

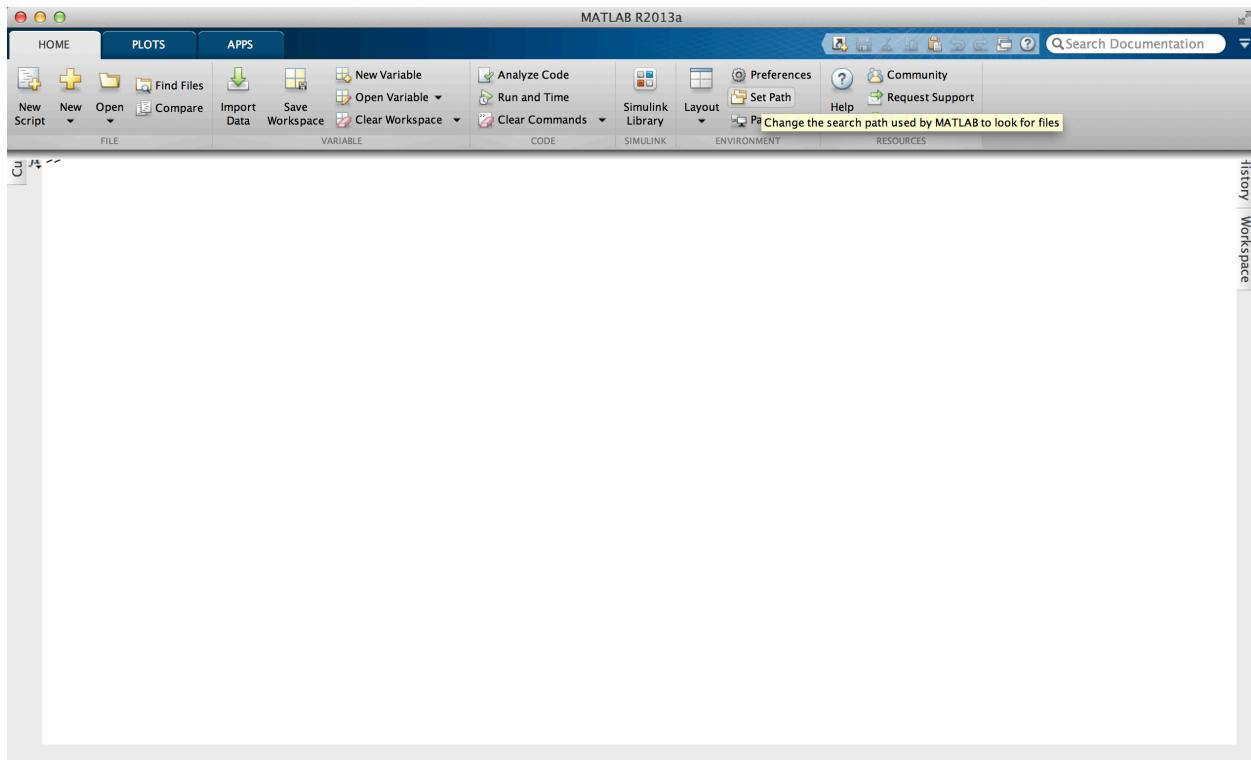
Simple user guide to Ariadne

by Nasso Sara

Ariadne's thread: a robust software solution leading to automated absolute and relative quantification of SRM data

It is advisable to run the code the first time with the provided data as from the publication on Matlab R2013a (further compatibility is not guaranteed).

First step: add the Ariadne code folder to the Matlab path:



Calibration experiment

This example uses the publication data. Browse to the folder “smooth – calibration exp”:

The screenshot shows the MATLAB interface with the 'Editor' window open. The current file is 'main.m'. The code in the editor is as follows:

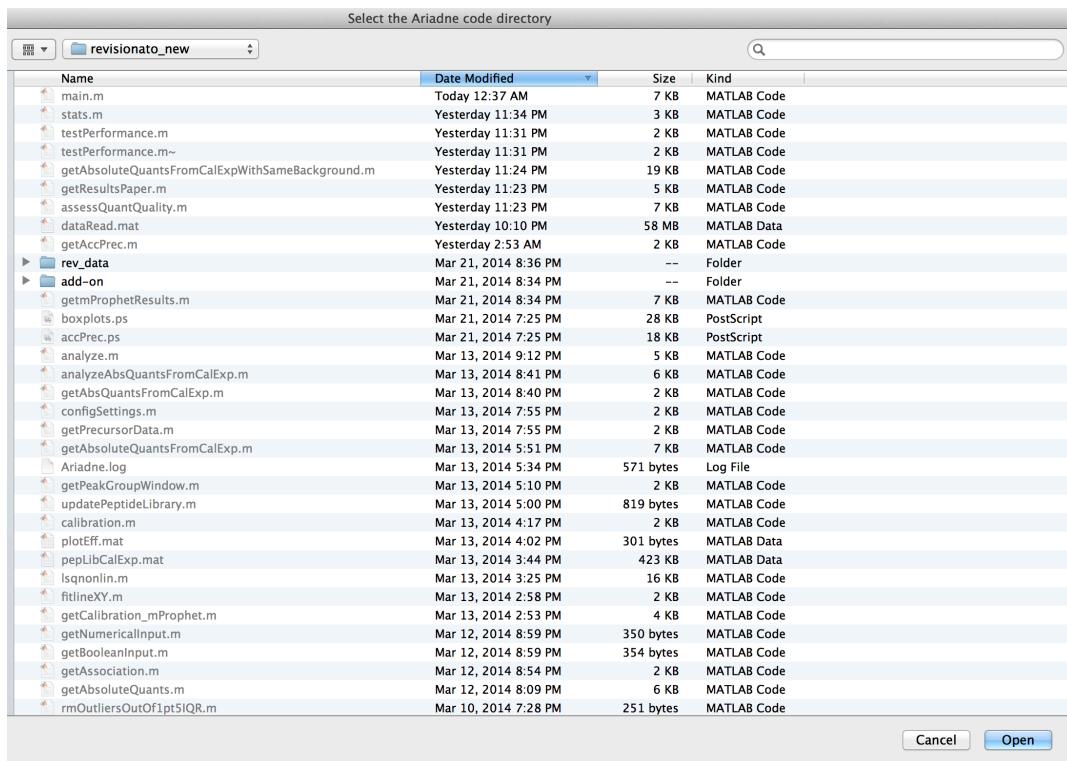
```
2 % This software is the implementation of the Ariadne algorithm by Nassos et al.
3 % Copyright (C) 2012 Sara Nassos
4 %
5 % Ariadne is free software; you can redistribute it and/or modify
6 % it under the terms of the GNU General Public License as published by
7 % the Free Software Foundation; either version 2 of the License, or (at
8 % your option) any later version.
9 %
10 % Ariadne is distributed in the hope that it will be useful, but
11 % WITHOUT ANY WARRANTY; without even the implied warranty of
12 % MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU
13 % General Public License for more details.
14 %
15 % You should have received a copy of the GNU General Public License
16 % along with this program; if not, write to the Free Software
17 % Foundation, Inc., 59 Temple Place, Suite 330, Boston, MA 02111-1307
18 % USA
19 % $ $ $ #####
20 %
21 - clear
22 - close all
23 - clc
24 - try
25 - matlabpool open
26 - catch
27 - disp('Warning: could not run the parallel computing option!')
28 - end
29 %
30 %% adding Ariadne path to Matlab path
31 dataDir = uigetdir(pwd, 'Select the Ariadne code directory');
32 addpath dataDir
33 %
34 %% config
35 [settings pathSettings] = uigetfile('.m', 'Select the file configSettings.m for this dataset');
36 settingsFilePath = [pathSettings settings];
37 run(settingsFilePath)
38 %
39 %% loading calibration experiment results (pepLibCalExp.mat) when needed
40 %
41 if settings.absoluteQuantification && ~settings.calibration
42 [calExp pathCalExp] = uigetfile('.mat', 'Select the file pepLibCalExp.mat', 'MultiSelect');
43 calExpFilePath = [pathCalExp calExp];
44 load(calExpFilePath)
45 end
```

