


2017

Data File Format Conversion

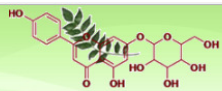


Tandem Mass Spectrum Database

CSIR - Central Drug Research Institute, India

Funded by Council of Scientific & Industrial Research (CSIR), India

Saturday, January 07, 2017



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Password:

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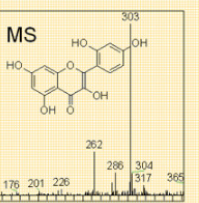
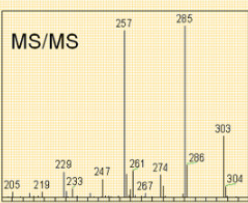
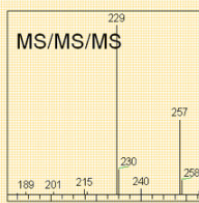
Tandem Mass Spectrum Database

TMS database is a library of MS/MS spectrum of naturally occurring compounds (Natural products). It is Designed and Developed by CSIR - Central Drug Research Institute, India. The analytical data/spectra /information are provided only for Research & Development purposes. These can't be used as certificates in legal disputes.

Search Options

General Searches	Mass Spectrometry Based Searches
<ul style="list-style-type: none">NameFormulaMolecular WeightCAS Registry Number	<ul style="list-style-type: none">MS/MS Ion SearchAdvanced SearchComprehensive Search

