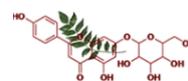


2025

Data File Format Conversion



Tandem Mass Spectrum Database
CSIR - Central Drug Research Institute, India



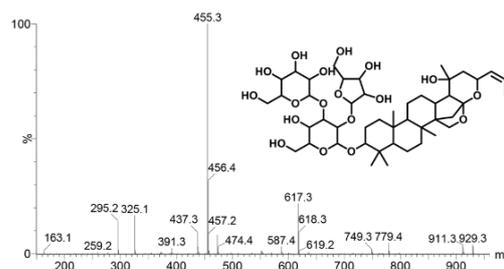
[HOME](#) [OVERVIEW](#) [SEARCH](#) [CONTRIBUTOR](#) [PLANT METABOLITES](#) [UTILITIES](#) [CONTACT US](#)

[SIGNIN](#)

Tandem Mass Spectrum Database

A library of the MS/MS spectrum of naturally occurring compounds (Natural products). This is Designed and Developed by CSIR - Central Drug Research Institute, U.P., India. The analytical data/spectra /information is provided only for Research & Development activity. These can't be used as certificates in legal disputes.

[Know More](#)



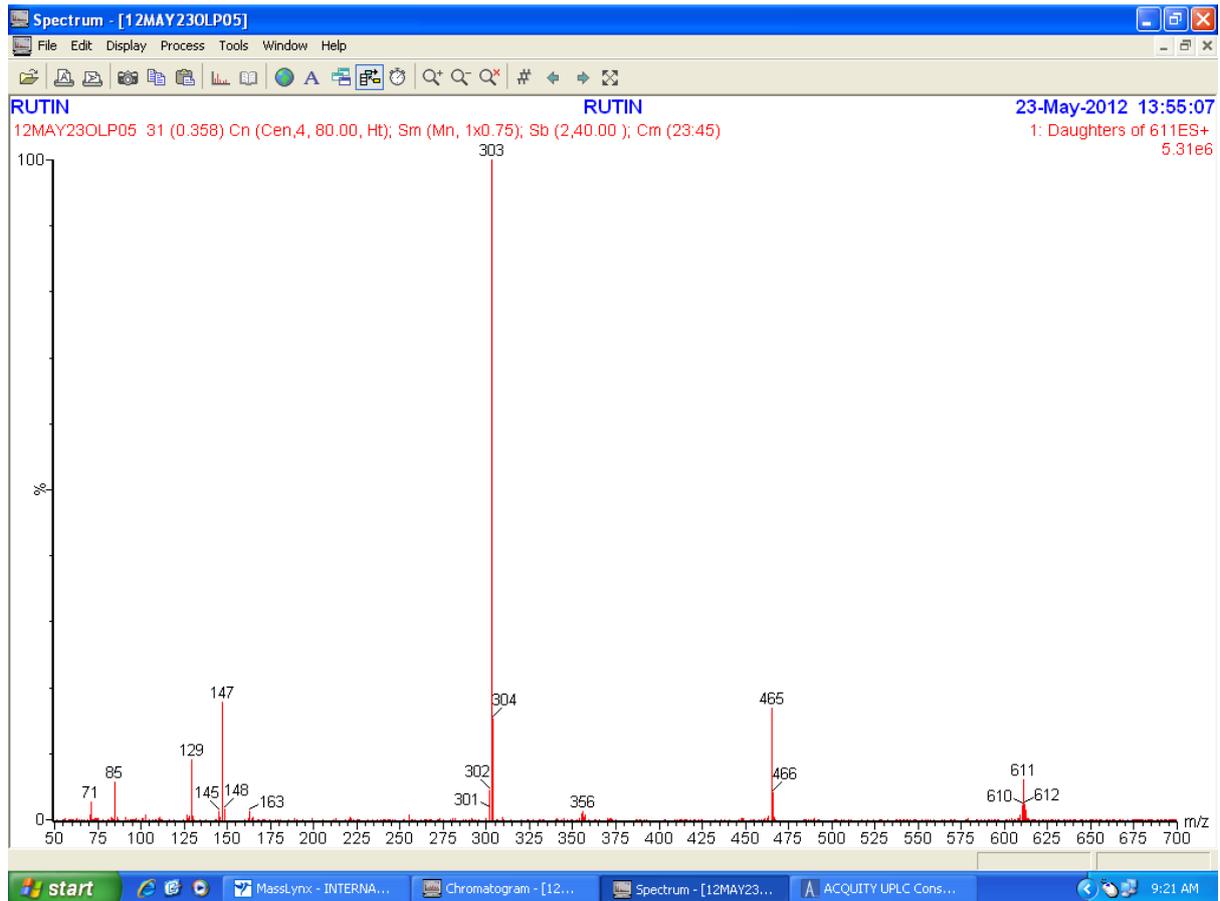
www.tmsdatabase.org

1/1/2025

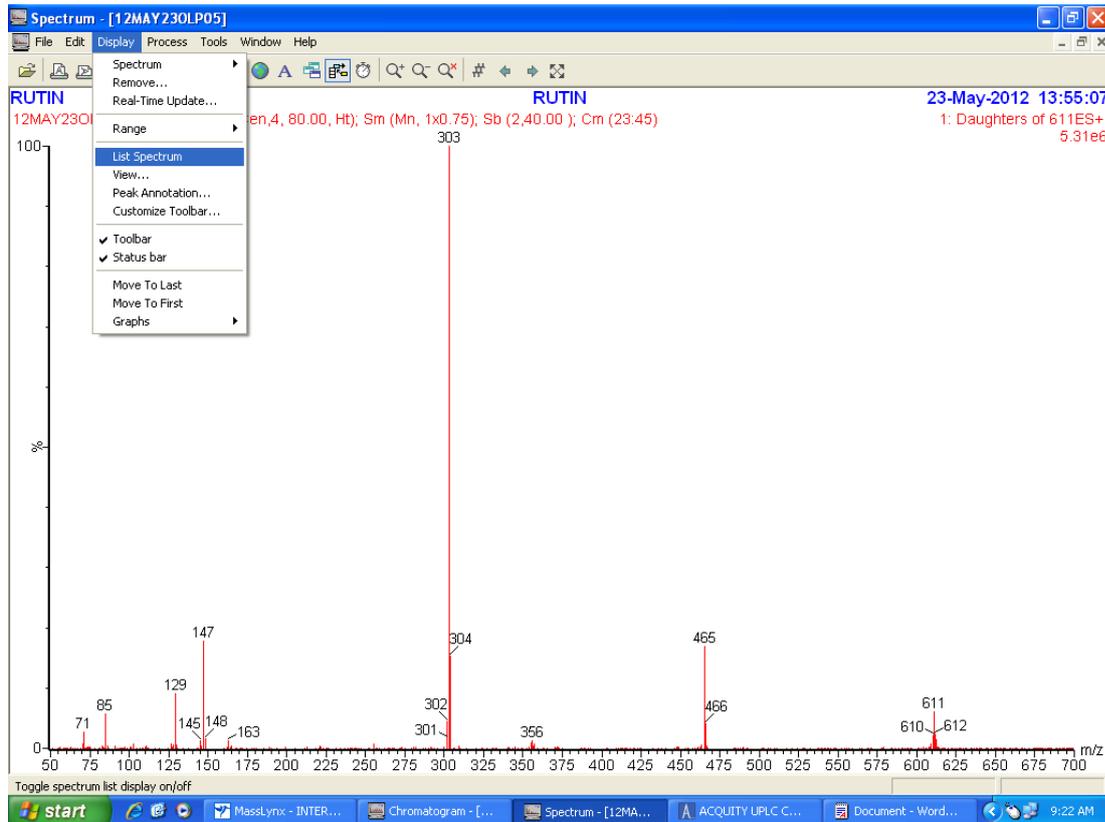
How to convert MS/MS spectrum to tms data format