The 'Command Window' tab is selected in the top right, showing the command `f1 >>`. The status bar at the bottom indicates 'Ln 23 Col 4'.

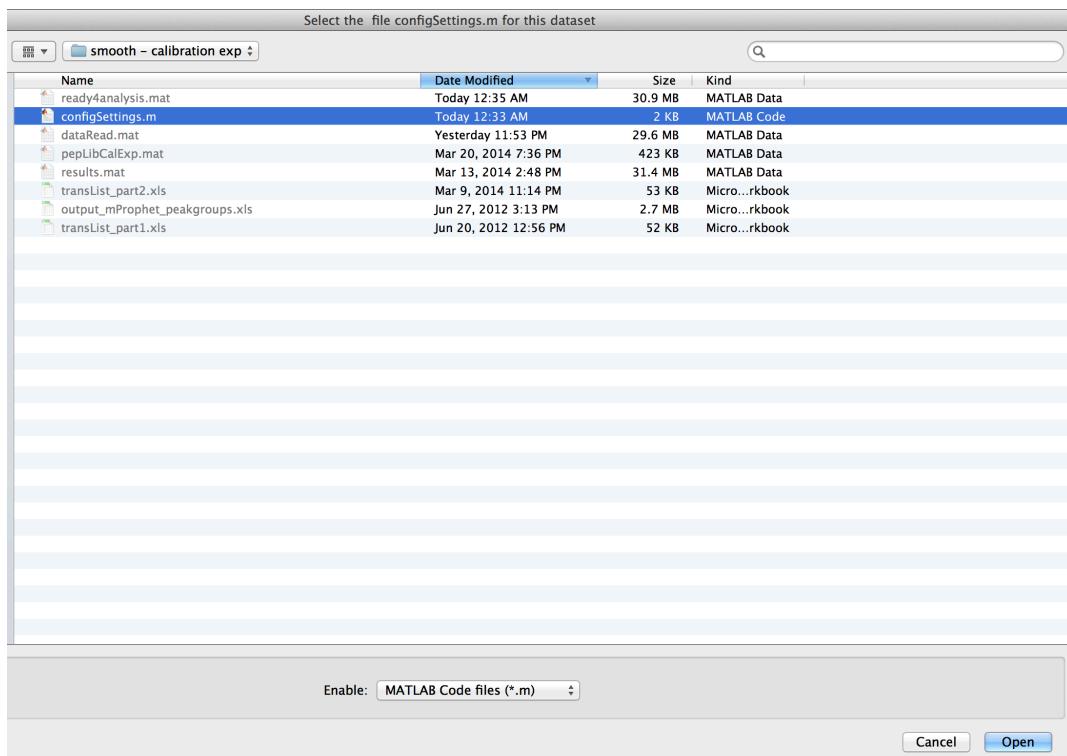
Run the main.m script and you will be prompted to input some data files as follows.

The screenshot shows the MATLAB interface with the 'Editor' window open. The current file is 'main.m'. The code in the editor is identical to the one in the previous screenshot. The 'Command Window' tab is selected in the top right, showing the command `f1 >> main`. The status bar at the bottom indicates 'Ln 23 Col 4'.

