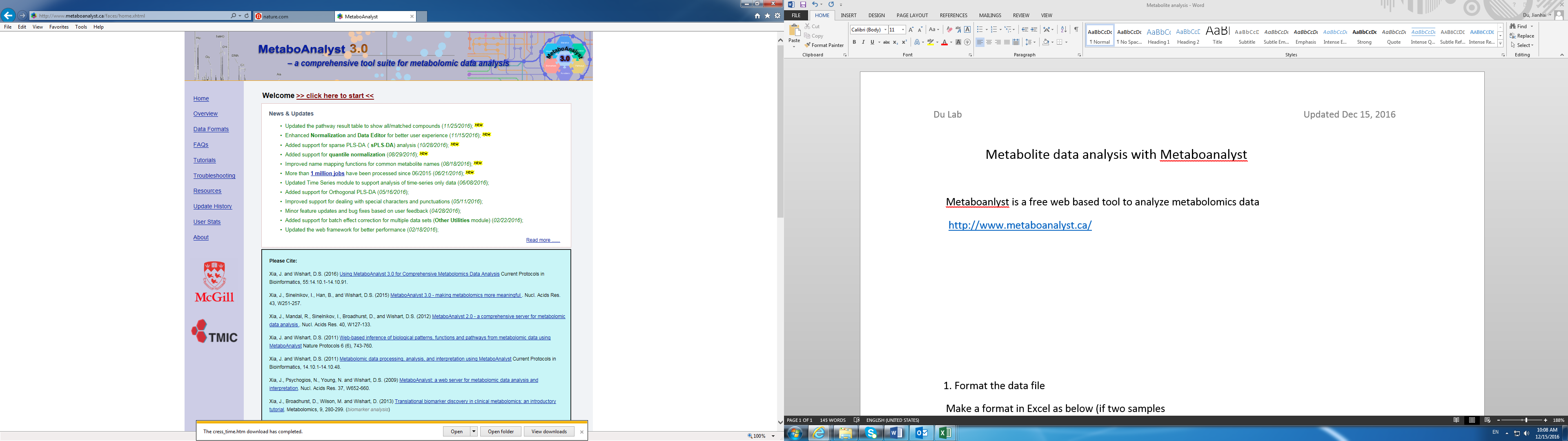
Metabolite data analysis with Metaboanalyst

Metaboanlyst is a free web based tool to analyze metabolomics data

<http://www.metaboanalyst.ca/>



There are more resources on the website in the left side.

