

Warp2d tutorial

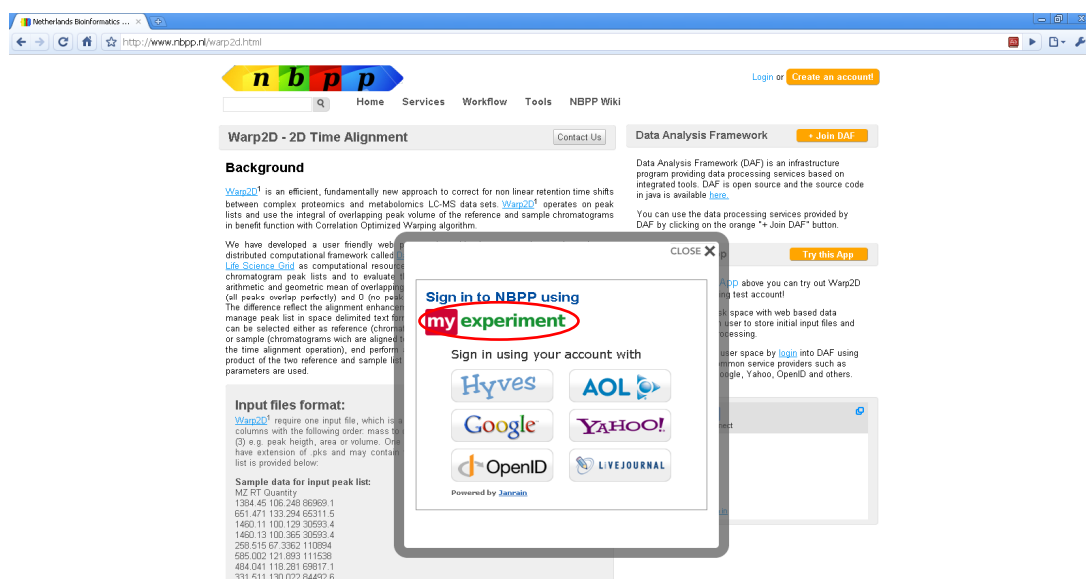
Warp2D is a time alignment method of LC-MS peak lists optimizing the overlap of peaks in retention time, mass to charge ratio and intensity dimensions. The input/output file formats as well the parameters are explained at <http://www.nbpp.nl/warp2d.html> page. This tutorial provides insight on the use of the Warp2D web based tool to perform many references to many samples and one reference to many sample alignment.

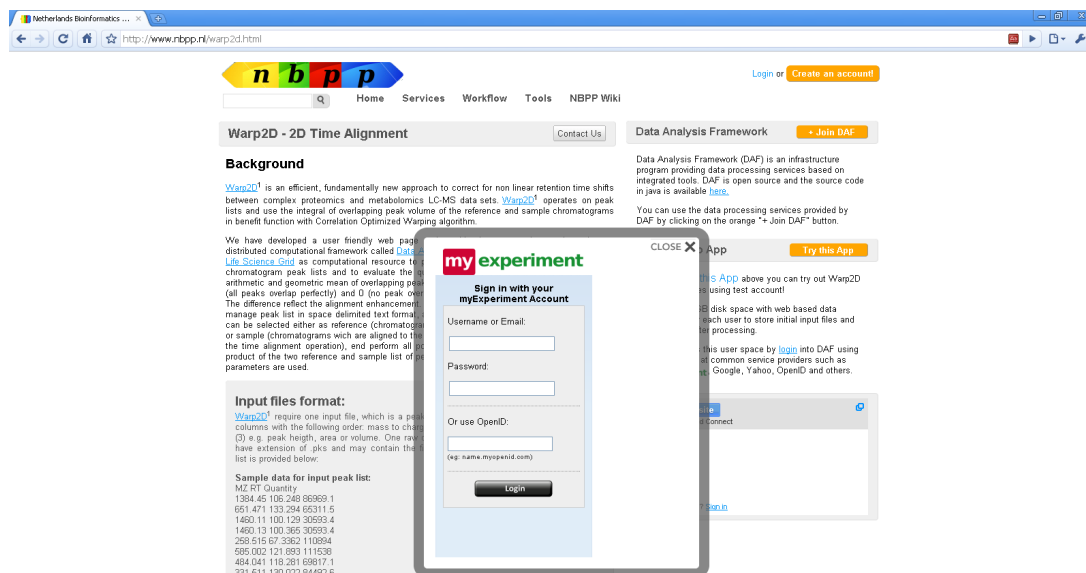
Login

The web application can be securely used by login with one of the account of the most popular community portals (see above in more details). Users may login on the portal main web page at <http://www.nbpp.nl/> or Warp2D processing service description web page at <http://www.nbpp.nl/warp2d.html> by clicking the login link at the top of the page:



Then login using one of the popular community portal authentication sites such as My experiment, Hyves, AOL, Yahoo, Live journal, Google or by using OpenID.

