AstraZeneca

Automate your own HTE workflow

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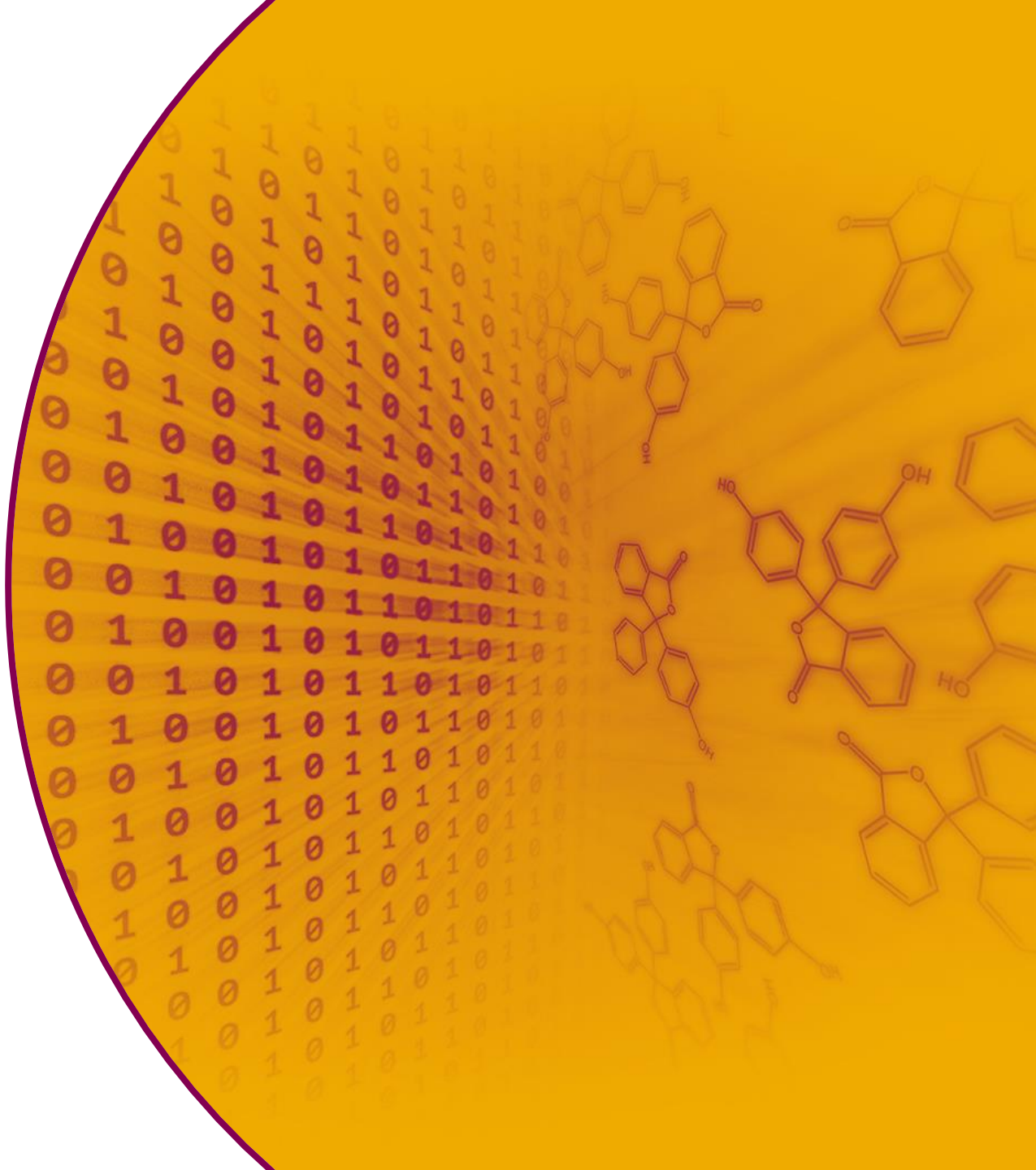
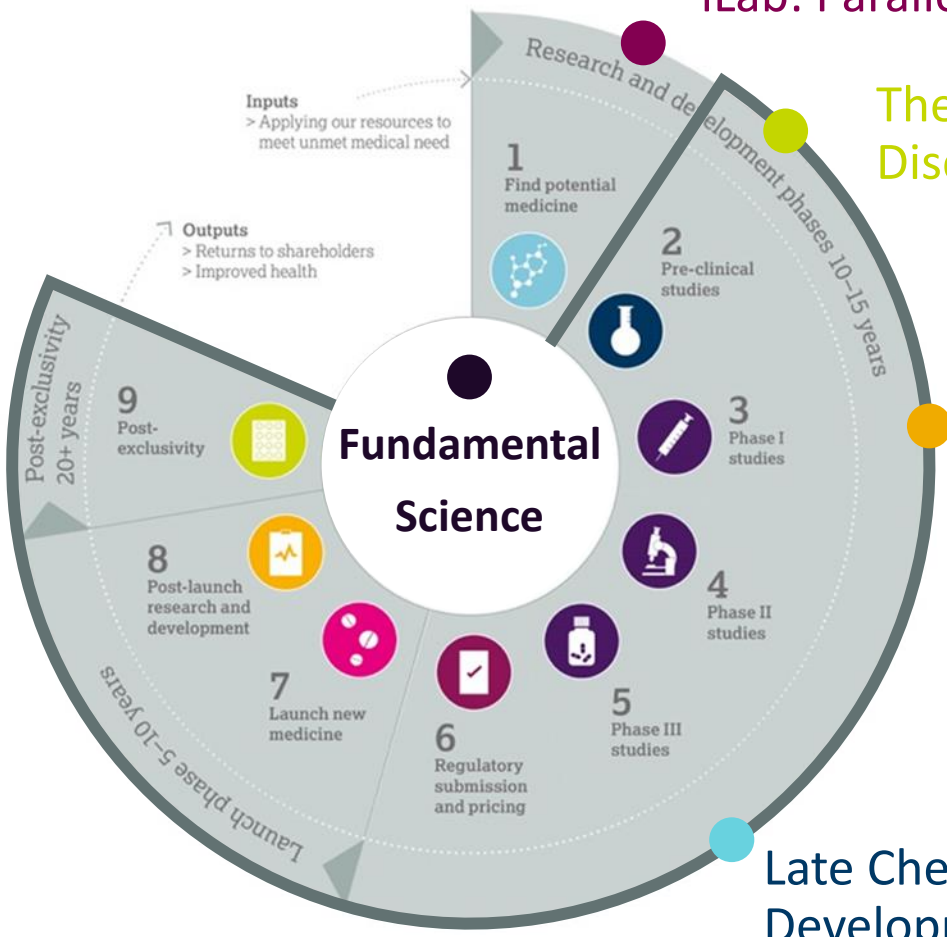


