# 2017

# Data File Format Conversion

| Tanden<br>CSIR - Cer      | CSIR - Central Drug Research Institute, India |                                |  |  |  |  |  |  |  |  |  |
|---------------------------|---|--------------------------------|--|--|--|--|--|--|--|--|--|
|                           | Funded by Council of Scientific 8             | Industrial Research (CSIR),    | India 🚯 Saturday, January 07, 2017                       |  |  |  |  |  |  |  |  |
| 🔒 Login                   | 229   | 257                            | 285 303  |  |  |  |  |  |  |  |  |
| User Name                 | MS/MS/MS                                      | MS/MS                          | MS но он   |  |  |  |  |  |  |  |  |
| Password                  |   |                                | HOLLEGOLOH   |  |  |  |  |  |  |  |  |
| Remember Me               | 257   |                                | 303<br>262   |  |  |  |  |  |  |  |  |
| LOGIN    Forget Password? | 230 259                                       | 229 247 261 2                  | 74 286 286 304   |  |  |  |  |  |  |  |  |
| New User? Register Here   | 189 201 215 240                               | 205 219 233 267                | 304 176 201 226 317 309                                  |  |  |  |  |  |  |  |  |
| 🕌 Home                    | Tandem Mass Spectrum Databa                   | se                             |  |  |  |  |  |  |  |  |  |
| 🚯 Overview                | TMS database is a library of MS/MS s          | nectrum of naturally occurri   | na compounds (Natural products). It is Designed and      |  |  |  |  |  |  |  |  |
| 🔏 Inventor                | Developed by CSIR - Central Drug Res          | earch Institute, India. The ar | alytical data/spectra /information are provided only for |  |  |  |  |  |  |  |  |
| Advisory Board            | Research & Development purposes. The          | se can't be used as certificat | es in legal disputes.                                    |  |  |  |  |  |  |  |  |
| 🔀 Collaborator            |   |                                |  |  |  |  |  |  |  |  |  |
| 🚱 Plant Metabolites       | Search Options                                |                                |  |  |  |  |  |  |  |  |  |
| 🧳 Contact Us              | General Searches                              | Mas                            | s Spectrometry Based Searches                            |  |  |  |  |  |  |  |  |
| 🧊 Download                | • Name  |                                | MS/MS Ion Search   |  |  |  |  |  |  |  |  |
| 🐼 Utility                 | Formula                                       |                                | Advanced Search  |  |  |  |  |  |  |  |  |
| 🕜 On-Line Help            | Molecular Weight     CAS Registry Number      | • (                            | Comprehensive Search                                     |  |  |  |  |  |  |  |  |

[ Available Database

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

| 🔜 Sp | ectru      | ım - [12  | MAY23      | OLPO   | 5]         |         |          |        |         |         |            |                  |          |      |       |         |        |        |         |           |      |           | _ 7    | ×    |
|------|------------|-----------|------------|--------|------------|---------|----------|--------|---------|---------|------------|------------------|----------|------|-------|---------|--------|--------|---------|-----------|------|-----------|--------|------|
| 📃 Fi | le Edil    | t Displa  | y Proce    | ss To  | ols Window | v Hel   | p        |        |         |         |            |                  |          |      |       |         |        |        |         |           |      |           | - ć    | 5 ×  |
