My Experience of Teaching with Schrödinger

Schrödinger

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ASTBURY CENTRE

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About Me

- Lecturer in Structural Pharmacology at University of Leeds
- **2005-2008** PhD in Medicinal Chemistry- Design, Synthesis and Biological Evaluation of Mur Enzyme Inhibitors- early days of *in silico* design work (SPROUT)
- Have been using Schrödinger software for design work since ~2007
- >20 publications using Schrödinger software

nature chemical biology

EMBO

PNAS

About Me

- My research group focuses on the identification of bioactive molecules for early-stage lead discovery on a number of challenging targets involved in disease areas such as cardiometabolic disorders, epilepsy and bunyaviruses.

- We use a range of computational methods to discover novel ligands for these target proteins, coupled with small molecule synthesis and assay development-collaborating with colleagues at the University of Leeds and beyond.

- Our primary aim is to identify therapeutic leads and to partner with industrial collaborators to further these leads as drug candidates.

Teaching with Schrödinger

- Using Schrödinger software for teaching for >10 years
- Using web-based Teaching with Schrödinger software for 4 years
- Use for teaching 3rd year BSc (final year projects) and MSc students (MSc Drug Discovery & Development)
- Varied student backgrounds- Chemistry, Pharmacology, Biomedical Sciences
- Developed a series of 3, 2-hour workshops to train how to use the Maestro GUI and Glide docking
- Final assessment using Glide docking and other in silico tools

Adapting to using TwS

- Had previously used Schrödinger software mounted on individual PCs
- Problematic and limited student numbers- needed updating yearly
- Hard to predict student numbers when renewing research license
- Much easier to use the online web platform- can be used anywhere across campus
- Can be used by students off-campus (a huge benefit!)
- Have used for classes up to 90 students

Learning Outcomes

- **Workshop 1-** learn how to use Maestro GUI, load and prepare a protein. Examine protein-ligand interactions and understand how mutations affect ligand binding

Short formative assessment to check understanding, image creation etc.

- **Workshop 2-** learn how to prepare ligand structures and carry out a small glide docking run (200 ligands), understand how Glide docking scores compliment visual protein-ligand interactions. Carry out a conformational analysis of ligands.

- **Workshop 3-** carry out a larger docking run (2000 compounds) and triage compounds based on docking scores and other properties using CheMBL and SwissADME (basis of assessment)

Learning Outcomes

- Students able to work at their own pace-great for groups with mixed backgrounds
- Ability to tailor learning outcomes to different groups of students
- Students can start work before session and use as a ‘drop-in’ if they like
- This can mitigate the only problem we have seen- sometimes slow to login to webserver (especially with large groups)
- Not sure if this is due to UoL internet of TwS…..

Student Engagement

- Improved student engagement as timetabled sessions are not always suitable for all students
- Co-taught so hard to fit to all student timetables
- Ability to use off campus great for students with disabilities or caring responsibilities
- Students find software intuitive to use
- Upskill students to engage with research version of Schrödinger software for projects

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Student Testimonial

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- Final year MChem Medicinal Chemistry student:

I found Maestro very easy to use as an all-in-one workflow, making docking and result analysis much more straightforward. Compared to other platforms I have used in my Undergraduate degree, it felt more detailed, robust, and reliable."