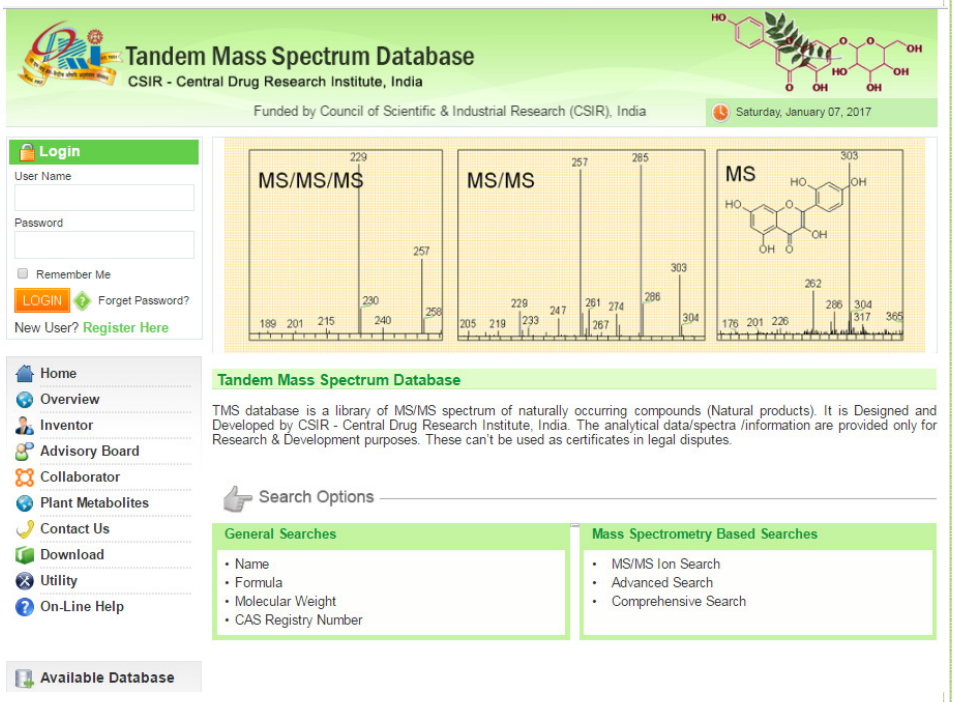
2017

Data File Format Conversion



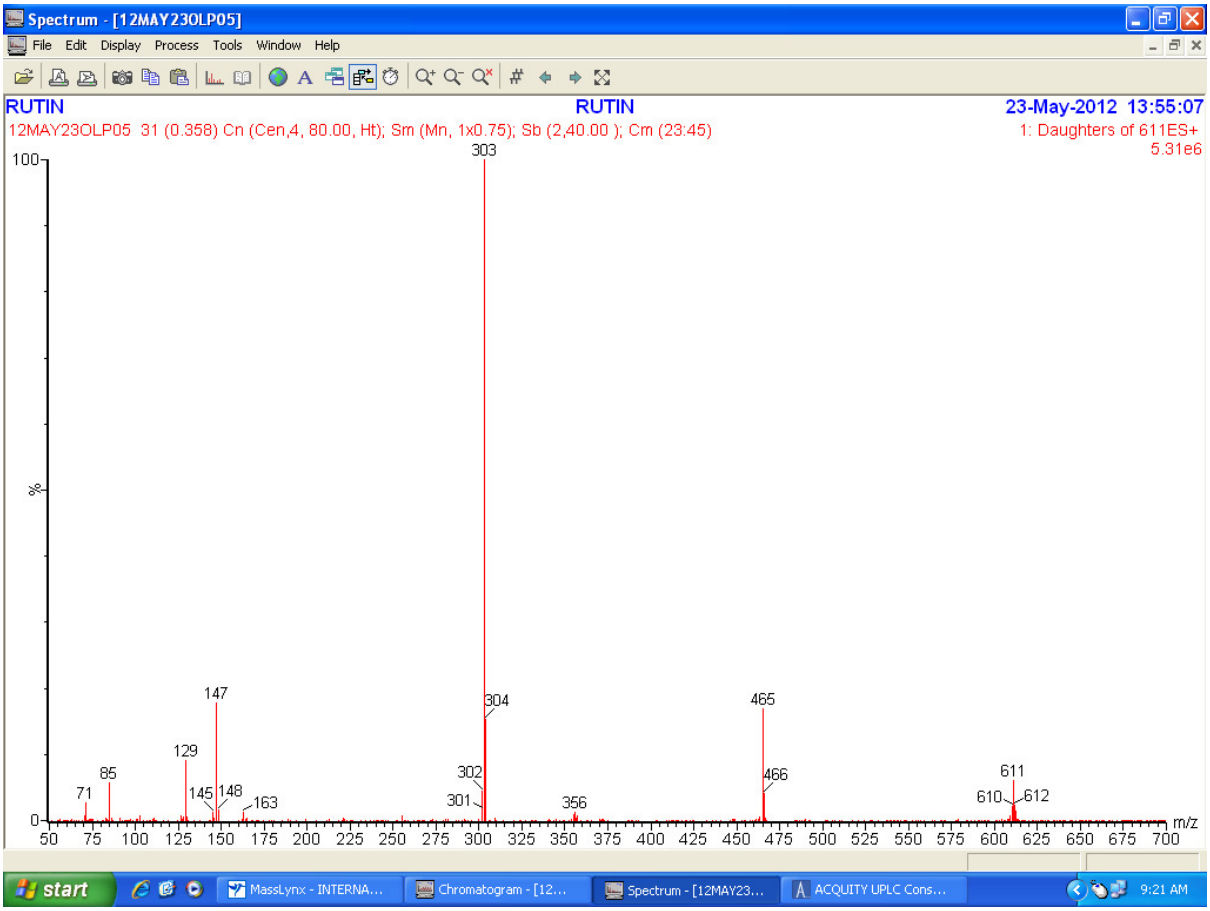
www.tmsdatabase.org

1/7/2017

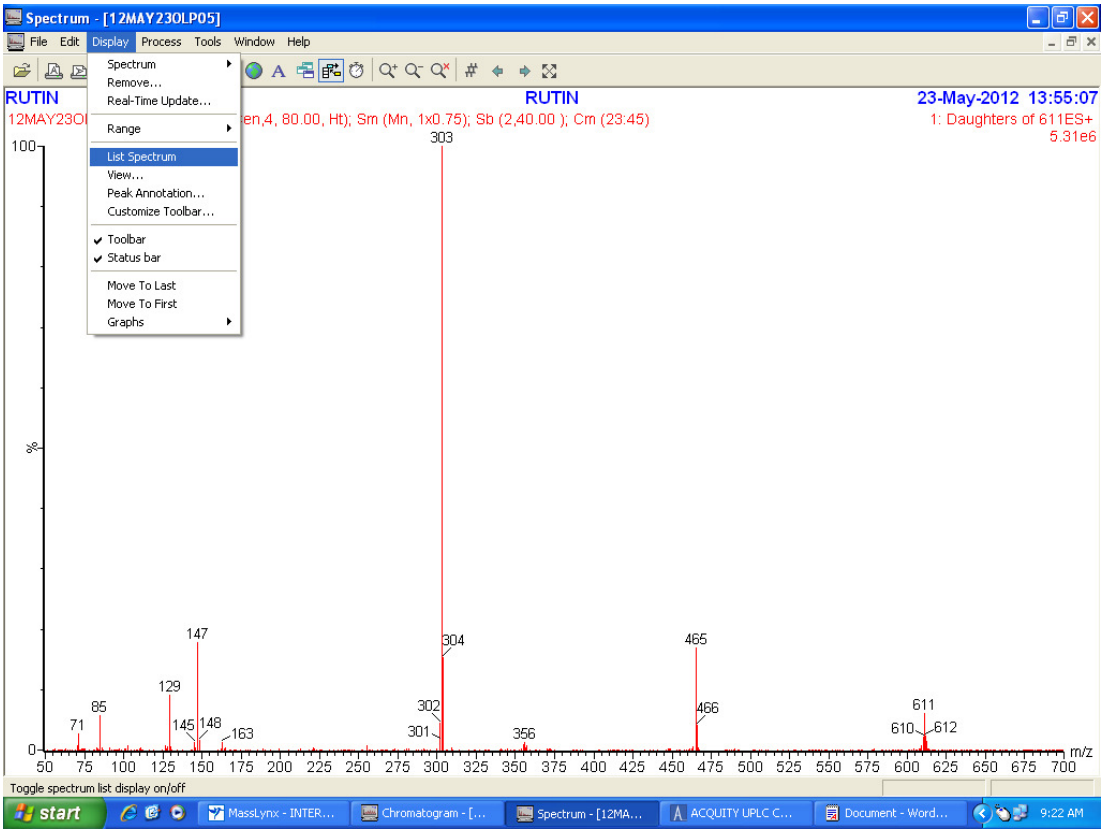
How to convert MS/MS spectrum to tms data format

1. **By the Waters MassLynx software**
   http://www.waters.com/waters/en_IN/MassLynx-Mass-Spectrometry-Software-/nav.htm?cid=513164&locale=en_IN

