

Volume 9 Nr. 3 December 2003

Training and education with EMBnet

- Australian & New Zealand undergraduate
- degrees in Bioinformatics

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- Bioinformatics in Latin America
- MacOSX and Bioinformatics (part 3)
- EMBnet E-meeting portal

HITAI

Volume 9 Nr. 3

ditorial

Education is one of the key component of the EMBnet community. Not only we have thousands of users around the world that are participants in our EMBnet courses and training sessions, but most of us organise and participate in the teaching of many academic degrees in bioinformatics.

Two articles in this issue examplify this. One describes the current situation of the bioinformatics degrees in Australia and New-Zealand, whereas the second explains the role of the E&T PC (Education and Training Program Committee) and details our new web submission tool for course organisers. Latin America is also very active in the Bioinformatics fields as demonstrated by a review of the non-EMBnet groups.

Don't miss also the last part of our MacOSX and Bioinformatics series. Finally a little report with some pictures of our last AGM in Poland.

The editorial board: Erik Bongcam-Rudloff, Laurent Falquet, Pedro Fernandes, Oscar Grau, Goncalo Guimaraes Pereira

Protein Spotlig

Protein Spotlight (ISSN 1424-4721) is a periodical electronic review from the SWISS-PROT group of the Swiss Institute of Bioinformatics (SIB). It is published on a monthly basis and consists of articles focused on particular proteins of interest. Each issue is available, free of charge, in HTML or PDF format at http://www.expasy.org/spotlight

We provide the EMBnet community with a Oscar Grau, IBBM, AR printed version of issue 40. Please let us know if you like this inclusion.

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Cover picture: a zinc cast of the sculpture by Konstanty Hegel, made in 1855. Syrena, Old Town (Stare Miasto) Warsaw, September 2003 [® Laurent Falquet]

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New **Zealand** Australian 8 undergraduate degrees ĪN **Bioinformatics**



S.K. Cattley

Australian National Genomic Information Service University of Sydney Camperdown 2006, NSW, Australia

Abbreviations:

UWA (University of Western Australia), UNSW (University of New South Wales), USQ (University of Southern Queensland), UofW (University of Wollongong),USyd (University of Sydney), Flinders (Flinders University of South Australia), La Trobe (La Trobe University), Macquarie (Macquarie University), QUT (Queensland University of Technology), UQ (University of Queensland), ANU (Australian National University), Melbourne (University of Melbourne), Massey (Massey University, NZ), Auckland (University of Auckland, NZ).

In Australia and New Zealand there has been a movement away from general science to more specialized degrees. Bioinformatics has been a hot topic for the past 5 years and as such, a number of bioinformatics degrees have been instigated. For students in next years intake there are eight specialized undergraduate bioinformatic degrees to choose from and another seven bioinformatic streams/majors within existing Bachelor of Science degrees.

The subject content between and within these degrees is not uniform. In this analysis, the degrees were examined to enable a comparison of the relative strengths and weaknesses in the curricula. Most of the degrees included a number of electives. In some cases only one or two electives were permitted but in other instances electives consisted of more than 50% of the entire degree. A graph of the proportion of elective subjects in each of the degree is given in Figure 1. Five of the degrees allowed for no variation. The majority of the dedicated

L University of Queensland

N Massey University (NZ) O University of Auckland (NZ)

M Queensland University of Technology

different subject area (biology, computer, statistics, mathematics, bioinformatics, other). 100 A University of Sydney **B Flinders University** C University of New South Wales 80 D La Trobe University E University of Southern Queensland F University of Western Australia 60 G University of Wollongong H Macquarie University I University of Melbourne 40 J Australian National University (B.Biotechnology) K Australian National University (B.Computational Science)

Figure 1: Ratio of compulsory to elective subjects in undergraduate bioinformatic degrees in Australia and New Zealand Elective component indicates the portion of subjects that can be taken from

AΒ CDEFGHIJKLMN \cap # Bioinformatic stream within general computer science or biotechnology degree.

Compulsory subject %

Elective subject %

20

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course content to vary depending on the students own interest. Two degrees allow 50% or more of the subjects to be chosen by the student.

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The fifteen degrees were examined from the websites listed in the appendix and six subject areas were chosen as markers for course content. Due to the differences in the number and choice of electives between the degrees the compulsory curricula only were used in the comparison.

- Bioloaical Sciences includes biology and chemistry subjects.
- Computer Science includes programming, computer studies and other subjects generally taught by the Department of Computer Science.
- Statistics includes all statistic and probability subjects.
- Mathematics includes mathematical subjects not covered in the area of statistics.
- Subjects that included a combination of biology and computer science (e.g. or Bioinformatic project) and/or were titled bioinformatics were grouped into the area Bioinformatics.
- that ranged from ethics, project management, experimental design and language comprehension through general electives outside the Faculty of Science.

While each of the courses surveyed contains a number of biological science and computer science subjects, the number of mathematics, statistics and bioinformatic subjects vary greatly and are even absent in some degrees. Figure 2. Statistics as nations). a compulsory was absent from three degrees (Sydney, Flinders, Melbourne) while mathematics was absent from two degrees and Macauarie). (Sydney Dedicated Bioinformatic courses were not present in four degrees (Maquarie, La Trobe, USQ and Melbourne).

degrees allow around 10-20% of the total This last omission is surprising. In all cases the computer science and biological science subjects are taught by different departments. Only in the bridging bioinformatics subjects are the students exposed to a field of study where all the information they have learnt from biology, computer science, mathematics and statistics can be integrated together into one unit. Without this subject incorporated into the curricula the student is required to make these connections themselves.

