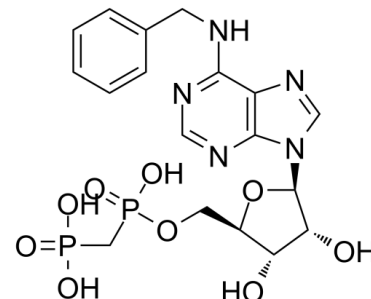


Data Sheet

Product Name:	PSB-12379
Cat. No.:	CS-7892
CAS No.:	1802226-78-3
Molecular Formula:	C ₁₈ H ₂₃ N ₅ O ₉ P ₂
Molecular Weight:	515.35
Target:	CD73
Pathway:	Immunology/Inflammation
Solubility:	H ₂ O : 7.14 mg/mL (13.85 mM; Need ultrasonic); DMSO : < 1 mg/mL (insoluble or slightly soluble)



BIOLOGICAL ACTIVITY:

PSB-12379 is a potent **Ecto-5'-Nucleotidase (CD73)** inhibitor with K_i s of 9.03 nM (rat) and 2.21 nM (human). IC₅₀ & Target: K_i : 9.03 nM (rat), 2.21 nM (human) (Ecto-5'-Nucleotidase)^[1]

References:

[1]. Bhattarai S, et al. α,β -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.

CAIndexNames:

Adenosine, N-(phenylmethyl)-, 5'-[hydrogen P-(phosphonomethyl)phosphonate]

SMILES:

O[C@@H]([C@H]1O)[C@@H](COP(CP(O)(O)=O)(O)=O)O[C@H]1N(C=N2)C3=C2C(NCC4=CC=CC=C4)=NC=N3

Caution: Product has not been fully validated for medical applications. For research use only.

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