Available Database

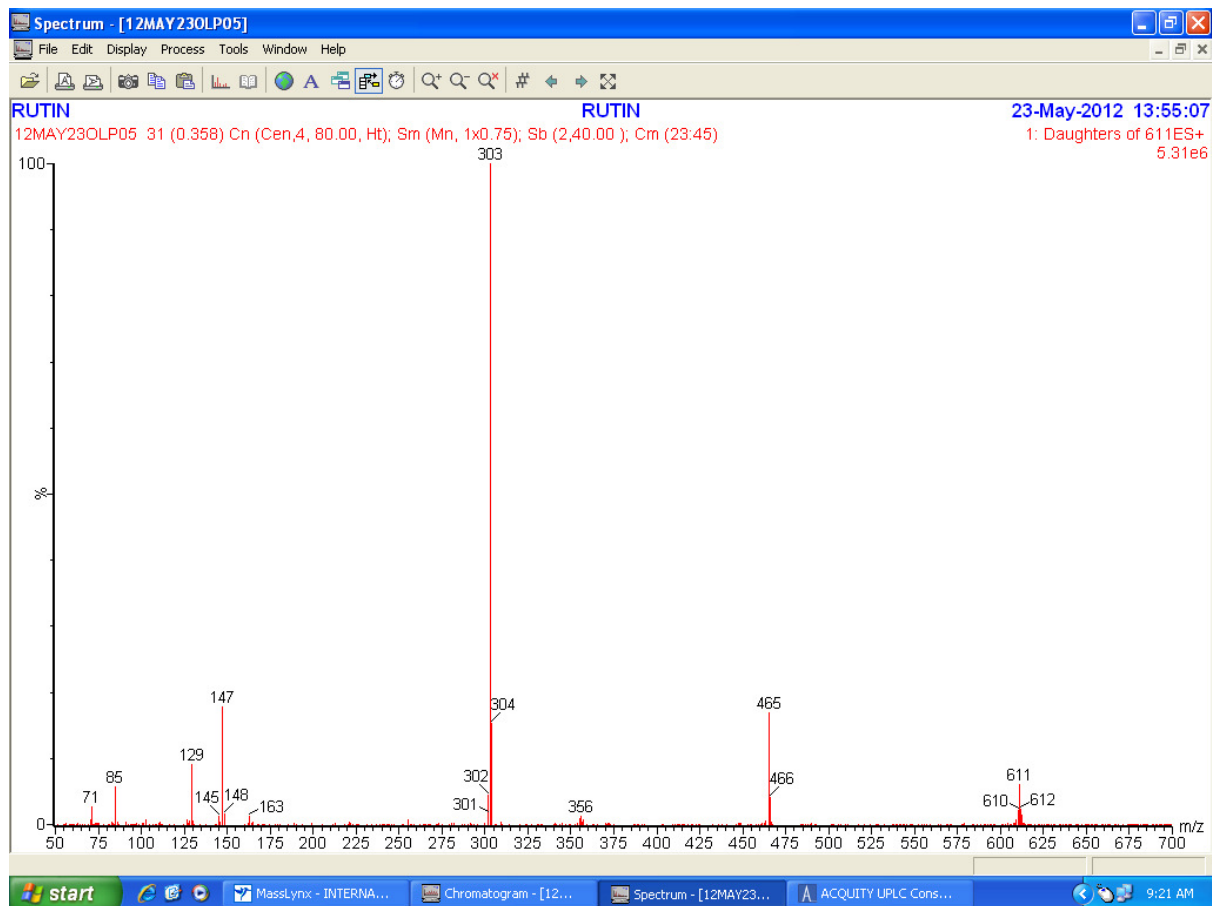


How to convert MS/MS spectrum to tms data format

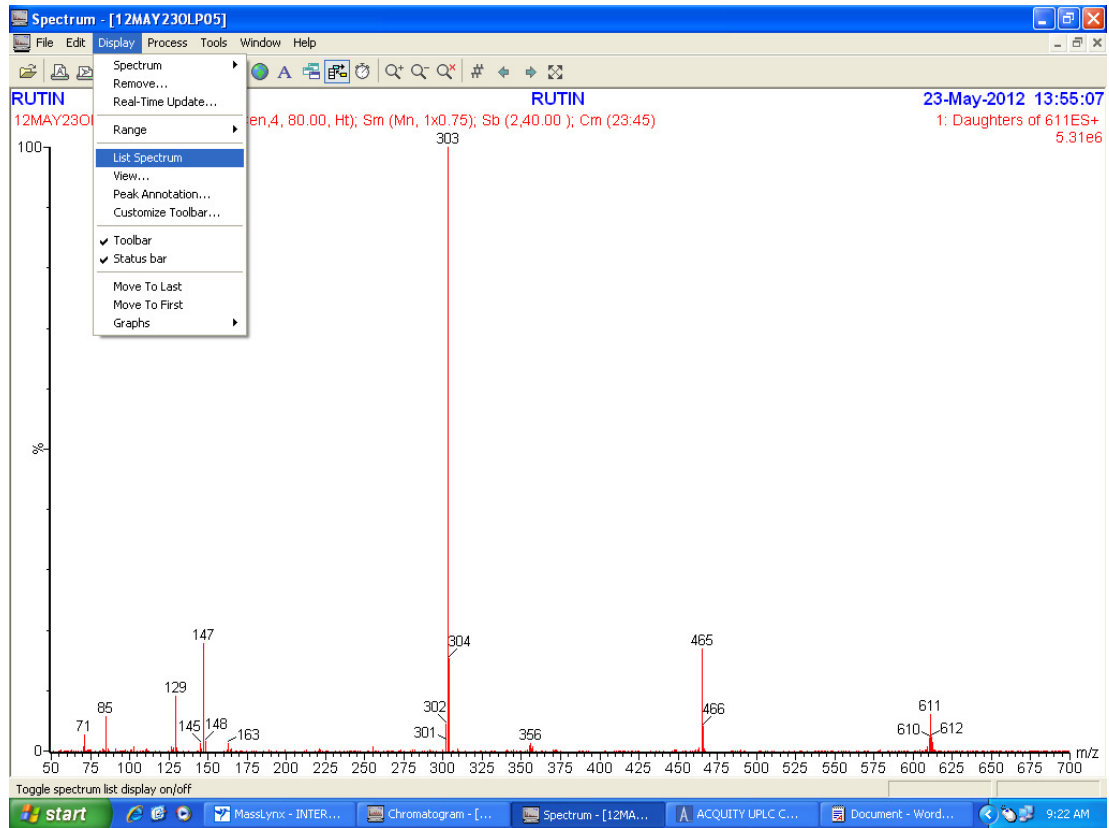
1. By the Waters MassLynx software

http://www.waters.com/waters/en_IN/MassLynx-Mass-Spectrometry-Software-/nav.htm?cid=513164&locale=en_IN

