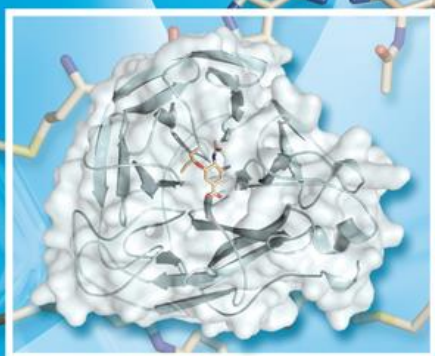




INTEGRATED PLATFORM FOR DRUG DESIGN AND DISCOVERY



CUSTOMIZED WORKFLOWS FOR DRUG DISCOVERY

Automated docking using FITTED

Filter by descriptors

Convert 2D to 3D

Prepare protein - pdb to mol2

Extract representative library

Create combinatorial library

Search for analogues

Easy integration of 3rd party programs

www.molecularforecaster.com

Molecular Forecaster Inc.

Forecaster 1.2 – Server Installation Guide

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CONTENTS

Windows.....	4
Linux	4
Installation Procedures	4
Windows Installation.....	4
Linux portable Installation	5
Extracting the Forecaster application	5
Extracting the Ruby Portable Application	5
Running the Application.....	5
Linux Ubuntu System Installation	6
Extracting the Forecaster application	6
Installing Ruby	6
Installing Rubygems	6
Installing the necessary libraries.....	7
Running the Application.....	7
Linux Centos 5 System Installation	8
Extracting the Forecaster application	8
Downloading and Installing Ruby.....	8
Installing Rubygems	8
Installing the necessary libraries.....	9
Running the Application.....	9
Linux Centos 6 System Installation	9
Extracting the Forecaster application	9
Installing Ruby	10
Installing Rubygems	10
Installing the necessary libraries.....	10

Running the Application.....	10
Troubleshooting.....	12
Linux host	12

Minimum System Requirements

WINDOWS

Windows XP, Vista, 7 or 8 (32 or 64 bits architecture)
6 Gb of RAM memory (8Gb recommended)
350 Mb of empty disk space (without user files)



LINUX

Ubuntu 10.04 LTS, CentOS 5.7 or CentOS 6.2 (32 or 64 bits architecture)
6 Gb of RAM memory (8Gb recommended)
500 Mb of empty disk space (without user files)



INSTALLATION PROCEDURES

The following sections provide detailed procedures to install ruby and the FORECASTER Platform. In the Windows environment, Ruby is provided as a folder and there is no system installation required. Under the Linux environment, there is two options offered: a system installation of Ruby or a self-contained folder. Please refer to either procedure according to your preferences.

WINDOWS INSTALLATION

Version recommended: Windows 7 64-bits



Executing the Forecaster platform on Windows is extremely simple and can be done in two steps. The first step is to unzip the Forecaster.zip into your favorite folder in the system. The second step is to run *start_forecaster.cmd*. The following command window will appear and the FORECASTER server will start on port 3000. As soon as this program runs, your computer acts as a server. You can modify the port by editing the *start_forecaster.cmd* script and changing the value in “-p 3000”.

```
C:\devzone\InstantRails\ruby\bin\ruby.exe
** Starting Mongrel listening at 0.0.0.0:3000
** Starting Rails with production environment...
** Rails loaded.
** Loading any Rails specific GemPlugins
** Signals ready. INT => stop (no restart).
** Mongrel 1.1.5 available at 0.0.0.0:3000
** Use CTRL-C to stop.
```

Finally, open your favorite browser and navigate to <http://127.0.0.1:3000> and the login screen will appear. The default user can login with login “admin” and password “fitted”. The forecaster application can be reached from another computer connected to the network by using the IP address of the server (ex: <http://168.192.0.11:3000>).

LINUX PORTABLE INSTALLATION

Version recommended: Linux 64-bits



Installation on Linux without any system installation is possible using the rubyportable package. The location of the rubyportable folder needs to be /opt/rubyportable or configured using the setup.sh script (see below). The following commands need to be executed in a terminal.