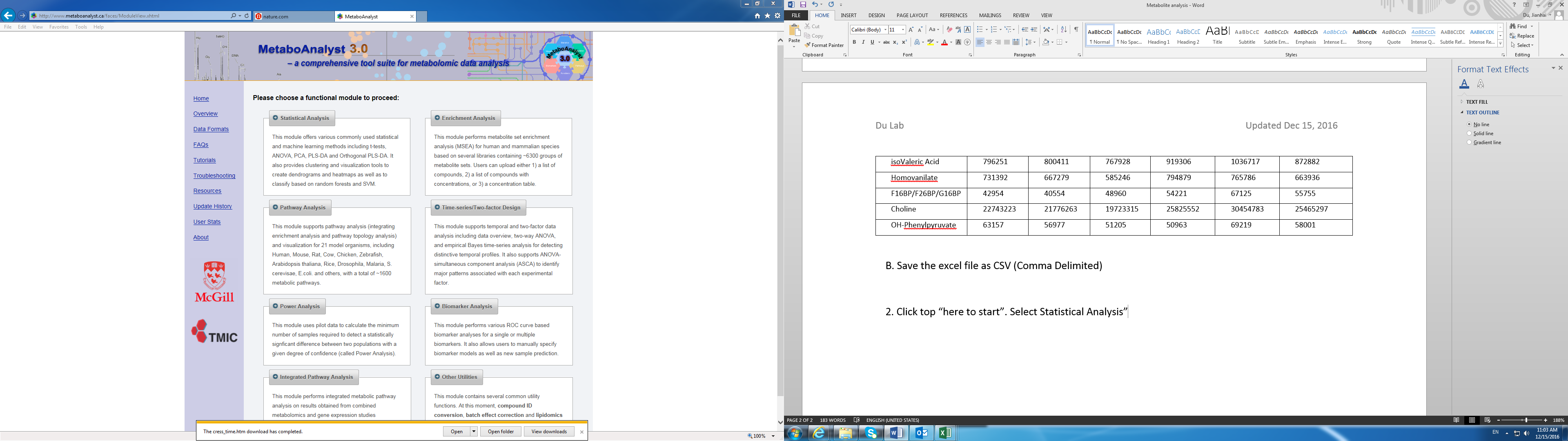
1. Format the data file

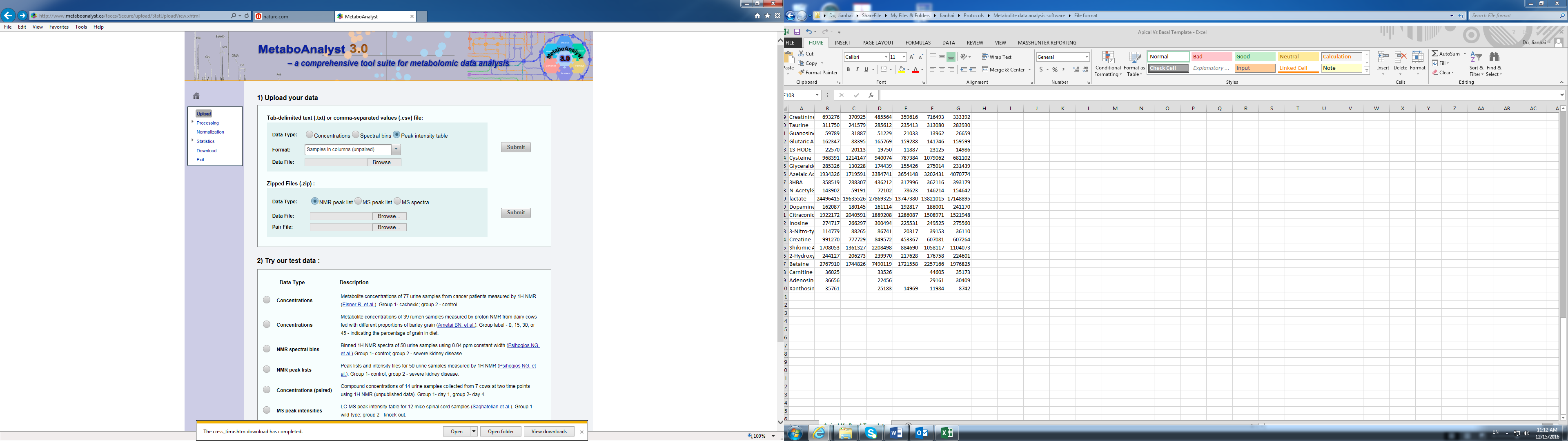
A. Make a format in Excel as below (if two groups). Here there are two groups (Apical and Basal)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sample** | **M1 1A** | **M1 2A** | **M1 3A** | **M1 1B** | **M1 2B** | **M1 3B** |
| **Label** | **Apical** | **Apical** | **Apical** | **Basal** | **Basal** | **Basal** |
| Proline | 59844441 | 33791551 | 23474213 | 119517656 | 136735841 | 128762485 |
| Allantoin | 19858 | 34695 | 29799 | 71271 | 62978 | 48100 |
| 4-Hydroxybutyrate | 2185475 | 1986435 | 2820447 | 3893676 | 2066648 | 3473576 |
| Ribose-5-P | 167070 | 197278 | 139778 | 195885 | 206918 | 130071 |
| Acetylcarnitine | 48707 | 62685 | 56021 | 51924 | 26663 | 41485 |
| Homoserine | 100250 | 102629 | 112778 | 151527 | 166205 | 156264 |
| Folic Acid | 15674 | 10762 | 15763 | 10833 | 21809 | 11802 |
| Arachidonate | 61729 | 66610 | 73376 | 79207 | 68003 | 54012 |
| isoValeric Acid | 796251 | 800411 | 767928 | 919306 | 1036717 | 872882 |
| Homovanilate | 731392 | 667279 | 585246 | 794879 | 765786 | 663936 |
| F16BP/F26BP/G16BP | 42954 | 40554 | 48960 | 54221 | 67125 | 55755 |
| Choline | 22743223 | 21776263 | 19723315 | 25825552 | 30454783 | 25465297 |
| OH-Phenylpyruvate | 63157 | 56977 | 51205 | 50963 | 69219 | 58001 |