> The greatest variation observed occurs with the proportion of each subject area. all Invariably the largest portions are dedicated to biological and computer science subjects. The actual proportions vary from between 25% (UNSW) through 60% (ANU) for biological science and 15% (ANU) through 50% (Melbourne) for computer science. The other subject areas also show variation. With selection of elective subjects, the proportions can change slightly. This can result in two students who undertake the same degree but graduate with vastly different levels of knowledge.

phylogenetics, micro array analysis. The explosion of bioinformatics degrees in Australia has already resulted in a casualty. In 2003, University of Western Sydney instigated a Bachelor of Science (Bioinformatics) but The area Other, included subjects this was cancelled after just one year. It is important that the bioinformatics degrees we already have fill a specific niche or produce a particular kind of graduate in order to guarantee themselves a long life. For instance, UNSW is a computer engineering designed towards producing degree computer programmers, USQ almost fills the niche of a distance education degree, Massey and Auckland fits in the geographic need for bioinformatics education New Zealand (and surrounding South Pacific

Appendix:

URL references bioinformatics degrees and streams:

Australian National University http://wwwmaths.anu.edu.au/bio.html

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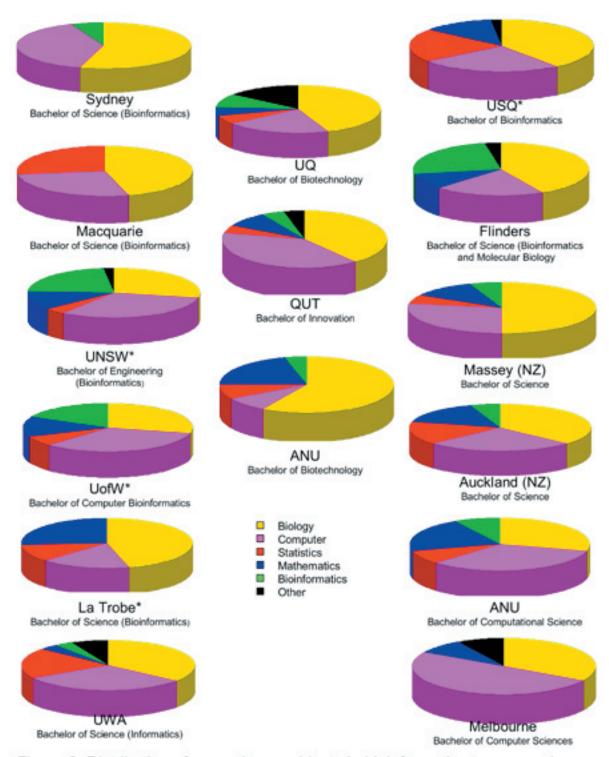


Figure 2: Distribution of compulsory subjects in bioinformatic streams and degrees available at Australian and New Zealand universities in 2004. All are 3 year degrees except those marked * which are 4 year

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Curtin University

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http://handbook.curtin.edu.au/
courses/30/301135.html

Flinders University

http://www.scieng.flinders.edu.au/

courses/bioinformatics/

La Trobe University

http://www.latrobe.edu.au/
handbook/scitech/stbsbb.htm

Macquarie University

http://www.hscandbeyond.com.au/ bio.htm

Massey University

http://study.massey.ac.nz/
major.asp?major_code=2511&prog_
code=92411

Queensland University of Technology

http://www.studyfinder.qut.edu.au/cgibin/WebObjects/StudyFinder

Use search term bioinformatics

Royal Melbourne Institute of Technology http://www.cs.rmit.edu.au/courses/

postgraduate/escience/

University of Melbourne

http://www.cs.mu.oz.au/courses/ugrad/ bcsbioinf.html

University of New South Wales

http://www.eng.unsw.edu.au/prospect/ ug/be/bio.htm

University of Queensland

http://www.uq.edu.au/study/
plan.html?acad_plan=BIOINX2055

University of Southern Queensland

http://www.usq.edu.au/handbook/2003/
BBIN.html

University of Sydney

http://www.science.usyd.edu.au/future/ ug/bsc-bio.html

http://www.scifac.usyd.edu.au/future/
pg/pgc bioinform.html

University of Western Australia

http://www.publishing.uwa.edu
.au/handbooks/2003/sciences/
BScInformatics.html

University of Wollongong

http://www.uow.edu.au/discover/ courses/yr2002/bcompbioinf.html

University of Auckland, New Zealand

http://www2.auckland.ac.nz/science/ subjects/bioinform.ptml

Bioinformatics in Latin America



Oscar Grau

EMBnet node manager IBBM, Facultad de Cs. Exactas, Universidad Nacional de La Plata Argentina

Introduction

Bioinformatics, as other emergent areas of science, has had a lag period to be established in the Region; however, in some countries it has sprung vigorously accompanying genetic engineering and genomic projects.

The contacts with members of EMBnet have been instrumental for the consolidation of the Cuban (http://www.cu.embnet.org/) and Argentinean (http://www.ar.embnet.org) nodes which had been providing services since the early 90s and later on for the Mexican (http://embnet.cifn.unam.mx), Colombian (http://bioinf.ibun.unal.e du.co), Chilean (http://www.embnet.cl) and Brazilean (http://www.br.embnet.org) nodes.

Inspired in the network organization of EMBnet and following the mandate of RELAB (Latin American Network of Biological Sciences) and with the sponsorship of FAO and BIOLAC a meeting was conveyed in Rio de Janeiro in June 2001. Then, a Latin American Bioinformatics Network project was elaborated and proposed to UNU-BIOLAC (United Nations University-Biotecnology for Latin America and the Caribbean, figure 1) for support. It includes members from Argentina, Bolivia, Brazil, Chile, Colombia, Cuba, Mexico and Venezuela, and provides an efficient clearhouse for information. http://www.lacbionet.org

In 2002 an Ibero-american network was proposed to CYTED (Ciencia y Tecnologia para el Desarrollo) and, as a consequence, a preparatory meeting was held in Buenos

a preparatory meeting was held in Buenos Aires in March 2003. A symposium, in which 24 members of 10 countries of Latin America

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and Spain presented their interests and results in Bioinformatics was held at the same time.

A project was elaborated and submitted to CYTED for support. All participants agreed to join efforts with the Latin American Network and coordinate activities. T. cruzi y G. lamblia proteins having capacity of interaction with the DNA or participation in the initiation complex. In the area of analysis of microarray data, they work in the

These iniciatives are fully operative at the moment and more details can be observed in the site http://portal-bio.ula.ve

Further information about EMBnet nodes from Argentina, Brazil, Colombia, Cuba, Chile and Mexico can be found on their respective web site and in the links provided by EMBnet at: www.embnet.org

A short description of other groups follows:

Argentina:

In Rosario, the Center of Computational Biology is a recent initiative of the Molecular Biology Institute and the Faculty of Exact

Sciences and Engineering of the National University of Rosario. They are interested in the design of motif detection algorithms for T. cruzi y G. lamblia proteins having capacity of interaction with the DNA or participation in the initiation complex. In the area of analysis of microarray data, they work in the design of classification algorithms based on error correcting codes and in the design of biclustering algorithms suitable for capturing coregulation mechanisms in circadian genes expression. In the present year the first course on Introduction to Bioinformatics will be offered.

