EMBnet.news

Volume 10 Nr. 2
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- embossRUNNER
- Workshops in Belgium and Sweden
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- New QuickGuides

and more...

Editorial

This issue perfectely reflects current EMBnet activities from workshops, international meetings, QuickGuides publications, to software tutorials. What is more convincing than real life experiences? Nothing, all the theoretical discussions are way behind the facts. If you ask all the participants of the courses and of the workshops, they praise the concept of practical work. Learn by doing! This demonstrates one of the principle roles of the EMBnet community better than a thousand words.

Teaching yes, but teaching allowing the students to practice immediately is much more satisfactory both for the teacher and for the students. This has some drawbacks though: the number of participants is obviously more limited than for a purely theoretical course, either by the number of available computers or even worse by the number of teachers.

EMBnet has the knowledge and the experience to carry at such workshops, we must fight to keep it running, so please give us your support!

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

Protein Spotlight

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 focusing 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 printed version of issues 46&47. Please let us know if you like this inclusion.

Cover picture: Aconcagua highest summit of the Andes, 6961m, April 2004 [® Erik Bongcam-Rudloff]

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Workshop: Bioinformatics System Management

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A workshop within the framework of the EMBCORE project

Gosselies, April 15 to 17, 2004

Background

The concept of organizing a workshop on the management of a Bioinformatics Workstation was inspired to Marc Colet while Robert Herzog reported the decision of the 2003 Annual General Meeting of the EMBnet about the need to run several workshops and courses during the year 2004, mainly financed by the European Union EMBCORE project. The goal would be to put the participants in a situation such that after a few days of guided work, they would have built from scratch a completely functional infrastructure allowing external users to run basic bioinformatic tasks. This would sufficiently mimic a real life situation so that when back at home, the participants would be able to install their own system for their local, regional or national users. Some of them might even become candidate EMBnet national nodes…!

A couple of years ago, a similar course was organised by our colleagues of Spain, under the leadership of J.R. Valverde. During this course, system management presentations were given by several speakers but there was no provision for extensive practice by the students. We decided to go for another kind of workshop, essentially concentrated on practice. No lengthy presentations of more or less abstract concepts but the possibility for the student to immediately reflect on his own workstation the operations demonstrated by the tutor. Naturally, this would not be fit for the total newcomer to UNIX and bioinformatics…

A computer room

The availability of a computer room is obviously of primary importance for such a project. Our neighbours on the Aeropole of Gosselies, the "Technopole", have gained a good reputation in teaching various informatics courses and they have several well equipped rooms for this purpose. Sadly, these rooms are under high demand and the perspective of having people needing root access to the machines was of some concern to the managers. As we happen to have a modest computer room in our own building, the management of which is directly under our control, this alternative was seriously considered, notwithstanding the fact that these are rather modest machines by today's standards (they were installed already three years ago, a long time in the life of microcomputers..) Still, we pursued the project and evaluated the technical possibilities: installing new hard disks and some more RAM would bring these machines in a reasonable shape to install a reduced set of data and we thought that the relative modesty of the configuration would give the students a good feeling of the needs of the various modules involved in building a functional system.

Teachers

Who would be the teachers ? Marc Colet would take over the function of general coordinator. As we are good friends with the Argentinean EMBnet Node (Martin Sarachu has been cooperating for months with Marc Colet in the development of wEMBOSS, Valérie Ledent from our node was in Buenos Aires a few weeks ago for a bioinformatics course), we thought that a concerted Belgo-Argentinean effort could be undertaken. Martin

Figure 1 Martin Sarachu from Argentina

would be with us during the Easter holidays, so that he could be part of the course staff. Naturally, our system and software managers David Coornaert and Guy Bottu would take their share of the work. And Robert Herzog would take his part of the work, and among other things the preparation of the course manual[1].

Software choices

Our project would concentrate on three major elements in order to obtain a functional system, ready to accept several simultaneous users like a real life EMBnet node :

- Ease to access databanks
- EMBOSS
- Web access to all services

Our solution is to install the databanks under the SRS system[2] that provides a very efficient, albeit computer intensive, indexing system, a good way to access the sequences by other software modules and a powerful and user-friendly web interface. As general purpose sequence analysis software package, we at BEN abandoned the too expensive GCG and took the option of providing EMBOSS[3], developed as Open Source within EMBnet. This is an obvious choice that gracefully integrates with the SRS formatted databanks. And to provide a web interface to sequence analysis, our local development of wEMBOSS[4] comes as the evident solution. A few additional software packages complete the picture: the unavoidable BLAST software, some useful datasets which are nice to have under EMBOSS, some wrappers to integrate "foreign" software under EMBOSS. All this will rely on the old faithful Apache web server.

Too ambitious a program ?

Whether a complete installation according to our dreams could be completed within three days by would-be system managers remained to be proven… We hoped that our participants would enjoy the experiment with us !

Participants

Due to its nature as a workshop entering the EMBCORE project, we started advertising the workshop amongst the EMBnet node, widening the coverage to the Belgian community of biologists and bioinformaticians during the following week. We announced a limit of 12 participants, as the room contains 15 workstations, and we wanted to keep a few not booked as reserves and for the teachers themselves. 13 participants did effectively turn up and attend the workshop, and among them 7 from outside Belgium. Five nationalities were present, namely Spain, Switzerland, Romania, Hungary and Belgium.

Program at a glance

Over the 3 day period, we went through the following program, physically completed personally by each participant on a personal computer:

Day 1

- install a purposely tuned Linux operating system based on our favourite SuSE distribution, including the compilers and all tools needed for development (gcc, g++, g77, make, automake, zlib, libpng and gd libraries, xfree, wget, etc.)
- install EMBOSS and BLAST so that the tools provided by these packages could be used to install some databanks
- install SwissProt and a subset of the EMBL databank (bacteria and phages only), as well as several small databanks (Prosite, Prints, Rebase)

1 This manual is available online in pdf format on the wEMBOSS website (see footnote 4)
2 Now property of Lion Biosciences, Heidelberg and Oxford
3 http://www.emboss.org
4 http://www.wemboss.org

- build the corresponding fasta- and blast-formatted datasets
- install and completely configure an SRS server and launch the indexation of the databanks overnight

Day 2

- terminate the installation of the SRS server and provide the web interface using the Apache server on each computer
- learn a little bit about how to use SRS at the command line and from the web interface
- install fastA and complete the installation of BLAST to run local databank similarity searches
- install several packages for EMBOSS (pftools, clutsalw, primer) as well as building configuring and installing EMBOSS wrappers to access the local BLAST and FastA servers
- install wEMBOSS as a web interface to EMBOSS
- use wEMBOSS to access EMBOSS, including the local wrappers to BLAST, etc
- access the databanks and sequences over the local SRS server and fasta formatted files

Day 3

- learn how to keep databanks up-to-date automatically on a day-by-day basis
- learn about databank "farms" (old GCG tradition !) and put them to use
- configure SRS for the support of "virtual" databanks, in order to provide a non-redudant search among release and daily updates of EMBL
- questions and answers

The afternoon of the last day was devoted to a visit of the "Fatal Attraction" exhibition (an original and widely applauded exhibition about the sexual behaviour in the animal world…) at the Museum of Natural Sciences. The evening of Saturday found everybody around the usual "closing dinner".