| 2    | <b>A</b> ( | 2 6       | <b>b C</b> | lulua. |            | A       |          | ð   Q+ | Q- Q    | × # <   | <b>6</b> • | 23               |          |      |       |         |        |        |         |           |      |           |        |      |
| RUT  | 'IN        |           |            |        |            |         |          |        |         |         |            | RUTIN            |          |      |       |         |        |        |         | 23-       | May- | 2012      | 13:55  | :07  |
| 12M/ | Y230       | DLP05     | 31 (0.3    | 358) C | On (Cen,4  | , 80.   | 00, Ht); | Sm (M  | n, 1x0. | 75); Sb | (2,40      | 1.00 ); C        | m (23    | :45) |       |         |        |        |         | 1:        | Dau  | anters o  | f 611E | ES+  |
| No   | Mass       | Inten     | %ÊPI       | %TÍC   | No         | Mass    | Inten    | %BÈI   | %TIC    | No I    | Mass       | Inten            | %ÈPI     | %TÍC | No    | Mass    | Inten  | %BPI   | %TIC    | No I      | 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    | 00.00  | 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    | 55         | 5.4283    | 0.10       | 0.05   | 43:        | 96      | 2.2001   | 0.00   | 0.00    | 81:     | 164        | 1.0364           | 0.19     | 0.09 | 119:  | 243     | 2.7263 | 0.05   | 0.02    | 157:      | 306  | 1.0363    | 0.02   | 0.0  |
| 0:   | 58         | 3.2201    | 0.00       | 0.00   | 44:        | 97      | 4.0983   | 0.08   | 0.04    | 82.     | 100        | 1.4984           | 0.28     | 0.13 | 120:  | 244     | 3.0360 | 0.00   | 0.00    | 158:      | 300  | 1.3462    | 0.00   | 0.0  |
| 6    | 59         | 4.62e1    | 0.00       | 0.00   | 40.        | 97      | 3 37e1   | 0.00   | 0.05    | 84      | 168        | 3.9401<br>8.02e1 | 0.00     | 0.00 | 121.  | 244     | 2.0001 | 0.00   | 0.00    | 160       | 310  | 1.7364    | 0.33   | 0.0  |
| 9    | 59         | 4.77e1    | 0.00       | 0.00   | 47         | 99      | 614e0    | 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         | 2.8963    | 0.05       | 0.03   | 56:        | 111     | 2.1964   | 0.41   | 0.19    | 94:     | 189        | 4.90e3           | 0.09     | 0.04 | 132:  | 265     | 4.0201 | 0.00   | 0.00    | 170:      | 334  | 5.04e1    | 0.00   | 0.0  |
| 19:  | 71         | 4.1284    | 0.78       | 0.36   | 57:        | 112     | 8.98e0   | 0.00   | 0.00    | 95:     | 190        | 1.5582           | 0.00     | 0.00 | 133:  | 200     | 4.5101 | 0.00   | 0.00    | 171:      | 340  | 1.7183    | 0.03   | 0.0  |
| 20.  | 72         | 2 2062    | 2.70       | 0.02   | 50:        | 117     | 1,4983   | 0.03   | 0.01    | 90.     | 194        | 6.11e1           | 0.00     | 0.00 | 134.  | 207     | 3.5783 | 0.07   | 0.03    | 172       | 241  | 5.0283    | 0.09   | 0.0  |
| 21.  | 72         | 7 8661    | 0.04       | 0.02   | 60:        | 110     | 1.0002   | 0.00   | 0.02    | 97.     | 205        | 3,7361           | 0.00     | 0.00 | 136   | 267     | 5 3061 | 0.07   | 0.00    | 174       | 342  | 2 1 8 0 1 | 0.00   | 0.0  |
| 23   | 73         | 7 98e3    | 0.00       | 0.07   | 61         | 125     | 4.61e3   | 0.00   | 0.04    | 99.     | 205        | 5.11e1           | 0.00     | 0.00 | 137   | 272     | 4 70e3 | 0.00   | 0.00    | 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     | 2.0663 | 0.04   | 0.02    | 184:      | 356  | 6.62e4    | 1.25   | 0.5  |
| 33:  | 84         | 4.6683    | 0.09       | 0.04   | 71:        | 143     | 3.6683   | 0.07   | 0.03    | 109:    | 226        | 2.7983           | 0.05     | 0.02 | 147:  | 291     | 6.0463 | 0.11   | 0.05    | 185:      | 357  | 2.0664    | 0.39   | 0.1  |
