The **EMBOSS** Administrators Guide

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This guide relates to **EMBOSS** 1.13.2
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1 Introduction

1.1 About this document
This guide has been written to assist system administrators and developers with the installation and configuration of **EMBOSS**. If you are reading this to find out how to do bioinformatics then you are wasting your time. You are referred instead to the Resources chapter below where there is a list of more relevant literature and web sites. Experienced users may find this document useful for configuring their own databases and customising their **EMBOSS** experience.

1.1.1 Credits
The principal author of this guide is David Martin\(^1\) at the Norwegian EMBnet node.\(^2\) It is however the result of a team effort. Thanks are due in particular to Alan Bleasby who answered a lot of silly questions, killed more than a few bugs, and provided clear explanations, and to the other **EMBOSS** developers at the ‘Hinxton triangle’. I would also like to thank Johann Visagie for the FreeBSD information and Peter Rice for the SRS information. Other contributors are acknowledged in the text.

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If you find this document useful and happen to meet the author or any of the other contributors at a meeting, they would be willing to accept a beer as a token of your appreciation.

1.2 What is **EMBOSS**?
**EMBOSS** is a freely available suite of bioinformatics applications and libraries. It can be downloaded via the internet, copied, customised, and passed on under the terms of the various General Public Licenses. **EMBOSS** has been developed in response to the need for a powerful, adaptable suite of software that can interface readily with many different situations and meet the need of professional bioinformaticists, particularly those needing high throughput and/or scriptable capabilities.

\(^1\)damartin@hgmp.mrc.ac.uk
\(^2\)http://www.no.embnet.org
EMBOSS has primarily been developed by those responsible for the public extensions to the GCG package. Whilst EMBOSS duplicates much of EGCG it includes far better database interaction and has the benefit of freely accessible source code so novel applications can be developed rapidly and at minimal cost.

EMBOSS is currently only available for Unix/Linux systems but it has been known to compile and run on Windows NT. This document will only consider the UNIX version and will assume the reader has some familiarity with UNIX system administration.

1.2.1 Where do I get it?

EMBOSS is available for download from the primary site at the UK EMBnet node by anonymous ftp.³ This directory contains the EMBOSS package and several associated packages (collectively known as EMBASSY) that are distributed with EMBOSS. Download these to a suitable location. Documentation is available on the WWW at the EMBOSS web site.⁴ FreeBSD distributions from 4.2 onwards now include EMBOSS as an optional package maintained by Johann Visagie.⁵ Please see section 2.5 for more information on installation on FreeBSD.

³ftp.uk.embnet.org/pub/EMBOSS/
⁴http://www.uk.embnet.org/Software/EMBOSS
⁵johann@egenetics.com
2 Installation

2.1 Retrieving EMBOSS by anonymous ftp

2.1.1 Interactive FTP

Change directory to the location in which you wish to download the EMBOSS source code. In this example we will download the source to /packages/EMBOSS. Then start your ftp client and point it to ftp.uk.embnet.org.

% ftp ftp.uk.embnet.org
Connected to tantalum.hgmp.mrc.ac.uk.
220 tantalum FTP server ready.
Name (ftp.uk.embnet.org:admmast):

We are using anonymous FTP so type the username anonymous.

Name (ftp.uk.embnet.org:admmast): anonymous
331 Guest login ok, send your complete e-mail address as password.
Password:

Enter your email address here as the password for user anonymous.

Password:
230-################################################################
230- 230- Welcome to the UK HGMP Resource Centre anonymous ftp service
230- 230- Please contact support@hgmp.mrc.ac.uk regarding
230- 230- any problems with this service
230- 230-################################################################
230- 230-Please read the file README
230- it was last modified on Wed Aug 13 15:40:25 1997 - 1093 days ago
230 Guest login ok, access restrictions apply.
Remote system type is UNIX.
Using binary mode to transfer files.
ftp>

Move to the EMBOSS directory and list the files. The output has been truncated a little to save space.

ftp> cd /pub/EMBOSS
ftp> ls
200 PORT command successful.
150 Opening BINARY mode data connection for /bin/ls.
total 5264
... 1871128 Aug  9 22:25 EMBOSS-1.1.0.tar.gz
... 133557 Aug  9 22:31 MSE-0.0.4.tar.gz
... 571095 Aug  9 22:31 PHYLIP-3.573c.tar.gz
Now download the source files

ftp> get EMBASSY-1.1.0.tar.gz
200 PORT command successful.
150 Opening BINARY mode data connection for EMBASSY-1.1.0.tar.gz
(1871128 bytes).
...
ftp>

And repeat for each file. Or use mget *gz to download all the files at once. Exit your ftp session with the command bye.

2.1.2 FTP using wget

The program wget can be used to download a remote directory noninteractively. More details on wget can be obtained from the Free Software Foundation. Assuming you have wget installed, use the following command which generates a lot of output on the screen:

```
% wget -m 'ftp://ftp.uk.embnet.org/pub/EMBOSS'
   => 'ftp.uk.embnet.org/pub/.listing'
Connecting to ftp.uk.embnet.org:21... connected!
Logging in as anonymous ... Logged in!
   => TYPE I ... done.  => CWD pub ... done.
   => PORT ... done.  => LIST ... done.
...
many pages truncated
...
FINISHED --15:04:55--
Downloaded: 2,657,366 bytes in 4 files
```

A new directory ftp.uk.embnet.org has been created and EMBASSY can be found at ftp.uk.embnet.org/pub/EMBOSS. You may wish to create a symbolic link to this from your /packages directory for convenience.

2.2 Unpacking

You will have downloaded the EMBOSS and EMBASSY packages to a suitable directory. For this example we will assume you have downloaded them to /packages so you should now have the following files (or similar) and maybe more packages in EMBASSY.

```
% ls
EMBOSS-1.0.0.tar.gz
PHYLIP-3.573c.tar.gz
MSE-0.0.4.tar.gz
TOPO-0.1.tar.gz
```

First unpack the EMBOSS distribution

---

1http://www.gnu.org
% gunzip EMBOSS-1.0.0.tar.gz
% tar xf EMBOSS-1.0.0.tar

This will create a new directory, EMBOSS-1.0.0 or similar. You may wish to use tar xpf for unpacking EMBOSS.

Enter the EMBOSS directory

% cd EMBOSS-1.0.0

create a directory for the EMBASSY packages

% mkdir embassy

Now copy the EMBASSY packages to the EMBASSY directory

% cp ../MSE-0.0.4.tar.gz PHYLIP-3.573c.tar.gz
   TOPO-0.1.tar.gz embassy

Go into the EMBASSY directory and unpack those packages.

% cd embassy

% gunzip MSE-0.0.4.tar.gz
% tar xf MSE-0.0.4.tar

and so on for each EMBASSY package.

Go back up one directory to the main EMBOSS package directory and prepare to start compilation.

2.3 Compilation

Building EMBOSS is easy. It follows the usual GNU style of ./configure, make, make install. We'll take these steps one at a time.

2.3.1 Configure

To accept the default configuration, just type ./configure and let EMBOSS get on with it. You may however want to make some changes to the configuration parameters according to your local policy. This section will not cover all the possibilities, just some of the more common. The configuration script will attempt to find the necessary components in your system to determine how to successfully build EMBOSS. It typically expects the GNU C compiler (gcc) and several standard libraries that should already be part of your Unix/Linux system. EMBOSS should configure, compile and run on most modern Linux distributions straight out of the box. For Mac OS X please read the separate section below.

