M1 ISDD - BI

PROTEIN DOCKING

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SOFTWARE INSTALLATION

(/home/sdv/all/protdocking/software/)

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1. GENERAL

Course directory accessible to all:

```
/home/sdv/all/protdocking/
```

Installation files will be in:

```
/home/sdv/all/protdocking/software/install/
```

Program directories will be in:

```
/home/sdv/all/protdocking/software/
```

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2.1. Installation of ZDOCK for Linux:

ZDOCK 2.1 linux distribution has been downloaded from:

```
http://zdock.umassmed.edu/software
```

Installation file:

```
/home/sdv/all/protdocking/software/install/zdock2.1_linux_p3.tar.gz
```

Within the `software` directory, uncompress and untar the file:

```
tar -zxvf install/zdock2.1_linux_p3.tar.gz
```

All needed ZDOCK files are located in the new created `IntelP3_Linux` directory.

WARNING: In classroom machines, we need to edit the first line in the file `create.pl` to set *perl* path to `/usr/bin/perl` (instead of the default `/usr/local/bin/perl`)

WARNING: before running zdock type the following in current shell (or in.bashrc):

```
export _POSIX2_VERSION=199209
```

(otherwise ZDOCK would not work on the classroom machines)

2.2. Installation of FTDock for Linux

The FTDock 2.0 linux installation files and instructions have been downloaded from:

```
http://www.sbg.bio.ic.ac.uk/docking/download.html
```

First we need to install the FFTW libraries, and then install the FTDock binaries, as follows.

2.2.1. Install FFTW libraries

FFTW libraries installation file:

```
/home/sdv/all/protdocking/software/install/fftw-2.1.5.tar.gz
```

Within the `software` directory, uncompress and untar the file:

```
tar -zxvf install/fftw-2.1.5.tar.gz
```

Compile the libraries:

```
cd ./fftw-2.1.5/
./configure --enable-float
make
```

We could move the `fftw-2.1.5` directory to any location, as long as we indicate such location in the next section *2.2.2*.

2.2.2. Install FTDock 2.0 executable

Installation file:

`/home/sdv/all/protdocking/software/install/gnu_licensed_3D_Dock.tar.gz`

Within the `software` directory, uncompress and untar the downloaded file:

```
tar -zxvf install/gnu_licensed_3D_Dock.tar.gz
```

```
cd ./3D_Dock/progs/
```

Open the *Makefile* file within the `progs` directory with a text editor and modify the following lines:

1) in the FFTW_DIR line, define the full path of the `fftw-2.1.5` directory created in the previous section *2.2.1.*

(usually `/home/sdv/all/protdocking/software/fftw-2.1.5`)

2) in the CC_FLAGS line, remove the `-malign-double` argument.

3) in the CC_FLAGS line, define `-mcpu=k8`

(instead of the default `-mcpu=pentiumpro`)

Now compile the program, within the `progs` directory:

```
make
```

(ignore WARNING messages)

All binary files are located in the `progs` directory.

2.3. ICM (optional)

ICM-browser 3.8.6a has been downloaded from www.molsoft.com, and installed with the proper libraries by the technicians at MTi, with the binary located in:

```
/opt/sdv/icm-browser-pro-3.8-6a/icmbrowserpro64
```

To launch the GUI version and automatically setup the `MOLBROWSERPROHOME` variable, a shell script has been created:

```
/opt/sdv/icm-browser-pro-3.8-6a/icm.sh
```

In order to run ICM with the proper libraries, we need to enter here:

```
ssh -X $USER@localhost
```

From there, ICM can be called from the soft link `/opt/sdv/bin/icm`. Assumming that `/opt/sdv/bin/` is in your PATH, then ICM can be called simply by:

```
icm
```

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3.1. pyDock

We will use here the version pyDock3.0.

Installation files:

```
/home/histidine/all/protdocking/software/install/pyDock3.tgz
```

Within the `software` directory, uncompress and untar the file:

```
tar -zxvf install/pyDock3.tgz
```

The pyDock binary is located in the `pyDock3` directory.

We need to change permissions to the `pyDock3/data` directory:

```
chmod go+rx data
```

Now we need to edit the following file:

```
/home/sdv/all/protdocking/software/pyDock3/etc/pydock.conf
```

And indicate the location of different external programs

```
ZDOCK=/home/sdv/all/protdocking/software/IntelP3_Linux/
FTDOCK=/home/sdv/all/protdocking/software/3D_Dock/
```

(some problems with ftdock module with elec on, it expects T26_rec.parsed file, so this has to be generated manually with FTDOCK... for the moment, we can copy T26_rec.pdb and T26_lig.pdb to T26_rec.parsed and T26_lig.parsed, respectively, and it will work)

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4.1. Installation of PatchDock for linux

The PatchDock executable has been downloaded from:

`http://bioinfo3d.cs.tau.ac.il/PatchDock/`

Installation file:

`/home/sdv/all/protdocking/software/install/patch_dock_download.zip`

Within the `software` directory, unzip the file:

```
unzip install/patch_dock_download.zip
```

All binary files are located in the `PatchDock` directory.

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5.1. Installation of FireDock for Linux

FireDock executable (statically compiled on Debian) is downloaded from:

```
http://bioinfo3d.cs.tau.ac.il/FireDock/
```

Installation file:

```
/home/sdv/all/protdocking/software/install/fire_dock_download.zip
```

Within the `software` directory, unzip the file:

```
unzip install/fire_dock_download.zip
```

All binary files are located in the `FireDock` directory.

For best use, set the following variable (for current shell, or in your .bashrc file):

```
export FIREDOCK=/home/sdv/all/protdocking/software/FireDock/
```

We need to edit the following file within the `FireDock` directory:

```
$FIREDOCK/PDBPreliminaries/prepareFragments.pl
```

and change the `/usr/local/bin/perl` in the first line to:

```
/usr/bin/perl
```

5.2. Installation of FlexDock for Linux

FlexDock executable is downloaded from:

```
http://bioinfo3d.cs.tau.ac.il/FlexDock/
```

Installation file:

```
/home/sdv/all/protdocking/software/install/flex_dock_download.zip
```

Within the `software` directory, unzip the file:

```
unzip install/flex_dock_download.zip
```

All binary files are located in the `FlexDock` directory. Some of the directories and files are not accessible to *others*, we need to change permissions*:*

```
chmod -R go+xr FlexDock
```

(to be more specific, x should be applied only to directories and .pl scripts, r also to all files)