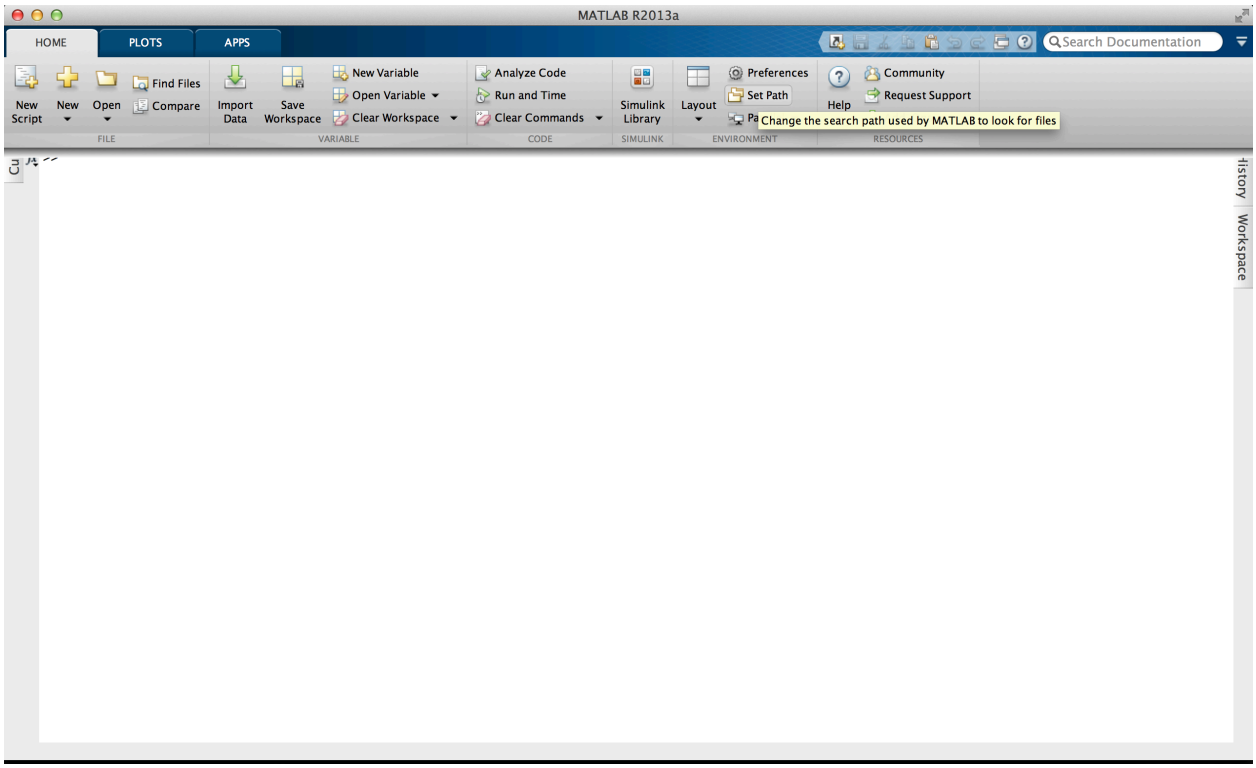
Simple user guide to Ariadne

by Nasso Sara

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

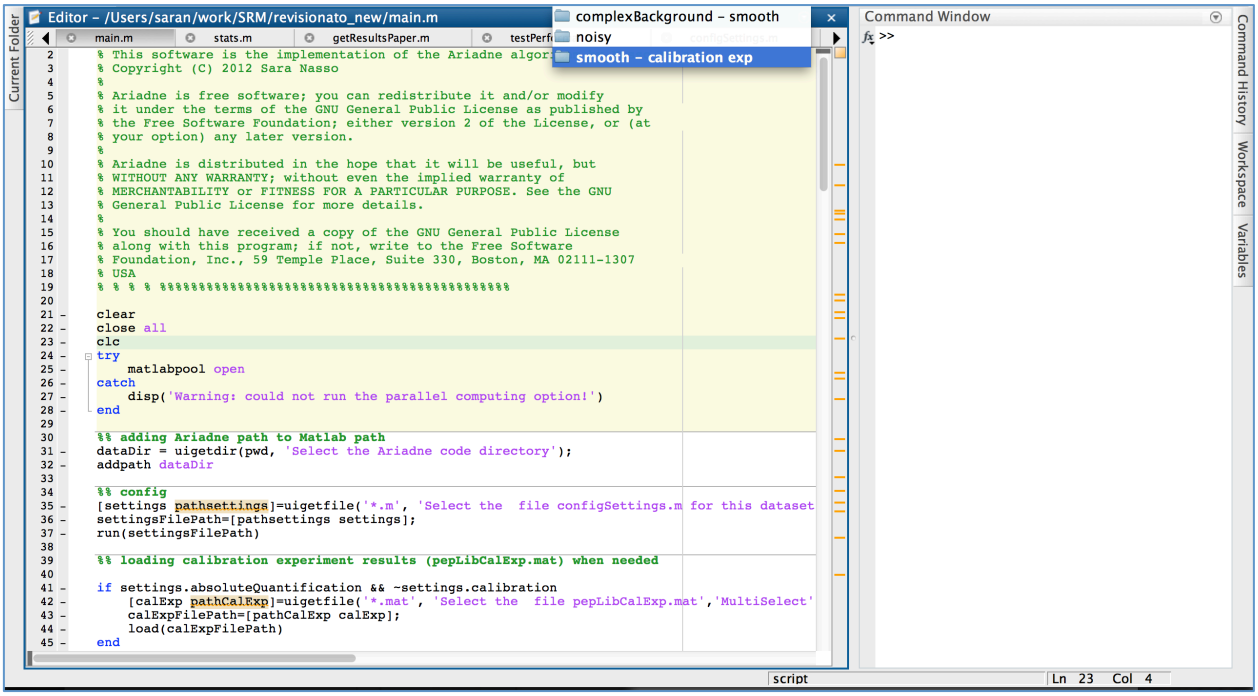
It is advisable to run the code the first time with the provided data as from the publication on Matlab R2013a (further compatibility is not guaranteed).

