In Silico insights on the electrode high sensitivity to salts.

Ser137 seem to play an important role in Coq10-Coq6 interaction. Therefore, comparative models of mutants at these positions and at additional polar residues in this pocket (S79A, S137A, S79A-S137A, S79A-W139A and S79A-S137A-W139A) were created using the program Modeller. A hundred different structures were generated for each mutation and the best models were chosen based on Ramachandran plot and PROSA analysis. Coq6 was docked in these structures using Autodock Vina and the results were analyzed in Pymol. When the mutation is made in SER79, SER137 and W139 there is not polar interactions between Coq10 an Coq6, as expected. Considering these results, we aim to validated them experimentally and to perform molecular dynamics to better understand the interaction between Coq10 and Coq6.

Poster #18
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Title/Abstract: In Silico insights on the electrode high sensitivity to salts

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Recent findings in sensing and biosensing based on electrical measurements point to a very high sensitivity, in which the introduction of one molecule of an analyte into one million (or more) molecules of water is already detectable. In some cases, the high sensitivity could be attributed to specific interactions between the analyte and the molecules on the sensing unit, but results have also been published of considerable sensitivity of bare electrodes for molecules with no molecular recognition capability[1]. This is the case of some electronic tongues reported in the literature. It seems that the presence of trace amounts of the analyte, e.g. a NaCl molecule, is sufficient to alter the properties of the water at the interface, particularly because the electrical measurements are very sensitive to interface changes. In this study, we

explore this hypothesis by calculating how the water properties in contact with a gold surface can be affected by incorporation of a NaCl molecule. The calculations are done within the Kohn-Sham Density Functional Theory[2] using Quantum ESPRESSO[3] code. It is found that the Fermi level has been changed in the presence of the NaCl molecule in the calculation. Although we cannot reproduce in the simulations the precise experimental conditions owing to computer power limitations, the significant changes observed may open the way for explaining the behavior of sensors and biosensors in unprecedented fashion.
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Title/Abstract: Lipid A is the outermost component of lipopolisaccharides of Gram-negative bacteria membranes, main responsible for bacteria endotoxicity and its chemical structure is basically composed of two phosphorylated N-acetylglucosamine rings attached to a variable number of acyl chains. Phenotypical modifications on the structure of Lipid A change its physical and biological properties in addition to its aggregation forms. Experimental evidences suggest a direct correlation between Lipid A membrane shape and the endotoxical bacterial activity. In order to test this hypothesis, we have performed molecular dynamics simulation of different phenotypes of Lipid A from Pseudomonas aeruginosa and Escherichia coli. To characterize the relationship between lipid phenotypical variation and its aggregate shape at a microscopic level. Simulations were carried out using