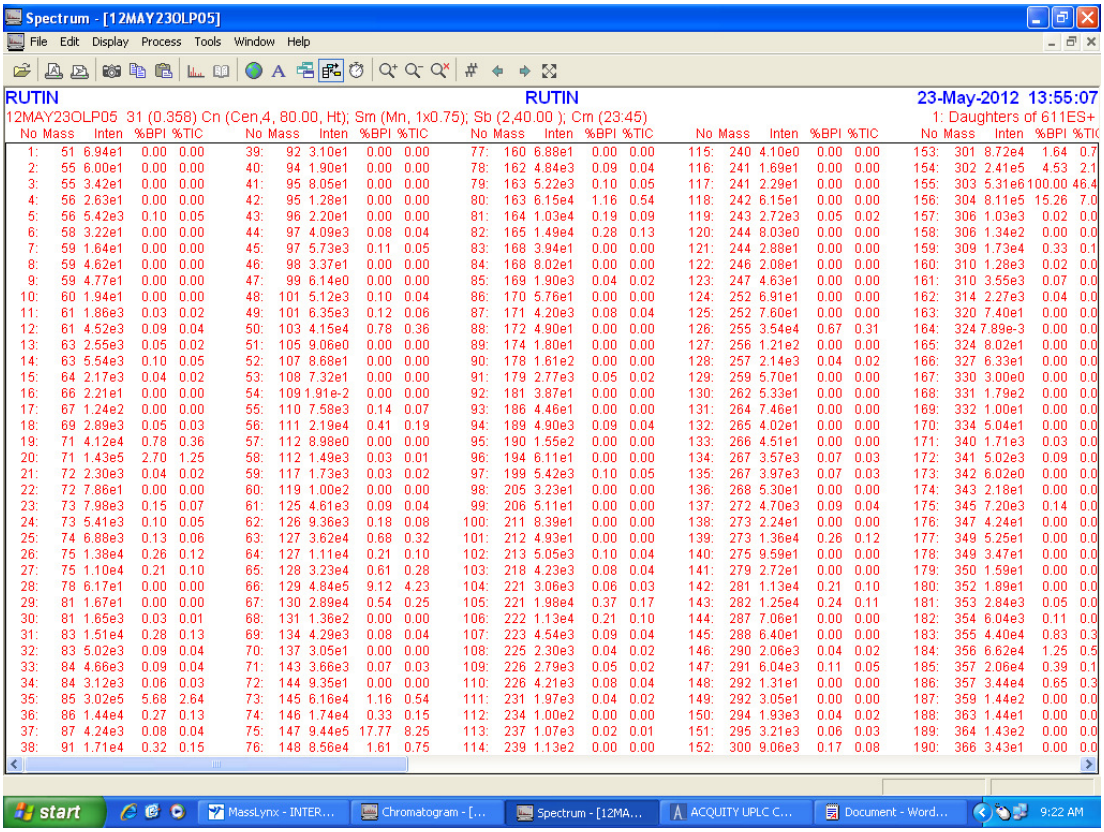
Open the MS/MS spectrum



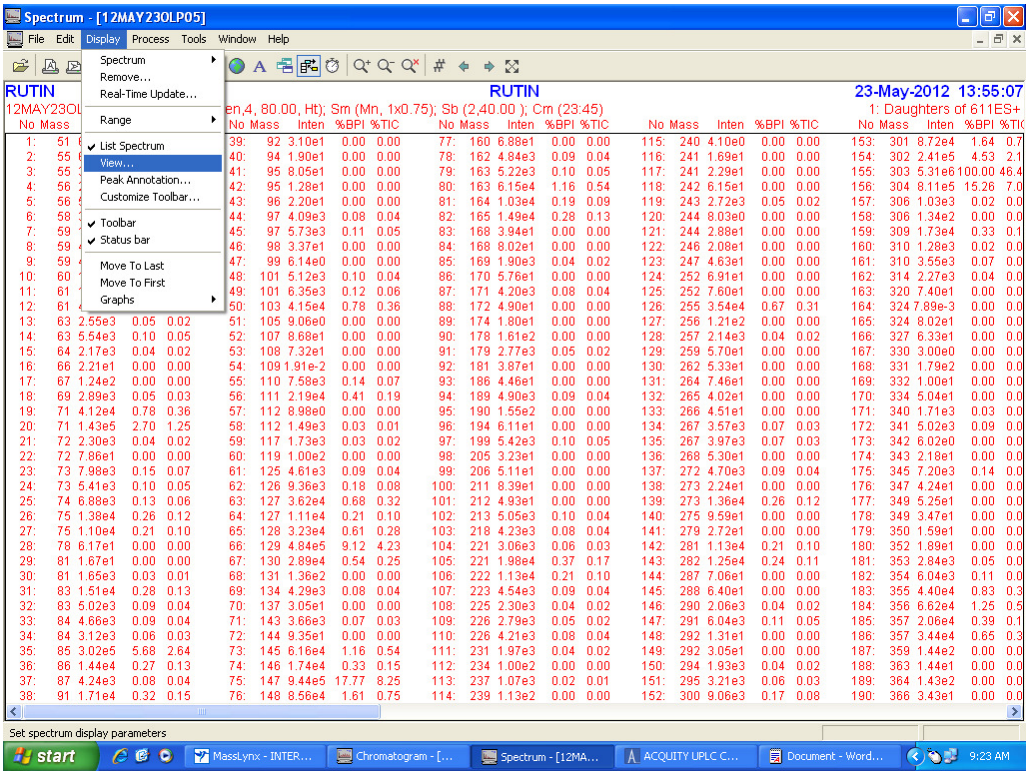
Go to display



