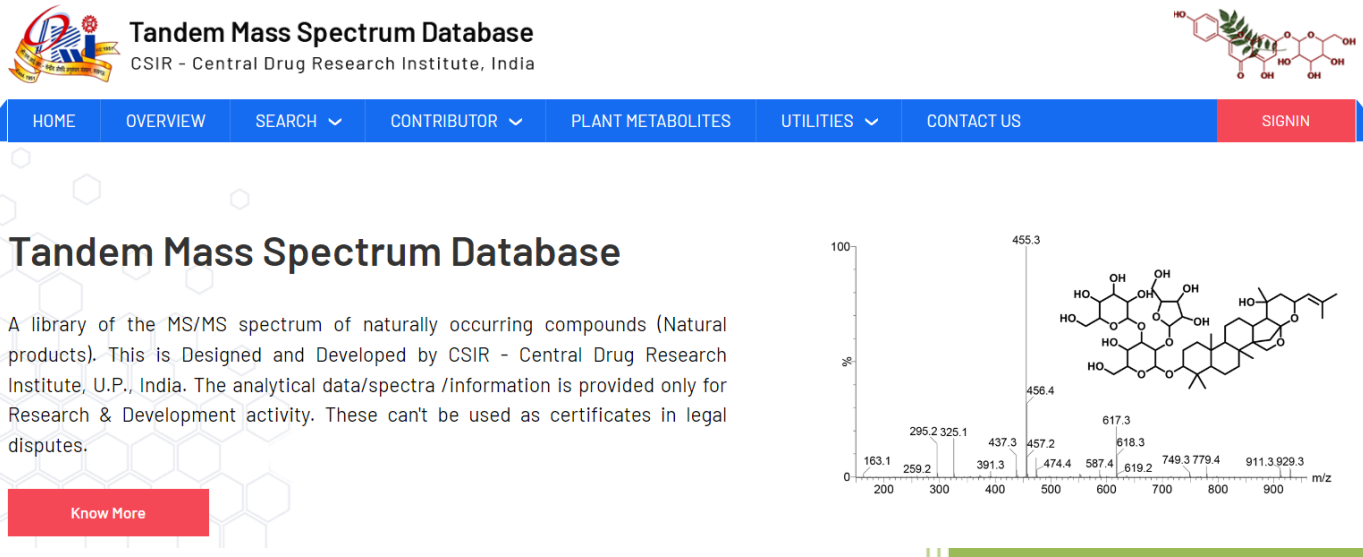
2025

# Data File Format Conversion



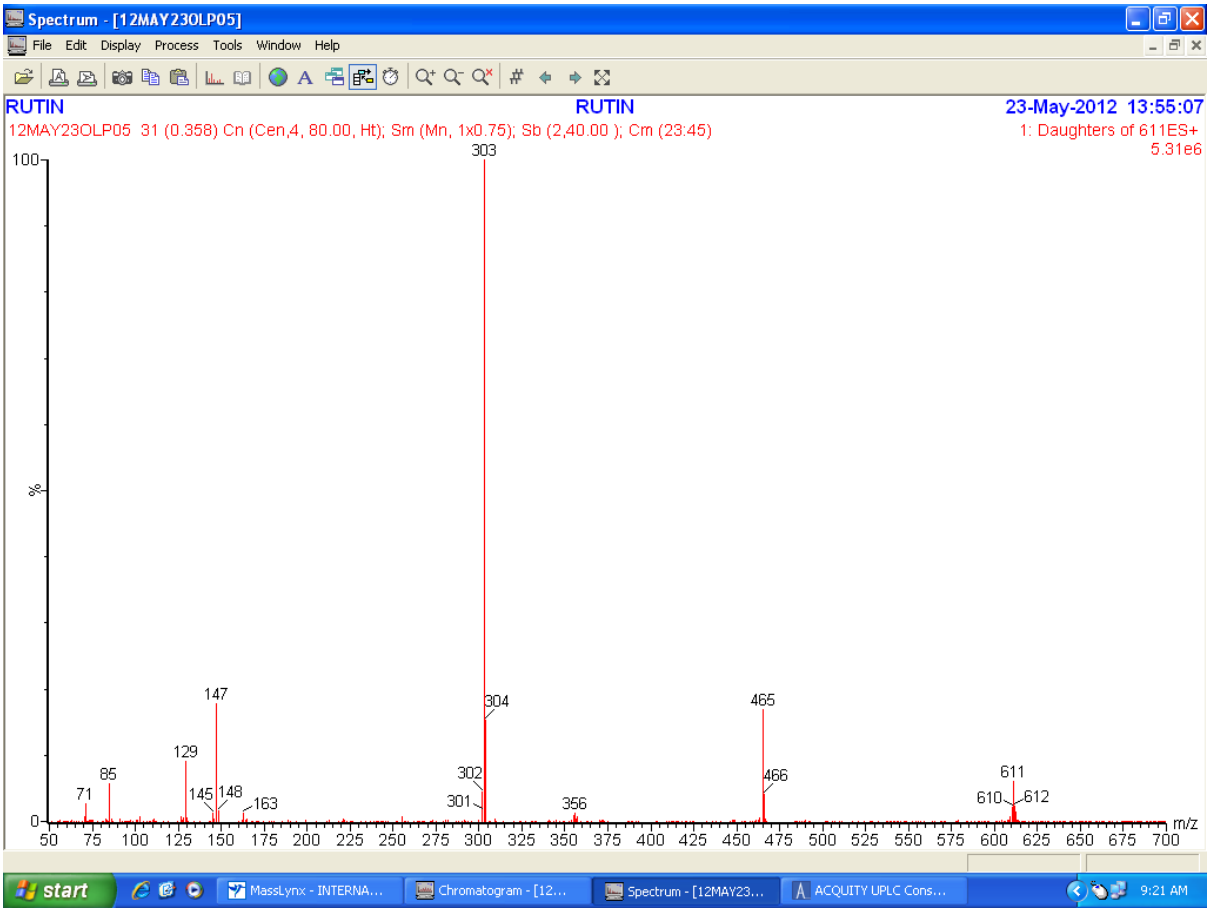

www.tmsdatabase.org

1/1/2025

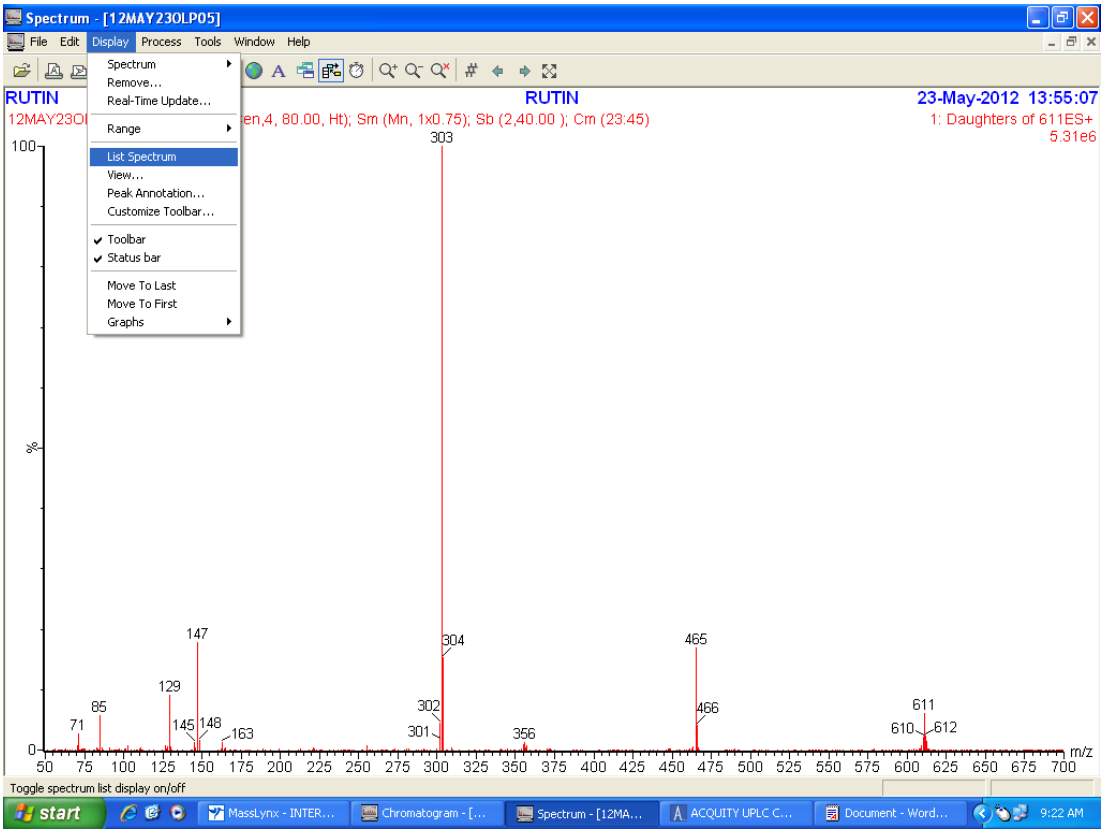