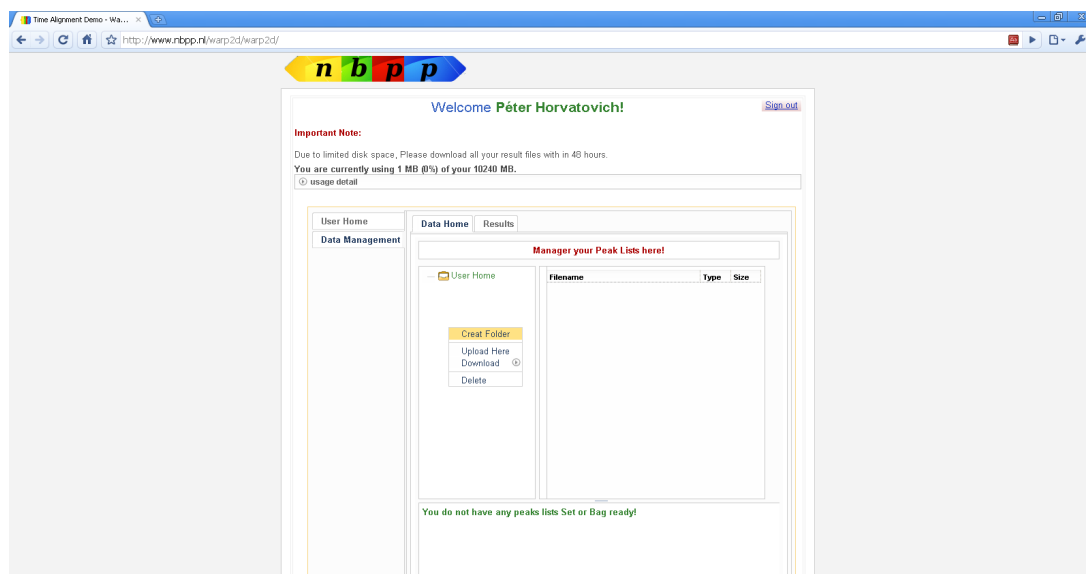




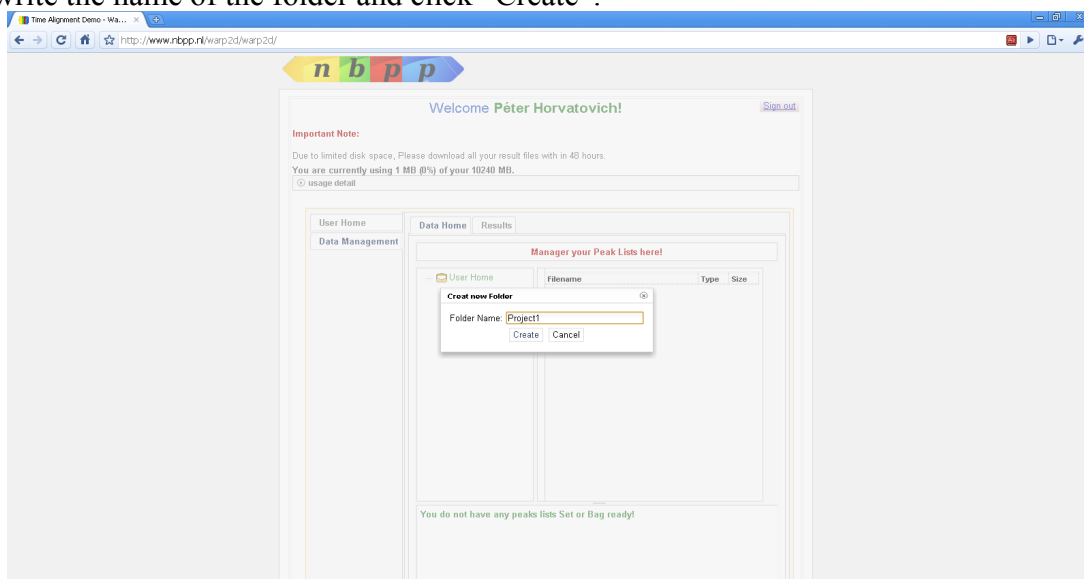
User Interface

The user interface is divided into 4 parts that are selectable by horizontal and vertical tabs: “*User Home*” and “*Data Management*” for vertical tabs and “*Data Home*” and “*Results*” horizontal tabs selectable with “*Data Management*” vertical tab and “*Desktop*” and “*Submission*” horizontal tabs selectable with “*User Home*” vertical tab.

To upload files go to “*Data Management*”/“*Data Home*”. Here you can create directory by right clicking the left part of the file manager panel and selecting “*Create Folder*” menu option:

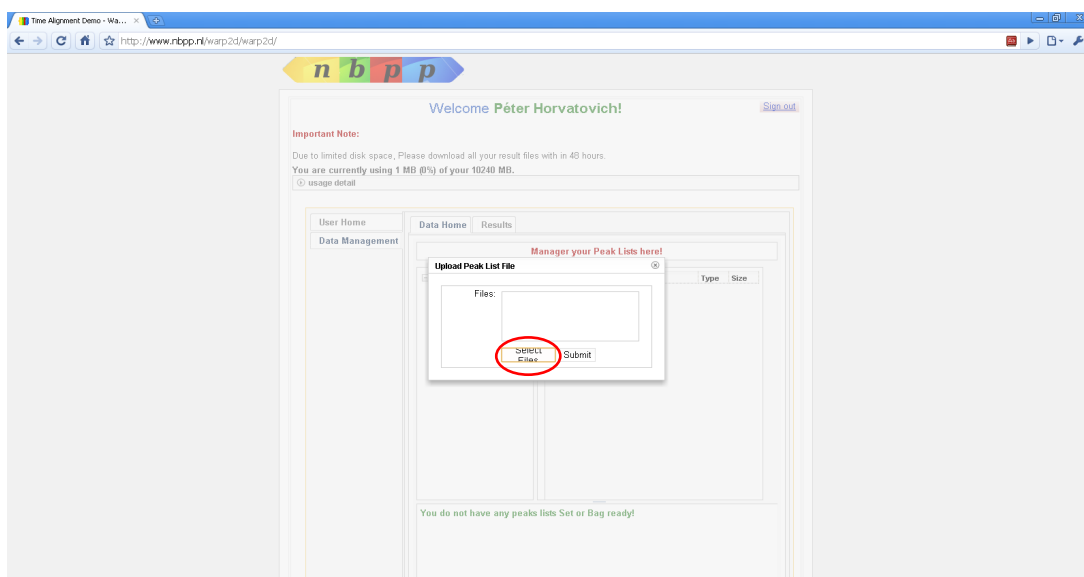


There write the name of the folder and click “Create”:

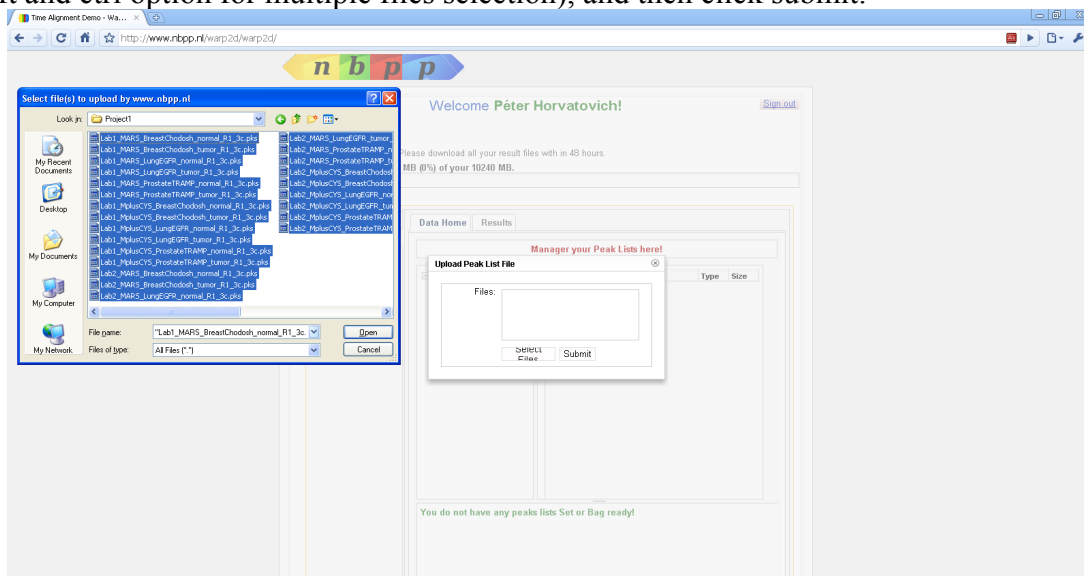


File upload

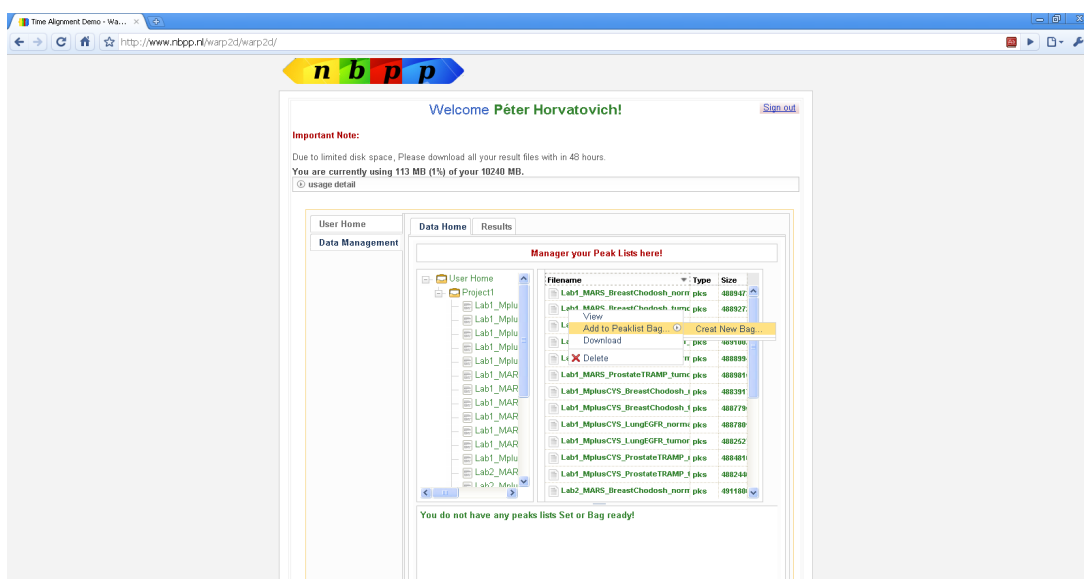
You can then upload your LC-MS peak list files (in a format described at “Input files format” section at <http://www.nbpp.nl/warp2d.html>) either to the home directory or any other available directory by choosing “upload here” from the popup menu obtained by right clicking the right file manager panel:



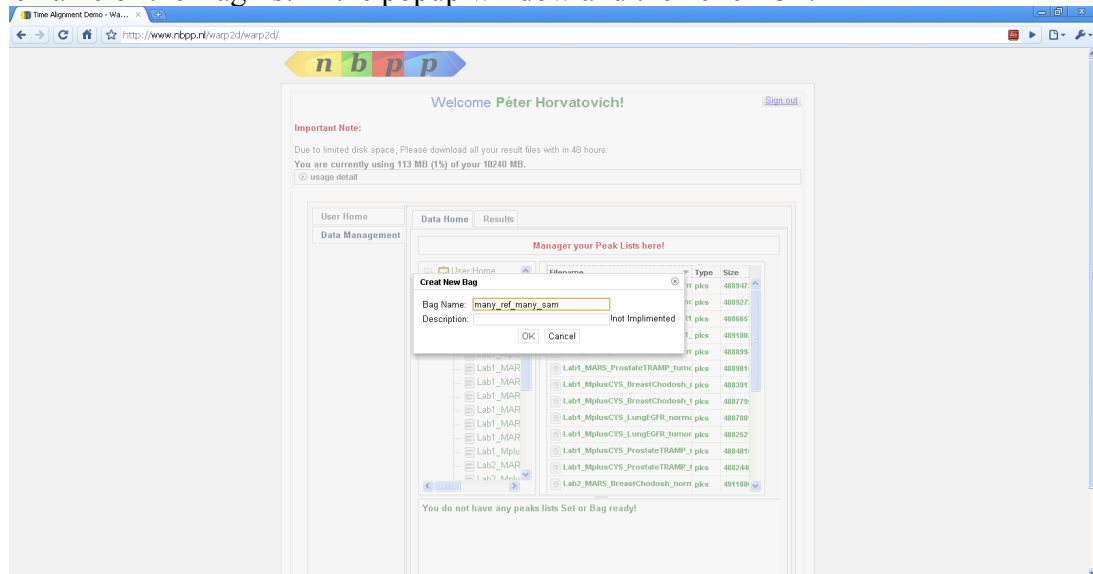
Click select files and from the popup many select the files that you would like to upload (you can use shift and ctrl option for multiple files selection), and then click submit:



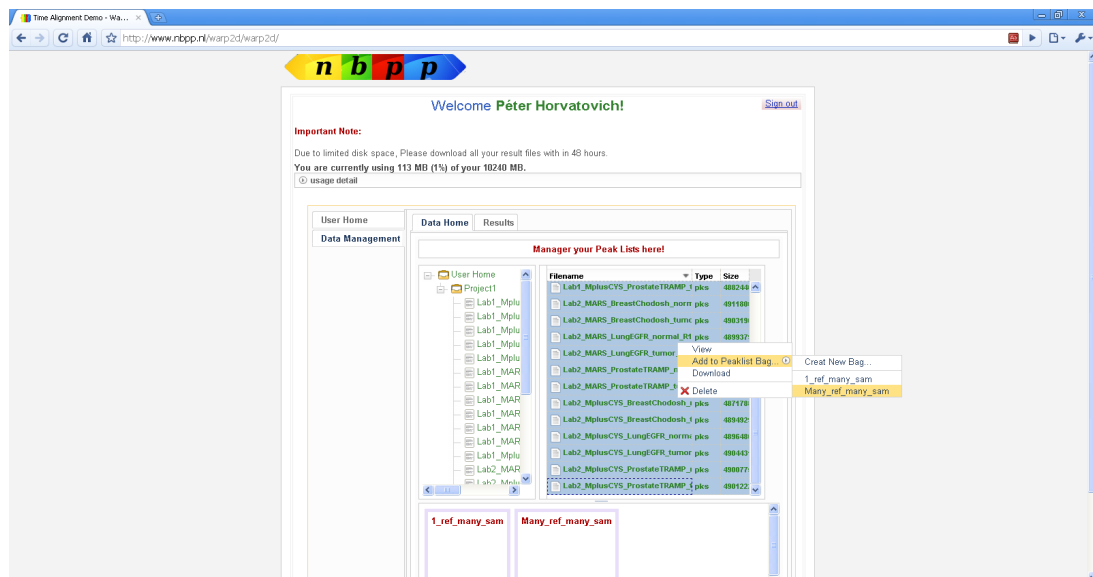
Once the files are uploaded you create bags (sets of peak lists) by right clicking the right panel of the file manager and selecting “Add to Peaklist Bag...”>>”Create New Bag”:



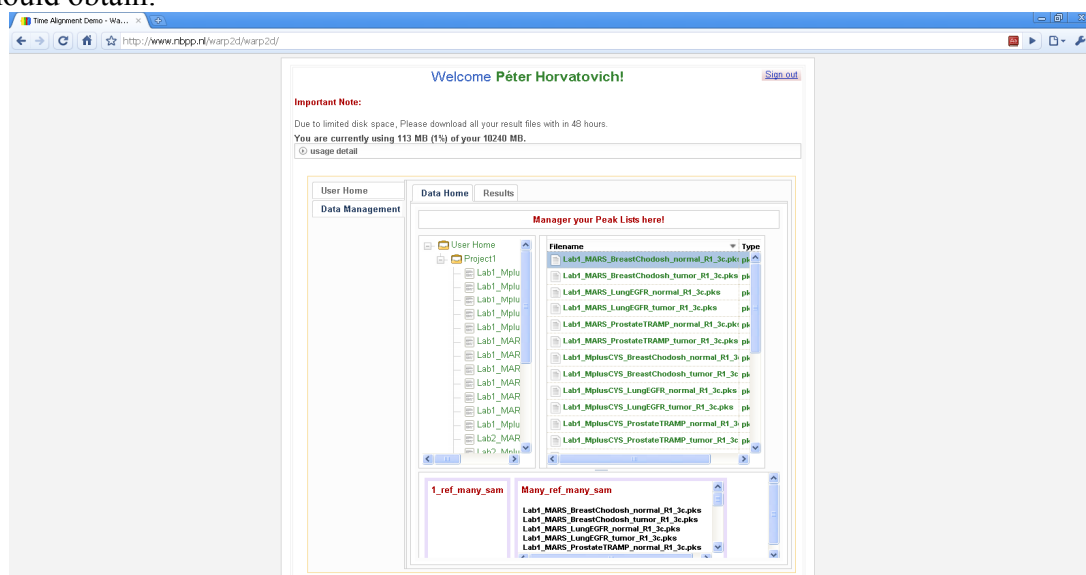
Enter the name of the Bag list in the popup window and then click Ok:



For example: create two bag lists with name of “Many_ref_many_sam” and “1_ref_many_sam”. Now insert files in “many_ref_many_samples” bag list by selecting all files on the right part of the file manager: You can use shift or ctrl for multiple selections. Then right click on the selected files and choose “Add to Peaklist Bag...” followed with the name of the bag list (“Many_ref_many_sam”):



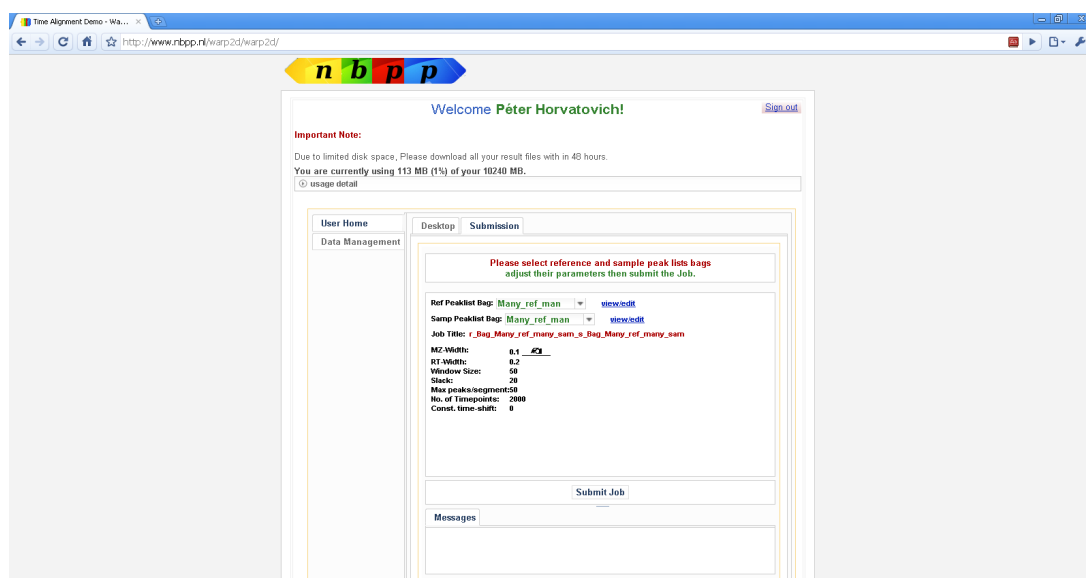
You should obtain:



Then select Lab1_MARS_BreastChodosh_normal_R1_3c.pks and place it in “1_ref_many_sam” bag.