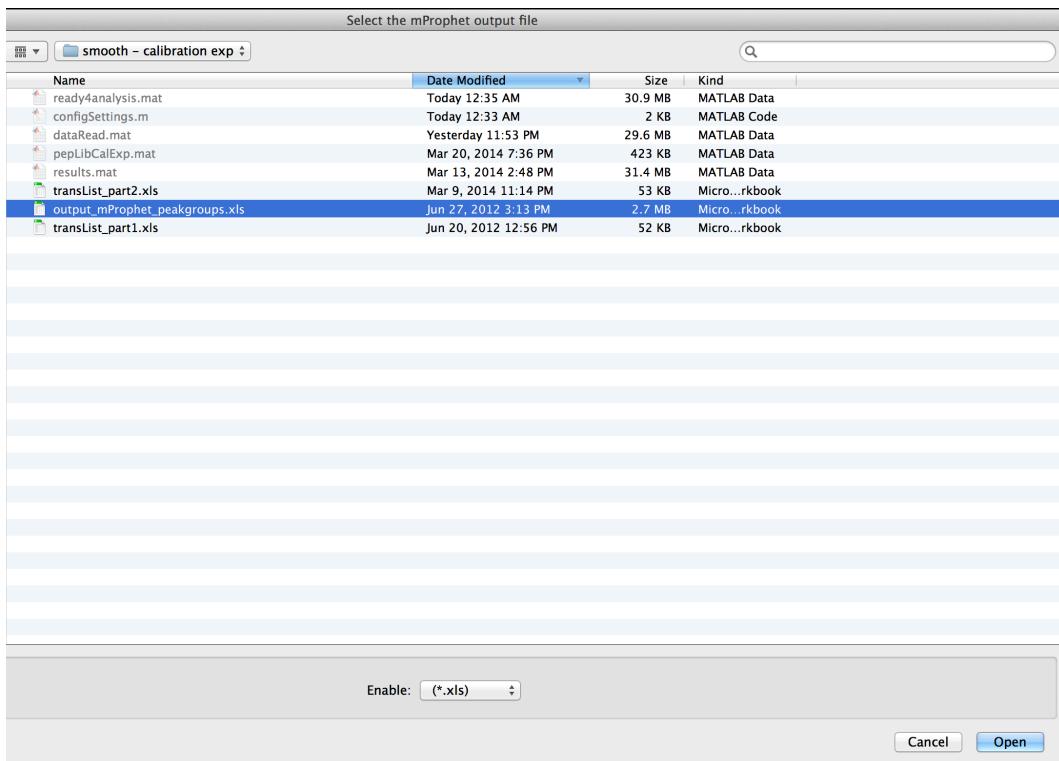
Browse to the folder where you saved the Ariadne code



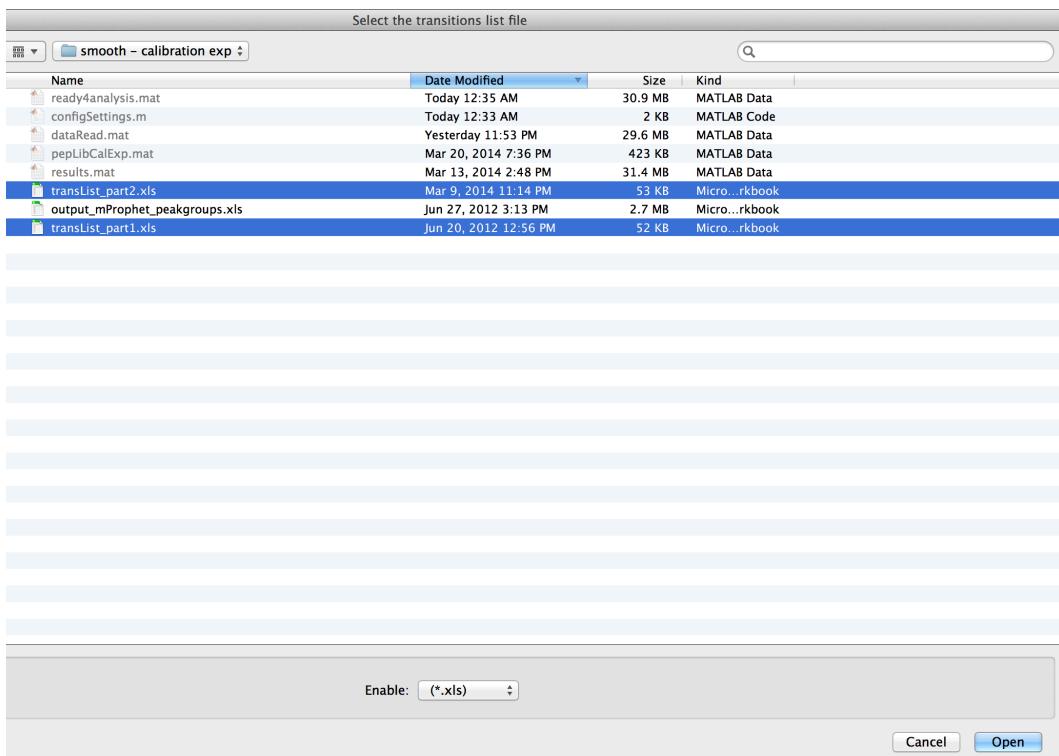
Select the configuration file for the current dataset "configSettings.m"



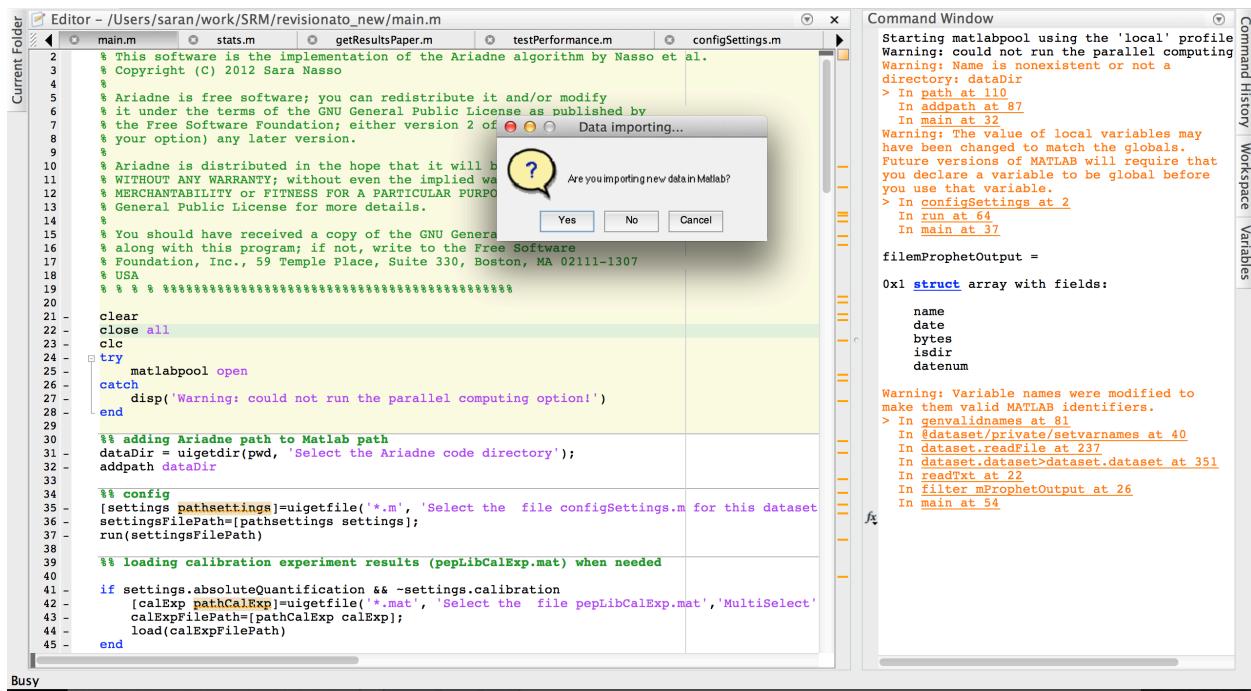
Select the mProphet output file (requested according to the configSettings.m settings)



