

REFERENCES

1. Schweitzer, B. I., Dicker, A. P., and Bertino, J. R. Dihydrofolate reductase as a therapeutic target., FASEB Journal 4, No., (1990): 2441-2452.
2. Knighton, D. R., Kan, C. C., Howland, E., Janson, C. A., Hostomska, Z., Welsh, K. M., and Matthews, D. A. Structure of and kinetic channelling in bifunctional dihydrofolate reductase-thymidilate synthase., Structural Biology 1(3), No., (1994): 186-194.
3. Bolin, J. T., Filman, D. J., Matthews, D. A., Hamlin, R. C., and Kraut, J. J.Biol.Chem. 257, No., (1982): 166-169.
4. Birdsall, B., Feeney, J., Tendler, S. J. B., Hammond, S., and Roberts, G. C. K. Biochemistry 28, No., (1989): 2297-2305.
5. Davies, J. F., Delcamp, T. J., Prendergrast, N. J., Ashford, V. A., Freisheim, J. H., and Kraut, J. Biochemistry 29, No., (1990): 9467-9479.
6. Bystroff, C. and Kraut, J. Biochemistry 30, No., (1991): 2227-223.
7. Bystroff, C., Oatley, S. J., and Kraut, J. Biochemistry 29, No., (1990): 3263-3277.
8. Champness, J. N., Achari, A., Ballantine, S. P., Bryant, P. K., Delves, C. J., and Stammers, D. K. Structure of *Pneumocystis-carinii* dihydrofolate-reductase to 1.9- angstrom resolution., Structure 2(10), No., (1994): 915-924.
9. Matthews, D. A., Bolin, J. T., Burridge, J. M., Filman, D. J., Volz, K. W., Kaufman, B. T., Beddell, C. R., Champness, J. N., Stammers, D. K., and Kraut, J. J.Biol.Chem. 260, No., (1985): 381-391.
10. Matthews, D. A., Bolin, J. T., Burridge, J. M., Filman, D. J., Volz, K. W., and Kraut, J. Dihydrofolate Reductase: The Stereochemistry of Inhibitor Selectivity., J.Biol.Chem. 260(1), No., (1985): 392-399.
11. Volz, K. W., Matthews, D. A., Alden, R. A., Freer, S. T., Hansch, C., Kaufman, B. T., and Kraut, J. J.Biol.Chem. 257, No., (1982): 2528-2536.
12. McTigue, M. A., Davies, J. F., Kaufman, B. T., and Kraut, J. Crystal structure of chicken liver dihydrofolate reductase complexed with NADP+ and biopterin., Biochemistry 31, No.32, (1992): 7264-7273.
13. McTigue, M. A., Davies, J. F., Kaufman, B. T., and Kraut, J. Biochemistry 32, No., (1993): 6855-6862.
14. Oefner, C., D'arcy, A., and Winkler, F. K. European Journal of Biochemistry 174, No., (1988): 377-385.

15. Cody, V., Wojtczak, A., Kalman, T. I., Freisheim, J. H., and Blakley, R. L. Chemistry and Biology of Pteridines and Folates, (1993): 481-486.
16. Cody, V., Galitsky, N., Luft, J. R., Pangborn, W., Blakley, R. L., and Gangjee, A. Comparison of ternary crystal complexes of F31 variants of human dihydrofolate reductase with NADPH and a classical antitumor furopyrimidine., Anti-Cancer Drug Design 13, No., (1998): 307-315.
17. Gangjee, A., Vidmans, A. P., Vasudevan, A., Queener, S. F., Kisliuk, R. L., Cody, V., Li, R. M., Galitsky, N., Luft, J. R., and Pangborn, S. Journal of Medicinal Chemistry 41, No., (1998): 3246-3434.
18. Davies, J. F., Delcamp, T. J., Prendergrast, N. J., Ashford, V. A., Freisheim, J. H., and Kraut, J. Crystal structures of recombinant human dihydrofolate reductase complexed with folate and 5-deazafolate., Biochemistry 29, No.40, (1990): 9467-9479.
19. Brown, K. A., Howell, E. E., and Kraut, J. Long-range structural effects in a second-site revertant of a mutant dihydrofolate reductase., Proceedings of the National Academy of Sciences USA 90, No.24, (1993): 11753-11756.
20. McTigue, M. A., Davies, J. F., Kaufman, B. T., and Kraut, J. Crystal structures of chicken liver dihydrofolate reductase: binary thioNADP⁺ and ternary thioNADP⁺. biopterin complexes., Biochemistry 32, No.27, (1993): 6855-6862.
21. McTigue, M. A., Davies, J. F., Kaufman, B. T., Xuong, N.-H., and Kraut, J. Crystal structures of organomercurial-activated chicken liver dihydrofolate reductase complexes., To be published, (1999).
22. Bolin, J. T., Filman, D. J., Matthews, D. A., Hamlin, R. C., and Kraut, J. Crystal structures of *Escherichia coli* and *Lactobacillus casei* dihydrofolate reductase refined at 1.7 angstroms resolution. I. General features and binding of methotrexate., Journal of Biological Chemistry 257, No., (1982): 13650.
23. Warren, M. S., Brown, K. A., Farnum, M. F., Howell, E. E., and Kraut, J. Investigation of the functional role of tryptophan-22 in *Escherichia coli* dihydrofolate reductase by site-directed mutagenesis., Biochemistry 30, No., (1991): 11092.
24. Bystroff, C. and Kraut, J. Crystal structure of unliganded *Escherichia coli* dihydrofolate reductase. Ligand-induced conformational changes and cooperativity in binding., Biochemistry 30, No.8, (1991): 2227-2239.
25. Bystroff, C., Oatley, S. J., and Kraut, J. Crystal structures of *Escherichia coli* dihydrofolate reductase. The NADP⁺ holoenzyme and the folate (dot)/