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

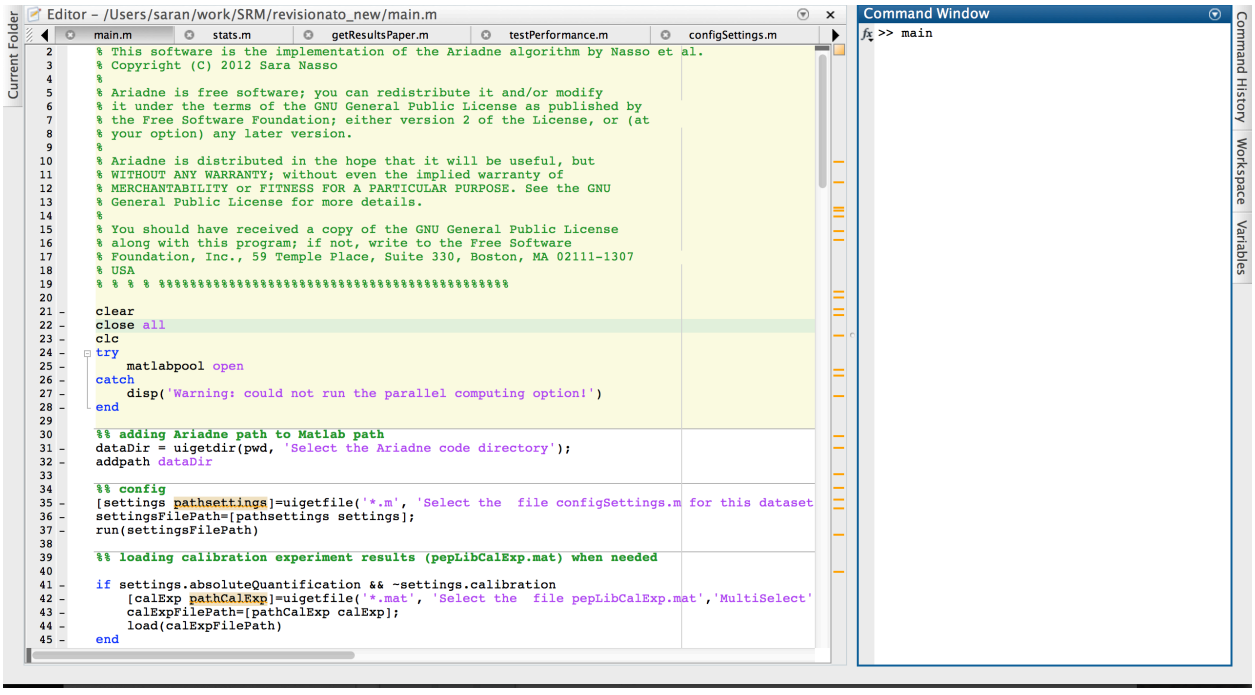


Calibration experiment

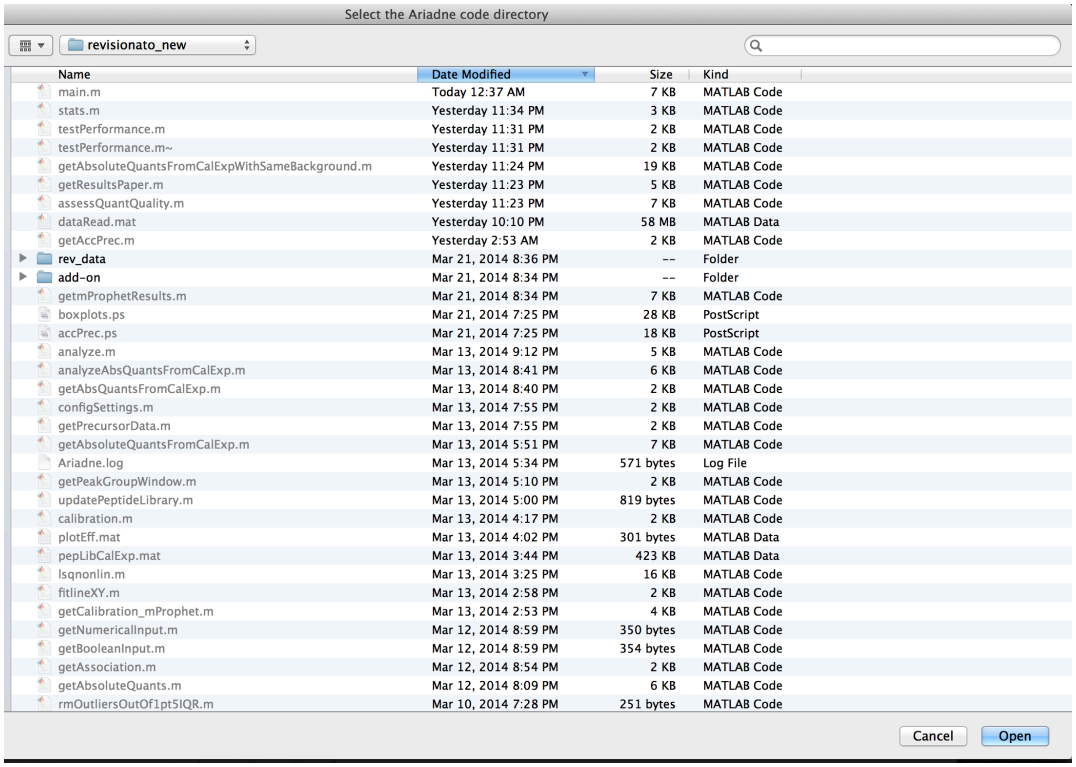
This example uses the publication data. Browse to the folder “smooth – calibration exp”:



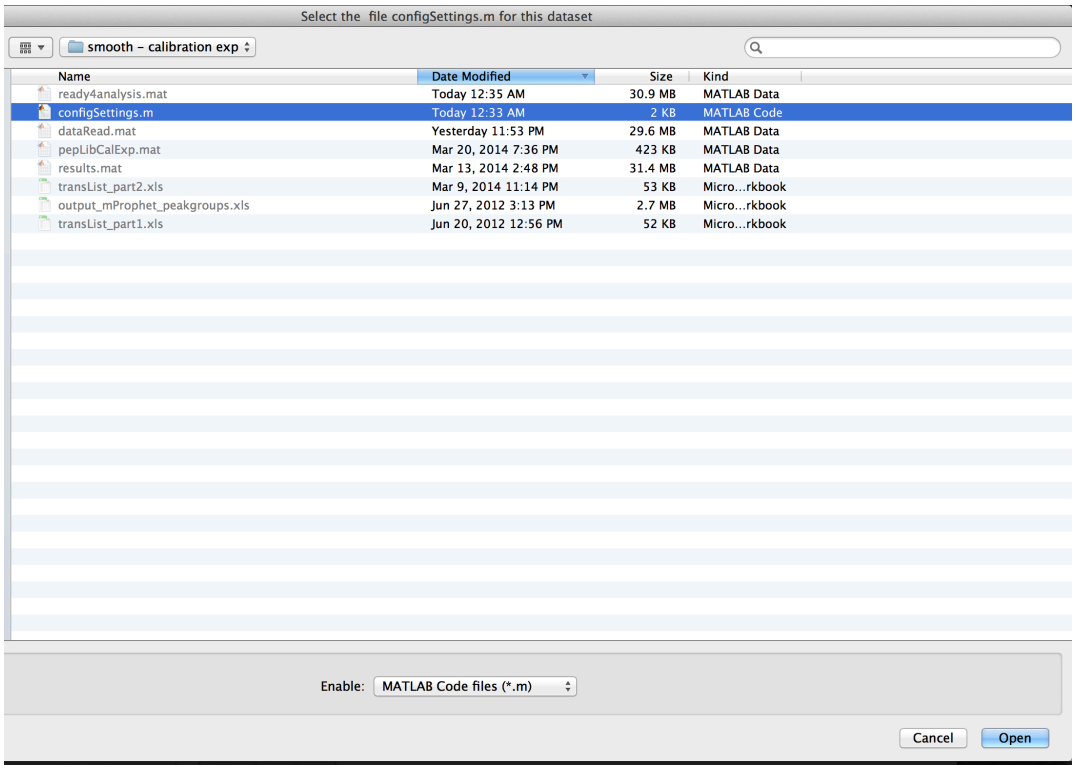
Run the main.m script and you will be prompted to input some data files as follows.



