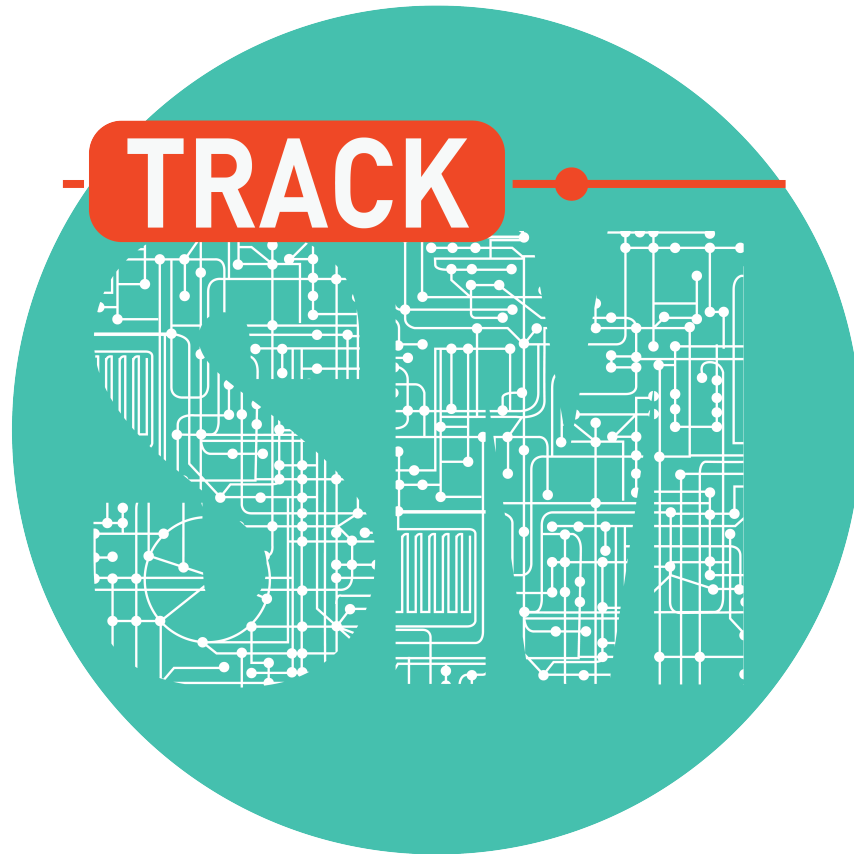


User Guide



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Availability and Requirements

Project home page: <http://metabolomics.pharm.uconn.edu/>

Operating System(s): Platform independent. TrackSM should work on any operating system (OS) including Windows, Linux/Unix Mac OSX or Solaris.

Other requirements: Java 1.6 or higher. Java standard edition (SE) run time (jre 1.6 / jre 1.7) can be freely downloaded from

<http://www.oracle.com/technetwork/java/javase/downloads/index.html>

Memory: We recommend at least 2 GB of RAM for java virtual machine. However, more RAM may be required depending on the number and size of structures being classified. The bundled program execution scripts (TrackSM.bat and TrackSM.sh for Windows and Linux respectively) found in the TrackSM folder will allocate 2GB of RAM for the java virtual machine. Please note that the RAM allocated for the java virtual machine can be easily changed. (See FAQ)

Processor: There are no processor requirements. However, faster (multi-core) processors will certainly help since TrackSM is designed to take advantage of modern multi-core architectures.

Restrictions to use by non-academics: NONE

Installation Instructions

No installation is required. Simply extract the downloaded zip file into a folder. To start TrackSM on

- Windows OS, double click on TrackSM.bat
- Linux/Mac OSX/Solaris, double click on TrackSM.sh or type `./TrackSM.sh` in the command prompt terminal.

Contents of the TrackSM Folder

Folders:

- *config*: contains configuration files.
- *input*: contains input files with candidate structures to be tested.
- *output*: contains individual output folders with results for each TrackSM run.

Files:

- *TrackSM.bat*: program startup script for Windows OS.
- *TrackSM.jar*: TrackSM platform independent executable file.
- *TrackSM.sh*: program startup script for Linux.

Frequently Asked Questions (FAQ)

1. **Nothing happens when I double click TrackSM.bat.**

This happens when operating system cannot locate the java run time (jre).

Add `C:\Program Files (x86)\Java\jre7\bin`

or

`C:\Program Files\Java\jre7\bin;`

to windows path. Please note that jre might be found at a different location. So search for `jre6\bin` or `jre7\bin` directories on your system.

2. **How do I know java runtime is correctly installed and java path is correctly set?**

Type `java -version` at the command prompt (dos prompt in Windows or terminal in Linux). This command should return the version number of java runtime.

3. **Why should I double click on the startup script (not the jar file) to start the program?**

Configuration files location and memory allocation information are passed on to TrackSM via startup scripts.

4. How do I change the amount of memory allocated to java virtual machine?

Use a text editor to open the startup script TrackSM.bat or TrackSM.sh. Change the highlighted number to desired amount. (Note: 1024m = 1 GB; m = mega bytes) `java -Xmx1024m -jar TrackSM.jar candidates.smiles 2 3`

Recommended text editors:

Windows OS: Notepad++, freely available at <http://notepad-plus-plus.org/>.

Mac OSX: TextEdit or TextWrangler.

Linux: gedit

5. How can I provide TrackSM with some candidate structures to classify?

Copy the input file (with candidate structures to examine) into the input folder in the TrackSM folder. Then use a text editor to open the startup script (TrackSM.bat or TrackSM.sh) and replace the highlighted text with the new file name. `java -Xmx1024m -jar TrackSM.jar candidates.smiles 2 3`

Please note that TrackSM is a computationally intensive program. Providing an input file with a large number of candidate structures might result in delayed responses.

6. How can I control the number of metabolic classes to be predicted by TrackSM?

Copy the input file (with candidate structures to examine) into the input folder in the TrackSM folder. Then use a text editor to open the startup script (TrackSM.bat or TrackSM.sh) and replace the highlighted text with the required number of class predictions.

```
java -Xmx1024m -jar TrackSM.jar candidates.smiles 2 3
```

7. How can I control the number of individual metabolic pathways to be predicted by TrackSM?

Copy the input file (with candidate structures to examine) into the input folder in the TrackSM folder. Then use a text editor to open the startup script (TrackSM.bat or TrackSM.sh) and replace the highlighted text with the required number of pathway predictions.

```
java -Xmx1024m -jar TrackSM.jar candidates.smiles 2 3
```

8. I can't find the results generated by TrackSM? The output folder has a lot of folders that I don't recognize.

Every time TrackSM is run, a new folder (labeled with run date_time:

yyyyMMdd_HHmms) is created in the output folder in the TrackSM folder.

That is where you would find the results.

9. I have a question that was not addressed in this user guide.

Please contact the authors with your question(s) for further assistance

ion@engr.uconn.edu or david.grant@uconn.edu
