# **KEMRI-Wellcome Trust Research Programme (KWTRP)**

### by Etienne de Villiers



The KEMRI-Wellcome Trust Research Programme, KWTRP (http://www.kemri-wellcome.org/), was formally established in 1989 as a partnership between the KEnyan Medical Research Institute (KEMRI), Oxford University and the Wellcome Trust.

It conducts basic, epidemiological and clinical research in parallel, with results feeding directly into local and international health policy, and aims to expand the country's capacity to conduct multidisciplinary research that is strong, sustainable and internationally competitive. Strong community links are at the heart of the Programme, with a particular

emphasis on capacity building and training to build scientific leadership.

The advent of Next Generation Sequencing (NGS) platforms has opened exciting new research avenues to life scientists. To support application of NGS within the Programme, the KWTRP-Bioinformatics Core (KBiC) was established with the aim to provide a single point of contact for computational biology, providing a venue for applying genomic approaches to basic biology, epidemiology and bioinformatics to develop novel approaches to improve human health. By providing KWTRP researchers with access to a bioinformatics infrastructure and expertise, the KBiC opens new areas of research, enhances the quality and consistency of high-throughput data analysis, and improves the Progamme's ability to support research in this area.

As a further important commitment, the core periodically organises courses and workshops in order to train biologists in the implementation of the main bioinformatics tools in their research.

#### Contact:

http://www.kemri-wellcome.org/index.php/en/contact\_page



## Protein structure databases and resources at the CMBI

### by Gert Vriend

Many of 'us' are involved in some form of analysis. but the **EMBnet** community also includes protein structure bioinformaticians. When crystallographers or NMR spectroscopists solve macromolecular structures, the coordinates must be made available before publication. The international wwPDB collects these structures, annotates them and releases them to the world in formatted, keyword-based PDB files - PDB's data collection started back when data storage was done with punched cards, so the PDB format is still fixed at 80 characters per line.

PDB files are routinely used in biomedical research. Unfortunately, they all contain errors owing to poor data, human error, the fact that supercomputers once had less CPU power than today's mobile phones, and that we didn't know so much about protein structures back then. We therefore set out to use today's software and computers to redo all PDB files [1]. The results are available in the PDB REDO database. We can't correct all errors, so we release error reports for all PDB files in the PDBREPORT database [2]; we also maintain DSSP [3], holding records of secondary structures for each proteincontaining PDB file, and HSSP [4], containing sequence alignments for all proteins. For those wanting to search the PDB, we maintain PDBFINDER [5], which holds the essential

metadata of PDB entries in an easy-to-parse format. And our user-friendly MRS [6] search engine can, in <1 second, query all these databases. For nucleic acid structures, where DSSP, HSSP, etc. files don't exist, the WHY\_NOT server [7] explains why a file is missing.

These databases (some from before the Internet) are regularly maintained. For users who want other things, we made a series of ~60 Web servers [8,9], and will make new servers upon request; and if you want to perform structure calculations on large numbers of files, you can get programmatic access to our software through Web services [10] – we also write Web services on request. All of these and other resources are available via http://swift.cmbi.ru.nl/gv/facilities/. It's no longer the same hardware, but swift was one of the first 2,000 computers attached to the Internet, and certainly the first computer ever on the Internet to provide bioinformatics services. I'm not sure if that makes me sad or happy.





### EMBnet Workshop & AGM 2014, Lyon, FR

#### by Teresa K. Attwood

EMBnet's 2014 AGM and associated events were hosted in the Hôtel de la Cité and on the Doua campus of the University of Lyon, from 26 to 30 May. Included were a 1-day tutorial entitled "From NGS data through the third dimension towards new agrochemicals and drugs"; the 2-day Bioinformatics for Environmental Genomics workshop of the Pluridisciplinary Thematic Network in Environmental Genomics; a 1-day EMBnet workshop; and the traditional business meeting.

These were stimulating events, serving to highlight the achievements of the last year, and how much remains to be done (full details will be reported in *EMBnet.journal*). Discussions were wide-ranging and productive: it was agreed to: i) review the structure and membership of the Committees, publish their current and future projects on the website, and deliver tangible outcomes; ii) create a Fellowship Programme; iii) formulate details of a Service Award scheme; iv) organise a meeting alongside the final AllBio AGM, to discuss development of global bioinformatics MSc curricula; v) invite members of target groups to join EMBnet, following the launch of the Fellowship Programme; and vi) develop a core for future tutorials, and ground rules for running and hosting them, aiming to expand the programme and recover costs.

The work of the last year has been led by a group of dedicated individuals, who are responsible for running *EMBnet.journal*, coordinating AllBio and SeqAhead, leading GOBLET, and championing EMBnet's PR activities. This year, we celebrated the arrival of a new individual member, Axel Thieffry, whom we hope will help to drive some of EMBnet's new initiatives forward, and especially to inspire and recruit more members!

As always, there's more to be done. We therefore warmly encourage you to contribute your energies and visions to EMBnet, to ensure its continued success as the Global Bioinformatics Network!





EMBnet.Spotlight is a quarterly release of InFocus sections published in EMBnet.digest (<a href="https://www.embnet.org/embnet-digest">www.embnet.org/embnet-digest</a>), EMBnet's monthly publication that provides a round-up of news from the community. The InFocus section features member activities, projects, initiatives, etc., especially from

new members, that may be of interest both to the network and to EMBnet's associated communities, societies and projects.