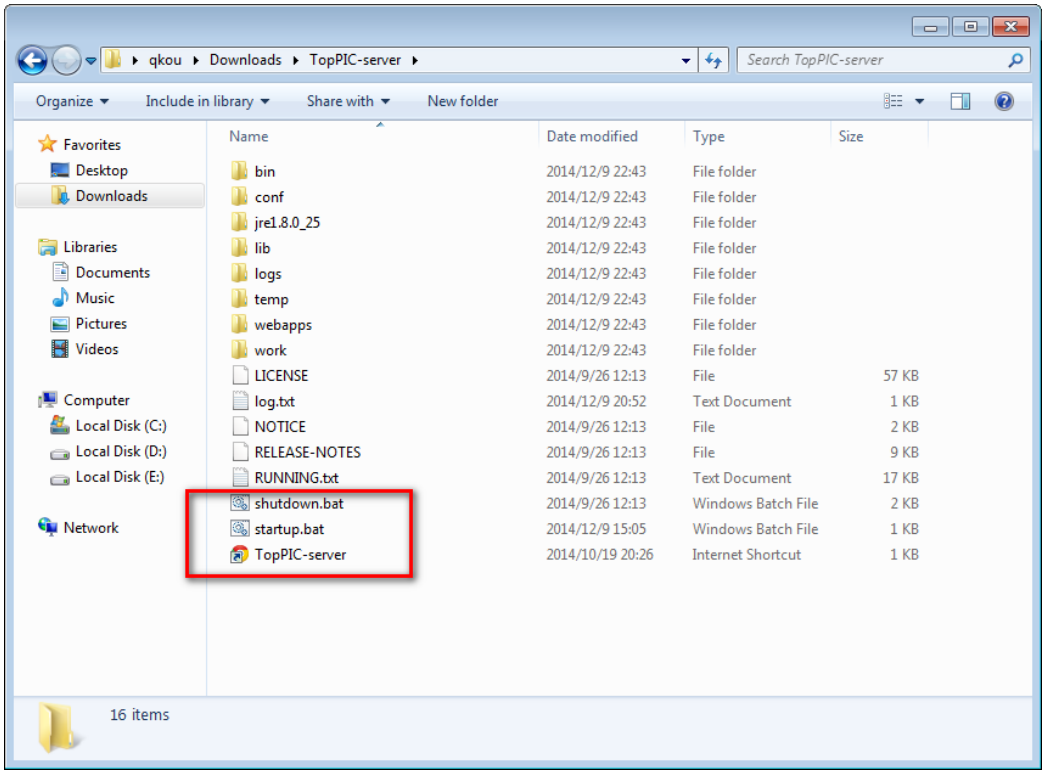
TopPIC-server User Manual

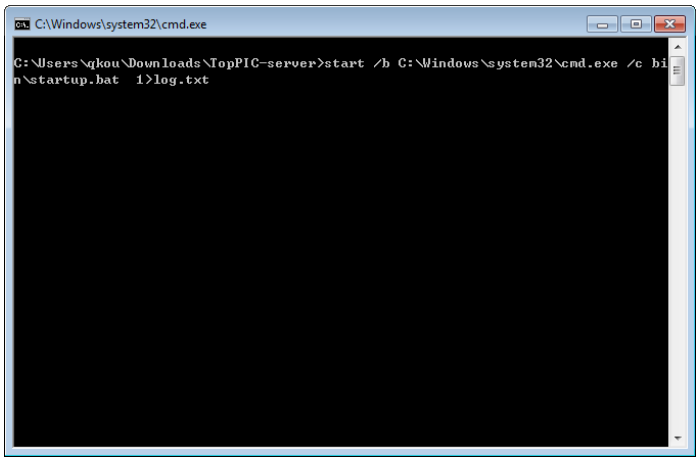
1 Installation

No installation is needed for TopPIC-server. Just download the zip file and unzip it, then you will find all files shown below. In most cases, we only use the last three files: **startup.bat** and **shutdown.bat** are used to start up and shut down the server respectively; the last one is the web link for the service.