The Bioinformatics Group at the Institute of Biotechnology, University of General San Martín, current interest is to develop an automated sequence analysis pipeline, customized to the unique features of singlepass sequences like ESTs and GSSs. This currently includes: clustering of sequence



Figure 1. LacBioNet home page

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data and analysis of the resultant nonredundant datasets to discover new genes. The focus is on annotation and prediction of function. Their laboratory is also interested in regulation of gene expression in trypanosomatids characterizing motifs and regulatory signals present in the UTRs of mRNAs. They provide access to two standalone sequence analysis suites through a web server: Paul Stothard's 'Sequence Manipulation Suite (SMS)' and Malay Basu's 'Sequence analysis using Web Resources (SeWer)'.

At the computing department of the University of Buenos Aires there is a database of repeat elements for Trypanosoma Cruzi, T. brucei and Leismanias and they offer undergraduate and postgraduate courses on Bioinformatics.

At the University of Quilmes, a course for graduate students in offered and an enterprise "Digital genes" offers access to EMBOSS and a limited group of services.

Bolivia

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Universidad Católica Boliviana, Cochabamba IIIA - Instituto de Investigación en Informática Aplicada.

They have developed the PC version MELANIE (Medical ELectrophoresis ANalysis Interactive Expert) project in collaboration with several Swiss institutions.

Also, they have migrated the protein database EXPASY to a Linux platform and installed a mirror at http://bo.expasy.org

They have also developed new Bioinformatics tools for sequencing and identifying proteins by mass spec.

Brazil

Besides the four laboratories that constitute the EMBnet node there are very many sites developing Bioinformatics.

For brevity only a list is included, but their coordinates can be found at http://www.lacbionet.org

- **Belo Horizonte**: DCC - Departamento de Ciências da Computação da Universidade Federal de Minas Gerais, Laboratório de Biologia Computacional do Departamento

de Bioqúimica e Imunologia da Universidade Federal de Minas Gerais, Laboratório de Computação Heurística, Núcleo de Bioinformática da Universidade Federal de Minas Gerais.

- **Brasília**: Embrapa - Genetic Resources and Biotechnology - Bioinformatics Laboratory, Bioinformatics Laboratory at Universidade Católica de Brasília, Projeto de BioInformática do Laboratório de Química Computacional da Universidade Federal de Brasilia.

- **Campinas**: Departamento de Genética e Evolução - IB - Unicamp. Instituto de Computação Universidade Estadual de Campinas, Laboratório de Bioinformática da Universidade de Campinas, Laboratório Nacional de Luz Síncrotron,. Sting Millennium Suite - Structural Bioinformátics Group - EMBRAPA/CNPTIA

- **Curitiba**: Laboratório de Bioinformática do CEFET - PR, Tecpar -Instituto de Tecnologia do Paraná.

- Florianópolis: Laboratório de Bioinformática da Universidade Federal de Santa Catarina.

- **Foz do Iguaçu**: LABI - Laboratório de Bioinformática.

- **Recife**: CIn - Centro de Informática da Universidade Federal de Pernambuco GENOMA/PE - cana-de-açúcar.

- **Rio de Janeiro**: Biologia Matemática e Computacional, LNCC - Laboratório Nacional de Computação Científica, Federal University of Rio de Janeiro, Instituto Virtual de Bioinformatica e Modelagem de Biossistemas, Pontifícia Universidade Católica do Rio de Janeiro - Departamento de Informática, FIOCRUZ - Fundação Oswaldo Cruz.

- **Porto Alegre**: LabBioInf - Laboratório de Bioinformática da Universidade Federal do Rio Grande do Sul, Ana Lúcia C. Bazzan -Laboratório de Informática da Universidade Federal do Rio Grande do Sul, Federal University Rio Grande do Sul.

- **São Carlos**: Laboratório de Inteligência Computacional.

- São Leopoldo: Laboratório de Bioinformática e Biologia Computacional.

- **São Paulo**: ICMC - Instituto de Ciências Matemáticas e da Computação

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da Universidade de São Paulo, IME - Instituto de Matemática da Universidade de São Paulo, Laboratorio de Bioinformatica do Instituto de Química da Universidade de São Paulo, Laboratório de Bioinformática - Hospital do Câncer - AC. Camargo, Laboratório de Biologia Computacional do Instituto Ludwig, LEMB - Laboratório de The University of Talca has implemented Evolução e Bioinformática, NIB - Núcleo de Informática Biomédica da Universidade de Campinas, BIOINFO - Núcleo de Pesquisas em Bioinformática da USP.

- Vicosa: Biologia Molecular Computacional da Universidade Federal de Vicosa

Cuba

The Centro Nacional de Bioinformática informaticians (BIOINFO, http://www.bioinfo.cu) was created in October 2001 in the Ministerio de Ciencia Tecnología y Medio Ambiente (CITMA). Their interests are focused in developing artificial intelligence tools for data mining, interaction databases and annotation. They have a server (http: //www.bioinfo.cu/iPPI.html) for the prediction and modelling of proteins and their particular interest is the prediction of the affinity of peptides to MHC class II.

Chile

The "Laboratorio de Bioinformática Matemática del Genoma" (LBMG) is located Calculo Científico Universidad de Los Andes in the Centro de Modelamiento Matemático (CMM) from Facultad de Ciencias Físicas v de Matemáticas, Universidad de Chile, Its main interests are: automatic genome annotation, microarrays analysis, metabolic pathway modelling and regulation, in particular The server offers support for analyzing DNA in bacteria involved in biolixiviation of minerals.

http://www.dim.uchile.cl/~genoma/ proyectos.shtml

At the Pontificia Universidad Catolica de Chile, Facultad de Ciencias Biologicas, Depto. Genetica Molecular y Microbiologia, at CeCalCULA in Mérida, Venezuela Molecular Bioinformatics Laboratory, the http://www.cecalc.ula.ve/bioinformatica. main interest is focused in Computational Biology, Protein Structure and Function, Prediction and interaction of them with other

elements. They provide access to ANOLEA, a program to assess the quality of a threedimensional protein structure that uses a statistical potential at the atomic level and gives an energy profile as output.

http://protein.bio.puc.cl/index.html

an undergraduate career in Bioinformatics based on the Faculty of Engineering and the Institute of Plant Biology and Biotechnology. The aroup is interested in data mining and visualization of macromolecules.

