



A Szerkezeti Kémia és Biológia Laboratórium szeretettel
meghív minden kedves érdeklődőt

Computational Medicinal Chemistry.

Searching peptides acting as antimicrobial agents

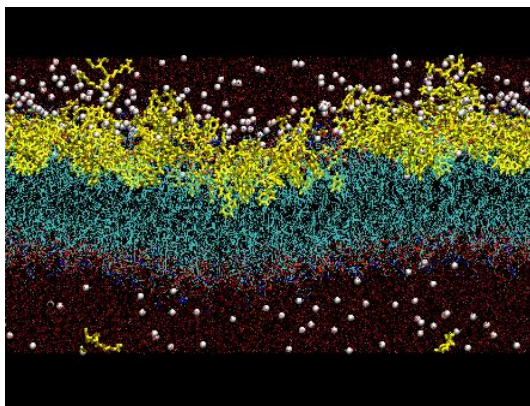
című előadásra.

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Összefoglaló: The synthesis, *in vitro* evaluation, and conformational study of penetratin and structurally related derivatives acting as antimicrobial agents are reported. Among the compounds evaluated, two methionine sulfoxide derivatives exhibited the strongest antibacterial and antifungal effects in this series. In order to better understand the antimicrobial activity obtained for these peptides we performed an exhaustive conformational analysis using different approaches. Molecular dynamics simulations were carried out using two different media (water and TFE/water). The results of these theoretical calculations were corroborated using experimental CD measurements. The electronic study for these peptides was carried out using molecular electrostatic potentials. The molecular modeling study allowed us to reduce in size these bioactive peptides from 16 to 11 and to 9 amino acid residues in total. Despite their reduction, they still maintained and even enhanced the antimicrobial activity detected for penetratin. Our results lead to the proposal of a peptide-induced lipid segregation model as the mechanism of action of these antimicrobial peptides.