B. Save the excel file as CSV (Comma Delimited)

2. Click top “here to start”. Select Statistical Analysis”

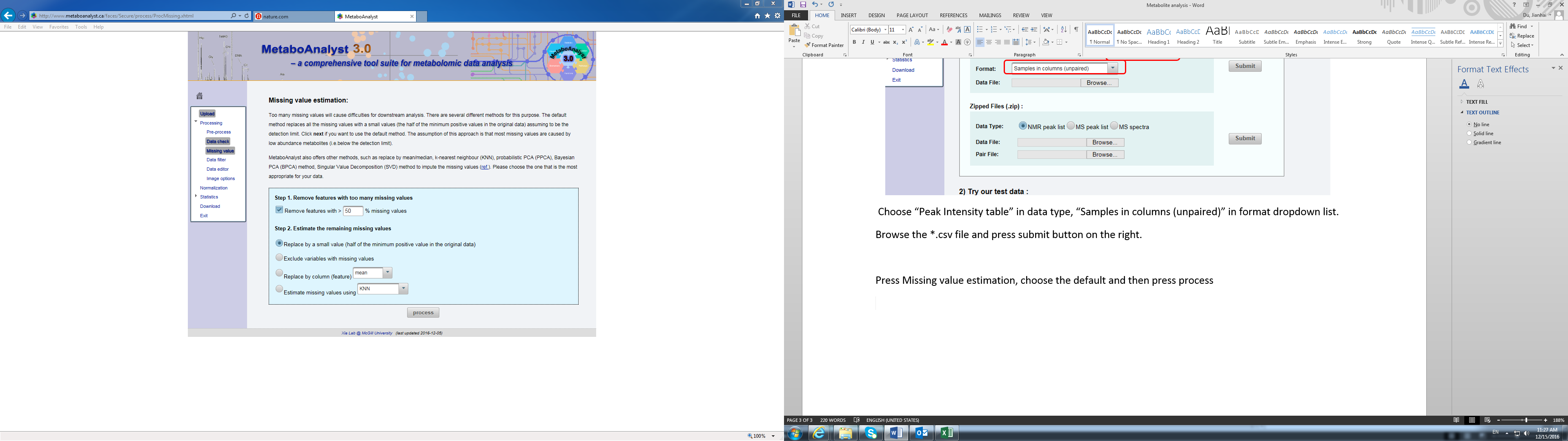


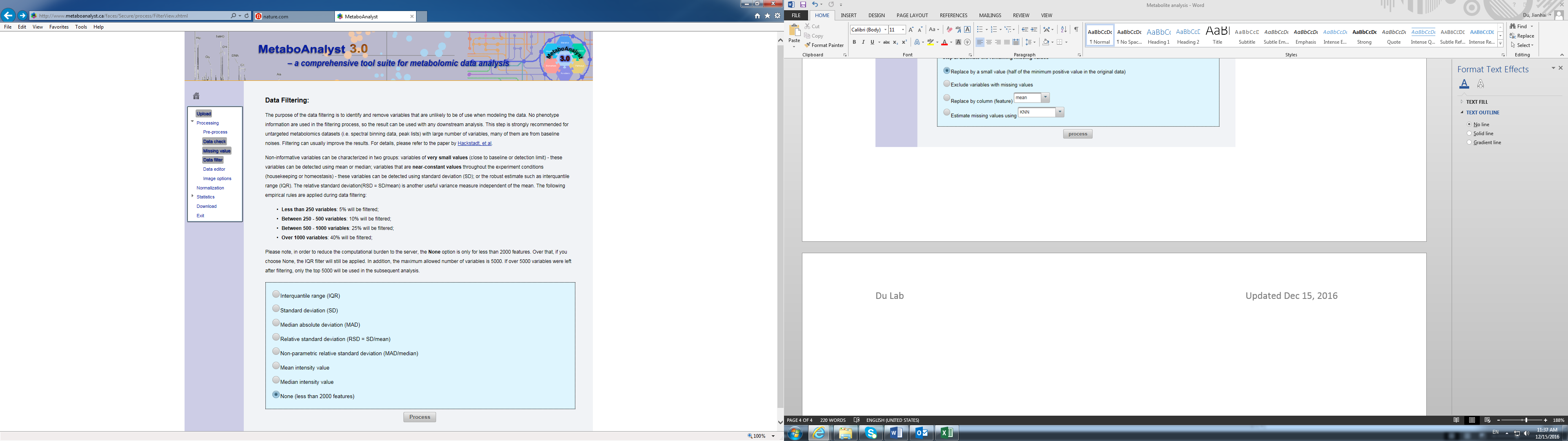


Choose “Peak Intensity table” in data type, “Samples in columns (unpaired)” in format dropdown list.

