

Data science tools in the pharmacy bachelor program

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#### Structure of presentation

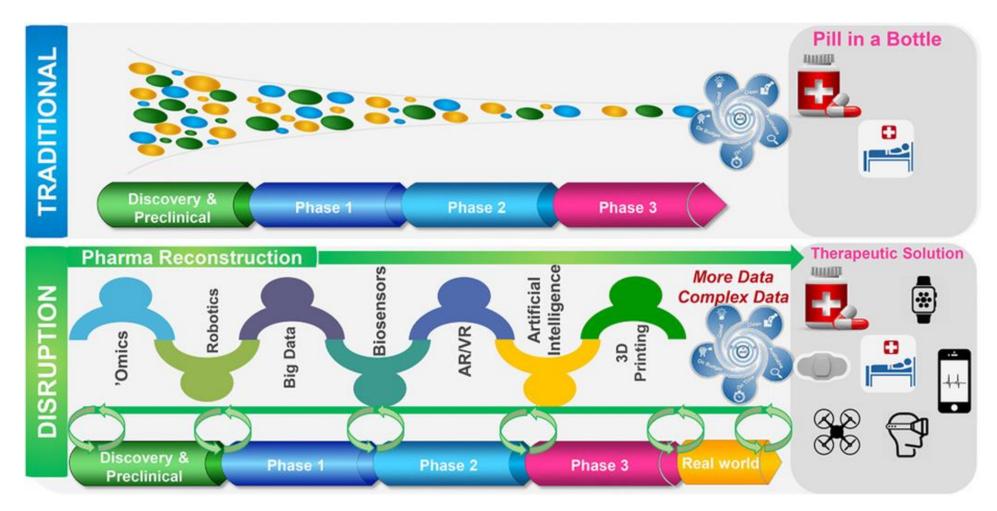
- Why is digitalization and data science important for our graduates?
- Ambition for transformation
- Overall implementation
- Focus on first semester Bachelor implementation 2022 and 2023
- Preliminary student evaluation

#### Current PharmaSchool graduate's contributions to Life Science and health care sectors



- Ideas for new medicines
- Medicinal chemistry
- Pharmacology
- Formulation design
- Production
- Clinical studies
- Benefit-risk assessment
- Optimal use of medications

# Are competences within data science and digitalisation important for future drug experts?



#### Swift et al, Clin Transl Sci (2018) 11, 450–460

# Pharmaceutical data science transformation at PharmaSchool

• Ambitions:

- To educate drug experts capable of using life science and health data – in collaboration with others – to make pharmaceutical relevant decisions
- Drug experts: More "comfortable" with data



- 3. Pharmaceutical data science researchers (PhDs & postdocs) Research training programme
- 2. Data-driven pharmaceutical science students (MSc students)

Elective courses in pharmaceutical data science MSc track/specialty in pharmaceutical data science

- **1. Bilingual pharmaceutical science students** Digitalization across the compulsory curriculum
- **0.** Today's pharmaceutical science students

### Considerations behind the data science implementation plan

- One single compulsory course or integrated into more courses?
- New curriculum or integration into existing?
- Introduction in BSc semester 1 or semester 5? (Fundamental changes in program or scratch in the surface?)
- As supplement/add-on/replacement for current ways of training students to work with data. (Not a substitute for Excel)



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## BSc courses with data science elements – Initial brainstorm

1. semester	2. semester		3. semester		4. semester		5. semester
Cellulær og molekylær biologi	Farmaceutisk biologi	Kvalitetsvurdering af farmaceutiske råvarer	Basal farmakologi	Farmaceutisk fysisk kemi II	Farmaceutisk analytisk kemi	Farmaci I	Farmaci II
<ul> <li>Data science:</li> <li>Hvad er data?</li> <li>Data I Farmaci</li> <li>Forståelse af data og filformater</li> <li>Data dimensionalitet</li> <li>Data baser</li> <li>Intro programmering</li> <li>Gennemgang af færdig kode</li> </ul> Fagspecifik: <ul> <li>Visuel simulering af cellulære processer (fx Enzymkinetik)</li> <li>Kode til vurdering af eksperimentelle data</li> </ul>	<ul> <li>Data science:</li> <li>Samle data fra databaser</li> <li>Behandling og rensning af data</li> <li>Lineær regression</li> <li>Visualisering af F-test og t-test</li> </ul> Fagspecifik: <ul> <li>Opsamling, rensning og undersøgelse af data fra fødevare- database (FRIDA)</li> <li>Rensning fra eksperimentelle målinger (fx cytokine ekspressionsniveauer)</li> <li>Modellering (fx effekt af medicin på cytokiner)</li> </ul>	<ul> <li>Data science:</li> <li>Måling af egne data, rensning og dataundersøgelse</li> <li>Statistiske tests på egne data samt på større datasæt</li> <li>Brug af visualisering af statistiske tests for bedre forståelse</li> <li>Fagspecifik:</li> <li>Data fra den kemiske analyse af råvarer evalueres statistisk og præsenteres grafisk</li> </ul>	<ul> <li>Data science:</li> <li>Visualisering (fx Scatterplot, histogram, density, o.s.v.)</li> <li>Transformation af data (fx normalisering)</li> <li>Non-lineær regression</li> <li>Kurvetilpasning</li> <li>Brug af data fra offentlige databaser</li> <li>Fagspecifik:</li> <li>Modellering (fx PKPD parametre)</li> <li>Opsamling data fra offentlige DBs med eksperimentelle målinger (fx ChEMBL)</li> </ul>	<ul> <li>Data science:</li> <li>Automatiseret datanalyse af større datasæt vha. python</li> <li>Fagspecifik:</li> <li>Stort datasæt opnået i øvelse vedr. diffusion databehandles vha. python in Jupyter Notebook.</li> </ul>	<ul> <li>Data science:</li> <li>Fortsættelse og udvidelse af brugen af Jupyter notebooks i forbindelse med databehandling og statistiske tests. Fx med øget fokus på adaptering af python scripts til brug med det givne datasæt</li> <li>Fagspecifik:</li> <li>Analystisk-kemiske data behandles og visualiseres vha. python</li> </ul>	<ul> <li>Data science:</li> <li>Dataopsamling</li> <li>Format/skabelon/strukturering</li> <li>Datahåndtering/analyse</li> <li>Benytte/køre kode</li> <li>Automatisering</li> </ul> Fagspecifik: <ul> <li>Opsamling af egendatafx opløselighed af lægemiddelformulering)</li> <li>t-test (sammenlign to batches)</li> </ul>	<ul> <li>Data science:</li> <li>Dataopsamling</li> <li>Identifikation af outliers ved hjælp af PCA</li> <li>PCA analyse af variable importance</li> <li>Visualisering af data med høj dimensionalitet ved hjælp af PCA</li> </ul> Fagspecifik: <ul> <li>Opsamling, rensning og undersøgeles af data</li> <li>Modellering</li> </ul>
Jupyter		Brug af	Python kode i Ju	pyter notebooks h	nele vejen igenner	n	<b>→</b>

