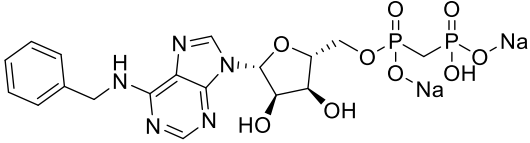


# Product data sheet



MedKoo Cat#: 526930 Name: PSB-12379 disodium CAS: To be determined Chemical Formula: C <sub>18</sub> H <sub>21</sub> N <sub>5</sub> Na <sub>2</sub> O <sub>9</sub> P <sub>2</sub> Exact Mass: 515.0971 Molecular Weight: 559.32	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.

## 1. Product description:

PSB-12379 is a potent and selective ecto-5'-nucleotidase (CD73) inhibitor. PSB-12379 displayed high selectivity versus other ecto-nucleotidases (NTPDase 1–3 and NPP 1–3) and ADP-activated P2Y1 and P2Y12 receptors.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
To be determined	To be determined	To be determined

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.79 mL	8.94 mL	17.88 mL
5 mM	0.36 mL	1.79 mL	3.58 mL
10 mM	0.18 mL	0.89 mL	1.79 mL
50 mM	0.04 mL	0.18 mL	0.36 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

## 6. Recommended literature which reported protocols for in vitro and in vivo study

### In vitro study

- Schmies CC, Rolshoven G, Idris RM, Losenkova K, Renn C, Schäkel L, Al-Hroub H, Wang Y, Garofano F, Schmidt-Wolf IGH, Zimmermann H, Yegutkin GG, Müller CE. Fluorescent Probes for Ecto-5'-nucleotidase (CD73). ACS Med Chem Lett. 2020 Sep 3;11(11):2253-2260. doi: 10.1021/acsmchemlett.0c00391. PMID: 33214837; PMCID: PMC7667873.
- Bhattarai S, Freundlieb M, Pippel J, Meyer A, Abdelrahman A, Fiene A, Lee SY, Zimmermann H, Yegutkin GG, Sträter N, El-Tayeb A, Müller CE.  $\alpha,\beta$ -Methylene-ADP (AOPCP) Derivatives and Analogues: Development of Potent and Selective ecto-5'-Nucleotidase (CD73) Inhibitors. J Med Chem. 2015 Aug 13;58(15):6248-63. doi: 10.1021/acs.jmedchem.5b00802. Epub 2015 Jul 30. PMID: 26147331.

### In vivo study

To be determined

## 7. Bioactivity

### Biological target:

PSB-12379 is a selective high affinity ecto-5'-nucleotidase/CD73 inhibitor (K<sub>i</sub> values are 2.21 and 9.03 nM at human and rat CD73, respectively). PSB-12379 blocks ecto-5'-nucleotidase-mediated adenosine production by preventing the conversion of AMP to adenosine.

# Product data sheet



## In vitro activity

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PSB-12379 demonstrated significant in vitro activity as an eN, CD73 inhibitor. It exhibited a  $K_i$  value of 9.03 nM. PSB-12379 showed high selectivity against other ecto-nucleotidases and ADP-activated P2Y receptors and demonstrated high metabolic stability.

Reference: J Med Chem. 2015 Aug 13;58(15):6248-63. <https://pubmed.ncbi.nlm.nih.gov/26147331/>

## In vivo activity

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To be determined

*Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.*