# How to convert MS/MS spectrum to tms data format

## 1. By the Waters MassLynx software

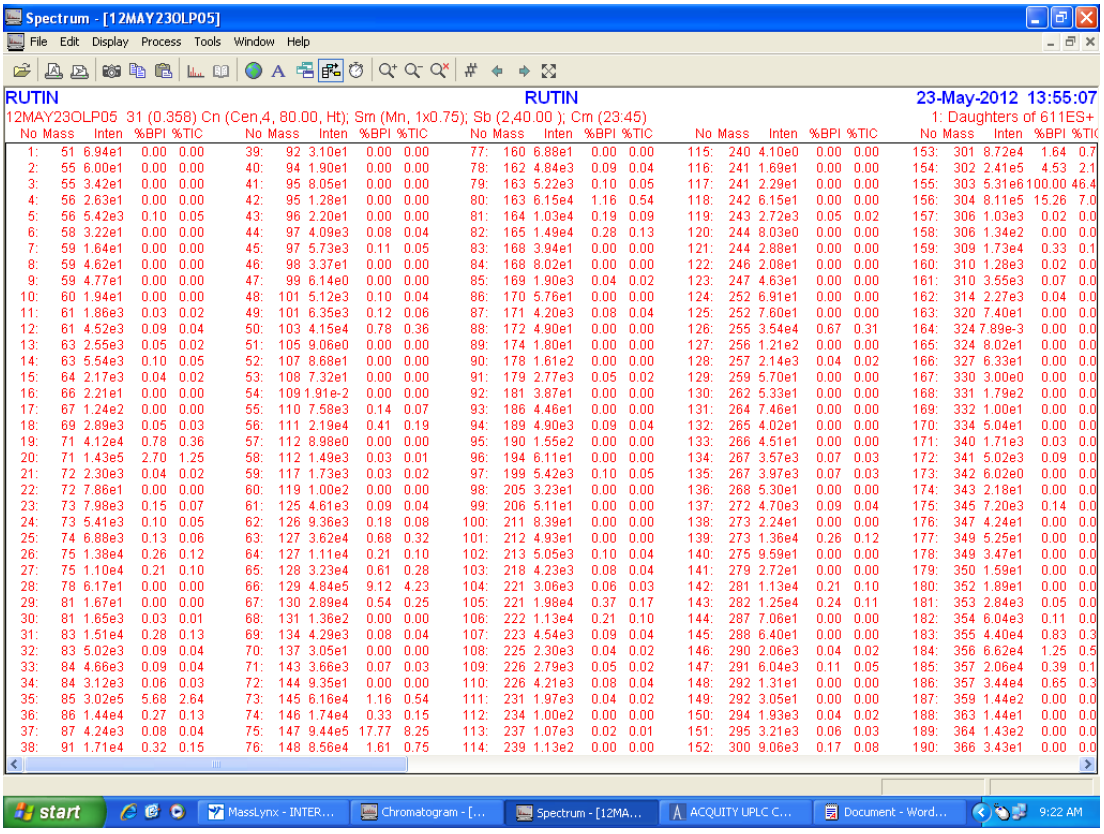
### Open the MS/MS spectrum using MassLynx software



