Voltammetric, spectroscopic and Computational molecular docking studies of two dithiole-3-thione derivatives interacting with DNA

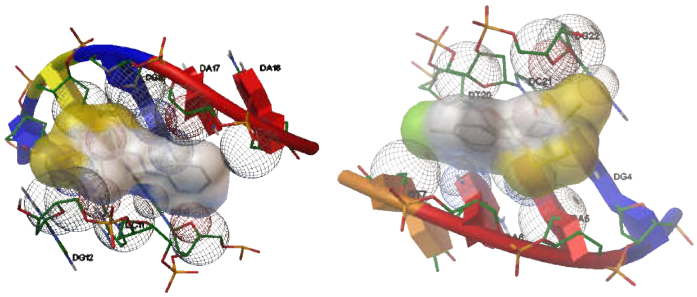
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Abstract

Cyclic voltammetry (CV) and UV-Visible spectroscopy (UV-Vis) techniques were used to calculate binding parameters of 4-methyl-5-((phenylimino)methyl)-3H-1,2-dithiole-3-thione (MPDT) and 5-(4-fluorophenyl)-3H-1,2-dithiole-3-thione (FPDT) with DNA. The results obtained from both techniques were confirmed by computational molecular docking using AutoDock molecular docking software. The anodic peak potential shift in CV indicated an intercalative mode of binding. The binding constants (M^{-1}) of the adducts MPDT-DNA and FPDT-DNA obtained from voltammetric measurements were found to be 8.0×10^{4} and 2.4×10^{4} , respectively, with binding free energy being -27.99 and -25.01 KJ mol^{-1}, respectively. These results are in good agreement with to those obtained from UV-Visible spectroscopic studies Vis. The diffusion coefficients of MPDT and FPDT i.e. (2.06×10^{-10} and 2.42×10^{-9}, respectively) were found to be higher than those of DNA-bounded compounds (1.27×10^{-10} and 1.65×10^{-9} cm^2/s, respectively). The binding free energy of MPDT and FPDT to DNA was also calculated by molecular docking study. The docking study gave excellent approximation with experimental results, shedding light and gave information on the sites of binding.



(a) (b)

Figure1. Three-dimensional model of interactions of MPDT (a) and FPDT (b) with DNA, the DNA is presented by secondary structure, by CPK, and by lines colored by atom type (C: gray; polar H: sky blue; and O: red). MPDT and FPDT are depicted by sticks and balls having green colored surface

Recent Publications

1. Barbaglia GA. Ueber den Sulfovaleraldehyd. Ber Dtsch Chem Ges. 1884;17:2654-2665.
2. Prestera T, Talalay P. Electrophile and antioxidant regulation of enzymes that detoxify carcinogens. Proc. Natl. Acad. Sci. USA. 1995;92(19):8965-8969.
3. Bange A, Halsall HB, Heineman WR. Microfluidic immunosensor systems. Biosens Bioelectron. 2005;20:2488-2503.
4. Saidi M, thèse de doctorat, Université Renne I. 1988:123-124.
5. Aslanoglu M, Ayne G. Voltammetric studies of the interaction of quinacrine with DNA. Anal. Bioanal. Chem, 2004;380(4):658-663.
6. Atkins PW. Physical Chemistry. Oxford University Press, Oxford, UK. 1986; 263-265.



Biography

Prof. Touhami LANEZ is a Professor at the University of El Oued, Algeria and the head of Laboratory of Valorisation and Technology of Sahara Resources (VTRS). He majored in organic chemistry at the University of Constantine, Algeria, and received a PhD in organic chemistry from the Strathclyde University, 1989. His research activities are focused on organometallic synthesis, electroanalytical chemistry, pharmacological sciences and antioxidant activity.

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