Reunião Anual do INCT-FCx - 2022

De 26 a 29/Outubro de 2022,
Hotel Estância Atibainha, Nazaré Paulista/SP

MOLECULAR SIMULATIONS OF THE NUCLEOTIDE CAPTURE BY THE POLYMER BRUSH PDMAEMA

Santos, V. F.[1]; Santos, D. E. S.[2]; Soares, T. A.[1]

[1]*Dept. de Química, Universidade de São Paulo, Ribeirão Preto, Brazil;*
[2]*Dept. de Química Fundamental, Universidade Federal de Pernambuco, Recife, Brazil;*

Abstract: It has been previously reported that the poly(dimethylaminoethyl methacrylate) (PDMAEMA) polymer brush can capture high loads of small nucleic acid sequences. It is particularly puzzingly that the PDMAEMA exhibits a much higher affinity, and thus higher load capture of RNA than DNA [1], but the molecular basis for this preference is not well understood. To investigate the influence of nucleotides chemistry and structure on this phenomenon we performed molecular dynamics and metadynamics simulations of the PDMAEMA brushes in presence of the nucleotides deoxyadenylate and deoxythymidylate present in the DNA, and adenylate and uridylate present in RNA. The metadynamics simulations were performed to estimate the energies needed to dissociate the nucleotides from the polymer brush structure. The dissociation free energies calculated for adenylate (-21,45 ± 4.94 kJ/mol) and deoxyadenylate (-13,74 ± 1,17 kJ/mol) suggests that the presence of an extra hydroxyl group in the RNA nucleotides contributes to a greater interaction with the polymeric brush, which may explain the greater loading of RNA. The high standard deviation values obtained made it difficult to find a significant difference between dissociation free energies for uridylate (-20,00 ± 5,54 kJ/mol) and deoxythymidylate (-23,66 ± 8,87 kJ/mol). So a higher precision methodology is needed to infer the influence of these nucleotides in the loading of nucleic acids by the PDMAEMA polymer brush. Determination of dissociation free energies for the remaining nucleotides present in DNA (deoxycytidylate and deoxyguanylate) and RNA (cytidylate e guanylate) will also be performed to confirm the role of the extra hydroxyl group in greater loading of RNA.

Key-words: Molecular dynamics, Metadynamics, Polymer brush.
Support: FNDE, CNPq and CAPES

References:

[1] D. Li, A. S. Sharili, J. Connelly, J. E. Gautrot, *Biomacromolecules. 19* (2), 606–615 (2019).