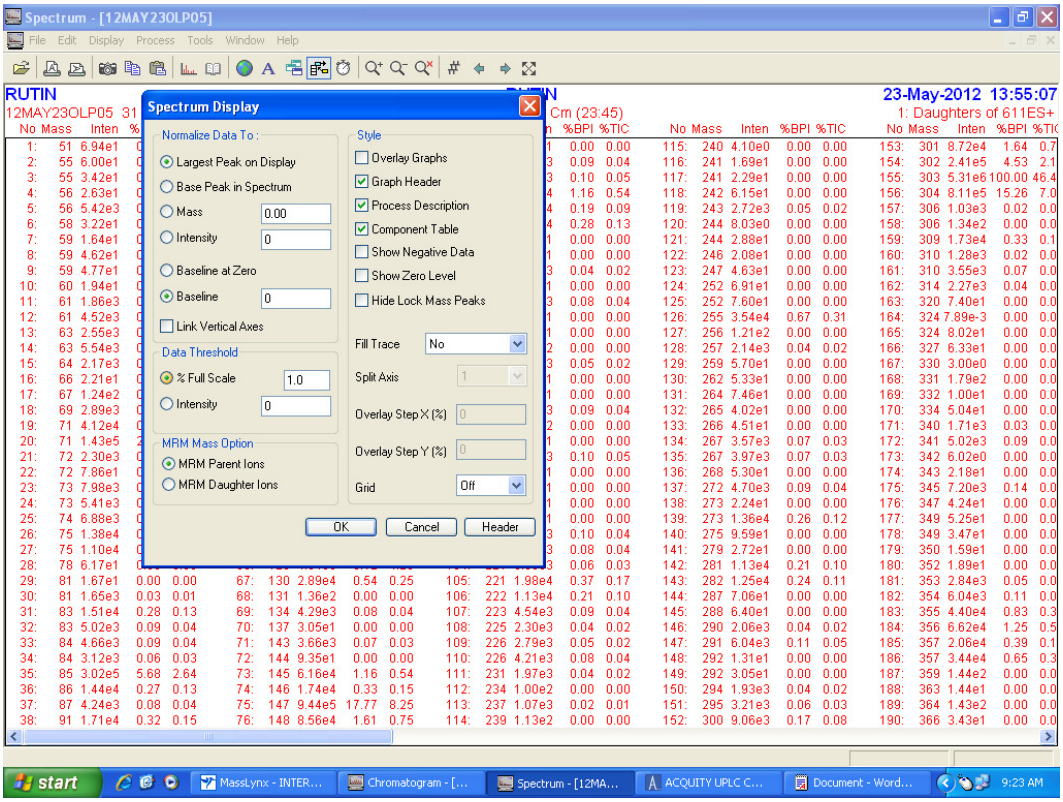
Select list spectrum



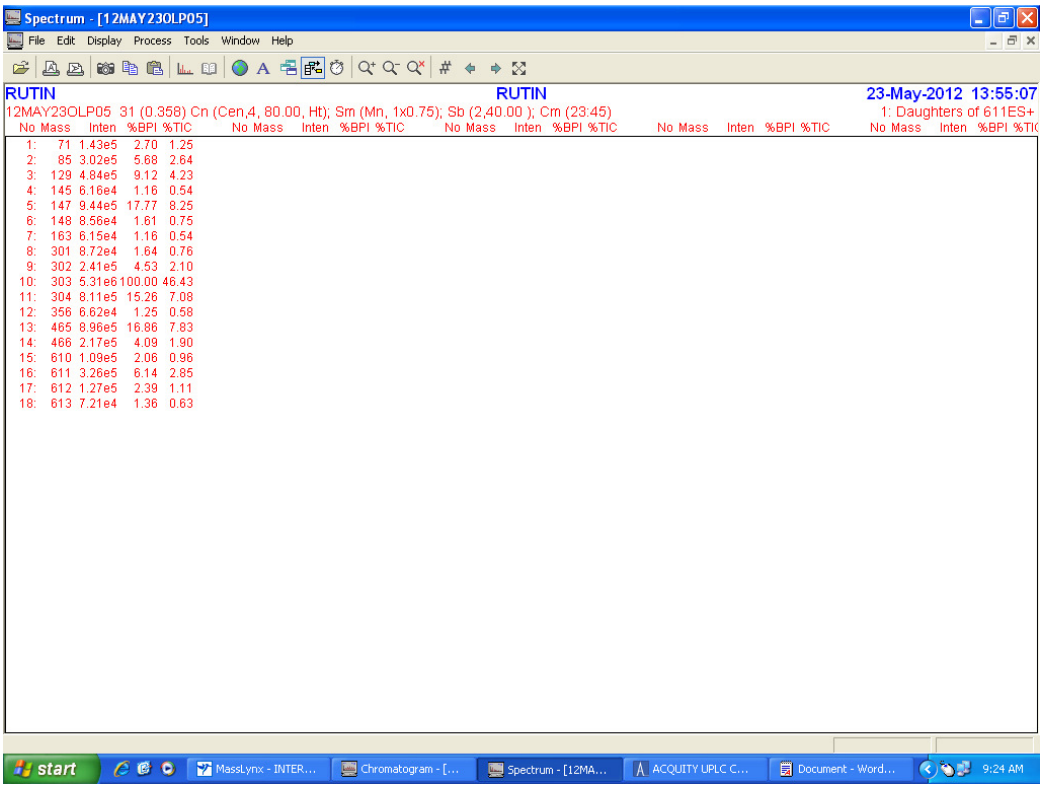
Select view



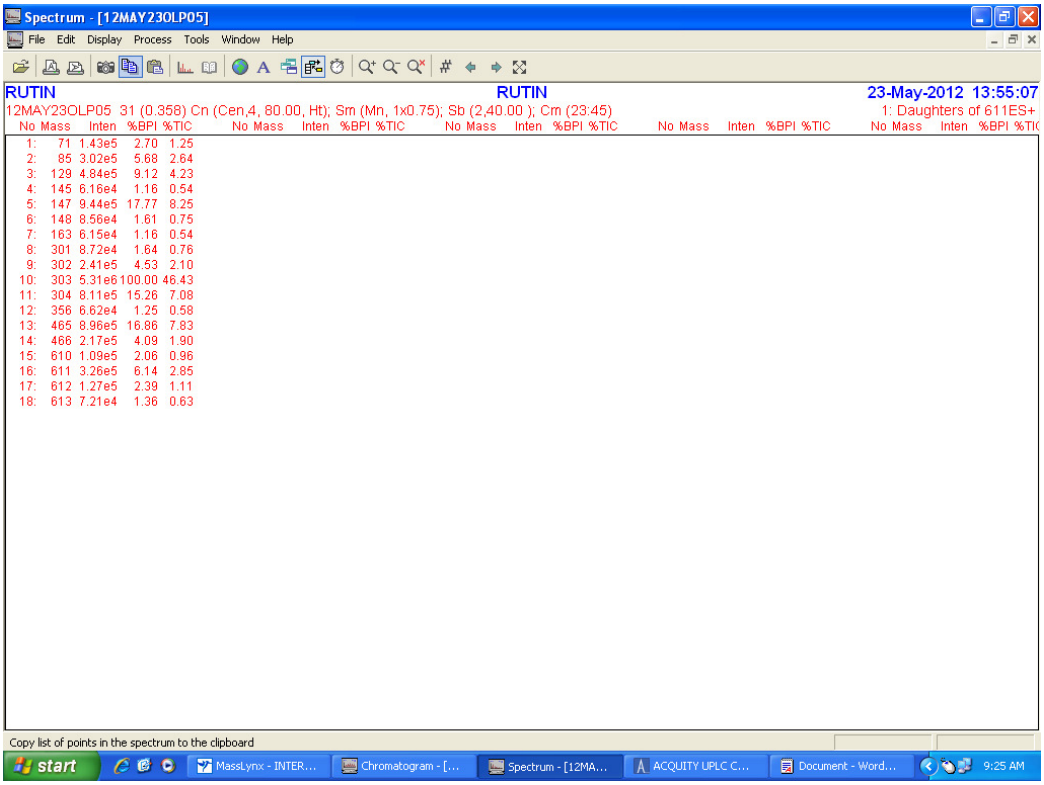