Peak alignment

To start the peak alignment go to the “*User Home*”/“*Submission*” and choose “Many_ref_many_sam” the “Ref Peaklist Bag” and “Samp Peaklist Bag”. Change the default value of “MZ-Width” to 0.1 and “Slack” to 20 as the example files were acquired with QTOF and the default values are provided for low resolution iontrap mass spectrometer and click the “Submit” button:



Then monitor the progression status with the following order:

The following screenshots illustrate the progression status of a job in the nbpp web interface:

Screenshot 1: Submission Status

Important Note: Due to limited disk space, Please download all your result files with in 48 hours. You are currently using 113 MB (1%) of your 10240 MB.

ID	Status	Title	Message
1	submitting	r_Bag_Many_ref_m	Newly created job, in Pre-processing Phase

Screenshot 2: Running Status

Important Note: Due to limited disk space, Please download all your result files with in 48 hours. You are currently using 1319 MB (13%) of your 10240 MB.

ID	Status	Title	Message
1	running	r_Bag_Many_ref_m	Job is running

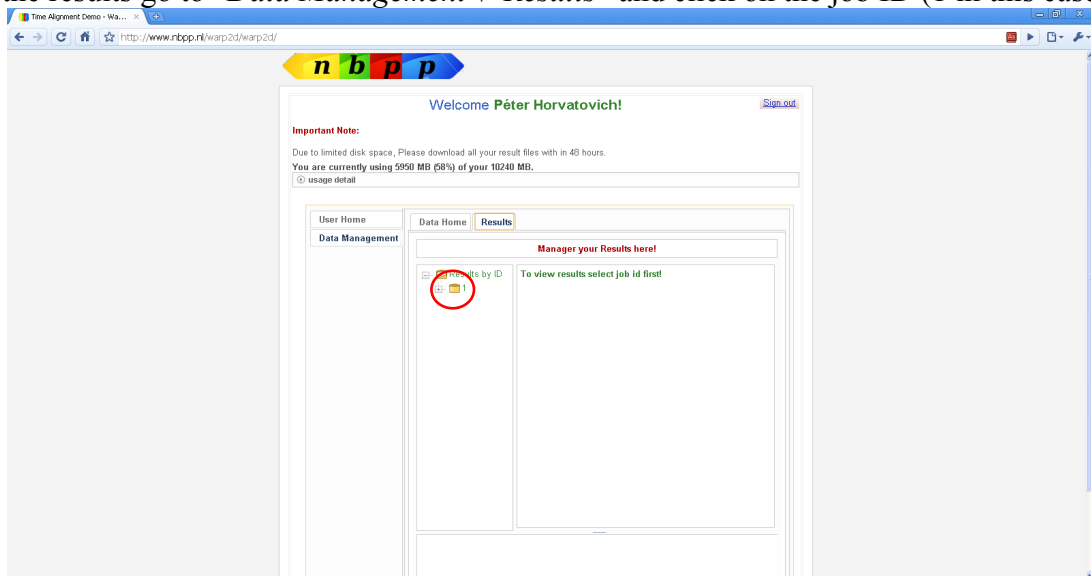
Screenshot 3: Completed Status

Important Note: Due to limited disk space, Please download all your result files with in 48 hours. You are currently using 5950 MB (58%) of your 10240 MB.

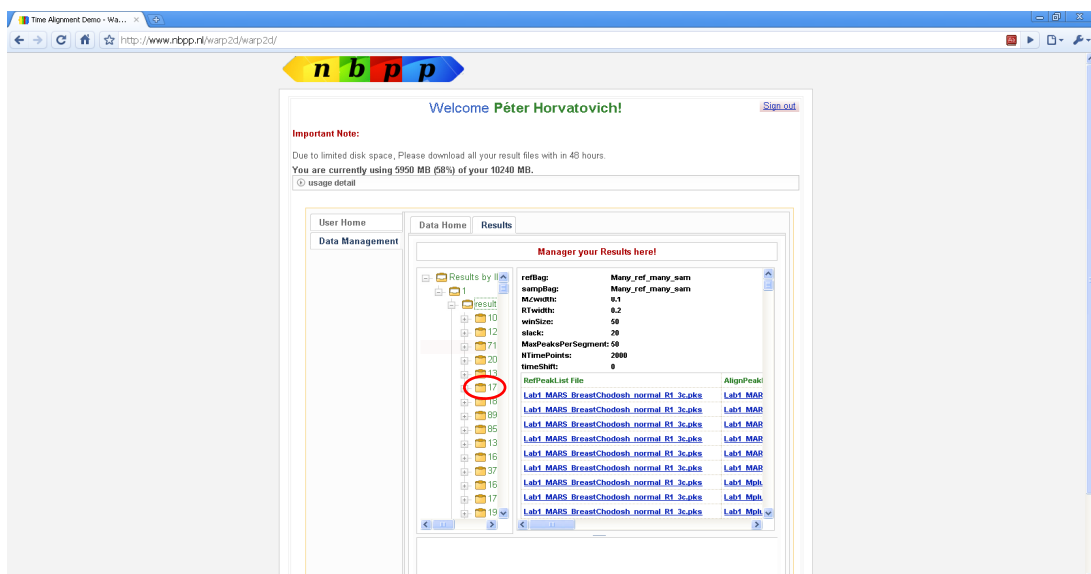
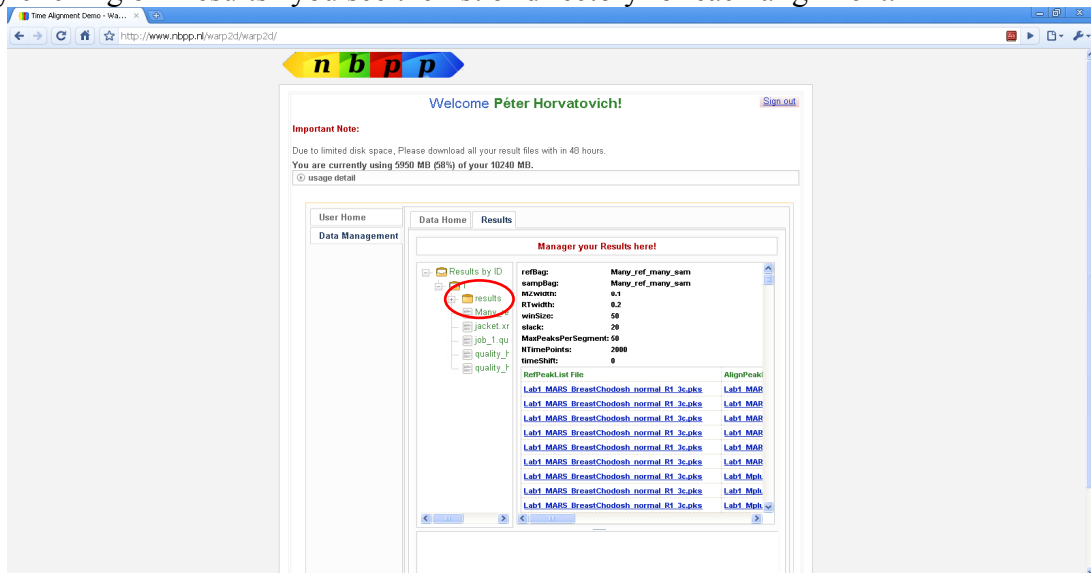
ID	Status	Title	Message
1	completed	r_Bag_Many_ref_m	Job is completed successfully