1. By the Waters MassLynx software

Open the MS/MS spectrum using MassLynx software



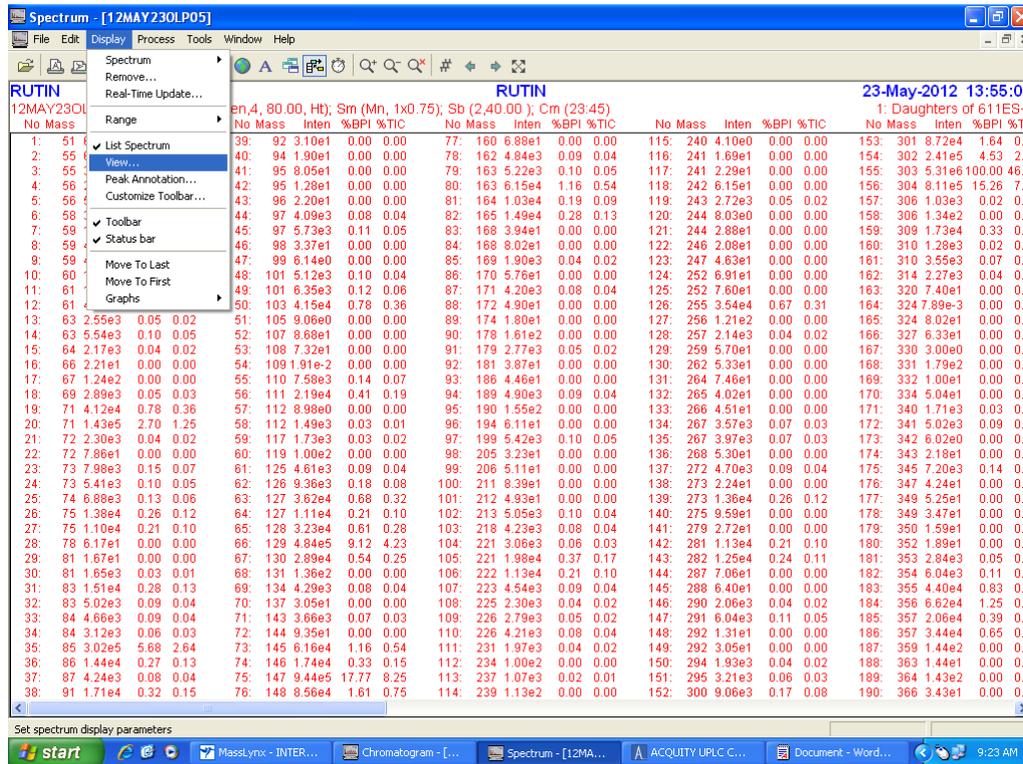
Go to display



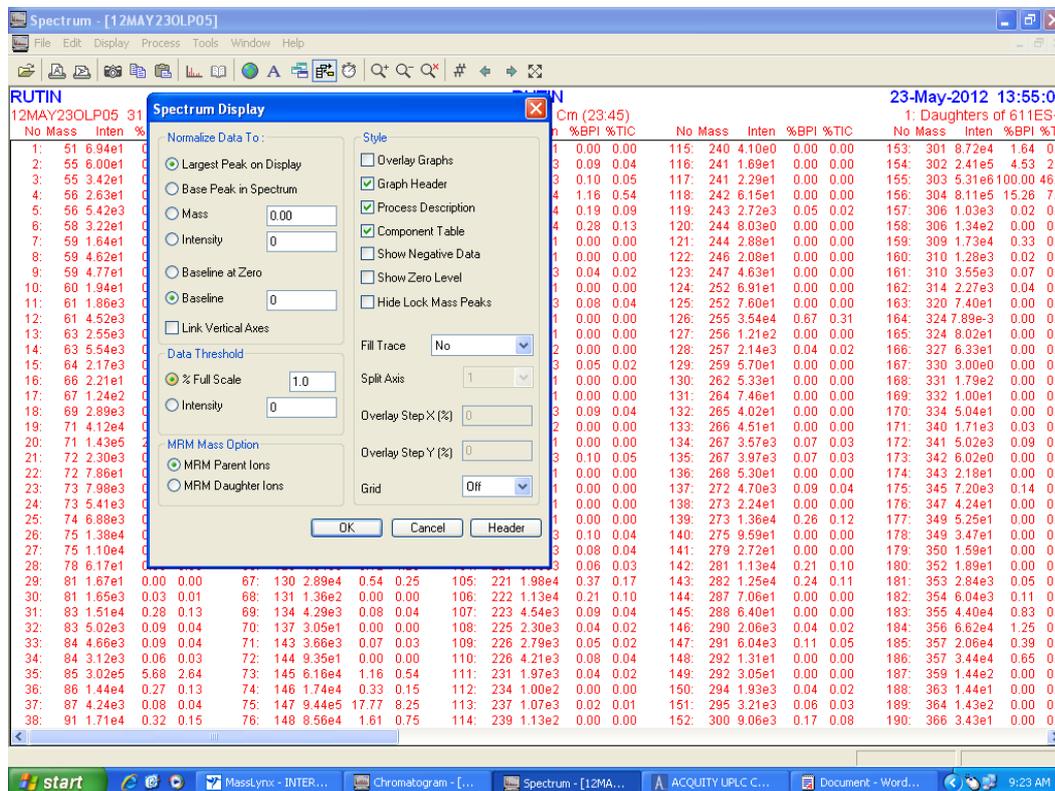
Select list spectrum

RUTIN					RUTIN					RUTIN				
No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	51	6.94e1	0.00	0.00	39:	92	3.10e1	0.00	0.00	77:	160	6.88e1	0.00	0.00
2:	55	6.00e1	0.00	0.00	40:	94	1.90e1	0.00	0.00	78:	162	4.84e3	0.09	0.04
3:	55	3.42e1	0.00	0.00	41:	95	8.05e1	0.00	0.00	79:	163	5.22e3	0.10	0.05
4:	56	2.63e1	0.00	0.00	42:	95	1.28e1	0.00	0.00	80:	163	6.15e4	1.16	0.54
5:	56	5.42e3	0.10	0.05	43:	96	2.20e1	0.00	0.00	81:	164	1.03e4	0.19	0.09
6:	58	3.22e1	0.00	0.00	44:	97	4.09e3	0.08	0.04	82:	165	1.49e4	0.28	0.13
7:	59	1.64e1	0.00	0.00	45:	97	5.73e3	0.11	0.05	83:	168	3.94e1	0.00	0.00
8:	59	4.62e1	0.00	0.00	46:	98	3.37e1	0.00	0.00	84:	168	8.02e1	0.00	0.00
9:	59	4.77e1	0.00	0.00	47:	99	6.14e0	0.00	0.00	85:	169	1.90e3	0.04	0.02
10:	60	1.94e1	0.00	0.00	48:	101	5.12e3	0.10	0.04	86:	170	5.76e1	0.00	0.00
11:	61	1.86e3	0.03	0.02	49:	101	6.35e3	0.12	0.06	87:	171	4.20e3	0.08	0.04
12:	61	4.52e3	0.09	0.04	50:	103	4.15e4	0.78	0.36	88:	172	4.90e1	0.00	0.00
13:	63	2.55e3	0.05	0.02	51:	105	9.06e0	0.00	0.00	89:	174	1.80e1	0.00	0.00
14:	63	5.54e3	0.10	0.05	52:	107	8.68e1	0.00	0.00	90:	178	1.61e2	0.00	0.00
15:	64	2.17e3	0.04	0.02	53:	108	7.32e1	0.00	0.00	91:	179	2.77e3	0.05	0.02
16:	66	2.21e1	0.00	0.00	54:	109	1.91e2	0.00	0.00	92:	181	3.87e1	0.00	0.00
17:	67	1.24e2	0.00	0.00	55:	110	7.58e3	0.14	0.07	93:	186	4.46e1	0.00	0.00
