Developing a tool for streamlined molecular weight analysis

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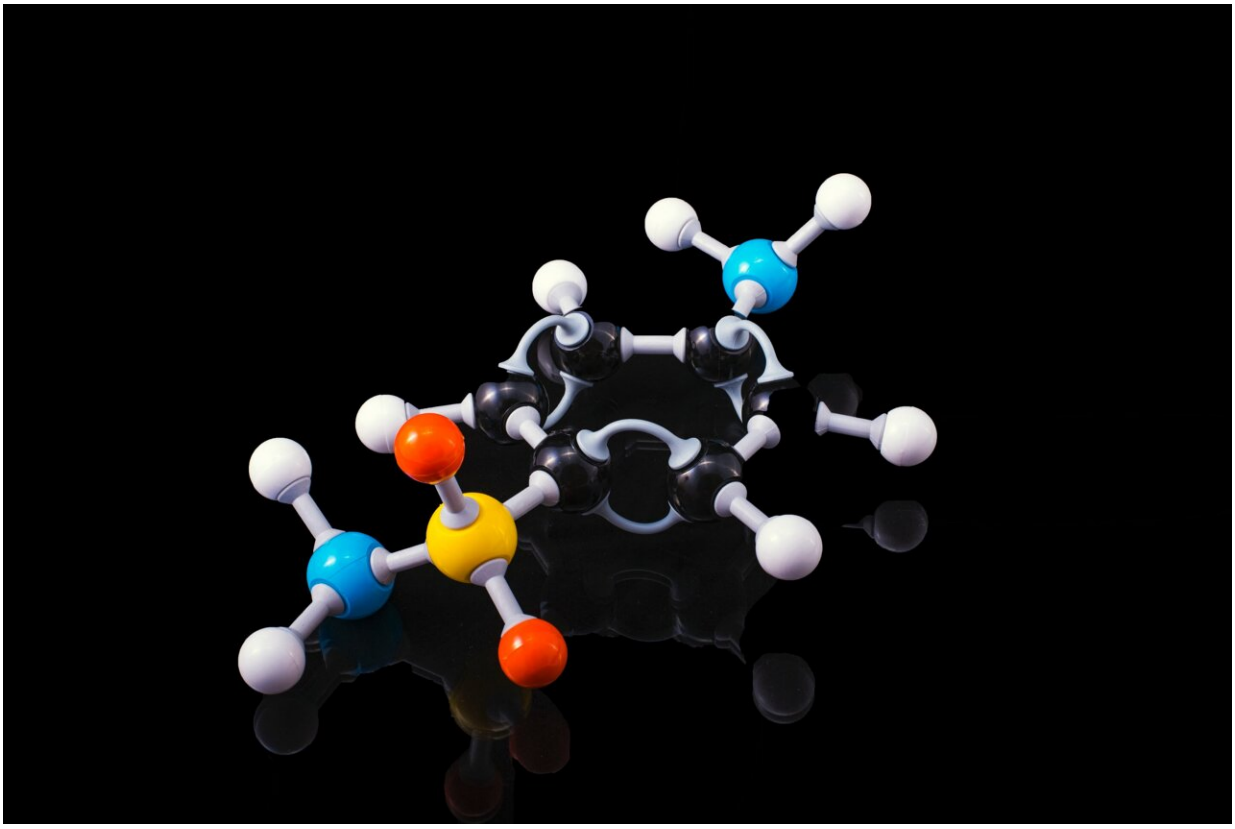

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New world-first Griffith University-led research has streamlined the process of identifying the structure and molecular weight of compounds, which could have positive implications for scientists working in the

fields of drug discovery, pollution analysis, food security and more.

Published in Royal Society of Chemistry's flagship journal *Chemical Science,* the team developed a novel Nuclear Magnetic Resonance-based (NMR) method to assign the molecular weight of compounds in mixtures which is a key asset for fields where individual components in complex mixtures need to be characterized.

The research, led by Professor Anthony Carroll from Griffith's School of Environment and Science and Griffith Institute for Drug Discovery with Ph.D. graduate Guy Kleks and Ph.D. candidates Darren Holland and Joshua Porter, is a breakthrough for scientists working on organic molecules.

"Currently you need two orthogonal techniques, mass spectrometry and NMR spectroscopy, to work out the molecular structure of a compound," Professor Carroll said.

"We've now condensed that into only needing one technique to work out the structure of the molecule."

The use of NMR, a similar method used in MRIs to image body parts, allows scientists to look at the unique "fingerprint of a compound." It is the leading method used to identify the molecular structure of an unknown molecule.

"But if you don't know the compounds molecular weight, then using NMR techniques gets you a certain distance towards identifying what the structure of a molecule is but doesn't get you all the way. Up until now this molecular weight was determined using mass spectrometry," Professor Carroll said.

Professor Carroll and his team have now developed an NMR method

that can predict the molecular weight of the compound. This "all in one" method now means that the molecular structure can be confirmed more quickly so that the compound can be used for further developments.

"What we've developed is actually a quick diagnostic tool that can help a whole range of areas including health and the environment," Professor Carroll said.

"Previously, it was like trying to find a needle in a haystack where one molecule out of a complex mixture was responsible for the effect that we see in, for example, cancer cells. That process generally requires us to do a whole lot of separation of molecules, which means a lot of time involved in doing purification and identification.

"Every molecule has its own molecular weight. If you don't know what that is, then then it's difficult to know what that compound is.

"What we've developed is a technique where we can look directly at this complex mixture and identify the individual molecules within it."

Professor Carroll hoped this world-first diagnostic method could become the adopted approach in the analysis of complex mixtures.

The research, "Natural Products Dereplication by Diffusion Ordered NMR Spectroscopy (DOSY)," has been published in *Chemical Science*.

More information: Guy Kleks et al, Natural Products Dereplication by Diffusion Ordered NMR Spectroscopy (DOSY), *Chemical Science* (2021). DOI: 10.1039/D1SC02940A

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