

# Autophaser improves sample analysis in areas such as cancer, Alzheimer's and oil spills

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(Phys.org) —A new software package allows researchers to vastly improve the performance of one of the key tools used to analyse medical and environmental samples.

Autophaser, developed by the University of Warwick and Aberystwyth University, enables researchers to make use of significantly more data when using Fourier transform [ion cyclotron resonance mass spectrometers](#) (FT-ICR MS).

FT-ICR is a powerful tool for identifying chemicals and biochemical components in complex mixtures and is used by scientists analysing substances across a wide range of sectors including medical, environmental, and commercial areas such as the [petroleum industry](#).

The software, which is free for academic purposes, will allow much greater confidence in interpreting results. For commercial purposes, the software is available to licence from Warwick Ventures, the commercial arm of the University of Warwick.

The normal method of processing data from FT-ICR MS – magnitude mode – effectively ignores half of the information generated, so mass accuracy and resolution are not as high as they could be.

However Autophaser allows researchers to make use of this otherwise

discarded data by converting FT-ICR MS results to absorption mode. This gives an improvement in [spectral resolution](#) of up to three times and a 41% improvement in the signal-to-noise ratio.

Using Autophaser, researchers will see more peaks in the spectrum, get better sequence coverage in proteins and have more confidence in peak assignments.

Dr David Kilgour of the Department of Chemistry at the University of Warwick said: "Major decisions are made every day in commercial, medical, and environmental settings on the basis of FT-ICR MS so it's vital that researchers have access to the most accurate processing methods.

"Autophaser unleashes the full potential of this type of mass spectrometry and really pushes back the barriers to the kinds of problems it can tackle.

"By making this software available for free to academic researchers, we envisage its benefits will be felt across many biomedical areas, for example cancer, Alzheimer's, and Parkinson's, the pharmaceutical and polymer industries, as well as in environmental analysis such as detecting pollution after oil spills."

Although the advantages of absorption mode FT-ICR MS have been known for nearly 40 years, the technique is still not widely used because a key mathematical hurdle presented a barrier.

The researchers at the University of Warwick and Aberystwyth University solved the problem using a kind of artificial intelligence known as a genetic algorithm.

The research behind the software was conducted by David Kilgour and

Peter O'Connor at the University of Warwick and Mark Neal at Aberystwyth University; based on earlier work by Peter O'Connor and a student in his group, Yulin Qi.

Autophaser was recently presented at the forthcoming American Society for [Mass Spectrometry](#) annual conference in the US.

**More information:** [www.warwick.ac.uk/autophaser](http://www.warwick.ac.uk/autophaser)

Provided by University of Warwick

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