18:	69	2.89e3	0.05	0.03	56:	111	2.19e4	0.41	0.19	94:	189	4.90e3	0.09	0.04
19:	71	4.12e4	0.78	0.36	57:	112	8.98e0	0.00	0.00	95:	190	5.55e2	0.00	0.00
20:	71	1.43e5	2.70	1.25	58:	112	1.49e3	0.03	0.01	96:	194	6.11e1	0.00	0.00
21:	72	2.30e3	0.04	0.02	59:	117	1.73e3	0.03	0.02	97:	199	5.42e3	0.10	0.05
22:	72	7.86e1	0.00	0.00	60:	119	1.00e2	0.00	0.00	98:	205	3.23e1	0.00	0.00
23:	73	7.98e3	0.15	0.07	61:	125	4.61e3	0.09	0.04	99:	206	5.11e1	0.00	0.00
24:	73	5.41e3	0.10	0.05	62:	126	9.36e3	0.18	0.08	100:	211	8.39e1	0.00	0.00
25:	74	6.88e3	0.13	0.06	63:	127	3.62e4	0.68	0.32	101:	212	4.93e1	0.00	0.00
26:	75	1.38e4	0.26	0.12	64:	127	1.11e4	0.21	0.10	102:	213	5.05e3	0.10	0.04
27:	75	1.10e4	0.21	0.10	65:	128	3.23e4	0.61	0.28	103:	218	4.23e3	0.08	0.04
28:	78	6.17e1	0.00	0.00	66:	129	4.84e5	9.12	4.23	104:	221	3.06e3	0.06	0.03
29:	81	1.67e1	0.00	0.00	67:	130	2.89e4	0.54	0.25	105:	221	1.98e4	0.37	0.17
30:	81	1.85e3	0.03	0.01	68:	131	1.36e2	0.00	0.00	106:	222	1.13e4	0.21	0.10
31:	83	1.51e4	0.28	0.13	69:	134	4.29e3	0.08	0.04	107:	223	4.54e3	0.09	0.04
32:	83	5.02e3	0.09	0.04	70:	137	3.05e1	0.00	0.00	108:	225	2.30e3	0.04	0.02
33:	84	4.66e3	0.09	0.04	71:	143	3.66e3	0.07	0.03	109:	226	2.79e3	0.05	0.02
34:	84	3.12e3	0.06	0.03	72:	144	9.35e1	0.00	0.00	110:	226	4.21e3	0.08	0.04
35:	85	3.02e5	5.68	2.64	73:	145	6.16e4	1.16	0.54	111:	231	1.97e3	0.04	0.02
36:	86	1.44e4	0.27	0.13	74:	146	1.74e4	0.33	0.15	112:	234	1.00e2	0.00	0.00
37:	87	4.24e3	0.08	0.04	75:	147	9.44e5	17.77	8.25	113:	237	1.07e3	0.02	0.01
38:	91	1.71e4	0.32	0.15	76:	148	8.56e4	1.61	0.75	114:	239	1.13e2	0.00	0.00