# Go to display

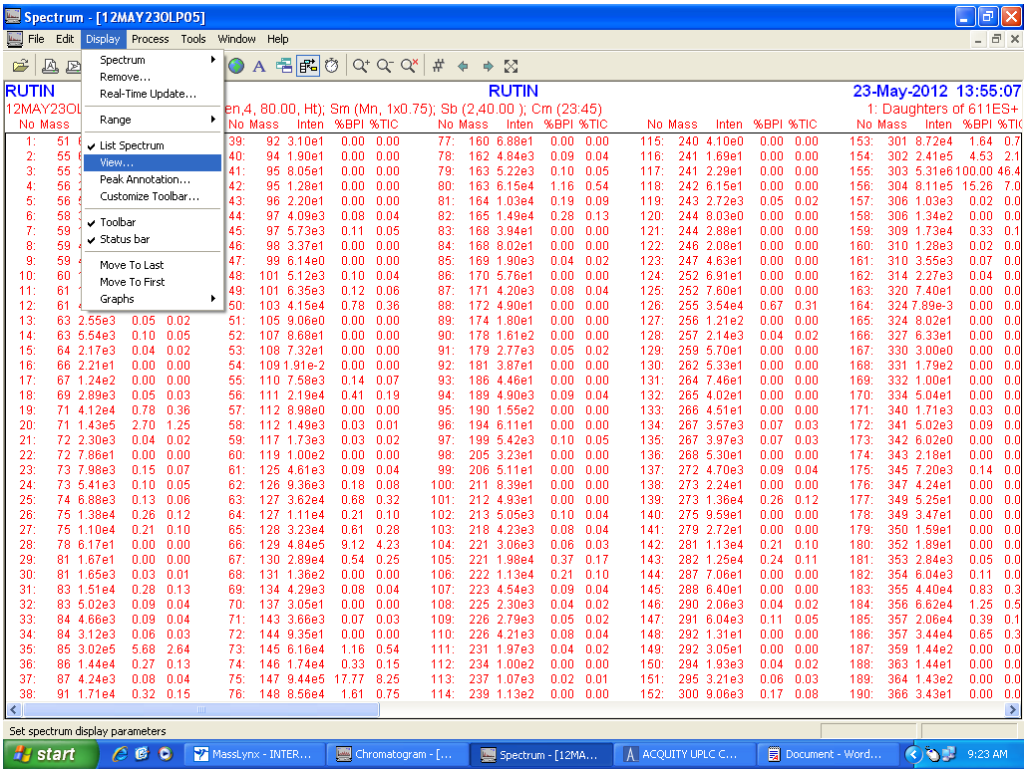



# Select list spectrum

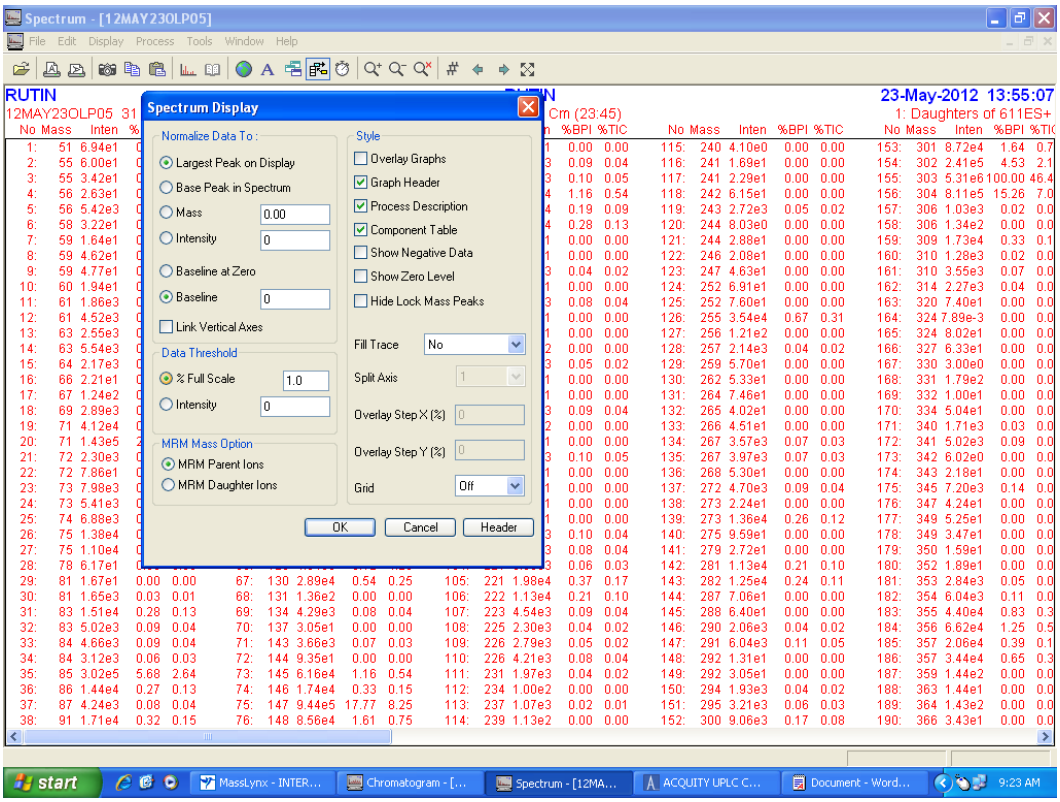



| No | Mass | Inten | %BPI | %TIC | No | Mass | Inten | %BPI | %TIC | No | Mass | Inten | %BPI | %TIC | No | Mass | Inten | %BPI | %TIC | No | Mass | Inten | %BPI | %TIC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1: | 51 | 6.94e1 | 0.00 | 0.00 | 39: | 92 | 3.10e1 | 0.00 | 0.00 | 77: | 160 | 6.88e1 | 0.00 | 0.00 | 115: | 240 | 4.10e0 | 0.00 | 0.00 | 153: | 301 | 8.72e4 | 1.64 | 0.7 |
| 2: | 55 | 6.00e1 | 0.00 | 0.00 | 40: | 94 | 1.90e1 | 0.00 | 0.00 | 78: | 162 | 4.84e3 | 0.09 | 0.04 | 116: | 241 | 1.69e1 | 0.00 | 0.00 | 154: | 302 | 2.41e5 | 4.53 | 2.1 |
| 3: | 55 | 3.42e1 | 0.00 | 0.00 | 41: | 95 | 8.05e1 | 0.00 | 0.00 | 79: | 163 | 5.22e3 | 0.10 | 0.05 | 117: | 241 | 2.29e1 | 0.00 | 0.00 | 155: | 303 | 5.31e6 | 100.00 | 46.4 |
| 4: | 56 | 2.63e1 | 0.00 | 0.00 | 42: | 95 | 1.28e1 | 0.00 | 0.00 | 80: | 163 | 6.15e4 | 1.16 | 0.54 | 118: | 242 | 6.15e1 | 0.00 | 0.00 | 156: | 304 | 8.11e5 | 15.26 | 7.0 |
| 5: | 56 | 5.42e3 | 0.10 | 0.05 | 43: | 96 | 2.20e1 | 0.00 | 0.00 | 81: | 164 | 1.03e4 | 0.19 | 0.09 | 119: | 243 | 2.72e3 | 0.05 | 0.02 | 157: | 306 | 1.03e3 | 0.02 | 0.0 |
| 6: | 58 | 3.22e1 | 0.00 | 0.00 | 44: | 97 | 4.09e3 | 0.08 | 0.04 | 82: | 165 | 1.49e4 | 0.28 | 0.13 | 120: | 244 | 8.03e0 | 0.00 | 0.00 | 158: | 306 | 1.34e2 | 0.00 | 0.0 |
| 7: | 59 | 1.64e1 | 0.00 | 0.00 | 45: | 97 | 5.73e3 | 0.11 | 0.05 | 83: | 168 | 3.94e1 | 0.00 | 0.00 | 121: | 244 | 2.88e1 | 0.00 | 0.00 | 159: | 309 | 1.73e4 | 0.33 | 0.1 |
| 8: | 59 | 4.62e1 | 0.00 | 0.00 | 46: | 98 | 3.37e1 | 0.00 | 0.00 | 84: | 168 | 8.02e1 | 0.00 | 0.00 | 122: | 246 | 2.08e1 | 0.00 | 0.00 | 160: | 310 | 1.28e3 | 0.02 | 0.0 |
| 9: | 59 | 4.77e1 | 0.00 | 0.00 | 47: | 99 | 6.14e0 | 0.00 | 0.00 | 85: | 169 | 1.90e3 | 0.04 | 0.02 | 123: | 247 | 4.63e1 | 0.00 | 0.00 | 161: | 310 | 3.55e3 | 0.07 | 0.0 |
| 10: | 60 | 1.94e1 | 0.00 | 0.00 | 48: | 101 | 5.12e3 | 0.10 | 0.04 | 86: | 170 | 5.76e1 | 0.00 | 0.00 | 124: | 252 | 6.91e1 | 0.00 | 0.00 | 162: | 314 | 2.27e3 | 0.04 | 0.0 |
| 11: | 61 | 1.86e3 | 0.03 | 0.02 | 49: | 101 | 6.35e3 | 0.12 | 0.06 | 87: | 171 | 4.20e3 | 0.08 | 0.04 | 125: | 252 | 7.60e1 | 0.00 | 0.00 | 163: | 320 | 7.40e1 | 0.00 | 0.0 |
| 12: | 61 | 4.52e3 | 0.09 | 0.04 | 50: | 103 | 4.15e4 | 0.78 | 0.36 | 88: | 172 | 4.90e1 | 0.00 | 0.00 | 126: | 255 | 3.54e4 | 0.67 | 0.31 | 164: | 324 | 7.89e-3 | 0.00 | 0.0 |
| 13: | 63 | 2.55e3 | 0.05 | 0.02 | 51: | 105 | 9.06e0 | 0.00 | 0.00 | 89: | 174 | 1.80e1 | 0.00 | 0.00 | 127: | 256 | 1.21e2 | 0.00 | 0.00 | 165: | 324 | 8.02e1 | 0.00 | 0.0 |
| 14: | 63 | 5.54e3 | 0.10 | 0.05 | 52: | 107 | 8.68e1 | 0.00 | 0.00 | 90: | 178 | 1.61e2 | 0.00 | 0.00 | 128: | 257 | 2.14e3 | 0.04 | 0.02 | 166: | 327 | 6.33e1 | 0.00 | 0.0 |
| 15: | 64 | 2.17e3 | 0.04 | 0.02 | 53: | 108 | 7.32e1 | 0.00 | 0.00 | 91: | 179 | 2.77e3 | 0.05 | 0.02 | 129: | 259 | 5.70e1 | 0.00 | 0.00 | 167: | 330 | 3.00e0 | 0.00 | 0.0 |
| 16: | 66 | 2.21e1 | 0.00 | 0.00 | 54: | 109 | 1.91e-2 | 0.00 | 0.00 | 92: | 181 | 3.87e1 | 0.00 | 0.00 | 130: | 262 | 5.33e1 | 0.00 | 0.00 | 168: | 331 | 1.79e2 | 0.00 | 0.0 |
| 17: | 67 | 1.24e2 | 0.00 | 0.00 | 55: | 110 | 7.58e3 | 0.14 | 0.07 | 93: | 186 | 4.46e1 | 0.00 | 0.00 | 131: | 264 | 7.46e1 | 0.00 | 0.00 | 169: | 332 | 1.00e1 | 0.00 | 0.0 |
| 18: | 69 | 2.89e3 | 0.05 | 0.03 | 56: | 111 | 2.19e4 | 0.41 | 0.19 | 94: | 189 | 4.90e3 | 0.09 | 0.04 | 132: | 265 | 4.02e1 | 0.00 | 0.00 | 170: | 334 | 5.04e1 | 0.00 | 0.0 |