Set data threshold 1-2% (for significant peak)



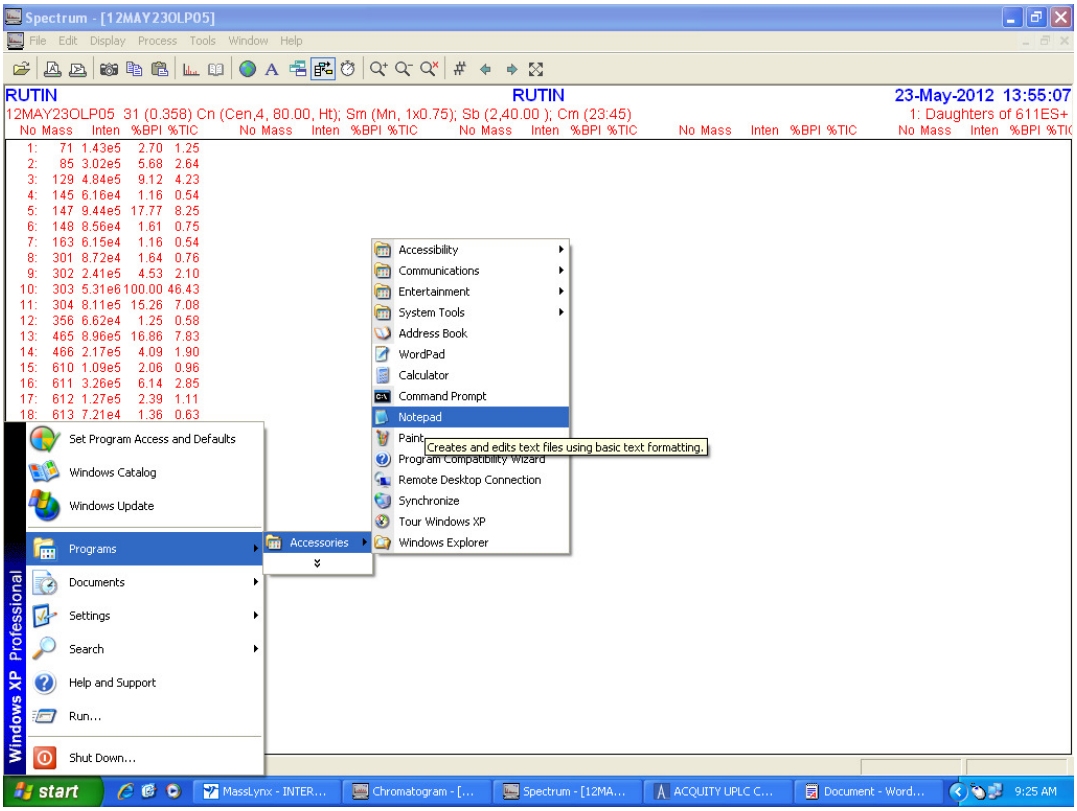
Press ok (list out major 25-30 peaks, if available)



