



***FTrees* in Moe v.0.4**

for

***FTrees* version 1.5.4**

and

Moe version 2006.08

User Guide

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About *FTrees*

See www.biosolveit.de/FTrees.

FTrees in Moe

In this version *FTrees* is used for virtual HTS. One molecule will be compared to many molecules.

We force *FTrees* *for the entire input library file* to be computed (i.e., converted) every time again. this results excess computation time and excess I/O activity. in a final version, the re-use of compound libraries will be much faster because the transformation of *FTrees* is saved and only similarity is computed.

Because the path of the svl script is used as a work-directory, each user needs a own copy in a writable directory. The GUI of the installation uses a File-Prompt to select the svl script. If all user want to use the same copyi, the svl script needs to be changed. A Directory-Prompt needs to be implemented and used for choosing work-directory.

Installation

1. Download from www.biosolveit.de/download/ and install the newest version of *FTrees* to your system. Linux and windows can be used to run *FTrees* .

2. Create a clean directory! This directory will be the work-directory of *FTrees* GUI.

3. Copy all files from the package into the work-directory!

Examples:

`/home/user/ftrees_in_moei` (linux)

`C:\Programme\FTrees` (windows)

Note: The current *FTrees* version can't work with paths containing spaces like "`C:\programe files\FTrees`"!

4. Start Moe:

(a) Go to File-Open.

(b) Browse to work-directory and choose `ftrees.svl`.

(c) 3 Files needed to set up:

(Please confirm each file through OK button)

(The located file you confirm will be checked!)

- First: locate `ftrees` executeable

Example:

`/software/ftrees1.5.1/bin/ftrees` (linux)

`C:\Programme\FTrees\bin\ftrees.exe` (windows)

- Second: locate `config_ft.dat`

Example:

`/software/ftrees1.5.1/config_ft.dat` (linux)

`C:\Programme\FTrees\config_ft.dat` (windows)

- Third: locate work-directory and choose `ftrees.svl`

Usage

4.1 Calculate Feature Tree Similarities

1. start MOE.
2. Go to file->open and choose a query mol2 file. An example is given in the work-directory: "query.mol2".
3. Select the hole molecule.
4. Right click with the mouse.
5. Select "use as FTrees query".
6. Locate a mol2 library and choose it. An example is given in the work-directory: "tiny.mol2". certainly you can emplay *any other* mol2 library file.
7. After Calculation optionally save the result through File->Save As... (standart file format is dbv)
8. Finally you open saved results through File->Open...

Uninstall

1. Delete work-directory
2. Delete `.fim.linux.cfg` or `fim.windows.cfg` in your home dir.
3. Open `/moe-menus` and delete the new option. (You can search for "FTREES MENU" to find the entry.)

Bibliography