

Publications:

1. **McKenna, R.**, R. Kuroda, S. Neidle, P. Serafinowski. 1987. A structural study of 3'-deoxytubercidin and 3-deaza-3'-deoxyadenosine. *Acta Cryst.*, C43:1790-1793.
2. **McKenna, R.**, S. Neidle, P. Serafinowski. 1987. The structure of 3'-deoxyformycin hydrochloride. *Acta Cryst.*, C43:2358-2361.
3. **McKenna, R.**, T. C. Jenkins, S. Neidle. 1988. Structures of the anticancer compounds *N*-(2-hydroxyethyl)-2-(3-nitro-1,2,4-triazol-1-yl)-acetamide (RB-6110) and 5-(1-aziridinyl)-3-nitro-1-(3-oxo-1-butyl)-1,2,4-triazole (RB-6162). *Acta Cryst.*, B44:672-676.
4. **McKenna, R.**, A. J. Beveridge, T. C. Jenkins, S. Neidle, W. A. Denny. 1989. Molecular modelling of DNA-antitumour drug intercalation interactions: Correlations of structural and energetic features with biological properties for a series of phenylquinoline-8-carboxamide compounds. *Mol. Pharma.*, 35:720-728.
5. **McKenna, R.**, S. Neidle, R. Kuroda, B. W. Fox. 1989. Structures of three DNA cross-linking agents, ethane-1,2-di(methylsulfonate), propane-1,3-di(methylsulfonate) and *n*-butane-1,4-di(methylsulfonate). *Acta Cryst.*, C45:311-314.
6. Deadman, J. J., M. Jarman, R. McCague, **R. McKenna**, S. Neidle. 1989. A benzoquinone di-imine from the oxidation of pentafluoroaniline by hypochlorite. X-ray crystal structure and possible formation via pentafluorophenylnitrene. *J. Chem. Soc. Perkin Trans., II*:971-975
7. **McKenna, R.**, S. Neidle, P. Serafinowski. 1990. The crystal structure of 5'-chloro-3',5'-dideoxyformycin A monohydrate. The effects of protonation on formycin structure and conformation. *Acta Cryst.*, C46:2448-2450.
8. Willingmann, P., S. Krishnaswamy, **R. McKenna**, T. J. Smith, N. H. Olson, M. G. Rossmann, P. L. Stow, N. L. Incardona. 1990. Preliminary investigation of the phage \square X174 crystal structure. *J. Mol. Biol.*, 212:345-350.
9. Laughton, C. A., **R. McKenna**, S. Neidle, M. Jarman, R. McCague, M. G. Rolands. 1990. Crystallographic and molecular modelling studies on 3-ethyl-3-(4-pyridyl)piperidine-2,6-dione and its butyl analogue, inhibitors of mammalian aromatase. Comparison with natural substrates: Prediction of enantioselectivity for N-alkyl derivatives. *J. Med. Chem.*, 33:2673-2679.
10. Agbandje, M., **R. McKenna**, M. G. Rossmann, S. Kajigaya, N. S. Young. 1991. Preliminary X-ray crystallographic investigation of human parvovirus B19. *Virology*, 184:170-174.
11. **McKenna, R.**, S. Neidle, W. D. Wilson. 1991. Structures of 1-(3,3-dimethylamino)propyl naphtho[2,1-b]thiophene-4-carboxylate and N-(3,3-dimethylamino)propyl-8-methoxynaphtho[2,1-b]thiophene-4-carboxamide, intercalators into double-helical DNA. *Acta Cryst.*, C47:2511-2513.
12. **McKenna, R.**, D. Xia, P. Willingmann, L. L. Ilag, S. Krishnaswamy, M. G. Rossmann, N. H. Olson, T. S. Baker, N. L. Incardona. 1992. The atomic structure of the single-stranded DNA bacteriophage \square X174 and its functional implications. *Nature*, 355:137-143.