View and download results

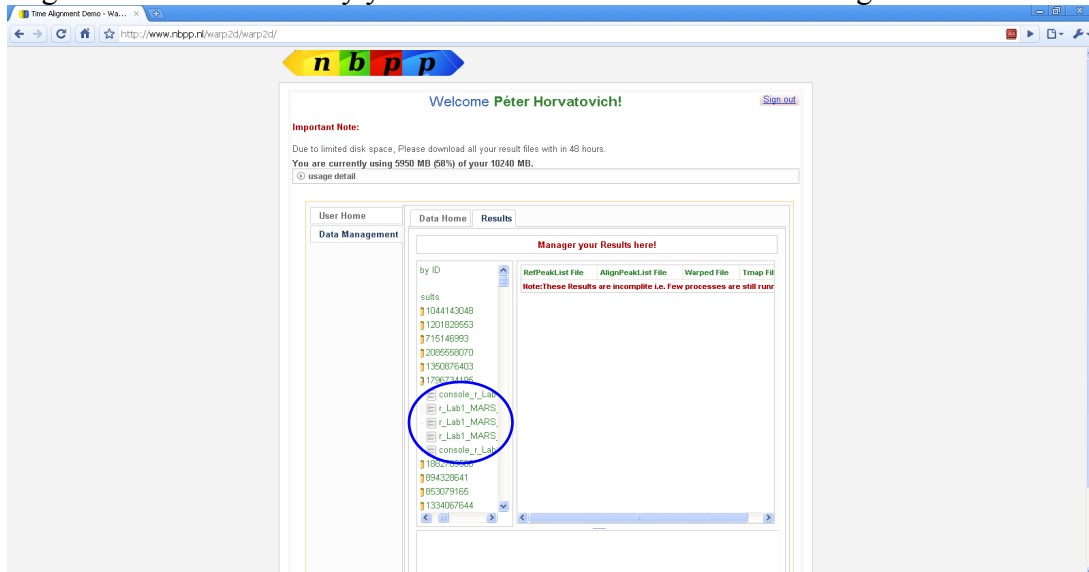
To see the results go to “Data Management”/“Results” and click on the job ID (1 in this case):



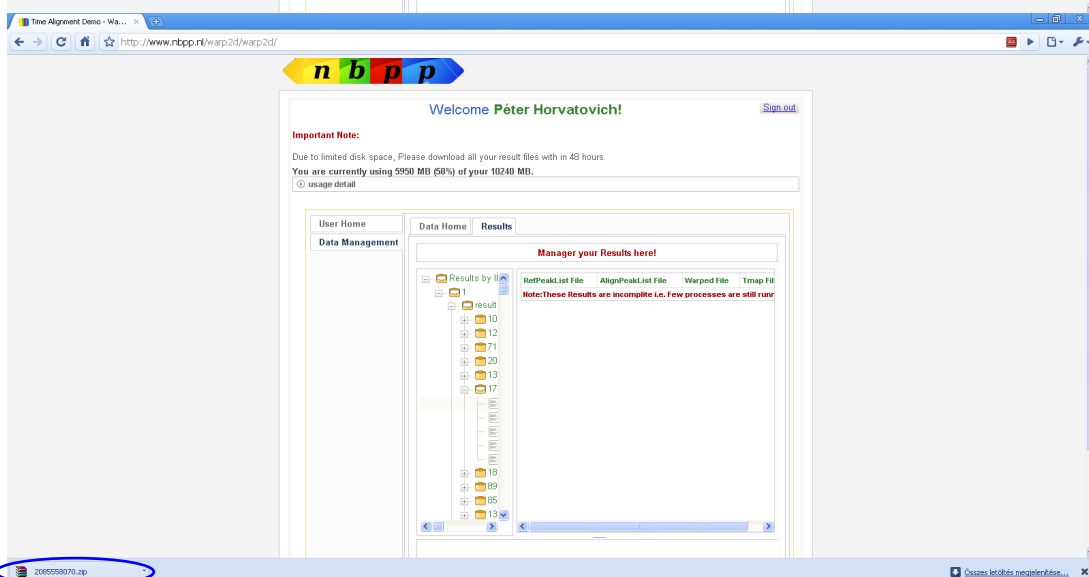
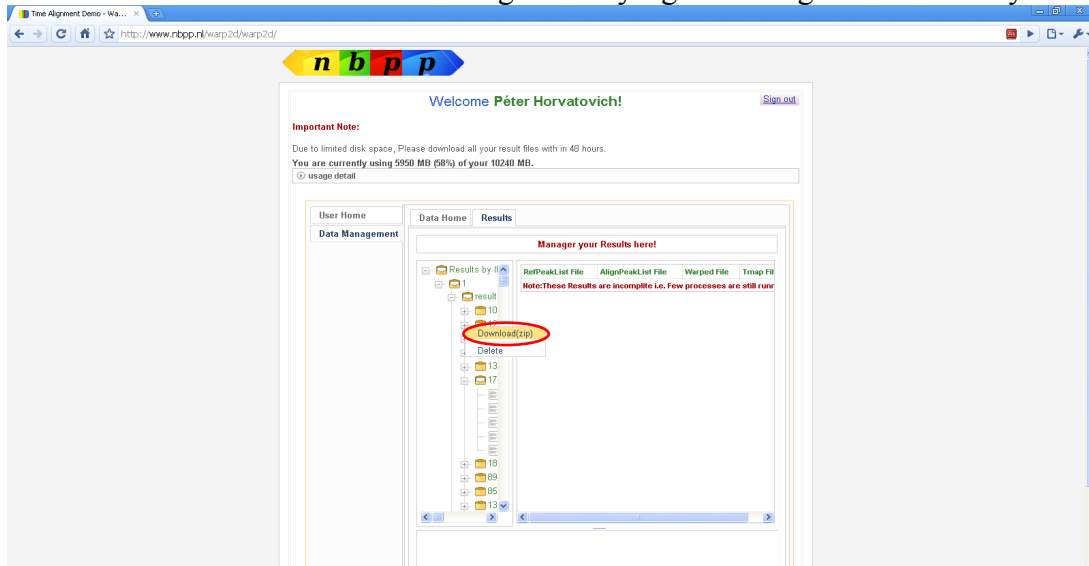
Here by clicking on “results” you see the list of directory for each alignment.



