



Analysing big data sets from small molecules

The Separation Science and Metabolomics Laboratory (SSML) at Murdoch University is located in Perth, Western Australia. Led by A/Prof. Robert Trengove, they have been using the Unscrambler since 2008. Having recently upgraded to the latest version of the software, the group is now enjoying the benefits of the enhanced features. Dr Garth Maker is a lecturer in Pharmaceutical Chemistry at Murdoch University and a group leader in the SSML.

Combining world-class expertise with leading-edge technology

The SSML focuses on metabolite research - small molecules such as sugar and amino acids. The group is a key node of Metabolomics Australia (MA) a Bioplatforms Initiative that supports life science research through technology and infrastructure investment in platform 'OMICS technologies.

After the initial excitement surrounding the potential of genomics and proteomics, Garth feels that people are cautious about over-hyping metabolomics, but interest in the field is steadily growing. "Metabolomic analysis can be applied to anything from blood to fungus, and our projects range from clinical studies to agricultural biosecurity." This exciting new field is increasingly being used for biomarker discovery and diagnostics in medicine, for example identification of metabolites that may indicate the presence of cancer cells.

Making sense of complex data

The SSML use pattern recognition to separate treatments from control and identify which metabolites are contributing to variance, highlighting which biochemical pathways are involved. "Essentially, we use the Unscrambler to make sense of the large data sets we generate from very complex samples" explains Garth.

"We often profile over 400 different analytes in a single sample. Picking the patterns in that data would be impossible without the Unscrambler" says Garth. "We recently had a case where a client had data but couldn't make sense of the results. After coming to us, we put their data into the Unscrambler and immediately could analyze patterns and were able to determine what was causing the difference between the samples."

The SSML have recently upgraded to the latest version of the Unscrambler and are already enjoying the significant improvements in the current release. "We've used the Unscrambler for a while, but we should have upgraded sooner. It's unbelievable the difference between versions 9 and 10," he says. "The price isn't an issue, the upgrade fee is very reasonable compared to what you're getting and straight away we are seeing the benefits of the new version."

Industry:

- ▶ Higher Education / Research

Product:

- ▶ The Unscrambler® X

Executive Summary:

- ▶ Conduct research into human, animal, plant, fungal and bacterial metabolomics, with extensive use of high resolution mass spectrometry
- ▶ Part of a group of universities and research institutes supported by Metabolomics Australia (MA), delivering world-class small molecule analysis to a wide range of industries
- ▶ Network licence of the Unscrambler X gives the group access to the software for analyzing complex data sets which could otherwise be very difficult
- ▶ Upgraded to current version of the Unscrambler X and already seeing benefits including time saving, more powerful analytics and improved ease of use

At a glance:

- ▶ Founded in 1974 in Perth, Western Australia
- ▶ Over 18,000 students and 1400 staff currently enrolled or working
- ▶ Offer more than 200 undergraduate degrees and postgraduate courses
- ▶ Recognised as one of Australia's leading research institutions

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Free TestDrive 

“The new version is even more intuitive and easy to use, especially for new users.”

Dr Garth Maker
Lecturer in Pharmaceutical Chemistry
Murdoch University

Easier to use and more powerful than ever

“The integrated workflow in the left hand task bar makes everything accessible. The new version is even more intuitive and easy to use, especially for new users. You don’t have to save every analysis individually, plus there are lots of handy new features, like integrated shortcuts, and the Sample Grouping function. You just drag, click, done!”

As a University lecturer, the use of software that is student-friendly is an important consideration for Garth. “We had a lab meeting the other day and you could hear the ‘oh’s’ and ‘aahs’ from the students,” he says. “The SSML has a network version so people can access it from where they are. This saves us lots of time rather than having scientists fighting to use the Unscrambler!” he continues “Especially in the summer, when it’s a ten minute walk across the campus in forty degree heat!”

Another of the reasons Garth is a loyal Unscrambler user is the reliability and stability of the program. “We find it to be very low maintenance software. We don’t need to talk to Support like we do with some other packages, which are also excellent, but more difficult to use and require more support.”

As a long-time user of the Unscrambler, Garth sums it up by saying “We’re breaking new ground and doing some very exciting data analysis, and the new version of Unscrambler is the perfect tool to help us understand our data better.”



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