| 34.  | 04         | 3.1283    | 0.00       | 2.64   | 12.        | 144     | 9.3581   | 0.00   | 0.00    | 110.    | 220        | 4.2183           | 0.08     | 0.04 | 148.  | 292     | 2.0561 | 0.00   | 0.00    | 180.      | 307  | 3.4484    | 0.00   | 0.3  |
| 36   | 88         | 1 4 4 6 4 | 0.27       | 0.13   | 7.5.       | 140     | 1 7/04   | 0.33   | 0.15    | 112     | 234        | 1.0062           | 0.04     | 0.02 | 140.  | 292     | 1.0363 | 0.00   | 0.00    | 199       | 262  | 1.4462    | 0.00   | 0.0  |
| 37   | 87         | 4 24e3    | 0.08       | 0.04   | 75         | 147     | 9 44 65  | 17.77  | 8.25    | 113     | 237        | 1.07e3           | 0.02     | 0.00 | 151   | 295     | 3.21e3 | 0.04   | 0.02    | 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  |
| <    |            |           |            |        | 10         |         |          |        |         |         |            | 1.00             |          |      |       | 1000    |        | 100000 |         |           |      |           |        | >    |
|      |            |           |            |        |            |         |          |        |         |         |            |                  |          |      |       |         |        |        | Γ       |           |      |           |        | _    |
| -    | star       |           | 6 6        | 0      | Massi vr   | nx - IN | TER      | Ch     | omatogr | am - Г  | Į.         | Spectrum         | o - [12M | Α    | A ACO | JITY UP | ιc c   |        | Documer | nt - Word | 1    | 50.2      | 9:22.4 | M    |

| Sel | ect | view  |  |
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| JCI | CLL | VICVV |  |

| Sner     | ctrum       | - F12M        | AY 230   | DI P051 |         |        |           |       |         |          |          |                  |          |       |        |     |                  |        |        |           |      |          | ीन     |       |
|----------|-------------|---------------|----------|---------|---------|--------|-----------|-------|---------|----------|----------|------------------|----------|-------|--------|-----|------------------|--------|--------|-----------|------|----------|--------|-------|
| File     | Edit        | Display       | Proces:  | s Tools | Windov  | v Hel  | D         |       |         |          |          |                  |          |       |        |     |                  |        |        |           |      |          | - 6    | J X   |
| ~ 5      | 2) ISA      | Specti        | rum      | •       |         |        |           | 3 0   | 0-0     | × #      | <u> </u> | <b>K</b> .3      |          |       |        |     |                  |        |        |           |      |          |        |       |
|          | ය සෙ        | Remo          | ve       |         |         | AH     |           | 9 4   | 40      | <   m    | ~ ~      | к'я              |          |       |        |     |                  |        |        |           |      |          |        |       |
| RUTIN    | •           | Real-1        | Time Upo | date    |         |        |           |       |         |          |          | RUTIN            |          |       |        |     |                  |        |        | 23-       | May- | 2012     | 13:55  | :07   |
| 12MAY    | 2301        | Range         | •        | •       | en,4    | , 80.0 | 00, Ht);  | Sm (M | n, 1x0  | .75); Sb | (2,40    | 1.00 ); C        | m (23    | :45)  | NI-    |     | Indexe           | or DDL | or TIO | 1:        | Daug | ghters c | f 611E | BS+   |
| 11       | ass<br>61.0 |               |          |         | 20-     | 02     | 2 1 0 0 1 | %BPI  | 0.00    | 77:      | 160      | 6 00o1           | %BPI     | 20110 | 115    | 240 | 4 1 0 o 0        | %8PI   | 20110  | 162       | 901  | 9 72o4   | 208PT  | 20110 |
