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## A simulation to support experiment design in an open ended investigation of an enzyme-catalysed reaction

COVID social distancing restrictions and absences due to self-isolation have caused significant issues for implementation and assessment of undergraduate laboratory classes. Here we describe a pre-laboratory simulation to support an open ended undergraduate chemistry practical class. The simulation also provides students who are unable to complete the laboratory work with personalised model data so that learning outcomes relating to experimental design, interpretation and reporting can be achieved.

Ordinarily, the year 2 biological chemistry laboratory experiment consists of two dedicated laboratory sessions in which students work in small groups to conduct an open ended investigation of an enzyme-catalysed reaction using a microplate-based assay with a coloured visual readout. As well as the practical experience of pipetting small volumes in microplates, the learning outcome of the exercise include being able to propose hypotheses, plan reaction conditions and appropriate control experiments. Under COVID restrictions, the available laboratory time was reduced to approximately one third. Due to the constraints on laboratory time, it was desirable that all planning was conducted prior to arriving at the laboratory. A simulation was devised in Microsoft Excel that gives students a free choice of volumes of enzyme, buffer, substrates and cofactor and layout of reactions in the 96-well microplate. After setting time and temperature, a visual display of the predicted colours in the microplate wells is generated. Warnings of common errors such as running out of solutions or overfilling the wells are given. The simulation was used with a cohort of ~200 undergraduates. Feedback was obtained via a survey and responses were largely positive, with a majority of respondents reporting that they had found the simulation useful for planning their laboratory work. Students who missed the laboratory session were able to use the simulated data to complete their assessed report.

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