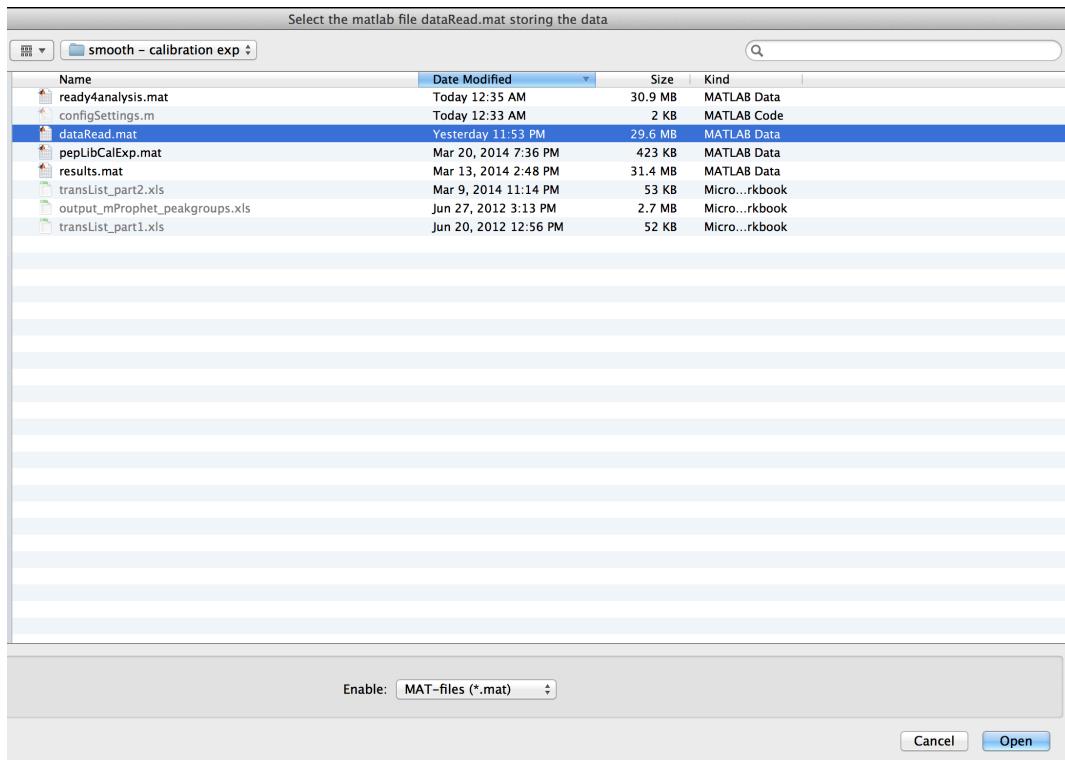
Select the transitions list (multiple selection: Ctrl/Command + click)



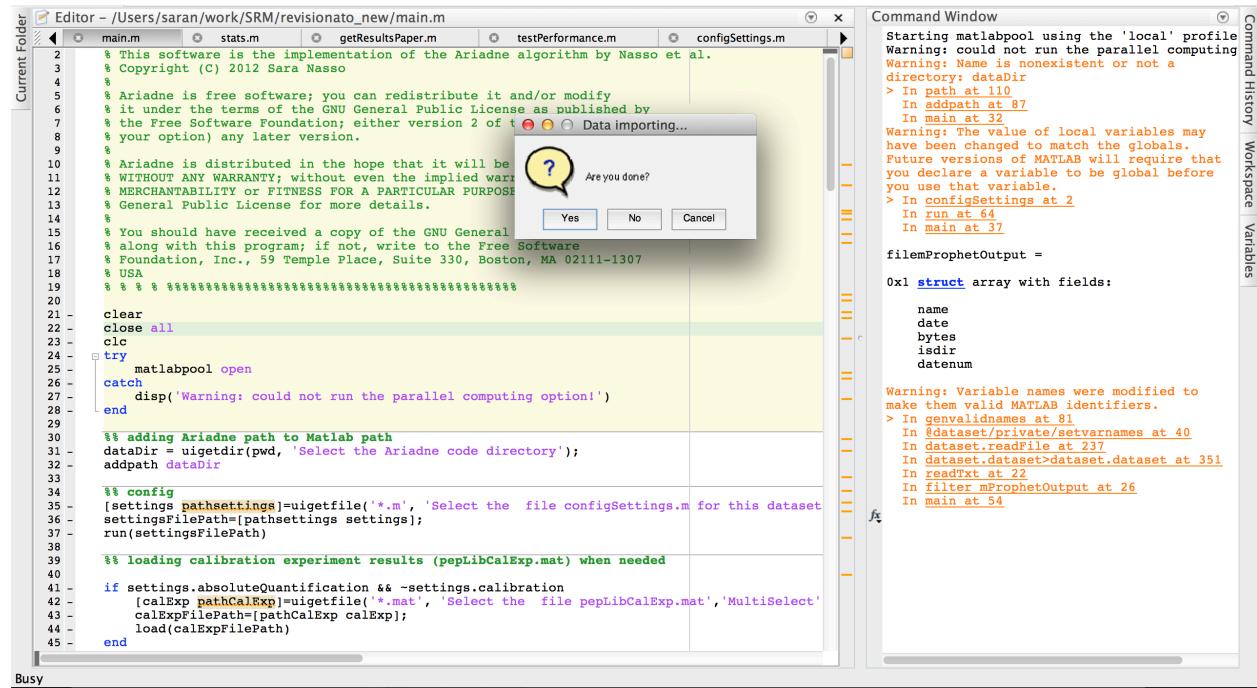
If you are importing new data click “Yes” and consider it takes some time (~h) to import them