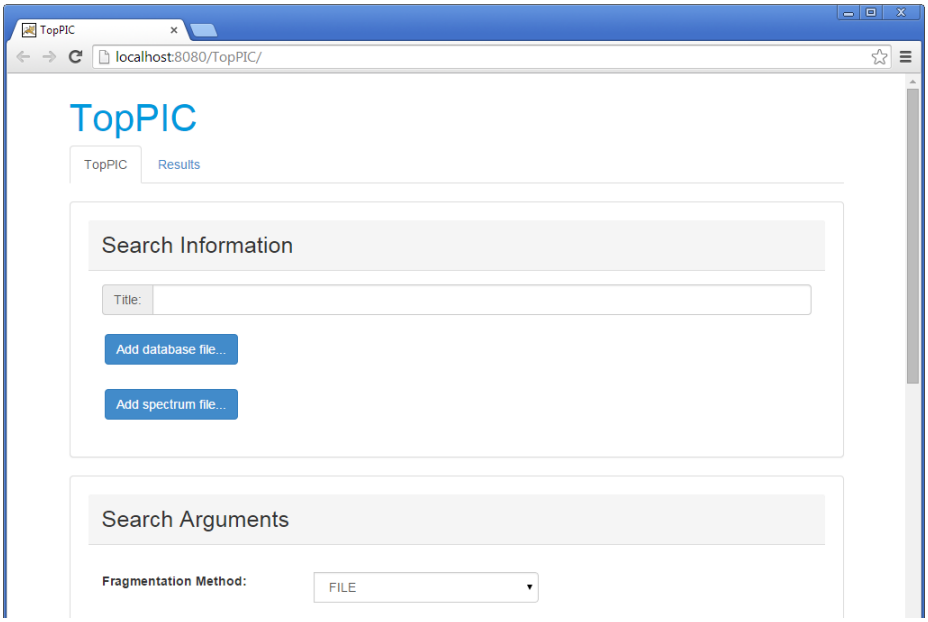


2 Start up the server

To start the TopPIC-server, please double click the "startup". A command line console like below will pop out, which means the server begins to run. You can close the console window and the server will be running in background until you shut it down.

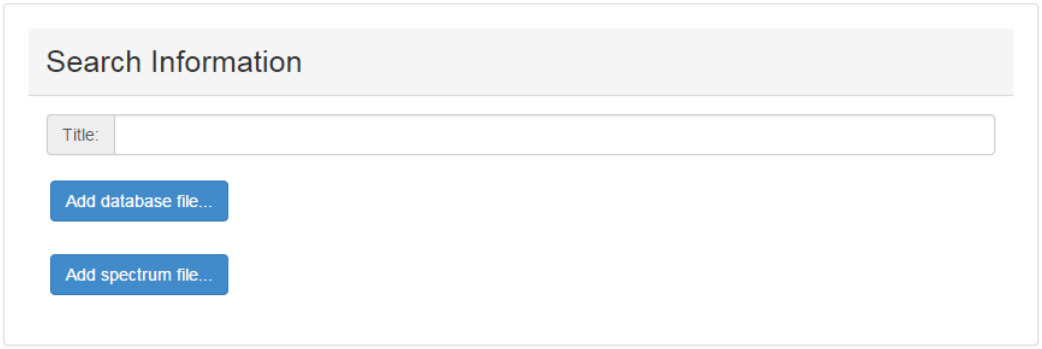


Also, the web page `http://localhost:8080/TopPIC` will be opened. You can bookmark the web page or use the link we provide in the folder. It will take more time for the first-time startup due to the service deployment.