13. Rossmann, M. G., **R. McKenna**, L. Tong, D. Xia, J. Dai, H. Wu, H. Choi, R. E. Lynch. 1992. Molecular replacement real space averaging. *J. Applied Cryst.*, 25:166-180.
14. **McKenna, R.**, M. Agbandje, S. Neidle. 1992. Structure of 9-amino-2,7-di-tert-butylacridine. *Acta Cryst.*, C48:188-190.
15. Agbandje, M., T. C. Jenkins, **R. McKenna**, A. Reszka, S. Neidle. 1992. Anthracen-9,10-diones as potential anti-cancer agents. Studies on a series of 2,6-disubstituted anthracen-9,10-diones. *J. Med. Chem.*, 35:1418-1429.
16. **McKenna, R.**, D. Xia, P. Willingmann, L. L. Ilag, M. G. Rossmann. 1992. Structure determination of the bacteriophage \square X174. *Acta Cryst.*, B48:499-511.
17. Agbandje, M., **R. McKenna**, M. G. Rossmann, M.C. Strassheim, C.R. Parrish. 1993. Structure determination of feline panleukopenia virus empty particles. *Proteins*, 16:155-171.

18. **McKenna, R.**, L. L. Ilag, M. G. Rossmann. 1994. Analysis of the single-stranded DNA bacteriophage \square X174, refined at a resolution of 3.0Å. *J. Mol. Biol.*, 237:517-543.
19. Agbandje, M., S. Kajigaya, **R. McKenna**, M. G. Rossmann, N. S. Young. 1994. The structure of human parvovirus B19 at 8 Å resolution. *Virology*, 203:106-115.
20. Ilag, L. L., **R. McKenna**, M. P. Yadav, J. N. Bemiller, N. L. Incardona, M. G. Rossmann. 1994. Calcium ion induced structural changes in phage \square X174. *J. Mol. Biol.*, 244:291-300.
21. Ilag, L. L., N. H. Olson, T. Dokland, C. L. Music, R. H. Cheng, Z. Brown, **R. McKenna**, M. G. Rossmann, T. S. Baker, N. L. Incardona. 1995. DNA packaging intermediates of bacteriophage \square X174. *Structure*, 3:353-363
22. **McKenna, R.**, B. Bowman, L. L. Ilag, M. G. Rossmann, B. A. Fane. 1996. The atomic structure of the degraded procapsid particle of the bacteriophage G4. *J. Mol. Biol.*, 256:736-750.
23. Dokland, T., **R. McKenna**, L. L. Ilag, B. R. Bowman, N. L. Incardona, B. A. Fane M. G. Rossmann. 1997. Structure of a viral procapsid molecular scaffolding. *Nature*, 389:308-313.
24. Chipman, P.R., **R. McKenna**, T.S Baker. 1997. Cryo-electron microscopy of spiroplasma virus SpV4. *Microscopy and Microanalysis*, Vol. 3, supplement 2:87-88.
25. Olson, N.H., P.R. Chipman, M. E. Bloom, **R. McKenna**, M. Agbandje-McKenna, T. F. Booth, T.S. Baker. 1997. Automated CCD data collection and 3D reconstruction of Aleutian mink disease parvovirus. *Microscopy and Microanalysis*, Vol. 3, supplement 2:1117-1118.
26. Chipman, P.R., M. Agbandje-McKenna, J. Renaudin, T.S. Baker, **R. McKenna**. 1998. Structural analysis of the *Spiroplasma* virus, SpV-4, implications for evolutionary variation to obtain host diversity among the *Microviridae*. *Structure*, 6:135-145.
27. Dokland, T., **R. McKenna**, D. Sherman, B. R. Bowman, W. F. Bean, M. G. Rossmann. 1998. Structure determination of the \square X174 closed procapsid. *Acta Cryst.*, D54: 878-890.
28. **McKenna, R.**, P.R. Chipman, N.H. Olson, T.S. Baker, T.F. Booth, J. Christensen, B. Aasted, M.E. Bloom, M. Agbandje-McKenna. 1999. The three-dimensional structure of Aleutian mink disease parvovirus: Implications for disease pathogenicity. *J. Virol.*, 73: 6882-6891.
