

# Proteus

An interactive Laboratory Journal Application for Gel-based Proteomics



Konstantin Otte<sup>1</sup>, Nils Hoffmann<sup>1,2</sup>, Fabian Schulte<sup>3</sup>, Karsten Niehaus<sup>3</sup>, Jens Stoye<sup>1</sup>

<sup>1</sup> Genome Informatics, Faculty of Technology, Bielefeld University  
<sup>2</sup> Graduate School in Bioinformatics and Genome Research, CeBiTec, Bielefeld  
<sup>3</sup> Proteomics and Metabolomics, CeBiTec, Bielefeld University

## Introduction

We present a stand-alone, platform-independent application for 2D-gel-based proteomics data management. Our software intends to bridge the gap between physical sample preparation and post-hoc analysis with software, such as Delta2D (Decodon GmbH, Greifswald), and mass-spectral analysis of gel-spots, i.e. with matrix-assisted laser-desorption-ionization (MALDI) for peptide and protein identification.

## Project Creation and Browsing

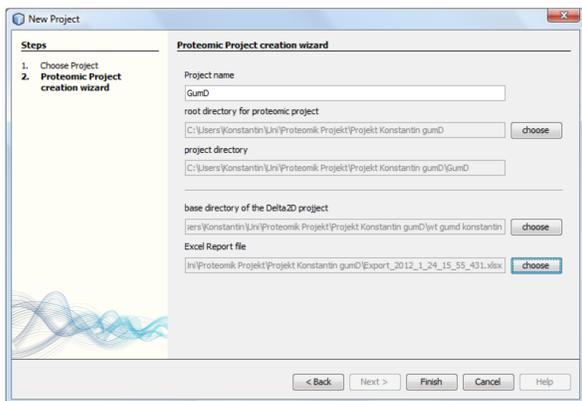


Figure 1: Project creation with data import from Delta2D projects.

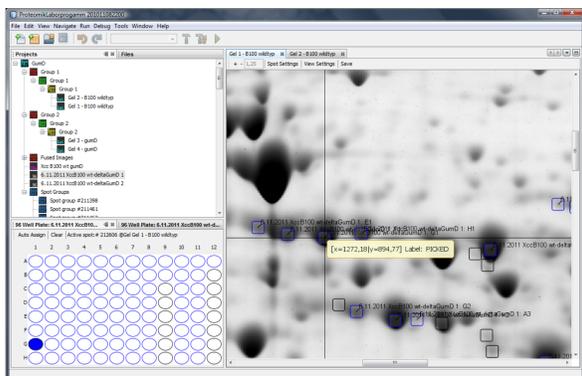


Figure 2: Overview of an open project (top-left), with an open gel view and selected spot (right) and highlighted picked spot location on a 96-well microtiter plate (bottom-left).

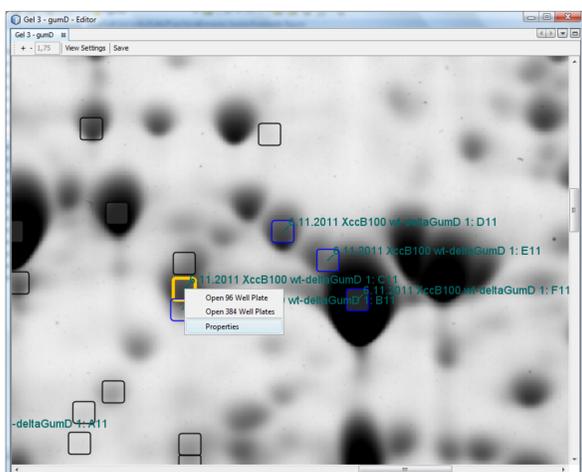


Figure 3: Gel viewer zoom in with spot selection, customized label colors and opened context menu for gel spots.

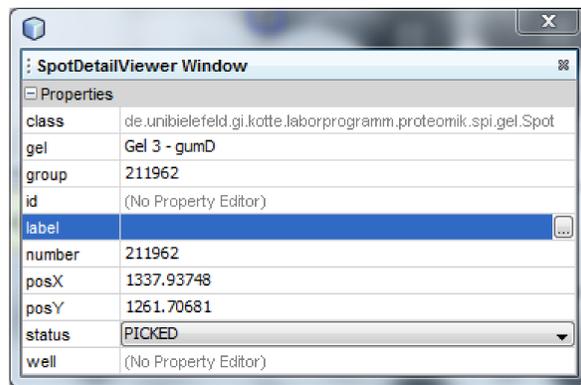
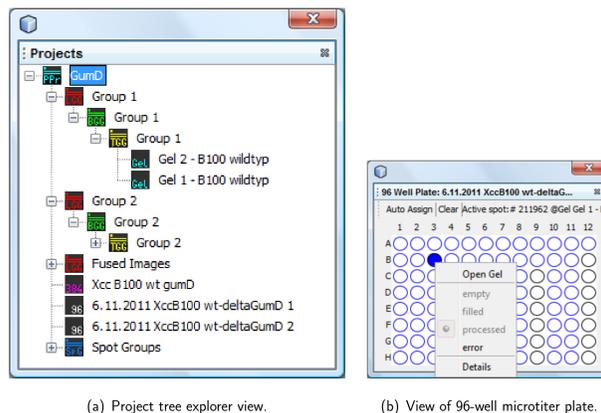


Figure 4: Detailed view of selected gel spot with editable properties.

