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Using structure to predict function in protein biochemistry: a combined computational and wet lab approach

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We have developed an undergraduate biochemistry lab curriculum based on authentic inquiry. The Biochemistry Authentic Scientific Inquiry Lab (BASIL) uses a combined computational and wet lab approach to study proteins of known structure but unknown function. There are over 3800 structures in the Protein Data Bank (PDB) that have unknown function. Students use a combination of sequence and structure alignment tools to study these structures with the goal of identifying possible enzymes. They then use molecular docking to predict what model substrates fit near a proposed active site. Students can produce the target enzymes in the lab using standard wet-lab biochemistry techniques for expression and purification, and they then perform kinetic assays with model substrates selected from their docking studies. We assess their learning as students and their growth as scientists in terms of research methods, visualization, biological context, and mechanisms of protein function. We have successfully used this curriculum in biochemistry lab courses for majors and non-majors. The curriculum is modular and can be used as a whole or individual parts may be incorporated into an existing course - either lecture or lab. The course modules are available for no charge via GitHub. We welcome new collaborators who are interested in adopting the curriculum in full or in part. We can offer synchronous support via virtual meetings and asynchronous support via Slack. This project is supported in part by NSF IUSE 1709355.

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