Conclusion

The teaching staff consisted of : Martin Sarachu from the Argentinean EMBnet node, and Marc Colet, Guy Bottu, David Coornaert and Robert Herzog from BEN. The students were a spread of informaticians, bioinformaticians and biologists, all of whom found that our program was of great value and a good balance of bioinformatic techniques, more computer-oriented stuff (like script management of the databanks) and biology with the assignment of a few "real world" bioinformatics tasks by the students once their machine became functional. The return from the participants was very positive, they claimed that what was promised was effectively reached, and we were even able to follow closely the timetable that we had set up for ourselves. The critical intermediary goals, like having most basic tools installed by the evening of first day, so that the time-consuming SRS indexing phase could be run overnight, could indeed be reached by all participants. By the end of day 2, most had a web-connected and functional workstation offering the databanks with full access to both SRS over the web, and EMBOSS at the command line and over the web through the wEMBOSS interface.

We are eager to run a similar course next year, where we could accept up to 20 participants, if we can settle a larger computer room with the adequate hardware. All participants got a purpose written 50 pages manual, a CDROM for network booting the OS installation, and another one with all the packages, as well as a copy of the EMBnet UNIX and EMBOSS quick guides.

The idea of preparing a purpose-built self-bootable BioKnoppix-like CDROM that would do all the magic automatically had to be dropped, due to lack of time. We leave this project for the Austrian node ! (Hi Martin !)

Greetings from Belgium

Robert Herzog

Workshop report:

May 6-7, 2004, LCB Uppsala Sweden. Organized by EMBnet Sweden and sponsored by EMBCORE project.

The Workshop took place at the Linnaeus Centre for Bioinformatics (LCB). The centre is a joint initiative between Uppsala University and the Swedish University of Agricultural Sciences. The workshop was organized by EMBnet Sweden.
The goal of the workshop was to have discussions and demonstrations of:
Promoter Databases, Promoter Prediction systems, Motif Search, Gene Expression Databases, Transcription Factors, Binding Site & Motif Databases.

Day 1: a day for lectures

The first day was dedicated to lectures with time for discussion. The lectures were of high quality and the subsequent discussions were very long and intensive. The first day surpassed the participant limits and we had more than 30 attendees. See Figure 1.

Figure 1 Dr. Philipp Bucher during his lecture (Day 1).

Figure 2 Shows the "hands-on" tutorials in the computer lab. Dr Jacques van Helden instructing Dr. Eija Korpelainen (Day 2).

Day 2: a day for "hands-on" tutorials

A- Signal Search Analysis Server, conducted by Dr. Philipp Bucher, Swiss Institute of Bioinformatics and Swiss Institute for Experimental Cancer Research, Switzerland.

B- Regulatory Sequence Analysis Tools. This tutorial was held by Jacques van Helden, Service de Conformation des Macromolécules Biologiques et de Bioinformatique, Université Libre de Bruxelles , Belgium.

This section was limited to 24 participants and we reached this maximum. The tutorials were on a modern Unix-based environment (MacOSX), see Figure 2.

The workshop was attended by people coming from nine different European countries.
It was a complete success and all participants agreed that this workshop should be repeated at least once more.

Assoc. Prof. Erik Bongcam-Rudloff

Related links

The workshops page:
`http://liv.bmc.uu.se/RSMD`
Regulatory Sequence Analysis Tools:
`http://liv.bmc.uu.se/rsa-tools/`
Signal Search Analysis Server:
`http://www.isrec.isb-sib.ch/ssa/`

embossRUNNER: Desktop Bioinformatics on MacOSX

Erik Bongcam-Rudloff
Associate Professor
Swedish University of Agricultural Sciences
The Linnaeus Centre for Bioinformatics, Uppsala

Introduction

We received several e-mails from people around the world having eBiotools installed and asking: "where are the applications"? For Unix people this is not an issue because they know how to work using command line tools. But from people using Windows or Macintoshes this is a big problem. We are working on this issue and we are creating a more "cut & paste" common "Graphic User Interface" (GUI).

During our frequent reviews of new nice bioinformatics applications we found a very good GUI namely "embossRUNNER" created by Rudi and Suksiri Grams. By installing this application you will get a very useful bioinformatics desktop environment. This is a free bioinformatics package for your desktop computer.

To work, embossRUNNER requires functional installations of: EMBOSS 2.8.0 and Ghostscript. You can install both, using some MacOSX easy-to-install packages (skip this step if you have EMBOSS already installed).

