**Product Data Sheet**

### Chemical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Product Name:</strong></td>
<td>Pralatrexate</td>
</tr>
<tr>
<td><strong>Cas No.:</strong></td>
<td>146464-95-1</td>
</tr>
<tr>
<td><strong>M.Wt:</strong></td>
<td>477.47</td>
</tr>
<tr>
<td><strong>Formula:</strong></td>
<td>C23H23N7O5</td>
</tr>
<tr>
<td><strong>Chemical Name:</strong></td>
<td>(2S)-2-[[4-[1-(2,4-diaminopteridin-6-yl)pent-4-yn-2-yl]benzoyl]amino]pentanedioic acid</td>
</tr>
<tr>
<td><strong>Canonical SMILES:</strong></td>
<td>C#CCC(CC1=CN=C2C(=N1)C(=NC(=N2)N)N)C3=CC=C(C=C3)C(=O)NC(CCC(=O)O)C(=O)O</td>
</tr>
<tr>
<td><strong>Solubility:</strong></td>
<td>≥23.85 mg/mL in DMSO, &lt;2.4 mg/mL in EtOH, &lt;2.29 mg/mL in H2O</td>
</tr>
<tr>
<td><strong>Storage:</strong></td>
<td>Store at -20°C</td>
</tr>
<tr>
<td><strong>General tips:</strong></td>
<td>For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.</td>
</tr>
<tr>
<td><strong>Shopping Condition:</strong></td>
<td>Evaluation sample solution: ship with blue ice&lt;br&gt;All other available size: ship with RT, or blue ice upon request</td>
</tr>
</tbody>
</table>

### Biological Activity

**Targets:** Metabolism  
**Pathways:** DHFR  
**Description:**  
Pralatrexate is an inhibitor of DHFR with Ki value of 45 nM [1]. Dihydrofolate reductase (DHFR) is an enzyme that reduces dihydrofolic acid to tetrahydrofolic acid, a methyl group shuttle required for the synthesis of purines, thymidylic acid, and certain amino acids.
Pralatrexate is a DHFR inhibitor with high affinity for folylpolyglutamate synthetase (FPGS) and reduced folate carrier 1 (RFC-1), resulting in extensive internalization and accumulation in tumour cells. In 15 human cancer cell lines, pralatrexate showed antiproliferative effects with IC50 < 0.1 μM in PC3, SCC61, DU145, HT29, HOP62, SQ20B, HOP92, HEP2 and IGROV1 cells. While it showed antiproliferative effects with IC50 ≥ 9 μM in Colo205, HCC2998, MCF7, HCT116, OVCAR3 and MDA-MB-435 cells [2].

In MV522 human non-small cell lung cancer (NSCLC) xenograft, pralatrexate showed increased antitumor activity. In the 2 mg/kg pralatrexate-treated group, the 38% tumor growth inhibition (TGI) was observed. In NCI-H460 NSCLC xenograft, pralatrexate showed antitumor activity in a dose-dependent way. TGI of 1 mg/kg and 2 mg/kg pralatrexate-treated groups was 34% and 52%, respectively. In the two xenografts, pralatrexate resulted in weight loss, which suggested its toxicity [1].

Reference:

Protocol

Cell experiment:

Cell lines
Cancer cell lines, NCI-H460 human NSCLC cells, MV522 human metastatic human NSCLC cells

Preparation method
The solubility of this compound in DMSO is > 23.9 mg/mL. General tips for obtaining a higher concentration: Please warm the tube at 37 °C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Reacting conditions

Applications
Pralatrexate showed antiproliferative activity against 15 cancer cell lines with the IC50 values ranged from 0.01 ± 0.002 μM for the prostate cancer cell line PC3 to > 350 μM for the MDA-MB-435 cell line. Pralatrexate dose-dependently inhibited the activity of DHFR. In NCI-H460 cells, treatment with pralatrexate for 15 or 60 min resulted in a short-term uptake of radiolabeled antifolates.

Animal experiment [3]:

Animal models
Female nude mice (nu/nu) bearing NCI-H460 or MV522 tumor cells
Dosage form
Intraperitoneal injection, 1 and 2 mg/kg, every day×5, for two cycles of 5 days

Applications
In MV522 human non-small cell lung cancer (NSCLC) xenograft, pralatrexate showed increased antitumor activity. In the 2 mg/kg pralatrexate-treated group, the 38% tumor growth inhibition (TGI) was observed. In NCI-H460 NSCLC xenograft, pralatrexate showed antitumor activity in a dose-dependent way. TGI of 1 mg/kg and 2 mg/kg pralatrexate-treated groups was 34% and 52%, respectively. In NCI-H460 and MV522 human tumor xenografts, pralatrexate resulted in dose-dependent weight loss, which suggested its toxicity.

Other notes
Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

Reference:

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Short-term storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.