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Computational Design of a Biosensor Based On Silicon Dioxide Nanoneedles Selective To *Fusarium Oxysporum*

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Extended Abstract

The idea of using silico dioxide nanoneedles (SIN) as a model of optical fibers as a sensor is today beneficial to detect molecules with applications in chemistry and biomedical areas. To perform a *Fusarium oxysporum* detector based on SIN, the need to know first a molecular analysis of the proteins of *Fusarium* and last analyses of the interactions with this and the SIN. Regarding the above, the present work performed the computational modeling of functionalized silicon dioxide nanoneedles with a biopolymer and evaluated their interactions with *Fusarium* proteins through computational methods.

Fusarium oxysporum is a phytopathogen with some strain that causes vascular wilting, crown, and root rots in several crops [1].

The docking assays were a computational method that predicted the possible ligand (SIN) target (*Fusarium* protein) interaction.

The selected target was a cutinase of *F. oxysporum*, an enzyme produced by the microorganism. Its primary function is to degrade the cellular wall of the plants that this infects [2]. The above protein was obtained from the protein data bank (PDB) with the PDB code 5AJH [3]. On the other hand, the selected ligands were the alginate, APTES, and APTES-alginate, which were modeled using the Avogadro package [4]. The docking assay was performed using the Molegro Virtual Docker (MVD) package [5] with the MoldockScore [6].

The results show a favorable target-ligand interaction. Regarding quantitative results, APTES was the better ligand, with a ligand efficiency (LE) of -5.75 kcal/mol, resulting in the more efficient ligand against *F. oxysporum*.

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