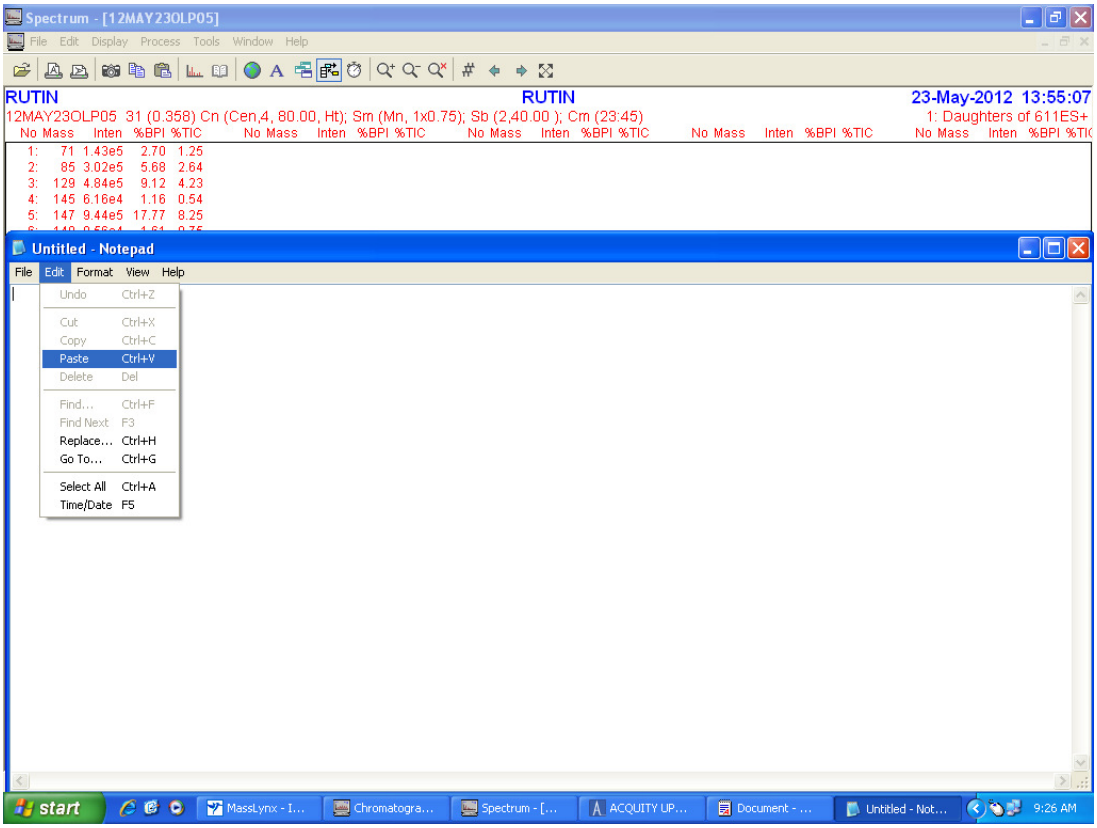
Copy the list of ions



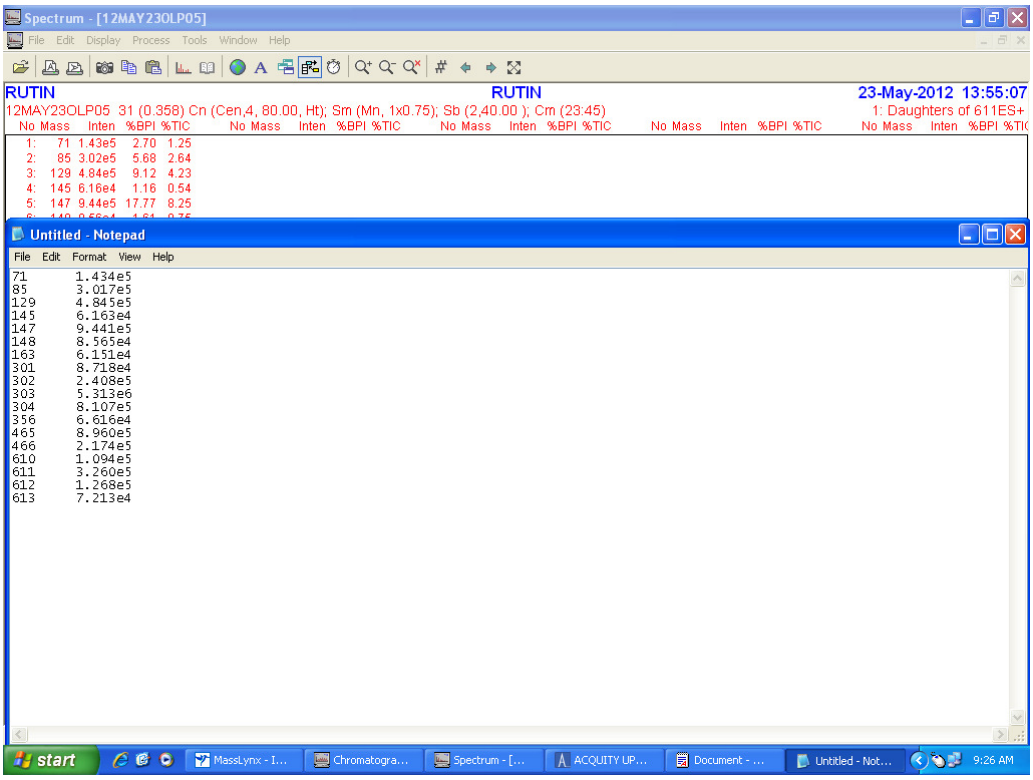
Open note pad



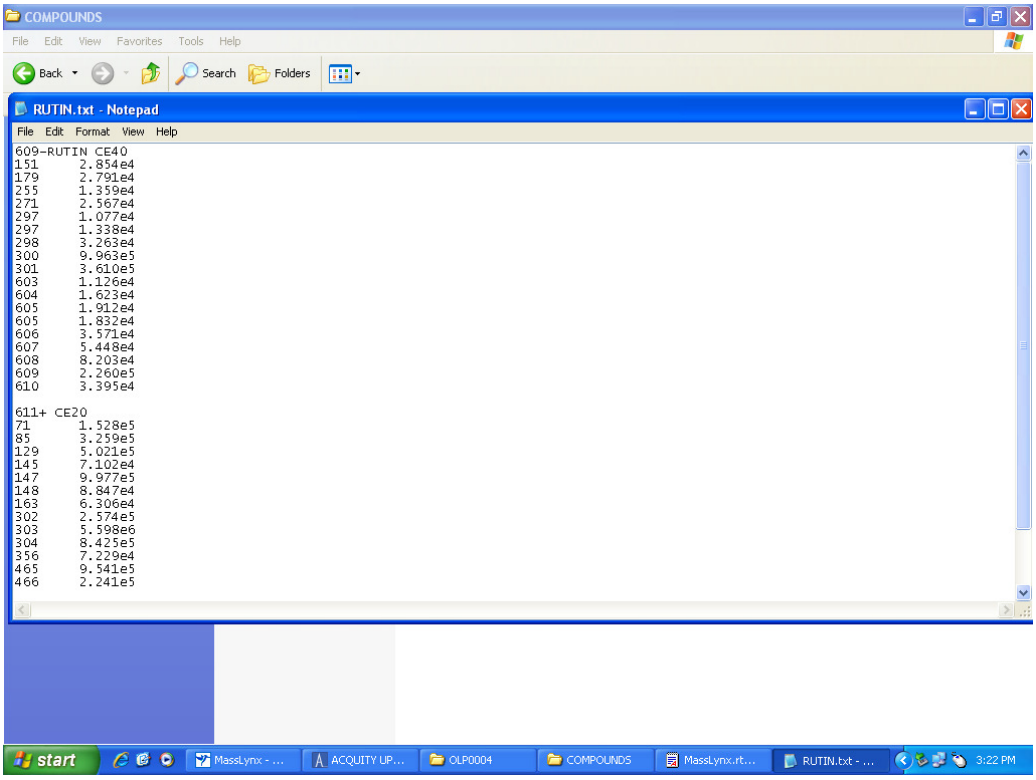
Paste the ions list on note pad