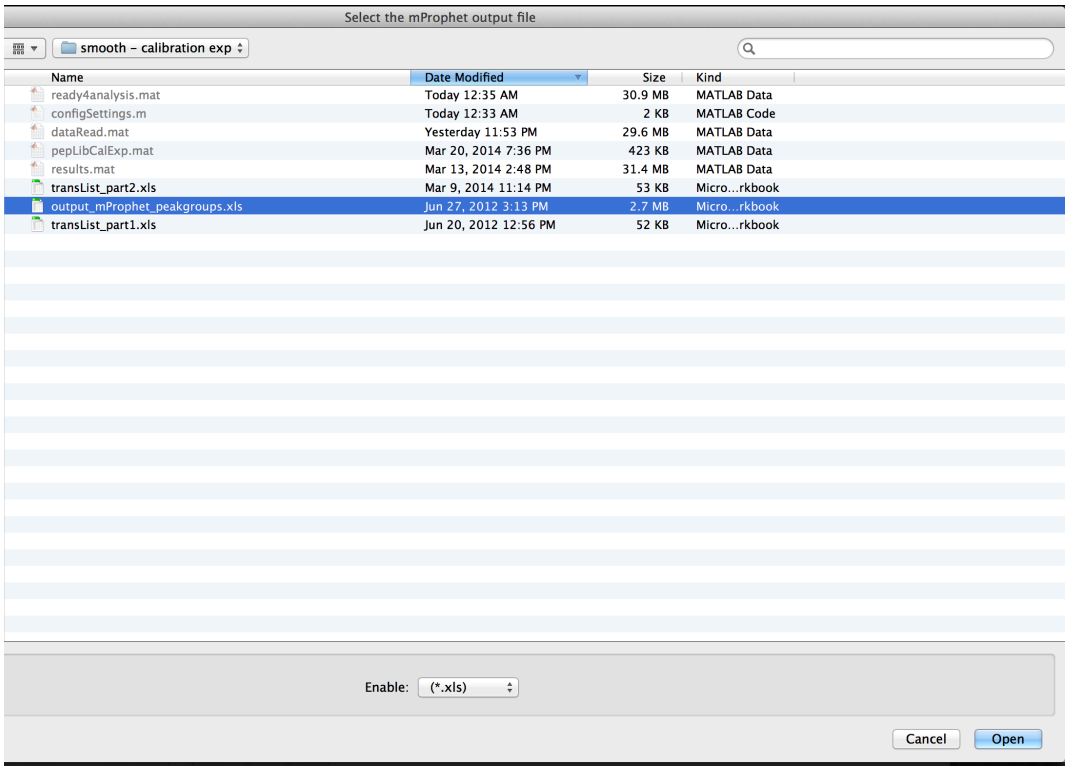
Browse to the folder where you saved the Ariadne code



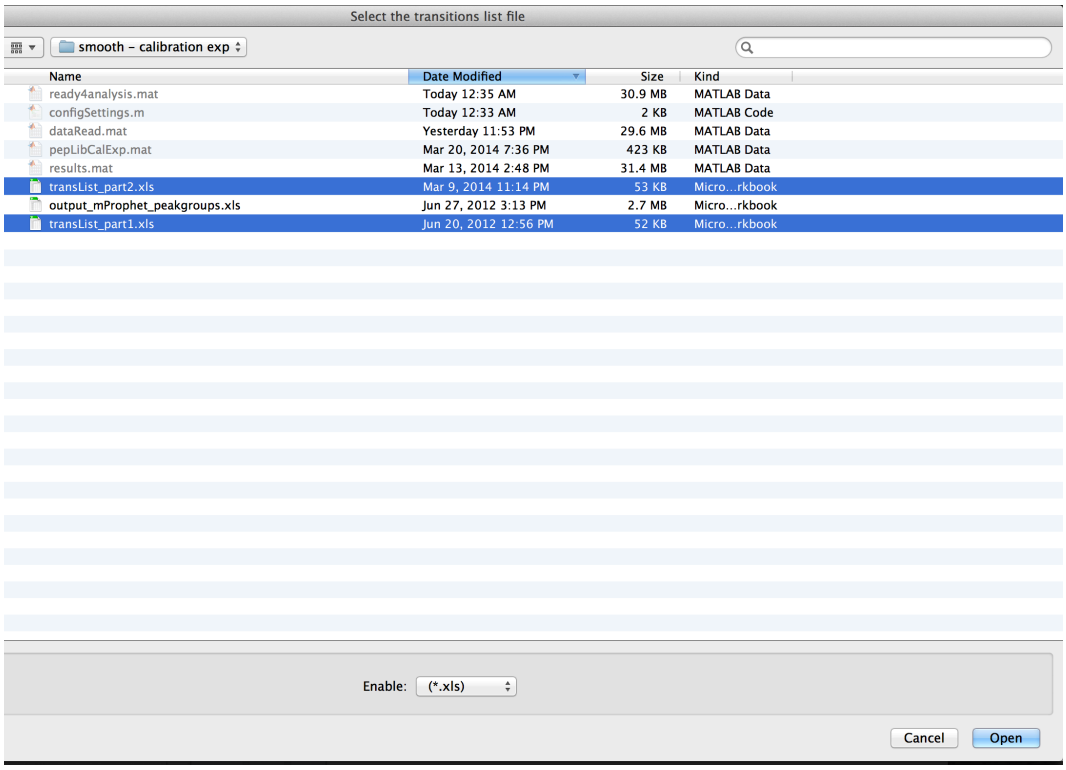
Select the configuration file for the current dataset “configSettings.m”