EXTRACTING THE FORECASTER APPLICATION

The first step is to uncompress the *forecaster.tgz* (tar gzip file) into the folder of your choice. Once the application is ready, open a terminal and type the commands required for each step as described below.

EXTRACTING THE RUBY PORTABLE APPLICATION

The first step is to uncompress the rubyportable.tgz file to the /opt/ folder (root required).

```
$ sudo su
# cd /opt/
# tar xvf rubyportable.tgz
# exit
```

Alternatively, if you don't have root permission to the /opt folder, you can run the script setup.sh to configure the ruby portable files according to your actual path (root not required).

```
$ tar xvf rubyportable.tgz
$ sh setup.sh
$ cp start_forecaster.sh <path to your FORECASTER installation/gui-revXXXX >
```

Once you execute the setup.sh script, it will generate a startup script (start_forecaster.sh) that has to be copied in your FORECASTER installation.

RUNNING THE APPLICATION


The application can be started. Once the installation is complete, go to the forecaster directory and start the rails server using

```
$ sh start_forecaster.sh
```

You can modify the port changing the value in “-p 3000” by editing the start_forecaster.sh script.

Once the server starts, open your favorite browser and navigate to <http://127.0.0.1:3000> and the login screen will appear. The default user can login with login “admin” and password “fitted”. The forecaster application can be reached from another computer connected to the network by using the IP address of the server (ex: <http://168.192.0.11:3000>).

LINUX UBUNTU SYSTEM INSTALLATION

Version recommended: Ubuntu 64-bits 10.04 LTS 

Installation on Ubuntu requires installing Ruby and all the required libraries. The following commands need to be executed in a terminal (sudo credentials required).

EXTRACTING THE FORECASTER APPLICATION

The first step is to uncompress the *forecaster.tgz* (tar gzip file) into the folder of your choice. Once the application is ready, open a terminal and type the commands required for each step as described below.

INSTALLING RUBY

Installing the required packages:

```
$ sudo aptitude install ruby1.8-dev ruby1.8 ri1.8 rdoc1.8 irb1.8  
libreadline-ruby1.8 libruby1.8 libopenssl-ruby sqlite3 libsqlite3-ruby1.8
```

Creating the symbolic links:

```
$ sudo ln -s /usr/bin/ruby1.8 /usr/bin/ruby  
$ sudo ln -s /usr/bin/ri1.8 /usr/bin/ri  
$ sudo ln -s /usr/bin/rdoc1.8 /usr/bin/rdoc  
$ sudo ln -s /usr/bin/irb1.8 /usr/bin/irb
```

INSTALLING RUBYGEMS

Prior to the installation of rubygems, the sources directory is created:

```
$ mkdir ~/sources  
$ cd ~/sources
```

Then rubygems are downloaded:

```
$ wget http://rubyforge.org/frs/download.php/55066/rubygems-1.3.2.tgz
```

The file is next unpacked and moved to the new directory:

```
$ tar xzvf rubygems-1.3.1.tgz
$ cd rubygems-1.3.1
```

At this point, the setup process can start:

```
$ sudo ruby setup.rb
```

And the symbolic link is created:

```
$ sudo ln -s /usr/bin/gem1.8 /usr/bin/gem
```

INSTALLING THE NECESSARY LIBRARIES

Rails and the required gems are next installed:

```
$ sudo gem install -v=2.1.0 rails
$ sudo gem install -v=0.8.1 hpricot
$ sudo gem install rubyzip
$ sudo gem install mongrel
```

RUNNING THE APPLICATION

The application can be started. Once the installation is complete, go to the forecaster directory and start the rails server using

```
$ ruby script/server -e production -p 3000
```

You can modify the port changing the value in “-p 3000”.

Once the server starts, open your favorite browser and navigate to <http://127.0.0.1:3000> and the login screen will appear. The default user can login with login “admin” and password “fitted”. The forecaster application can be reached from another computer connected to the network by using the IP address of the server (ex: <http://168.192.0.11:3000>).

