# Data Sheet (Cat.No.T78084)

TargetMol

## PSB 0777 ammonium hydrate

### Chemical Properties

CAS No. :

Formula: C18H20N5O7S2.NH4.1.75H2O

Molecular Weight: 532.09

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

### Biological Description

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|---|---|
| Description | PSB 0777 ammonium hydrate is a potent and selective adenosine A2A receptor full agonist, with K i values of 44.4 nM for rat A2A receptors and 360 nM for human A2A receptors. For rat and human A1 receptors, it has significantly lower affinity, with K i values of ≥10000 nM and 541 nM, respectively. The compound exhibits poor brain penetration and is not orally absorbable. It is of interest in research related to inflammatory bowel disease (IBD) [1] [2] [3]. |
| Targets(IC50) | Adenosine Receptor |
| In vitro | PSB 0777 ammonium hydrate (compound 7) exhibits high specificity for A2A adenosine receptors (A2A AR), demonstrating over 225-fold selectivity compared to other AR subtypes, with K i values above 10000 nM for A2B AR and even higher for A3 AR. As a full agonist at A2A AR, it has an EC50 of 117 nM in CHO-K1 cells [1]. It also binds to human β1 and β3 adrenergic receptors, with K i values of 4.4 μM and 3.3 μM, respectively [2]. In ex vivo experiments, PSB 0777 ammonium hydrate enhances acetylcholine-induced contractions in both untreated and inflamed rat ileum/jejunum preparations in a concentration-dependent manner at 0.1 μM, 1 μM, and 10 μM [1]. |
| In vivo | PSB 0777 ammonium hydrate administered at 0.4 mg/kg/day orally from day 5 to 10 significantly decreases inflammatory cell infiltration and improves colonic mucosal structure [3]. Dose-dependent hypothermia and reduced activity levels in C57BL/6J mice are observed with intraperitoneal injections of 0.03, 0.3, and 3 mg/kg of the compound [2]. Following oral administration, PSB 0777 ammonium hydrate is not systemically absorbed by the digestive mucosa. Plasma concentrations in rats peak at sub-5 nM levels 30 minutes after oral dosing with 0.4 mg/kg/day and are undetectable at 60 minutes. Conversely, intraperitoneal injection at the same dosage yields significant plasma concentration at 30 minutes, which diminishes by the 60-minute mark and is non-detectable at both 120 and 240 minutes [3]. |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|---|---|---|---|
| 1 mM | 1.8794 mL | 9.3969 mL | 18.7938 mL |
| 5 mM | 0.3759 mL | 1.8794 mL | 3.7588 mL |
| 10 mM | 0.1879 mL | 0.9397 mL | 1.8794 mL |
| 50 mM | 0.0376 mL | 0.1879 mL | 0.3759 mL |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.



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