Uruguay

Very recently, a group of experimental and theoretical biologists as well as created consortium a named CUBIC (Consorcio Universitario de Bioinformática y Biología Computacional) to develop infrastructure, an undergraduate carreer in Bioinformatics and a postgraduate programme in computational biology.

http://bioinformatics.fq.edu.uy/cubic/ index.shtml

Venezuela

"Servidor de Bioinformatica" a Venezuelan Bioinformatics Server is a strategic alliance involving an interdisciplinary partnership of four Venezuelan institutions. It is a shared y effort between the Centro Nacional de (CeCalCULA), The Instituto Venezolano Investigaciones Cientificas (IVIC), Corporacion Parque Tecnologico de Merida (CPTM), and Universidad de Los Andes (ULA).

data, protein sequences, prediction of three-dimensional structures (protein and epitopes), development of web interfaces for biological software, data-mining of genomic data, and informatics tools for educational and research exchange among collaborators. This server is physically located

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E&T PC Training with EMBnet

The Education and Training Committee currently comprises four members based at three different institutes. Martin Bishop and Lisa Mullan are resident at the HGMP-RC (Human Genome Mapping Project Resource Centre), UK, where Martin is head of the Bioinformatics Division, and Lisa is involved in coordinating and teaching the various courses in the HGMP-RC training schedule. Janet Kelso is involved in the Stack Database at SANBI (South African National Bioinformatics Institute) and Isabel Margues coordinates administration for the Bioinformatics courses at the Gulbenkian Institute in Oeiras, Portugal alongside assisting researchers across the country with their bioinformatics queries.

Our mission is to hold the funds that are reserved for training from the EMBCORE grant and offer them to EMBnet members wishing to run bioinformatics training courses for students in their own, and EMBnet communities. Many successful courses have been run over the years, emphasis is slowly shifting away from introductory courses and more towards specialist courses. This is indicative of a community becoming more familiar with the area of bioinformatics tools.

Further money (Stichting funding) is available for those nodes outside the EU member countries, although it is not in such plentiful supply and subject to greater revision.

Courses tend to offer training to at least 20 students (although in the case of China, 120 students were taught by six trainers) and the training is generally conducted by two or three colleagues. Specialist courses may involve a lower ratio of trainers to students.

I have personally been involved in several courses across the world due to invitations to teach from the EMBnet community, and I am grateful to them all. It is a pleasure to be hosted by those interested in both enhancing the range of training offered in their country and wanting to explain their culture and customs to a foreigner. Also the students

must be applauded for their willingness to be taught in English. As a member of the ET committee, it is also important for me to see that the money has been well spent!

Last year (2002) the ETPC supported seven courses at a grand total cost of \notin 40,800 this represented courses supported by both EMBCORE and Stichting funding. Only six institutes applied for this support.

We now have an absolute fortune of more than €100K to spend and we must do so before December 2004. We have already funded several courses but we need applications for more! Specialist courses would be nice, but we understand that introductory courses still play a very important role in the training for students of all countries. We offer to cover 50% of the course costs and there is no restriction on the funding, however each application is reviewed by the training committee who will exercise judgment on the necessity for the award. Come and join the regular band who use EMBnet money to support their training!

Fortunately the process for proposing a course is now made easy by a web interface. First of all we set up a list of available lecturers with their topic of interest. This can be very

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	fane	Donate of experime	Languages	inside the
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		Sequence Analysis, Protein domains and function, EMBOSS, Per Foster member of the PROSITE team	Franch, English	Extent Instanted
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	The second	Sequence Analysis, EXECUS, Searcherg delationer, Parnine sequence compariser, Sequence databast searching by similarity Base interaction to the 3D structure of proteins	English	Deuro EMBort Stole
	1888 A.B. Laurineen 월 -31 317 484214 쇼 -31 317 48534	Beaurice Analysis, Phylogen, COSESCO, ERE, ODECHNIK, UNXYME	Datin, English, Damat, very dim Famph	Centra Sar Mancula and Bucculaular Informatica Control

Figure 1. Lecturers list

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Figure 2. Index page

useful when a course organiser is looking for a teacher in a particular domain (figure 1): http://www.embnet.org/php/lecturers.php

Every node manager can propose a course using its authentification (username/ password) to access our internal pages: http://www.embnet.org/php/index.php

Please follow this rule:

- File a course proposal
- Wait for approval by ETPC
- Fill out the contract
- Run the course
- File the report for the course
- Send a formal reimbursement request

By clicking on the button "Create course proposal" (figure 2), you will be asked to fill a form (figure 3) and click the "Send course proposal to ETPC" button. After a while you will receive an email from the ETPC to inform

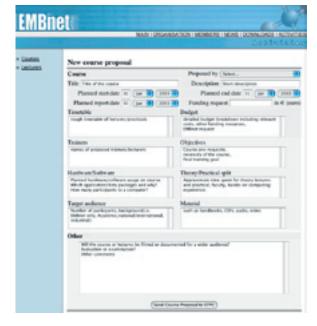


Figure 3. Course proposal form



Figure 4. Courses status page

you about the status of your proposal. Should you not receive this email, you can check the current status of your course on the courses page (figure 4):

http://www.embnet.org/ET/courses.php

Once your course is approved you must fill in the contract with either EMBCORE (EU countries) or Stichting (non-EU countries). http://www.embnet.org/EMBCORE/GrantMa nagementstructure.php

You can now run your course, ask your participants to fill in the evaluation form http://www.embnet.org/ET/questionnaire.php

Finally you must file a report (figure 5) using the web form accessible from the index page (figure 2) and send a reimbursement request to EMBCORE or Stichting manager.

Lisa Mullan & Laurent Falquet



Figure 5. Course report form

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AGM03:EMBnet annual general meeting 2003 in Poland

The EMBnet community met in Warsaw beginning of last september for its 17th Annual General Meeting (AGM03).

The meeting was hosted by the Polish EMBnet node team and its node manager, Piotr Zielenkiewicz, did a great job. The meeting was held at the Institute of Biochemistry and Biophysics of the Polish Academy of Sciences.

