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Targeting TMPRSS2 with carbon nanostructures: an in silico study

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TMPRSS2 (transmembrane serine protease 2) is a key protein involved in SARS-CoV-2 entry into host cells by participating in membrane fusion. Therefore, TMPRSS2 represents a promising therapeutic target with a lower risk of resistance development as a host factor compared to viral proteins.

In this study, the in silico investigation was conducted to evaluate the possibility of interaction between C60 fullerene and TMPRSS2. First, four potential binding pockets were predicted by using the p2Rank tool. Based on structural features and residue decomposition, three pockets were selected for further analysis. The molecular docking simulations suggested strong interactions within pocket 1. However, long-scale (1000 ns) MD simulations indicate C60 fullerene migration from pocket 1 to pocket 2, showing thermodynamic stability insight that pocket.

RMSD and RMSF analyses confirmed the overall structural stability of the complexes, while PCA analysis indicated a significant reduction in conformational flexibility upon fullerene binding compared to the apo-TMPRSS2 structure. The MM/PBSA approach has shown that van der Waals interactions dominate in the binding between C60 fullerene and TMPRSS2. Pocket 2 exhibited the most favourable binding energy ($\Delta G \approx -30.7$ kcal/mol), whereas binding in the other pockets was weak.

To conclude, C60 fullerene can interact with TMPRSS2 via a non-classical, hydrophobic-driven mechanism and stabilize via van der Waals interactions. Obtained results suggest C60 fullerene as potential antiviral scaffolds targeting the TMPRSS2 protein. To find more details about this work, use this link: https://doi.org/10.3390/molecules30234586

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