# Waters<sup>™</sup>

#### Applikationsbericht

# TransOmics Informatics Powered by Nonlinear Dynamics

Lee A. Gethings, Martha D. Stapels, Ian Mons, Jackson Pope, James I. Langridge

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# Abstract

In this application note, we introduce the workflow of TransOmics Informatics Software that has been specifically developed for the larger scale analysis of ion mobility MS data from proteomics and metabolomics data sets, comprising technical and biological replicates.

#### Benefits

- Perform large scale analysis of ion mobility MS data from proteomics and metabolomics data sets using TransOmics Informatics Software.
- · Provides 100% matching of all LC-MS features with no missing values.

# Introduction

MS<sup>E</sup> and HDMS<sup>E</sup> are LC-MS-based acquisition strategies for life sciences that can be used for a variety of

research focused applications and applied to the ACQUITY UPLC System and oa-Tof-based mass spectrometry platforms, including the SYNAPT G2-S HDMS System. In LC-HDMS<sup>E</sup>-based acquisitions, ions are separated in the gas phase by ion mobility and subsequently, the energy applied to the collision cell is alternated between a low and elevated state on a scan-to-scan basis, providing both qualitative and quantitative accurate mass precursor and product ion information that is retention and drift time aligned. The challenge is to make use of the high quality ion mobility resolved data that are generated. In this application note, we introduce the workflow of TransOmics Informatics Software that has been specifically developed for the larger scale analysis of ion mobility MS data from proteomics and metabolomics data sets, comprising technical and biological replicates.

## Experimental

Three replicates of each E.coli sample, differentially spiked with bovine serum albumin (BSA), alcohol dehydrogenase (ADH), Enolase and Glycogen phosphorylase B were analyzed. The injected on-column amounts for the spike protein in the first sample (Mixture 1) were 500 attomoles each and 4000, 500, 1000 and 250 attomoles for the second sample (Mixture 2), respectively. The peptides were separated and analyzed using a nanoACQUITY UPLC System coupled with a SYNAPT G2-S, operating at a mass resolution of >20k FWHM. The data were acquired in either LC-MS<sup>E</sup> or HDLC-MS<sup>E</sup> mode, an unbiased acquisition method in which the mass spectrometer switches between low and elevated energy on alternate scans with or without including ion mobility separation, respectively.

#### **Results and Discussion**

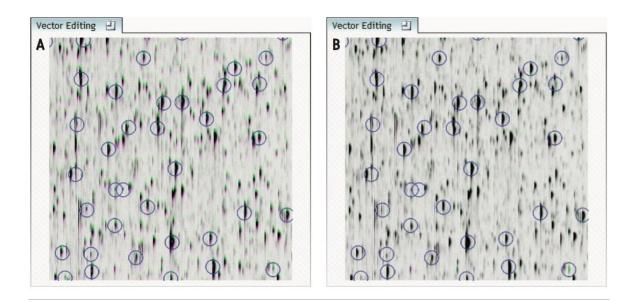
#### Peak modeling

Online LC-MS instrumentation can generate considerable volumes of raw data, which often makes it impractical to run large numbers of biological and technical replicates. To overcome this, Nonlinear Dynamics developed an intelligent peak-modeling algorithm that can reduce data files by an order of magnitude. Using a wavelet-based approach, peaks are identified and peak models are created, and all relevant quantification and positional information is retained. TransOmics Informatics Software supports a number of common raw and processed data

generated by LC-MS instruments.

#### **Run Alignment**

The ability to combine data from multiple data independent analysis (DIA), UPLC-MS<sup>E</sup> or UPLC-HDMS<sup>E</sup> is required for comparative expression profiling studies. This enables the comparison of different experimental conditions or time-course studies using a high number of replicates. To combine and compare results from different runs, TransOmics Informatics Software aligns injections to compensate for between-run variations in the LC separation technique, shown in Figures 1 and 2. This results in increased reliability and reproducibility.