The session was conducted by the chairman Jack Leunissen. The usual administrative procedure took place with a very dense discussion on the future of EMBnet organisation. Several proposals were discussed and the nodes agreed to organise workshops on different topics in 2004 (see list next page).

Elections:

Executive Board

Erik Bongcam-Rudloff (SE) chairman (new) Martin Grabner (AT) secretary Sandor Pongor (ICGEB) treasurer Terri Attwood (UMBER) member



Education & Training PC

Martin J. Bishop (UK) chairman Isabel Marques (PT) secretary Lisa Mullan (UK) treasurer Rob Harper (FI) member (new)

Technical Management PC

José R. Valverde (ES) chairman Nils-Einar Eriksson (SE) secretary Kristian Vlahovicek (ICGEB) treasurer Endre Barta (HU) member (new)

Publications & Public Relation PC

Gonçalo Guimarães Pereira (BR) chairman Pedro Fernandes (PT) secretary Laurent Falquet (CH) treasurer Oscar Grau (AR) member (new)



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Planned Activities for 2004

Workshops

January 29: EMBER - a European Multimedia Bioinformatics Educational Resource, Amsterdam NL. attwood@bioinf.man.ac.uk

February 2-5: EMBOSS, ICGEB Trieste IT. kristian@icgeb.org

April 22-23: Videoconferencing systems, CSC Espoo FI. eija.korpelainen@csc.fi

May 5-7: Regulatory sequence motif discovery, LCB Uppsala SE. Erik.Bongcam@lcb.uu.se

May 27-28: Web-services, ETI NL. marc@eti.uva.nl

August 30-31: BioMinT - Biological Text Mining Summer School, Geneva CH. attwood@bioinf.man.ac.uk

September 16: Collaborative EMBnet workshop day. In connection with the AGM. Brussels, BE. rherzog@dbm.ulb.ac.be

date to be announced

Federating the SRS servers within the EMBnet infrastructure, BE or UK. rherzog@dbm.ulb.ac.be

Meetings

February 25-27: EMBnet Interim meeting, Volendam NL. asfra@asfra.nl

September 16-19: Annual General Meeting ment
(AGM), Brussels, BE.
rherzog@dbm.ulb.ac.beCiner

For more detailed information, consult our from: web site: http://www.embnet.org

Announcements

Visitor at BEN

BEN (Belgium EMBnet Node) welcomes Viorica Ghita who will act as bioinformatics teacher within the EMBER project. She will be with us between November 1 2003 and January 31 2004.

CINEMA 5 beta release

Cinema 5 (Colour INteractive Editor for Multiple Alignments) is an interactive visual tool for the interpretation and manipulation of protein and DNA sequences. Cinema 5 allows the user to interactively construct and edit and visualise multiple sequence alignments. It provides a highly intuitive, flexible and userfriendly interface with many features:

Intuitive mouse-controlled interface for navigating and editing an alignment
Optimised rendering for large sequences
Multiple different alignments may be opened for editing simultaneously

- Many views can be created simultaneously onto a single alignment

- Support for many popular protein file formats

- Breakpoints allow aligned sections to be protected from edits elsewhere in the sequence

- Flexible zoom controls allow an alignment to be visualised at varying levels of detail

- Hierarchical grouping to simplify editing tasks

- Flexible sub-sequence searching allowing wildcard and fuzzy searching using customisable substitution matrices

- Advanced editing tools, such a hierarchical sequence groups & search-guided alignment

Cinema 5 is available for Linux, Windows and Mac OS X, and can be downloaded for free from:

http://aig.cs.man.ac.uk/utopia/download

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Aquide on how to install Bioinformatics version number is 10.3 and its code name is tools on MacOSX (part III)





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Introduction

Today, the desktop of a typical researcher in Life Sciences has two or more computers: a UNIX workstation for research and analysis applications and a PC or a Macintosh for mainstream applications such as writing, Web-surfing or creating Power-point presentations. With the arrival of MacOSX and the new 64 bit G5 computers, a researcher can now run both productivity applications and high-performance UNIX applications on a single system.

Apple is not known for server or super computer production but these past months have changed all that. As an example: Virginia Tech has built one of the Top Supercomputers in the world from approximately 1,100 of Apple's new Dual 2.0GHz PowerMac G5s.

This cluster achieved the #3 spot according to: http://www.top500.org/.

The Virginia Tech built their 10.2 Tflop/s X11 and Perl 5.8 obsolete for Panther. cluster in a few weeks for \$5.2 million, while Japan's 35.9 Tflop/s Earth Simulator, currently the fastest system in the world, costs around \$350 million.

Introduction to Panther

During the development of our bioinformatics tutorials and packages Apple released a major update of its OS and presented a new computer architecture. The new Mac OS

Panther.



Figure 1. A schematic picture of MacOSX Panther system architecture.

Panther comes on four CDs: three discs for installing the OS and one disc containing the developer tools. For our purposes be sure to install the developer tools.

Panther is now synchronized with FreeBSD 5, and has adopted gcc 3.3 as its default compiler. The new version of gcc gives better optimized code for the PowerPC architecture. More importantly, it includes performance profiles for the G5 (PowerPC 970), including native 64-bit integer arithmetic as well as features like the G5's hardware sauare-root function. Worth mentioning is the fact that Panther was compiled using acc 3.3 and and this produced more optimized code for the G5.

Panther improves the open-standard, UNIXbased foundation of MacOSX and now includes X11 for Mac OS X. Along comes an enhanced Terminal and updated open source projects such as Python, FreeBSD 5 commands and libraries. New is also that 10.3 has Perl 5.8.1RC3 and Java 1.4.1 as default. This makes our previous packages of

G5

The Power Mac G5 is the first to bring a 64bit architecture to the personal computer market. This new G5 is a-new implementation of the PowerPC architecture, the G5 processor is based on IBM's 64-bit POWER4 processor. More practical and useful for bioinformatics applications, the Power Mac G5 can be configured with 8GB of RAM,

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four times more than what is supported by a typical PC. The G5 also has a 1GHz frontside bus, an advanced system controller, fast 400MHz 128-bit memory and Serial ATA disks.

New package system

In previous issues of EMBnet.news we provided two releases of bioinformatics tools, namely Packages Version 0.9 and Packages Version 2.0.