| 19: | 71 | 4.12e4 | 0.78 | 0.36 | 57: | 112 | 8.98e0 | 0.00 | 0.00 | 95: | 190 | 1.55e2 | 0.00 | 0.00 | 133: | 266 | 4.51e1 | 0.00 | 0.00 | 171: | 340 | 1.71e3 | 0.03 | 0.0 |
| 20: | 71 | 1.43e5 | 2.70 | 1.25 | 58: | 112 | 1.49e3 | 0.03 | 0.01 | 96: | 194 | 6.11e1 | 0.00 | 0.00 | 134: | 267 | 3.57e3 | 0.07 | 0.03 | 172: | 341 | 5.02e3 | 0.09 | 0.0 |
| 21: | 72 | 2.30e3 | 0.04 | 0.02 | 59: | 117 | 1.73e3 | 0.03 | 0.02 | 97: | 199 | 5.42e3 | 0.10 | 0.05 | 135: | 267 | 3.97e3 | 0.07 | 0.03 | 173: | 342 | 6.02e0 | 0.00 | 0.0 |
| 22: | 72 | 7.86e1 | 0.00 | 0.00 | 60: | 119 | 1.00e2 | 0.00 | 0.00 | 98: | 205 | 3.23e1 | 0.00 | 0.00 | 136: | 268 | 5.30e1 | 0.00 | 0.00 | 174: | 343 | 2.18e1 | 0.00 | 0.0 |
| 23: | 73 | 7.98e3 | 0.15 | 0.07 | 61: | 125 | 4.61e3 | 0.09 | 0.04 | 99: | 206 | 5.11e1 | 0.00 | 0.00 | 137: | 272 | 4.70e3 | 0.09 | 0.04 | 175: | 345 | 7.20e3 | 0.14 | 0.0 |
| 24: | 73 | 5.41e3 | 0.10 | 0.05 | 62: | 126 | 9.36e3 | 0.18 | 0.08 | 100: | 211 | 8.39e1 | 0.00 | 0.00 | 138: | 273 | 2.24e1 | 0.00 | 0.00 | 176: | 347 | 4.24e1 | 0.00 | 0.0 |
| 25: | 74 | 6.88e3 | 0.13 | 0.06 | 63: | 127 | 3.62e4 | 0.68 | 0.32 | 101: | 212 | 4.93e1 | 0.00 | 0.00 | 139: | 273 | 1.36e4 | 0.26 | 0.12 | 177: | 349 | 5.25e1 | 0.00 | 0.0 |
| 26: | 75 | 1.38e4 | 0.26 | 0.12 | 64: | 127 | 1.11e4 | 0.21 | 0.10 | 102: | 213 | 5.05e3 | 0.10 | 0.04 | 140: | 275 | 9.59e1 | 0.00 | 0.00 | 178: | 349 | 3.47e1 | 0.00 | 0.0 |
| 27: | 75 | 1.10e4 | 0.21 | 0.10 | 65: | 128 | 3.23e4 | 0.61 | 0.28 | 103: | 218 | 4.23e3 | 0.08 | 0.04 | 141: | 279 | 2.72e1 | 0.00 | 0.00 | 179: | 350 | 1.59e1 | 0.00 | 0.0 |
| 28: | 78 | 6.17e1 | 0.00 | 0.00 | 66: | 129 | 4.84e5 | 9.12 | 4.23 | 104: | 221 | 3.06e3 | 0.06 | 0.03 | 142: | 281 | 1.13e4 | 0.21 | 0.10 | 180: | 352 | 1.89e1 | 0.00 | 0.0 |
| 29: | 81 | 1.67e1 | 0.00 | 0.00 | 67: | 130 | 2.89e4 | 0.54 | 0.25 | 105: | 221 | 1.98e4 | 0.37 | 0.17 | 143: | 282 | 1.25e4 | 0.24 | 0.11 | 181: | 353 | 2.84e3 | 0.05 | 0.0 |
| 30: | 81 | 1.65e3 | 0.03 | 0.01 | 68: | 131 | 1.36e2 | 0.00 | 0.00 | 106: | 222 | 1.13e4 | 0.21 | 0.10 | 144: | 287 | 7.06e1 | 0.00 | 0.00 | 182: | 354 | 6.04e3 | 0.11 | 0.0 |
| 31: | 83 | 1.51e4 | 0.28 | 0.13 | 69: | 134 | 4.29e3 | 0.08 | 0.04 | 107: | 223 | 4.54e3 | 0.09 | 0.04 | 145: | 288 | 6.40e1 | 0.00 | 0.00 | 183: | 355 | 4.40e4 | 0.83 | 0.3 |
| 32: | 83 | 5.02e3 | 0.09 | 0.04 | 70: | 137 | 3.05e1 | 0.00 | 0.00 | 108: | 225 | 2.30e3 | 0.04 | 0.02 | 146: | 290 | 2.06e3 | 0.04 | 0.02 | 184: | 356 | 6.62e4 | 1.25 | 0.5 |
| 33: | 84 | 4.66e3 | 0.09 | 0.04 | 71: | 143 | 3.66e3 | 0.07 | 0.03 | 109: | 226 | 2.79e3 | 0.05 | 0.02 | 147: | 291 | 6.04e3 | 0.11 | 0.05 | 185: | 357 | 2.06e4 | 0.39 | 0.1 |
| 34: | 84 | 3.12e3 | 0.06 | 0.03 | 72: | 144 | 9.35e1 | 0.00 | 0.00 | 110: | 226 | 4.21e3 | 0.08 | 0.04 | 148: | 292 | 1.31e1 | 0.00 | 0.00 | 186: | 357 | 3.44e4 | 0.65 | 0.3 |
| 35: | 85 | 3.02e5 | 5.68 | 2.64 | 73: | 145 | 6.16e4 | 1.16 | 0.54 | 111: | 231 | 1.97e3 | 0.04 | 0.02 | 149: | 292 | 3.05e1 | 0.00 | 0.00 | 187: | 359 | 1.44e2 | 0.00 | 0.0 |
| 36: | 86 | 1.44e4 | 0.27 | 0.13 | 74: | 146 | 1.74e4 | 0.33 | 0.15 | 112: | 234 | 1.00e2 | 0.00 | 0.00 | 150: | 294 | 1.93e3 | 0.04 | 0.02 | 188: | 363 | 1.44e1 | 0.00 | 0.0 |
| 37: | 87 | 4.24e3 | 0.08 | 0.04 | 75: | 147 | 9.44e5 | 17.77 | 8.25 | 113: | 237 | 1.07e3 | 0.02 | 0.01 | 151: | 295 | 3.21e3 | 0.06 | 0.03 | 189: | 364 | 1.43e2 | 0.00 | 0.0 |
| 38: | 91 | 1.71e4 | 0.32 | 0.15 | 76: | 148 | 8.56e4 | 1.61 | 0.75 | 114: | 239 | 1.13e2 | 0.00 | 0.00 | 152: | 300 | 9.06e3 | 0.17 | 0.08 | 190: | 366 | 3.43e1 | 0.00 | 0.0 |

