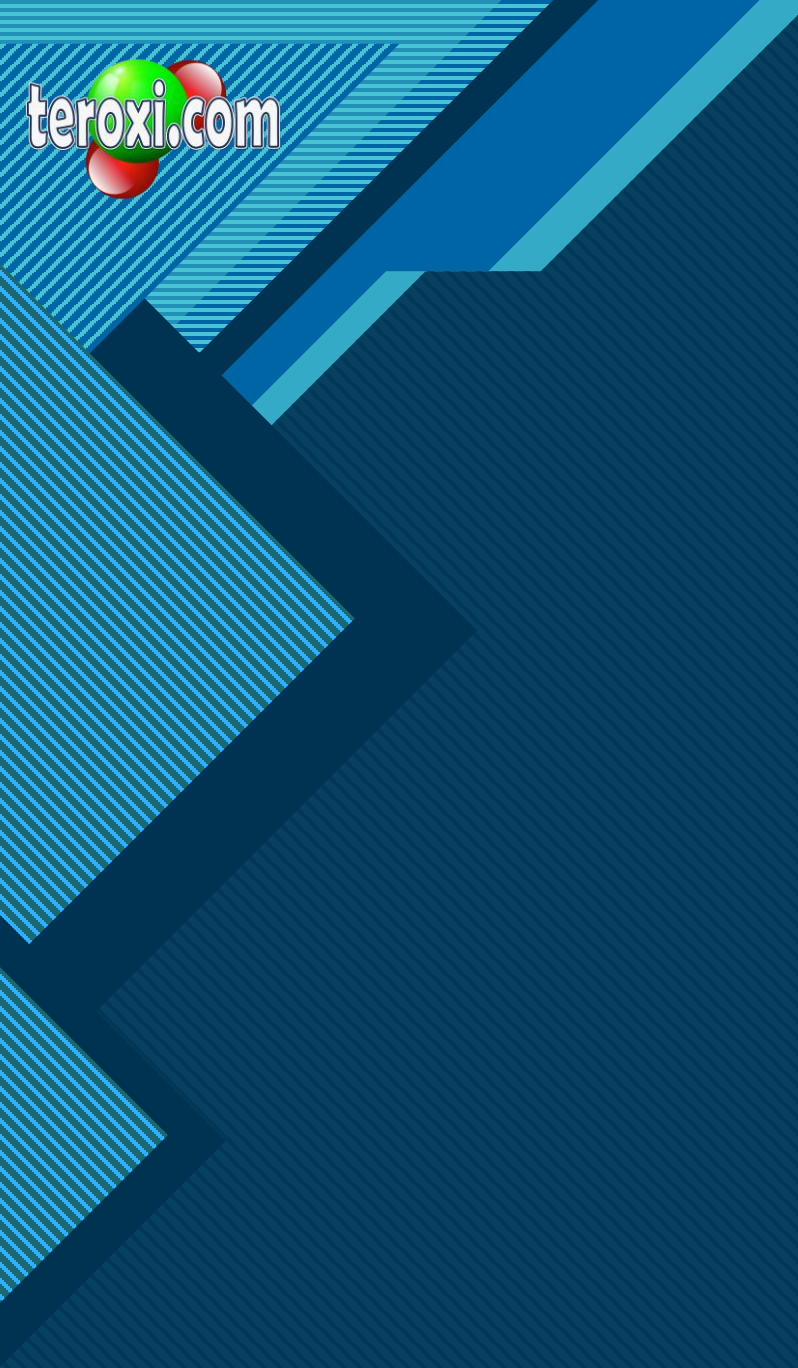


Terapias Oxigenativas 14



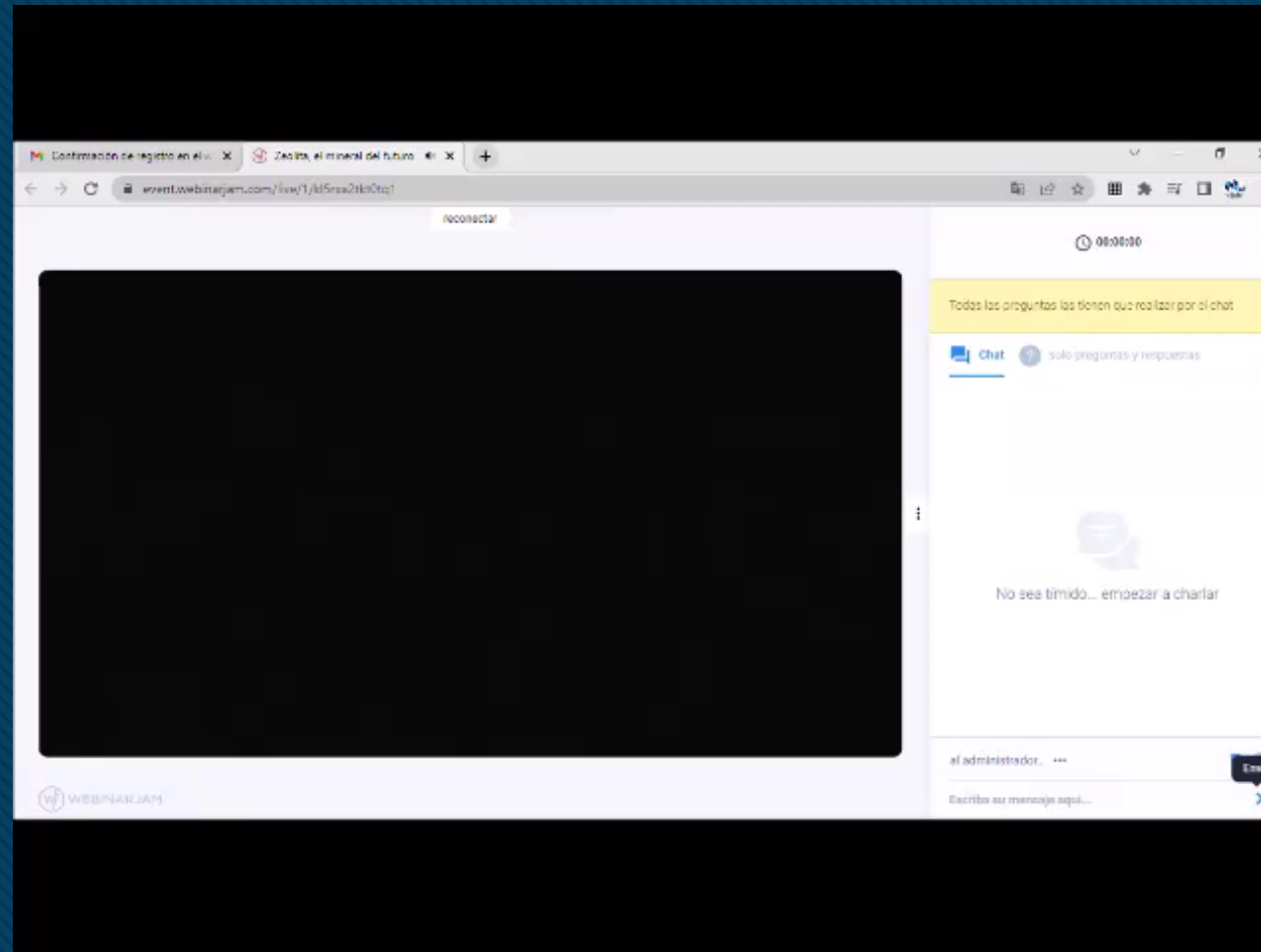
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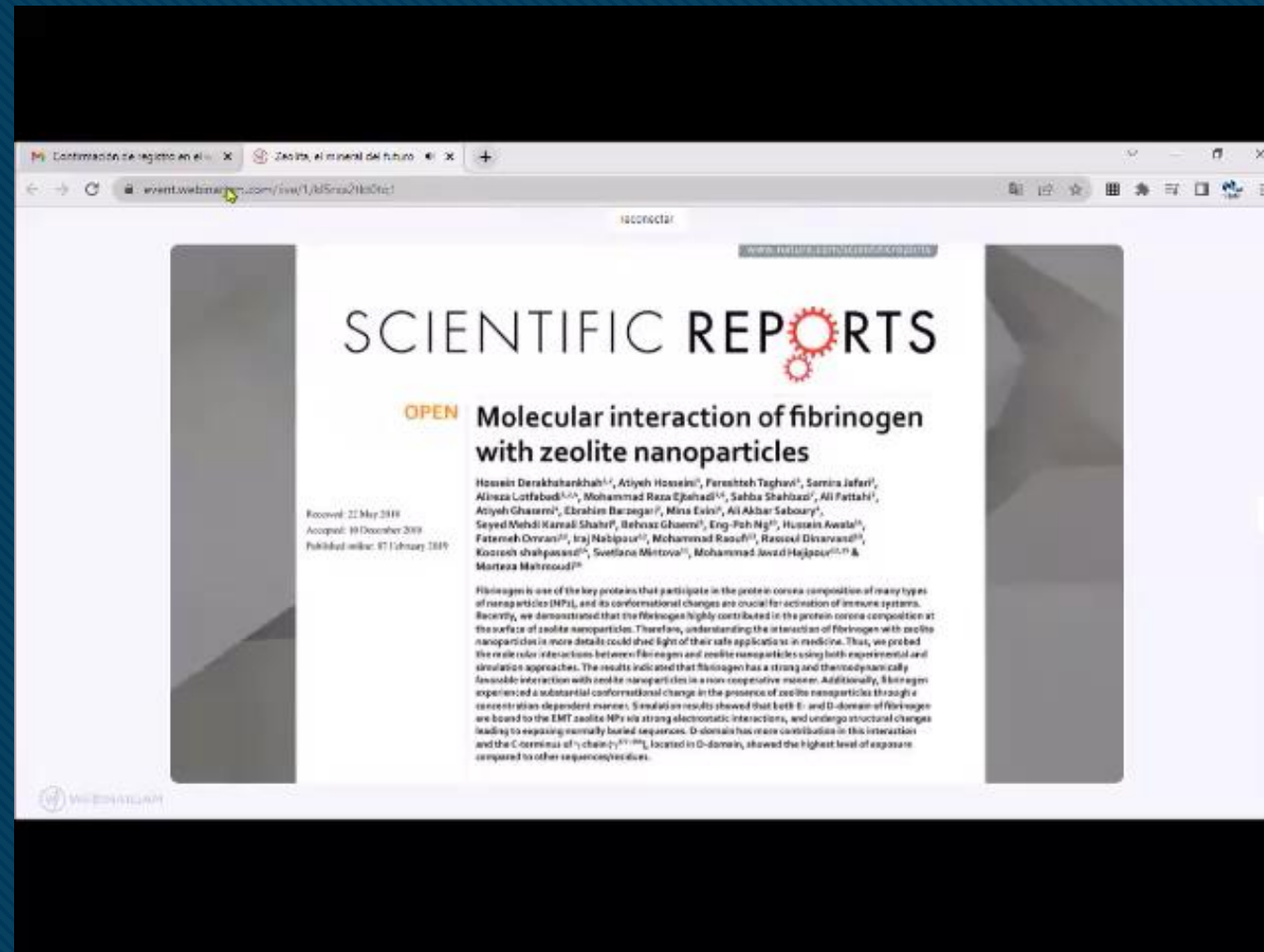


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Molecular interaction of fibrinogen with zeolite nanoparticles

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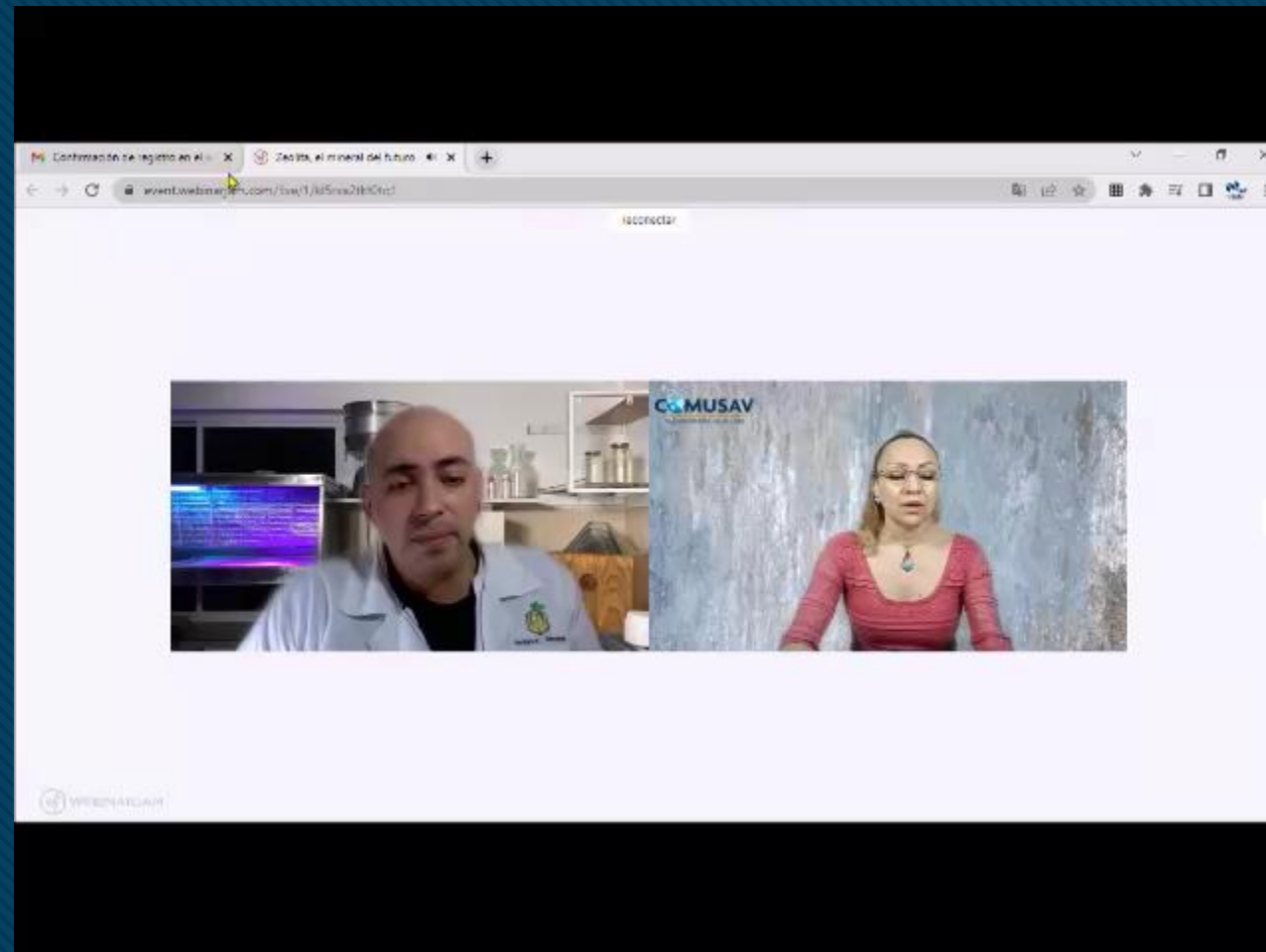