Now we have created a single, uniform installation package installing the following bioinformaticsprograms/packages:EMBOSS, NCBI-blast, T-coffee, Staden, ClustalW1.8.2, wwwtools, wise, primer3, HMM 2.2g (Altivec optimized) and Phylip.

The installation also installs nedit , the QT libraries, kaptain., and other necessary libraries.

New in this release is that this installation does not need Fink(an Open Source project that adapts Unix software so that it compiles Figure 3. You must have administrator rights on your and runs on Mac OS X ("port" it)). The X11 (for Panther, optional for Jaguar) and Perl 5.8, are already installed in Panther. New also is that we adopted a new destination for all packages: /usr/ebiotools. This will make it easier for the user to remove the packages or to install our new releases. Another change is the inclusion of a Staden license, no need to apply for one (please read this information: http://www.mrc-lmb.cam.ac.uk/pubseq/ news.2003.html).

The requirements for the package are MacOS X 10.2 (Jaguar) or 10.3 (Panther) and Figure 4. The installation starts Apples X11.app (beta 3 for Jaguar or version 1 for Panther). It also runs under XDarwin with XFree86 4.3.

How to install our new release:

Go to our site 1-

http://www.ebioinformatics.org/downloads/ 2-Download a single package, choose your MacOSX: Jaguar or Panther.

- 3-Unpack
- 4-Click twice on the icon

5-This action will start a visual install procedure, all Unix commands will run in the background.



Figure 2. This is the window that starts the easy install.



machine. Please fill in and press "install".





Figure 5. The installation will take around 15 minutes on a single 400 Ghz G4 or less than one minute on a dual 2Ghz G5.

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Notes

You will need to read our previous tutorial (EMBnet.news 9.2) to make the wwwtools to work. First of all you must start your Macs web-sharing and then modify the Apache configuration file httpd.conf to be able to execute the web-blast scripts. Later on you should also configure your blast databases following the instruction in EMBnet.news 9.2.

For addendum and updates (always on development): www.ebioinformatics.org. If you want to adapt your environment follow the instructions on EMBnet.news 9.2, (pp 16-22) and create a ".cshrc" file in your home directory.

Most packages work directly from the command line and the GUI through the X-Windows system (X11).

Blast comparison

To test the power of our new systems we performed a series of Basic Local Alignment Search Tool (blast) tests. The blast experiments were conducted on a G4 Xserve (Dual 1Ghz G4, 2GB RAM, MacOSX 10.2.8 (Jaguar) and a G5, dual 2Ghz G5, 4 GB RAM and 10.3.1 (Panther). The executable used was ncbi-blast 2.2.6 compiled on the individual machines. The databases were downloaded from EBI in blast format.

Blasts were run in a fashion similar to the Apple-genentech-blast described at:

http://developer.apple.com/hardware/ ve/acgresearch.html

http://developer.apple.com/hardware/ ve/pdf/PerfData18Apr02.pdf

With an increasing word size as the only variable parameter, the BLOSUM62 matrix and an e-value of 0.000001 was used. Three randomly selected human ests were used as guery strings for all searches.

Plots depict the time taken for a blast-run with the word count W on the x-axis and time in seconds on the Y-axis. Databases plotted are nt, est, other genomic and sts.

Our tests are only comparisons between different MacOSX versions and computers based on different PowerPC architectures. The reader will also wonder how this architecture compares with other systems.

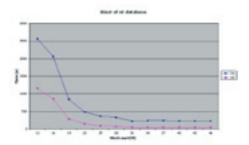


Figure 6. Comparison of blast runs on a Jaguar Xserve (G4) and a Panther G5. Parameter Word (x-axis) count plotted against run time (y-axis). The G5 has run times that range from more than twice as fast as the G4 for low Word count values, and up to 6,5 times as fast for higher word counts.

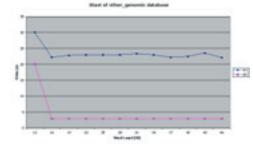


Figure 7. Comparison of blast runs on a Jaguar Xserve (G4) and a Panther G5. Parameter Word (x-axis) count plotted against run time (y-axis). The G5 is 4,5 times faster for all values of W.

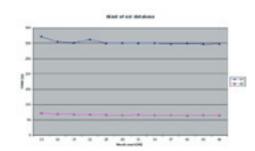


Figure 8. Comparison of blast runs on a Jaguar Xserve (G4) and a Panther G5. Parameter Word (x-axis) count plotted against run time (y-axis). The G5 is consistently about 8 times faster than the G4.

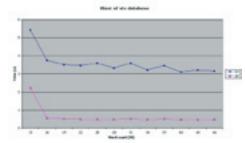


Figure 9. Comparison of blast runs on a Jaguar Xserve (G4) and a Panther G5. Parameter Word (x-axis) count plotted against run time (y-axis). The G5 is about 7,5 times as fast for the small sts database.

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We did not have the time to do our own tests and we can only present a figure showing an experiment done by Apple. This is shown for your information only, we are planning to run our own comparisons in the future. To demonstrate the performance advantages of the Power Mac G5 for processor-intensive scientific analysis Apple used blast. All Power Mac G5 systems were tested using A/G BLAST. 2 The Dell Dimension XPS, Alienware Aurora and Dell Precision 650 ran NCBI BLAST on Red Hat Linux.

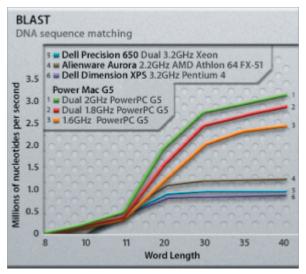


Figure 10. In common searches using a word size of more than 11 the Power Mac G5 far outperformed the Pentium 4-, dual Xeon- and Athlon 64 FX-51-based systems

Conclusion

The improvements in the last MacOSX version make an upgrade to Panther a significant performance boost. Together with our new installation package you will easily build a "Bioinformatics Workbench" on your desktop machine. Our new approach will also make it easy to enhance and upgrade the whole system. We are at the moment compiling a list of Open Source bioinformatics tools to add as modules to our system.