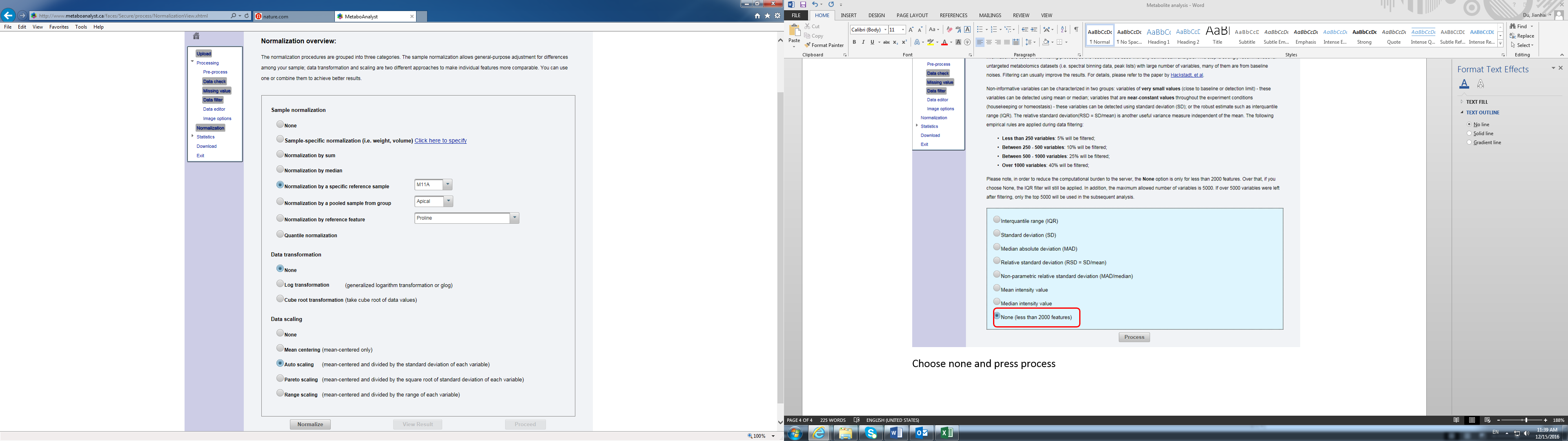
Browse the \*.csv file and press submit button on the right.

Press Missing value estimation, choose the default and then press process





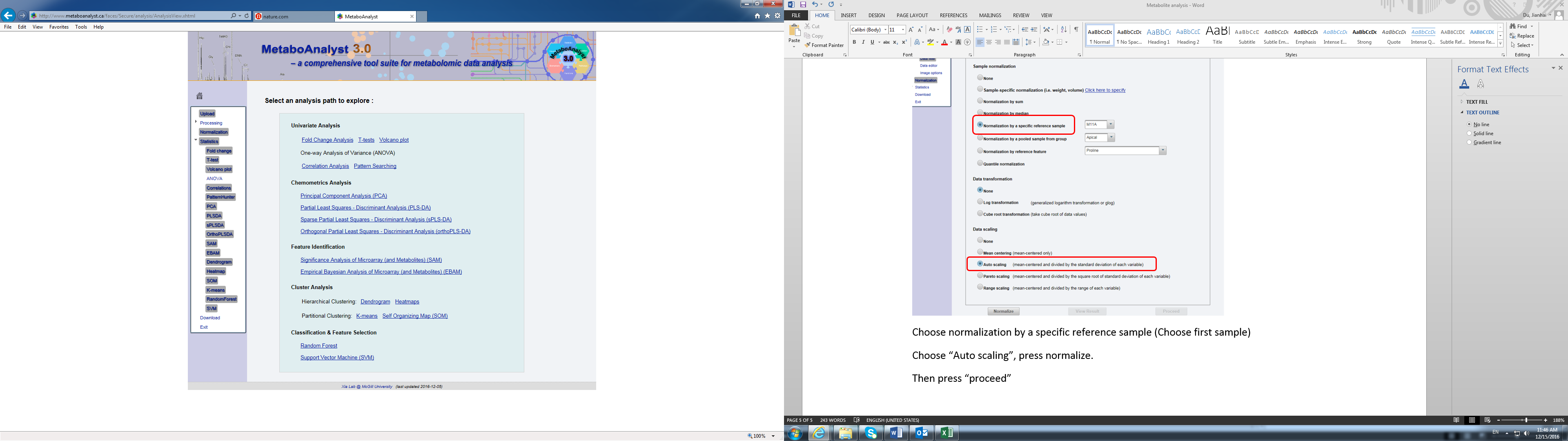
Choose none and press process



Choose normalization by a specific reference sample (Choose first sample)

Choose “Auto scaling”, press normalize.

Then press “proceed”



Press the option on the left for “fold change, T test, PCA, PLSDA and look at the imp. Feature, correlation. Finally, press download to download .zip for all the report.

Press “upload” on the left top and go the home page. For enrichment and pathway analysis, just paste the changes in T test