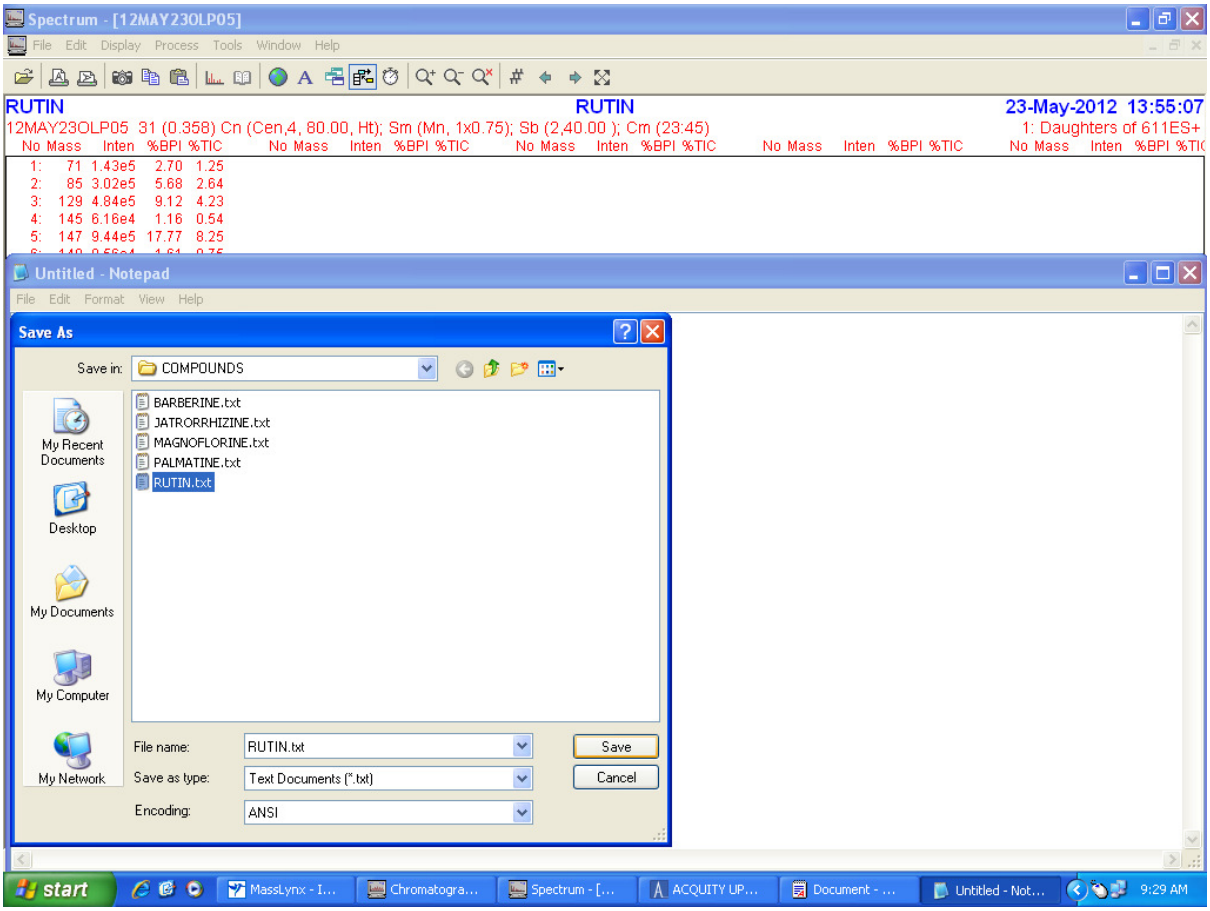
List of ions on note pad



Edit the note pad file with precursor ion value, charge state and collision energy as given below (611+ CE 20) or (609 – CE 40)

