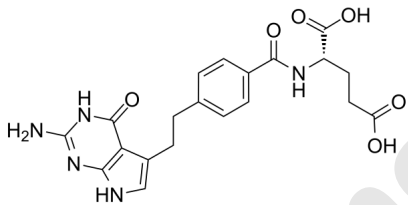


Data Sheet

Product Information

Catalog Number	BP12436
Product Name	Pemetrexed
Description	Pemetrexed, a guanine-derived antineoplastic agent, binds to and inhibits the enzyme thymidylate synthase (TS).
Targets&IC50	thymidylate synthase (TS):1.3 nM(ki), dihydrofolate reductase (DHFR):7.2 nM(ki), glycineamide ribonucleotide formyltransferase (GARFT):.65 nM(ki)
In vitro	Pemetrexed (LY231514) disodium is a novel classical antifolate, the antitumor activity of which may result from simultaneous and multiple inhibition of several key folate-requiring enzymes via its polyglutamated metabolites. Pemetrexed (LY231514) is one of the best substrates that is known for the enzyme FPGS ($K_m=1.6 \mu M$ and $V_{max}/K_m=621$). It is likely that polyglutamation and the polyglutamated metabolites of LY231514 play profound roles in determining both the selectivity and the antitumor activity of this novel agent. Whereas LY231514 only moderately inhibits TS ($K_i=340 \text{ nM}$, recombinant mouse), the pentaglutamate of LY231514 is 100-fold more potent ($K_i=3.4 \text{ nM}$), making LY231514 one of the most potent folate-based TS inhibitors.
In vivo	The group of mice treated with PC61 plus Pemetrexed demonstrates statistically longer survival than other groups. In a survival analysis, significantly better survival is observed in the group of mice treated with PC61 plus Pemetrexed compared with those treated with PC61 alone, rat IgG plus Pemetrexed, or no treatment.
Synonyms	LY231514, Pemetrexed acid, LY-231514 Disodium Hydrate
CAS No.	137281-23-3

Chemical Formula	C ₂₀ H ₂₁ N ₅ O ₆
Molecular Weight	427.41
Solubility	DMSO: 100 mg/mL (233.97 mM)
Storage	Powder: -20°C for 2 years In solvent: -80°C for 1 year
Chemical Structure OR Tested Image	 <p>The chemical structure shows a purine-like core (a fused bicyclic system with an amino group and a carbonyl group). This core is connected via a methylene chain to a benzene ring. The benzene ring is further connected to a side chain that includes a carboxylic acid group and a hydroxyl group. The side chain is: -CH₂-CH₂-C(=O)-NH-CH(OH)-CH₂-COOH.</p>

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