Installation directory

You need to have write permission on the directory in which you eventually wish to install EMBOSS. You may also wish to put it somewhere else other than the standard location of /usr/local/emboss.

The installation directory is controlled by the --prefix argument. In my case I have all my applications owned by a non-priviledged user and installed in a package specific directory under /site/prog

% ./configure --prefix=/site/prog/emboss
will install EMBOSS under `/site/prog/emboss`. The binaries will be installed in `/site/prog/emboss/bin` with shared libraries installed in `/site/prog/emboss/lib`. System wide data are installed in `/site/prog/emboss/share/EMBOSS/data`, and the configuration files (ACD files) for the applications will be installed in `/site/prog/emboss/share/EMBOSS/acd` (or for EMBASSY in directories corresponding to the package name.) Documentation is installed in `/site/prog/emboss/share/EMBOSS/doc`. The installation directory should be specified using a full path otherwise interesting failures may occur.

The individual directories for installation can be modified with other configuration commands but this is usually not necessary. Run `./configure --help` to get more information on the directories that can be changed and other configuration options.

Run `./configure` with the options you wish to use. This may take a short time as various messages scroll up the screen.

Depending on your system you may need to explicitly configure the graphics. Please see the section 'Configuring EMBOSS graphics' below.

As I am not an expert in the use of Gnu tools I have not yet worked out how to persuade `make` to look in non standard directories for include files.

All should be well with this and configure should exit with a message like this:

```
... much output skipped
creating ./config.status
creating plplot/Makefile
creating plplot/lib/Makefile
creating nucleus/Makefile
creating ajax/Makefile
creating emboss/Makefile
creating emboss/acd/Makefile
creating test/Makefile
creating test/data/Makefile
creating test/embl/Makefile
creating test/pir/Makefile
creating test/swiss/Makefile
creating test/swnew/Makefile
creating test/wormpep/Makefile
creating emboss/data/Makefile
creating emboss/data/CODONS/Makefile
creating emboss/data/REBASE/Makefile
creating emboss/data/PRINTS/Makefile
creating emboss/data/PROSITE/Makefile
creating Makefile

Configuration is now complete.
```

Reconfiguration

If at first you don’t succeed, try, try and try again. It is not uncommon to make typos or other mistakes when running `./configure`. If you want to run configure again you should delete the file `config.cache` and run `make clean` before running `./configure` with (hopefully) the correct options.

Configuring EMBOSS graphics

The PLPLOT library can produce output to many devices but requires certain libraries that are NOT distributed with EMBOSS

To get X-windows based output you must have X installed else PLplot will not build the required driver. You may need to specify the location of your X-windows library with the configuration
options:  --x-includes=DIR (X include files are in DIR)  --x-libraries=DIR (X library files are in DIR)

To explicitly configure PLPLOT without X-windows, use --without-x.

To get PLPLOT to produce PNG images you will need to have the z\(^2\), png\(^3\) and gd\(^4\) libraries installed. gd version \(\geq 1.6.3\) must be used as the older versions support GIF which is NOT supported in later versions. If for some reason you do not have the required libraries and your system support group will not update them for the system then install all three latest versions (z,gd,png) to a new directory and then add this new directory to your configure line for EMBOSS — ./configure --with-pngdriver=my_dir where the z, png and gd libraries were each installed using ./configure --prefix=my_dir

It may also be helpful to ensure that the LD_LIBRARY_PATH environment variable is set appropriately to include the libraries in the path.

You can explicitly tell EMBOSS to not include PNG support with --without-pngdriver You can tell if ./configure has found a suitable PNG library by watching for something like the following when running ./configure:

checking if png driver is wanted... yes
checking for inflateEnd in -lz... (cached) yes
checking for png_destroy_read_struct in -lpng... (cached) yes
checking for gdImageCreateFromPng in -lgd... (cached) yes

This means that the configuration script has located the PNG libraries on your system. If you see a message indicating that ./configure could not find the libraries or that the version of gd was too old then you should install the latest versions of the libraries yourself and rerun configure with the correct --with-pngdriver value.

2.3.2 Configuring for 64 bit systems

EMBOSS configure looks for gcc and uses this of preference when compiling EMBOSS. This is not ideal for those who wish to have a compiled and linked 64 bit version of EMBOSS. The current version is NOT 64 bit clean (i.e. it does not necessarily use 64 bit representation internally) but will compile and run quite happily on 64 bit systems.

Additional notes are appended below for the various operating systems I have information on.

IRIX 6.5.10

In order to compile for 64 bit on IRIX you have to specify the native compiler in 64 bit mode (cc -64) and the linker in 64 bit mode (/bin/ld -64). The following notes were provided by Jose Ramon Valverde\(^5\).

I have succeeded in compiling EMBOSS for IRIX using 64 bit compilation.
It required some tweaking, but works. The recipe for those willing to give it a try is:

- remove 'gcc' from your path
- define COMPILER_DEFAULTS_PATH appropriately (see pe_envir) to look for a compiler.defaults file containing e.g. :abi=64:isa=4:proc=r10k
- ./configure in EMBOSS and all EMBASSY subdirs
- search in all files for 'CC = cc' and substitute it for 'CC = cc -64'
- same for 'LD = /bin/ld' to 'LD = /bin/ld -64'

\(^2\)http://www.info-zip.org/pub/infozip/zlib/
\(^3\)http://libpng.sourceforge.net/
\(^4\)http://www.boutell.com/gd/
\(^5\)jrvalverde@cnb.uam.es
• make

The reason is that compiling depends on the Makefile and on libtool, as well as linking. I didn’t
spend much in looking at configure since the above steps were so straightforward. I know I should
look into the configure script and add an option for 64-bit-irix-compile or some such, but that’ll have
to wait till I have time for it.

Yes, I know, the search and substitute thing looks tedious, but it isn’t, honest: create a ‘chfile.sh’
out of the EMBOSS source hierarchy containing:

#!/bin/sh
cp $1 $1.orig
mv $1 tmpfile
sed -e 's/CC="cc"/CC="cc -64"/g' tmpfile | \ 
sed -e 's/CC = cc/CC = cc -64/g' | \ 
rm tmpfile
## if you are sure, uncomment this
#rm $1.orig

'cd' to the emboss directory and run

find . -type f -exec /path/to/chfile.sh {} \; -print

and you are done with the CC changes. Libtool requires special treatment since it uses quotes.

Configuring for Mac OS X

The latest release of the Macintosh operating system is a Unix-like system based on a BSD Unix
framework with some tweaks and modifications. Configuring EMBOSS requires a small number
of changes. I am grateful to Don Gilbert ⁶ for the changes in ./configure. You will need the free
Developer Tools package installed. I tested this with OS X 10.0.0.4 and the 10.0.1 release of the
developer toolkit.

