

Supporting information for

A multi-disciplinary team-based classroom exercise for small molecule drug discovery

Charlotte A Dodson ^{1*}, Stephen E Flower ^{2*} & Mark Thomas ³

¹ Department of Life Sciences, ² Department of Chemistry, ³ Department for Health, University of Bath, Claverton Down, Bath BA2 7AY, UK

* c.a.dodson@bath.ac.uk, s.e.flower@bath.ac.uk

	Summary sheet of software and assay simulation information.docx Summary sheet of software and assay simulation information.pdf (text taken from main manuscript)
Supporting file S1:	Brief instructions for docking ligands into Chk1.docx Brief instructions for docking ligands into Chk1.pdf
Supporting file S2:	Team brief and fragment screen.docx Team brief and fragment screen.pdf
Supporting file S3:	Example of compound progression.pdf
Supporting file S4:	Example of excellent student work.pdf
Supporting file S5:	Blank Team Charter.docx Blank Team Charter.pdf
Supporting file S6:	Example team rules and commitments.docx Example team rules and commitments.pdf
Supporting file S7:	Sample slides for workshop 1.pptx Sample slides for workshop 1.pdf
Supporting file S8:	Workshop 2 nomenclature.pdf (Short classroom exercise on protein nomenclature)
Supporting file S9:	Fragment screen hits.pse (Structure of Chk1 bound to initial fragments)
Supporting file S10:	Team submission document.docx
Supporting file S11:	Blank physicochemical data form.docx
Supporting file S12:	Example data provided to students.xls
Supporting file S13:	Summative assessment template.docx
Supporting file S14:	Peer assessment and feedback.docx Peer assessment and feedback.pdf
Supporting file S15:	Peer evaluation.xlsx
Supporting file S16:	Example mark scheme.docx Example mark scheme.pdf
Supporting file S17:	Chk1.pdb (Chk1 kinase prepared for docking using GOLD) Chk1.mol (Chk1 for docking using more recent release of GOLD)
Supporting file S18:	gold.conf (Configuration file for compound docking in GOLD)
Supporting file S19:	cavity.atoms (Cavity file for compound docking in GOLD)
Supporting file S20:	Template Prism file for data simulation.pzf
Supporting file S21:	Python code for simulating experimental data.zip (Jupyter notebook (python) and tools file as an alternative to GraphPad Prism)