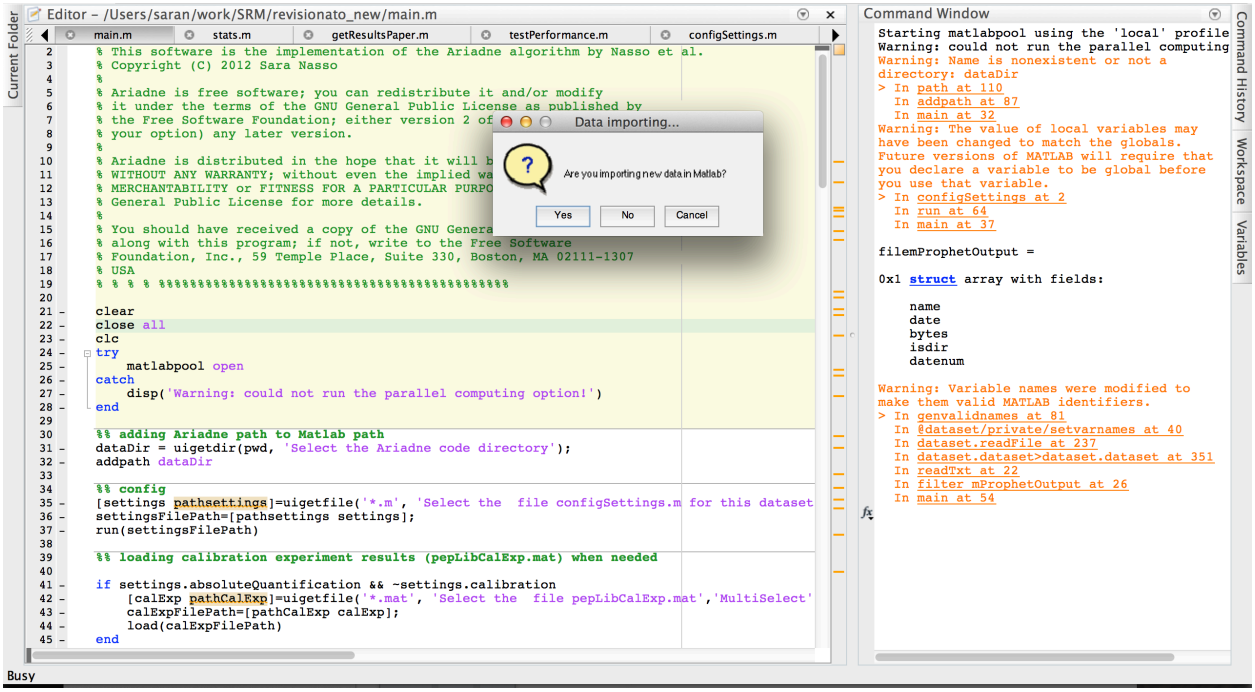
Select the mProphet output file (requested according to the configSettings.m settings)



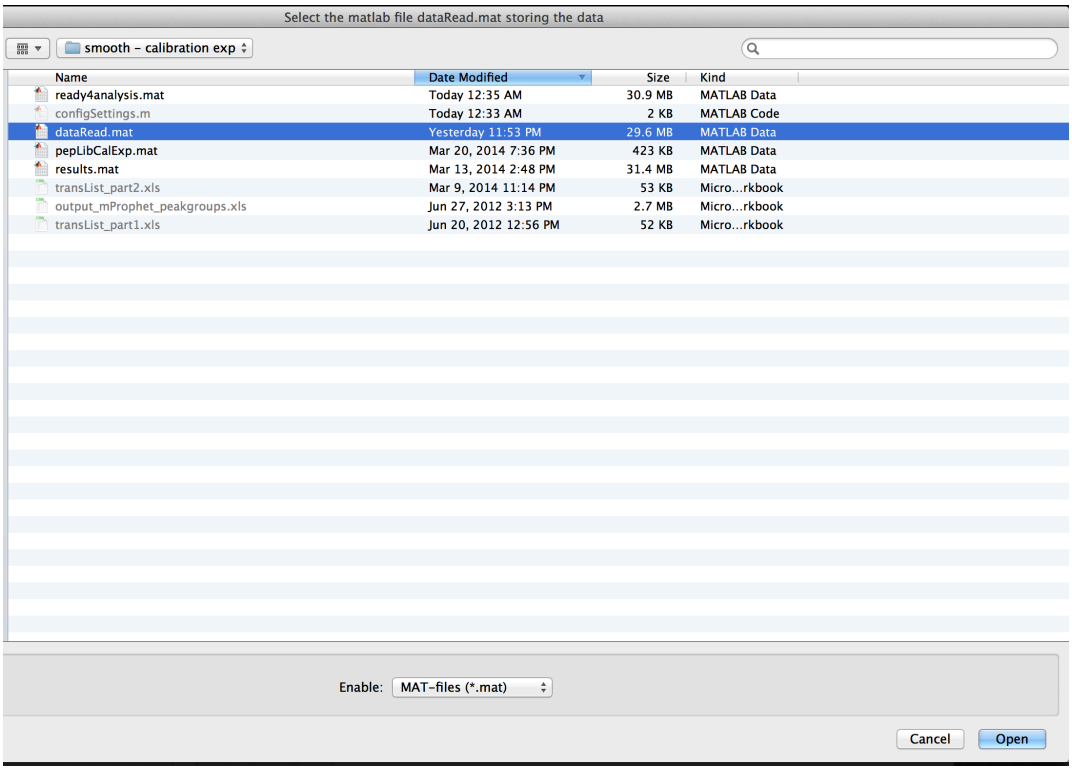
Select the transitions list (multiple selection: Ctrl/Command + click)



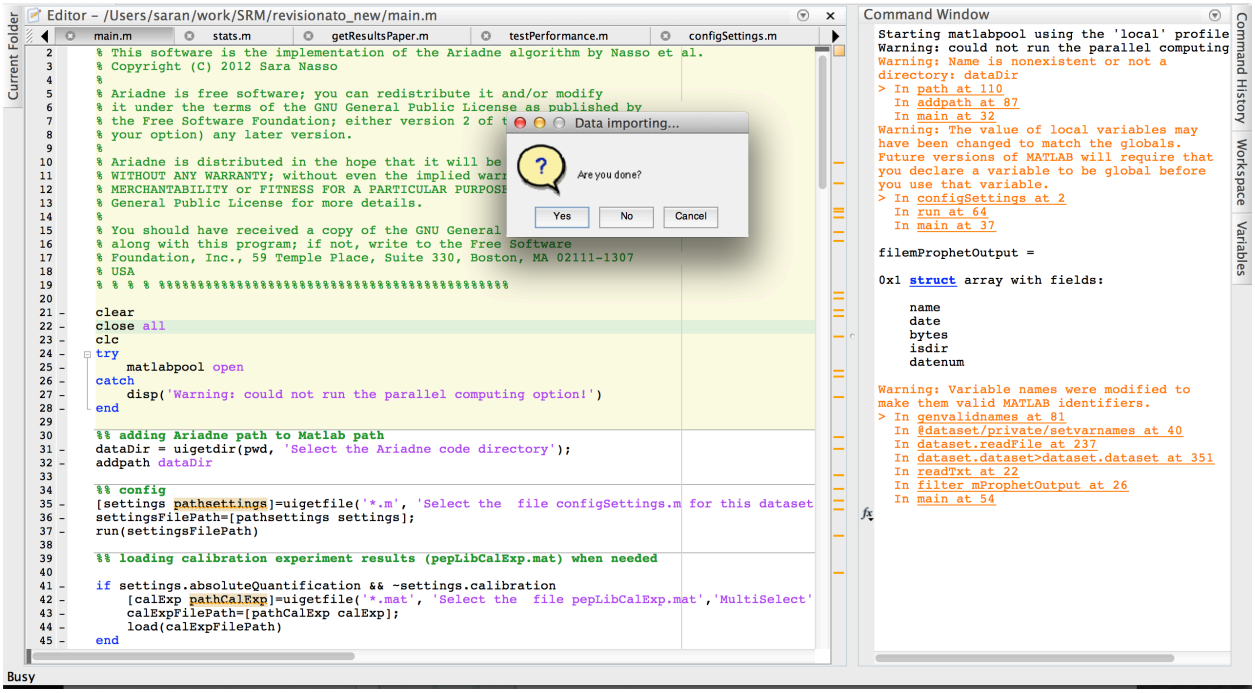
If you are importing new data click “Yes” and consider it takes some time (~h) to import them