If you click “No” you can load already imported data, as provided in “dataRead.mat”

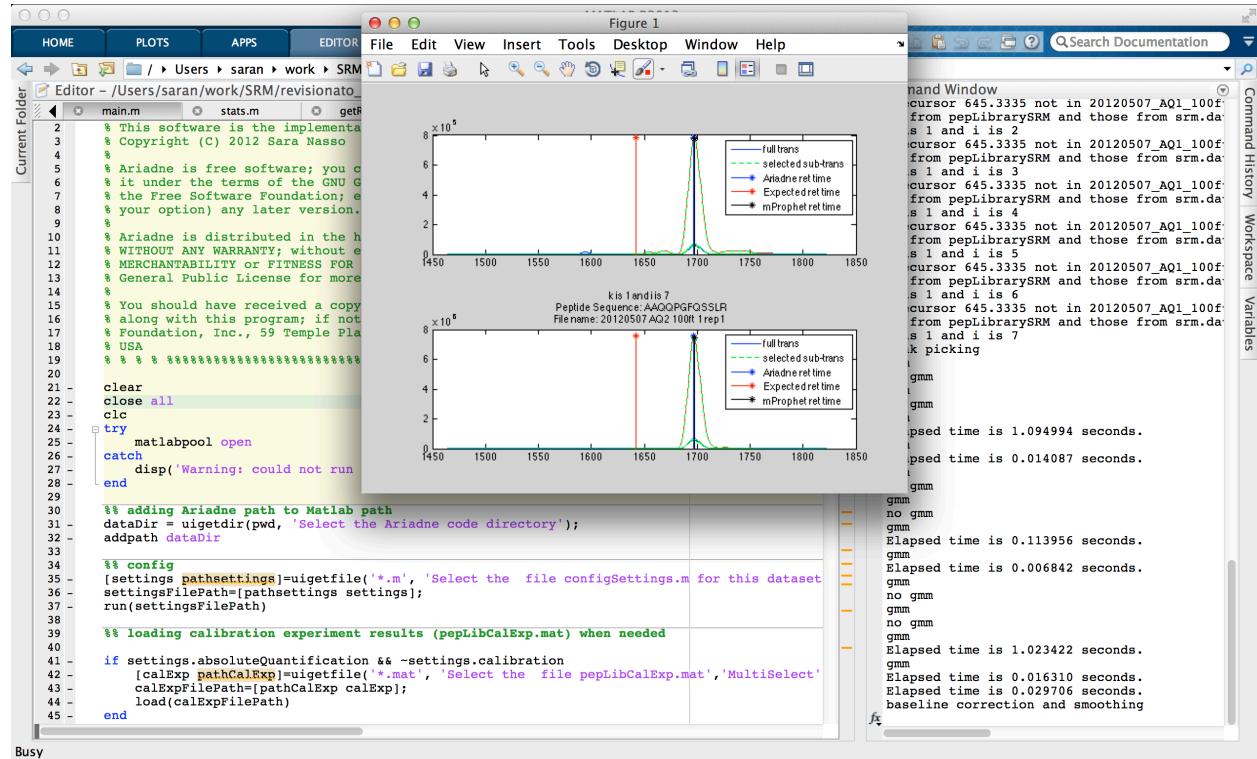


You could also select another .mat data file if necessary



There you go, let it run!

You can roughly estimate the required time as: Time(1pep) x #files x #pep per file



Absolute Quantification experiment

The noisy and complex background datasets allow performing absolute quantification using the smooth data from the above calibration experiment as calibrants.

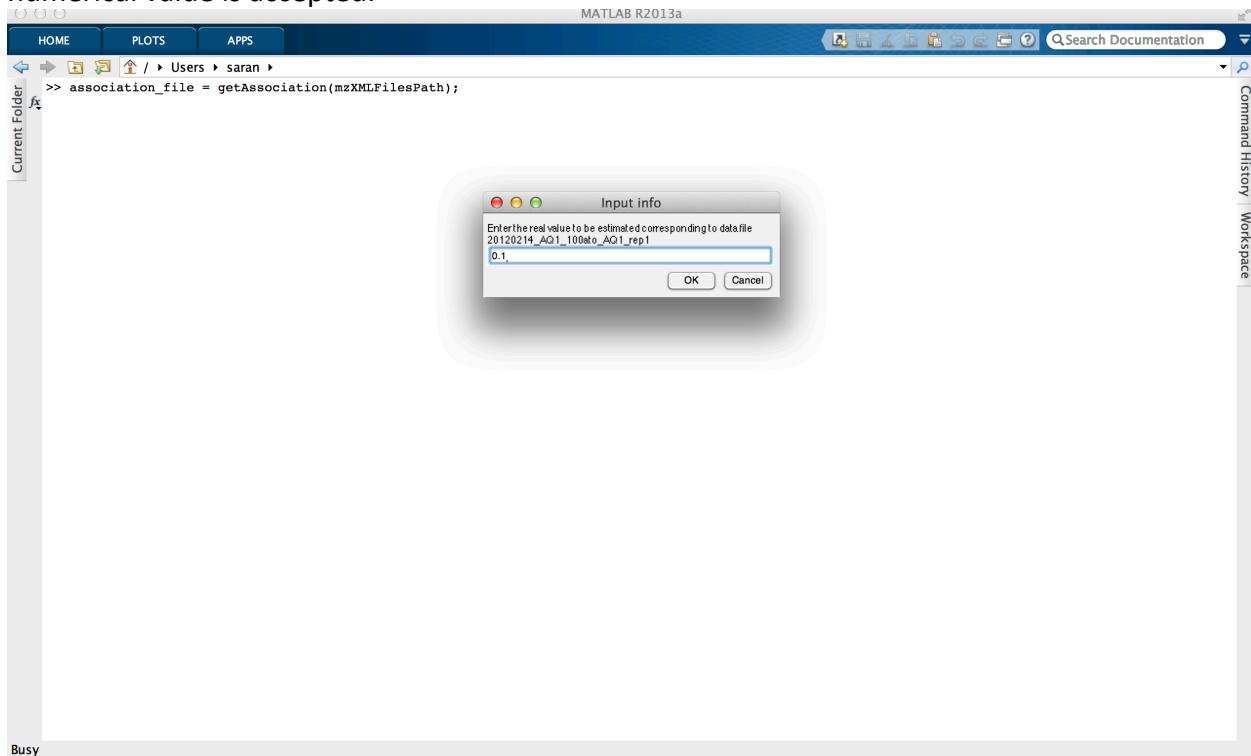
As before, run the main.m but load the inputs from either the noisy or complex background folder, depending on which dataset you may want to analyze: complex background dataset is smaller, so analysis will be faster while on the noisy data you can appreciate the effectiveness of the smoothing procedure.