If you want X-windows support then you will need to get a version of X-windows. The Darwinfo
site ⁷ has links to several X-windows implementations. I have only tested the XFree86 4.1 X server
with the Quartz desktop client. This can be downloaded from the XFree86 project ⁸ and contains
comprehensive instructions for installation. Install this including the optional programmers and
quartz packages before configuring EMBOSS.⁹

Having installed XFree86 (or not if you do not wish for an X interface), edit the EMBOSS
configure script as follows:

Find line 1455 (or thereabouts)

$libtool_flags --no-verify $ac_aux_dir/ltmain.sh $host \ 

and edit this to

$libtool_flags --no-verify $ac_aux_dir/ltmain.sh darwin \ 

Find line 2203 (or thereabouts)

X_CFLAGS= X_PRE_LIBS= X_LIBS= X_EXTRA_LIBS=
else
if test -n "$x_includes"; then

and insert the following

⁶gilbertd@bio.indiana.edu
⁷http://www.darwinfo.org
⁸http://www.xfree86.org
X_CFLAGS= X_PRE_LIBS= X_LIBS= X_EXTRA_LIBS=
else
  X_LIBS=-lX11
  if test -n "$x_includes"; then
    Find line 4400 (it will be 4401 now)
    XLIB="$X_LIBS -lX11 $X_EXTRA_LIBS"
    and delete the X11 reference
    XLIB="$X_LIBS $X_EXTRA_LIBS"
  fi
Save the file. Because OS X is quite new, the automatic configuration file config.guess cannot
cope so the --host option has to be specified on the command line.
You will need to install the following libraries in order to get PNG support to work: LIBPNG\textsuperscript{10},
LIBGD\textsuperscript{11} and LIBJPEG\textsuperscript{12}. Download each package to a temporary directory and uncompress them.
Install LIBJPEG first. cd into the jpeg-6b directory and run the following sequence of commands in
this order (the jpeg-6b % is the prompt and should not be typed):
\begin{verbatim}
jpeg-6b % ./configure
jpeg-6b % make
\end{verbatim}
then as root (superuser)\textsuperscript{13}
\begin{verbatim}
jpeg-6b % mkdir -p /usr/local/man/man1
jpeg-6b % make install
jpeg-6b % cp *.h /usr/local/include
\end{verbatim}
Now install the LIBPNG library. Change to the libpng-1.0.12 directory into which the libpng
archive unpacked. Copy the standard makefile to this directory with cp scripts/makefile.std
makefile and edit it to point ZLIBINC and ZLIBLIB to /usr/include and /usr/lib. Save the makefile
and type make and, as root, make install. The library will now install. Before it can be used one
further command needs to be run on it. As root run ranlib -c /usr/local/lib/libpng.a.
The LIBGD library is installed last of all. In the gd-1.8.4 directory run make then, as root, make
install and, as for LIBPNG, ranlib -c /usr/local/lib/libgd.a.
You can now change back to the EMBOSS directory.
Configure EMBOSS with ./configure --host=darwin and everything should configure just
fine. There will be some errors but these are not fatal. Building and installing follows the standard
procedure.

2.3.3 Building EMBOSS

Building EMBOSS is a matter of typing 'make' and going to find something else to do for the next
ten minutes to half an hour depending on the speed of your system. EMBOSS will first build the
shared libraries (PL_PLOT, AJAX, and NUCLEUS) and then build the applications.
You may see plenty of warnings (especially on SGI systems) complaining about libraries not
being used to resolve any symbols. These can be safely ignored.
If all goes according to plan you should have built EMBOSS successfully. If not you will have
to try to work out why the build failed. If you can’t work it out yourself, send an email describing
the problem to emboss-bug@embnet.org with a copy of the config.status and config.cache files from
\textsuperscript{10}http://libpng.sourceforge.net
\textsuperscript{11}http://www.boutell.com/gd/
\textsuperscript{12}ftp://ftp.uu.net/graphics/jpeg/jpegsrc.v6b.tar.gz
\textsuperscript{13}If you do not have root access to your system you will have to install these libraries in a different directory. Use
the --prefix option to configure to specify a different directory for LIBJPEG and edit the makefiles for the other
libraries to include the installation locations. Then use the --with-pngdriver= option when configuring EMBOSS.
your EMBOSS directory. (These will tell the developers what state your system was in when compilation failed).

Assuming that compilation was successful, you can now type `make install`. After a few minutes and many pages of messages, EMBOSS should be installed where you specified in the `--prefix` option (or in the default location of `/usr/local/emboss` if `--prefix` was not specified).

### 2.3.4 Post compilation setup

You will now need to make a few adjustments to your environment to ensure that EMBOSS runs smoothly. EMBOSS looks for certain environment variables to determine where the libraries and data are found. These instructions assumed you installed EMBOSS in `/site/prog/emboss`. Adjust these instructions to suit your installation. Insert the following lines at the end of `/etc/cshrc` (or `.cshrc` for a personal installation)

```bash
setenv PLPLOT_LIB /site/prog/emboss/lib
set path=( /site/prog/emboss/bin ${path} )
```

Or for bash/ksh/sh users, insert the following at the end of `/etc/profile` or `.bashrc`

```bash
PLPLOT_LIB=/site/prog/emboss/lib
PATH=/site/prog/emboss/bin:$PATH
export PLPLOT_LIB PATH
```

EMBOSS should now be ready for use. If you want to place your data files elsewhere or have a separate set of datafiles you wish to use you can set the `EMBOSS_DATA` variable, either as an environment variable in your `cshrc`/`profile` or in `emboss.default`. It is essential to set `EMBOSS_DATA` otherwise EMBOSS will as default install the data files (including those installed with REBASEEXTRACT, PROSEXTRACT or PRINTSETRACT) in the default directory `emboss/data` in the unpacked source code. This ‘feature’ is due to the definition

```
AJAX_FIXED_ROOT ="\\"pwd\\"/emboss\\""
```

in `Configure`. This will probably be altered in future versions to be

```
AJAX_FIXED_ROOT="\\"${datadir}/${PACKAGE}\\""
```

which will remove the need for specifically defining `EMBOSS_DATA`.

### 2.3.5 Testing your EMBOSS installation

You can test your EMBOSS installation by trying the program `wossname`

```bash
% wossname -auto | more
```

This should give a long list of programs that are available. Press space to page down through the list. This is just the EMBOSS programs and doesn’t include any of the EMBASSY programs.

### 2.4 Installing EMBASSY

As well as the base libraries and standard EMBOSS distribution, various extra packages (EMBASSY) are distributed with EMBOSS.

To install an EMBASSY package, go to the relevant directory. For example to install PHYLIP (which was unpacked into `/packages/EMBOSS-1.0.0/embassy/PHYLIP-3.573c` earlier) go to the relevant directory.

---

14You don’t have to do this. You can leave EMBOSS where it is and just add the path to the `emboss` directory to your `PATH`
% cd /packages/EMBOSS-1.0.0/embassy/PHYLIP-3.573c
% ./configure --prefix=/site/prog/emboss
   ... output not shown
% make
   ... output not shown
% make install
   ... output not shown

Note. You MUST use the same arguments for ./configure that you used for the installation of the main EMBOSS package. It may be necessary to add other options as required by individual packages (see below).

Repeat as necessary for the other EMBASSY packages. It should also be noted that certain EMBASSY packages may require additional libraries.

You should now find that running wossname as before lists the EMBASSY programs.

2.4.1 EMBASSY package specific notes

If a package has no notes below then it either should compile without a hitch or I don’t know about it/haven’t written it up yet. So far TOPO, MEME, PHYLIP and MSE appear to install without a problem using the same arguments to configure.

