Spin-Labelled DNA Oligomers: Simulations and Experiment

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Modern spectroscopic and microscopic techniques are of immense importance for studying biological macromolecules. Important information can be obtained using "spectroscopic rulers", like fluorescence resonance energy transfer (FRET) or electron paramagnetic resonance (EPR) spectroscopy, which are used to measure distances between chromophores or spin labels.
We present extensive GPU-accelerated MD simulations of oligonucleotides with covalently conjugated spin labels. These simulations provide insight into the conformations of the labelled nucleosides and a possible influence on DNA structure. The simulations are essential for understanding the experimental distance distributions obtained from EPR (DEER/PELDOR) measurements, especially as X-ray- or NMR-structural data are not (yet) available for all oligonucleotide/spin-label combinations of interest.
We believe that such a close combination of experiment and simulation is a promising approach to elucidating structural and spectroscopic features of complex and flexible biomolecules like DNA- or RNA-conjugates.

[1] M. M. Haugland, A. H. El-Sagheer, R. J. Porter, J. Pena, T. Brown, E. A. Anderson, J. E. Lovett, *2'-Alkynylnucleotides: A Sequence- and Spin Label-Flexible Strategy for EPR Spectroscopy in DNA, J. Am. Chem. Soc.* **2016**, *138,* 9069-9072.