By clicking on one of the directory you can see the results files for this alignment:



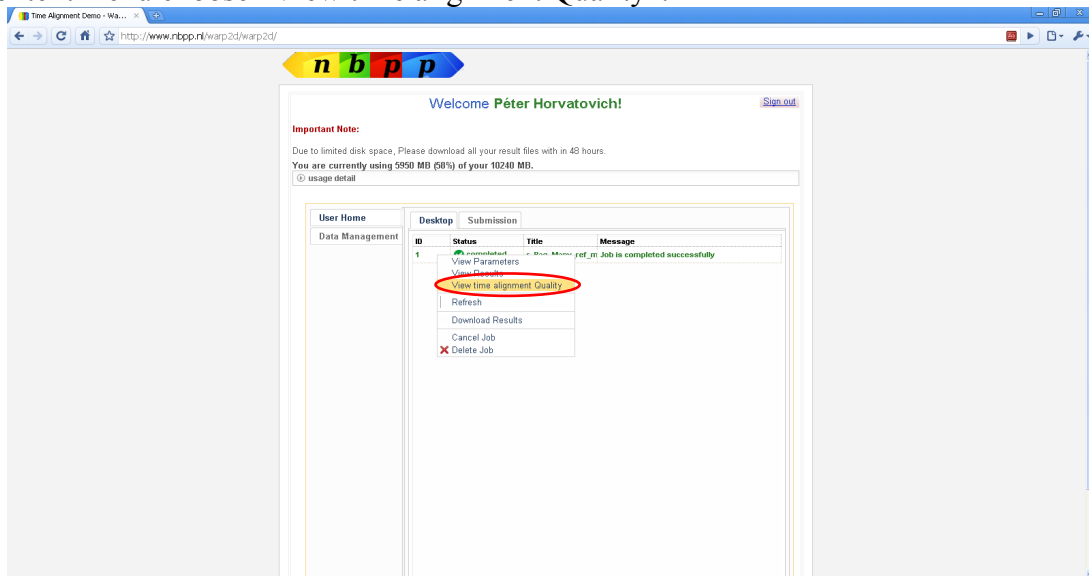
You can download result files for one time alignment by right clicking on the directory tree:



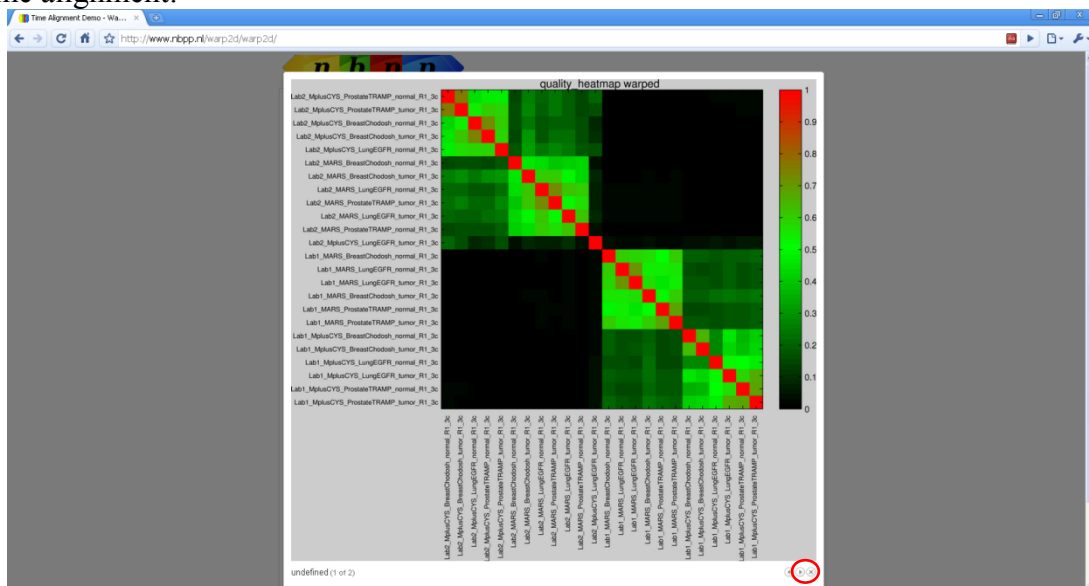
You can also download all result files of one job by clicking on the job ID or right clicking at the status line of particular finished job at “User Home”/“Desktop”.