EMNU

EMNU requires the curses or ncurses libraries that come as standard on most Unix-like systems. In particular EMNU requires two header files form.h and menu.h that are not distributed with all implementations. If your curses/ncurses library is installed in a strange place then you may need to instruct configure with the option

--with-curses=/path/to/curses

2.5 Installing EMBOSS in package format

EMBOSS can be installed on almost all Unix/Linux operating systems using the instructions above, but the package format can be far more convenient. A package is a precompiled set of binaries with installation instructions that can be set up on your system with a minimum of work. In some cases the package will check for the correct libraries and install those as necessary.

Brief instructions are given here for the packages of which I am aware. These are maintained separately from the main source tree and may also install some files in operating system standard locations instead of the locations used by the ‘raw’ EMBOSS distribution. Please read the more detailed instructions that accompany each package.

2.5.1 Installing EMBOSS on FreeBSD

A FreeBSD EMBOSS package has been created by Johann Visagie\(^\text{15}\) of Electric Genetics. This will be distributed on the installation CD’s and through the normal distribution channels from FreeBSD version 4.2 onwards.

For the FreeBSD user with an up-to-date ports tree\(^\text{16}\), installing EMBOSS reduces to two simple commands (as root):

```
# cd /usr/ports/biology/emboss
# make install
```

\(^\text{15}\) johann@egenetics.com

\(^\text{16}\) FreeBSD users can update their ports tree through a variety of mechanisms. Please see the FreeBSD specific guide produced by Johann for more information
The FreeBSD specific parts of the port are that `emboss.default` is included with the other configuration files under `/usr/local/etc` as `emboss.default.sample`, and the EMBOSS documentation is installed in `/usr/local/share/doc/EMBOSS` instead of the default location. For further information on installation under FreeBSD you are referred to the Resources chapter.
3 Configuration

EMBOSS can be readily configured to match your requirements. In a standard installation of EMBOSS the configuration directives are looked for in the following locations and in the following search order:

1. A file `emboss.default` in the `share/EMBOSS` subdirectory of your EMBOSS installation.\(^1\)
2. A file `.embossrc` in the directory specified by the `EMBOSSRC` environment variable.
3. A file `.embossrc` in the users home directory.

`emboss.default` and `.embossrc` are plain text files that can readily be edited to suit.\(^3\) Redefinitions of configuration parameters will override those previously defined. In the descriptions that follow only `.embossrc` will be mentioned but all directives can be placed in `emboss.default` for site wide configuration.

Several aspects of EMBOSS can be defined. These are:

- EMBOSS environment variables
- EMBOSS databases
- Default behaviour of EMBOSS programs

Databases are by far the most complex of these.

EMBOSS will ignore blank lines in the `emboss.default` and `.embossrc` files. It will also ignore any lines beginning with `#` or `!` allowing comments to illuminate the declarations in the file.

3.1 EMBOSS environment variables

EMBOSS environment variables are set with an `env` or a `set` declaration. `env` and `set` are interchangeable. The most important environment variable is the location of the `.acd` files that describe each program.

```
set emboss_acdroot /site/prog/emboss/share/EMBOSS/acd
```

Environment variables are useful for simplifying maintenance of your `.embossrc`. For example you may want to specify the location of your databases as an environment variable. Then if you move the databases you only have to update one line in the configuration file.

```
set emboss_database_dir /data/databases/flatfiles
```

This would then be referred to later in `.embosrc`as

```
$emboss_database_dir/embl
```

for the directory `/data/databases/flatfiles/embl`

---

\(^1\)This location may have been redefined in installations of EMBOSS that have been packaged for specific operating systems. See section 2.5 for further information on OS specific package installations.

\(^2\)EMBOSS will also look in the `emboss` directory under the EMBOSS source distribution for `emboss.default` if it is not found under the installation directory.

\(^3\)A sample `emboss.default` is located in `emboss/acd` under the source distribution.
3.1.1 Configuring EMBOSS differently for different groups of users

It may be the case that you have users who need to share a specific setup. Maybe to have access to different sets of databases or need to use a different data directory.

It can be time consuming and error prone to maintain a series of individual .embosrc files or to cause users to have to work in the same directory or to copy an .embosrc to each directory they wish to work in. The environment variable EMBOSSRC can be set to point to an arbitrary directory containing an .embosrc which can then be used to give workgroup specific configuration. Each user then only needs to set EMBOSSRC in their .cshrc (C Shell) or .profile (Bash) to get the workgroup specific setup.

In my case I have several groups of researchers for whom I maintain biological sequence databases. These databases have been made available under restrictive licenses so that I cannot allow researchers outside the groups to access the databases. Using $EMBOSSRC I can set up a common configuration for the members of each group by defining the databases in the $EMBOSSRC/.embosrc file.

3.2 Databases

3.2.1 Database access modes

EMBOSS offers three modes for accessing databases:

Single: EMBOSS retrieves a single sequence indexed by ID or accession number.

Query: EMBOSS retrieves a set of sequences corresponding to a wildcard query.

All: EMBOSS returns all the sequences in the database in no particular order

Each database definition can configure one or many of these modes for database access.

Typically EMBOSS uses variations on the EMBLCD system of database indexing to provide rapid access in single and query modes to flat file databases. The EMBLCD method is implemented in a variety of ways depending on the original format of your database. The EMBLCD method assumes that you have one or both of ID and accession number in each record and that they are unique for the whole database index. EMBOSS also provides methods for retrieving sequences via the WWW and a specific method for interaction with SRS\(^4\). For other non-flat file databases or flat file databases in formats not currently supported by EMBOSS you will have to configure an external application to retrieve sequences.

3.2.2 General database configuration.

Each database is configured using a DB declaration.

The generalised form is

```
DB databasename [Configuration options]
```

The configuration options are tag/value pairs and must contain at least a description of the access method (using method: or one or more of method: single:, method: query: and method: all:) and a description of the original format of the sequences (using format:). In addition to these tags there will be other tags that are needed for particular methods and other tags that are optional.

\(^4\)http://www.lionbio.co.uk
Database access methods

The scope of each method is:

**Single mode** - *s* Supports retrieval of a single sequence.

**Query mode** - *q* Supports retrieval of a subset of the sequences in the database specified using a wild card query in the USA\(^5\)

**All mode** - *a* Supports retrieval of all sequences in the database as a stream of data.

An example entry for each access method is shown.

**DIRECT**  
Modes: *a*  
Direct accesses the flatfile directly. It returns all the database entries, one after the other. It assumes no indexing.

```
DB mydb [
  #required parameters
  method: direct
  format: fasta
  dir: $emboss_db_dir/mydb
  file: *.dat
  #optional parameters
  type: N
  release: 63.0
  comment: "My own database with no indices"
  exclude: "est*.dat"
]
```

**SRS**  
Modes: *a q s*  
SRS returns entries from a local installation of SRS using the -e switch to getz to return entries in the original format.

```
DB mydb [
  #required parameters
  method: srs
  format: embl
  app: getz
  #optional parameters
  dbalias: embl
  type: N
  comment: 'My srs indexed database'
  release: '63.0'
]
```

**SRSFASTA**  
Modes: *a q s*  
As SRS but returns the sequences in FASTA format.

---

\(^5\)Please see the EMBOSS documentation for description of Uniform Sequence Address format
URL Modes: s
URL uses a defined web server to retrieve a specific entry. EMBOSS may fail if the HTML causes complications with parsing of the entry.