*Figure 1. LC-MS runs represented as m/z versus retention time overlaid: (A) unaligned runs; (B) aligned runs.* 

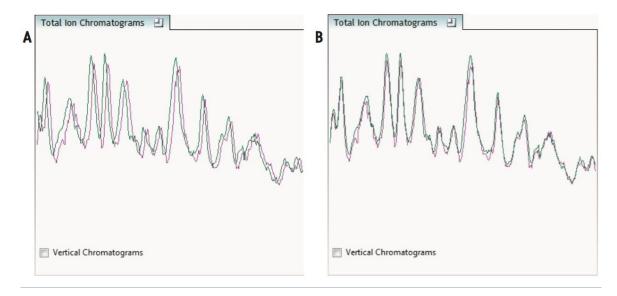


Figure 2. Total ion chromatogram view: (A) unaligned runs; (B) aligned runs.

#### Peak Picking

To ensure consistent peak picking and matching across all data files, an aggregate data set is created from the aligned runs. This data set contains all peak information from all sample files, allowing the detection of a single map of peptide ions. This map is applied to each sample, giving 100% matching of all chromatographic peaks with no missing values, enabling the application of multivariate statistical tools to explore data and measure differential analysis.

The peak picking algorithm handles complex samples and can discern overlapping isotopic peptide ion distributions. The end result is highly accurate detection, which saves time further down the workflow. The ion mobility separation of chromatographically co-eluting isotopic distributions is shown in Figure 3. It also generates complete datasets that contain no missing values, which allows obtaining reliable results from the multivariate statistical tools.

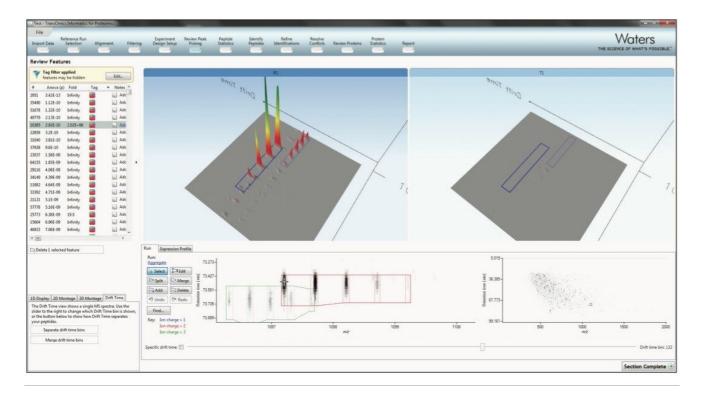


Figure 3. Ion abundance quantification.

For the most accurate measurements, survey scan or low energy MS<sup>E</sup> data is used for quantitation. This significantly outperforms spectral counting, and allows for quantitation of peptide ions without (DIA) MS<sup>E</sup> or data directed analysis (DDA) MS/MS data. Additional fragmentation data can be gathered after the data analysis, using either a targeted DDA inclusion list or a non-targeted DIA experiment. After measuring each of the runs, the data are then normalized, so comparisons can be made between the runs.

#### Statistical analysis of peptide ions

Using advanced statistical tools – including ANOVA, power analysis, and q-values (for false discovery rate) – peptides can be user selected for identification.

#### Peptide identification

MS<sup>E</sup> and HDMS<sup>E</sup> search results can be appended to the aggregate and quantitative results. Alternatively, once a list of peptide ions has been selected to be identified, the fragmentation data can be exported for searching using any of the search engines (e.g. PLGS, MASCOT, etc.) and databases supported.

For any features that do not have fragmentation data, a targeted inclusion list can be exported for a subsequent sample injection to gather further targeted MS/MS data, to increase the identification coverage for the peptides of interest.

#### Review the proteins of interest

Quantitative data and qualitative fragmentation spectra search results are brought together to produce a peptide-based view of potentially interesting proteins in the experiment, with the ability to resolve conflicts when a peptide sequence is associated with more than one protein. It is easy to tag unique peptides and select the best ones as candidates for future MRM studies.

