New calculations solve an old problem with DNA

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The normal (B-form) DNA will switch to left-handed DNA when it is physically twisted, or when a lot of salt is added to the solution. Researchers at the University of Luxembourg were able to accurately calculate for the first time the amount of salt which is required to do this. Z-DNA in the cell leads to loss of function and cancer.

In a recent publication, researchers achieved new accuracy in the ability to measure energy differences between states of molecules, thus predicting which states will be observed.

It has been known since the seventies that excessive salt causes DNA to reverse its twist, from a right-handed spiral to a left-handed one. DNA in the Z form is treated by our natural repair enzymes as damaged, and is therefore usually deleted from the cell. Deletion of genetic material can lead to cancer or to other problems, so the B-Z transition is no mere curiosity. However such is the complexity of the DNA molecule that a theoretical explanation which correctly predicts the amount of salt to do this has never before been found.

Dr. Josh Berryman and Professor Tanja Schilling of the University of Luxembourg have now been able to find a method of calculation which predicts this transition with unprecedented accuracy. With this success in describing the most enigmatic of molecules, the team is optimistic that they will be able to perform similar mathematical analyses for a variety of other substances. "It will enable us to predict material properties such as melting temperatures or elasticity. And this will be done with high

accuracy using our new technique. Hence, we can now design new materials and biomaterials on the computer more effectively than before," said Prof. Schilling.

Prof Schilling and Dr Berryman are physicists at the University's Physics and Material Sciences Research Unit, which comprises a team of 50 researchers.

More information: "Free Energies by Thermodynamic Integration Relative to an Exact Solution, Used to Find the Handedness-Switching Salt Concentration for DNA", Joshua T. Berryman and Tanja Schilling, J. Chem. Theory Comput., Article ASAP, DOI: 10.1021/ct3005968 , Publication Date (Web): November 19, 2012, *Journal of Chemical Theory and Computation*, pubs.acs.org/doi/abs/10.1021/ct3005968

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