DB mydb [
  # required parameters
  method: url
  format: genbank
  url: "http://www.infobiogen.fr/srs5bin/cgi-bin/wgetz?-e+[genbank-id:%s]"
  #optional parameters
  type: N
  comment: "Genbank by ID from InfoBiogen"
]

The %s in the URL string indicates where EMBOSS will insert the identifier portion of the USA.

EMBLCD Modes: a q s
EMBLCD uses EMBLCD indices created with dbiflat or dbifasta to access flatfile databases in the original format.

DB mydb [
  method: emblcd
  format: embl
  dir: $emboss_db_dir/embl
  file: *.dat
  #optional parameters
  type: N
  release: 63.0
  comment: "my comment"
  exclude: est*.dat
  indexdir: $emboss_db_dir/indices
]

This method can require careful setup. Please read the more specific descriptions below.

GCG Modes: a q s
GCG uses EMBLCD indices created with dbigcg to access databases in GCG format. This method uses the .seq and .header files created by the GCG suite of programs.

DB mygcgdb [
  method: gcg
  format: embl
  dir: $emboss_db_dir/gcgembl
  file: *.seq
  #optional parameters
  type: N
  release: 63.0
  comment: "my comment"
  exclude: est*
  indexdir: $emboss_db_dir/indices
]

BLAST Modes: a q s
BLAST uses EMBLCD indices created with dbiblast to access databases in BLAST format.
EXTERNAL Modes: a q s
EXTERNAL uses an external application to retrieve sequences. The ID is passed as an argument to
the application, either replacing %s in the command string (if present) or as an additional argument
(if there is no %s). EXTERNAL expects the application to return the sequence on STDOUT.

DB mydb [  
  #required parameters  
  method: app  
  format: fasta  
  app: "getfromdb mydb"  
  #optional parameters  
  type: P  
  comment: "my own protein database with a custom retrieval program"  
]

APP Modes: a q s
APP is the same as EXTERNAL.

For any given method: declaration, EMBOSS will use that method for those access modes
supported by the method.

If you wish to specify which access mode (all, query or single) should be handled by which
database retrieval method then the methodsingle:, methodquery: and methodall: declarations
should be used instead of method:

DB mydb [  
  methodsingle: app  
  format: fasta  
  app: "customapp myproteindb"  
  methodall: direct  
  dir: $emboss_db_dir/myproteindb  
  file: myproteindb.dat  
  type: P  
  comment: "single and all access for myproteindb"  
]

3.2.3 Indexing and configuring flatfile databases

Flatfile databases are plain text files in a defined format such as those released by EMBL, Swissprot
and so on. The EMBOSS program dbiflat is used to generate EMBLCD indices that can be
used for all types of database access. DBIFLAT can process databases in EMBL, SWISSPROT and
GENBANK format. Pseudo EMBL format databases which do not have unique ID and AC entries
may cause DBIFLAT to do mysterious things and should be avoided.

DBIFLAT (and the EMBLCD access method) requires the databases to be uncompressed. The
examples given here will not probe the deeper secrets of DBIFLAT (for which the reader is referred to
the documentation, or failing that the source code) but will show a typical installation for a common
database.

We assume that EMBOSS has been installed and works. This can be tested with the command
wossname -auto which should list all the programs available.

In this example we will index and configure the EMBL database for use with EMBOSS.

First download and unpack the EMBL database. This will require a considerable amount of disk
space. If you do not have sufficient space available then just download a subset of the database.

Use cd to move the directory in which you have unpacked EMBL. This should look something
like this when you run ls:

% ls
est_fun.dat
Run dbiflat to create the EMBLCD indices.

% dbiflat

Index a flat file database
  EMBL : EMBL
  SWISS : Swiss-Prot, SpTrEMBL, TrEMBLnew
  GB : Genbank, DDBJ
Entry format [SWISS]: EMBL
Database name: embl
Database directory [-]:
Wildcard database filename [*.dat]:
Release number [0.0]: 63.0
Index date [00/00/00]: 31/07/00

DBIFLAT should happily chug away for some considerable time (up to a few hours depending on the speed of your machine) and will generate (eventually) the following index files:

% ls
  acnum.hit
  acnum.trg
  division.lkp
  entrynam.idx

Now we create an entry in the EMBOSS configuration files to access the database. It is probably a good idea to try new database definitions in your local configuration file first.

Put the following entry in your .embossrc

DB embl [
  type: N
  method: emblcd
  format: embl
  dir: $emboss_db_dir/embl
  file: "*.dat"
  release: "63.0"
  comment: "EMBL release 63.0"
]

you will have needed to redefine $emboss_db_dir using a directive such as

set emboss_db_dir /path_to_databases

somewhere in your emboss.default or .embossrc.

Save .embossrc and try SHOWDB. You should see a line that looks like:

% showdb
  .. output deleted
  embl    N   OK OK EMBL release 63.0
  .. output deleted
3.2.4 Fine tuning the installation:

It is probably a good idea to set up subsections of the database so that end users can search just the regions they wish to search. This section applies to all access methods that use EMBLCD style indexes and probably to others as well.

Files can be included with the declaration file: or excluded with the declaration exclude:. It is a good idea to put the wild card directory specifier (/) in front of the filename to ensure that any path that may be included in division.lkp will be matched. Please note especially the notes for GcG formatted databases indexed with dbigcg.

In order to just take the EST files in our EMBL database try the following:

```plaintext
DB emblest [
  type: N
  method: emblcd
  format: embl
  dir: $emboss_db_dir/embl
  file: "est*.dat"
  release: "63.0"
  comment: "EMBL release 63.0"
]
```

Files can also be given as a space separated list enclosed in quotes. For example to set up a database of all mammalian sequences (except genomes) try the following:

```plaintext
DB emballmam [
  type: N
  method: emblcd
  format: embl
  dir: $emboss_db_dir/embl
  file: "rod*.dat hum*.dat mam*.dat"
  release: "63.0"
  comment: "EMBL release 63.0"
]
```

As you can see from these two examples, the file: tag takes a space delimited list of filenames enclosed in quotes that can contain normal wildcard (?*) characters.

It can be quite tedious to set up a long list of sequences to search. In many cases you can use the exclude: tag to make things easier.

```plaintext
DB embnoest [
  type: N
  method: emblcd
  format: embl
  dir: $emboss_db_dir/embl
  file: "*.dat"
  exclude: "est*.dat"
  release: "63.0"
  comment: "EMBL release 63.0"
]
```

This configures the embnoest database to contain all of EMBL except the EST’s.

3.2.5 Indexing and configuring GCG format databases

EMBOSS can access GCG formatted databases, thus avoiding having multiple copies of the same databases in different formats for those who still use GCG alongside the flatfiles. EMBOSS creates EMBLCD like indices for the GCG format databases using the program dbigcg. This runs in much
the same way as dbiflat. You will need the GCG format .seq and .header files in order to create an EMBLCD indexed database.

Move to the GCG database directory containing your data and run dbigcg

Index a GCG formatted database

EMBL : EMBL
SWISS : Swiss-Prot, SpTrEMBL, TrEMBLnew
GB : Genbank, DDBJ
PIR : NBRF
Entry format [EMBL]:
Database name: embl
Database directory [.]:
Wildcard database filename [*.seq]:
Release number [0.0]: 63.0
Index date [00/00/00]: 31/07/00

The program will chug along for a while and will then generate the EMBLCD index files for the GCG format database.