Example of absolute and relative quantification results exported in a .txt file:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Protein	Peptide	Charge	RetentionT	FileName	Ratio	AbsoluteQuant									
2	BAP60	AAQQPQFQSSLR	2	1568.678936	20121126_AQ2_100ft_1_rep1	0.136746941	131.7774142									
3	BAP60	AAQQPQFQSSLR	2	1557.51888	20121126_AQ2_100ft_1_rep2	0.135910584	131.7774142									
4	BAP60	AAQQPQFQSSLR	2	1592.771232	20121126_AQ2_100ft_1_rep3	0.134515548	131.7774142									
5	BAP60	AAQQPQFQSSLR	2	1557.458992	20121126_AQ2_10ft_1_rep1	1.673388573	10.20822563									
6	BAP60	AAQQPQFQSSLR	2	1548.604986	20121126_AQ2_10ft_1_rep2	1.62575045	10.20822563									
7	BAP60	AAQQPQFQSSLR	2	1558.514118	20121126_AQ2_10ft_1_rep3	1.529423341	10.20822563									
8	BAP60	AAQQPQFQSSLR	2	1575.779944	20121126_AQ2_1ft_1_rep1	19.74553518	0.764128387									
9	BAP60	AAQQPQFQSSLR	2	1568.656975	20121126_AQ2_1ft_1_rep2	27.74283766	0.764128387									
10	BAP60	AAQQPQFQSSLR	2	1561.624538	20121126_AQ2_1ft_1_rep3	13.59024398	0.764128387									
11	hyc	AILDYDVDSRK	2	1872.059916	20121126_AQ2_100ft_1_rep1	0.401971545	103.7701687									
12	hyc	AILDYDVDSRK	2	1855.848151	20121126_AQ2_100ft_1_rep2	0.369680613	103.7701687									
13	hyc	AILDYDVDSRK	2	1894.401794	20121126_AQ2_100ft_1_rep3	0.354930611	103.7701687									
14	hyc	AILDYDVDSRK	2	1865.658764	20121126_AQ2_10ft_1_rep1	3.610019186	10.71710415									
15	hyc	AILDYDVDSRK	2	1848.024118	20121126_AQ2_10ft_1_rep2	3.687115132	10.71710415									
16	hyc	AILDYDVDSRK	2	1843.781709	20121126_AQ2_10ft_1_rep3	3.38385993	10.71710415									
17	hyc	AILDYDVDSRK	2	1874.176975	20121126_AQ2_1ft_1_rep1	38.75359601	0.899655051									
18	hyc	AILDYDVDSRK	2	1863.08437	20121126_AQ2_1ft_1_rep2	39.68827605	0.899655051									
19	hyc	AILDYDVDSRK	2	1848.999664	20121126_AQ2_1ft_1_rep3	188.5282904	0.899655051									
20	ARM	AISNSNDESTIK	2	1398.168627	20121126_AQ1_100ft_2_rep1	0.051285146	103.9275853									
21	ARM	AISNSNDESTIK	2	1399.009693	20121126_AQ1_100ft_2_rep2	0.028309627	103.9275853									
22	ARM	AISNSNDESTIK	2	1399.098875	20121126_AQ1_100ft_2_rep3	0.036378496	103.9275853									
23	ARM	AISNSNDESTIK	2	1408.199804	20121126_AQ1_10ft_2_rep2	0.429653413	6.083529256									
24	ARM	AISNSNDESTIK	2	1410.197563	20121126_AQ1_10ft_2_rep3	0.587026896	6.083529256									
25	ARM	AISNSNDESTIK	2	1405.201064	20121126_AQ1_1ft_2_rep1	5.746704879	1.703326106									
26	ARM	AISNSNDESTIK	2	529.79112	20121126_AQ1_1ft_2_rep2	0	1.703326106									
27	ARM	AISNSNDESTIK	2	1402.142745	20121126_AQ1_1ft_2_rep3	2.627543155	1.703326106									
28	pont	ALLLAGPPGTGK	2	2044.109606	20121126_AQ1_100ft_2_rep1	0.131563054	118.9614164									
29	pont	ALLLAGPPGTGK	2	2001.578961	20121126_AQ1_100ft_2_rep2	0.125811993	118.9614164									
30	pont	ALLLAGPPGTGK	2	2009.789748	20121126_AQ1_100ft_2_rep3	0.124320327	118.9614164									
31	pont	ALLLAGPPGTGK	2	2118.212437	20121126_AQ1_10ft_2_rep2	1.610928253	8.178921256									
32	pont	ALLLAGPPGTGK	2	2193.445294	20121126_AQ1_10ft_2_rep3	1.625609794	8.178921256									
33	pont	ALLLAGPPGTGK	2	2076.994454	20121126_AQ1_1ft_2_rep1	13.63668081	1.039435598									
34	pont	ALLLAGPPGTGK	2	2042.046443	20121126_AQ1_1ft_2_rep2	14.95246941	1.039435598									
35	pont	ALLLAGPPGTGK	2	2036.997059	20121126_AQ1_1ft_2_rep3	14.2364199	1.039435598									
36	ccdc2	APEVLLGSPR	2	1809.304706	20121126_AQ1_100ft_2_rep1	0.250125321	118.8106293									
37	ccdc2	APEVLLGSPR	2	1788.874202	20121126_AQ1_100ft_2_rep2	0.260450123	118.8106293									

Importing new data and associating a group

When you are importing new data you will be prompted to associate data files to groups. For each file, this has to be inserted manually. If the absolute abundances are known, as in a dilution experiment, files have to be grouped by their abundance values. Otherwise, any other numerical value is accepted.