1- Download eBiotools

To install EMBOSS 2.8.0 download the latest

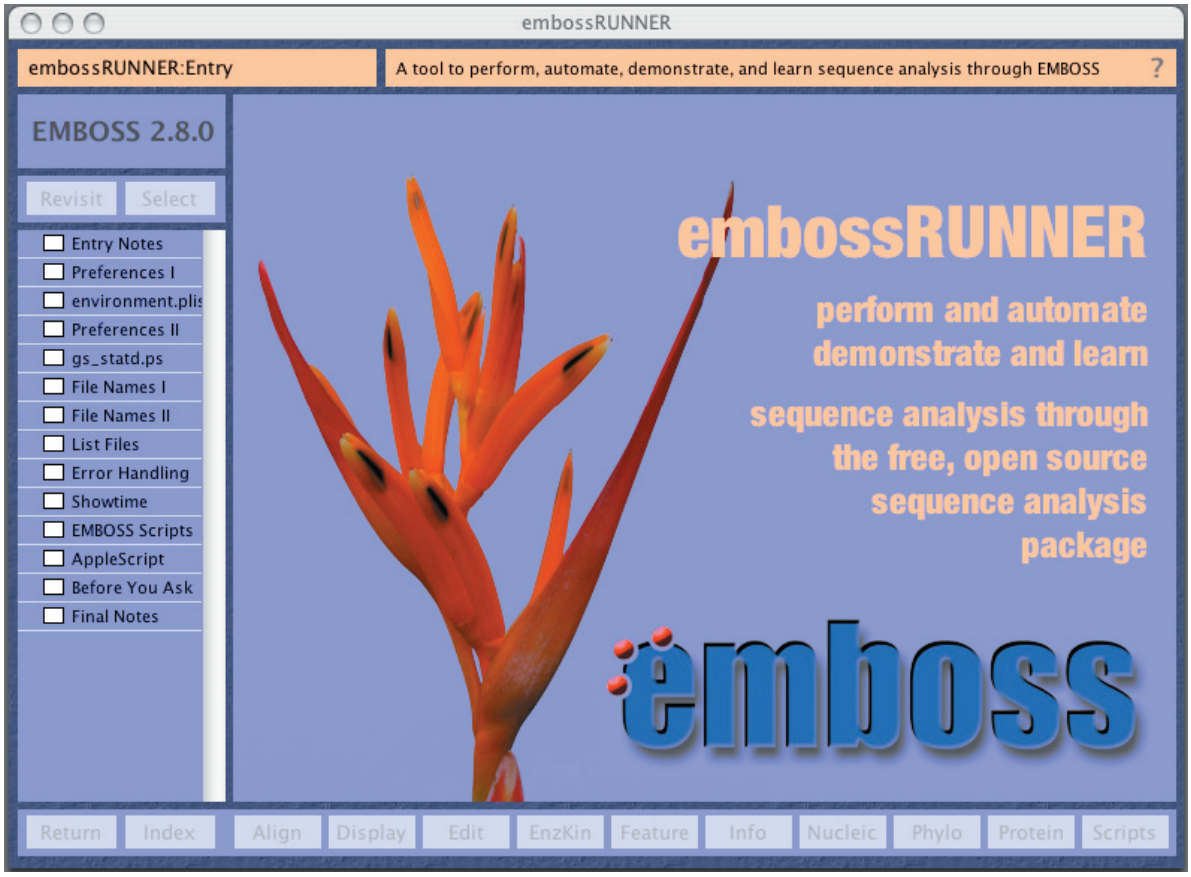


Figure 1 This is what you see when you start embossRUNNER. On the left side you will find useful information on how to configure your system. On the bottom wou will find a panel for selection of the main analysis groups.

eBiotools (at this moment packages version 040324). The package contains EMBOSS 2.8.0, you can download it from:
`http://www.ebioinformatics.org`
or from:
`http://liv.bmc.uu.se/macosx/software4.htm`
Please be sure to download the latest package. We keep the old ones only for the record!

Install and adapt the environment variables as described in previous EMBnet.news issues. You can always use EMBOSS using the other tools described in previous EMBnet.news issues, e.g., Kaptain GUI and of course directly from the command-line using the "Terminal" (you find the Terminal in `/Applications/Utilities`).

You can find previous EMBnet.news issues on `http://www.embnet.org/download/embnetnews`

2- Download embossRUNNER

When eBiotools have been installed it is time to download the latest embossRUNNER (at this moment 1.1.1) from:
`http://hyperarchive.lcs.mit.edu/HyperArchive/Archive/sci/emboss-runner-111.hqx`
We also have a mirror of this file at `http://www.ebioinformatics.org`

This part is very simple, just download and unpack it (use Stuffit Expander). Copy the embossRUNNER-1.1.1 folder to your Applications directory. For fast retrieval put the application icon of embossRUNNER on the dock. See Figure 2.

(You can build a nice collection of desktop-tools on your Mac, more information at `www.embnet.org`)

3- Set up the environment

Now you have to create the environment rules for this application. This is done in two steps, first you create a `.MacOSX` directory (please be aware of the "." in front of the MacOSX) in your home directory secondly you must create a text file containing the environment variables. If you want more details you can read the instructions on the first pages of embossRUNNER (Preferences, environment.plist, etc).
All is done in the Terminal (open it, it is located on `/Applications/Utilities`) and type:

```
mkdir .MacOSX
cd  .MacOSX
pico environment.plist
```

Then within pico type:

```
<?xml version="1.0" encoding="UTF-8"?>
<!DOCTYPE plist PUBLIC "-//Apple Computer//DTD PLIST 1.0//EN" "http://www.apple.com/DTDs/PropertyList-1.0.dtd">
<plist version="1.0">
<dict>
        <key>PATH</key>
          <string>/usr/ebiotools/bin:/usr/local/bin:/usr/bin:/bin:/usr/local/sbin:/usr/sbin:/sbin:/usr/X11R6/bin</string>
        <key>PLPLOT_LIB</key>
        <string>/usr/ebiotools/share/EMBOSS</string>
        <key>embossManual</key>
```

Figure 2 Shows some useful bioinformatics tools made for the MacOSX.

```
        <string>/usr/ebiotools/share/
EMBOSS/doc/programs/html</string>
        <key>graphViewer</key>
        <string>Preview.app</string>
        <key>showViewer</key>
        <string>Safari.app</string>
        <key>textViewer</key>
              <string>TextEdit.app</
string>
</dict>
</plist>
```

Save and exit (ctrl-O, ctrl-X) from pico, then quit the terminal. **Log out** from your session and **log in** again.

Hint: To avoid typos, you can also download the file «environment.plist» directly from `http://www.ebioinformatics.org` (look under download -> software).

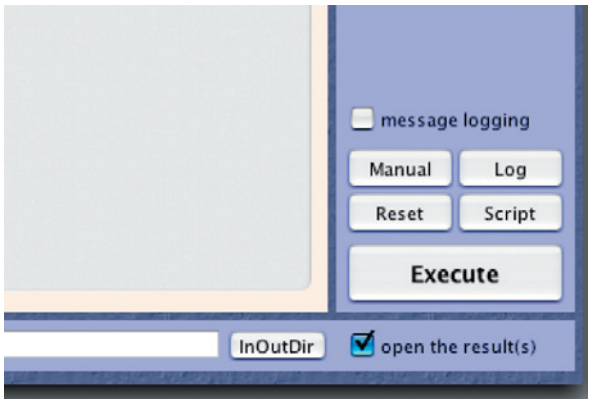


Figure 3 The results will not be presented if you selected a program that produces images e.g., "plotorf". To view them you must install the Ghostscript package. This is easily done with the help of another installation tool.

Now you can test your new application. You will immediately be able to produce nice text documents. Select main group then program, select a sequence file and press Execute. Please check the box "open the result(s)" to see the results immediately, if you expect a graphical output and don't get the result, see Figure 3 and proceed to next step.

4- Install Ghostscript 8.0 (skip if it has already been done).

First we download the i-Installer application. This application will be used to install Gerben Wierda's free binary distribution of AFPL Ghostscript 8 for Mac OS X.

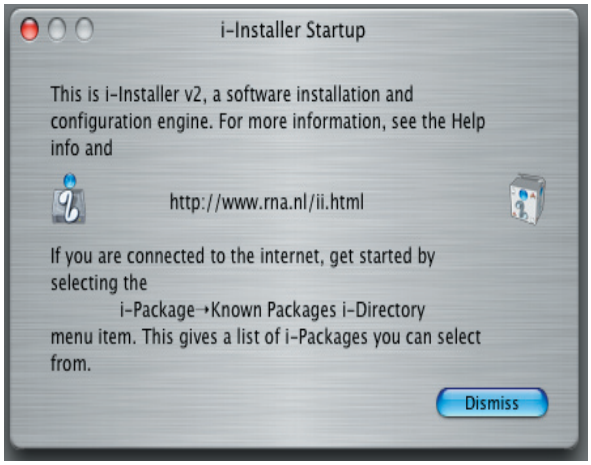


Figure 4 Start information for i-Installer version 2 used to install Ghostscript. You can use it to install other packages e.g TeX, ImageMagick etc.

Follow the links to i-installer from
`http://www.rna.nl/`
or you can download it directly from:
`ftp://ftp.nluug.nl/pub/comp/macosx/volumes/ii2/II2.dmg`

This will download a disk image, that you can double-click to open. Copy the i-Installer application to the folder `/Applications/Utilities`. Run i-Installer (see Figure 4) and select the Known Packages i-Directory submenu as shown in Figure 5. If you are

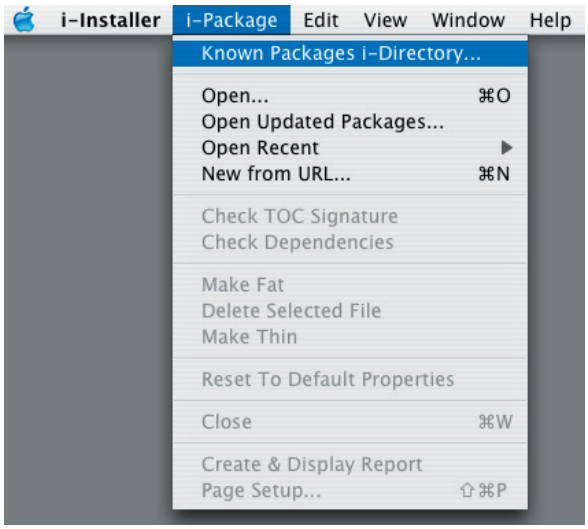


Figure 5 First you must choose the known Packages i-Directory as shown.

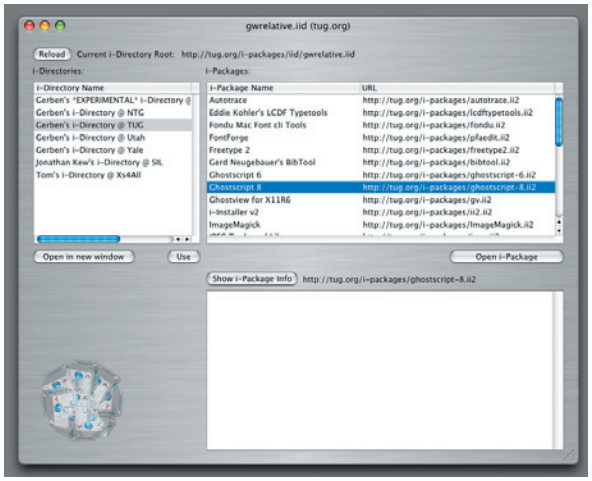


Figure 6 Next you must choose the Ghostscript 8.0 package and click twice on it.

Figure 7 Now you will get information about the package. To install it press on "Install & Configure".
Figure 8 See next page.

connected to the internet you will be presented with a list of known packages.

Select Ghostscript package and install it by following the steps described (see Figures 6-8).

Once you have Ghostscript installed you can go back to embossRUNNER and select any program you like. Those with graphic

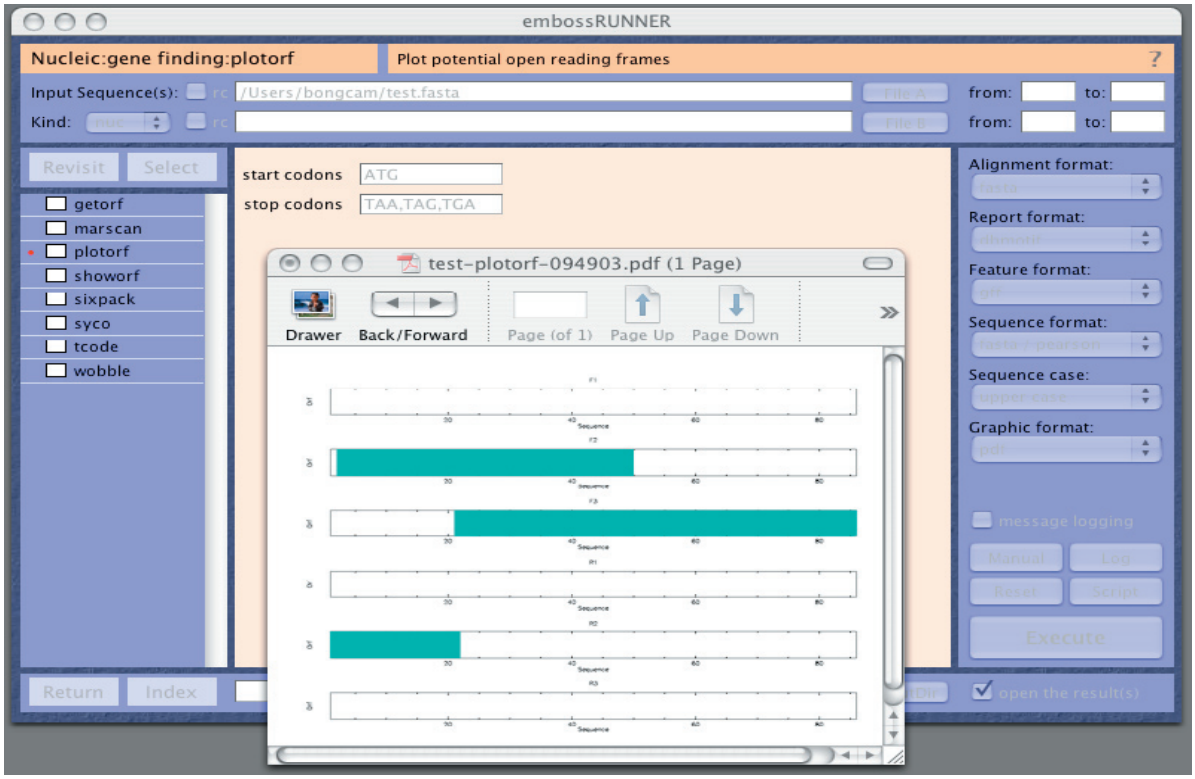


Figure 9 Shows a result produced by executing plotorf. The PDF image is shown by Preview. It is possible to save this image in other formats (e.g tif, png, jpg, bmp) using the export function of Preview.

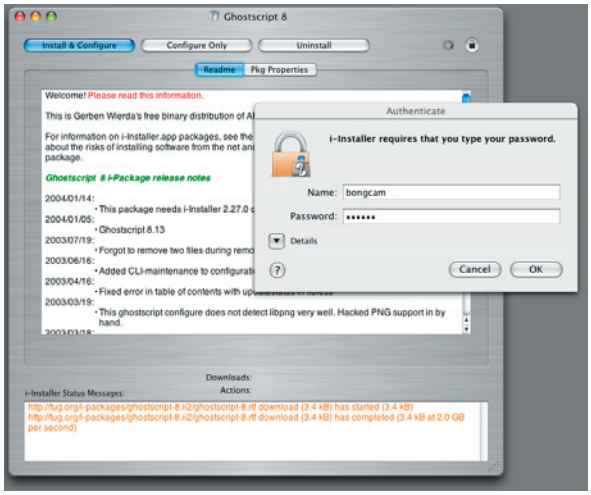


Figure 8 The package will ask for the administrator password. The package will install and configure Ghostscript 8.0 for you.

output will produce nice PDF files. If you select Postscript the application Preview will convert them automatically for you to PDF files as shown in Figure 9.

After installing eBiotools, embossRUNNER and Ghostscript it is time to start exploring your new, free bioinformatics Desktop package with a nice GUI interface!!

Acknowledgements

The authors of embossRUNNER are biologists working on trematode parasites in Thailand. As old Mac users they wanted to make the handling of EMBOSS a bit more user friendly in the daily work routine. You can contact them at: `rgrams@gmx.net`

We also use this occasion to do the same as the authors of embossRUNNER and thank everyone involved in the development of EMBOSS, especially Alan Bleasby!

Short meeting report

China - Europe meeting in the UK.

It was a beautiful weekend in the early spring in England. The Watson room of the Hinxton Conference Centre looks rather busy. Sponsored by the European Federation of Biotechnology and China National Centre of Biotechnology Development, the China-EU bioinformatics workshop was held here on February 20-22, 2004. A delegation of 12 Chinese bioinformaticians from various institutions and universities flew here, to meet with colleagues from France, UK, Germany, Spain, Switzerland, the Netherlands, Denmark and other European countries.

The workshop started with an opening address by David Bennett, the secretary of the Public Perceptions of Biotechnology, one of the five task groups under the European Federation of Biotechnology. Participants from both sides reported their progress in several research areas and the main focus was on genome annotation, functional genomics, protein resource, microarray data interpretation, phylogenetic analysis, sequence motif prediction, etc. Staffs from the European Bioinformatics Institute and the Sanger Institute were also spending the weekend with the two delegations. The main goal of this workshop was to build bridges between partners from both sides, and to identify possible collaborations. A draft of guidelines for research projects were proposed and follow-up email messages are being actively exchanged and hopefully, this will lead several groups to partner for the application to the Sixth Framework Programme of the EU grants.

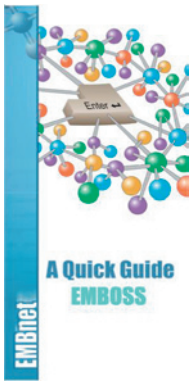
Prof. Jingchu Luo

Four new EMBnet QuickGuide available !

We are happy to announce that our famous QuickGuide family has seen the birth of 4 new members.

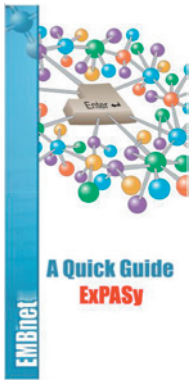
A QuickGuide to EMBOSS

Designed by Lisa Mullan of the UK EMBnet node, this guide describes the EMBOSS package in detail and provides the user with an extensive list of useful commands and advices.



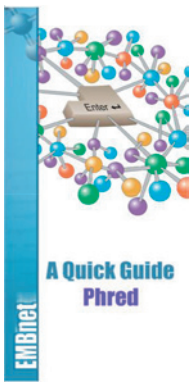
A QuickGuide to ExPASy

Designed by Elisabeth Gasteiger of the Swiss Institute of Bioinformatics, to celebrate the web site's 10th anniversary, this guide summarizes the content of one of the oldest and most famous web sites: www.expasy.org.



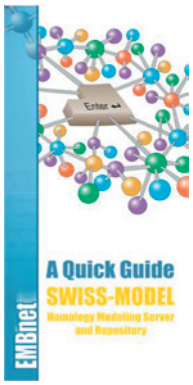
A QuickGuide to Phred

Designed by Marcos R. Araujo and several members of the Brasilian EMBnet node, this guide describes the Phred program of the phred/phrap package. A second companion guide is in preparation to describe the Phrap software.



A QuickGuide to SWISS-MODEL Homology Modeling Server & Repository

Designed by Lorenza Bordoli of the Swiss EMBnet node in collaboration with colleagues of the Swiss Institute of Bioinformatics, this guide describes the SWISS-MODEL web server.



All these new guides and older versions are freely availllable from our web site `http://www.embnet.org/download/guides.html`

Planned Activities for 2004

Workshops

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

September 14-15:
Federating the SRS servers within the EMBnet infrastructure, Brussels, BE.
`rherzog@dbm.ulb.ac.be`

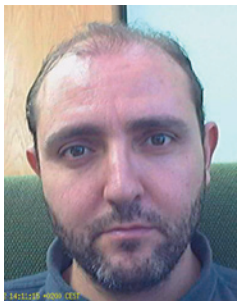
September 16: Collaborative EMBnet workshop day. In connection with the AGM. Brussels, BE.
`rherzog@dbm.ulb.ac.be`

Meetings

September 17-19: Annual General Meeting (AGM), Brussels, BE.
`rherzog@dbm.ulb.ac.be`

For more detailed information, consult our web site: `http://www.embnet.org/TM/workshops.php`

Project Management (part 2): project conception



José R. Valverde
EMBnet/CNB,
Centro Nacional de Biotecnología, CSIC
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Cantoblanco, Madrid
28049, Spain

This article elaborates on the initial phase of Project Management (PM) or **How Do I Get My Project Approved**. Here we will elaborate on how a project is first conceived and started and what are the roles of different parties in this phase of the process.
In this phase you must identify what the project wants to achieve, and gain the client's commitment to support the project. In other words you must identify the needs, justify the project in terms of those needs, define what benefits are to be expected and get relevant stakeholders to sign in.

Along the way we will refer to a number of technical terms (in **bold** face). You will feel familiar with most of the concepts, but knowing the appropriate technical term will allow you to communicate effectively with other Project Managers from any discipline.

Getting started

When one starts, it is always better to go by the book and try to follow every step carefully. A good deal of self-discipline will be needed to avoid vices in the early learning stages. As experience and confidence grow, it becomes easier and one may recognize shortcuts and exceptions for what they are worth.

It is important to *get into PM as early as possible* into your career. This doesn't mean you should fight to get a promotion (much less disposing of your boss to take his position, no matter how attractive the idea may seem), but rather that you should think of yourself as a Project Manager and of your boss as the client. Being your own PM entails exercising relevant abilities: you must find out ways to justify and organize work, build up morale, confidence, interest, etc... which you can only do by *careful introspection*, thus learning first hand the basic principles involved.

Finally, you must get used to the fact that *PM requires an **integrated approach***: you must be aware of all the implications of the project you are managing as well as the effects that it, its success or its failure may have on the environment and the effects of the environment on the process itself.

The start

Your involvement with a project will usually start after the *initial need* has arisen. Someone, the client (which may be a funding agency, or other department in your company, your boss, or even yourself), has identified some need that they want to cover.

Initially, *this perception of a need is often diffuse*. You discover something is missing, and want it fixed, but not having the knowledge or time to do it yourself, you go out and look for some expert to do it instead. That expert is the **Project Manager** that will cater to your needs.

Identifying the client

Now, if you are the Project Manager, you must be aware that *the client expects you to understand the problem for them and come up with the solution*.

The first task that you, as Project Manager, must take, is to *make it clear what it is exactly that the client needs* and define the **goal** of the project. From the initial diffuse conception you must work out its exact meaning within the client's existential context.

The first step in refining the need involves *identifying the client and establishing a successful, relaxed and confident communication* among all parties involved. These parties will be your client, and you.

Note that **client** here means everybody on the client side that will be involved in using the final product or that will have a say in the decision; it means *anybody having any stake or interest in the outcome* (good or bad) of

the project. Similarly, **you** means you and everybody else in your environment that will be involved in the production and delivery of the final product. Your role (and that's really **you** as Project Manager) is to enable an efficient communication path among both parties.

Understanding the need

For instance, your client may say he needs a break in his work. But, why? What does he want a break for? Many people have stressful jobs and having a break may help them release stress and come back with renewed strength to finish the work. But, what does it really mean? What is a break for your client? What kind of activities do actually allow him to disconnect from work and relax? Every person has a different notion of leisure. Is it for him only or for everybody in the team? In the company? And, how long would such a break take? 15', 1h, 1day, 1week, 1 month, a sabbatical year? And most of all, what does he expect from you?

The final solution may be to build a coffee room in the office for everyone in the department to share, where they may break 15 minutes a day and have a nice cup of expresso, may be with some cookies, small talk and a whiteboard to post jokes, pet peeves or relevant leisure events.

Or it might simply be planning holidays for him and his wife at some exotic place where they may relax, sunbathe and drink daikiris if they are so inclined or perhaps some dangerous site where they may go bungee jumping, whitewater rafting and having an altogether miserable but exciting time for themselves.

How could you possibly know from their initial statement "*I need a break*"?

You must *identify all people with a relevant interest* in the project and find out what their actual needs and expectations are regarding the project. You should identify conflicts of interest and try to solve them before defining exactly what it is that the project will try to achieve, weighting in the relative relevance of the various stakeholders.

Who is your client?

Naïvely it might be a funding Agency which has stated some general research policy guidelines. And you may want to shape your project proposal to fit within these guidelines. But if you don't want to be short sighted you must recognize that beyond the Agency there are advisory experts and ultimately users, voting taxpayers who direct the Agency's actions.

A better strategy is to talk to the Agency experts and discover what it is that they intended to state with their general policies. And even better yet, once you have a closer idea, go directly to the end users and ask them what it is that they expect and would like to get from your research. Try to identify what is *really needed*, and not just sell what you perceive or think or would like to produce (even if you are the lucky guy who always turns out to be right).

Clients are waking up and smarting-up quickly. You too should smarten-up.

Note that you must be ready to repeat all this work and actualize your conceptions and inventory of client expectations as the project evolves into later phases, being able to reconsider everything if and when you need to adapt to changes as the project goes along and until its final completion.

The goal

The *goal is a general statement of what is to be achieved*. In the example above, the call was to "*have a break*", but actually, the final goal was to "increase productivity by releasing stress". The goal statement is a general description that must be clearly and unambiguously stated and defined. The goal statement must identify and consider all the expectations of the different stakeholders, clarifying what it means for each of the different parties involved and what it is that they expect from the final product.

The scope

Once you have a clear idea of what it is that you want to achieve, you must refine it by defining the **scope** of the project. This is *a general description of what the project is expected to achieve in terms of features and results, its quality, time and cost constraints and any other relevant influences* that may affect its outcome. In other words, we must define the scope, cost, quality and time constraints (what, how much, how well and when is to be done) of the project and determine where it stands among them.

More specifically, we need to clarify the overall **goals** to be achieved (e.g. "increase quality of life"), the **needs** that we must satisfy (e.g. "reduce AIDS morbidity"), what are the **expectations** of the client regarding the final product in terms of features and quality (e.g. "developing an AIDS vaccine or enhanced anti-AIDS drugs"), the **resources** available to reach the goal (e.g. "research teams, infrastructure, knowledge, etc."), the **deadline** for delivery of the product (e.g. "two to three years") and any **other** constraints and considerations that may affect the quality, cost, features and timely delivery of the final product (e.g. "relevant risks like sickness leave of workers, extinction of AIDS or appearance of a new, more dangerous plague requiring your resources").

Note that we are talking all the time of **client** needs and expectations. You may want to build the ultimate and definitive solution, you may even have the best solution ever for their problem, but it is not up to you to decide. Other people will often have their own priorities and be ready to sacrifice quality, cost, time or features that to you may look not negotiable. It is seldom so, and even if it were, *it is their choice and they must be free* to take chances despite all your good advice.

It is neither wise nor ethical to let them loose either. *Sometimes, user needs may become very complex*, and understanding them is a serious challenge both for you and for users themselves. Remember that you are the expert and that's why they called on you. In these instances you should *consider building a **task force*** to study and understand thoroughly the user needs, and ***educate*** *your users* so that they understand better their needs and possible solutions. Workshops and end-user meetings may do for an effective means to prepare and understand a project needs.

In defining what is to be achieved, it is important to *make it clear what is **critical*** to the outcome of the project and what features are not. These may be nice to have in the final product, and will probably be accepted by most stakeholders, but impose an additional burden and you must be ready to sacrifice any of them if need be. Your role is to help clients and sponsors discriminate between **critical** (must have) and **disposable** (nice) features so they may take an educated decision.

Furthermore, there are many ways to skin a cat, and you should be prepared to consider as many of them as possible, and *present any relevant alternatives to your stakeholders* for negotiation, with their viability, cost, quality and impacts so they may make their choice. Not only it will make them happy to make the decision, it will allow for better, more informed decision-making and, most of all, may provide alternative accomplishment paths should the initially agreed method prove unsatisfactory. Being flexible is the hallmark of a **good professional**. Putting all your eggs in a single basket is rarely a good strategy.

Talking of professionalism: besides specifically stating what you intend to achieve, please *make sure to be **realistic***, for goodness sake, about what can be achieved (promising the moon may work for you today but will undercut our way tomorrow) *and state clearly how project progress can be **measured*** (vague or no promises are just as bad).

Approval

Once it is clear what we want to achieve, we need to *get approval and support by the relevant sponsoring authority* to carry out the project. While in principle you may go around with just approval from the authorities, it is rarely enough for success.

You should also get all relevant stakeholders to agree and sign-off the project definition, lest some disgruntled party play against you and undermine all your work.

If you identified everybody with an interest in the project -anyone that will be affected by the project- then you can try to reach a consensus and make them happy. It may not always be so (e.g. if getting support for you means depriving others of resources they relish) and in these cases it is of the utmost importance that you identify the relative weight of each stakeholder and make sure you gather enough support to ensure the continued viability of the project. In other words, *identify key stakeholders and continuously cater for their needs*.

Again, who is your client?

Funding agencies will review you work and project evolution. They won't just look at whether you produce deliverables or papers. They will conduct reviews to see if it is timely, appropriate and useful. While there may be a contract in between, if they perceive at any time that they are not getting what they wanted, or that they are wasting their money, because users or peers complain, if they think you fooled them into signing a contract that didn't fit their expectations, they will seriously consider cancelling your contract and shifting your funding to wherever they think it may be better put to work.

Watch out for users and make sure you promise and manage to deliver to meet their needs, and keep in contact to ensure their continued satisfaction with your deliverables and support for your work.

Think of competitors and others who may have a stake against you: are you well shielded against their complaints? Can you justify that your project is better than theirs? On enough grounds?