29. Hernando, E., A. L. Llamas-Saiz, C. Foces-Foces, **R. McKenna**, I. Portman, M. Agbandje-McKenna, J. M. Almendral. 2000. Biochemical and physical characterization of parvovirus minute virus of mice virus-like particles. *Virology*, 267:299-309.
30. Bennett, M., A. Krah, F. Wien, E. Garman, **R. McKenna**, M. Sanderson, S. Neidle. 2000. A DNA-porphyrin minor-groove complex at atomic resolution: The structural consequences of porphyrin ruffling *Proc. Natl. Acad. Sci. USA*, 97:17, 9476-9481.
31. Zhang, W., N.H. Olson, T. S. Baker, L. Faulkner, M. Agbandje-McKenna, M. I. Boulton, J. W. Davies, **R. McKenna**. 2001. Structure of the maize streak virus geminate particle. *Virology*, 279: 471-477.
32. Duda, D. M., C. Tu, M. Qian, P. Laipis, M. Agbandje-McKenna, D. N. Silverman, **R. McKenna**. 2001. Structural and kinetic analysis of the chemical rescue of the proton transfer function of carbonic anhydrase II. *Biochemistry* 40: 1741-1748.
33. Duda, D. M., C. Tu, D.N. Silverman, A.J. Kalb, M. Agbandje-McKenna, **R. McKenna**. 2001. Ultra-high resolution X-ray diffraction from crystals of the kinetic mutant of human carbonic anhydrase II, His64Ala, and its complexes with proton acceptor/donors. *Protein and Peptide letters*, 1: 63-67.
34. Bloom, M.E., P. Yaciuk, S. F. Hayes, S. M. Best, J. Lukszo, J. B. Wolfenbarger, **R. McKenna**, M. Agbandje-McKenna. 2001. Identification of Aleutian mink disease parvovirus capsid sequences mediating antibody-dependent enhancement of infection, virus neutralization and immune complex formation. *J. of Virol.*, 75: 11116-11127.
35. Brentlinger, K., S. Hafenstein, C.R. Novak, B.A. Fane, R. Borgon, **R. McKenna**, M. Agbandje-McKenna. 2002. Microviridae, a family divided. Isolation, characterization and genome sequence of a ϕ MH2K, a bacteriophage of the obligate intracellular parasitic bacterium *Bdellovibrio bacteriovorus*. *J. Bact.*, 184: 1089-1094.

36. An, H., C. Tu, D. M. Duda, I. Montanez-Clemente, K. Math, **R. McKenna**, P. J. Laipis, & D. N. Silverman. 2002. Chemical rescue in catalysis by human carbonic anhydrases II and III. *Biochemistry*, 41: 3235-3242.
37. Duda, D. M., C. Yoshioka, L. Govindasamy, H. An, C. Tu, D. N. Silverman, **R. McKenna**. 2002. Crystallization and preliminary X-ray analysis of human carbonic anhydrase III. *Acta Cryst.*, D58:849-852.
38. Bubb, M. R., L. Govindasamy, E. G. Yarmola, S. M. Vorobiev, S. C. Almo, T. Somasundaram, M. S. Chapman, M. Agbandje-McKenna, **R. McKenna**. 2002. Polylysine induces an antiparallel actin dimer that nucleates filament assembly. *JBC.*, 277:20999-21006.
39. Lian, W., L. Govindasamy, Y. Gu, T. Kukar, M. Agbandje-McKenna, **R. McKenna**, D. Wu. 2002. Crystallization and preliminary x-ray crystallographic studies on recombinant human carnitine acetyltransferase. *Acta Cryst.*, D58:1193-1194.
40. Tu, C., M. Qian, H. An, N. R. Wadhwa, D. M. Duda, C. Yoshioka, Y. Pathak, **R. McKenna**, P. J. Laipis, and D. N. Silverman 2002. Kinetic analysis of multiple proton shuttles in the active site of human carbonic anhydrase. *JBC.*, 277:38870-38876.
41. Reutzler, R., S. K. Boehlein, L. Govindasamy, R. B. Brenes, M. Agbandje-McKenna, S. M. Schuster, **R. McKenna**. 2002. Crystallization and preliminary X-ray analysis of the tumor metastasis factor p37. *Acta Cryst.*, D58: 2141-2144.
42. Duda, D.M., L. Govindasamy, C. Tu, M. Qian, M. Agbandje-McKenna, D. N. Silverman, **R. McKenna**. 2003. The refined atomic structure of carbonic anhydrase II at 1.05Å resolution: Implications of chemical rescue of proton transfer. *Acta Cryst.*, D59:93-104.
43. Kaludov, N., E. Padron, L. Govindasamy, **R. McKenna**, J. A. Chiorini, M. Agbandje-McKenna. 2003. Production, purification and preliminary X-ray crystallographic studies of Adeno-associated virus serotype 4. *Virology*, 306:1-6.
44. Wu, D., L. Govindasamy, W. Lian, Y. Gu, T. Kukar, M. Agbandje-McKenna, **R. McKenna**. 2003. Structure of human carnitine acetyltransferase: Molecular basis for fatty acyl transfer. *JBC.*, 278:13159-13165
45. Gumz, M. L., D. Duda, **R. McKenna**, C. S. Wingo, B. D. Cain. 2003. Molecular modeling of the rabbit colonic (HK α 2a) H⁺, K⁺, ATPase. *J. Mol. Model*, 9:283-289.
46. Lian W., Y. Gu, B. Pedersen, T. Kukar, L. Govindasamy, M. Agbandje-McKenna, S. Jin, **R. McKenna**, D. Wu. 2004. Crystallization and preliminary X-ray crystallographic studies on recombinant rat choline acetyltransferase. *Acta Cryst.*, D60: 374-375.
47. Casado, C.G., G.J. Ortiz, E. Padron, S. Bean, **R. McKenna**, M. Agbandje-McKenna, M. I. Boulton. 2004. Isolation and characterization of subgenomic DNAs encapsidated in "single" icosahedral particles of Maize streak virus. *Virology*, 323:164-171.
48. Reutzler, R., C. Yoshioka, L. Govindasamy, E. G. Yarmola, M. Agbandje-McKenna, M. R. Bubb, **R. McKenna**. 2004. Actin crystal dynamics: Structural implications for F-actin nucleation, polymerization and branching mediated by the anti-parallel dimer. *J. Structural Bio.*, 146:291-301.
49. Govindasamy, L., T. Kukar, W. Lian, B. Pedersen, Y. Gu, M. Agbandje-McKenna, **R. McKenna**, D. Wu. 2004. Structural and mutational characterization of L-carnitine binding to human carnitine acetyltransferase. *J. Structural Bio.*, 146:416-424.
50. Govindasamy, L., R. Reutzler, M. Agbandje-McKenna, **R. McKenna**. 2004. Structural determination of a partial hemihedral twinned actin crystal. *Acta Cryst.*, D60:1040-1047.
51. Govindasamy, L., B. Pedersen, W. Lian, T. Kukar, M. Agbandje-McKenna, D. Wu, **R. McKenna**. 2004. Structural insights and functional implications of choline acetyltransferase. *J. Structural Bio.*, 148:226-235.
52. Clemente, J.C., R. E. Moose, R. Hemrajani, L. R. S. Whitford, L. Govindasamy, R. Reutzler, **R. McKenna**, M. Agbandje-McKenna, M. M. Goodenow, B. M. Dunn. 2004. Comparing the accumulation of active site and non-active site mutations in the HIV-1 protease. *Biochemistry*, 43:12141-12151.

53. Padron, E., V. Bowman, N. Kaludov, L. Govindasamy, P. Nick, **R. McKenna**, J. A. Chiorini, T. S. Baker, M. Agbandje-McKenna. 2005. The structure of adeno-associated virus. *J. Gen. Virol.*, 79:5047-5058.