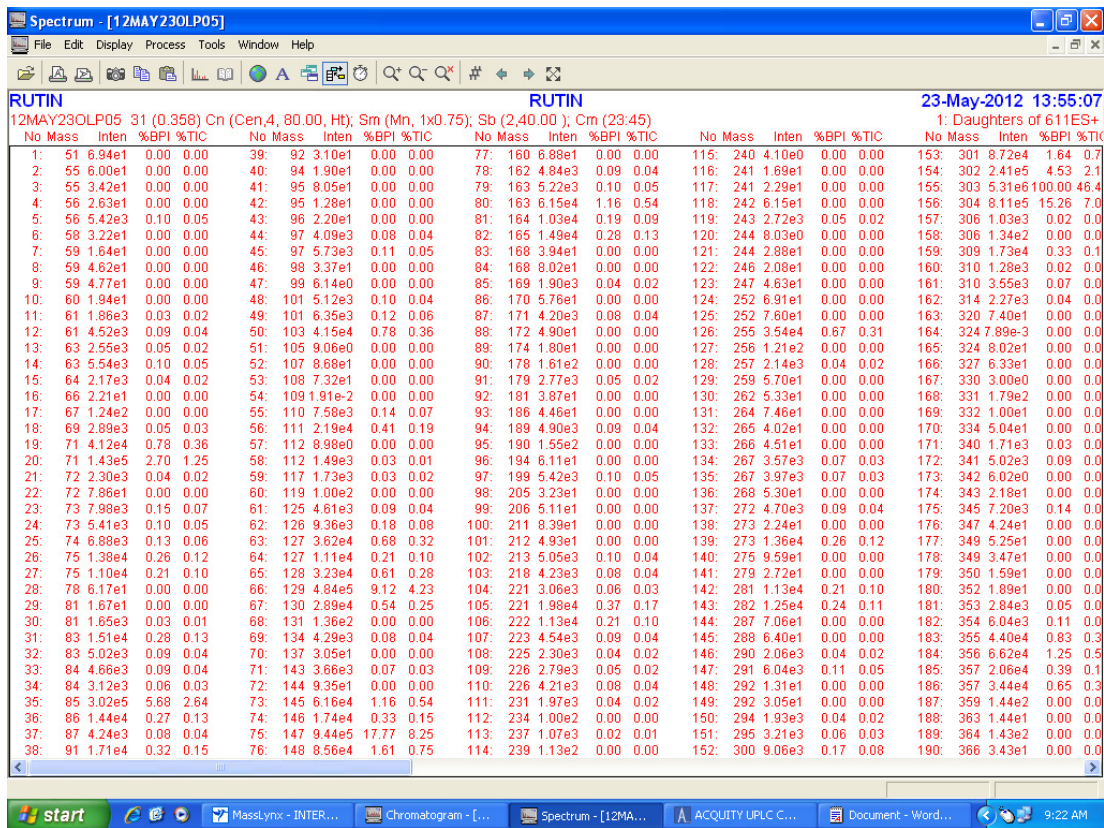
Open the MS/MS spectrum



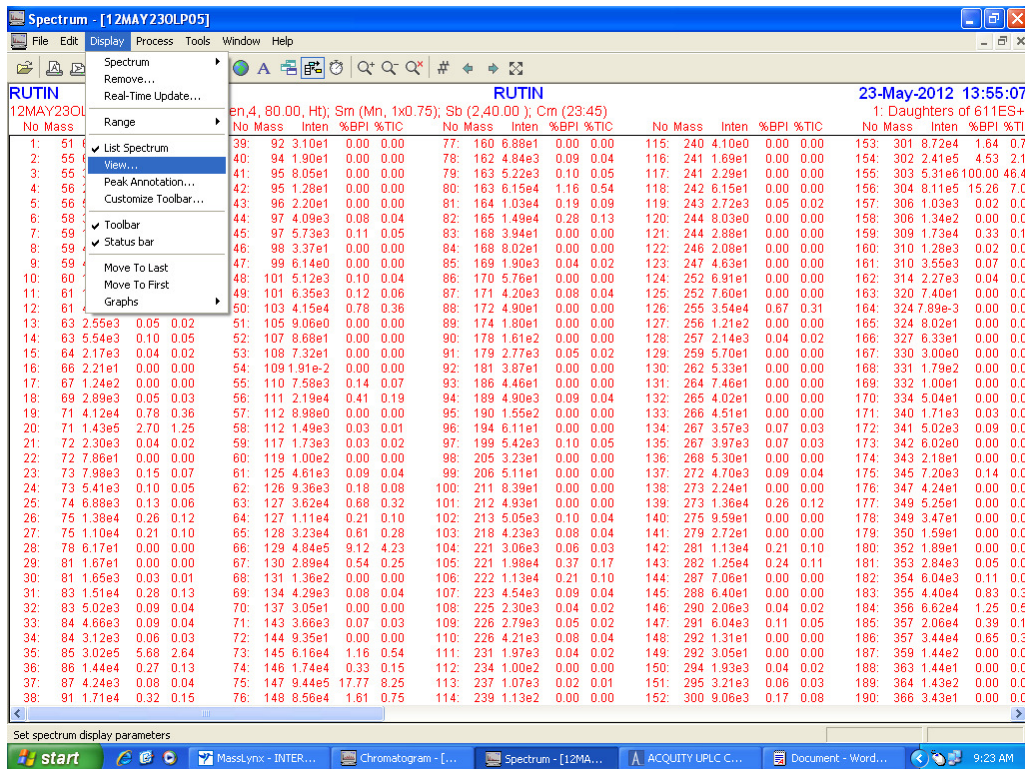
Go to display