| 2:       | 55 6        | ✓ List Sp     | oectrum  |         | 40:     | 94     | 1.90e1    | 0.00  | 0.00    | 78:      | 162      | 4.84e3           | 0.00     | 0.00  | 116:   | 240 | 4.10e0           | 0.00   | 0.00   | 153.      | 302  | 2.41e5   | 4.53   | 2.1   |
| 3:       | 55 :        | View          |          |         | 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   | 00.00  | 46.4  |
| 4:       | 56 1        | Peak          | Annotat  | ION     | 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 (        | Custo         | mize i o | olbar   | 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   |
| 5        | - 58 i      | 🗸 Toolba      | ar       |         | 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   |
| 8        | 59 4        | 🗸 Status      | s bar    |         | 40.     | 98     | 3.37e1    | 0.00  | 0.05    | 84       | 168      | 3.94e1<br>8.02e1 | 0.00     | 0.00  | 121.   | 244 | 2.00e1<br>2.08e1 | 0.00   | 0.00   | 160:      | 310  | 1.7364   | 0.33   | 0.1   |
| 9:       | 59 4        | Move          | To Last  |         | 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        | Move          | To First |         | 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        | Graph         | is is    |         | 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        | 66.00         | 0.05     | 0.00    | 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   |
| 1.3.     | 62.4        | 6463          | 0.05     | 0.02    | 52      | 105    | 9.0000    | 0.00  | 0.00    | 00.      | 179      | 1.6162           | 0.00     | 0.00  | 127.   | 200 | 21462            | 0.00   | 0.00   | 166:      | 324  | 6.2261   | 0.00   | 0.0   |
| 15:      | 64 2        | 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        | 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        | 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        | 4205          | 0.78     | 0.36    | 570     | 112    | 8.98e0    | 0.00  | 0.00    | 95:      | 190      | 1.5582           | 0.00     | 0.00  | 133:   | 266 | 4.5101           | 0.00   | 0.00   | 171:      | 340  | 1./103   | 0.03   | 0.0   |
| 20.      | 72 3        | .4365<br>30e3 | 0.04     | 0.02    | 59      | 117    | 1.4363    | 0.03  | 0.01    | 97       | 199      | 5.47e3           | 0.00     | 0.00  | 135    | 267 | 3.9763           | 0.07   | 0.03   | 173       | 347  | 6.02e3   | 0.05   | 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        | 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 8        | 5.88e3        | 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   |
| 20:      | 75 1        | .3864         | 0.20     | 0.12    | 65      | 127    | 3,2364    | 0.21  | 0.10    | 102:     | 213      | 5.05e3<br>4.23e3 | 0.10     | 0.04  | 140:   | 2/5 | 9.5981           | 0.00   | 0.00   | 178:      | 349  | 3.4781   | 0.00   | 0.0   |
| 28       | 78 6        | 17e1          | 0.21     | 0.00    | 661     | 129    | 4 84e5    | 9.12  | 4 23    | 104      | 2210     | 3.06e3           | 0.08     | 0.04  | 142    | 281 | 1.13e4           | 0.00   | 0.00   | 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:      | 04 7        | 0.0283        | 0.09     | 0.04    | 70:     | 137    | 3.0561    | 0.00  | 0.00    | 108:     | 225      | 2.3083           | 0.04     | 0.02  | 140:   | 290 | 2.0683           | 0.04   | 0.02   | 184:      | 355  | 0.0204   | 1.25   | 0.5   |
| 34       | 84 3        | 12e3          | 0.09     | 0.04    | 72      | 143    | 9.35e1    | 0.07  | 0.03    | 110      | 220      | 4 21 983         | 0.05     | 0.02  | 147.   | 291 | 0.04e5           | 0.11   | 0.05   | 186       | 367  | 3.44e4   | 0.59   | 0.1   |