54. Fisher, S. Z., J. A. Hernandez Prada, C. Tu, D. M. Duda, C. Yoshioka, H. An, L. Govindasamy, D. N. Silverman, **R. McKenna**. 2005. Structural and kinetic characterization of active-site histidine as a proton shuttle in catalysis by human carbonic anhydrase II. *Biochemistry*, 44:1097-1105.
55. Beyer, B. B., J. V. Johnson, A. Y. Chung, T. Li, A. Madabushi, M. Agbandje-McKenna, **R. McKenna**, J. B. Dame, B. M. Dunn. 2005. Active site specificity of digestive aspartic peptidases from the four species of plasmodium that infect humans using chromogenic combinatorial peptide libraries. *Biochemistry*, 44:1768-1779.
56. Madabushi, A., S. Chakraborty, S. Z. Fisher, J.C. Clemente, C. Yowell, M. Agbandje-McKenna, J. B. Dame, B. M. Dunn, **R. McKenna**. 2005. Crystallization and preliminary X-ray analysis of the aspartic protease plasmepsin 4 from the malarial parasite *P. malariae*. *Acta Cryst.*, F61:228-231.
57. Elder, I., C.K. Tu, L.-J. Ming, **R. McKenna**, D. N. Silverman, 2005. Proton transfer from exogenous donors in catalysis by human carbonic anhydrase II. *Archives of Biochemistry and Biophysics*, 437: 106-114.
58. Ketcham, C. M., S. Anai, R. Reutzel, S. Sheng, S. M. Schuster, R. B. Brenes, M. Agbandje-McKenna, **R. McKenna**, C. J. Rosser, S. K. Boehlein. 2005. P37 Induces tumor invasivity. *Molecular Cancer Therapeutics*, 4:1031-1038
59. Bhatt, D., C. Tu, Z. S. Fisher, J. A. Hernandez Prada, **R. McKenna**, D. N. Silverman. 2005. Proton Transfer from His200 in Human Carbonic Anhydrase II. *PROTEINS: Structure, Function, and Bioinformatics*, 61:239-245.
60. Lane, M. D., N. Hyun-Joo, E. Padron, B. Whitaker, E. Kohlbrenner, G. Aslanidi, B. Byrne, **R. McKenna**, N. Muzyczka, S. Zolotukhin, M. Agbandje-McKenna. 2005. Production, Purification, Crystallization, and preliminary X-ray analysis of Adeno-Associated virus serotype 8. *Acta Cryst.*, F61: 558-561.
61. Kontou, K., L. Govindasamy, H-J Nam, N. Bryant, A. L. Llamas-Saiz, C. Foces-Foces, E. Hernando, M.-P. Rubio, **R. McKenna**, J.M. Almendral, M. Agbandje-McKenna. 2005. Structural determinants of tissue tropism and in vivo pathogenicity for the parvovirus minute virus of mice. *J. of Virology*, 79:10931-10943.
62. Duda, D.M. C.K. Tu, S.Z. Fisher, H. An, C. Yoshioka, L. Govindasamy, P. J. Laipis, M. Agbandje-McKenna, D. N. Silverman, **R. McKenna**. 2005. Human carbonic anhydrase III: Structural and kinetic study of catalysis and proton transfer. *Biochemistry*, 44:10046-10053.
63. DiMattia, M., L. Govindasamy, H. C. Levy, B. Gurda-Whitaker, A. Kalian, E. Kohlbrenner, J. A. Chiorini, **R. McKenna**, N. Muzyczka, S. Zolotukhin, M. Agbandje-McKenna. 2005. Production, Purification, Crystallization, and preliminary X-ray structural studies of Adeno-Associated virus serotype 5. *Acta Cryst.*, F61: 917-921.
64. Quint, P, R. Reutzel, R. Mikulski, **R. McKenna**, D. N. Silverman. 2006. Structure and catalytic inhibition of nitrated human Mn superoxide dismutase: Mechanism of inactivation in conditions of oxidative stress. *Free Radical Biology and Medicine*, 40:453-458.