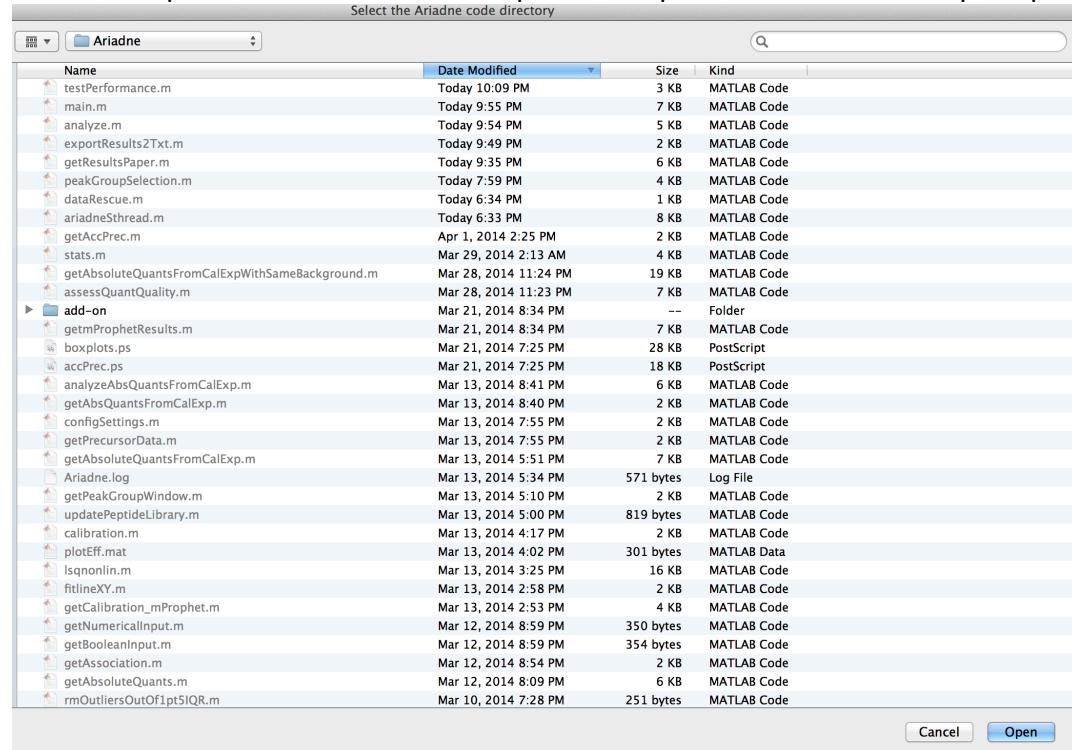


Testing the performance/ Reproducing published results

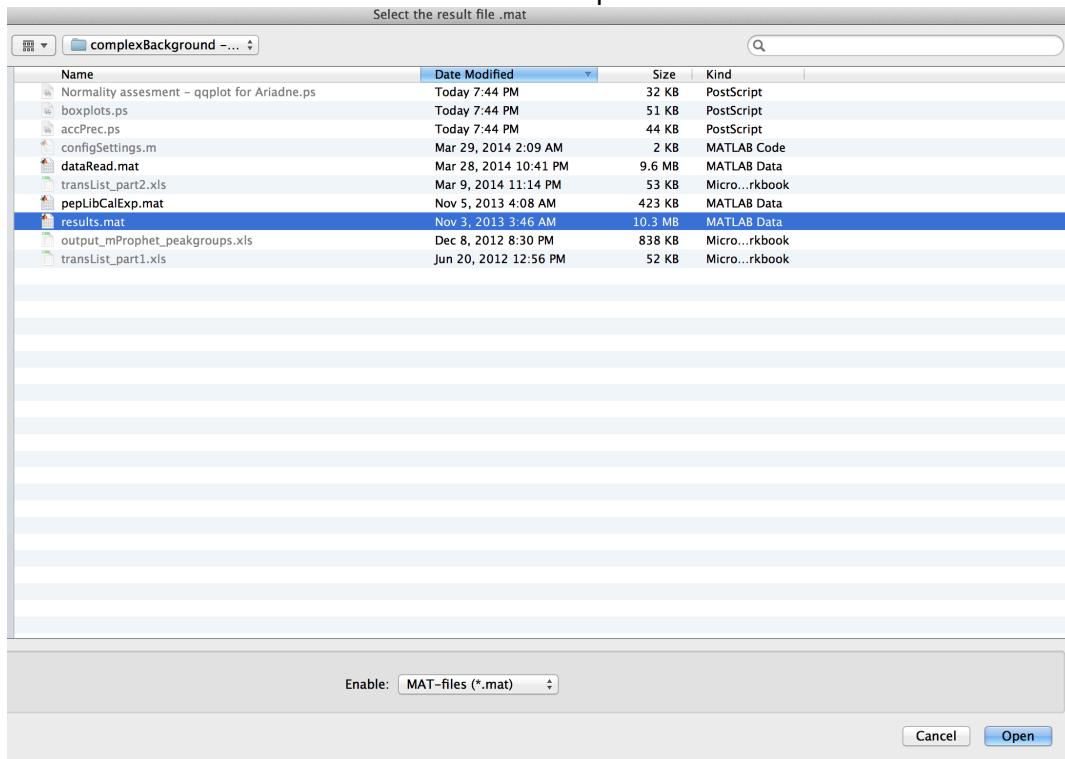
If comparing to mProphet or Skyline please refer to the corresponding Ariadne code package and accompanying data folder that would be better placed inside the code folder. Next releases will only integrate with Skyline and support the comparison to Skyline as it already implements the mProphet package and provides with superior quantification performance compared to mProphet.

