Supporting information for

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

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[Summary sheet of software and assay simulation information.docx](Summary%20sheet%20of%20software%20and%20assay%20simulation%20information.docx)

[Summary sheet of software and assay simulation information.pdf](Summary%20sheet%20of%20software%20and%20assay%20simulation%20information.pdf) *(text taken from main manuscript)*

Supporting file S1: [Brief instructions for docking ligands into Chk1.docx](File%20S1%20Brief%20instructions%20for%20docking%20ligands%20into%20Chk1.docx)

[Brief instructions for docking ligands into Chk1.pdf](File%20S1%20Brief%20instructions%20for%20docking%20ligands%20into%20Chk1.pdf)

Supporting file S2: [Team brief and fragment screen.docx](File%20S2%20Team%20brief%20and%20fragment%20screen.docx)

[Team brief and fragment screen.pdf](File%20S2%20Team%20brief%20and%20fragment%20screen.pdf)

Supporting file S3: [Example of compound progression.pdf](File%20S3%20Example%20of%20compound%20progression.pdf)

Supporting file S4: [Example of excellent student work.pdf](File%20S4%20Example%20of%20excellent%20student%20work.pdf)

Supporting file S5: [Blank Team Charter.docx](File%20S5%20Blank%20Team%20Charter.docx)

[Blank Team Charter.pdf](File%20S5%20Blank%20Team%20Charter.pdf)

Supporting file S6: [Example team rules and commitments.docx](File%20S6%20Example%20team%20rules%20and%20commitments.docx)

[Example team rules and commitments.pdf](File%20S6%20Example%20team%20rules%20and%20commitments.pdf)

Supporting file S7: [Sample slides for workshop 1.pptx](File%20S7%20Sample%20slides%20for%20workshop%201.pptx)

[Sample slides for workshop 1.pdf](File%20S7%20Sample%20slides%20for%20workshop%201.pdf)

Supporting file S8: [Workshop 2 nomenclature.pdf](File%20S8%20Workshop%202%20nomenclature.pdf) *(Short classroom exercise on protein nomenclature)*

Supporting file S9: [Fragment screen hits.pse](File%20S9%20Fragment%20screen%20hits.pse) *(Structure of Chk1 bound to initial fragments)*

Supporting file S10: [Team submission document.docx](File%20S10%20Team%20submission%20document.docx)

Supporting file S11: [Blank physicochemical data form.docx](File%20S11%20Blank%20physicochemical%20data%20form.docx)

Supporting file S12: [Example data provided to students.xls](File%20S12%20Example%20data%20provided%20to%20students.xlsx)

Supporting file S13: [Summative assessment template.docx](File%20S13%20Summative%20assessment%20template.docx)

Supporting file S14: [Peer assessment and feedback.docx](File%20S14%20Peer%20assessment%20and%20feedback.docx)

[Peer assessment and feedback.pdf](File%20S14%20Peer%20assessment%20and%20feedback.pdf)

Supporting file S15: [Peer evaluation.xlsx](File%20S15%20Peer%20evaluation.xlsx)

Supporting file S16: [Example mark scheme.docx](File%20S16%20Example%20mark%20scheme.docx)

[Example mark scheme.pdf](File%20S16%20Example%20mark%20scheme.pdf)

Supporting file S17: [Chk1.pdb](File%20S17%20Chk1.pdb) *(Chk1 kinase prepared for docking using GOLD)*

[Chk1.mol](File%20S17%20Chk1.mol) *(Chk1 for docking using more recent release of GOLD)*

Supporting file S18: [gold.conf](File%20S18%20gold.conf) *(Configuration file for compound docking in GOLD)*

Supporting file S19: [cavity.atoms](File%20S19%20cavity.atoms) *(Cavity file for compound docking in GOLD)*

Supporting file S20: [Template Prism file for data simulation.pzf](File%20S20%20Template%20Prism%20file%20for%20data%20simulation.pzfx)

Supporting file S21: [Python code for simulating experimental data.zip](File%20S21%20Python%20code%20for%20simulating%20experimental%20data.zip) *(Jupyter notebook (python) and tools file as an alternative to GraphPad Prism)*