Received: 22 May 2018

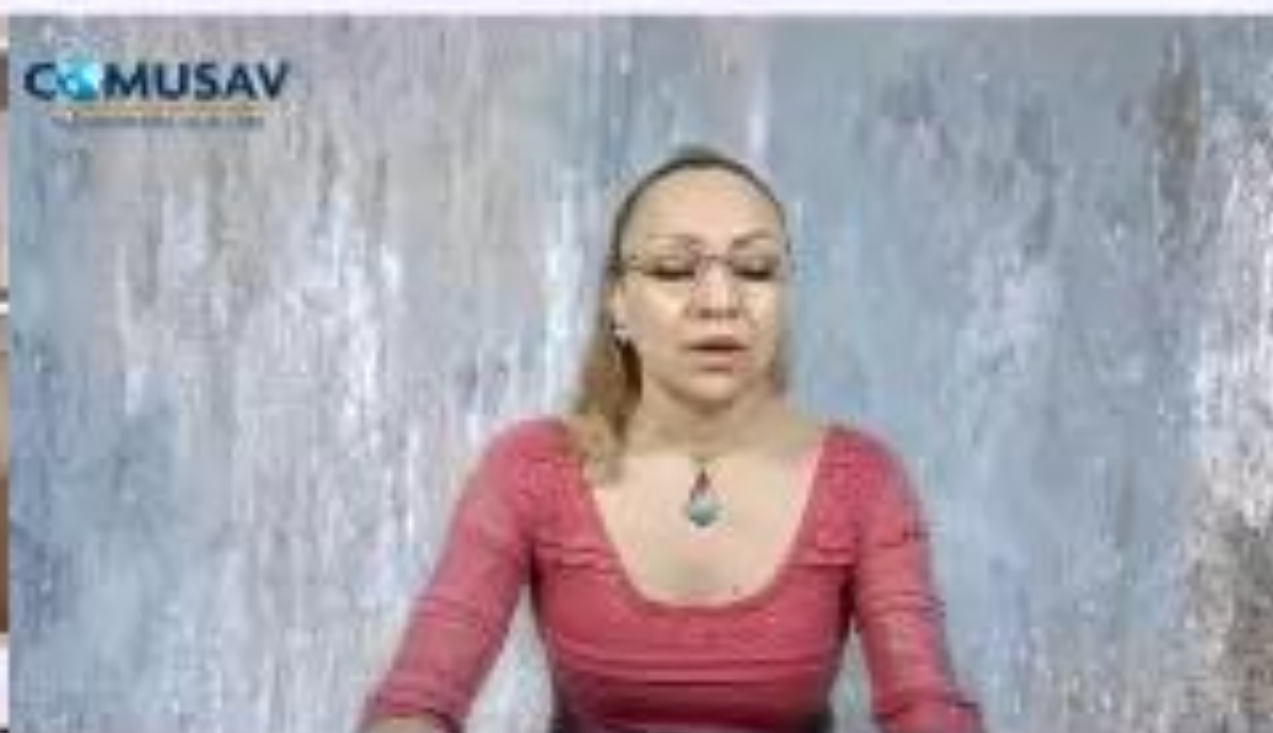
Accepted: 10 December 2018

Published online: 07 February 2019

Fibrinogen is one of the key proteins that participate in the protein corona composition of many types of nanoparticles (NPs), and its conformational changes are crucial for activation of immune systems. Recently, we demonstrated that the fibrinogen highly contributed in the protein corona composition at the surface of zeolite nanoparticles. Therefore, understanding the interaction of fibrinogen with zeolite nanoparticles in more details could shed light of their safe applications in medicine. Thus, we probed the real-time interactions between fibrinogen and zeolite nanoparticles using both experimental and simulation approaches. The results indicated that fibrinogen has a strong and thermodynamically favorable interaction with zeolite nanoparticles in a non-cooperative manner. Additionally, fibrinogen experienced a substantial conformational change in the presence of zeolite nanoparticles through a concentration-dependent manner. Simulation results showed that both E- and D-domain of fibrinogen are bound to the EMT zeolite NPs via strong electrostatic interactions, and undergo structural changes leading to exposing normally buried sequences. D-domain has more contribution in this interaction and the C-terminus of γ_2 chain ($\gamma_2^{371-386}$), located in D-domain, showed the highest level of exposure compared to other sequences/residues.

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Gracias