References

- 1 http://www.top500.org/
- 2 http://www.apple.com/ downloads/macosx/math_science/ appleanenteebblast html
- applegenentechblast.html
- 3 http://www.ebioinformatics.org

Addendum

Free/Open Source Packages for the MacOSX (a preliminary list):

• EMBOSS, ClustalW, Staden, T-coffee, Fasta, HMMer, NCBI Toolkit, Phylip, Primer3, Wise2 (Protein comparison):

- www.ebioinformatics.org
- Amber:
- amber.scripps.edu
- Apollo Genome Browser:
- www.ensembl.org/apollo
- AutoDock Toolkit:

www.scripps.edu/pub/olson-web/doc/ autodock

- BASE:
- base.thep.lu.se
- BioPerl, BioJava, BioXML, BioCorba,
- BioRuby, BioPython open-bio.org
- BLAT:
- DLAI.
- contact kent@soe.ucsc.edu
- CINEMA 5:
- aig.cs.man.ac.uk/utopia/download
- Cn3D:
- www.ncbi.nlm.nih.gov/Structure/CN3D/ cn3dinstall.shtml
- Glimmer2, MUMmer
- www.tigr.org/software
- GROMACS:
- www.gromacs.org/
- MacGDE 1.3:
- www.msu.edu/~lintone/macgde
- MolMol, O:

www.msg.ucsf.edu/local/programs/ MacOSX/MACOSX_Downloads.htm

- OmniGene/OmniView
- omnigene.sourceforge.net
- Prhed-Phrap-Consed:
- www.phrap.org
- PyMOL:

fink.sourceforge.net/pdb/package.php/
pymol

- Python Molecule Viewer:
- www.scripps.edu/~sanner/python/pmv/ webpmv.html
- RasMOL:
- proclus.tripod.com/darwin/
- Scilab:
- scilabsoft.inria.fr
- VMD:
- www.ks.uiuc.edu/Research/vmd

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EMBnet E-meeting portal



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The EMBnet organization is more global than ever. We have an increasing need for fast and personal contacts as a complement to our usual meetings (AGM, PC-meetings, courses and workshops). The telephone and E-mail are useful, but we need ways to meet face to face with node managers and PC-members (to see the facial reactions) without spending all our time and money on airlines and hotels!

The solution we were looking for is The Marratech Work Environment consists of videoconferencing. Using the Internet for the Marratech E-meeting Portal server and videoconferencing isn't a new concept; the free Marratech Pro client software. different projects have tried for years to create The steps to connect to an E-meeting are:

such applications. But videoconferencing applications from five years ago, like CUseeMe and early versions of Microsoft NetMeeting, proved too difficult to set up for mainstream use, and they tended to work badly. Many people at EMBnet have had bad experiences with these media.

We did a quick research of newly developed software and we found one that fulfilled our pre-requisites. Easy of use, clients for all major OS (Linux, Windows, MacOSX and Solaris), encrypted communication and good sound and video quality. The software we found is Marratech. (www.marratech.se)

The next-most-important consideration was whether the application works from behind a firewall, after testing we can state that Marratech does without problems.

EMBnet has now a Video-conferencing portal server (Marratech E-meeting Portal server) and the only thing an EMBnet member need to connect to an E-meeting is a Webcamera, a hedset and client software.

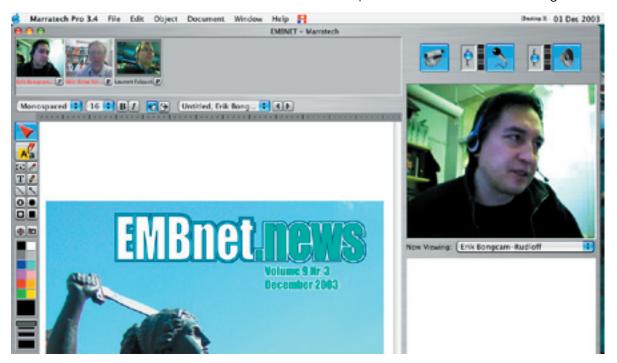


Figure 1 Shows a typical session with 3 participants and one shared document page. This meeting place can easily accommodate 20 simultaneous participants.

nemat**naws**

1- Download the Marratech client at:

http://www.marratech.se/download/

2- Install Marratech Pro on your computer my classroom over the Internet by having (Windows, Mac, Sun or Linux), connect a headset and a web camera (it is possible to only communicate with sound!). Start Marratech or point your web browser to the EMBnet E-meeting Portal link. Marratech Pro will then start and let you securely interact with other EMBnet node managers or PCmembers. You will need a username and a password for the meeting room. That's all!

Embnet's Executive Board (EB) has made use of the system and we can report that three virtual meetings have taken place during the past 3 months. The system works rather well in our hands.

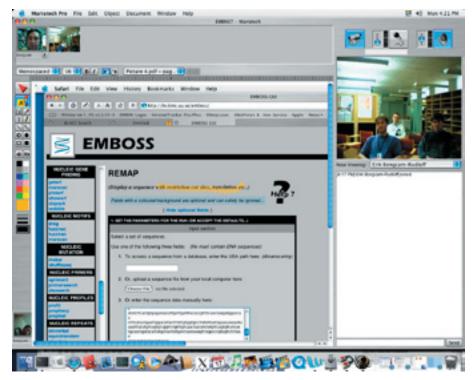
The E-meeting room allows you to share documents as: Power-point presentations, PDF-files, pictures, text files etc. All the participants can move and control the meeting-room, this of course requires some meeting discipline among users.

I have personally used the Marratech system the audience. I have used this system several

on The Linnaeus Centre for Bioinformatics (LCB) own server installation. I distributed students join via LCBs meeting portal. Before the class started, I imported my PDF-files and other material to the meeting room's electronic whiteboard. When the class begun, all the students had the material pre-loaded into their Marratech Pro clients; changing slides took then a fraction of a second.

This environment enables truly interactive elearning, and students could ask questions (Marratech uses proprietary algorithms for high quality sound) and use the whiteboard to show me problems.

The system can also be used to give remote seminars, the teacher and the audience connects then to the portal (see Figure 2). The seminar room needs a computer beam and good speakers for the audience to see and hear the teachers lecture. To make the experience truly interactive is a good idea to have a couple of microphones to handle to



times in Sweden and from Sweden Norway. to The first time it is rather strange to look into the camera not to the and screen showing the audience, but after a while everyone can learn to act as a pro. All sessions can be recorded to the hard disk making it possible for the students to review the lecture afterwards.