Getting approval to proceed requires that you do your homework: sometimes you may go away by selling a concept with enthusiasm to the authorities, but this rarely works more than once unless you are the special kind of visionary that always is right. In most cases, an exercise in humility is called for, and your best course of action is to *make a **Business Case***, a serious analysis of the value to be delivered by the project, conducting a cost-benefit analysis and actually proving that the project is justified and to which extent it is advantageous by itself and over other projects and why it should be funded in preference to those (even if they are not direct competitors for the same goal). *A continued, strong Business Case is paramount to convince the **Project Sponsor*** (who must provide the resources for the project success) of its utility, returns and viability so that you can steer his support throughout the project.

Indeed, before getting on with the project it is wise to perform what is known as a **Gate Review** and, as a matter of fact, you may have no choice but to conduct it anyway. In a Gate Review your performance to date is analyzed before going ahead, *assessing whether it makes sense to cross the gate to the next phase* of the project.

A Gate Review usually involves an **Executive Project Portfolio Team** (which decides which projects are funded among many competing ones), a **Project Change Control Board** (which approves changes to ongoing projects) or an **Executive Funding Review Board** (which reviews project funding). You should *identify the audience in advance and prepare to state your case* in front of them describing clearly the goal and expectations of your project, its scope, constraints, alternative solutions, their cost, assumptions, risks, value, trade-offs, their viability and generally justify the need for your project. The **Review Board** will assess your performance, make comments and recommendations for changes and future activities and possibly agree to allocate funding for your next phase and until the next Gate Review.

The Project Charter

The **Project Charter** is the general definition of what the project wants to achieve, signed off by all relevant stakeholders. Passing the Gate Review should *not make you confident* that you got everything right. It only means that the Review Board (the Executive Project

Portfolio Team at this stage) has evaluated your project, possibly among many others, and was convinced to allocate the funds to undertake your project.

Fleeting a ship

Getting the ship owner agreement is not enough to fleet a ship. There are many parties involved in a project, and unless you can secure them on board, it won't make sense to sail the ship, for you will have a difficult time to safely dock.

Before you start sailing there is a lot to do: you need to secure provisions, the merchants' goods for shipment, proficient sailors, etc... It would be unwise for a ship owner to let you sail off on a venture without first making sure there are goods to carry on board and trade with and securing all the needed resources to reach your destination.

So, yeah right, we all agreed that a shipment of trading goods to the New World is a good business opportunity for the Company, but you can't start on a statement of interest from merchants, you need them to really compromise and commit their goods to the shipment before going ahead. Otherwise they might think better and let you down with a fully equipped ship, a lot of costs and compromises and nothing to carry on board.

Your next step is to *get* ***executive approval*** *of the Project Charter,* i.e., get every key stakeholder to sign off the charter contents. Their signature implies a legal commitment to the Project Charter: it means they have read, understood and accepted its contents, certifies that it represents their expectations, that they are willing to commit to it and that there are no impediments on their side against the agreement.

Your client (a Company, a Funding Agency, an Organization, your boss or yourself) must now *evaluate the proposal and* ***prioritize*** *it* among their whole Executive Project Portfolio. As Project Manager, you are highly interested in the outcome of this process: the client often has many projects to manage and must rank this one against many others evaluating its relevance to their interests. The higher the ranking your project gets, the greater the interest of your client will be in seeing your work succeed and hence you can expect greater and quicker involvement and support for your work.

Once your Project Charter has been definitively approved you will be given *formal notification and authorization to proceed* and move on to the next phase. It is now your turn to notify other involved project managers of the approval and start all of them allocating resources to the project and building the Project Team.

Want to know more?

We will keep this information up for public discussion in the EMBnet/CNB portal (see "Table of Contents: Bioinformatics: Project Management"), where you may add your comments, experiences and questions. We intend to keep the posted information up to date and extend it as suitable, adding examples, notes and additional information to clarify the concepts. Please, feel free to visit the portal and contribute to build a useful resource for the community.

The PMI publishes the PMBoK, the Project Management Body of Knowledge, a PM resource acknowledged all over the World. Additional links and pointers are available on EMBnet/CNB portal directory page.

If you are interested specifically on Bioinformatics Project Management, then the Atlantic Systems Guild (`http://www.systemsguild.com/`) has useful resources for Requirements Analysis and Software Engineering.

A SMALL BLAST FROM THE PAST

By Vivienne Baillie Gerritsen

'What's a fossil Mum?' A question to which most Mums would answer, 'A fossil, sweetie, is bone which has become stone because it's been lying somewhere for a very very long time.' The process of bone diagenesis is just that little more complicated but on the whole Mum's answer is not incorrect. At least…this is what we have always been taught. However, before the bone becomes absolute stone, some organic parts – depending on the environment – can actually survive quite a long time. Millions of years actually. Scientists have already managed to extract DNA from fossil bone - though in terrible shape. A pity, because DNA, though minute, can stash huge amounts of information. Something not quite so delicate had to be found; something which could also offer biological information from the past. A protein perhaps? Yes. In the 1980s, the existence of a bone protein, osteocalcin, was detected in bovid bones dating back 13 million years and rodent teeth dating back 30 million years! In the 1990s, osteocalcin was detected in 75 million-year-old fossils such as the duck-billed dinosaur. The tricky part was to extract the protein from the bone intact and in sufficient quantities to be able to sequence it. This was only achieved a decade later in fossil bison bone. But what an achievement. And little did osteocalcin know that it would become such a famous molecule.

Bone is an exceptional organic tissue in that it is largely mineral (70-90%). The organic part is mainly collagen. Noncollagenous matrix proteins make up for the rest, of which osteocalcin represents just a tiny fraction. What an interesting fate for such a humble protein! Osteocalcin is a small protein, barely 50 amino acids long. Also known as the bone Gla-protein, because it has a number of γ-carboxyglutamic acid (Gla) residues in its sequence. It is found in bone only, secreted there by osteoblasts, where it binds to the bone minerals. And it is the tight bonds it makes with the bone minerals, which most probably protect it from vanishing in the process of fossilization. It is directly associated with bone formation and mineralization – though in what way exactly still remains unclear. What has been discovered is that impaired osteocalcin expression causes bone calcification to spread into nearby cartilaginous structures, so it must somehow have a role in directing and controlling bone formation.

Fig.1 One of the bison drawn in the Altamira Cave in Spain.

The osteocalcin that became a star was extracted from fossilized bison bone, *Bison priscus*, which was radiocarbon-dated back almost 60'000 years. *Bison priscus*, more commonly known as the steppe bison, though now extinct is quite well known thanks to prehistoric paintings in Paleolithic caves and fossils found in permafrost – in particular, a near intact carcass of an 8 to 9 year-old male carcass found in 1979 in Alaska and known as 'Blue Babe'. 'Blue' because the specimen was almost entirely coated with vivianite, a blue iron-phosphate, and 'Babe' from the North American tales of Paul Bunyan, a lumberjack who once brought up a blue ox… Steppe bison stampeded the steppe-like grasslands of northern Eurasia and North America during the Pleistocene (2 million to 10'000 years ago); the bone fossils from which were extracted the to-be-sequenced osteocalcin were found in Alaskan and Siberian permafrost.

