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Using mass spectrometry to isolate guanine-rich DNA ions

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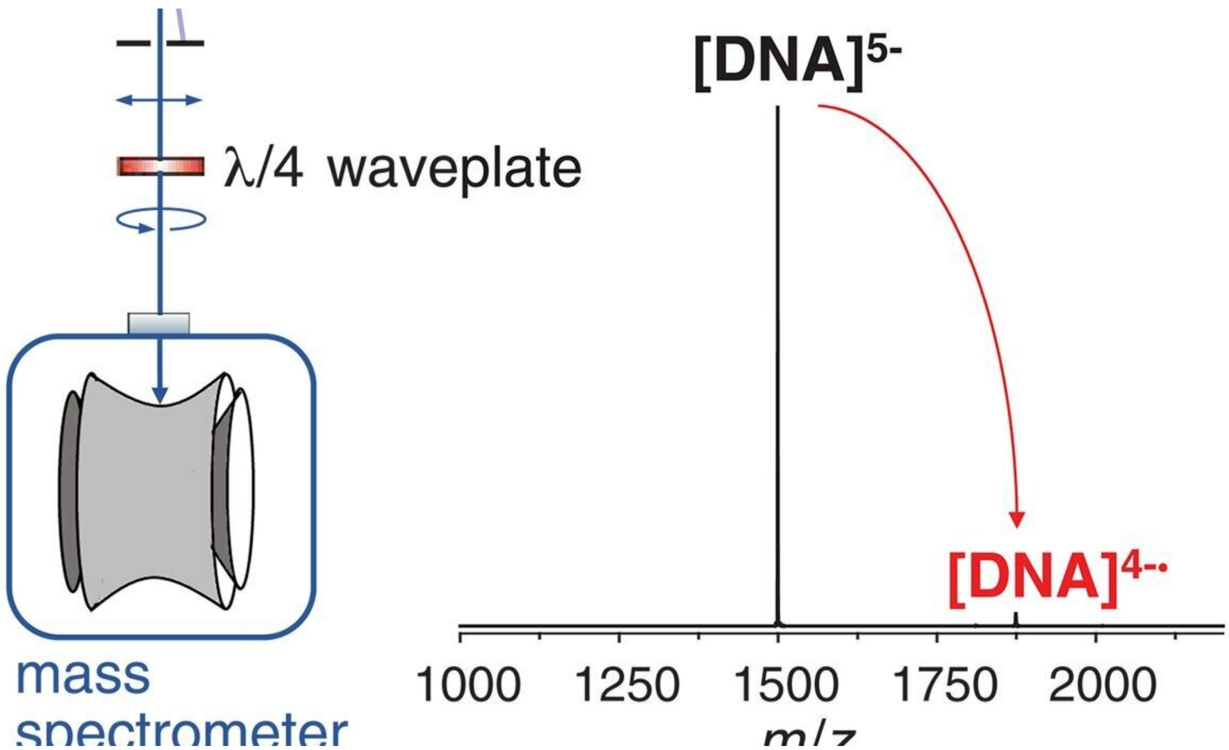

Experimental setup for generating circularly polarized laser pulses. Also shown is the typical mass spectrum after isolation of D-$[(dTGGGGT)_4{\bullet}(NH_4^+)_3]^{5-}$ ions and irradiation with left circularly polarized (LCP) light at 260 nm. See supplementary materials for setup details. Credit: *Science* (2020). DOI: 10.1126/science.abb1822

A team of researchers at Université de Bordeaux has developed a way to use mass spectrometry to isolate guanine-rich DNA ions. In their paper published in the journal *Science*, the researchers describe their method and how it might be used to expand the capabilities of mass spectrometry for structural analysis. Perdita Barran with the University of Manchester has published a Perspective piece outlining the history of the study of molecular chirality in crystals in the same issue, and also provides an overview of the work by the team in France.

The researchers note that circular dichroism spectroscopy is the primary tool for distinguishing between nonidentical mirror-image molecules. Circular dichroism is where a medium has the property of unequal absorption of left and right plane-polarized light—resulting in elliptically polarized emergent light. Circular dichroism spectroscopy techniques are based on taking advantage of the differences in absorption of right versus left circularly-polarized light. But it requires the use of solution-phase samples, which makes interpreting the results difficult and also limits its use to small molecules. In this new effort, the researchers have developed a new way to achieve the same goal with more easily interpreted results.

The work involved combining circular dichroism with mass spectrometry. They first used mass spectrometry to isolate guanine-rich DNA sequences rich in ions. They then irradiated the DNA with blasts from a laser—that forced the DNA ions to lose an electron, which changed their charge state. Then, by measuring the extent of the response, they were able to determine the chirality of the ion and the polarization of the light. That allowed the researchers to obtain a mass spectrum of ions—then, by switching between the different light polarizations, they were able to calculate circular dichroism. The researchers also undertook a study of DNA complexes with ammonium and potassium counterions, and as a result, gained a new perspective on individual molecule solvation.

In reviewing their work, the researchers found that reconstructed circular dichroism ion spectra looked very much like conventional solution-phase counterparts. They suggest their technique will provide researchers with another tool for conducting mass spectrometry during structural analysis efforts.

More information: Steven Daly et al. Mass-resolved electronic circular dichroism ion spectroscopy, *Science* (2020). DOI: 10.1126/science.abb1822