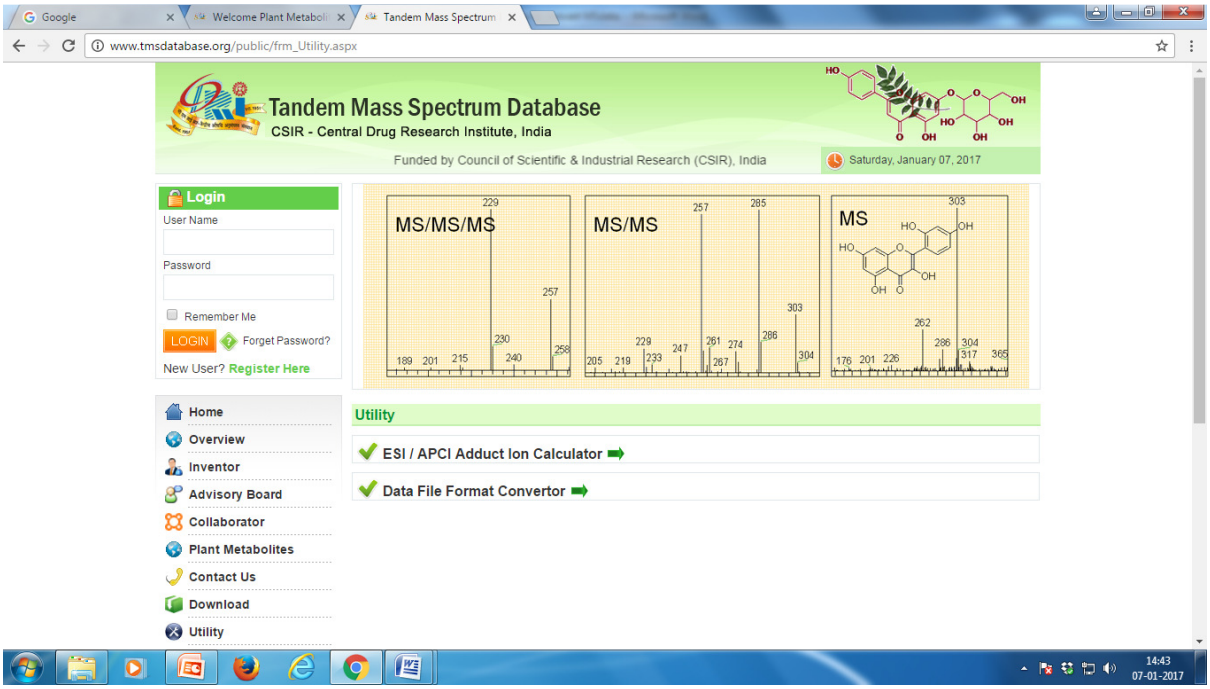


Save the note pad file in *.txt format

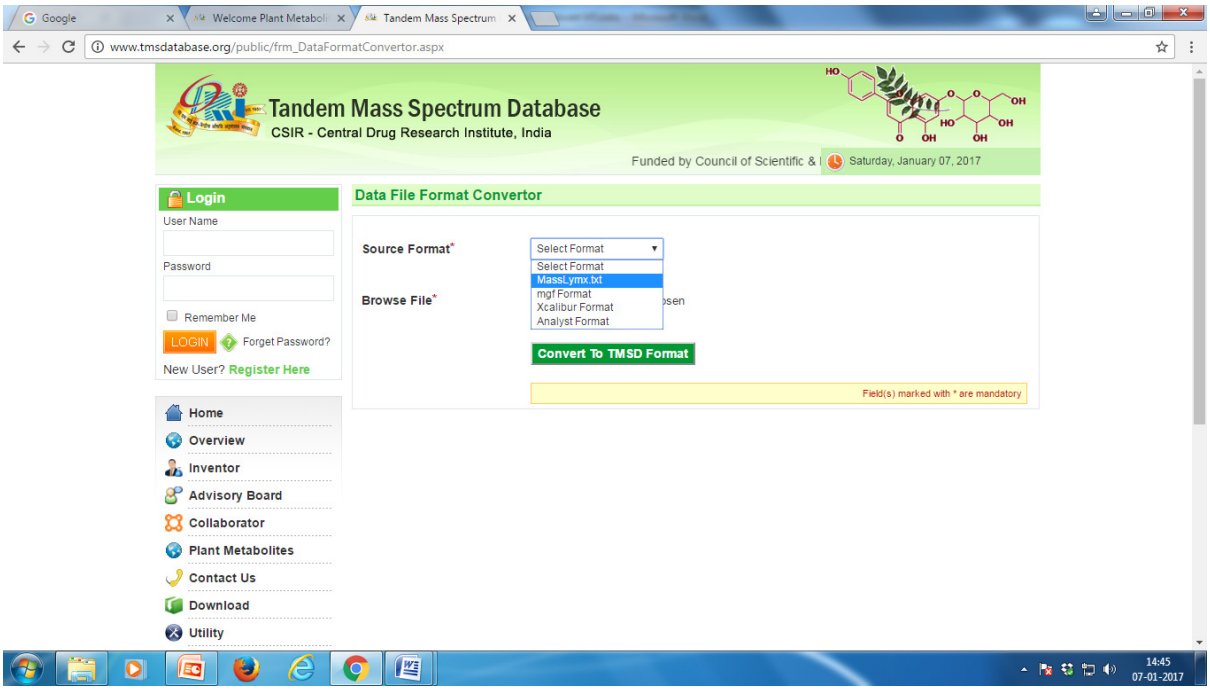


Go to the www.tmsdatabase.org select utility section

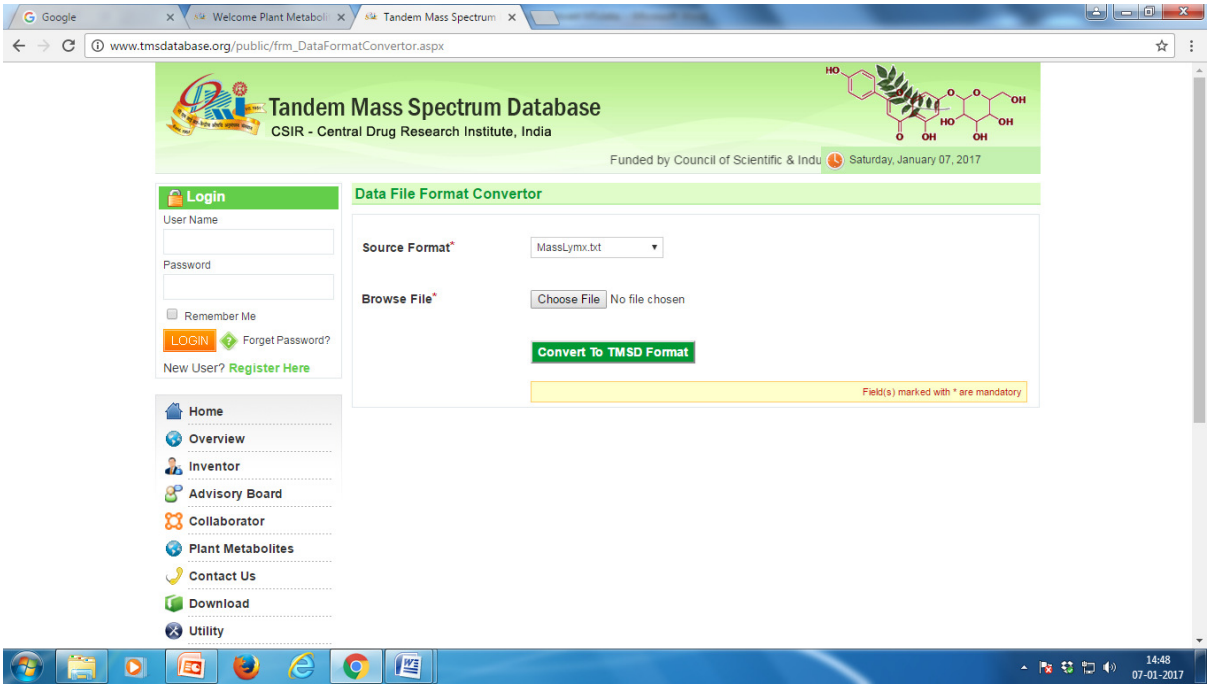
http://www.tmsdatabase.org/public/frm_Utility.aspx



