | | | |
|---|---|---|---|
| Cas. No. | 1644645-32-8 | | |
| Formula | $C_{16}H_8ClFN_4$ | M.Wt | 310.71 |
| Solubility | DMSO : 12.5 mg/mL (40.23 mM; Need ultrasonic) | Storage | Store at -20°C |
| General tips | For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months. | | |
| Shipping Condition | Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request. | | |
| Structure | | | |




## Background

HTL14242 (HTL0014242) is an advanced and orally active mGlu5 NAM with a pKi and a pIC50 of 9.3

and 9.2, respectively[1]. HTL14242 can be used for the research of parkinson's disease[2].

HTL14242 is stable in rat plasma, inactive at the hERG ion-channel, and has a clean profile in vitro assays of cytotoxicity in HepG2 cells, the TC50 is >90 μM[1].

HTL14242 (oral administration; 1, 3, or 10 mg/kg; sacrificed 1 h postdose) emonstrates an excellent, dose-dependent occupancy of mGlu5 receptors from an oral dose, with an estimated ED50 of 0.3 mg/kg[1]. HTL14242 (oral administration; 1 mg/ml) exhibits an oral PK Profile, the t1/2, AUCinf and F% are 6.5 hours, 3946 ng/h/mL and 80%, respectively in dog[1].

[1]. Kirstie A Bennett, et al. Structure-based Discovery and Development of Metabotropic Glutamate Receptor 5 Negative Allosteric Modulators. Adv Pharmacol. . 2020;88:35-58.
[2]. John A Christopher, et al. Fragment and Structure-Based Drug Discovery for a Class C GPCR: Discovery of the mGlu5 Negative Allosteric Modulator HTL14242 (3-Chloro-5-[6-(5-fluoropyridin-2-yl)pyrimidin-4-yl]benzonitrile). J Med Chem. . 2015 Aug 27;58(16):6653-64.