Select view



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



Press ok (List out the major 25–30 peaks, if available.)

Spectrum - [12MAY230LP05]
File Edit Display Process Tools Window Help

RUTIN **RUTIN** **23-May-2012 13:55:07**
12MAY230LP05 31 (0.358) Cn (Cen,4, 80.00, Ht); Sm (Mn, 1x0.75); Sb (2,40.00); Cm (23.45)
1: Daughters of 611ES+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	71	1.43e5	2.70	1.25																				
2:	85	3.02e5	5.68	2.64																				
3:	129	4.84e5	9.12	4.23																				
4:	145	6.16e4	1.16	0.54																				
5:	147	9.44e5	17.77	8.25																				
6:	148	8.56e4	1.61	0.75																				
7:	163	6.15e4	1.16	0.54																				
8:	301	8.72e4	1.64	0.76																				
9:	302	2.41e5	4.53	2.10																				
10:	303	5.31e6	100.00	46.43																				
11:	304	8.11e5	15.26	7.08																				
12:	356	6.62e4	1.25	0.58																				
13:	465	8.96e5	16.86	7.83																				
14:	466	2.17e5	4.09	1.90																				
15:	610	1.09e5	2.06	0.96																				
16:	611	3.26e5	6.14	2.85																				
17:	612	1.27e5	2.39	1.11																				
18:	613	7.21e4	1.36	0.63																				

start | MassLynx - INTER... | Chromatogram - [...] | Spectrum - [12MA... | ACQUITY UPLC C... | Document - Word... | 9:24 AM

