



VABILO NA PREDAVANJE V OKVIRU DOKTORSKEGA ŠTUDIJA KEMIJSKE ZNANOSTI

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z naslovom: FOLDIT: Scientific Discovery by Protein Folding Game Players

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Vljudno vabljeni!

Abstract

Can the brainpower of humans worldwide be brought to bear on critical problems posed in computational biology, such as the structure determination of proteins and designing novel enzymes? Yes! We have worked with and studied how citizen scientists, most of whom have little or no prior biochemistry experience, have uncovered knowledge that eluded scientists for years. Players of the online protein folding video game Foldit have been able to determine a crystal structure of a previously unsolved protein, as well as enhancing the activity of a designed enzyme. In the protein folding field, game-playing humans have been most successful in the refinement of partially correct models. As this restricts the usefulness of player-driven folding to starting models that are already close to the native, we recently set out to see if the participants of Foldit could benefit from using electron density data that was too poor for PHENIX AutoBuild to refine. Despite starting Foldit players with an extended chain as a starting model—the exact opposite of refinement—a select group of players have been able to produce very accurate models using electron density information not good enough for PHENIX AutoBuild. These exciting results demonstrate the combined power of humans and computers by introducing a new approach: distributed computing driven by human intuition.