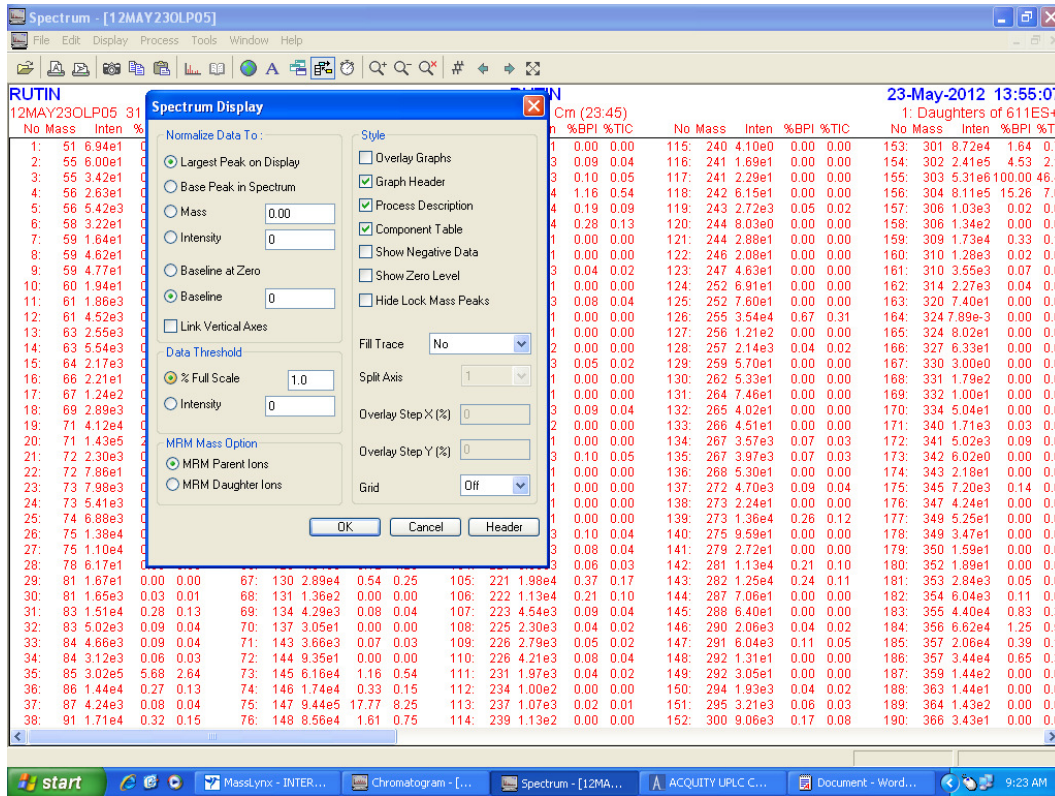
Select list spectrum



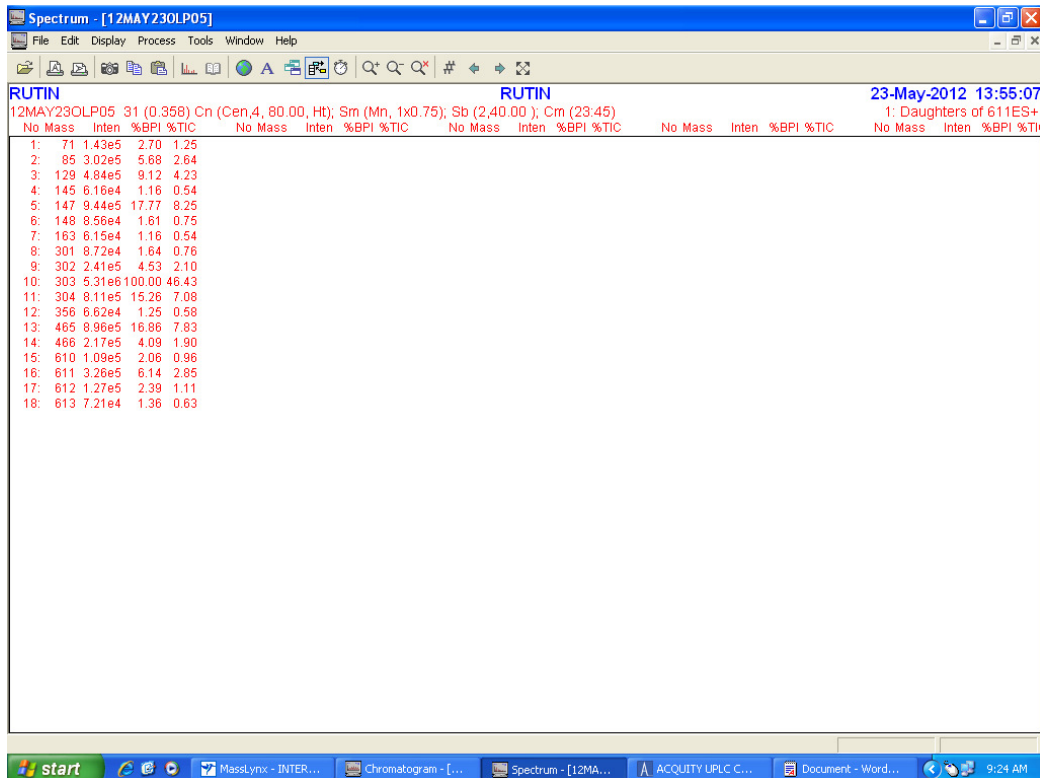
Select view



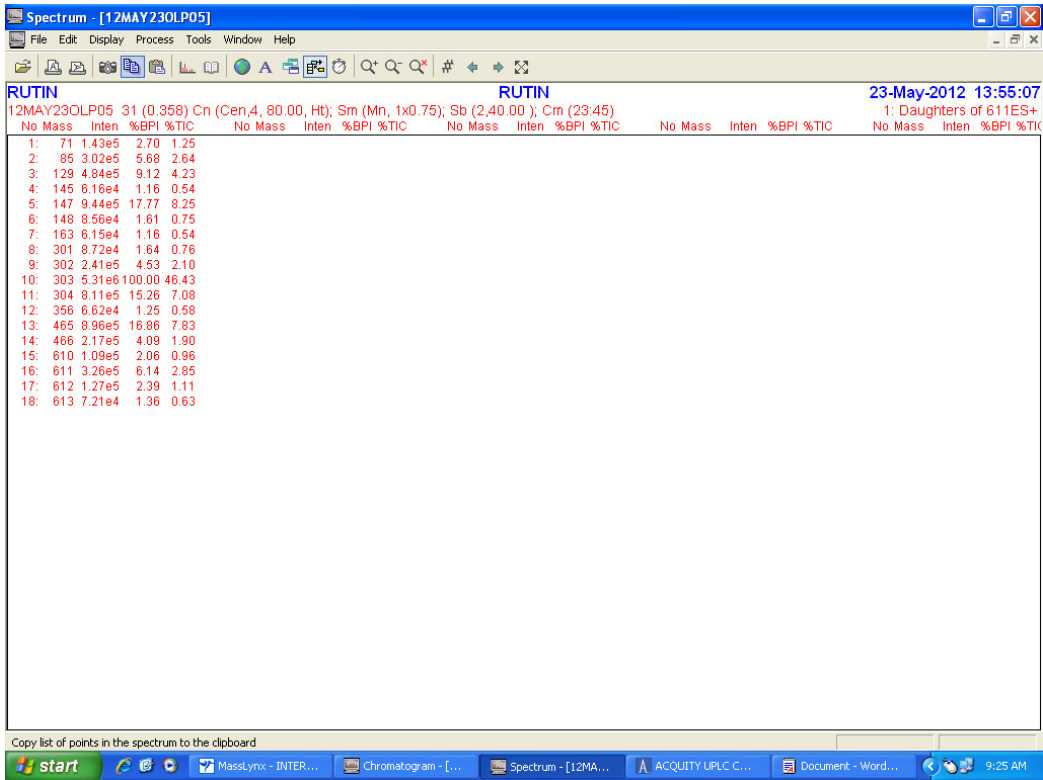