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

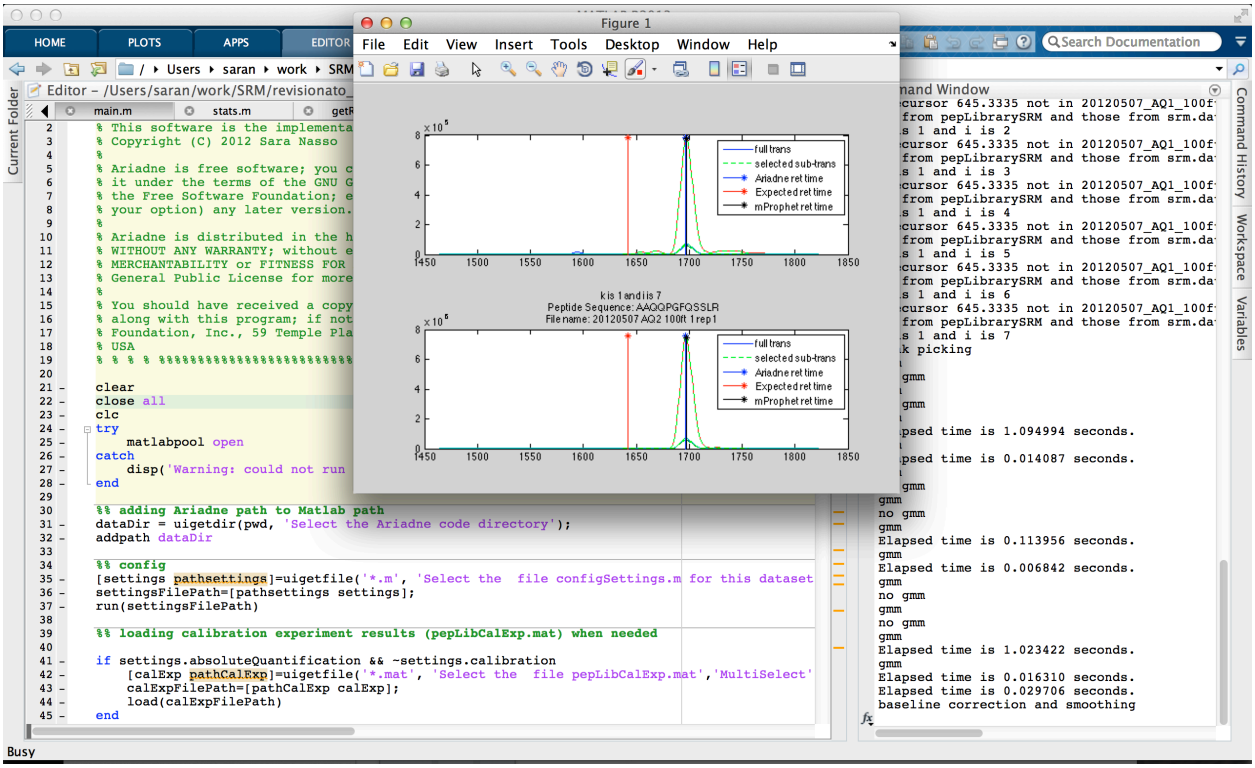


You could also select another .mat data file if necessary



There you go, let it run!

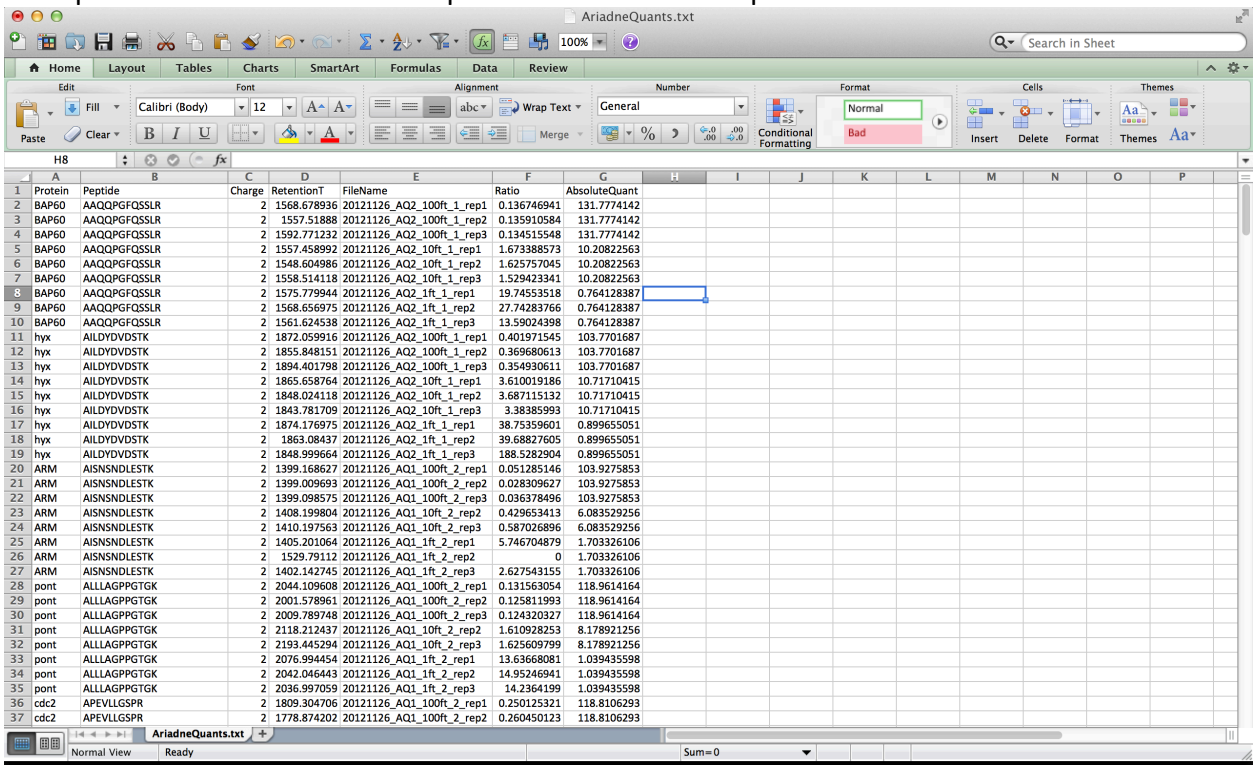
You can roughly estimate the required time as: Time(1pep) x #files x #pep per file



