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Computational investigation of interactions of Pemetrexed and Pazopanib anticancer drug molecules conjugated with small peptide link with magnetite (Fe_3O_4) surface

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Pharmacologically active anticancer drugs reach to tumor tissue with low specificity and they have dose-dependent toxicity in chemotherapy applications. Classical drug administration routes are oral and intravenous. Orally taken tablets or capsules result in irregular pharmacokinetic due to the metabolic pathways and they frequently damage healthy tissues due to low specificity. After the developments in nanotechnology, it is possible to reduce these harmful side effects by using nanoparticular drug delivery systems. When iron oxide (magnetite) nanoparticles are loaded with some anticancer drugs, the drug loaded iron oxide nanoparticles can be directed to tumor tissues via an external magnetic field and this may mostly eliminate the side effects of classical oral treatment. In the present study, we computationally investigate interactions of Fe_3O_4 (magnetite) surface with pemetrexed and pazopanib drug molecules that are both separately conjugated with small specifically designed peptide link. In particular, we present thermodynamic, geometrical and electronic properties of the drug-peptide complex interacting with model Fe_3O_4 surface predicted by several molecular modelling methods (including semi empirical methods and DFT).

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Biography

Senay Sanlier has completed her PhD in 2000 at Ege University, Faculty of Science Biochemistry Department on 'Encapsulation of enzyme systems in erythrocytes'. In 2007, she was appointed as an Assistant Professor and in 2013 she was appointed as a Professor at Ege University Faculty of Science Biochemistry Department. She is also a Consultant in Ege University Pharmacokinetic Drug Development & Research Center (ARGEFAR) since 2013. Her main research interests are nanoparticular drug delivery systems for cancer therapy, proteomics, enzymology and drug design.

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