Set data threshold 1-2% (for significant peak)



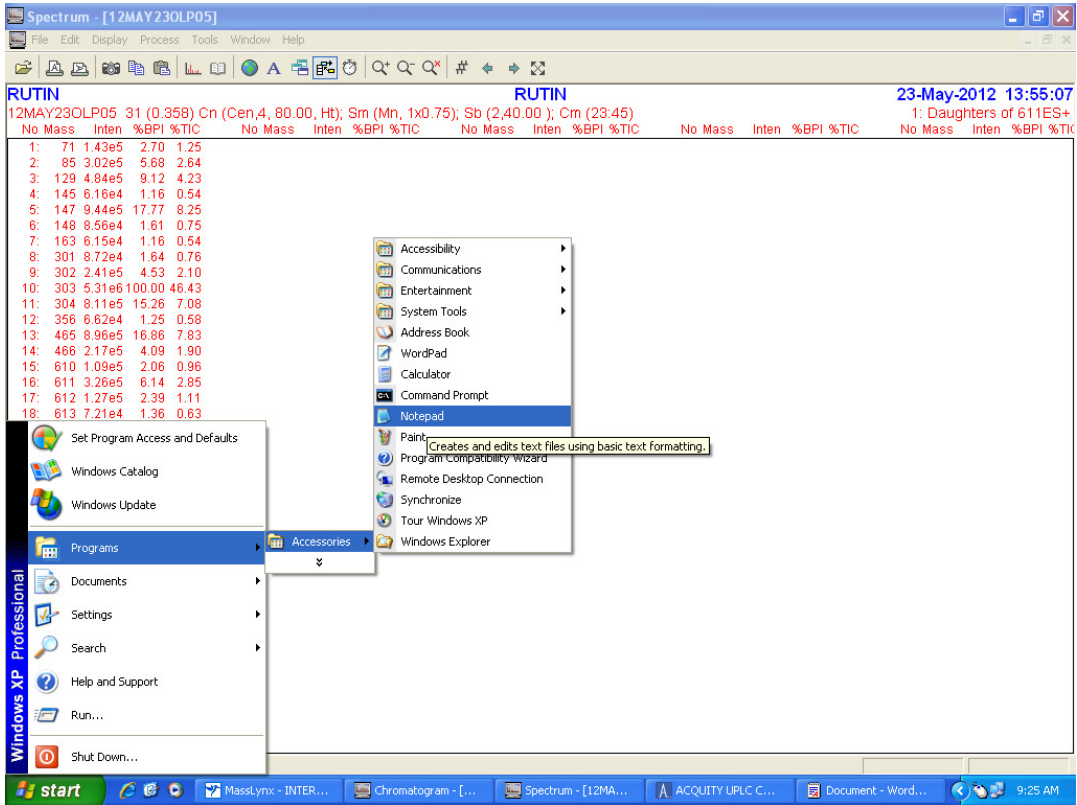
Press ok (list out major 25-30 peaks, if available)



