

Product Name: PSB 0777 ammonium salt

Catalog No.: 4334

Batch No.: 3

CAS Number: 2122196-16-9

IUPAC Name: 4-[2-[(6-Amino-9-b-D-ribofuranosyl-9H-purin-2-yl)thio]ethyl]benzenesulfonic acid ammonium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₀N₅O₇S₂.NH₄.1³/₄H₂O

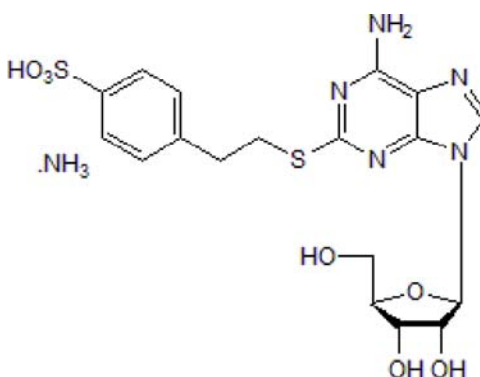
Batch Molecular Weight: 532.07

Physical Appearance: Off White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	40.63	5.21	15.79
Found	40.19	5.12	15.48

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Potent adenosine A_{2A} receptor full agonist (K_i = 44.4 nM for rat brain striatal A_{2A} receptors). Exhibits subtype selectivity for A_{2A} receptors over A₁, A_{2B} and A₃ receptors (K_i ≥ 10 000 nM for rat A₁, human A_{2B} and human A₃ receptors). Potentiates acetylcholine-induced contractions in ex vivo rat ileum/jejunum segments.

Physical and Chemical Properties:

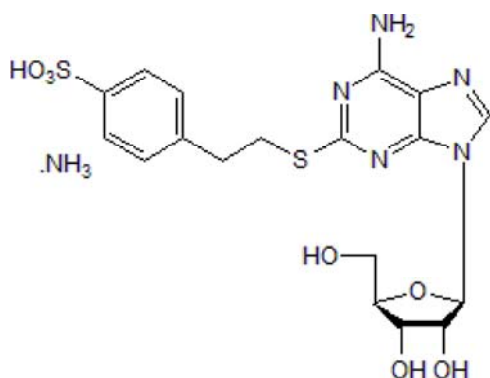
Batch Molecular Formula: C₁₈H₂₀N₅O₇S₂.NH₄.1³/₄H₂O

Batch Molecular Weight: 532.07

Physical Appearance: Off White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

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:

El-Tayeb *et al* (2012) Development of polar adenosine A_{2A} receptor agonists for inflammatory bowel disease: synergism with A_{2B} antagonists. ACS Med.Chem.Lett. 2 890.

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