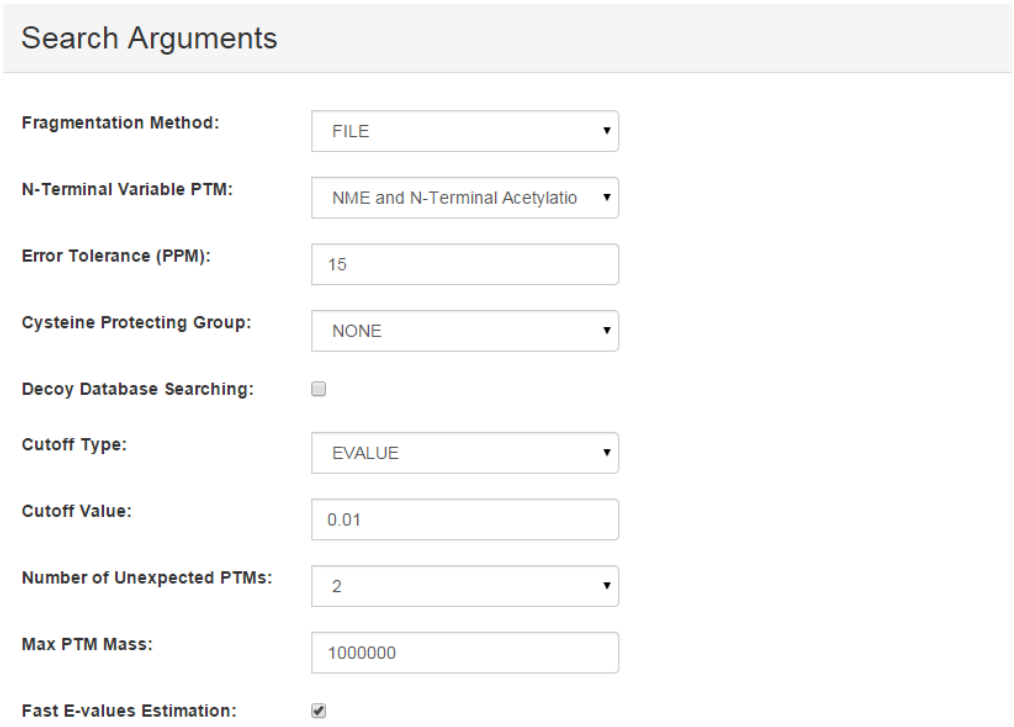


3 Submit tasks

The web page is used to submit tasks and view task status. In submitting task, you need to provide the task title and upload database and spectrum file in **Search Information** part. Only **fasta** format is accepted for database and **msalign** format for spectrum file.

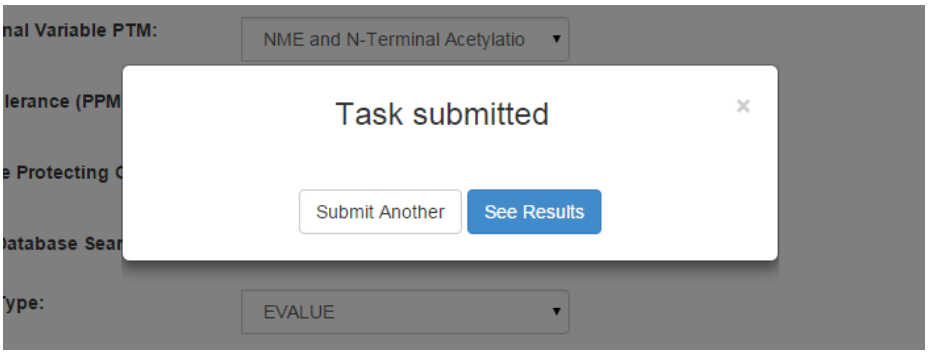


You can set searching arguments in **Search Arguments** part. Detailed explanation is provided below.



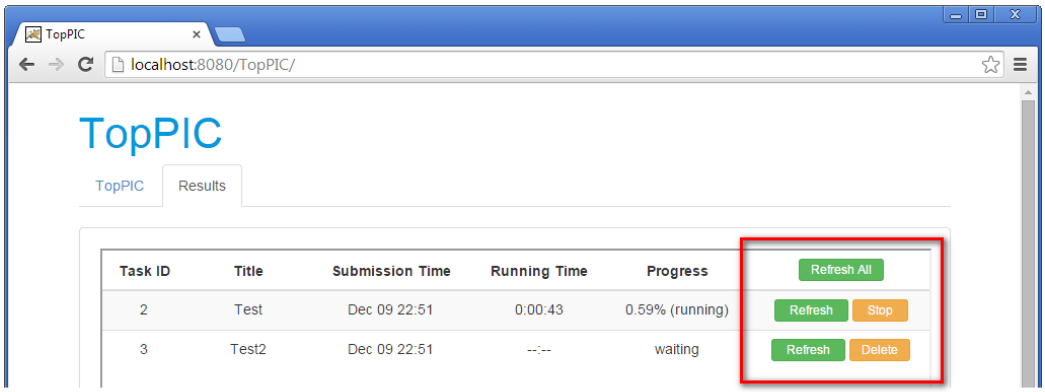
- Fragmentation Method. Four options are provided: FILE, CID, ETD, HCD. The default value is FILE, which means getting fragmentation method from the spectrum file.
- N-Terminal Variable PTM. Three options are provided: NME and N-Terminal Acetylation, NONE, NME.
- Error Tolerance (PPM). Error tolerance for precursor and fragment masses in parts per million.
- Cysteine Protecting Group. Three options are provided: NONE, Carbamidomethylation (C57), Carboxymethylation (C58). The default value is NONE.
- Decoy Database Searching. When selected, a shuffled decoy protein database will be used to estimate false discovery rates.
- Cutoff Type. The cutoff type are support: EVALUE and FDR. The Decoy Database Searching option must be selected, if you want to use FDR.
- Cutoff Value. Cutoff value for reporting proteoform-spectrum-matches.
- Number of Unexpected PTMs. Maximum number of unexpected post-translational modifications in a proteoform-spectrum-match.
- Max PTM Mass. Maximum absolute value of masses (in Dalton) of unexpected post-translational modifications in proteoforms.
- Fast E-values Estimation. When selected, precomputed estimation will be used to save time. The error tolerance can only be 15, 10, or 5 when this option selected.