| 35:      | 85 3        | 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           | U.00     | U.00  | 152:   | 300 | 9.06e3           | 0.17   | 0.08   | 190:      | 366  | 3.43e1   | 0.00   | 0.0   |
|          | 0. 44       |               |          |         | _       |        | -         | _     |         | _        | -        | _                | _        | _     | _      | _   | _                | _      | -      |           | _    | -        | _      | >     |
| Set spec | trum d      | isplay par    | ameters  |         |         |        |           |       |         |          | _        |                  |          |       |        |     | _                |        |        |           | _    |          |        |       |
| 🦰 🛃 Si   | tart        | C             | 6        | 3 7     | MassLyn |        |           | Ch 🔤  | romatog | ram - [  |          | Spectru          | m - [12M | A     | A ACQL |     |                  |        | Docume | nt - Word |      | 000      | 9:23 A | аM    |

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

| 🔜 Spectrum - [12MAY230LP05]  |   |  |                                    |                |                                   |           |  |  |  |  |  |
|--|---|--|------------------------------------|----------------|-----------------------------------|-----------|--|--|--|--|--|
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| RUTIN 23-May-2012 13:55:07   |   |  |                                    |                |                                   |           |  |  |  |  |  |
| 12MAY23OLP05 31 Spectrum Display   |   | Cm (23:45)                                   |                                    |                | 1: Daughters of                   | f 611ES+  |  |  |  |  |  |
| No Mass Inten % Normalize Data To :                                      | Style   | n %BPI %TIC                                  | No Mass Inten                      | %BPI %TIC N    | lo Mass Inten                     | %BPI %TIC |  |  |  |  |  |
| 1: 51 6.94e1 0   | Dverlau Graphs                                  | 1 0.00 0.00                                  | 115: 240 4.10e0                    | 0.00 0.00 15   | 3: 301 8.72e4                     | 1.64 0.7  |  |  |  |  |  |
| 2: 55 5.00001 U Cargest Peak on Display                                  |   | 3 0.09 0.04                                  | 110. 241 1.0901                    | 0.00 0.00 15   | 4. 302 2.4100<br>6: 202 5.21e61   | 4.53 2.1  |  |  |  |  |  |
| 4: 56 2.63e1 Base Peak in Spectrum                                       | Graph Header                                    | 4 1.16 0.54                                  | 118: 242 6.15e1                    | 0.00 0.00 15   | 6: 304 8.11e5                     | 15.26 7.0 |  |  |  |  |  |
| 5: 56 5.42e3 C Mass 0.00   | Process Description                             | 4 0.19 0.09                                  | 119: 243 2.72e3                    | 0.05 0.02 15   | 7: 306 1.03e3                     | 0.02 0.0  |  |  |  |  |  |
| 6: 58 3.22e1 C   | Component Table                                 | 4 0.28 0.13                                  | 120: 244 8.03e0                    | 0.00 0.00 15   | 8: 306 1.34e2                     | 0.00 0.0  |  |  |  |  |  |
| 7: 59 1.64e1 O Intensity 0   | Chou Magative Data                              | 1 0.00 0.00                                  | 121: 244 2.88e1                    | 0.00 0.00 15   | 9: 309 1.73e4                     | 0.33 0.1  |  |  |  |  |  |
| 8: 59 4.6201 U   | Show wegative bata                              | 1 0.00 0.00                                  | 122: 246 2.0861                    | 0.00 0.00 16   | 0: 310 1.2863                     | 0.02 0.0  |  |  |  |  |  |
