

A Profile of the CCP13 R.A., Dr Mark Shotton



Mark Shotton graduated in physics from Imperial College, University of London, in 1992, and then went on to spend 18 months as an accountant before coming to his senses and commencing postgraduate work in the Keele University Physics Department in 1994. His time at Keele was spent in the molecular biophysics group, studying DNA structure and hydration by complementary neutron and X-ray fibre diffraction, under the guidance of Dr Trevor Forsyth and Professor W. Fuller.

Mark's main research interest was in analysing the specific patterns of ordered water that stabilise the various conformations adopted by the DNA double helix. Ordered water networks surrounding DNA were identified through high-angle neutron fibre diffraction experiments conducted using instrument D19 at the Institut Laue-Langevin with a monochromatic beam of neutrons of wavelength $\approx 2.4\text{\AA}$ (the D19 instrument is described in detail on pages 17 to 24). These experiments all utilised the ability to isotopically replace H_2O by D_2O in the sample, leading to decreased sample absorption and incoherent scattering and making use of the large coherent neutron scattering length of deuterium in order to image ordered water sites. The A and B conformations of natural DNA [1-3] and the A and D conformations of poly[d(A-T)].poly[d(A-T)] were all studied using this technique. Figures 3 and 4 on pages 20 and 21 show the ordered water sites

identified around the A conformation of perdeuterated *E. Coli* DNA and the B conformation of hydrogenated calf thymus DNA.

Mark began work as the CCP13 R.A. in May 1998. A description of the software that has been developed since then is included on pages 40 to 44. Additionally, in response to increasing user demand, it has been possible to release Linux versions of all programs in the CCP13 suite and it is in Mark's brief to support Linux versions of all future CCP13 software. The news of software upgrades is e-mailed to the CCP13 bulletin board (to subscribe, send "subscribe ccp13bb" to majordomo@dl.ac.uk) and is included in the *Latest News* section of the new-look CCP13 web pages at

<http://www.dl.ac.uk/SRS/CCP13>.

If you encounter any difficulties with CCP13 software, or have any suggestions for possible improvements, please contact Mark by e-mail to m.shotton@dl.ac.uk, or phone (01925) 603626.

References

- [1] Shotton, M.W., Pope, L.H., Forsyth, V.T., Langan, P., Denny, R.C., Giesen, U., Dauvergne, M.-Th. and Fuller, W., *Biophysical Chemistry* (1997) **69** (1), 85-96.
- [2] Pope, L.H., Shotton, M.W., Forsyth, V.T., Langan, P., Denny, R.C., Giesen, U., Dauvergne, M.T. and Fuller, W., *Physica B* (1998) **241-243**, 1156-1158.
- [3] Shotton, M.W., Pope, L.H., Forsyth, V.T., Langan, P., Grimm, H., Rupprecht, A., Denny, R.C. and Fuller, W., *Physica B* (1998) **241-243**, 1166-1168.

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