The impact of carbon-based nanoparticle on the progression of Alzheimer's Disease in the presence of ammonium nitrate salt of various concentrations

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## Abstract

According to the recent research studies, nanoparticles (NPs) can be absorbed to human blood and have toxicological effect on human organisms. Due to the small particle size, NPs can translocate to the human brain and contribute to the progression of neurodegenerative diseases. In this work, molecular dynamics study was performed to investigate the impact of carbon-based NP on the aggregation of amyloid beta  $(A\beta)$  peptides, a symbol of Alzheimer's Disease. Moreover, the synergistic effect of NP and environmental pollutants was investigated at various concentrations of the ions found in the environmental realm. In particular the effect of C<sub>60</sub> on the aggregation kinetics of eight A $\beta_{16-21}$  peptides, the segment of A $\beta$  peptide, was studied in the presence of ammonium and nitrate ions with the concentrations varied from 50 mM to 150 mM. The results showed that the aggregation of  $A\beta_{16-21}$  peptides was slower in the presence of carbon NP at all concentrations of ammonium nitrate salt. In addition, in the absence of carbon nanoparticle, the slowest aggregation was observed at 100 mM salt concentration among other salt concentrations. While in the presence of  $C_{60}$ , no significant effect of the salt concentration on the aggregation kinetics of the peptides was observed. Moreover, the amounts of hydrogen bonds and beta sheets in the secondary structures of  $A\beta$  peptides were calculated to identify the type of the interactions involved in the aggregation of peptides.