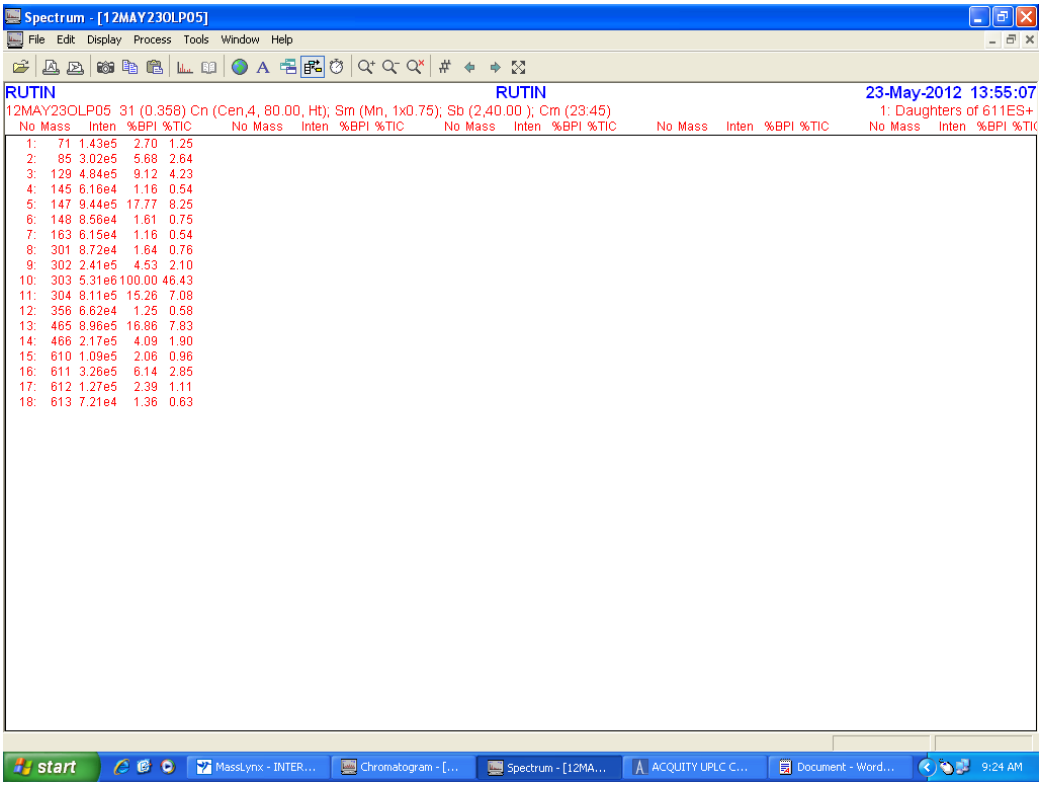
# Select view



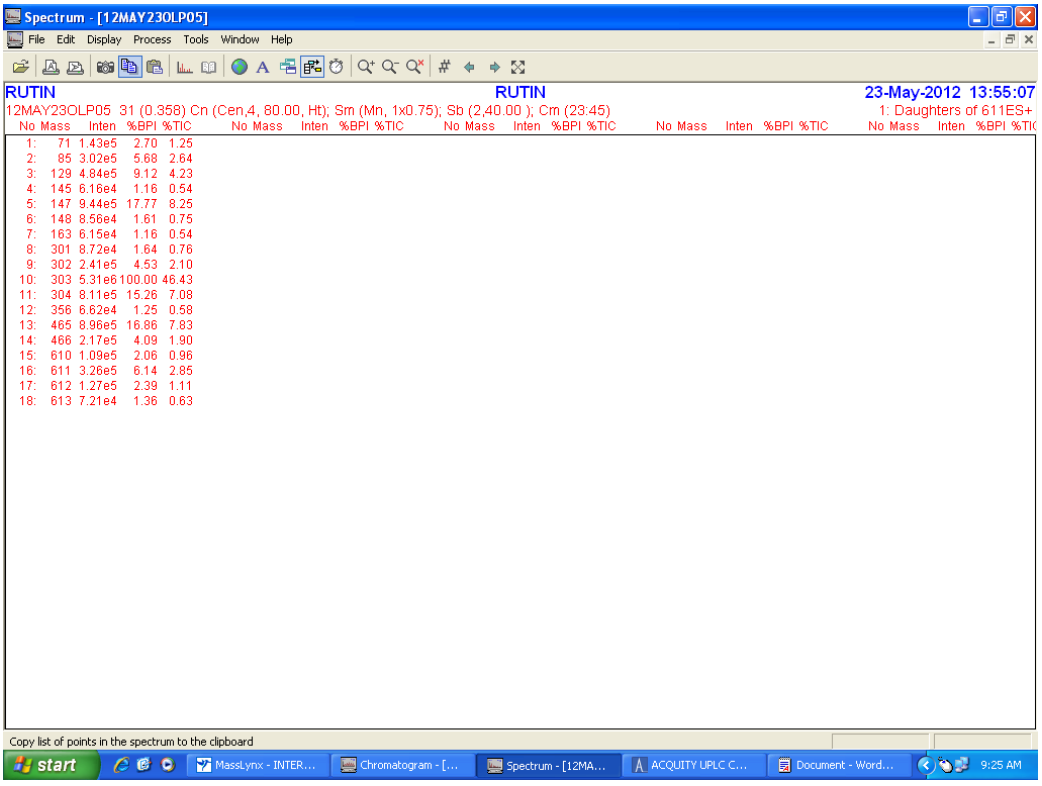

# Set data threshold 1-2% (for significant peak)



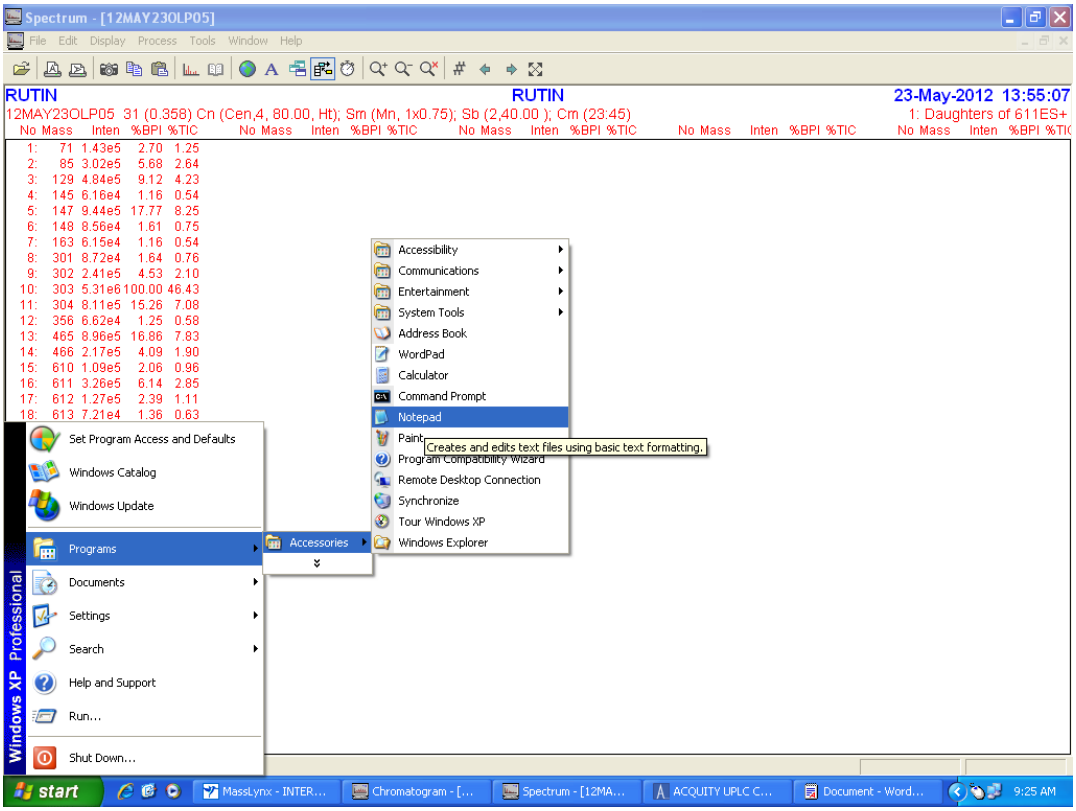
## Press ok (List out the major 25–30 peaks, if available.)