When dbigcg prompts for the entry format (Entry format [EMBL]:) you should enter the original database format before you ran embltogo or similar to generate the GCG databases.

The following entry should be put in your .embosrc

DB gcgeemb1 [
  type: N
  method: gcg
  format: embl
  dir: $emboss_db_dir/embl
  file: "*.dat"
  release: "63.0"
  comment: "EMBL release 63.0"
]

SHOWDB should show your newly configured database.

You can configure subsets of the databases in the same way as for the original format databases, described in section 3.2.4 above. One difference to dbiflat indexing is that both the .seq and .header files are listed in the division.lkp file. file: and exclude: directives should therefore be of the form exclude: */em*est* instead of just */em*est*.seq.

3.2.6 Indexing and configuring BLAST databases

BLAST format databases are generated for efficient homology searching using the BLAST programs. It can be convenient to avoid redundant copies of databases so EMBOSS provides a mechanism for accessing these databases.

BLAST format databases are those generated using the tools distributed with NCBI-BLAST or with WU-BLAST. For indexing of one BLAST database, move to the directory containing your BLAST format databases and run dbiblast

Index a BLAST database

Database name: blastsw
Database directory [.]:
database base filename [blastsw]:
Release number [0.0]:
Index date [00/00/00]:
  N : nucleic
  P : protein
  ? : unknown
Sequence type [unknown]: p
  1 : wublast and setdb/pressdb
  2 : formatdb
  0 : unknown
Blast index version [unknown]: 2

The program will chug along for a while and will then generate the EMBLCD index files for the BLAST format database.

The following entry (or one like it that is more appropriate to your particular installation) should be put in your .embossrc

```
DB blastsw [
  type: P
  method: blast
  format: ncbi
  dir: $emboss_db_dir/blastsw
  file: "blastsw"
  release: "38.9"
  comment: "BLAST format Swissprot"
]
```

SHOWDB should show your newly configured database.

Because of the way BLAST works, many sites may group their BLAST databases in the same directory. You can index these in situ with DBIBLAST but this may require some extra steps if your databases are not of the same type as generation of subsequent index files will overwrite those that already exist. To avoid overwriting of index files you can index many databases with one set of index files, or you can use the indexdir options to place the indices in a different directory.

There are two requirements for indexing several databases together in one index. The first is that the databases are the same type (protein/nucleic acid) and generated with the same tool (pressdb or formatdb); the second is that all the ID and accession numbers in the combined databases are unique.

Run DBIBLAST as before but specify all the databases you wish to be included when prompted for the database filename.

Index a BLAST database
Database name: alldbs
Database directory [.]:
database base filename [alldbs]: dbone dbtwo dbthree dbfour
Release number [0.0]:
Index date [00/00/00]:
  N : nucleic
  P : protein
  ? : unknown
Sequence type [unknown]: p
  1 : wublast and setdb/pressdb
  2 : formatdb
  0 : unknown
Blast index version [unknown]: 2

These can then be configured as described in section 3.2.4 above by using the 'file:' and 'exclude:' tags as appropriate.6

6There is one difference to the standard EMBLCD access method in that the database indexes will not allow the generation of exclusive subsections of the combined database. If an ID or accession number is specified that is present in the index then the sequence will be returned irrespective of which database it is in.
When you have databases of different types, generated with different programs or where the ID/accession numbers are duplicated between databases the preferred strategy is probably to keep the source data for the individual databases in separate directories and index them there.  

Alternatively you can place the index files in a separate directory. This requires that you run dbiblast with the -indexdirectory option and set the indexdir: tag in the database configuration to point to the correct database. The example below illustrates database configuration using the indexdir options.

```
% dbiblast -indexdir=/databases/indices/mydb
Index a BLAST database
Database name: mydb
Database directory [.]:
database base filename [mydb]:
Release number [0.0]:
Index date [00/00/00]:
    N : nucleic
    P : protein
    ? : unknown
Sequence type [unknown]: p
    1 : wublast and setdb/pressdb
    2 : formatdb
    0 : unknown
Blast index version [unknown]: 2
```

The corresponding entry in .embossrc (or emboss.default) would look like:

```
DB mydb [
    type: P
    method: blast
    format: ncbi
    dir: $emboss_db_dir/blastsw
    indexdir: /databases/indices/mydb
    file: mydb
    release: "1.0"
    comment: "My BLAST DB with an index in a different directory"
]
```

Again, multiple indices cannot coexist in the same directory so care should be taken when using the indexdir options that an existing database index is not overwritten.

### 3.2.7 Indexing and configuring FASTA databases

The FASTA specifications just define the sequence file as a header line that begins with > and subsequent lines containing the sequence. The header line can be present in an almost infinite number of formats, several of which can be processed by EMBoss. EMBoss attempts to determine the accession number and/or ID for each sequence. For indexing purposes there is no semantic difference between an accession number and an ID. In the real world, accession numbers are immutable, ie. they do not change with subsequent releases of the database, but ID’s may change. In any case IDs and accession numbers are unique, and that is all that matters for database indexing EMBoss.

The program used to process FASTA format databases is dbifasta. It can recognise the following header line formats:

---

7Keeping one directory with symbolic links for your BLAST installation will ensure that BLAST continues to function correctly if you set BLASTDB to point to the directory containing the symbolic links. The EMBoss indices can be placed wherever you wish as long as you remember to run dbiblast with the appropriate options and put an appropriate indexdir tag in the DB configuration in your .embosrc
Other header formats will not be recognised by DBIFASTA and will cause indexing and/or database lookup to fail. If you have a different header format that DBIFASTA cannot yet handle you have two options:

1. (The preferred option) Get a C programmer to modify the source code for DBIFASTA and recompile. If you are a community spirited person you will also contribute these changes to the main EMBOSs source tree. (email emboss-dev@embnet.org for more information on contributing changes to the EMBOSs source code and/or read the EMBOSs developers documentation)

2. (The quick hack) Write a custom script (using e.g. BioPerl\(^\text{10}\)) to access your database and use method: external to configure it. This is less desirable as you may be limited in the access modes you can use.

To index a FASTA format database, run DBIFASTA.

```bash
% dbifasta
Index a fasta database
  simple : >ID
  idacc : >ID ACC
  gcgid : >db:ID
  gcgidacc : >db:ID ACC
  ncbi : >blah|...[|ACC]|ID
ID line format [idacc]:
Database name: mydb
Database directory [.]:
Wildcard database filename [*.dat]: mydb.fasta
Release number [0.0]:
Index date [00/00/00]:

DBIFASTA will chug along for a little while and will produce the index files. You can use the same indexdir options as for DBIFLAT, DBIGCG and DBIBLAST to place the indices in a different directory.

Place the following entry in your .embossrc

```bash
DB mydb [
  type: P
  method: emblcd
  format: fasta
  dir: $emboss_db_dir/mydb
  file: mydb.fasta
    comment: "My database"
]
```

format: should be dbid, ncbi or fasta (for every format except dbid or ncbi. The same file: and include: tags can be used as for the other database indexing programs.

\(^8\)db is one word

\(^9\)The ID is always taken to be the characters after the last bar (|). The previous field is also indexed but ONLY if it looks like an accession number (e.g. AC00001).

\(^10\)http://www.bioperl.org
3.2.8 Configuring EMBOSS to use SRS for database lookup.

**method: srs** is really a special case of **method: external** with some additional features.

SRS is a powerful database querying system that can cross reference between different databases, launch applications and so on. SRS can be run either through a web interface (see the description of the URL method above for an example) or via the command line program **getz**. Indexing and configuring databases for SRS is outside the scope of this document which will describe how to connect to preconfigured and indexed SRS databases.\(^{11}\) If **getz** is already in your **PATH** environment variable then insert the following (or similar) in your .embossrc:

```
DB emblgetz [
    type: N
    method: srs
    release: "63"
    format: embl
    comment: 'EMBL using getz'
    dbalias: embl
    app: getz
]
```

This will provide access to the SRS database 'embl' as **emblgetz:acc**. If the SRS database has a different name to the EMBOSS database (as is the case here) then the **dbalias: tag** should be used to access the correct SRS database.

This configuration can be extremely slow for the all access mode. It is probably a better idea to set up the database as follows:

```
DB emblgetz [
    type: N
    methodquery: srs
    release: "63"
    format: embl
    comment: 'EMBL using getz'
    dbalias: embl
    app: getz
    methodall: direct
    file: ".*.dat"
    dir: $emboss_db_dir/embl
]
```

which will use **method: srs** for the query access mode but will use **method: direct** for the all access mode, thus speeding up reading of the whole database.

The SRSFASTA access method is identical to the normal SRS method except that it returns the sequence in FASTA format and so does not need a **format:** tag.

3.2.9 Indexing and configuring other databases

Many institutions may have local databases set up in their own Laboratory Information Management System. EMBOSS provides a simple mechanism for interfacing with such systems.

As long as a program is available that can be called noninteractively and returns the specified sequence on standard output, EMBOSS can interface with it. Use method: app or external (the two are equivalent) and app: "program command". The ID given in the USA will be appended to the command used to run the program. It is probably best to specify the methods available using the method subsets, methodall:, methodquery: and methodsingle: rather than using the generic method: tag.

\(^{11}\)For information on configuring and indexing SRS databases please look at the SRS administrators guide [www/doc/srsadmin.pdf](http://www/doc/srsadmin.pdf) in your SRS 6 installation
3.3 Other data

EMBOSS can be integrated with some common biological databases. These are described in this section.

3.3.1 REBASE

Rebase is the restriction enzyme database maintained by New England Biolabs. It is needed for programs such as remap and restrict.

The latest version of Rebase can be obtained by anonymous FTP.\textsuperscript{12} EMBOSS needs the \texttt{withrefm} file. The data is extracted for EMBOSS with the program \texttt{rebaseextract}.

If you installed EMBOSS with the \texttt{--prefix} option you may need to create the REBASE directory under the EMBOSS data directory (\texttt{/site/prog/emboss/data} in this example) This directory only needs creating once.

\begin{verbatim}
% mkdir /site/prog/emboss/data/REBASE
% rebaseextract
Extract data from REBASE
Full pathname of WITHREFM: /data/rebase/withrefm.008
\end{verbatim}

Rebase is now installed and ready to use.

3.3.2 TRANSFAC

Transfac is the transcription factor binding site database. It is available by anonymous FTP.\textsuperscript{13} Unpacking the distribution reveals a file called \texttt{site.dat}. This is the one EMBOSS needs.

Run \texttt{tfextract} to extract the data from TRANSFAC.

\begin{verbatim}
% tfextract
Extract data from TRANSFAC
Full pathname of transfac SITE.DAT: /databases/transfac/site.dat
\end{verbatim}

\texttt{TFSCAN} can now access the TRANSFAC database.

3.3.3 PROSITE

Prosite is a database of regular expressions that match potentially diagnostic regions for structural/functional classification of proteins. EMBOSS needs this database for the \texttt{patmatmotifs} program.

PROSITE can be obtained via anonymous FTP.\textsuperscript{14} You may need to create a PROSITE subdirectory under data in the EMBOSS installation directory.

Then run \texttt{prosextract} to build the EMBOSS Prosite database.

\begin{verbatim}
% prosextract
Builds the PROSITE motif database for patmatmotifs to search
Enter name of prosite directory: /data/prosite
\end{verbatim}

PROSITE is now integrated into your EMBOSS installation.

\textsuperscript{12}ftp://ftp.ebi.ac.uk/pub/databases/rebase
\textsuperscript{13}ftp://transfac.gbf.de/pub/transfac/ascii/
\textsuperscript{14}ftp://ftp.ebi.ac.uk/pub/databases/prosite
3.3.4 PRINTS

Prints is a database of diagnostic patterns of blocks of sequence homology in protein families. The PRINTS database can be searched using the EMBOSS program pscan.

PRINTS can be obtained via anonymous FTP.\(^{15}\) The database is made available as compressed files which should be uncompressed using gzip before integrating them into EMBOSS.

PRINTS is integrated with EMBOSS using the program printsextract:

```
% printsextract
Extract data from PRINTS
Input file: /data/prints/prints27_0.dat
```

The PRINTS database is now integrated with EMBOSS.

3.3.5 Miscellaneous data files

Other data files should be kept in the data directory under the main EMBOSS installation. Individual users personal data files can be kept in the current working directory, a subdirectory .embossdata of the current directory, their home directory or a subdirectory .embossdata of their home directory. EMBOSS will search these locations in this order and will stop as soon as it finds a matching file. If the personal directories do not contain the desired file, EMBOSS will search the system wide data directory, /site/prog/emboss/data in this example.

Apparently inexplicable errors when running EMBOSS programs may be caused by the system not using the data files one expects. The search path can be displayed in search order using the command embossdata.

3.4 Default program settings

As with many other areas, the default behaviour of programs can be controlled by setting appropriate values in .embossrc.

All general qualifiers\(^ {16}\) can be specified as

```
set emboss_QUALIFIER 1
```

where QUALIFIER is one of the general qualifiers and the value can be 1 or 0 for true or false respectively. Setting the qualifier value to true has the effect of running every program with that qualifier set.\(^ {17}\) multiple qualifiers can be set and will work in the same way as if you set them when running the program. For example you can set emboss_verbose 1 and the program will run normally, but when the program is run with the -help qualifier, the output will be in verbose form.

Qualifiers that can be set:

HELP Print help text.

VERBOSE Causes -help to print verbose text.

ACDTABLE Causes -help to print HTML formatted table of options.

STDOUT Causes all output to go to STDOUT as default.

ACDPRETTY Rewrites the ACD file in a nicely formatted way.

ACDLOG Enables ACD file processing to be logged. Useful for hunting bugs.

DEBUG Writes debugging output to a file. Also useful for finding bugs.

\(^ {15}\)ftp://ftp.ebi.ac.uk/pub/databases/prints

\(^ {16}\)See the EMBOSS Quick Guide or the web documentation (or use wossname -help -verbose) for an overview of general qualifiers.

\(^ {17}\)You can specifically unset it by using the -noQUALIFIER command line option.
OPTIONS Enable prompting for optional parameters.

FILTER Take input from STDIN and send it to STDOUT.

AUTO Do not prompt for any options but accept the defaults if no values are given.

These qualifiers are typically used by advanced users (-options, -verbose) or by developers (-debug -acdlog).

Other program options that can be set are emboss_format, emboss_acdroot, and emboss_data. The value of emboss_format determines which default sequence format to use for output. For example, if you are running EMBOSS alongside GcG you may wish to have the following entry in your .embossrc:

```
set emboss_FORMAT gcg
```

which has the effect of using GcG format by default.¹⁸ emboss_acdroot /path/to/acd can be set if you wish to use a different directory for the ACD files, and emboss_data /path/to/data if you wish to use a separate data directory.

3.5 Logging

Many system administrators may wish to make use of the logging facilities of EMBOSS. Setting the variable emboss_logfile in emboss.default or .embossrc allows the system to keep a log of which programs are used when and by whom.

