

An open-source software for fast and automatic processing of 2D-gel and MALDI-based mass spectrometry protein data

J. Eduardo Araújo¹, Hugo López-Fernández^{1,2}, Daniel Glez-Peña², Miguel Reboiro-Jato², Florentino Fdez-Riverola², José L. Capelo-Martínez¹

¹BIOSCOPE Group, UCIBIO-REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Portugal.

²SING Research Group, Escuela Superior de Ingeniería Informática, University of Vigo, Edificio Politécnico, Campus Universitario As Lagoas s/n, 32004 Ourense, Spain.

Introduction

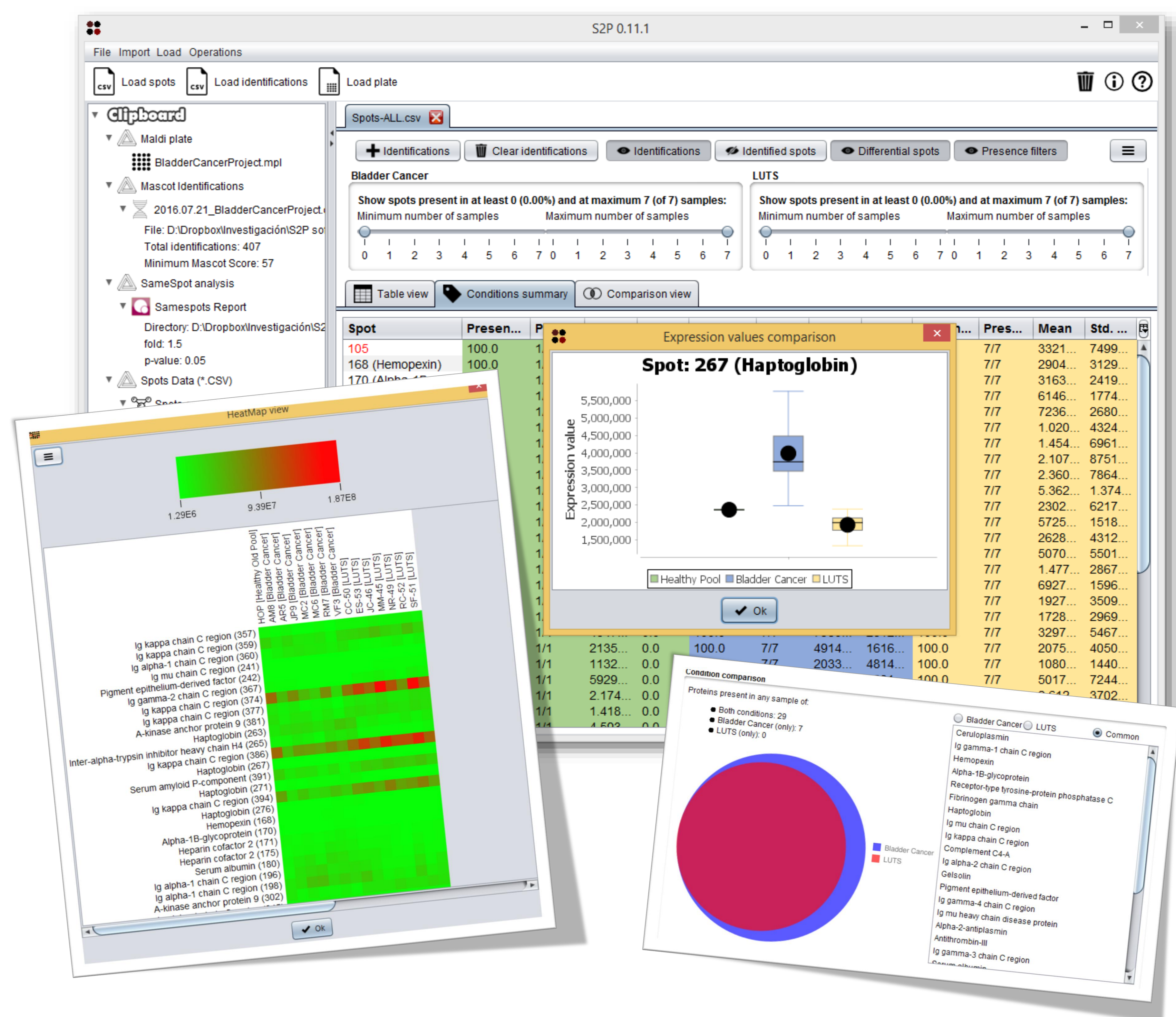
2D-gel electrophoresis and *MALDI-TOF-MS* (mass spectrometry using matrix assisted laser desorption ionization coupled to time of flight analysers) are usually employed together in experimental workflows. While *2D-gel electrophoresis* allows obtaining a set of differentially expressed spots, *MALDI-TOF-MS* allows identifying the proteins associated with such spots. Such processes involve large data processing in order: (i) to analyze *2D-gels* across samples to obtain the differentially expressed spots using *Progenesis SameSpots* software, (ii) to excise such spots and to treat them for protein identification and (iii) to bind those protein identifications to the *2D-gel* spots. Such procedure is done in an intensive handling and time consuming way. Moreover, doing this repetitive process in a non-automated manner is error-prone, threatening study reliability and reproducibility.

In order to fast and automatically perform these tasks we are developing the **S2P** software application (www.sing-group.org/s2p), to help researchers to overcome this tedious but necessary data processing. The purpose of this work is to present this open software.

Results: S2P

S2P (*Spot to Proteomics*) is a desktop application specifically created to perform fast processing of *2D-gel* and MALDI-based mass spectrometry protein identification data. Currently, **S2P** allows researchers: (i) to collect *Progenesis SameSpots* reports into a full table where all samples can be compared and analyzed, (ii) to link spots to protein identifications obtained with Mascot, and (iii) to export and explore data in different ways (such as heatmaps or Venn Diagrams).

Try **S2P** now!
www.sing-group.org/s2p



Conclusions

S2P is completely free, distributed under license GPLv3, and provide a friendly graphical user interface designed to allow researchers saving time in data processing tasks related to 2D and MALDI mass spectrometry protein identification-based data.

Acknowledgements

H. López-Fernández is supported by a post-doctoral fellowship from Xunta de Galicia and thanks CINBIO (*Centro De Investigaciones Biomédicas*) for financial support. SING group thanks CITI (*Centro de Investigación, Transferencia e Innovación*) from University of Vigo for hosting its IT infrastructure. J. L. Capelo acknowledges *Associação Científica ProteoMass* for financial support. J. E. Araujo acknowledges the financial support given by the Portuguese Foundation for Science and Technology under doctoral grant number SFRH/BD/109201/2015. The Nova Medical School is also acknowledged for financial support under project “Discovery of biomarkers for bladder carcinoma diagnosis”.