Copy the list of ions

Spectrum - [12MAY230LP05]
File Edit Display Process Tools Window Help

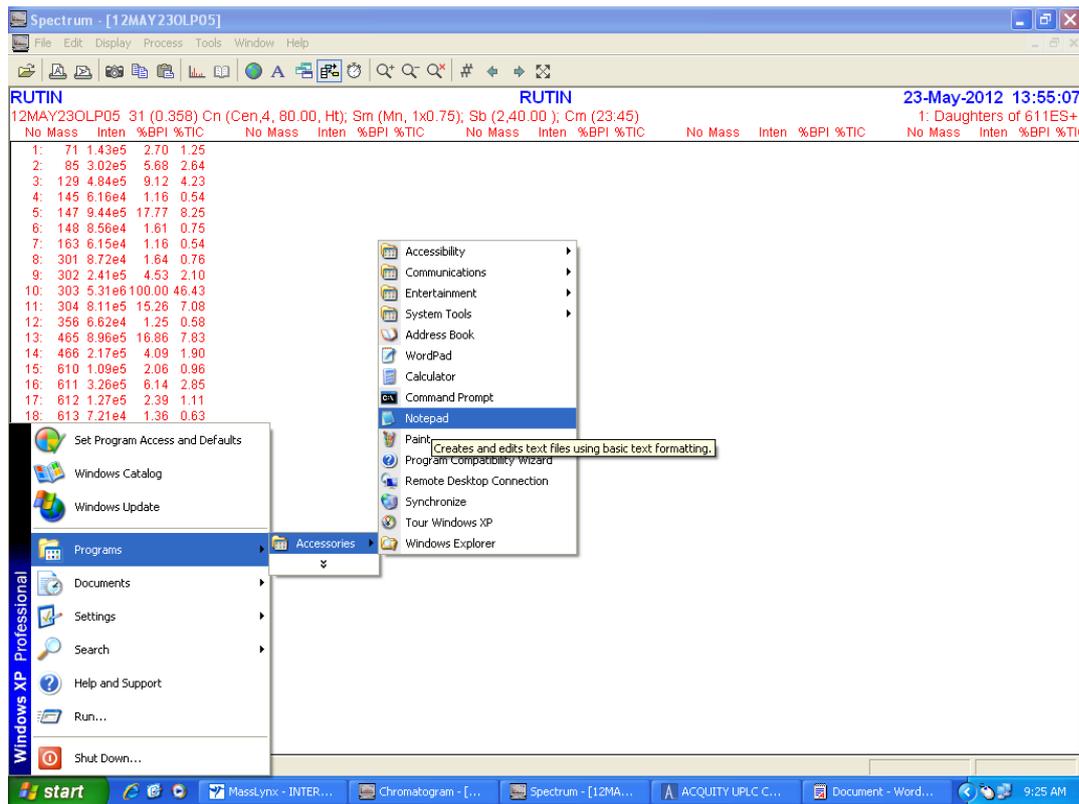
RUTIN **RUTIN** **23-May-2012 13:55:07**
12MAY230LP05 31 (0.358) Cn (Cen,4, 80.00, Ht); Sm (Mn, 1x0.75); Sb (2,40.00); Cm (23.45)
1: Daughters of 611ES+

No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC	No	Mass	Inten	%BPI	%TIC
1:	71	1.43e5	2.70	1.25																				
2:	85	3.02e5	5.68	2.64																				
3:	129	4.84e5	9.12	4.23																				
4:	145	6.16e4	1.16	0.54																				
5:	147	9.44e5	17.77	8.25																				
6:	148	8.56e4	1.61	0.75																				
7:	163	6.15e4	1.16	0.54																				
8:	301	8.72e4	1.64	0.76																				
9:	302	2.41e5	4.53	2.10																				
10:	303	5.31e6	100.00	46.43																				
11:	304	8.11e5	15.26	7.08																				
12:	356	6.62e4	1.25	0.58																				
13:	465	8.96e5	16.86	7.83																				
14:	466	2.17e5	4.09	1.90																				
15:	610	1.09e5	2.06	0.96																				
16:	611	3.26e5	6.14	2.85																				
17:	612	1.27e5	2.39	1.11																				
18:	613	7.21e4	1.36	0.63																				