A final list of interesting proteins and their measurements, including a display of quantitative profiles in each group is automatically generated, as shown in Figure 4. Protein quantitation is based solely upon unique peptides. This provides reliable quantification for biological studies and publications.

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20     1308     5%     4     107548     1.23     1.84     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     2     1.307-64     3     0     1.207-26     1.307-64     3     0     1.207-26     1.307-64     3     0     1.207-26     1.307-64     3     0     1.207-26     1.307-64     3     0     1.207-26     0     1	Protect actions - Trend Tee Tee Tee Protectus Control - Teens Control - Teens	Paptor Cont Paptor Cont 10 00 1 10 0 0 1 10 0 0 1 10 0 0 0	facts         Scare           0         83           0         83           1         82           2         25           1         88           1         28           2         23           3         28           3         24           4         38           1         28           9         Perceptioned           9         Perceptioned           1170         Perceptioned	Comm. Top • Abundan * 10-06 7020-05 3021-05	#         Sci           V         100         1           V         200         1           V	Him         Mass           62         2         1049407           42         2         1049407           42         2         1049407           42         2         1049407           42         2         1049407           43         4         1042307           45         3         1040,201           46         1         1042,201           45         3         1040,201           46         3         1040,201           47         3         1040,201           48         3         1040,201           49         PEPP carbinary         149           100         7         3           101         7         3           1149         PEPP carbinary           May Status         X	248 4.86 2.96 3.87 3.83 4.87 4.80 9.86 9.85 9.83 9.83 9.84 9.85 9.85 9.85 9.85 9.85 9.85 9.85 9.85	8.4 9.3 754 424 9.7 723 848 848 848 848 848 849 97 97 97 98 97 98 97 98 97 98 97 98 97 97 97 97 97 97 97 97 97 97 97 97 97	Change 7 to 2 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	4.825-04 1.001-04 2.01-04 2.01-04 2.01-04 2.01-04 0.011-04 0.011-04 0.011-04 0.011-04 0.011-04		Section Complete With the section of works the section of works the section of works the section of works the section of the section the section of the section of the section the section of the section of the section of the section the section of the secti
10     2004     0     1     107.00     10.5     2     5.06-00     2     0	Protections - Trend For Protection Protectio	Papelates for     Papelates     Papelat	facts         Score           0         801           0         801           0         202           2         205           1         181           0         203           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         172           1         208           1         170           1         170           1         208           1         170	Emme.           Tap         - Mandae           18-88         3216-95           3216-95         3216-95      <	#         Soc           10         200         1           10         200         1         1           10         200         1         1         1           10         200         1         1         1         1           10         200         1	PB         Mass           0         3         Detext           42         2         Detext           42         2         Detext           43         4         Detext           44         Detext         Detext           45         4         Detext           45         1         Detext           46         2         Detext           47         2         Detext           48         2         Detext           49         2         Detext           40         2         Detext         Detext           40         2         Detext <td>248 4.86 258 4.67 363 4.67 363 4.67 363 4.67 363 4.67 363 363 363 363 363 363 363 363 363 3</td> <td>8.4 8.3 284 848 848 848 848 849 850 7 7 8 8 8 8 8 8 8 9 7 8 8 8 8 8 8 8 8 8</td> <td>Charge Tag</td> <td>* Algorithms Latter 2.27-34 2.27-34 2.27-34 2.27-34 2.27-34 4.27-34 4.27-34 1.</td> <td></td> <td>Section Campi With Comments In the sectores of works In the sectores of works In the sectores of works In the sectores of works In the sectores of the sectores In the sectores of the sectores of the sectores In the sectores of the sectores of the sectores of the sectores In the sectores of the sectores</td>	248 4.86 258 4.67 363 4.67 363 4.67 363 4.67 363 4.67 363 363 363 363 363 363 363 363 363 3	8.4 8.3 284 848 848 848 848 849 850 7 7 8 8 8 8 8 8 8 9 7 8 8 8 8 8 8 8 8 8	Charge Tag	* Algorithms Latter 2.27-34 2.27-34 2.27-34 2.27-34 2.27-34 4.27-34 4.27-34 1.		Section Campi With Comments In the sectores of works In the sectores of works In the sectores of works In the sectores of works In the sectores of the sectores In the sectores of the sectores of the sectores In the sectores of the sectores of the sectores of the sectores In the sectores of the sectores