First, add the desired Ariadne package folder to the Matlab path.

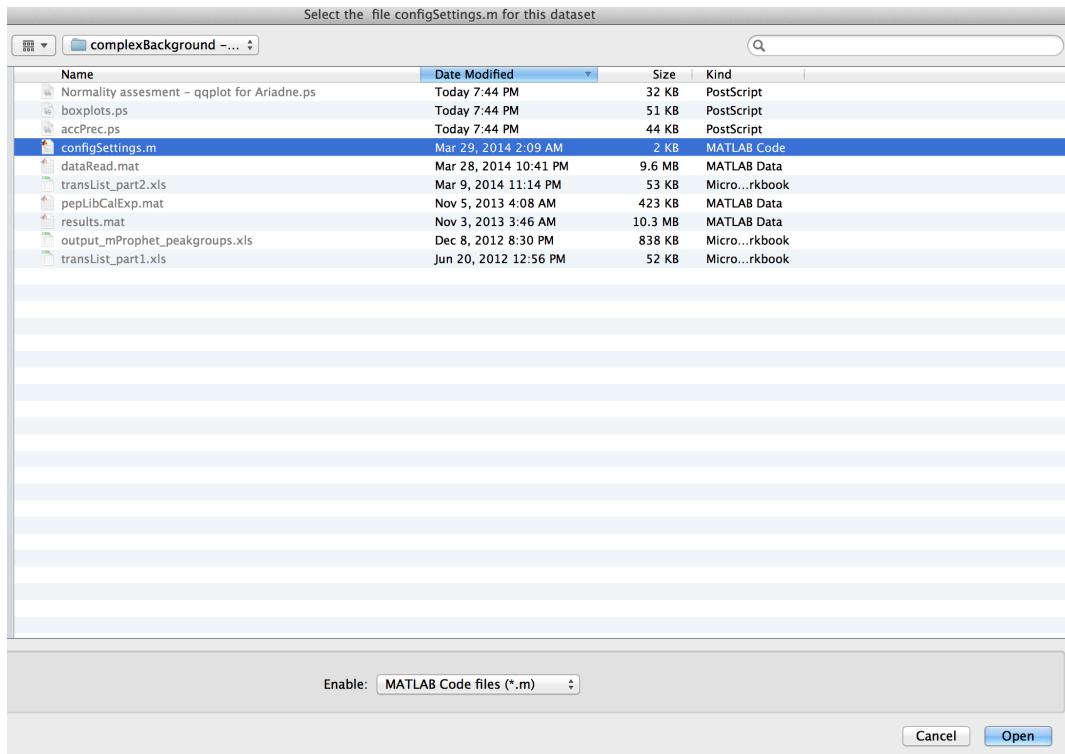
Run the script testPerformance.m and provide requested information as prompted.



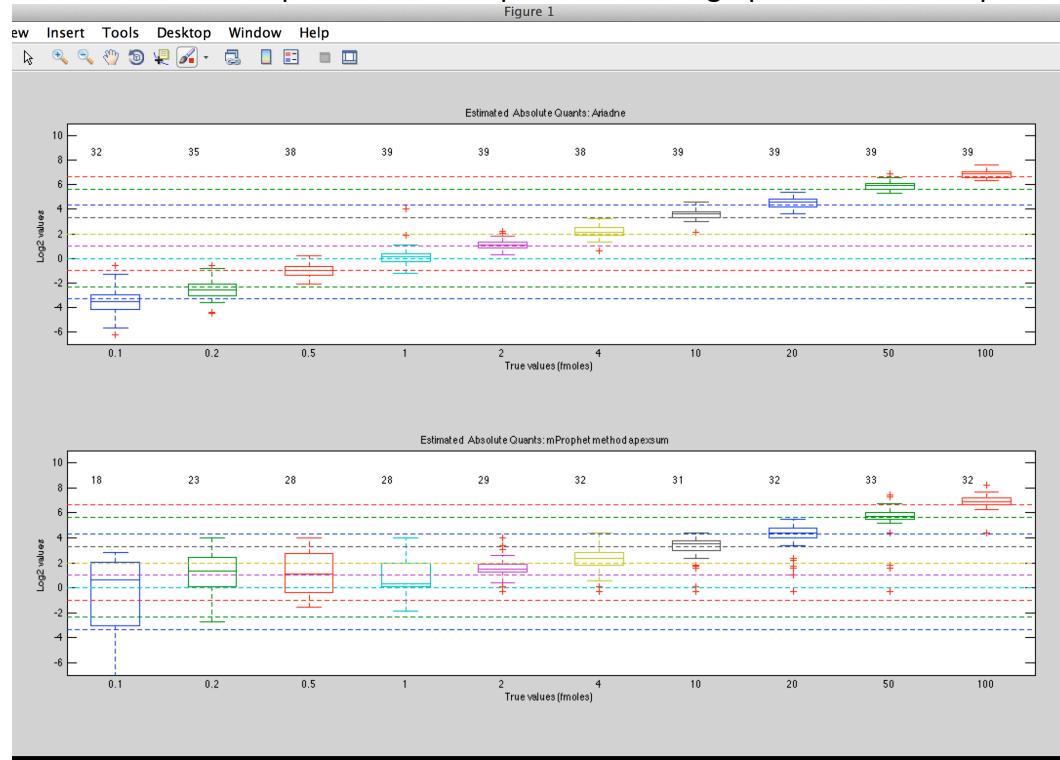
Select the result file of which to evaluate the performance:



Select the configuration file for the current dataset "configSettings.m":



The results will be represented in boxplots and other graphs and saved in .ps files.



Footnotes

This work was supported, in whole or in part, by the PRIME-XS Project, funded by the European Union Seventh Framework Program. For any enquiries please contact the developer:
sara.nasso@gmail.com.