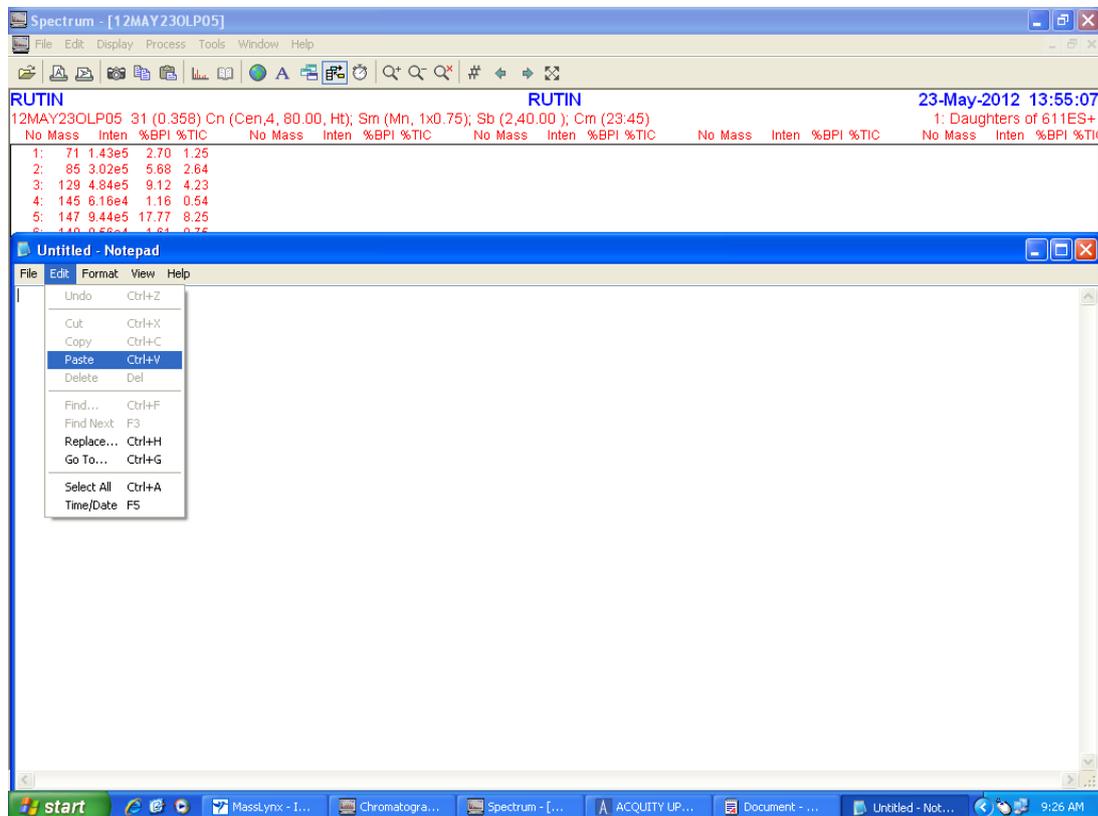
Copy list of points in the spectrum to the clipboard

start | MassLynx - INTER... | Chromatogram - [...] | Spectrum - [12MA... | ACQUITY UPLC C... | Document - Word... | 9:25 AM

Open Notepad



Paste the ions list on note pad



Paste the ion list on a notepad.

The screenshot shows a mass spectrometer software window titled "Spectrum - [12MAY230LP05]". The main display area shows a mass spectrum for "RUTIN" with the following data:

No	Mass	Inten	%BPI	%TIC
1	71	1.43e5	2.70	1.25
2	85	3.02e5	5.68	2.64
3	129	4.84e5	9.12	4.23
4	145	6.16e4	1.16	0.54
5	147	9.44e5	17.77	8.25
6	148	8.56e4	1.61	0.72

Below the spectrum, a "Daughters of 611ES+" section shows a list of ions. An "Untitled - Notepad" window is open in the foreground, containing the following ion data:

71	1.434e5
85	3.017e5
129	4.845e5
145	6.163e4
147	9.441e5
148	8.565e4
163	6.151e4
301	8.718e4
302	2.408e5
303	5.313e6
304	8.107e5
356	6.616e4
465	8.960e5
466	2.174e5
610	1.094e5
611	3.260e5
612	1.268e5
613	7.213e4

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

The screenshot shows a mass spectrometer software window titled "COMPOUNDS". The main display area shows a mass spectrum for "RUTIN" with the following data:

No	Mass	Inten	%BPI	%TIC
1	71	1.43e5	2.70	1.25
2	85	3.02e5	5.68	2.64
3	129	4.84e5	9.12	4.23
4	145	6.16e4	1.16	0.54
5	147	9.44e5	17.77	8.25
6	148	8.56e4	1.61	0.72

Below the spectrum, a "Daughters of 611ES+" section shows a list of ions. An "Untitled - Notepad" window is open in the foreground, containing the following ion data:

609--RUTIN	CE40
151	2.854e4
179	2.791e4
255	1.359e4
271	2.567e4
297	1.077e4
297	1.338e4
298	3.263e4
300	9.963e5
301	3.610e5
603	1.126e4
604	1.623e4
605	1.912e4
605	1.832e4
606	3.571e4
607	5.448e4
608	8.203e4
609	2.260e5
610	3.395e4
611+	CE20
71	1.528e5
85	3.259e5
129	5.021e5
145	7.102e4
147	9.977e5
148	8.847e4
163	6.306e4
302	2.574e5
303	5.986e6
304	8.425e5
356	7.229e4
465	9.541e5
466	2.241e5

Save the note pad file in *.txt format

The screenshot shows a Windows desktop environment. The main application window is titled "Spectrum - [12MAY23OLP05]". It displays a mass spectrum analysis for "RUTIN". The analysis parameters are: 12MAY23OLP05 31 (0.358) Cn (Cen,4, 80.00, Ht); Sm (Mn, 1x0.75); Sb (2,40.00); Cm (23:45). The spectrum shows several peaks, with the most prominent one at m/z 147. The table below the spectrum lists the following data:

No	Mass	Inten	%BPI	%TIC
1:	71	1.43e5	2.70	1.25
2:	85	3.02e5	5.68	2.64
3:	129	4.84e5	9.12	4.23
4:	145	6.16e4	1.16	0.54
5:	147	9.44e5	17.77	8.25
6:	149	0.56e4	1.61	0.75

Below the spectrum, there is a "1: Daughters of 611ES+" section. In the foreground, a Notepad window is open with a "Save As" dialog box. The dialog box shows the file name "RUTIN.txt" and the save location "COMPOUNDS". The file type is set to "Text Documents (*.txt)" and the encoding is "ANSI".

Go to <https://tmsdatabase.cdri.res.in> and select utility section:

The screenshot shows the homepage of the Tandem Mass Spectrum Database. The page header includes the date "Wednesday, November 22, 2023 11:00:19 AM" and the site name "Tandem Mass Spectrum Database" with the affiliation "CSIR - Central Drug Research Institute, India". The navigation menu includes "HOME", "OVERVIEW", "SEARCH", "CONTRIBUTOR", "PLANT METABOLITES", "UTILITIES", and "CONTACT US". The "UTILITIES" menu is expanded, showing options: "UTILITY", "FAQ", "DOWNLOAD", "ESI / APCI ADDUCT ION CALCULATOR", and "DATA FILE FORMAT CONVERTOR". The main content area features a large heading "Tandem Mass Spectrum Database" and a description: "A library of the MS/MS spectrum of naturally occurring compounds (Natural products). This is Designed and Developed by CSIR - Central Drug Research Institute, U.P., India. The analytical data/spectra /information is provided only for Research & Development activity. These can't be used as certificates in legal disputes." There is a "Know More" button. To the right, there is a mass spectrum plot with a chemical structure of a polyphenolic compound. The x-axis is labeled "m/z" and ranges from 60 to 320. The y-axis is labeled "Abundance". The base peak is at m/z 122.0. Other significant peaks are at m/z 147.1, 165.1, 180.0, 181.2, 207.1, 249.2, 273.2, and 291.1. The footer includes "News", "General Search", "MS Based Search", and a note "The project is funded by the Council of Sci".

Choose /browse note pad *.txt file

The screenshot shows the web interface of the Tandem Mass Spectrum Database Data File Format Converter. The page title is "Data File Format Converter" and the URL is "172.16.0.65:8080/DataFileFormatConverter". The interface includes a navigation menu with options like HOME, OVERVIEW, SEARCH, CONTRIBUTOR, PLANT METABOLITES, UTILITIES, CONTACT US, and SIGNIN. The main content area has a form with the following fields:

- Source Format: MassLymx.txt
- Total No. Of Values: 25
- Browse File: Choose File (No file chosen)

A red button labeled "Convert to TMSD Format" is located below the form. The footer contains the CSIR logo and text in Hindi and English, along with contact information for CSIR-Central Drug Research Institute, Lucknow.

Click to convert to tmsd format

File will open as tmsd format in *.txt format

The screenshot shows a Notepad window titled "Rutin - Notepad" 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:

- The TMS file format can be made by direct MS/MS Spectrum, as shown in the script shown above.
- Multiple scripts can be generated through this method for each spectrum.