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Adaptable online Team-Based Learning in a capstone simulation "Hit-to-Lead" Drug Discovery exercise

Drug discovery, particularly at the early stages, involves an understanding of both the chemistry of the potential drug molecule and the biological environment with which it interacts. This exercise pulls together all these different components that they have been taught across their degree programme into one capstone coursework exercise over eight weeks. The simulation allows students to synthesise and use material from all years of their degree to experience how this fits together in the pharmaceutical industry. The work is entirely open-ended allowing teams to address the problem in very different ways. The students also develop skills in use of PyMol and GOLD to visualise x-ray structures of target proteins and dock their potential leads. The simulation uses Team-Based Learning (TBL) exercises in the early stages of the coursework to help cement the team environment and peer-to-peer learning. Teams give justifications for modifications for compound modifications and interpret those data they receive from their changes. They then must propose a synthesis of their lead compound searching chemical databases and literature, to plan a route bearing in mind cost, efficiency, scale-up concerns, and green chemistry principles. The assessment has a team component, a peer mark, and an individual mark for the report. Students also include a reflection on their own development during the exercise. In the pandemic the exercise was carried out entirely online, using Teams to facilitate separate areas for the groups to work in. The exercise has been developed using computational modelling, however it can be run entirely as a paper-based exercise and we are currently working with colleagues at the University of Leicester who have been trialling this. We will describe how to run the exercise and how it can be modified for differing circumstances.

Key words

Drug Discovery, Team-Based Learning, Remote Teaching

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