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:

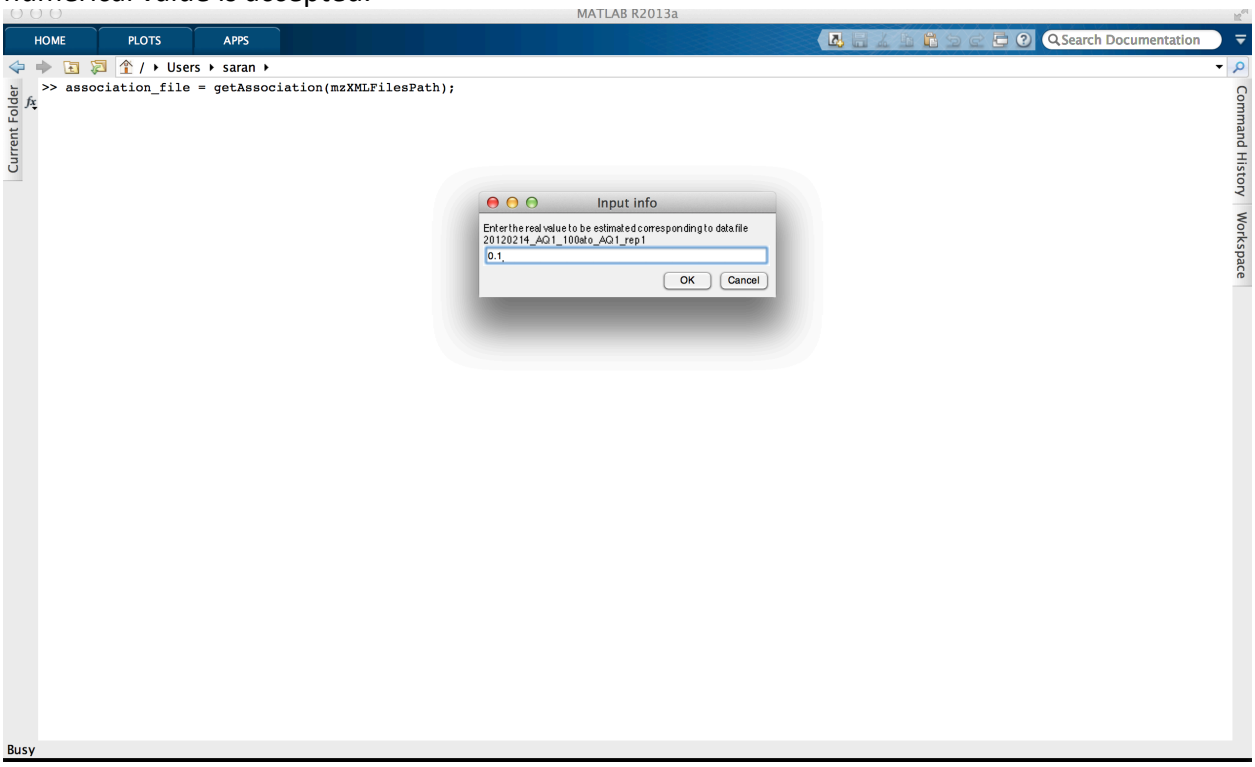


AriadneQuants.txt

Protein	Peptide	Charge	RetentionT	FileName	Ratio	AbsoluteQuant
BAP60	AAQQPGFQSSLR	2	1568.678936	20121126_AQ2_100ft_1_rep1	0.136746941	131.7774142
BAP60	AAQQPGFQSSLR	2	1557.51888	20121126_AQ2_100ft_1_rep2	0.135910584	131.7774142
BAP60	AAQQPGFQSSLR	2	1592.771232	20121126_AQ2_100ft_1_rep3	0.134515548	131.7774142
BAP60	AAQQPGFQSSLR	2	1557.458992	20121126_AQ2_10ft_1_rep1	1.673388573	10.20822563
BAP60	AAQQPGFQSSLR	2	1548.604986	20121126_AQ2_10ft_1_rep2	1.625757045	10.20822563
BAP60	AAQQPGFQSSLR	2	1558.514118	20121126_AQ2_10ft_1_rep3	1.529423341	10.20822563
BAP60	AAQQPGFQSSLR	2	1575.779944	20121126_AQ2_1ft_1_rep1	19.74553518	0.764128387
BAP60	AAQQPGFQSSLR	2	1568.656975	20121126_AQ2_1ft_1_rep2	27.74283766	0.764128387
BAP60	AAQQPGFQSSLR	2	1561.624538	20121126_AQ2_1ft_1_rep3	13.59024398	0.764128387
hyx	AILDYDVDSTK	2	1872.059916	20121126_AQ2_100ft_1_rep1	0.401971545	103.7701687
hyx	AILDYDVDSTK	2	1855.848151	20121126_AQ2_100ft_1_rep2	0.369680613	103.7701687
hyx	AILDYDVDSTK	2	1894.401798	20121126_AQ2_100ft_1_rep3	0.354930611	103.7701687
hyx	AILDYDVDSTK	2	1865.658764	20121126_AQ2_10ft_1_rep1	3.610019186	10.71710415
hyx	AILDYDVDSTK	2	1848.024118	20121126_AQ2_10ft_1_rep2	3.687115132	10.71710415
hyx	AILDYDVDSTK	2	1843.781709	20121126_AQ2_10ft_1_rep3	3.38385993	10.71710415
hyx	AILDYDVDSTK	2	1874.176975	20121126_AQ2_1ft_1_rep1	38.75359601	0.899655051
hyx	AILDYDVDSTK	2	1863.08437	20121126_AQ2_1ft_1_rep2	39.68827605	0.899655051
hyx	AILDYDVDSTK	2	1848.999664	20121126_AQ2_1ft_1_rep3	188.5282904	0.899655051
ARM	AISNSNDLESTK	2	1399.168627	20121126_AQ1_100ft_2_rep1	0.051285146	103.9275853
ARM	AISNSNDLESTK	2	1399.009693	20121126_AQ1_100ft_2_rep2	0.028309627	103.9275853
ARM	AISNSNDLESTK	2	1399.098575	20121126_AQ1_100ft_2_rep3	0.036378496	103.9275853
ARM	AISNSNDLESTK	2	1408.199804	20121126_AQ1_10ft_2_rep2	0.429653413	6.083529256
ARM	AISNSNDLESTK	2	1410.197563	20121126_AQ1_10ft_2_rep3	0.587026896	6.083529256
ARM	AISNSNDLESTK	2	1405.201064	20121126_AQ1_1ft_2_rep1	5.746704879	1.703326106
ARM	AISNSNDLESTK	2	1529.79112	20121126_AQ1_1ft_2_rep2	0	1.703326106
ARM	AISNSNDLESTK	2	1402.142745	20121126_AQ1_1ft_2_rep3	2.627543155	1.703326106
pont	ALLLAGPPGTGK	2	2044.109608	20121126_AQ1_100ft_2_rep1	0.131563054	118.9614164
pont	ALLLAGPPGTGK	2	2001.578961	20121126_AQ1_100ft_2_rep2	0.125811993	118.9614164
pont	ALLLAGPPGTGK	2	2009.789748	20121126_AQ1_100ft_2_rep3	0.124320327	118.9614164
pont	ALLLAGPPGTGK	2	2118.212437	20121126_AQ1_10ft_2_rep2	1.610928253	8.178921256
pont	ALLLAGPPGTGK	2	2193.445294	20121126_AQ1_10ft_2_rep3	1.625609799	8.178921256
pont	ALLLAGPPGTGK	2	2076.994454	20121126_AQ1_1ft_2_rep1	13.63668081	1.039435598
pont	ALLLAGPPGTGK	2	2042.046443	20121126_AQ1_1ft_2_rep2	14.95246941	1.039435598
pont	ALLLAGPPGTGK	2	2036.997059	20121126_AQ1_1ft_2_rep3	14.2364199	1.039435598
cdc2	APEVLLGSPR	2	1809.304706	20121126_AQ1_100ft_2_rep1	0.250125321	118.8106293
cdc2	APEVLLGSPR	2	1778.874202	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.