10     544     44     1     105.01     1.04     1     1061-01     1     90     91000000       10     7.08     7.02     7.0     1000000     41.0     41.7     2     44.07-64     0     9     91000000       10     6.00     7.08     7.02     1000000     10.1     2     14.07-64     0     9     910000000       10     6.00     900000     7.00     7.01     7.00     7.01     7.01     6     9     910000000       10     6.00     9000000     9.00     900000     7.00     7.01     7.00	Protections - Trend For Protection Protectio	Papelates for     Papelates     Papelat	facts         Score           0         801           0         801           0         202           2         205           1         181           0         203           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         172           1         208           1         170           1         170           1         208           1         170	Emme.           Tap         - Mandae           18-88         3216-95           3216-95         3216-95      <	#         So           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           3         100         1           4         1000         1           4         1000         1           4         1000         1	PB         Mass           0         2         1204407           42         2         1204407           42         2         1204407           42         2         1204407           42         2         1204407           43         2         1405107           45         3         1445407           45         2         144520           46         1         1442307           47         3         144520           48         2         144520           49         2         144520           40         3         144520           40         3         144520           40         3         144520           40         3         144520           40         7         144200           1         144520         1445400	248 448 258 467 461 467 463 467 463 466 466 467 463 467 463 467 467 467 467 467 467 467 467 467 467	8.4 8.3 724 824 824 827 823 844 824 827 823 844 844 845 845 845	Orange Trans 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	<ul> <li>4425-9</li> <li>1487-6</li> </ul>	Context	
10     7.08     7.02     0     100.002     10.0     4.07     2     4.061-46     0     9     9.0021071970420       10     8.0     6     100.179     5.00     10.1     2     7.004-46     0     9     9.012117131101719704       10     10.1     105.10     105.01     100     17     4     10.04     6     9     9.012111017197       10     100     7.07     5     105.01     100     17     5     1057.04     6     9     9.012110117197       10     100     5.00     107     4     10.04     6     9     9.012110117197       10     100     5.00     107.7     4     10.04     6     9     9.0212101101797       10     100     5.00     107.7     5     1057.64     6     9     7121210101797       10     100     7     10.04     6     9     7121210101797     100     100     7     100.04     6     9     7121210101797       10     100     7.00     10.04     10     10.01     100.01     100.01     100.01     100.01     100.01     100.01     100.01     100.01     100.01       10     100     10	Protections - Trend For Protection Protectio	Papelates for     Papelates     Papelat	facts         Score           0         801           0         801           0         202           2         205           1         181           0         203           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         172           1         208           1         170           1         170           1         208           1         170	Emme.           Tap         - Mandae           18-88         3216-95           3216-95         3216-95      <	#         Soc           0         200         200         200           0         200         200         200         200           0         200	Hits         Mass           0         3         204407           42         2         1070407           42         2         1070407           43         2         1070407           44         2407207         30           45         104208         3           46         2         104208           48         2         104208           49         2         104208           48         2         104208           49         2         104208           40         2         104208           40         2         104208           40         2         104208           40         2         104208           40         2         104208           40         2         104208           40         2         104208           1         304208         1           1         304208         1           1         304208         1           1         304208         1           1         304208         1	248 648 258 547 547 548 547 548 547 548 547 548 547 547 548 547 548 547 548 547 548 547 547 548 548 547 548 547 548 547 548 547 548 547 548 547 548 548 548 548 548 548 548 548	8.4 8.3 244 8.4 8.4 8.4 8.4 8.4 73 73 73 73 73 73 73 73 73 73 73 73 73	Course Process 2 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	4.021-9     1.001-0     1.001-0     1.001-0     1.001-0     1.011-0     1.011-0     1.011-0     1.011-0     1.011-0     1.011-0     1.011-0     1.011-0     1.011-0     1.011-0	Cardian 1	
10     1017     707     6     1075.05     107     6     1110.04     0     0     VERTIFICATION CONTRACT       10     2005     107     6     1075.07     5     1205.04     0     VERTIFICATION CONTRACT       10     100     5.01     5.00     107.7     7     1205.04     0     VERTIFICATION CONTRACT       10     100     5.01     5.00     107.7     1     1205.04     0     VERTIFICATION CONTRACT       10     100     5.01     5.00     100.01     0     0     0.01.000000000000000000000000000000000	Protections - Trend For Protection Protectio	Papelates for     Papelates     Papelat	facts         Score           0         801           0         801           0         202           2         205           1         181           0         203           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         172           1         208           1         170           1         170           1         208           1         170	Emme.           