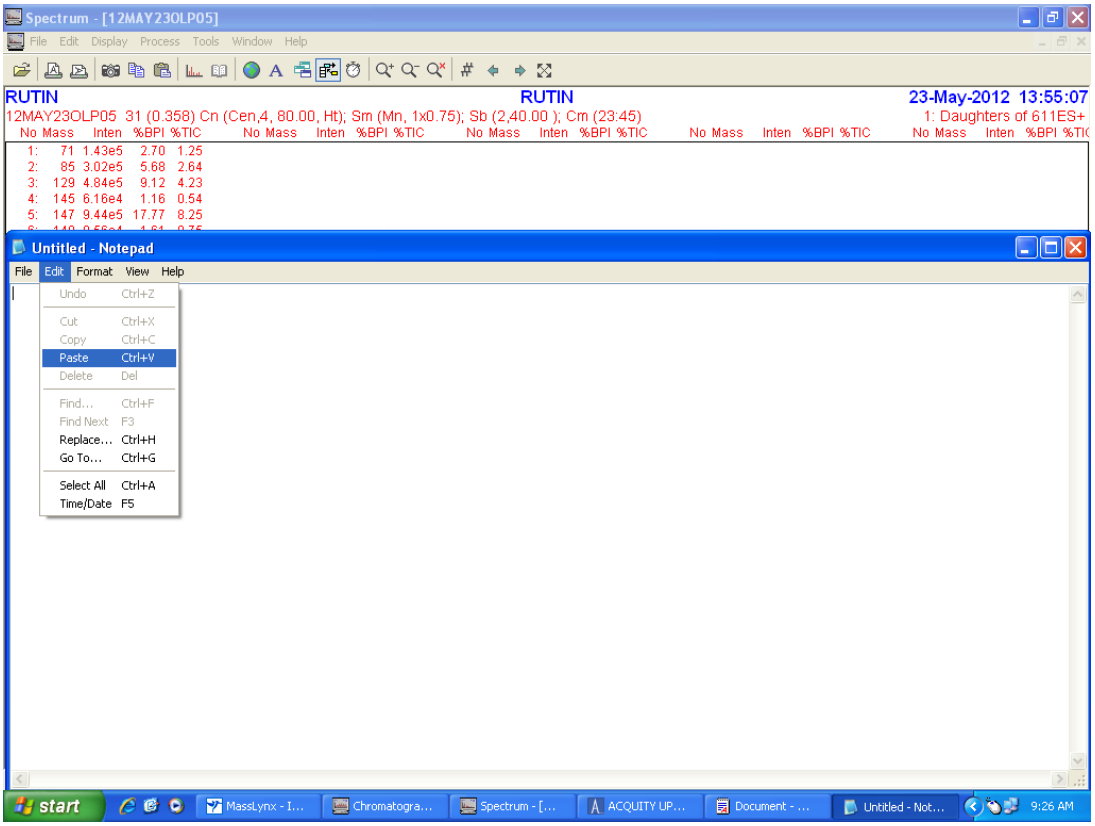

## Copy the list of ions



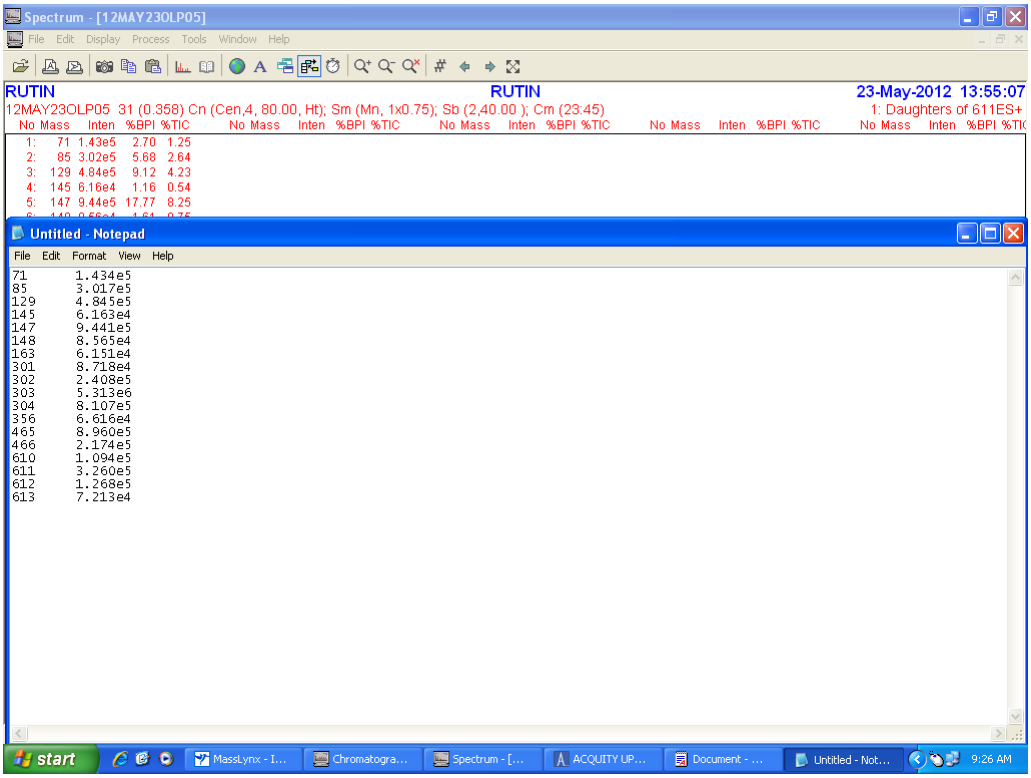
# Open Notepad