- NADP⁺ ternary complex. Substrate binding and a model for the transition state., Biochemistry 29, No., (1990): 3263.
26. Davies, J. F., Matthews, D. A., Oatley, S. J., Kaufman, B. T., Xuong, N. h., and Kraut, J. Refined crystal structures of chicken liver dihydrofolate reductase. 3 Angstroms apo-enzyme and 1.7 angstroms/ NADPH holo-enzyme complex., To be published, (1999).
 27. Matthews, D. A., Alden, R. A., Bolin, J. T., Freer, S. T., Hamlin, R., Xuong, N., Kraut, J., Poe, M., Williams, M., and Hoogsteen, K. Science 197, No., (1977): 452.
 28. Matthews, D. A., Alden, R. A., Bolin, J. T., Filman, D. J., Freer, S. T., Hamlin, R., Hol, W. G. L., Kisliuk, R. L., Pastore, E. J., Plante, L. T., Xuong, N., and Kraut, J. Journal of Biological Chemistry 253, No., (1978): 6946.
 29. Matthews, D. A., Alden, R. A., Freer, S. T., Xuong, N., and Kraut, J. Journal of Biological Chemistry 254, No., (1979): 4144.
 30. Feeney, J., Roberts, G. C. K., Birdsall, B., Griffiths, D. V., Ng, R. W., Scudder, P., and Burgen, A. S. V. Proc.R.Soc.London Ser.B 196, No., (1977): 267.
 31. Jorgensen, W. L., Chandrasekhar, J., Madura, J. D., Impey, R. W., and Klein, M. L. Comparison of simple potential functions for simulating liquid water., J.Chem.Phys. 79, No., (1983): 926-935.
 32. Pearlman, D. A., Case, D. A., Caldwell, J. W., Ross, W. S., Cheatham III, T. E., Debolt, S., Ferguson, D., Seibel, G., and Kollman, P. AMBER, a package of computer program for applying molecular dynamics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules., Comp.Phys.Commun. 91, No., (1995): 1-41.
 33. Berendsen, H. J. C., Postma, J. P. M., van Gunsteren, W. F., DiNola, A., and Haak, J. R. Molecular dynamics with coupling to an external bath., J.Chem.Phys. 81, No., (1984): 3684-3690.
 34. Case, D. A., Pearlman, D. A., Caldwell, J. W., Cheatham III, T. E., Ross, W. S., Simmerling, C. L., Darden, T. A., Merz, K. M., Stanton, R. V., Cheng, A. L., Vincent, J. J., Crowley, M., Ferguson, D. M., Radmer, R. J., Seibel, G. L., Singh, U. C., Weiner, P. K., and Kollman, P. A. AMBER 5., (1997).
 35. Insight II User Guide., (1995).
 36. Sayle, R. Rasmol, v. 2.6, Molecular Visualization Program., (1995).
 37. WebLab Viewer Version 2.1., (1997).

38. Kraulis, P. Journal of Applied Crystallography 24, No., (1991): 946.
39. Laskowski, R. A., MacArthur, M. W., Moss, D. S., and Thornton, J. M. PROCHECK: a program to check the stereochemical quality of protein structures., Journal of Applied Crystallography 26, No., (1993): 283-291.
40. Stockman, B. J., Nirmala, N. R., Wagner, G., Delcamp, T. J., DeYarman, M. T., and Freisheim, J. H. Sequence-Specific ^1H and ^{15}N Resonance Assignments for Human Dihydrofolate Reductase in Solution., Biochemistry 31, No., (1992): 218-229.
- 41 Jain, D. C.; Sapse, A. M.; Cowburn, D. J. Phys. Chem. 92, (1988): 6847-6849.
- 42 <http://www.pdb.bnl.gov>
- 43 HyperChem™ Computational Chemistry: Part I Practical Guide., (1992): 5-80.
- 44 Palmer, T. Understanding Enzymes., 3rd ed. West Sussex: Ellis Horwood, 1991.
- 45 Grant, G. H. and Richards, W. G. Computational Chemistry., 1st ed. Oxford: Oxford University Press Inc., 1995.
- 46 Rhodes, G. Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models., 1st ed. San Diego: Academic Press Inc., 1993.
- 47 Stryer, L. Biochemistry., 4th ed., 1995.
- 48 Leach, A. R. Molecular Modelling: Principles and Applications., 1st ed. Essex: Addison Wesley Longman Limited, 1996.
- 49 Brooks, C. L., III, Karplus, M., and Petitt, B. M. Proteins: A Theoretical Perspective of Dynamics, Structure and Thermodynamics., New York: John Wiley & Sons Inc. 1988.
- 50 Blakley, R. L., Folates and Pteridines. New York: John Wiley & Sons Inc. 1984.

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