Tap         - Mandae           18-88         3216-95           3216-95         3216-95      <	#         Sort           2         1236         3           2         1236         2         3           2         1236         2         3         3           2         1236         2         3         3         3           2         1236         3	PB         Mass           0         3         Linesco           42         2         Linesco           43         3         Linesco           43         3         Linesco           44         3         Linesco           45         3         Linesco           45         3         Linesco           45         3         Linesco           46         3         Linesco           47         1         Linesco           48         PEPC careboxy         Linesco           41         PEPC careboxy         Linesco           4         Linesco         Linesco           5         HICSNO         L           4         Linesco         Linesco	244 6.44 7.54 1.94 1.94 1.95 1.93 1.93 1.93 1.93 1.93 1.93 1.93 1.93 1.93 1.93 1.93 1.93 1.93 1.93 1.94 1	8.4 15.3 16.4 16.4 16.4 16.4 16.4 16.4 16.4 16.4 17.5 1	Charge Trans 2 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	4825-9     1885-9     1885-9     1885-9     1885-9     1885-9     1885-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9     1895-9	Conduction	
10     2005     7.07     6     107,47     6.08     107     7     1.207,44     0     0     VERUPUSION/VE	Protections - Trend For Protection Protectio	Papelates for     Papelates     Papelat	facts         Score           0         801           0         801           0         202           2         205           1         181           0         203           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         172           1         208           1         170           1         170           1         208           1         170	Emme.           Tap         - Mandae           18-88         3216-95           3216-95         3216-95      <	0         Soc           2         120         2           2         120         2         2           2         120         2         2         2           2         120         2         2         2         2           2         120         1         2         <	PB         Mass           0         3         Detext0           42         2         DOVED           42         2         DOVED           43         4         Detext0           44         Detext0         Detext0           45         2         DOVED           45         S         Detext0           45         S         Detext0           45         S         Detext0           106         3         Detext0           107         S         Detext0           108         2         Detext0           109         1         S         Detext0           100         1         S         Detext0           100         1         S         Detext0           100         1         S         Detext0           1         Max         N         Detext0           1         Max         N         Detext0           1         Max         N         Detext0           1         Max         Detext0         Detext0           1         Max         Detext0         Detext0           1         Max <td>248 6.08 2.98 2.98 3.99 3.93 3.17 3.07 3.07 5</td> <td>5.4 15.3 14.4 10.7 1</td> <td>Charge Tay 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3</td> <td>K01-9     L01-9     L</td> <td>Cardial Cardial 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1</td> <td></td>	248 6.08 2.98 2.98 3.99 3.93 3.17 3.07 3.07 5	5.4 15.3 14.4 10.7 1	Charge Tay 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	K01-9     L01-9     L	Cardial Cardial 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
IDM         AD         MAL         ADM         ADM         IDF         I         LAN-44         D         TEXTORY           ID         AD         AD         ADM         ADM         IDF         I         LAN-44         D         TEXTORY           ID         ADD         ADD         ADD         IDF         I         LAN-44         D         TEXTORY           ID         ADD         ADD         ADD         IDD	Protections - Trend For Protection Protectio	Papelates for     Papelates     Papelat	facts         Score           0         801           0         801           0         202           2         205           1         181           0         203           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         172           1         208           1         170           1         170           1         208           1         170	Emme.           Tap         - Mandae           18-88         3216-95           3216-95         3216-95      <	0         So           2         120         2           2         120         2         200         2           2         120         2         200         2           2         120         2         200         2           2         120         2         200         2           2         120         2         200         2           2         200         2         200         2           2         200         2         200         2           2         200         2         200         2           2         200         2         200         2           2         200         3         2         200         3           2         200         4         2         200         4           PopUsers         5         200         6         2         200         5           2         200         6         5         2         2         2         2         2         2         2         2         2         2         2         2         2         2         2         2         2	PB         Mass           0         3         LD4647           42         2         LD4647           43         2         LD4647           100         3         SD4648           101         1         LD4647           102         1         LD4647           103         2         LD4647           104         1         LD4647           105         2         LD4647           106         1         LD4647           1         LD4647         LD4647           1         LD4647         LD4647           1         LD4647         LD4647           1         LD4748         LD4748           1         LD404812         LD404812           1         LD404812         LD404812           1         LD404812         LD404812	348 428 128 128 129 121 121 122 124 123 123 123 123 123 123 123 123 123 123	8.4 10.3 10.4 40.4 10.7 1	Orang Tan 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	Algoridante     Algoridan	Cardial	
20         2010         7.02         8         2003555         8.714         21.4         2         1.878-40         0         0         0.010000000000000000000000000000000000	Protections - Trend For Protection Protectio	Papelates for     Papelates     Papelat	facts         Score           0         801           0         801           0         202           2         205           1         181           0         203           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         172           1         208           1         170           1         170           1         208           1         170	Emme.           Tap         - Mandae           18-88         3216-95           3216-95         3216-95      <	0         Soc           2         120         2           2         120         2         2           2         120         2         2         2           2         120         2         2         2         2           2         120         2         <	PB         Mass           0         3         Linet.47           42         2         Linet.47           42         2         Linet.47           43         4         Linet.47           43         4         Linet.47           45         3         Linet.47           46         3         Linet.47           47         2         Linet.47           48         2         Linet.27           49         2         Linet.27           45         1         Linet.27           45         2         Linet.27           45         Linet.27         Linet.27           45         Linet.27 <td< td=""><td>248 4.08 2.08 3.09 3.03 4.09 4.09 3.07 4.09 4.09 4.09 4.09 4.09 4.09 4.09 4.09</td><td>8.4 10.3 10.4 10.7 1</td><td>Charge Top 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3</td><td>Kurt-H     Life-H     Life-H</td><td>Cardhal Cardhal S S S S S S S S S S S S S S S S S S S</td><td></td></td<>	248 4.08 2.08 3.09 3.03 4.09 4.09 3.07 4.09 4.09 4.09 4.09 4.09 4.09 4.09 4.09	8.4 10.3 10.4 10.7 1	Charge Top 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	Kurt-H     Life-H	Cardhal Cardhal S S S S S S S S S S S S S S S S S S S	
Image         B         6         1001300         R0.3         R0.5         2         L201-04         8         0.5         L201000           Image         6.0         6.00         6.00         10.00         R0.5         10.7         2         5.00-64         8         0.0151000000           Image         6.00         10.00         1.00         1.00         10.7         2         5.00-64         8         0.0151000000           Image         6.00         1.00         1.00         1.00         10.0         10.7         10.0         10.0         0         0.0100000000           Image         6.00         1.000000         1.00         0.00         1.000000000000000000000000000000000000	Protections - Trend For Protection Protectio	Papelates for     Papelates     Papelat	facts         Score           0         801           0         801           0         202           2         205           1         181           0         203           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         208           1         172           1         208           1         170           1         170           1         208           1         170	Emme.           Tap         - Mandae           18-88         3216-95           3216-95         3216-95      <	#         Soc           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           2         120         1           3         120         1           4         12         10           1         12         10           1         12         10           1         10         10           1         10         10           1         10         10           1         10         10           1         10         10           1         10         10           1         10         10           1	PB         Mass           0         3         Linesard           42         2         Linesard           42         2         Linesard           42         2         Linesard           42         2         Linesard           43         3         Linesard           43         3         Linesard           44         2         Linesard           45         3         Linesard           45         3         Linesard           45         3         Linesard           46         3         Linesard           47         3         Linesard           48         PEPP carebases           41         PEPP carebases           41         Linesard           4         Lines	188 188 188 188 181 182 183 183 184 184 184 184 184 184 184 184	8.4 10.3 10.4 10.4 10.5 10.4 10.4 10.5 10.4 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 10.4 10.5 1	Orange Trans 2 3 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	* Alacolaus 1.00-9 2.10-9 2.10-9 2.10-9 1.01-9 4.01-9 4.01-9 4.01-9 4.01-9 4.01-9 1.01-9 4.01-9 1.01	Control 1	
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Figure 4. (A) Quantitative profiling of proteins and peptides; (B) Protein resolution information highlights

differing multi-protein identifications.

## Statistical analysis of protein data and report results

Multivariate statistical analysis on protein measurements can be performed to make confident conclusions and generate a protein-based report of the experiment, as shown by the power analysis, dendrogram and expression examples in Figure 5. Protein measurements can also be exported to any custom bioinformatics workflow, and supplementary data or new results can be imported back into the analyzed experiment.

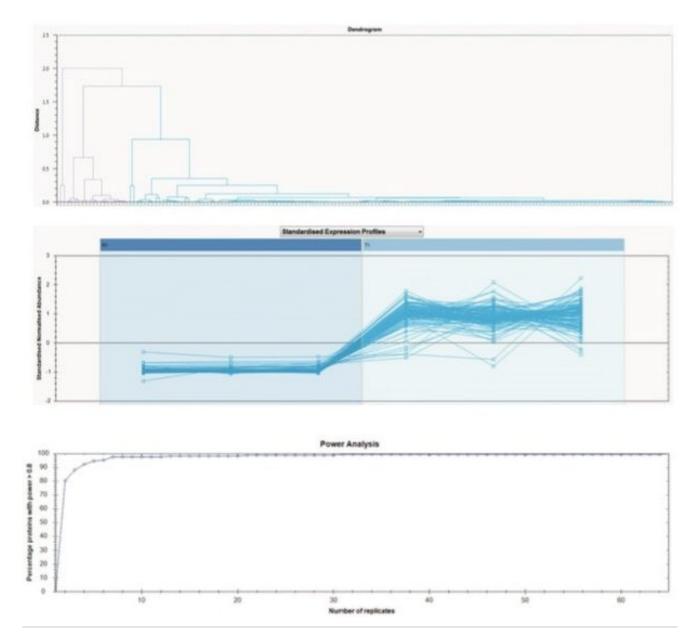


Figure 5. Integrated power analysis and statistical validation label-free LC-MS data and experiments.

# Conclusion

TransOmics Informatics Software has been specifically developed for large scale analysis of ion mobility MS data

from proteomics and metabolomics.

- TransOmics Informatics Software allows for all peak information from all sample files to be detected in a single map of peptide or metabolite ions.
- Obtain 100% matching of all chromatographic peaks with no missing values, for data to be explored and differential analysis to be measured.
- Gain quantitation of peptide ions without (DIA) MS<sup>E</sup> or data directed analysis (DDA) MS/MS results annotation.
- Export MS/MS data and search using any search engine.
- Bring together quantitative data and qualitative fragmentation spectra for a peptide-based view of potentially interesting proteins, metabolites, or lipids.

# **Featured Products**

Metabolomics & Lipidomics <https://www.waters.com/514526> ACQUITY UPLC M-Class System <https://www.waters.com/134776759>

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