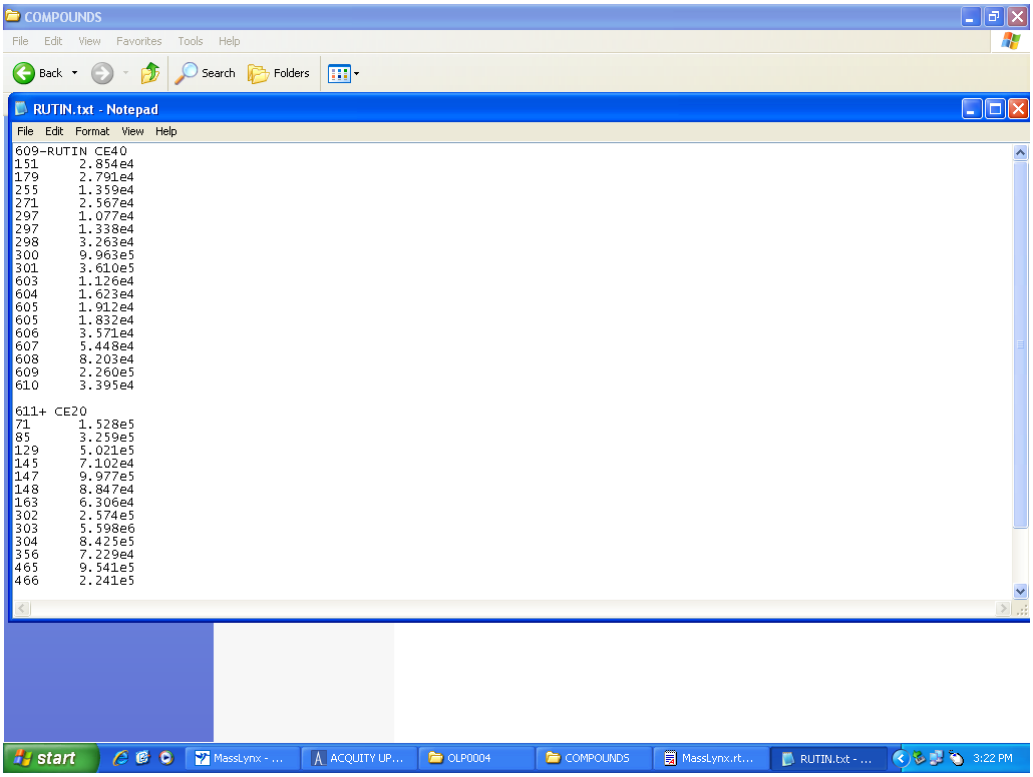

# Paste the ions list on note pad



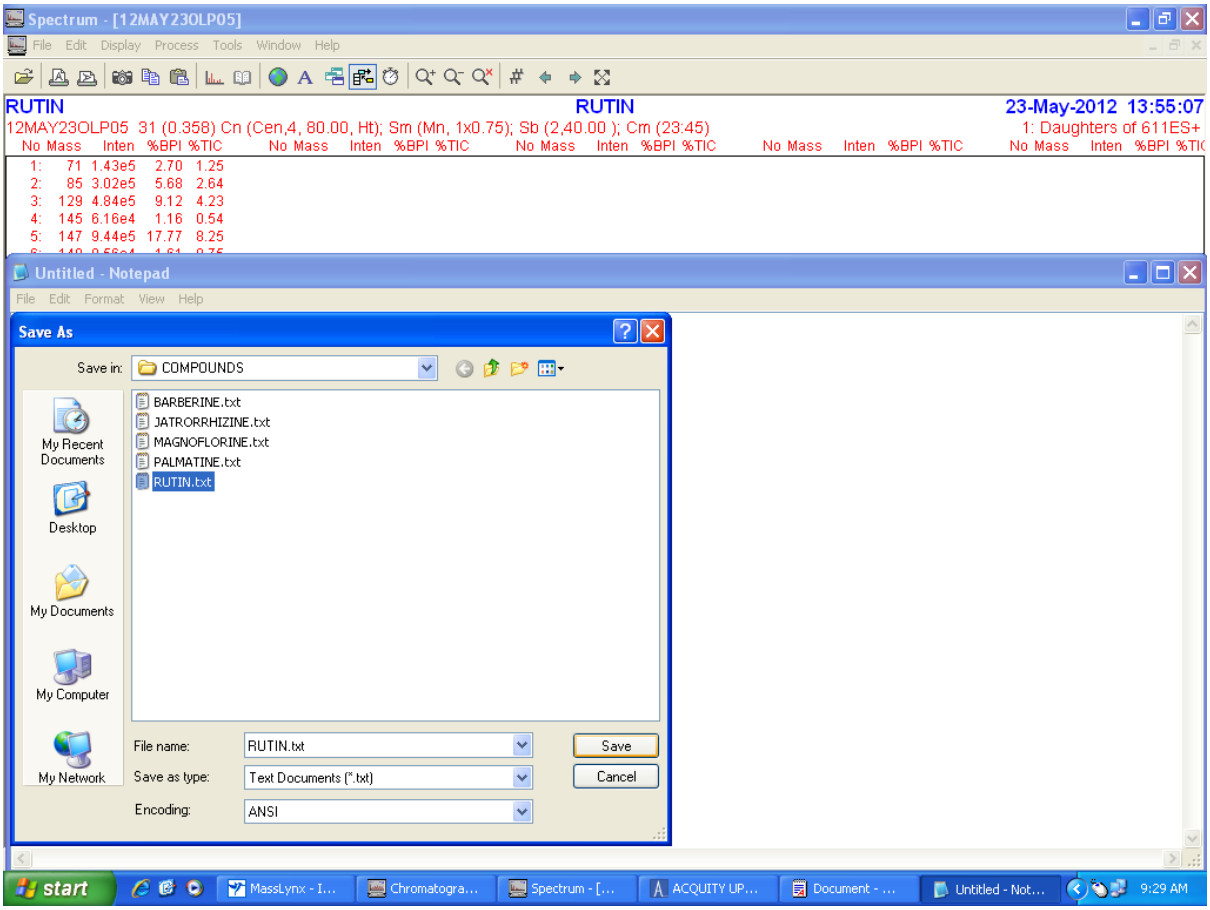
## Paste the ion list on a notepad.



