XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Title: Design of immunosensors assisted by computer simulations

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Abstract: Immunoglobulin oriented immobilization was conducted by means of molecular dynamic (MD) simulation in order to assist immunobiosensors experimental development. As a specific and well-defined interaction, antibody-antigen requires several protocols to concatenate clues in order to improve the methodology accuracy. Interactions between analyte and substrate can be measured both experimentally and theoretically through the Atomic Force Microscope (AFM) and Steered Molecular Dynamics (SMD), respectively. Six orientations were selected and studied to accomplish nanosensor requirements. The most promising of orientation (orientation 5 - P5) presented both a large number of possible hydrogen bonds (126) with silanol groups from the surface and a large surface contact area. The system was parameterized according to the CHARMM force field protocol for MD simulation. Within 100 ns, the lowest molecular fluctuations were verified for each configuration set. Then, molecular docking calculations in the presence of the ligand were performed within the active site. Docking favorable poses were again submitted to MD simulations followed by SMD to mimic the AFM experiments. Force values ranged from 1,950 pN to 2,430 pN using a spring constant of 7.34 kcal/mol/Å2. In order to establish a correlation between theoretical and experimental results, experimental analysis were conducted with the system. Experimental force values ranged from 641,60 ± 363,27 pN. Statistical analysis helped to make a correlation between experimental and theoretical results.

Key-words: Immunoglobulin, immobilization, SMD, MD and AFM
Support: This work has been supported by FAPESP: 2013/09746-5

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