| 10: 60 1 94e1  | Show Zero Level                                 | 1 0.00 0.02                                  | 124: 252 6.91e1                    | 0.00 0.00 16   | 2: 314 2 27e3                     | 0.07 0.0  |  |  |  |  |  |
| 11: 61 1.86e3 0 💿 Baseline 0   | Hide Lock Mass Peaks                            | 3 0.08 0.04                                  | 125: 252 7.60e1                    | 0.00 0.00 16   | 3: 320 7.40e1                     | 0.00 0.0  |  |  |  |  |  |
| 12: 61 4.52e3 C  |   | 1 0.00 0.00                                  | 126: 255 3.54e4                    | 0.67 0.31 16   | 4: 324 7.89e-3                    | 0.00 0.0  |  |  |  |  |  |
| 13: 63 2.55e3 C  | Fill Trace No.                                  | 1 0.00 0.00                                  | 127: 256 1.21e2                    | 0.00 0.00 16   | 5: 324 8.02e1                     | 0.00 0.0  |  |  |  |  |  |
| 14: 63 5.54e3 Data Threshold   | rii Hace  | 2 0.00 0.00                                  | 128: 257 2.14e3                    | 0.04 0.02 16   | 6: 327 6.33e1                     | 0.00 0.0  |  |  |  |  |  |
| 15. 64 2.1783 U<br>16: 66 2.21e1 U @ % Full Scale 1.0                    | Solit Axis                                      |  | 129. 209 0.7001<br>130: 262 5.33e1 | 0.00 0.00 16   | 7. 330 3.0000<br>8. 331 1.79e2    | 0.00 0.0  |  |  |  |  |  |
| 17: 67 1.24e2  |   | 1 0.00 0.00                                  | 131: 264 7.46e1                    | 0.00 0.00 16   | 9: 332 1.00e1                     | 0.00 0.0  |  |  |  |  |  |
| 18: 69 2.89e3 0 O Intensity 0  | Overlay Sten × (%)                              | 3 0.09 0.04                                  | 132: 265 4.02e1                    | 0.00 0.00 17   | 0: 334 5.04e1                     | 0.00 0.0  |  |  |  |  |  |
| 19: 71 4.12e4 C  |   | 2 0.00 0.00                                  | 133: 266 4.51e1                    | 0.00 0.00 17   | 1: 340 1.71e3                     | 0.03 0.0  |  |  |  |  |  |
| 20: 71 1.43e5 2 MRM Mass Option  | Overlau Step Y (%)                              | 1 0.00 0.00                                  | 134: 267 3.57e3                    | 0.07 0.03 17   | 2: 341 5.02e3                     | 0.09 0.0  |  |  |  |  |  |
| 21: 72 2.30e3<br>22: 72 7.96e1<br>MRM Parent Ions                        |   | 3 0.10 0.05                                  | 135: 267 3.9763                    | 0.07 0.03 17   | 3: 342 6.02e0                     | 0.00 0.0  |  |  |  |  |  |
| 22. 72 7.00e1 0<br>23. 73 7 98e3 0 OMRM Daughter lons                    | Grid Off  |  | 137: 272 4 70e3                    | 0.00 0.00 17   | <ol> <li>5: 345 7 20e3</li> </ol> | 0.00 0.0  |  |  |  |  |  |
| 24: 73 5.41e3  |   | 1 0.00 0.00                                  | 138: 273 2.24e1                    | 0.00 0.00 17   | 6: 347 4.24e1                     | 0.00 0.0  |  |  |  |  |  |
| 25: 74 6.88e3 C  | OK Council II                                   | 1 0.00 0.00                                  | 139: 273 1.36e4                    | 0.26 0.12 17   | 7: 349 5.25e1                     | 0.00 0.0  |  |  |  |  |  |
| 26: 75 1.38e4 C  |   | ade 3 0.10 0.04                              | 140: 275 9.59e1                    | 0.00 0.00 17   | 8: 349 3.47e1                     | 0.00 0.0  |  |  |  |  |  |
| 27: 75 1.10e4 0  |   | 3 0.08 0.04                                  | 141: 279 2.72e1                    | 0.00 0.00 17   | 9: 350 1.59e1                     | 0.00 0.0  |  |  |  |  |  |
| 28: 78 0.1781 0.00 0.00 67: 120 2.0                                      | 04 0.54 0.25 105: 2                             | 21 1 0004 0 27 0 17                          | 142: 281 1.1384                    | 0.21 0.10 18   | 0: 352 1.8981                     | 0.00 0.0  |  |  |  |  |  |