## Data Science implementation PharmaSchool 1<sup>st</sup> semester

#### Initiatives in Cellular and Molecular Biology 2022 – A PILOT STUDY

- 210 students, 7 teams.
- Lectures, theoretical class teaching, wet-lab experimental exercises on enzymes, enzyme kinetics and transport
- One inspirational lecture: "Data science: How to boost your digital CV"
- Drylab exercise (rudimentary introduction to Python + Jupyter notebook included)

#### Aims of this dry-lab exercise

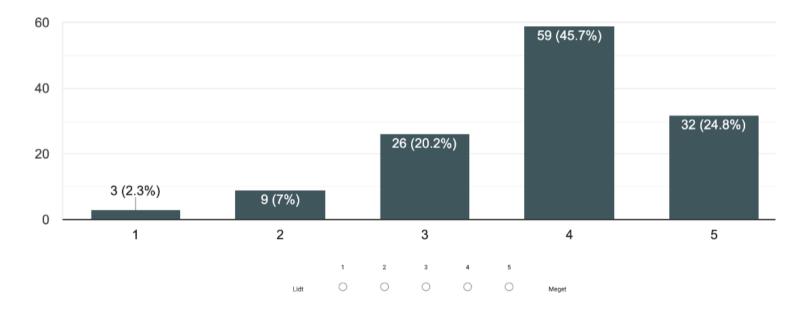
Going through the workflow in this notebook has two main aims:

- 1. Teaching about membrane transport proteins and kinectics of transport across the cell membrane
- 2. Giving an introduction to importing, handling, analyzing and visualizing data with the use of python code in a notebook format

## 2022 initiative: Well-received by the students

- More than half of the students have never experienced to read code.
- Appr. 2/3 of the students feel they have been well introduced to python code and to use the code
- A few students ask for more challenges

Har du efter dette modul (forelæsning + øvelse) fået en bedre forståelse for vigtigheden af digital dannelse i fremtiden? 129 responses



## Cellular and molecular biology 2023-initiative

- Inspirational lecture
- Online material in Absalon
  - Introduction to Python, libraries, simple coding
  - Developed in collaboration with KUB-datalab

# **KUB** Datalab



#### What is KUB Datalab?

KUB Datalab is Copenhagen University Library's centre for working with data. Our primary focus is to support students at the University of Copenhagen in regards to their work with data and digital methods.

KUB Datalab offers guidance, classroom teaching, datasprints, events, and workshops. Furthermore, we collaborate with teaching staff to support and advance the development of student skills and data literacy.

Through our learning activities, we support students in regards to:

- Harvesting data
- · Cleaning data
- · Analysing data
- Visualising data
- Considerations on format (screencasts, Notebook or on campus/on library teaching)
- Considerations on content and content complexity ("just in time")

#### Basic introduction to Python – sem 1 bachelor

#### Python Lessons

All the lessons below are made in Google Colab and specifically designed with the purpose of preparing you for the *dry-lab* exercise in CMB. However, each af the lessons describe aspects of Python which are also generally applicable and will help you develop skills with using Python code.

Each lesson is a link that wil open a new Colab notebook and you are encurage to make a local copy in your own Google Drive. This will allow you to modify and edit the notebook so that you can change or add code to see what happens.

- Data types
- Variables
- Built-in functions
- <u>Lists</u>
- Loops
- <u>Conditionals</u>
- <u>Writing functions</u>
- Libraries

While, or after, completing all the above lessons, you should also complete the quiz in Absalon.

## Cellular and molecular biology 2023-initiative

- Inspirational lecture
- Online material in Absalon (developed in collaboration with KUB-datalab)
  - Introduction to Python, libraries, simple coding
  - Tailormade to the course and the program
- Class tutorial ("code along" unfinished simple code) simple transformations of biological relevance
- Quiz in Absalon (mandatory) due next week
- Dry-lab exercise as in 2022 will be run in December hopefully with more time to focus on the subject matter

#### Status Student reactions 2023 (As of November)

- Almost all students have carried out the Quiz well before deadline
- The online material and the Quiz was "nothing special"
- No student resentment/complaints about having to work with code.
- Learning outcome better this year? Too early to say



#### Acknowledgement and thanks to



Osman Mirsa Niels Skotte Kasper Harpsøe



Daniel Pryn Christian B. Knudsen



Teaching development with digital elements



# Thank you for your attention



# Questions?

# Comments?

