

# **Data Sheet**

Product Name: Pseudothymidine

 Cat. No.:
 CS-7718

 CAS No.:
 65358-15-8

 Molecular Formula:
 C10H14N2O5

Molecular Weight: 242.23

Target:HIV; Nucleoside Antimetabolite/AnalogPathway:Anti-infection; Cell Cycle/DNA DamageSolubility:DMSO :  $\geq$  61.17 mg/mL (252.53 mM)

### **BIOLOGICAL ACTIVITY:**

Pseudothymidine is a C-nucleoside analog of thymidine. In Vitro: Pseudothymidine is a C-nucleoside analog of thymidine [1]. The calculated  $\Delta\Delta G^{\circ}_{50}/\text{mod}$  is -0.5 kcal/mol, with a  $\Delta T_{m}/\text{mod}$  of 0.82°C. For the duplexes containing nine dA-T/ $\psi$ T pairs, the  $\Delta T_{m}/\text{mod}$  is -0.9°C and a  $\Delta\Delta G^{\circ}_{50}/\text{mod}$  is +1.1 kcal/mol. The modification of the duplex containing 12 consecutive dA-T/ $\psi$ T base pairs produces a  $\Delta T_{m}/\text{mod}$  of -0.9°C and a  $\Delta\Delta G^{\circ}_{50}/\text{mod}$  of +1.2 kcal/mol<sup>[2]</sup>.

## PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: Thermal DNA duplex denaturation studies are performed with templates containing up to twelve consecutive dA residues that are paired with its complement template containing consecutive T or Pseudothymidine ( $\psi$ T) residues. Experiments are performed in a buffer (45 mM NaCl, 45 mM sodium citrate, pH 8.1, final vol. 1.5 mL) containing template and its complement (1.5  $\mu$ M of each). Absorbance (260 nm) is monitored over a range of 25.0 to 90.0°C with a change in temperature of 0.5°C/min for five heating cycles. The initial heating cycle is discarded and the T<sub>m</sub> is determined by averaging the temperatures of the remaining four cycles. The  $\Delta$ T<sub>m</sub> between similar duplexes is calculated by subtracting the T<sub>m</sub> of the duplex containing standard bases from the T<sub>m</sub> of the duplex containing C-glycosides (including Pseudothymidine)<sup>[2]</sup>.

### References:

[1]. S Lutz, et al. An in vitro screening technique for DNA polymerases that can incorporate modified nucleotides. Pseudo-thymidine as a substrate for thermostable polymerases. Nucleic Acids Res. 1999 Jul 1; 27(13): 2792-2798.

[2]. Havemann SA, et al. Incorporation of multiple sequential pseudothymidines by DNA polymerases and their impact on DNA duplex structure. Nucleosides Nucleotides Nucleic Acids. 2008 Mar;27(3):261-78.

#### **CAIndexNames**:

2,4(1H,3H)-Pyrimidinedione, 5-(2-deoxy-β-D-erythro-pentofuranosyl)-1-methyl-

### **SMILES:**

O = C(N1)C([C@@H]2O[C@H](CO)[C@@H](O)C2) = CN(C)C1 = O

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

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