Version recommended: CentOS 5.7 64-bits



Installation on Centos requires some steps to install Ruby from sources and all the required libraries since the ruby version from the CentOS repository is 1.8.5 and we need a newer version. The following list of commands allows the installation of the required version of ruby.

EXTRACTING THE FORECASTER APPLICATION

The first step is to uncompress the *forecaster.tgz* into the folder of your choice. Once the application is ready, open a terminal and type the commands required for each step as described below. You need to be root to perform the installation of ruby.

DOWNLOADING AND INSTALLING RUBY

First, as root, create the source folder and download the source files:

```
$ su -
# mkdir ~/sources
# cd ~/sources
# wget http://ftp.ruby-lang.org/pub/ruby/1.8/ruby-1.8.7.tar.gz
# tar xvfz ruby-1.8.7.tar.gz
```

Installing the dependencies:

```
# yum install gcc gcc-c++
# yum install zlib-devel
# yum install openssl-devel
# yum install readline-devel
# yum install sqlite-devel
```

Building the program and installation:

```
# cd ruby-1.8.7
# ./configure --with-openssl-dir=/usr/lib64/openssl
# make
# make install
```

INSTALLING RUBYGEMS

Downloading the rubygems sources:

```
# cd ~/sources
# wget http://rubyforge.org/frs/download.php/69365/rubygems-1.3.6.tgz
```



```
# tar xzvf rubygems-1.3.6.tgz
# cd rubygems-1.3.6
# ruby setup.rb
```

INSTALLING THE NECESSARY LIBRARIES

Rails and the required gems are installed:

```
# gem install -v=2.1.0 rails
# gem install hpricot
# gem install rubyzip
# gem install mongrel
# gem install -v=1.2.4 sqlite3-ruby
# exit
```

RUNNING THE APPLICATION

The application can be started. Once the installation is complete, go to the forecaster directory and start the rails server using (as a user, not root)

```
$ ruby script/server -e production -p 3000
```

You can modify the port changing the value in “-p 3000”.

Once the server starts, open your favorite browser and navigate to <http://127.0.0.1:3000> and the login screen will appear. The default user can login with login “admin” and password “fitted”. The forecaster application can be reached from another computer connected to the network by using the IP address of the server (ex: <http://168.192.0.11:3000>).

LINUX CENTOS 6 SYSTEM INSTALLATION

Version recommended: CentOS 6.2 64-bits



Installation on Centos requires to install from the CentOS. The following list of commands allows the installation of the required version of ruby.

EXTRACTING THE FORECASTER APPLICATION

The first step is to uncompress the *forecaster.tgz* into the folder of your choice. Once the application is ready, open a terminal and type the commands required for each step as described below. You need to be root to perform the installation of ruby.

INSTALLING RUBY

First, as root, install ruby:

```
# yum install ruby ruby-devel
```

Installing the dependencies:

```
# yum install gcc gcc-c++  
# yum install zlib-devel  
# yum install openssl-devel  
# yum install readline-devel  
# yum install sqlite-devel
```

INSTALLING RUBYGEMS

Installing rubygems:

```
# yum install rubygems
```

INSTALLING THE NECESSARY LIBRARIES

Rails and the required gems are installed:

```
# gem install -v=2.1.0 rails  
# gem install hpricot  
# gem install rubyzip  
# gem install mongrel  
# gem install sqlite3  
# exit
```

RUNNING THE APPLICATION

The application can be started. Once the installation is complete, go to the forecaster directory and start the rails server using

```
$ ruby script/server -e production -p 3000
```

You can modify the port changing the value in “-p 3000”.

Once the server starts, open your favorite browser and navigate to <http://127.0.0.1:3000> and the login screen will appear. The default user can login with login “admin” and password “fitted”.

The forecaster application can be reached from another computer connected to the network by using the IP address of the server (ex: <http://168.192.0.11:3000>).

TROUBLESHOOTING

LINUX HOST

1. **Ruby runs at >90% CPU all the time.** To correct this issue, simply reset the date by executing the following command (as root or sudo):

```
# date -s `date`
```