The great breakthrough is that osteocalcin was extracted from crushed bone fossil and ultimately fully sequenced, which is something that had met with hopeless failure until the year 2002. How was it done? Small amounts (20 mg) of osteocalcin were extracted thanks to techniques to which molecular geneticists

are largely accustomed and are used for DNA purification, not protein purification.

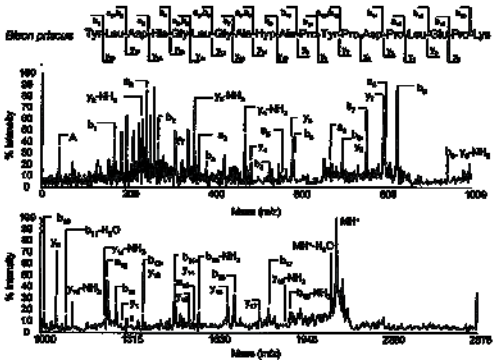

Fig. 2 The fossil *B.priscus* osteocalcin sequence appears above mass spectra.

Until then, large amounts of protein were needed but were very difficult to come by. This solved the 'quantity' problem. The sequencing was performed thanks to a technique (matrix-assisted laser desorption ionization mass spectrometry) which, unlike sequencing by Edman degradation, is not hindered by amino-terminal blockage. Thus solving the 'sequencing' problem. As a result, the protein was fully sequenced and the ancient bison protein was found to match the modern osteocalcin bison protein. It even predicted the single amino-acid substitution which makes the difference between cow and bison osteocalcin sequences.

What's the point of it all? Well…though DNA is far more informative from an evolutionary point of view than protein, and it is also far easier to sequence, it is also far more subject to lab contamination. What's more, DNA survives less well than protein in the process of fossilization. It has been estimated that protein could survive millions of years (whilst DNA being a more fragile molecule seems to survive only thousands) – an exciting prospect since this could take us right back to the beginnings of homan evolution. The key now would be to seek for proteins which are even more informative from an evolutionary and perhaps even animal behavior point of view. Besides paleontology, studies on the survivability of proteins – i.e. protein degradation – are obviously of great interest to those who work in the field of forensics. What is more, further research into osteocalcin itself could ultimately inspire the design of drugs for the treatment of bone diseases such as osteoporosis, in which osteocalcin may well have a role.

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MAD YEAST DISEASE?

By Vivienne Baillie Gerritsen

When referring to prions, most of us think 'Mad Cow disease' (Bovine Spongiform Encephalopathy or BSE). Which is not incorrect but rather narrow-minded. Indeed, the term 'prion' – coined in the early 1980s by the American biochemist Stanley Prusiner – simply means 'infectious protein', from which were derived the letters which make up the word. One may wonder which 'i', 'o' and 'n' were promoted but that is not the issue here… Prion proteins are not only found in cattle, sheep and humans, but also other vertebrates as well as yeast and certain fungi. And will no doubt continue to be discovered in many other organisms, if not all. The URE2 protein, a candidate prion in *Saccharomyces cerevisiae*, was the first prion to be crystallized. Clearly, the understanding of a prion's 3D structure and the conformational changes it undergoes – and passes onto its peers – is of great interest in the quest for therapeutic treatments of diseases caused by certain prions.

Scrapie, the fatal neurodegenerative disease which affects sheep and goats, and which could very well be named the 'Mad Sheep disease', was first described in the 1700s but its infectious nature was only recognized in the 1930s. It took a further 70 years before it was discovered that the infectious agent of such diseases was in fact a protein. Prusiner made the discovery and tentatively suggested it to the scientific community.

The concept that a protein could be infectious did not get a standing ovation and the media helped generously in kindling disagreement. It took some time before the idea seeped in and was finally accepted. Prusiner went through a rough time but was ultimately rewarded the Nobel Prize in Medecine in 1997 for his discovery, where he wisely asserted that '…while it is quite reasonable for scientists to be skeptical of new ideas that do not fit within the accepted realm of scientific knowledge, the best science often emerges from situations where results carefully obtained do not fit within the accepted paradigms.'

Contrary to popular belief, prion proteins do not necessarily bring on disease. They are not 'infectious' in the common sense. What a prion is capable of doing is undergoing a conformational change which, in turn, it can transmit – and in this sense it is being infectious – to a second identical protein, and so on. In the event of BSE, the prions form fibrillar structures in the cells, which are ultimately harmful to the organism. Such an affliction is also termed a conformational disease. On the other hand, a number of prions are absolutely harmless to the cell and the organism as a whole; despite the 'infection', there is no disease. It may be that some organisms actually use prion infection as regulator of a function. That is to say, the infection can actually switch on a function at a given time. In the event of *S.cerevisiae* and URE2, the protein's function is disrupted but causes no subsequent harm to the yeast.

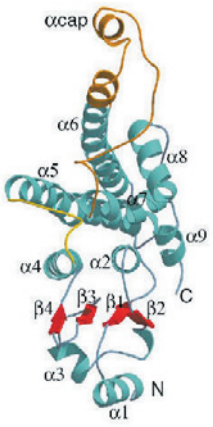

Fig.1 3D structure of the functional region of URE2p in its monomeric form (Source Ref.3).

What function does URE2 have in its native form? Well, no one knows for sure. It does have sequence similarity and even structural similarity to glutathione S-transferases but no one yet has been able to show that this is actually its function. Although it has been shown that URE2 is required for detoxification of glutathione S-transferase substrates and cellular oxidants. What is known, however, is that it has a role in nitrogen metabolism, where

it regulates a number of transcription factors. When there is plenty nitrogen, yeast turns off enzymes and transporters needed in the event of a poor nitrogen source. URE2 helps out in this process by binding to transcription factors in the cytoplasm, thereby preventing their entry into the nucleus where they would promote the transcription of a certain number of genes.

URE2 is a rather globular protein with a flexible cap region and a poorly structured N-terminal region. The belly of the protein does sport a cleft – like the glutathione S-transferases – and could well be there for an unknown ligand. In its active form, URE2 acts as a dimer, where it seems likely that the N-terminal region of one monomer interacts with the belly (functional) region of the other to hold the dimer together in an appealing embrace.

The poorly-structured N-terminal is also known as the prion region. It may be that the interaction of the latter with the globular functional region – within the same monomer – prevents the conversion of the protein into its prion form. What molecular changes occur to ease URE2 into its prion form, URE2p? No one knows. What happens though is that the structural change causes the subsequent loss of URE2 function altogether and promotes the assembly of URE2p into fibrils through the interaction of URE2p monomers. It is not known to date whether it is the subtle change in conformation which causes the loss of URE2 function or whether the novel fibril formation simply hinders the URE2/GLN3 interaction. How is the 'infection' propagated from one yeast cell to another? By cytoplasmic mixing. When yeast mates, the cytoplasm of the parental strains mix even though the nucleii do not fuse. When the URE2p of one strain flows into the other, it infects the second strain by transmitting the URE2p conformational change.

Naturally, the whole point in understanding how a prion protein such as URE2p becomes infectious and assembles into fibrils, how it loses its function and how it ultimately affects an organism is to help in the future design of drugs which could counter neurodegenerative diseases such as BSE and the unfortunate human form: Creutzfeldt-Jakob disease.

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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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