## Microtiter Plate Definition

The user can then define 96-well microtiter plates in order to associate physical spot locations on a gel with the physically picked spot within a well of the plate.



(a) Project tree explorer view. (b) View of 96-well microtiter plate.

Figure 5: (a) Details of the project tree explorer displaying gel groups, individual gels, a MALDI target plate and 96-well microtiter plates, along with spot group information. (b) View of a 96-well microtiter plate.

## MALDI Target Plate Definition

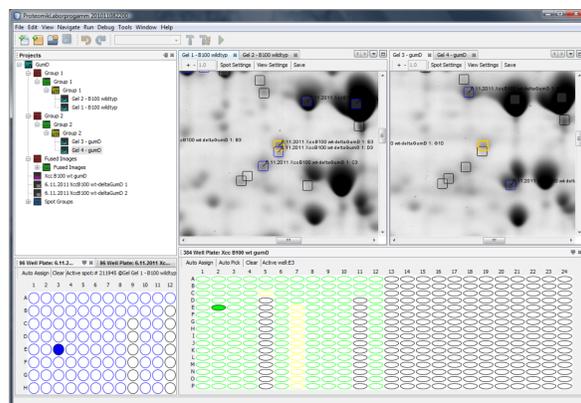


Figure 6: Program overview with Project Explorer (top-left), 96-well microtiter plates (bottom-left), 384 well MALDI target plate (bottom) and linked gel view (center). The gels are both centered on a spot from the same spot group. The corresponding wells belonging to the picked spot in the left gel are highlighted on the plates.

The user can assign each microtiter plate well to a position on a custom MALDI target plate. Currently, MS1 and MS2 report data in BTR format (Bruker Daltonik GmbH, Bremen) can be imported and associated to target plate locations, which are in turn associated to microtiter plate wells and ultimately to the originating gel spots.

Associated wells, target positions and gel spots are highlighted on user selection for easier comprehension. Spot identification data may be browsed and edited within the software and edited identifications can be reexported for use in Delta2D for labelling and downstream statistical analysis.

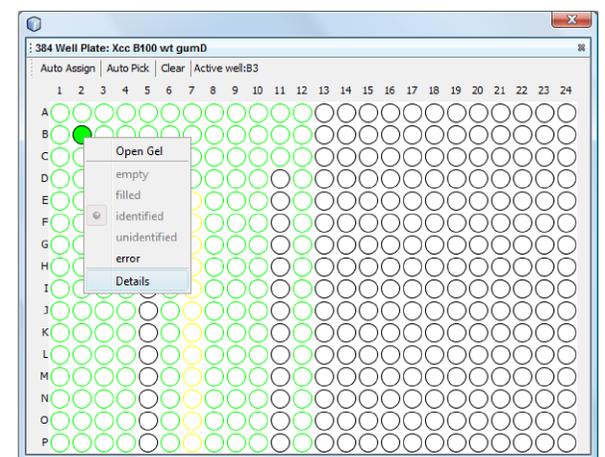


Figure 7: View of a MALDI target plate with opened well status menu. The wells are color coded according to their status.

## Spot Browsing and Identification

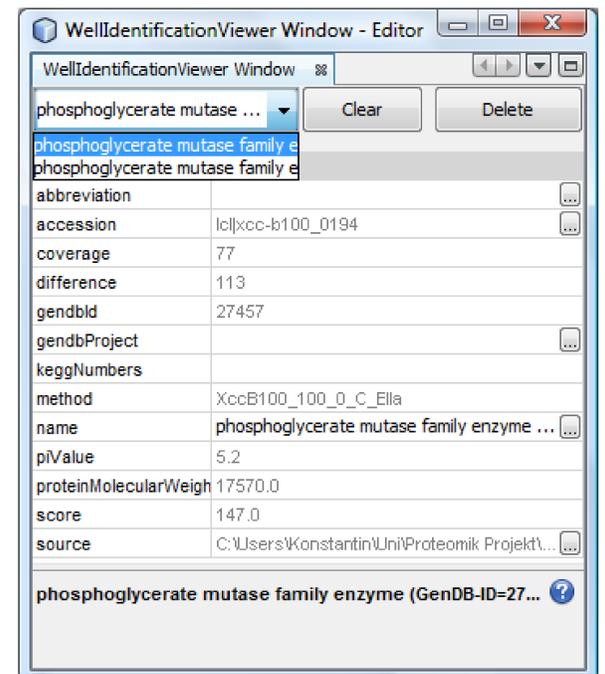


Figure 8: View on a MS identification of a MALDI target spot. Multiple identification results (i.e. from different methods) can be selected.

## Results and Outlook

The software is based on the NetBeans Rich Client Platform, which enforces a high level of modularity and leads to easy extensibility of core functionality through additional plugins. It will be available under the GNU L-GPL v3 OpenSource license.

Future work will integrate Proteus with our Metabolomics software Maui (<http://ma1tcms.sf.net>) and machine learning algorithms for combined time course data analysis.