# INVENTION RECORD **Project number: (for Isis use)**

The invention record is a written description of your invention. It fulfils several important purposes:

* It helps Isis to assess whether the work is patentable;
* It helps the patent attorney to prepare the draft patent, if Isis decides to proceed with patenting;
* It helps give Isis and the University’s Intellectual Property Due Diligence team an early indication as to the University’s ownership of your invention, and identify issues which will need to be addressed downstream; and
* It provides an important record of the date of invention, which can become important in future patent process.

IMPORTANT: Discussions between you and Isis about your invention are confidential. To avoid any inadvertent public disclosure of your invention please consider all discussions about the invention confidential. Please use Confidential Disclosure Agreements to protect discussions with anyone outside the University. Please ask Isis for advice.

Please answer the following questions, either on these two pages or on separate sheets.

1. Descriptive Title of the Invention.

UniDec: Universal Mass Spectrometry Deconvolution Software

1. Who was involved? Please tell us for each individual who contributed, invented or authored (if software):
   1. Their names and if any are foreign nationals;
   2. Who their employer is, and if this is not Oxford, are any contracts or arrangements in place?
   3. What they contributed to the development of the technology (e.g. came up with the original idea; designed experiments; carried out experimental work; wrote code)

|  |  |  |  |
| --- | --- | --- | --- |
| Name | Nationality | Employer(s) | What did this person contribute? |
| Michael Marty | USA | University of Oxford | Primary intellectual and code development |
| Andrew Baldwin | UK | University of Oxford | Significant intellectual contributions and some code |
| Erik Marklund | Sweden | University of Oxford | Helpful discussions on C code and code |
| Tim Allison | New Zealand | University of Oxford | Contributions of python code and discussions on GUI |

IMPORTANT NOTE: Inventors must be legal inventors according to the definition in patent law (please ask your Isis Technology Transfer Manager for guidance if necessary). Software Authors are those who actually wrote the code and thereby created the copyright. The University also has a mechanism for rewarding contributors who are not inventors or authors but who have made a significant and identifiable contribution to the intellectual property, and revenue distribution to all individuals is dealt with through the IP2 form. Please add rows or supply further detail on a separate sheet if there is not enough room.Please tell us about your invention:

What do you think your invention is? A new approach to analysis of mass spectrometry data based on a Bayesian deconvolution

What will your invention be used for? Analysis of mass spectrometry data

What are the advantages of your invention and how does it improve on the present situation? It is fast, robust, and capable of analysing complex data.

What is new about your invention? It is both a new algorithm and a new approach.

How and why does it work? What is the science behind the invention? It uses a Bayesian deconvolution algorithm similar to a Richardson-Lucy algorithm combined with smoothing of charge state and/or oligomer distribution.

Are there any other uses of the invention? Deconvolution of other types of data potentially.

Waters, Amgen

4. Are you aware of any companies who have an interest in the area, e.g. companies who sponsor research or who attend relevant conferences? If so, please supply the companies’ names (and contact details, if you have them).

**Marty, M.T.**; Zhang, H.; Cui, W.; Gross, M.L.; Sligar, S.G. “Interpretation and Deconvolution of Nanodisc Native Mass Spectra” *J. Am. Soc. Mass Spectrom.* **2014**, 25, 269-277.

5. Do you know of any published literature (including patents) relevant to your invention? Have you done any searching for published literature, and if so where? Please provide any details.

6. Please tell us the story of the development of the invention:

When and where was the invention first conceived? Michael Marty developed the initial specific case of the algorithm during my PhD, and it is published in the article cited above. At Oxford, Michael Marty expanded and generalized the algorithm to work for a variety of spectra. A number of small changes have been made to the algorithm to make it faster, more robust, and more universal.

When was the invention first reduced to practice? The generalized algorithm began to shape in February 2014.

What practical work has been done to date on the invention? Has the invention been tested in the laboratory or has it been used? If so please give results. The program has been developed and tested by the group. It works well on a number of spectra, and we are preparing a publication.

Who did what in the development of the invention? Michael Marty did most of the coding and intellectual development. Andrew Baldwin offered significant guidance and some early C code. Erik Marklund added a key insight in the development process to speed up the C code. Tim Allison contributed advice on the python code and several python classes used in the GUI.