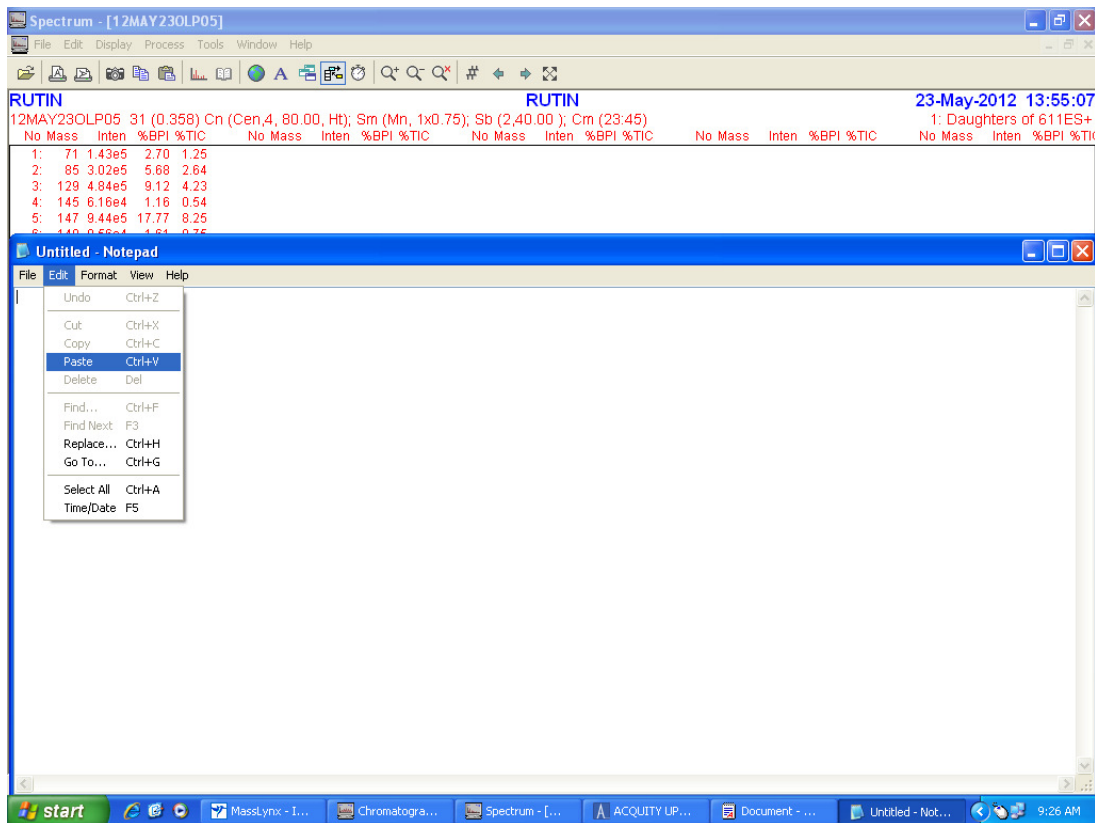
Copy the list of ions



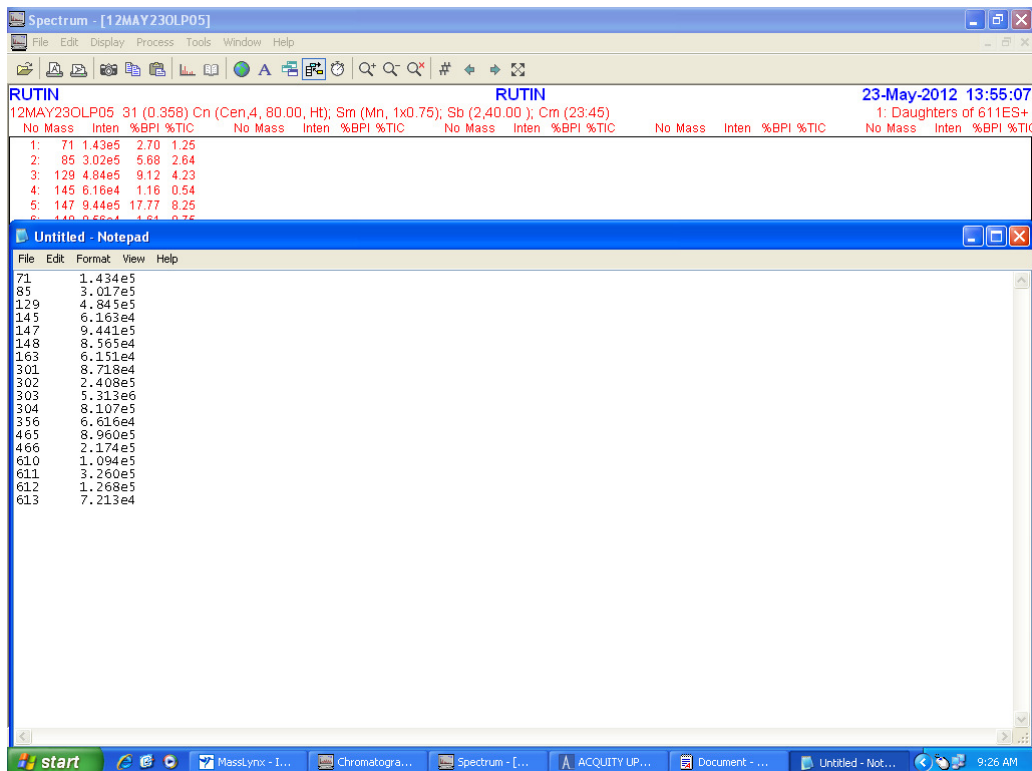
Open note pad



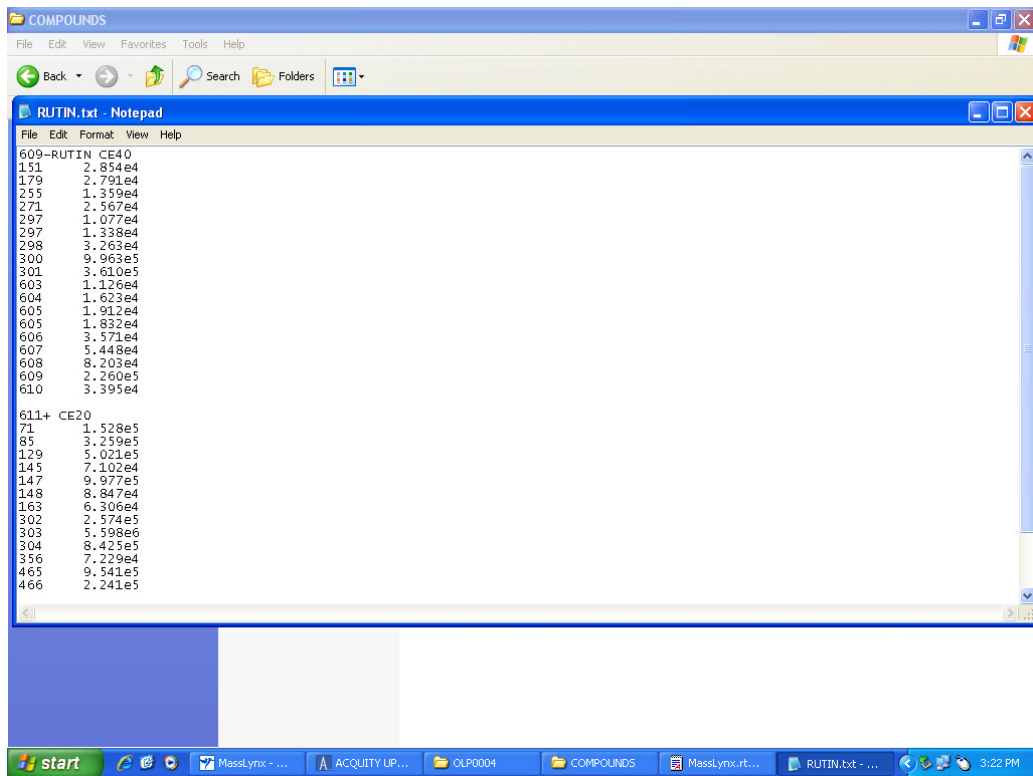
Paste the ions list on note pad



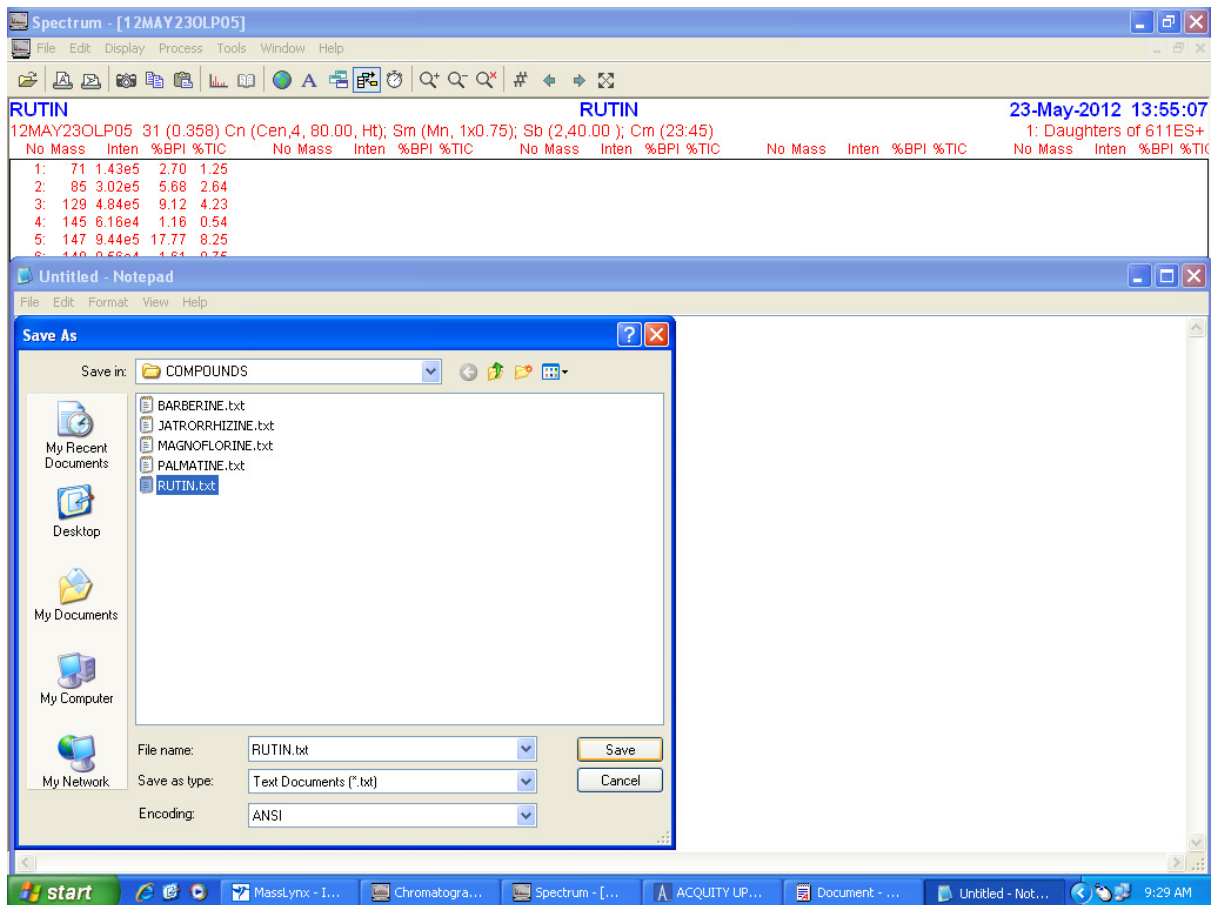
List of ions on note pad



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

The screenshot shows the 'Utility' section of the Tandem Mass Spectrum Database. On the left is a 'Login' form with fields for 'User Name' and 'Password', a 'Remember Me' checkbox, and buttons for 'LOGIN', 'Forgot Password?', and 'Register Here'. Below the login form is a navigation menu with links to Home, Overview, Inventor, Advisory Board, Collaborator, Plant Metabolites, Contact Us, Download, and Utility. The main content area features three mass spectra plots: 'MS/MS/MS', 'MS/MS', and 'MS'. The 'MS' plot includes a chemical structure of a polyphenolic compound. Below the plots is a 'Utility' section with two active options: 'ESI / APCI Adduct Ion Calculator' and 'Data File Format Converter', each with a green checkmark and a right-pointing arrow.

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