For more specific notes about recommended hardware please visit:

Figure 2 Depicts a typical lecture situation in this case between Uppsala, Sweden and Bergen, Norway.

http://www.marratech.se/support.shtml

IN VINO VITA? By Vivienne Baillie Gerritsen

For many, a prolonged – but of course healthy – life is a tempting prospect. Especially, in a day and age where there seems so little time to fulfill our ever-growing aspirations and the gift of an extra few hours a day is just not on. Researchers have been giving a lot of their time to the problem of longevity since the 1930s when it was first discovered that calorie restriction actually lengthened life expectation in mammals. It took many more years of research before scientists got a glimpse of the molecular pathway underlying such a process. And, for the time being, it really is just a glimpse but an encouraging one. A family of proteins, known as sirtuins (sir-too-ins) or SIRS, an abbreviation of Silent Information Regulators, known to exist from bacteria to humans, seem to have a definite role in the ageing process of cells, and hence the ageing process of organisms.



Fig.1 Bacchus, Hermitage, St. Petersburg Peter Paul Rubens (1610-1695)

It is now clear that the ageing pathway in different organisms is different. In yeast, for example, an accumulation of what is known as toxic extrachromosomal rDNA circles (ERCs) is a cause of cell senescence. Whilst in worms, interference in the insulin signaling pathway have an effect in the organism's longevity. The exciting discovery is that sirtuins have a direct effect in these different ageing processes. They may act in different molecular pathways but their mode of action is the same. Sirtuins are NADdependent protein deacetylases. What they do is remove acetyl groups from specific target proteins. Their function however depends on the intracellular concentration of nicotinamide adenine dinucleotide (NAD), which in the oxidized form greatly enhances sirtuin activity. In yeast for example, genomic instability and hence the accumulation of ERCs, stakes its fate. Sirtuins can brake this fate by acting on certain histones. Through deacetylation of the said histones, chromatin structure is modified, the lecture of rDNA disrupted and the formation of ERCs hindered.

What kind of event would delay cell senescence? Calorie restriction for one. It is thought that calorie restriction either shifts the ratio of oxidized/reduced NAD or alters its level, thereby having an effect on sirtuin activity. How? Well, a number of proteins which are also NADdependent may become less active and release their NAD which is then free to activate the sirtuins. Another hypothesis for an increase in NAD is a metabolic shift to respiration. Indeed, when glucose is limiting, respiration is preferred. An increase in respiration yields a higher rate of electron transport thereby increasing the overall cellular NAD/NADH ratio. Either way, an increase in NAD activates sirtuin activity and as a result, in the event of environmental stress, such as less food but also fungal infection for instance, organisms would be given a better chance to survive.

So, sirtuins do seem to have an overall role as regulators of programmed cell death and cell differentiation. As we have seen, they are more heavily summoned during environmental stress. In the quest for eternal youth and health, scientists set about to find out if they could pin down a molecule or two which could trigger off sirtuin activity, instead of just counting on calorie restriction. A number of chemical compounds examined amongst which a few were polyphenols, which are metabolites found in plants. The most potent activator turned out to be resveratrol, a plant metabolite found in the skins of red and white grapes for instance.... and in the eyes of the convivial 'grapes' spells 'wine'.... Another plant metabolite, quercetin, is also an activator of sirtuins, but to a lesser degree and is found in olive oil for example. Both compounds are synthesized in response to environmental stress and are already known for their health

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benefits, namely their antioxidant properties, their capacity to lower cholesterol levels and decrease blood clot formation.

There is a theory that, when there is a lack of nutrients, plants may have the power to 'say' so to other organisms via resveratrol for example. Various animals feeding on plants would assimilate the increased ratio of resveratrol and thereby transfer the warning message to their own organism; i.e. that reproduction has to be halted and survival means undertaken. However, there is no reason not to believe that organisms other than plants do not have their own sirtuin activity enhancers which have simply not been identified yet. Time will tell.

So should we all take to drinking a glass of red wine or two per day? Or adding olive oil to our diet? Certainly, statistics have shown that the French, who are generous drinkers of red wine, suffer less from the side effects of overweight than do the Americans for example. A Mediterranean diet, which includes not only red wine but also ample amounts of olive oil as well as fresh fruit and vegetables, is also statistically far kinder to humans than a more Western diet of coke, hamburgers and chips. Let us make a finer comparison for the gourmet readers: wines produced in cooler regions or areas where grapes are more prone to disease often have more resveratrol. Hence Pinot Noir, for instance, has rather high doses of the chemical while a Cabernet-Sauvignon is not so rich in the compound. What is more, resveratrol is unstable on exposure to air and goes off within 24 hours. Would it be wiser then to drink a bottle a day?

Well no. In fact, it has been shown that high doses of resveratrol stunts its effect on sirtuins so no point in overdrinking. Nothing has been proved yet. No one can say whether even one glass of wine a day keeps the doctor away or not. Furthermore, in human cells, resveratrol - via sirtuin activity - ultimately deactivates a tumor suppressor, thus fueling concerns that increasing resveratrol levels may predispose humans to cancer. Though a number of scientists disagree since calorie restriction per se has never proved to do so. Much more has to be done, sirtuin's 3D structure for one, before any conclusions can be made. Naturally, a lot of money could be involved in this kind of discovery. Yet another miracle diet: eat your cake and swill it down with a glass of wine enriched with resveratrol. Just imagine. However scientists insist that the findings are not so much to prolong life than to avoid the bothersome effects of ageing such as neurodegeneration, carcinogenesis and atherosclerosis. Well, the message is always the same isn't it? Just eat a healthy varied diet: some wine, some olive oil, fresh fruit and vegetables, cereals and even chocolate. Just don't eat too much of it and you should be all right.

Cross-references to Swiss-Prot

P06700: Saccharomyces cerevisiae (Baker's yeast) NAD-dependent histone deacetylase SIR2

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The team gives support to EMBnet nodes and helps them with maintenance and troubleshooting. The team is formed of experienced system administrators and programmers who ensure the availability of local services for all EMBnet users.

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Dear reader,

If you have any comments or suggestions regarding this newsletter we would be very glad to hear from you. If you have a tip you feel we can print then please let us know. Please send your contributions to one of the editors. You may also submit material by e-mail.

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