Visualize results

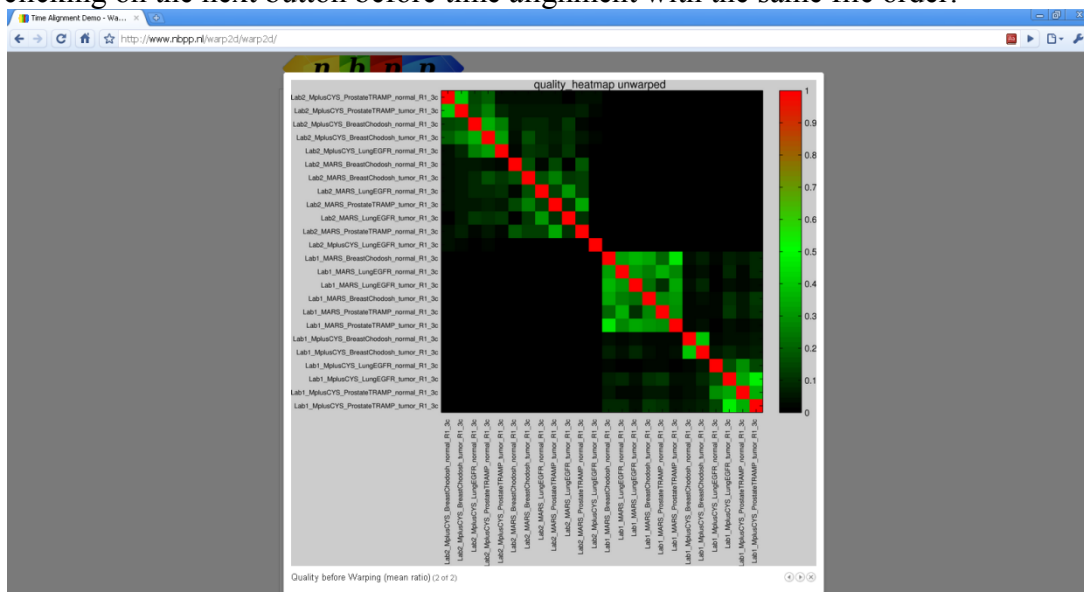
To visualise the quality of the time alignment go to “User Home”/“Desktop” and from the right click context menu choose “View time alignment Quality”:



And you can see the time alignment quality in matrix format rearranged with hierarchical clustering after time alignment:



and by clicking on the next button before time alignment with the same file order:



To perform alignment to one reference go back to “Data Management”/“Data Home” and select the first file (Lab1_MplusCYS_BreastChodosh_tumor_R1_3c.pks) and place it into 1_ref_many_samp bag:

Welcome Péter Horvátovich!

Important Note:
Due to limited disk space, Please download all your result files with in 48 hours.
You are currently using 5950 MB (58%) of your 10240 MB.

Data Management

Manager your Peak Lists here!

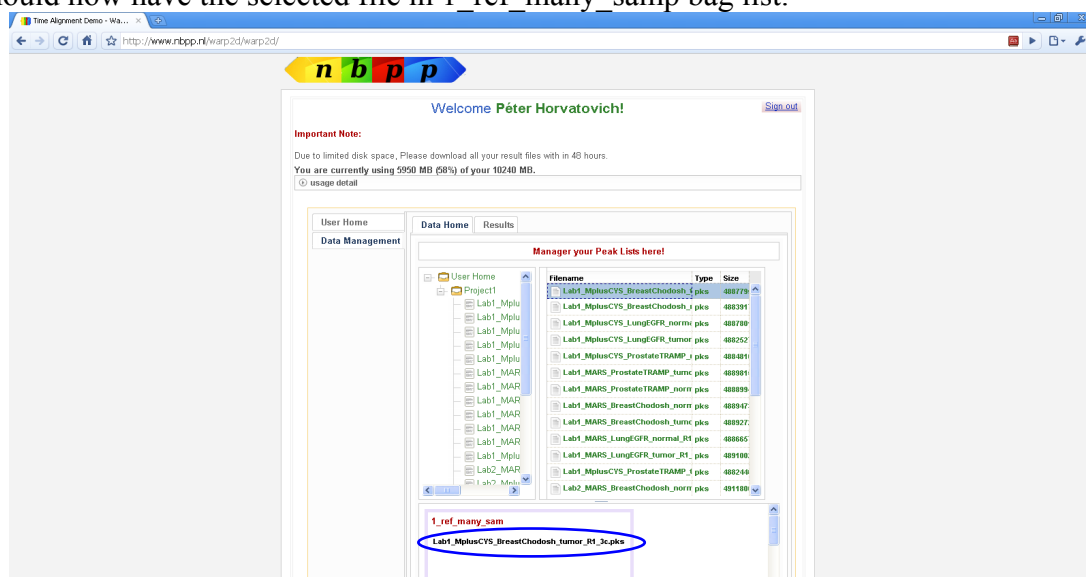
Filename	Type	Size
Lab1_M		489778
Lab1_M		489778
Lab1_M		489778
Lab1_M		489778
Lab1_MplusCYS_ProstateTRAMP_1.pks		489481
Lab1_MARS_ProstateTRAMP_tumor.pks		489891
Lab1_MARS_ProstateTRAMP_norm.pks		489893
Lab1_MARS_BreastChodosh_tumor.pks		489897
Lab1_MARS_BreastChodosh_norm.pks		489897
Lab1_MARS_LungGFR_normal_R1.pks		489865
Lab1_MARS_LungGFR_tumor_R1.pks		489100
Lab1_MplusCYS_ProstateTRAMP_1.pks		489240
Lab2_MARS_BreastChodosh_norm.pks		491159

1_ref_many_sam

Many_ref_many_sam

- Lab1_MARS_BreastChodosh_normal_R1_3c.pks
- Lab1_MARS_BreastChodosh_tumor_R1_3c.pks
- Lab1_MARS_LungGFR_normal_R1_3c.pks
- Lab1_MARS_LungGFR_tumor_R1_3c.pks
- Lab1_MARS_ProstateTRAMP_normal_R1_3c.pks

You should now have the selected file in 1_ref_many_samp bag list.



Then go to “User Home”/“Submission” and select 1_ref_many_samp bag list for reference and many_ref_many_samp bag list as sample. Change the default value of “MZ-Width” to 0.1 and “Slack” to 20 and click the “Submit Job” button as previously:

