Bioinformatics software for effective analysis of mass spectrometry data: *S2P*, *Mass-Up* and *LA-iMageS*

H. López-Fernández[1,2,3], M. Reboiro-Jato[1,2], G. de S. Pessôa[4,5], M. A. Z. Arruda[4,5], J.E. Araújo[3], H.M. Santos[3], F. Fdez-Riverola[1,2], D. Glez-Peña[1,2], J. L. Capelo-Martínez[3]

1 SING Research Group, Escuela Superior de Ingeniería Informática, University of Vigo, Edificio Politécnico, Campus Universitario As Lagoas s/n, 32004 Ourense, Spain.

2 CINBIO - Centro de Investigaciones Biomédicas, University of Vigo, Campus Universitario Lagoas-Marcosende, 36310, Vigo, Spain.

3 BIOSCOPE Group, UCIBIO-REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Portugal.

4 Group of Spectrometry, Sample Preparation and Mechanization (GEPAM), Institute of Chemistry, University of Campinas, UNICAMP, PO Box 6154, 13083-862, Campinas, SP, Brazil.

5 National Institute of Science and Technology for Bioanalytics, Institute of Chemistry, University of Campinas, UNICAMP, 13083-862, Campinas, SP, Brazil.

S2P

www.sing-group.org/s2p
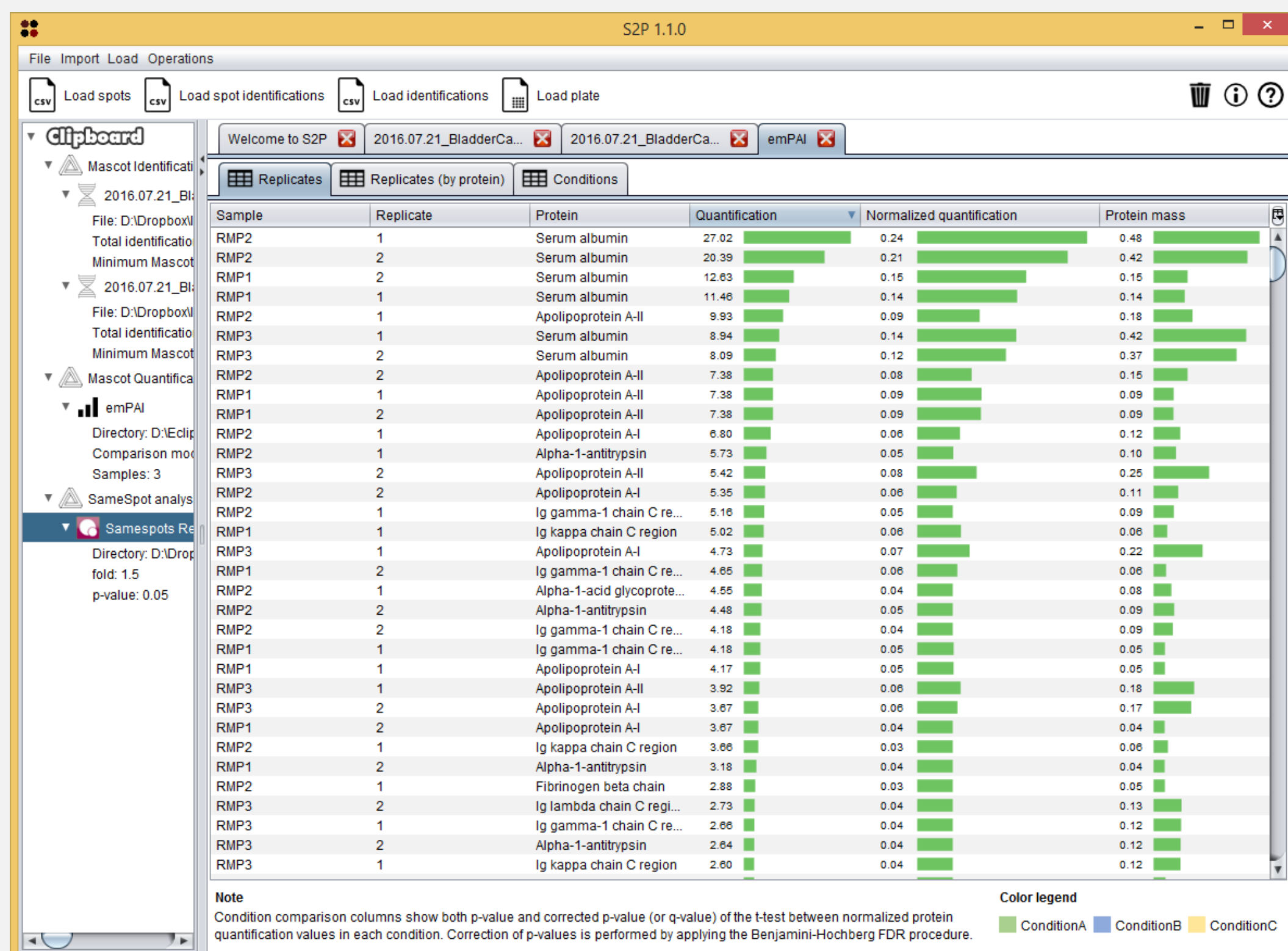
What is S2P? *S2P* is a desktop multiplatform application specifically created to perform fast and easy processing of 2D-gel and MS protein identification-based data.

Features: *S2P* allows researchers to:
- Import data from Progenesis SameSpots and save it as comma-separated values (CSV) files.
- Import, process and save Mascot reports.
- Create MALDI plate designs and export them as PDF or CSV files.
- Bind Mascot identifications to spots data.
- Visualize and explore spots data in different ways.

www.sing-group.org/mass-up

Mass-Up

What is Mass-Up? *Mass-Up* is an open-source software for proteomics designed to support the preprocessing and analysis of MALDI-TOF mass spectrometry data.

Features: *Mass-Up* allows researchers to:
- Load and visualize raw spectra from mzML, mzXML or CSV files.
- Preprocess raw spectra using well-known R libraries (MALDIquant and MassSpecWavelet).
- Perform different types of analysis (quality control, biomarker discovery, principal component analysis, hierarchical clustering, biclustering, and classification analysis) on the aligned peak lists.
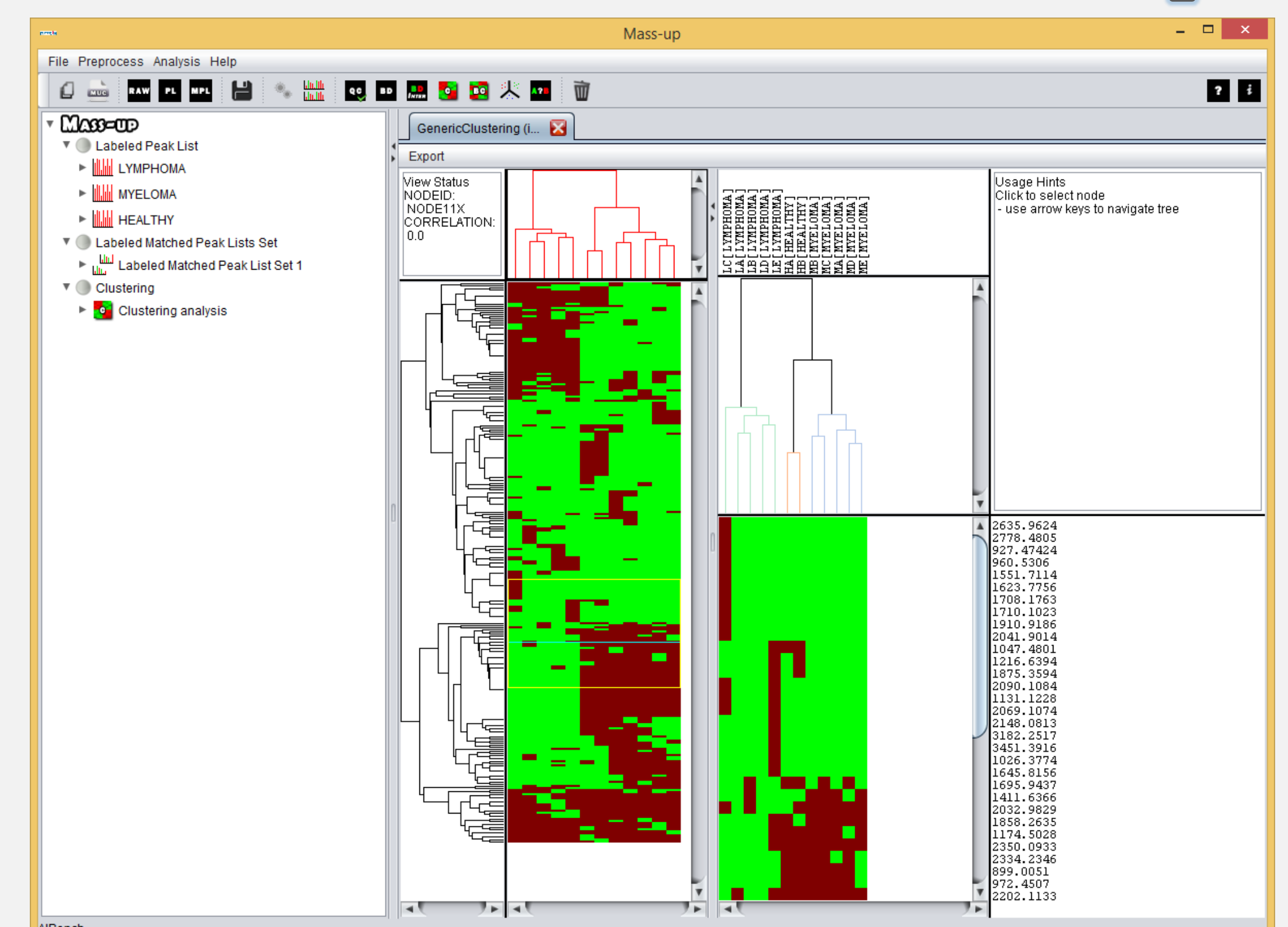
LA-iMageS

www.la-images-net

What is LA-iMageS? *LA-iMageS* is an open source application to generate 2D/3D elemental distribution bioimages from LA-ICP-MS spectra.

Features: *LA-iMageS* allows researchers to:
- Extract the elemental distributions of elements from LA-ICP-MS spectra.
- Normalize the elements by a standard.
- Generate custom 2D/3D representations of each element.
- Export the results into images and the elemental distributions to CSV files.