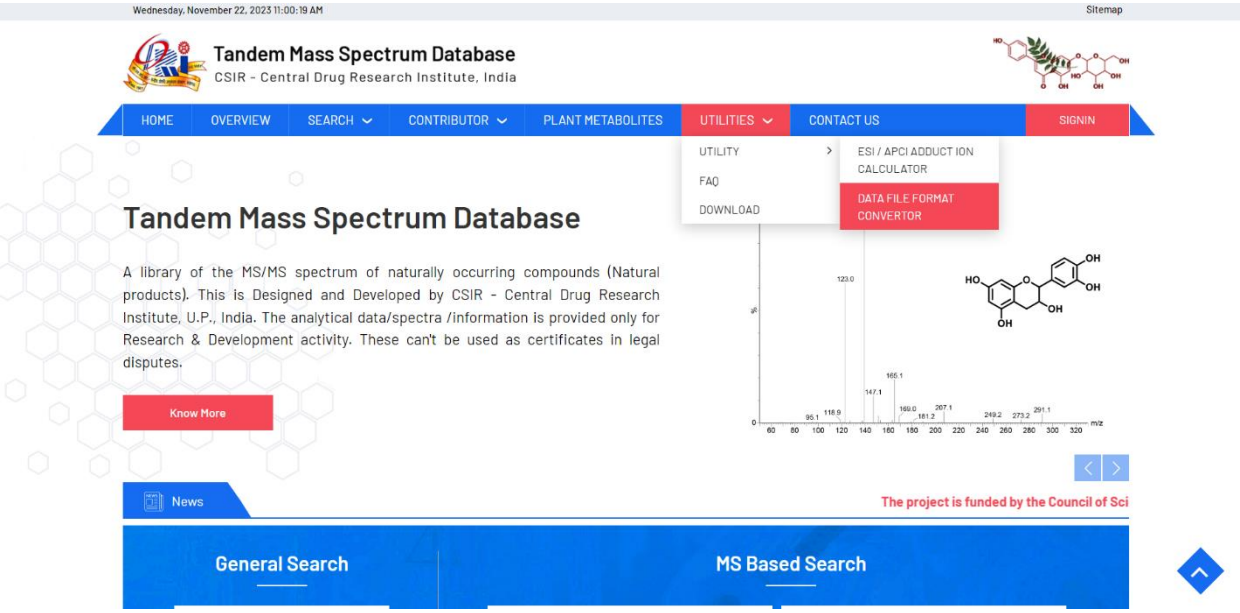

## Edit the notepad file with the precursor ion value, charge state, and collision energy as given below (611+ CE 20) or (609-CE 40).



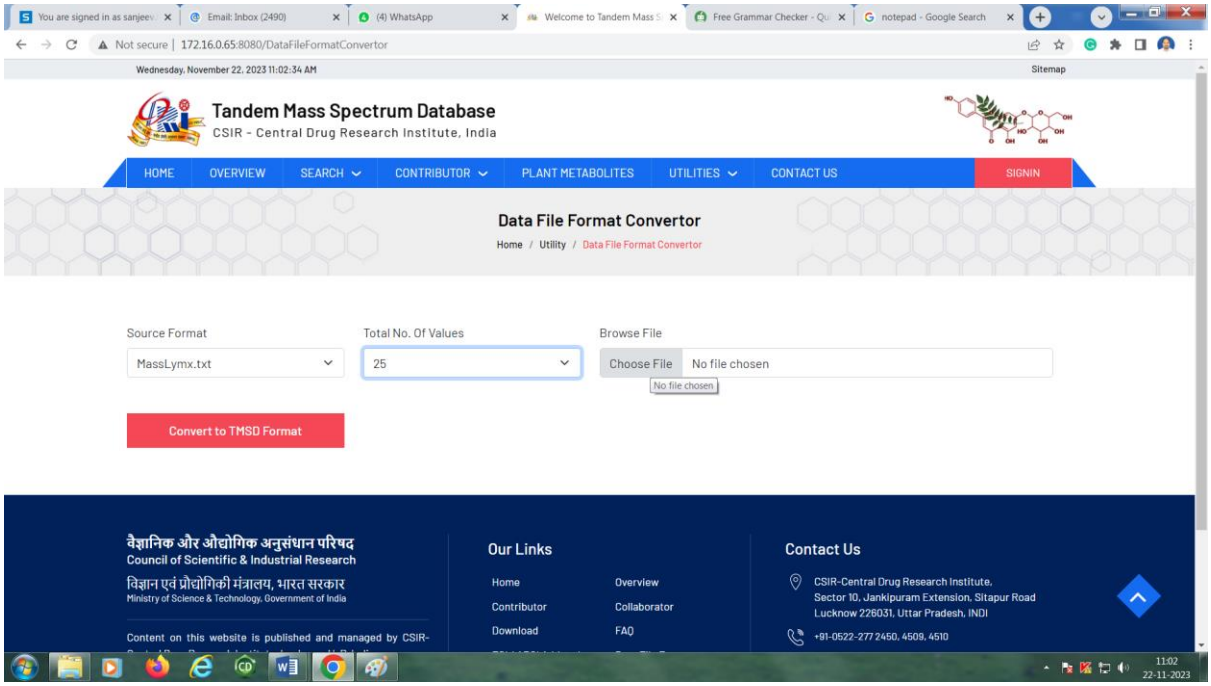

## Save the note pad file in *.txt format




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

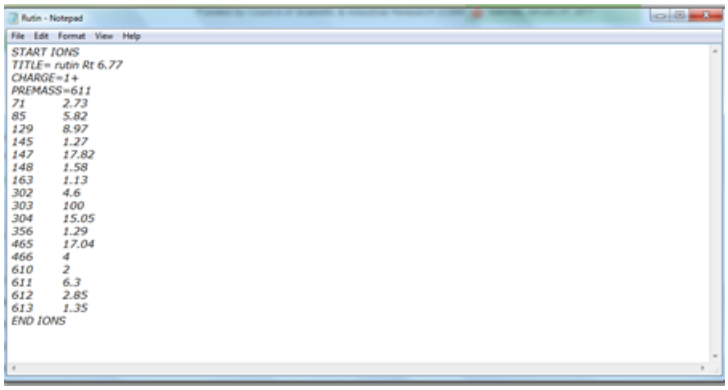


## Choose /browse note pad *.txt file




## 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:

- **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.**