```
set emboss_logfile /site/log/emboss.log
```

The log file structure is very simple. Three tab separated fields are stored, program name, user name, and the date and time.

```
prettyplot joeuser Wed Aug 02 14:29:13 2000
```

The file set in emboss_logfile should be world writable. The following command ensures logging can occur.

```
chmod +w /site/log/emboss.log
```

All settings can be overridden in a users .embossrc files by redefining the relevant variables. eg. to prevent my system usage being logged I can redefine emboss_logfile by putting the following entry in my .embossrc file.

```
set emboss_logfile /dev/null
```

This behaviour may change in the future to prevent users redefining some system settings.

¹⁸This can of course be overridden using the -osformat associated qualifier. See the EMBOSS Quick Guide for more information.
4 Graphical interfaces to EMBOSS

4.1 Web Interfaces

There are several web interfaces to EMBOSS available. Please see the main EMBOSS web site for more details on these.
5 Resources

5.1 Web sites

5.1.1 Programs

EMBOSS source code ftp://ftp.uk.embnet.org/pub/EMBOSS

EMBOSS Documentation http://www.uk.embnet.org/Software/EMBOSS

BLAST tools Tools for generating BLAST format databases are contained in the NCBI toolkit which can be obtained from NCBI at:


SRS software The SRS software can be obtained from Lion Bioscience. This is a commercial package but at the time of writing is available free of charge to academic institutions.

wget Various useful utilities including the wget program are available from the Free Software Foundation.

5.1.2 Databases

Most of the databases mentioned in the text along with many others can be obtained via anonymous ftp from the European Bioinformatics Institute (EBI) at:

ftp://ftp.ebi.ac.uk/pub/databases

Please use a mirror site where possible to avoid overloading of the EBI’s resources.

Other databases can be obtained from NCBI (Genbank, UniGene etc.)

5.1.3 Other Documentation

Please review the EMBOSS documentation available on the WWW at the URL above.

The EMBOSS Quick guide A pocket reference guide to using EMBOSS.

The EMBOSS Tutorial A tutorial to give an introduction to using EMBOSS for bioinformatics users.

The updated ABC guide This is a series of bioinformatics practicals based predominantly on EMBOSS.

EMBOSS-FreeBSD-HOWTO Detailed documentation on installation of EMBOSS on FreeBSD.

---

1http://www.lionbio.co.uk
2http://www.gnu.org
4http://www.hgmp.mrc.ac.uk/Registered/Option/emboss.html
5ftp://ftp.no.embnet.org/pub/ABC
5.2 Maintenance of your EMBOSS installation

EMBOSS is a rapidly evolving software package. It is constantly being improved, new features added and 'issues' resolved. In addition there are new applications added and you probably want to make use of these.

5.2.1 Automated installation of EMBOSS and EMBASSY

Once you have installed EMBOSS and got it to work you have solved the hardest part of the struggle. Updating EMBOSS as new releases appear can be quite tedious. UNIX is designed for the lazy, so here is my lazy man's guide to always having an up to the minute EMBOSS installation.

The following script can be run manually (it should probably be 'sourced' rather than executed directly) or can be fired off with cron (in the early hours of the morning is a good time). It assumes you are installing EMBOSS outside the source directory and have write permissions to do so.

EMBOSS will update EMBOSS distributed files but will not alter or overwrite your own datafiles or your emboss.default.

---

# This script should be sourced, not run.
# EMBOSS UPDATE.
# it assumes $packages_dir/EMBOSS is a symbolic link to
# $mirror_dir/ftp.uk.embnet.org/pub/EMBOSS
#

#site specific variables: season according to taste..

set mirror_dir=('/ftp/mirrors')
set packages_dir=('/site/newprog')
set emboss_config_options=\ ('--prefix=/site/prog/emboss --with-pngdriver=/site/lib')

# Now the script proper

set oldpwd='pwd'

cd $mirror_dir
echo 'updating EMBOSS'
if ( `wget -m ftp://ftp.uk.embnet.org/pub/EMBOSS |& \
    tail -1 | awk '/^Downloaded:/{print $5}'' != "0" ) then

    cd ${packages_dir}/EMBOSS
    echo 'new EMBOSS programs found .. installing'
    set latest_emboss='ls -t EMBOSS*|head -1'

    cd $packages_dir
    rm -Rf EMBOSS--
    tar zxf EMBOSS/$latest_emboss
    set emboss_dir='ls -dt EMBOSS-*[^z]|head -1'

    #the next line is necessary on my system but may not be for yours.
    setenv LD_LIBRARY32_PATH /site/lib

7 EMBOSS is rebuilt nightly from CVS, tested, and, assuming it passes the compilation tests, the latest version is posted to the EMBOSS FTP server.

8 Assuming of course that you haven’t overwritten EMBOSS datafiles with your own to begin with.

---
cd $emboss_dir

# If you have any site specific changes to the source code
# that you want to include, copy them in here

./configure $emboss_config_options &&
make && 
make install

# Now unpack and build EMBASSY

mkdir embassy

cd embassy

# Unpack and build each package one at a time

foreach embassadir ( 'ls ../../EMBOSS/*gz |grep -v EMBOSS-' )
tar zxf $embassadir
set embassadir_arch=$embassadir:t
set embassadir_root=$embassadir_arch:r

cd $embassadir_root:r
./configure $emboss_config_options &&
make && 
make install

cd ..

end
else
    echo 'No new version of EMBOSS available'
endif

cd $oldpwd

5.2.2 Automated database updating

In the same way, scripts can be written to automatically update the biological databases. An example
is given here for REBASE. As all the parameters for EMBOSS programs can be specified on the
command line it is a trivial matter to include index generation in your nightly update scripts. The
management of a bioinformatic resource is beyond the scope of this document, though EMBOSS
goes a long way towards easing the burden of management.

Automated update of REBASE

This script will look for a new version of REBASE and install it in EMBOSS using rebaseextract.

# This script should be sourced, not run.
# REBASE UPDATE. Should be run just after the beginning of the month.
set mirrors_dir=('/ftp/mirrors')
set oldpwd='pwd'

cd $mirrors_dir
if ( 'wget -m ftp://ftp.ebi.ac.uk/pub/databases/rebase/*' |&
    tail -1 | awk '/^Downloaded:/ {print $5}'' != "0" ) then
    cd ftp.ebi.ac.uk/pub/databases/rebase
    cp 'ls -t withrefm.*.Z|head -1' withrefm.Z
    uncompress withrefm.Z
    rebaseextract \
    ${mirrors_dir}/ftp.ebi.ac.uk/pub/databases/rebase/withrefm
    rm withrefm
endif

cd $oldpwd

I make no guarantees that these scripts will work correctly on your system. If it deletes all your
files, spams your associates, scratches your CD's and initiates a nuclear strike on a small unpopulated
pacific island it is NOT MY FAULT. It just happens to work for me.
6 Acknowledgements

The acknowledgements and credits are found at the front of this guide because no one ever reads them if they are at the back.