65. Clemente, J. C., L. Govindasamy, A. Madabushi, R. E. Moose, C. A. Yowell, K. Hidaka, T. Kimura, Y. Hayashi, Y. Kiso, M. Agbandje-McKenna, J. B. Dame, B. M. Dunn, **R. McKenna**. 2006. X-ray crystal structure of the aspartic protease plasmepsin 4 from the malarial parasite plasmodium malariae bound to an allophenylnorstatine based inhibitor. *Acta Cryst.*, D62:246-252.
66. López-Bueno, A., M. P. Rubio, N. Bryant, **R. McKenna**, M. Agbandje-McKenna, J. M. Almendral. 2006. Host selection of subtle topological changes at the sialic acid binding pocket of the parvovirus capsid modulating cell binding affinity drastically determine virulence. *J. Virol.*, 80:1563-1573.

67. Budayova-Spano, M., S. Z. Fisher, M.-T. Dauvergne, M. Agbandje-McKenna, D. N. Silverman, D. A. A. Myles, **R. McKenna**. 2006. Production and X-ray crystallographic analysis of fully deuterated human carbonic anhydrase II. *Acta Cryst.*, F62: 6-9.
68. Fisher, S. Z., L. Govindasamy, C. K. Tu, M. Agbandje-McKenna, D. N. Silverman, H. J. Rajaniemi, **R. McKenna**. 2006. Structure of human salivary α -amylase crystallized in a C-centered monoclinic space group. *Acta Cryst.*, F62: 88-93.

Accepted:

69. Clemente, J.C., R.M. Coman, M.M. Thiaville, L.K. Janka, J.A. Jeung, S. Nukoolkarn, L. Govindasamy, M. Agbandje-McKenna, **R. McKenna**, W. Leelamanit, M.M. Goodenow, B.M. Dunn. Analysis of HIV-1 CRF_01 A/E Protease inhibitor resistance: structural determinants for maintaining sensitivity and developing resistance to atazanavir. *Biochemistry*

Chapters:

1. Agbandje, M., **R. McKenna**. 1992. Comparative studies of intercalative DNA-drug interactions using molecular modelling and biophysical techniques. pp. 525-556. In Propst, C.L., Perun, T.J. (eds.). *Nucleic Acid Targeted Drug Design*. Marcel Dekker, Inc.
2. Rossmann, M. G., **R. McKenna**, L. Tong, D. Xia, J. Dai, H. Wu, H. Choi, D. Marinescu, R. E. Lynch. 1992. Molecular replacement real space averaging. In *Molecular Replacement*. pp. 33-48. In Dodson, E., Gover, S., Wolf, W. (eds.) *Proceedings of the CCP4 study weekend, 31 January - 1 February, 1992*. Science and Engineering Research Council, Daresbury, UK.
3. Chapman, M. S., E. Blanc, **R. McKenna**, S. Munshi, M. G. Rossmann, J. Tsao. 1998. Use of non-crystallographic symmetry for ab initio phasing of virus structures. pp. 433-442. In Fortier, S. (ed.), *NATO Advanced Study Institute on Direct Methods for Solving Macromolecular Structures*, Kluwer, Dordrecht, Netherlands, Erice, Italy.
4. **McKenna, R.**, L. Faulkner. 2000. *Virus Structure*. Encyclopedia of Life Science, Macmillan Reference Ltd.
5. Agbandje-McKenna, M., A. Edison, **R. McKenna**. 2003. Biophysical techniques. pp 269-290. In Davey, J., Lord, M. (ed.). *Essential Cell Biology Volume I: A Practical Approach*.
6. Duda, D. M., **R. McKenna**. 2004. Carbonic anhydrase, α -class, pp 249-263. In Messerschmidt, A. (ed.). *Handbook of metalloproteins*. John Wiley & sons, Ltd, New York. USA.