The screenshot shows the 'Data File Format Converter' page. It features the same 'Login' form and navigation menu as the previous page. The main content area is titled 'Data File Format Converter' and contains a 'Source Format*' dropdown menu with 'MassLynx.txt' selected. Below the dropdown is a 'Browse File*' button. A green 'Convert To TMSD Format' button is positioned below the 'Browse File' button. A yellow warning box at the bottom of the form states 'Field(s) marked with * are mandatory'. The Windows taskbar at the bottom shows the system time as 14:45 on 07-01-2017.

Choose /browse note pad *.txt file

The screenshot shows the Tandem Mass Spectrum Database website. The header includes the logo, the name 'Tandem Mass Spectrum Database', and the affiliation 'CSIR - Central Drug Research Institute, India'. Below the header, there is a 'Login' section with fields for 'User Name' and 'Password', a 'Remember Me' checkbox, and a 'LOGIN' button. To the right of the login section is a 'Data File Format Converter' section. It features a 'Source Format' dropdown menu set to 'MassLym.txt', a 'Browse File' button with the text 'No file chosen', and a green 'Convert To TMSD Format' button. A yellow warning box at the bottom of the converter section states 'Field(s) marked with * are mandatory'. The website is accessed via a browser window showing the URL 'www.tmsdatabase.org/public/fm_DataFormatConverter.aspx'.

Click to convert to tmsd format

This screenshot shows the same Tandem Mass Spectrum Database website, but with the 'Data File Format Converter' section updated. The 'Source Format' dropdown remains 'MassLym.txt', but the 'Browse File' button now shows 'Rutin.txt'. The green 'Convert To TMSD Format' button is still present, and a yellow warning box at the bottom of the converter section now contains a 'Click to Convert' button. The rest of the website, including the login section and navigation menu, remains the same as in the previous screenshot.

File will open as tmsd format in *.txt format

The screenshot shows a web browser window with the URL www.tmsdatabase.org/public/frm_DataFormatConveror.aspx. The page title is "Tandem Mass Spectrum Database" and it is from CSIR - Central Drug Research Institute, India. A chemical structure of Rutin is visible in the top right corner. A Notepad window titled "Rutin - Notepad" is overlaid on the page, containing the following text:

```

START IONS
TITLE= rutin Rt 6.77
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

```

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.**