1. PHYSICAL AND CHEMICAL PROPERTIES

   **Batch Molecular Formula:** \( C_{14}H_{14}N_4O_5S \cdot \frac{3}{4}H_2O \)

   **Batch Molecular Weight:** 363.86

   **Physical Appearance:** Light brown solid

   **Solubility:**
   - DMSO to 100 mM
   - Water to 20 mM with gentle warming

   **Storage:** Store at RT

   **Batch Molecular Structure:**

   ![Molecular Structure Image]

2. ANALYTICAL DATA

   **HPLC:** Shows 99.7% purity

   **\(^1\H NMR:** Consistent with structure

   **Mass Spectrum:** Consistent with structure

   **Microanalysis:**

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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<td>15.4</td>
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<tr>
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<td>46.34</td>
<td>4.56</td>
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</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
**Product Name:** PSB 1115  
**Catalog No.:** 2009  
**Batch No.:** 3

**CAS Number:** 152529-79-8  
**IUPAC Name:** 4-(2,3,6,7-Tetrahydro-2,6-dioxo-1-propyl-1H-purin-8-yl)-benzenesulfonic acid

**Description:**
Highly selective, water-soluble, human A_{2B} adenosine receptor antagonist. K_i values are 53.4, > 10000 and > 10000 nM at human A_{2B}, A_1 and A_3 receptors respectively. Also selective versus rat A_1 and A_{2A} receptors (K_i values are 2200 and 24000 nM respectively). Produces potent analgesic effects in vivo.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C_{18}H_{14}N_{4}O_{5}S.¾H_{2}O
- **Batch Molecular Weight:** 363.86
- **Physical Appearance:** Light brown solid
- **Minimum Purity:** >98%

**Storage:** Store at RT

**Solubility & Usage Info:**
- DMSO to 100 mM
- water to 20 mM with gentle warming

**Stability and Solubility Advice:**
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

- **SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.
- **SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**