7. What are your future plans for developing the technology? Do you have funds in place for this work, and what do you think you will achieve in this area in the next 12 months?

The general algorithm is largely complete. Small changes to the mechanics will be explored to improve it, but development will likely progress for making more specialized applications of the code. Some ideas include for isotopically resolved mass spectrometry and for other types of data, Images and NMR.

Michael Marty showed the program to Keith Richardson from Waters on 30/04/14. He has also informed Michael Gross and Stephen Sligar (coauthors on the original paper) that a generalized version of the algorithm existed and was performing well. I have corresponded and distributed a test copy to Iain Campuzano at Amgen on 12/08/14.

8. Who have you told about the invention? When did you do this and where?

There are some sparse personal notes, emails, and old versions of the code that track the development. Recent changes are logged on a subversion server.

9. When did you first describe the invention in writing or electronically? Do lab book records exist, or personal notes?

In addition to the published paper describing the initial specific version of the code, results from the program have been submitted for publication in Int. J. Mass Spectrom.: Shepherd, D.A.; **Marty, M.T.**; Giles, K; Baldwin, A.J.; Benesch J.L.P. “Combining Tandem Mass Spectrometry with Ion Mobility Separation to Determine the Architecture of Polydisperse Proteins”

However, this paper did not contain the details of the algorithm.

10. Have you published, verbally, electronically or in writing, anything relevant to the invention, and if so when and what? Please tell us about abstracts, web pages and presentations as well as any published articles.

11. Do you have plans to publish the work? If so, what is the timescale and where will the publication take place? If a draft paper exists please provide a copy.

We are planning on submitting a paper for publication before Sept 12.

I’m not sure what funding is relevant. We didn’t use any special materials, just a desktop computer.

1. What is the funding background of the work you’ve done on the invention? Did you use any equipment, materials, samples, gifts or other in kind support provided by third parties, or biological materials obtained from humans? If so, please give details; specifically: was patient consent obtained?

For inventions that include software please provide the following additional information.

UniDec Version 0.105

1. Please provide the software application name and version number.
2. For source code developed by the researchers identified in question 2 above:

What source files were used? Please provide a list.

UniDec.c

UniDec.h

Gui.py and a number of other python files to run the GUI

Which programming languages were used?

C and Python

Which development tools were used to create or generate the source files? Please provide a list.

Eclipse (C Development Environment)

PyCharm (Python development environment)

What copyright protection notices are included in the source files?

None.

For new versions, which source files have been changed, added or removed since the previous version?

What documentation or other files are required for others to use, develop and maintain the software? Please provide a list.

I have a PowerPoint presentation that print as a PDF as a manual. There are also some comments in the code.

Please indicate if the source files have been distributed outside the University, and if so, in what form and to whom?

No one outside the University has to my knowledge been given the source files.

Are the source files are available as a web download? If so, please provide the download URL and state the terms under which the download is available.

No

1. For other source files or libraries that are required to build the software application (external software):

Please list all external software (files and libraries) used that provide functions required by the application.

FFTW and GSL are used in the C code

C code is compiled with GCC and OpenMP

MatPlotLib, NumPy, SciPy, wxPython, ZoomSpan and ZoomBox, and python modules distributed with the standard python installation were used for the GUI

Python code was compiled using Pyinstaller

Which organization owns each piece of software?

ZoomSpan and ZoomBox are owned by Duke University (<https://scion.duhs.duke.edu/svn/vespa/trunk/>)

FFTW is owned by MIT and Matteo Frigo

Python is the Python Software Foundation.

Others are owned by random developers groups.

How was each piece of software obtained?

Free download from internet

Please provide details of the licence terms, or if it was a standard Open Source licence please provide the name of that licence.

Many are GPL. I have a folder with the license info for each.

Please sign and date the Invention Record below.

Signature:

## Name: Michael Marty

Date:

**The completed form should be returned to:**Isis Innovation Ltd, Ewert House, Ewert Place, Summertown, Oxford OX2 7SG

T +44 (0) 1865 280830  
F +44 (0) 1865 280831  
E [innovation@isis.ox.ac.uk](mailto:%20innovation@isis.ox.ac.uk)

The next steps are for an Isis Technology Transfer Manager to discuss the invention with you. Further detailed forms are required to establish correct legal ownership of the intellectual property rights.