After setting basic information and searching arguments, you can submit the task. If all the information and arguments are valid, you can submit another task or check the task status.



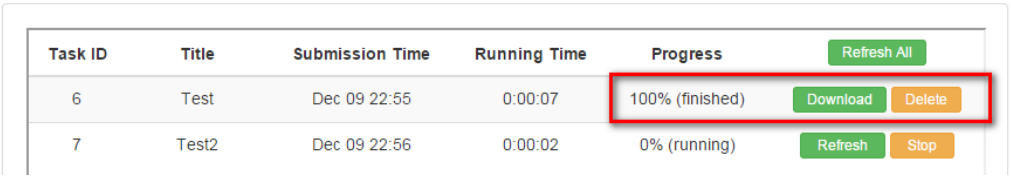
4 View task status

In the results tab, you can view the information about all the tasks submitted, including id, title, submission time, running time and progress. You can refresh the running progress, stop running task and delete waiting task by using corresponding buttons.

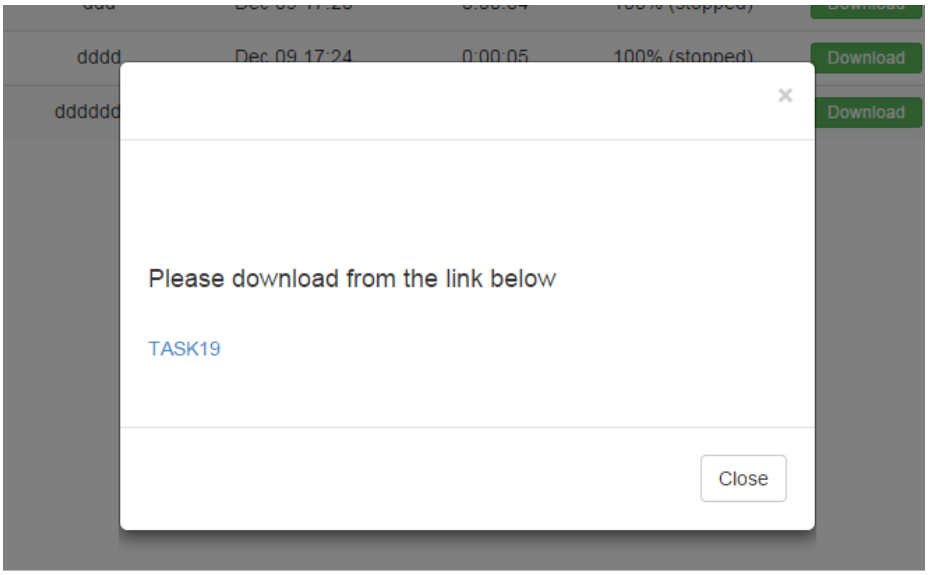


5 Download searching results

You can find the download button for each finished and stopped task.



The task result will be packaged into a zip file and you can download it using the link we provide. It may take some time for zipping all the results.



The result contains a tab delimited text file and a collection of html files for identified proteoforms. For example, when the input spectral data file is spectral.msalign, the tab delimited text file is spectral.OUTPUT_TABLE and the html files are in the directory spectral_html. Use a web browser, such as Chrome or Firefox, to open the file spectral_html/proteins.html to browse all identified proteoforms.

The result of *Salmonella typhimurium* and *Escherichia coli* data sets are shown as examples.