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Creation of a Poly-Nucleotide Reference Dataset for Circular Dichroism

Circular dichroism is a sensitive absorption spectroscopy probing the chirality of macromolecules such as proteins, nucleic acids and sugars. Widely used by molecular biologists and biophysics in industrial and academic research, it is a proven technique for protein -folding, -thermal stability, -dynamics as well as protein-protein interactions.
In the past 16 years protein CD/SRCD spectra and associated bioinformatics and experimental metadata have been gathered, deposited and archived in a publicly accessible database the PCDDB (BBK, UK).
For poly-nucleotides the spectral CD band is larger and more variable than for proteins.
Currently, no systematic open-access deposition site exists. Reasons for this include physically the difference of the electronic transitions excitable in the polarized ultraviolet light as well as the structural sensitivity of nucleotides to their environment (pH, salinity, temperature). Indeed, the attribution of electronic transitions within the nucleotides, pairing nucleotides to their corresponding absorption maxima and minima is far more complex compared to the well understood n-pi*and pi-pi* transitions of the peptide bond.
Based on the success of the PCDDB databank we are aiming at establishing a database for poly-nucleotide CD spectra. All entries will undergo validation and curation procedures to ensure completeness, redundancy and quality of the data included. An open-access web interface shall enable users to browse and query samples, meta-data including other biophysical assays. Ultimately spectra in graphical display and tabulation format shall be made accessible to experimentalists as well as theoreticians.
Here we will present the first steps and suggestions of how to accumulate and standardize CD spectra of nucleotides, their archiving and classification following the folding patterns of DNA and RNA macro-molecules.

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