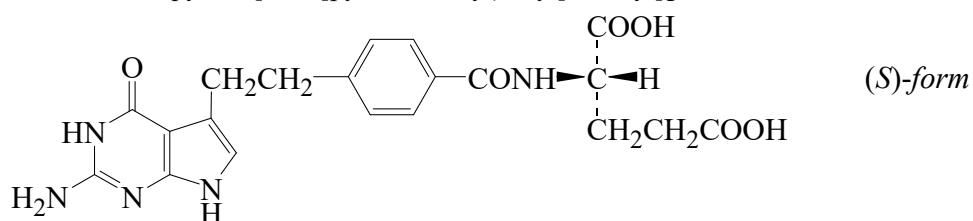




>>Entry Name: Pemetrexed, INN

Synonym(s): *N*-[4-[2-(2-Amino-4,7-dihydro-4-oxo-1*H*-pyrrolo[2,3-*d*]pyrimidin-5-yl)ethyl]benzoyl]glutamic acid, 9Cl. LY 231514



Molecular Formula: C₂₀H₂₁N₅O₆

Molecular Weight: 427.416

Accurate Mass: 427.149185

Percentage Composition: C 56.20%; H 4.95%; N 16.39%; O 22.46%

Biological Use/Importance: Thymidylate synthase inhibitor. Antineoplastic agent

Development Status: Phase II clinical trials (1997)

>>Variant: (*S*)-form

CAS Registry Number: 137281-23-3

Molecular Formula: C₂₀H₂₁N₅O₆

Molecular Weight: 427.416

Accurate Mass: 427.149185

Percentage Composition: C 56.20%; H 4.95%; N 16.39%; O 22.46%

Physical Description: Powder (MeOH/Me₂CO)

Melting Point: Mp 172-174°

>>Derivative: Di-Na salt

Synonym(s): Pemetrexed disodium, USAN

CAS Registry Number: 150399-23-8

References:

- Taylor, E.C. *et al.*, *J. Med. Chem.*, 1992, **35**, 4450-4454, (*synth, pmr, pharmacol*)
Miwa, T. *et al.*, *J.O.C.*, 1993, **58**, 1696-1701, (*synth, ir, pmr*)
Eur. Pat., 1994, *Eli Lilly*, 589 720; *CA*, **121**, 83363m, (*synth*)
Hamilton, C.L. *et al.*, *J. Chromatogr., B: Biomed. Appl.*, 1994, **654**, 297-303, (*hplc*)
Rinaldi, D.A. *et al.*, *J. Clin. Oncol.*, 1995, **13**, 2842-2850, (*clin trial*)
Shih, C. *et al.*, *Cancer Res.*, 1997, **57**, 1116-1123, (*pharmacol*)
Woodland, J.M. *et al.*, *Drug Metab. Dispos.*, 1997, **25**, 693-700, (*hplc, metab*)
Calvert, A.H. *et al.*, *Br. J. Cancer*, 1998, **78**, 35-40, (*rev*)
Graul, A. *et al.*, *Drugs of the Future*, 1998, **23**, 498-507, (*rev*)
Taylor, E.C. *et al.*, *Tet. Lett.*, 1999, **40**, 4023-4026, (*synth*)