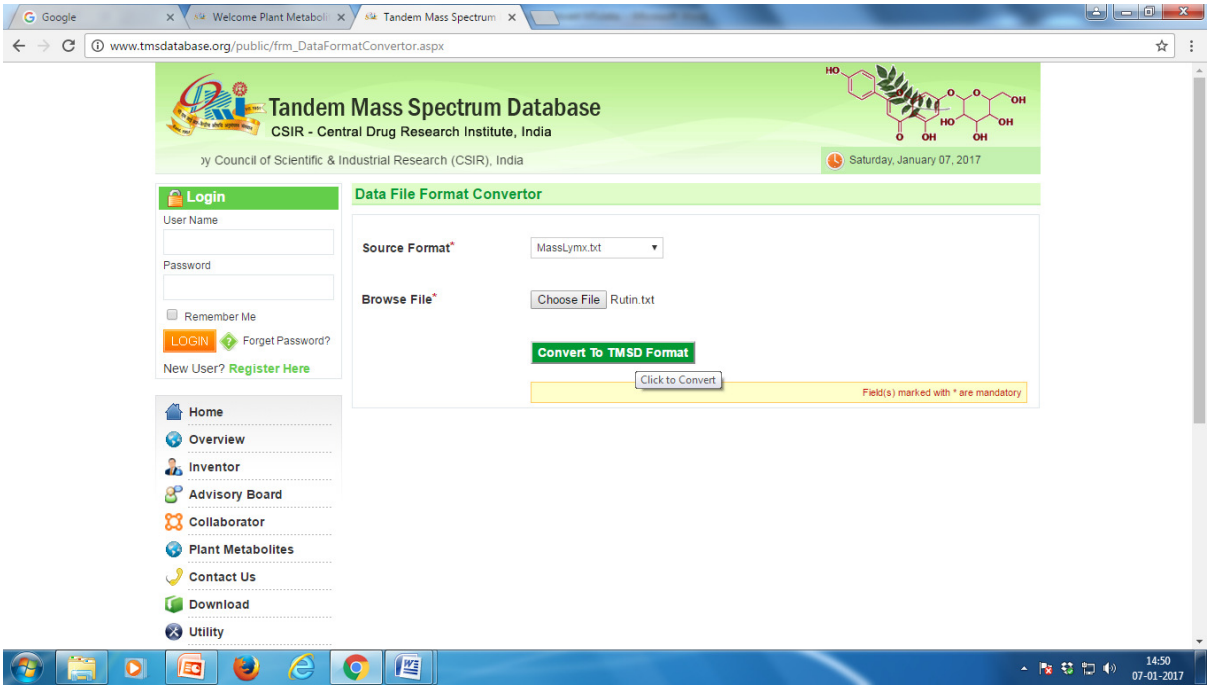
Click on data file format converter and select MassLynx.txt format



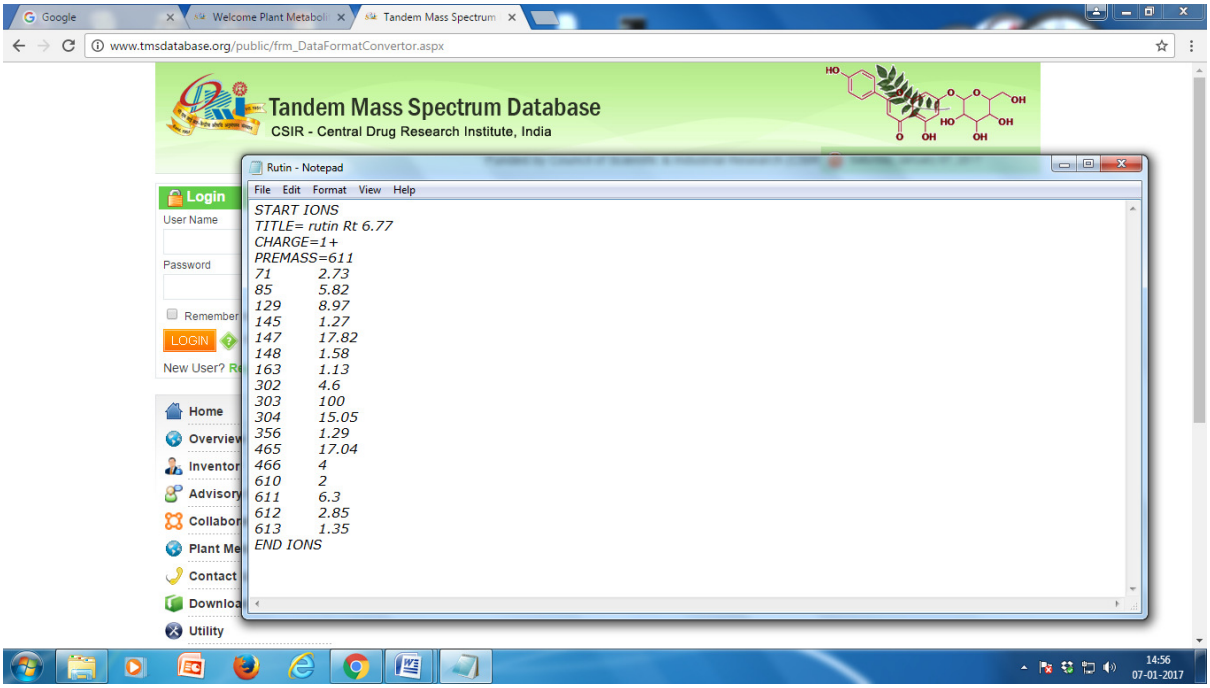
Choose /browse note pad *.txt file



Click to convert to tmsd format



File will open as tmsd format in *.txt format



Script with

START IONS
TITLE =
CHARGE = 1+
PREMASS = 611

71	2.73
85	5.82
129	8.97
145	1.27
147	17.82
148	1.58
163	1.13
302	4.6
303	100
304	15.05
356	1.29
465	17.04
466	4
610	2
611	6.3
612	2.85
613	1.35

END IONS

Note:

1. **Tmsd file format can be made by direct MS/MS spectrum also as script shown above.**
2. **Multiple scripts can be generated through this method.**