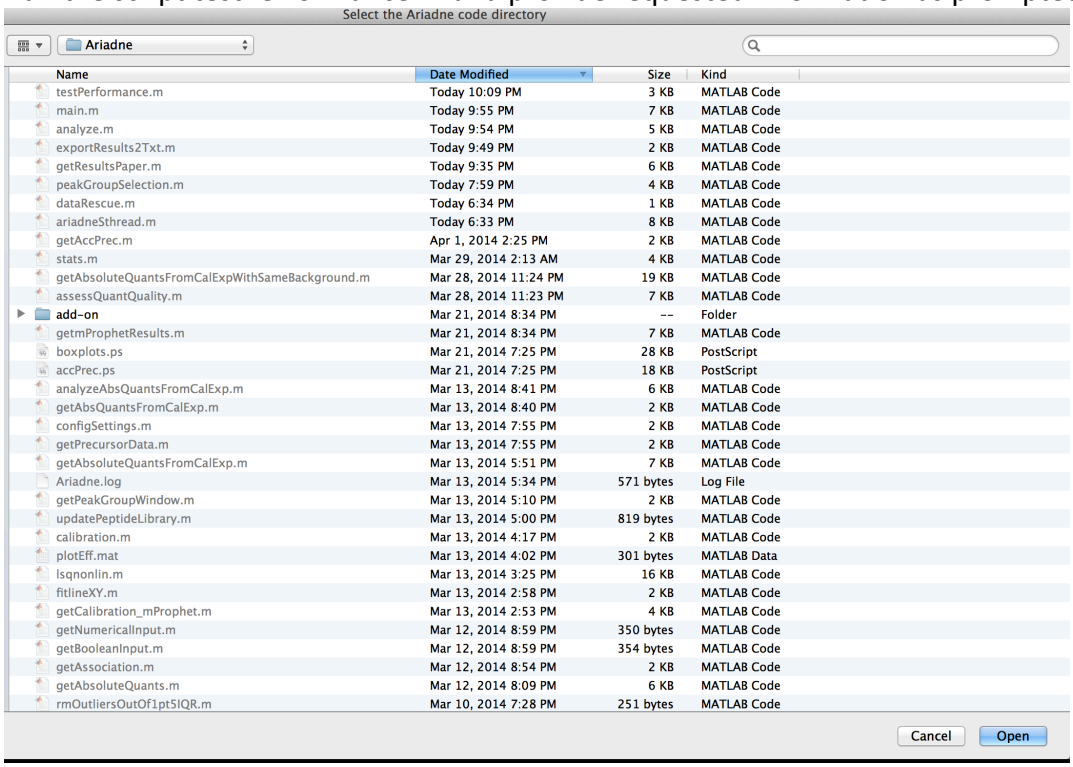


Testing the performance/ Reproducing published results

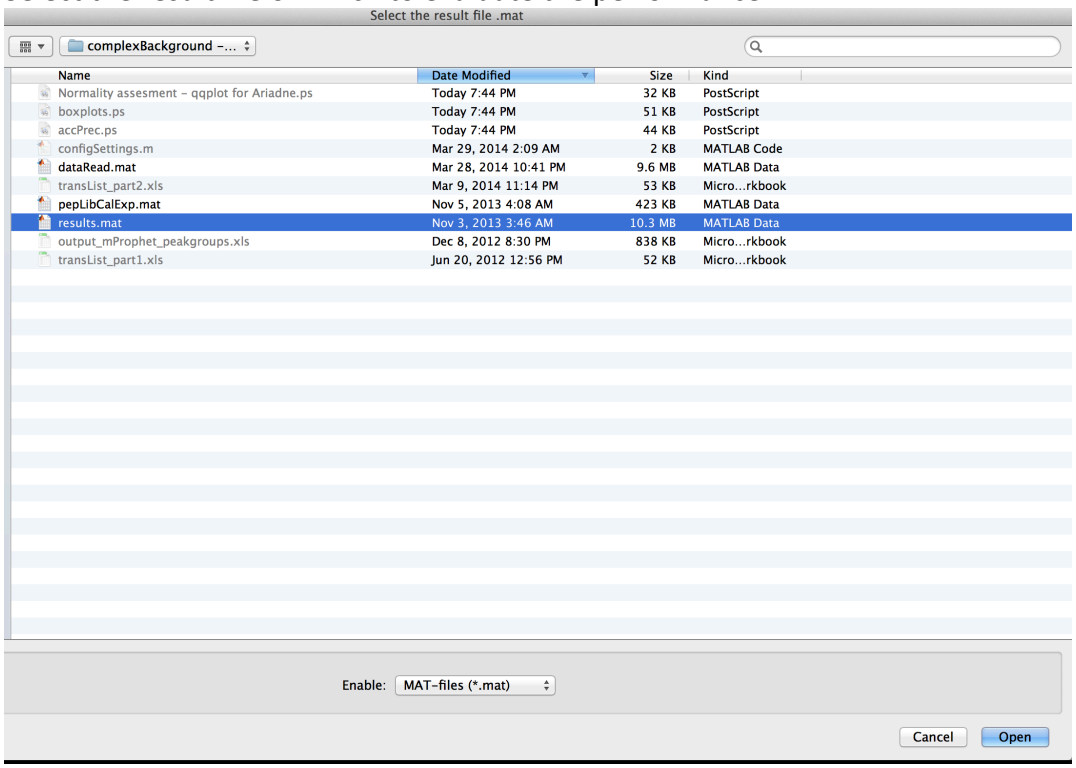
If comparing to mProphet or Skyline please refer to the corresponding Ariadne code package and accompanying data folder that would be better placed inside the code folder. Next releases will only integrate with Skyline and support the comparison to Skyline as it already implements the mProphet package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