| 30° 81 1.67e1 0.00 0.00 0.00 07. 130 2.0                                 | ie2 0.00 0.00 106 2                             | 221 1.3084 0.37 0.17                         | 144: 287 7 06e1                    | 0.00 0.00 18   | 2: 354 6.04e3                     | 0.03 0.0  |  |  |  |  |  |
| 31: 83 1.51e4 0.28 0.13 69: 134 4.29                                     | le3 0.08 0.04 107: 2                            | 23 4.54e3 0.09 0.04                          | 145: 288 6.40e1                    | 0.00 0.00 18   | 3: 355 4.40e4                     | 0.83 0.3  |  |  |  |  |  |
| 32: 83 5.02e3 0.09 0.04 70: 137 3.0                                      | ie1 0.00 0.00 108: 2                            | 25 2.30e3 0.04 0.02                          | 146: 290 2.06e3                    | 0.04 0.02 18   | 4: 356 6.62e4                     | 1.25 0.5  |  |  |  |  |  |
| 33: 84 4.66e3 0.09 0.04 71: 143 3.6                                      | ie3 0.07 0.03 109: 2                            | 26 2.79e3 0.05 0.02                          | 147: 291 6.04e3                    | 0.11 0.05 18   | 5: 357 2.06e4                     | 0.39 0.1  |  |  |  |  |  |
| 34: 84 3.12e3 0.06 0.03 72: 144 9.3                                      | e1 0.00 0.00 110: 2                             | 26 4.21e3 0.08 0.04                          | 148: 292 1.31e1                    | 0.00 0.00 18   | 6: 357 3.44e4                     | 0.65 0.3  |  |  |  |  |  |
| 30. 00 3.0200 0.08 2.04 73: 145 0.10 36: 86 1.44e4 0.27 0.13 74: 146 1.7 | e4 i.10 0.34 - 111: 2<br>.e4 0.33 0.15 - 112: 2 | 131 1.9783 0.04 0.02<br>234 1.00e2 0.00 0.00 | 149. 292 3.0581<br>150° 294 1.93e3 | 0.00 0.00 18   | 7. 309 1.4462<br>8: 363 1.4461    | 0.00 0.0  |  |  |  |  |  |
| 37: 87 4.24e3 0.08 0.04 75: 147 9.4                                      | e5 17.77 8.25 113: 2                            | 237 1.07e3 0.02 0.01                         | 151: 295 3.21e3                    | 0.06 0.03 18   | 9: 364 1.43e2                     | 0.00 0.0  |  |  |  |  |  |
| 38: 91 1.71e4 0.32 0.15 76: 148 8.5                                      | ie4 1.61 0.75 114: 2                            | 39 1.13e2 0.00 0.00                          | 152: 300 9.06e3                    | 0.17 0.08 19   | 0: 366 3.43e1                     | 0.00 0.0  |  |  |  |  |  |
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| RUTIN         RUTIN           12MAY230LP05         31 (0.358) Cn (Cen,4, 80.00, Ht); Sm (Mn, 1x0.75); Sb (2,40.00 ); Cm (23:45)<br>No Mass Inten %BPI %TIC         No Mass Inten %BPI %TIC | No Mass Inten    | 23-May-2<br>1: Daug<br>%BPI %TIC No Mass | 2012 13:55:07<br>hters of 611ES+<br>Inten %BPI %TI( |
| 1: /1 1.43eb 2./U 1.25<br>2: 85 302e5 5.68 2.64<br>3: 129 4.94e5 9.12 4.23<br>4: 145 6.16e4 1.16 0.54<br>5: 147 9.44e5 17.77 8.25<br>6: 449 0.65e4 1.62 3.5                                |                  |  |   |
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| 12: 356 6.62e4 1.25 0.58<br>13: 465 0.96e5 16.66 7.83<br>14: 466 2.17e5 4.09 1.90<br>15: 610 1.09e5 2.06 0.96<br>16: 611 3.26e5 6.14 2.85  |                  |  |   |
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| b: 148 8.5664 1.61 U./5<br>7: 163 61564 1.16 0.54  |  |
| 8: 301 87294 164 076   |  |
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| 10: 303 5.31e6100.00 46.43 m Entertainment   |  |
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| 14: 466 2.17e5 4.09 1.90   |  |
| 15: 610 1.09e5 2.06 0.96   |  |
| 16: 611 3.26e5 6.14 2.85   |  |
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#### 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.