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Combining Single-Walled Carbon Nanocones with Antioxidant Vitamins C and E Towards Neurotherapy-Based Nanomedicine

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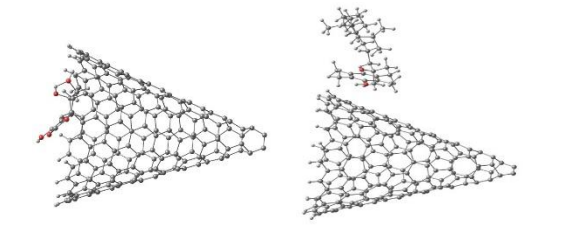
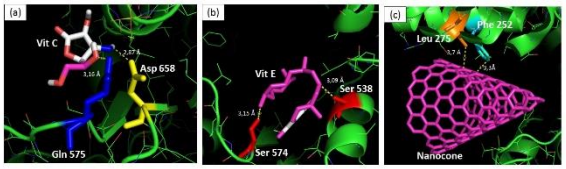
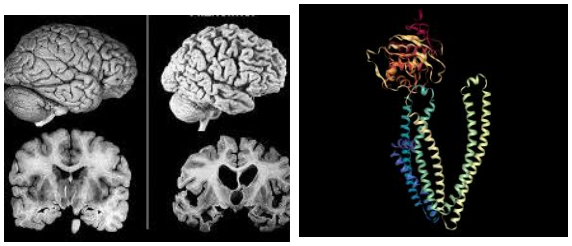
Graphical Abstract



***SWCNC* + Vit C** ***SWCNC* + Vit E**



***ABC*/Vit C** **ABC/Vit E** **ABC/SWCNC**



Neurotarget drug-discovery based mitochondrial nanomedicine

Abstract. Currently, a*ntioxidant compounds, such as vitamins C and E, are widely used to deactivate free oxygen radical species (ROS), playing an essential role in preventing chronic neurodegenerative diseases where ROS levels are significantly increased [1,2]. Herein, single-walled carbon nanocones (SWCNC), a nanocarbon allotrope with unique physico-chemical properties, was combined with antioxidant vitamins C and E toward exploring mitochondrial nanomedicine applications in molecular neurosciences [3,4].To this end, we carried out the study of SWCNCs interaction with vitamin C and vitamin E using ab initio calculations based on Density Functional Theory[5].Besides, molecular docking methodology was applied by selecting the human ABC-mitochondrial carrier ABCB10, PDB ID: 4ayt to address the study of molecular interactions with the antioxidant vitamins C and E [6]. The results obtained from ab initio study, showed that the most stable configuration was observed for the SWCNC interacting with vitamin C >> vitamin E, with DFT-binding energy of 0.98 and 0.56 eV, respectively. The results on molecular docking study provided a free binding energy (FEB) and rmsd for the neurotarget (4ayt) following the order of as: ABC-carrier/SWCNCs (-17.6 Kcal / mol and 0.931 Å)>>ABC-carrier/vitamin E (-5.4 Kcal / mol and 0.911 Å) and ABC-carrier/vitamin C (-4.5 Kcal / mol and 1.567 Å), and SWCNCs simultaneously interacting with vitamin E*

	on ABC-carrier was -18 Kcal /mol and r.m.s.d = 0.079 Å). Lastly, the results suggest that the potential therapeutic combination of SWCNTs with vitamins E > C, could be a new and promising alternative for neurotherapy-based nanomedicine.

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