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

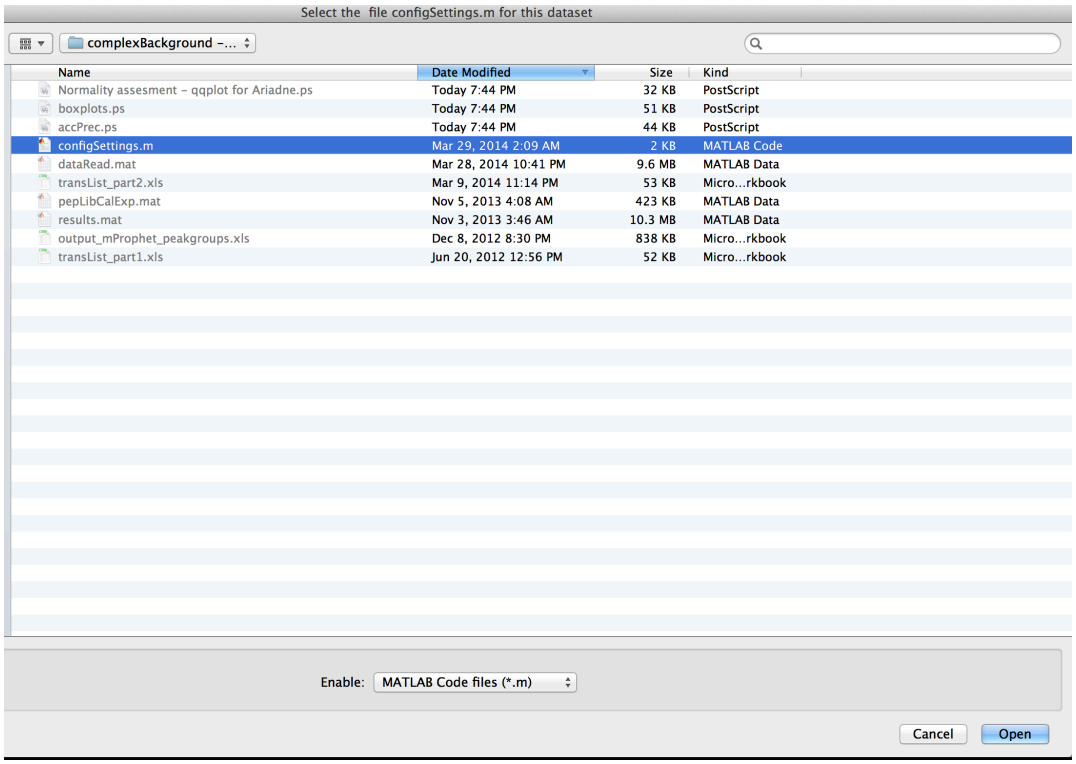
Run the script testPerformance.m and provide requested information as prompted.



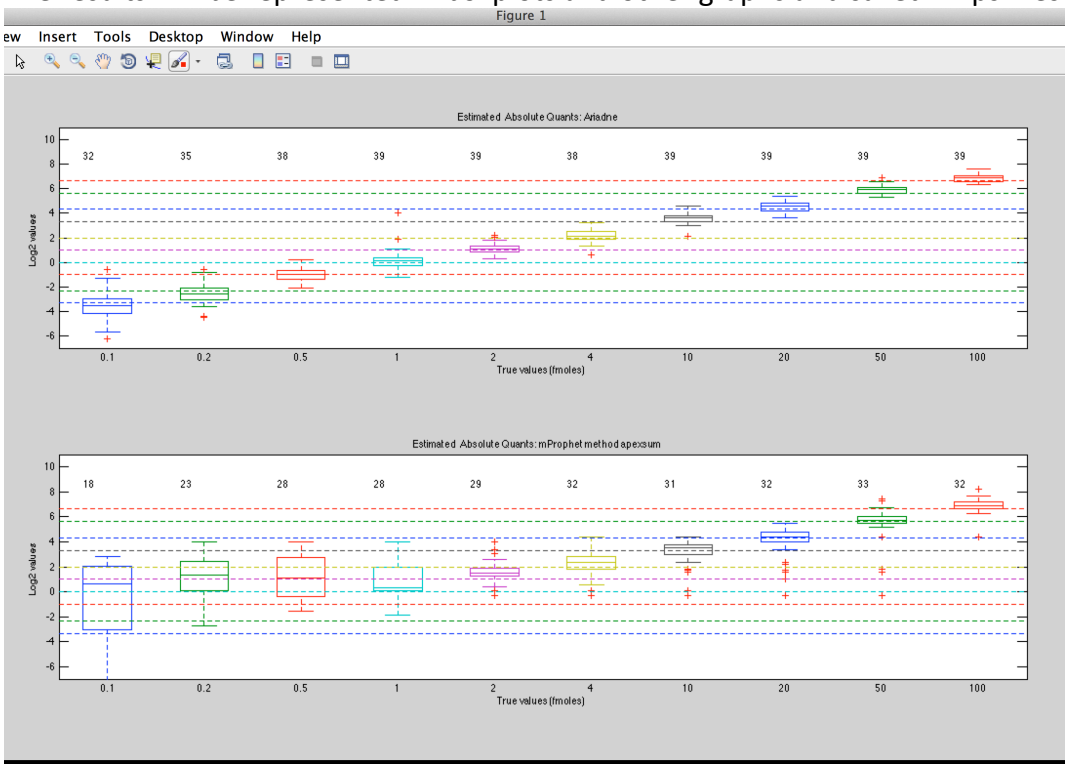
Select the result file of which to evaluate the performance:



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

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