18 Nov 2022

Current HTE landscape at AZ



iLab: Parallel chemistry

Therapy areas:
Discovery chemistry

Early Chemical Development

Late Chemical Development

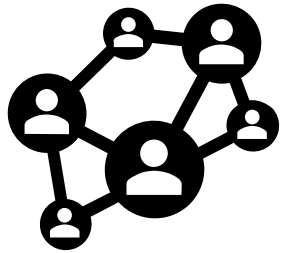
Specialists e.g.
- Biocatalysis
- Isotope chemistry
- New modalities

AZ HTE vision 2025

Expand specialist HTE in Macclesfield and at other sites

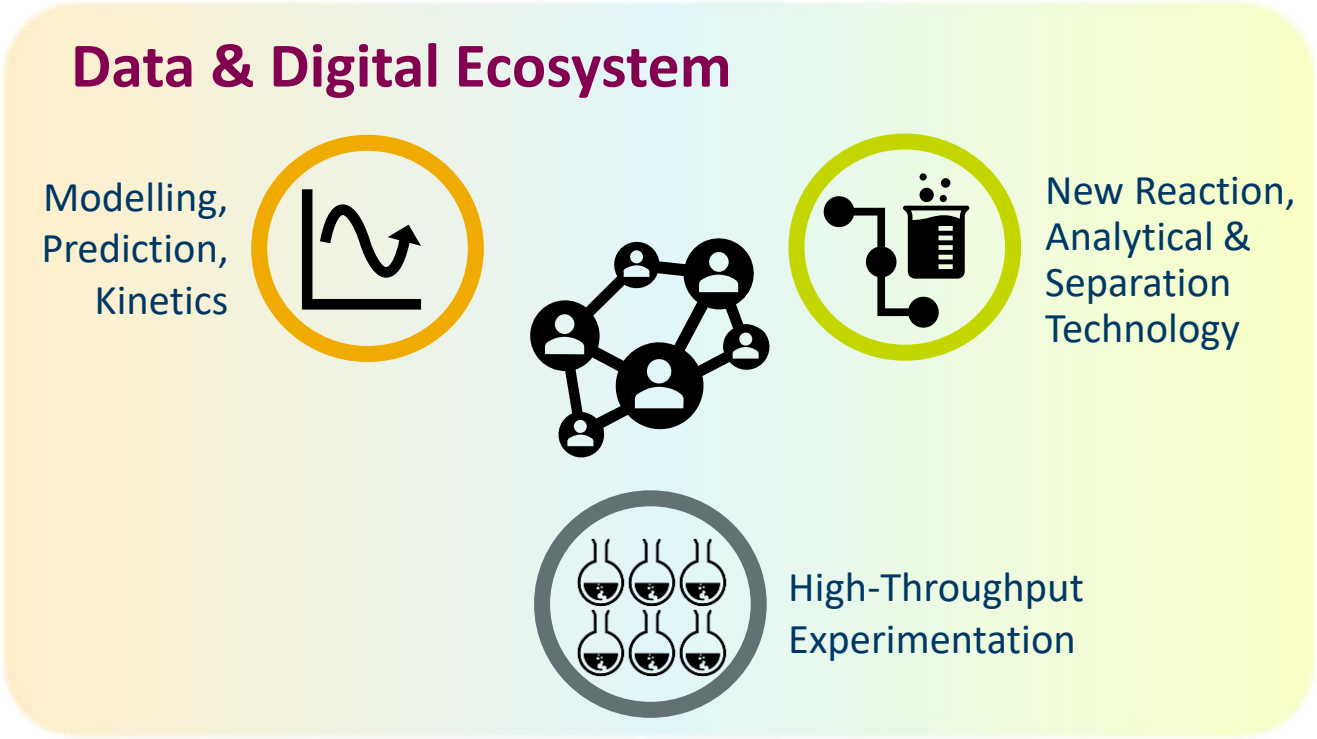
Expand and enable HTE methods and culture across all synthetic chemists

AstraZeneca will become carbon negative across the entire value chain by 2030



Culture Data Systems Training

Data flow enables enabling technology



- HTE runs on data science:
  data management is critical at all steps
- Data must be **FAIR** at all points
- Data collection must be:
  - **very fast** (automated)
  - user-friendly
  - also FAIR

Graphic by James Douglas & Simon Yates

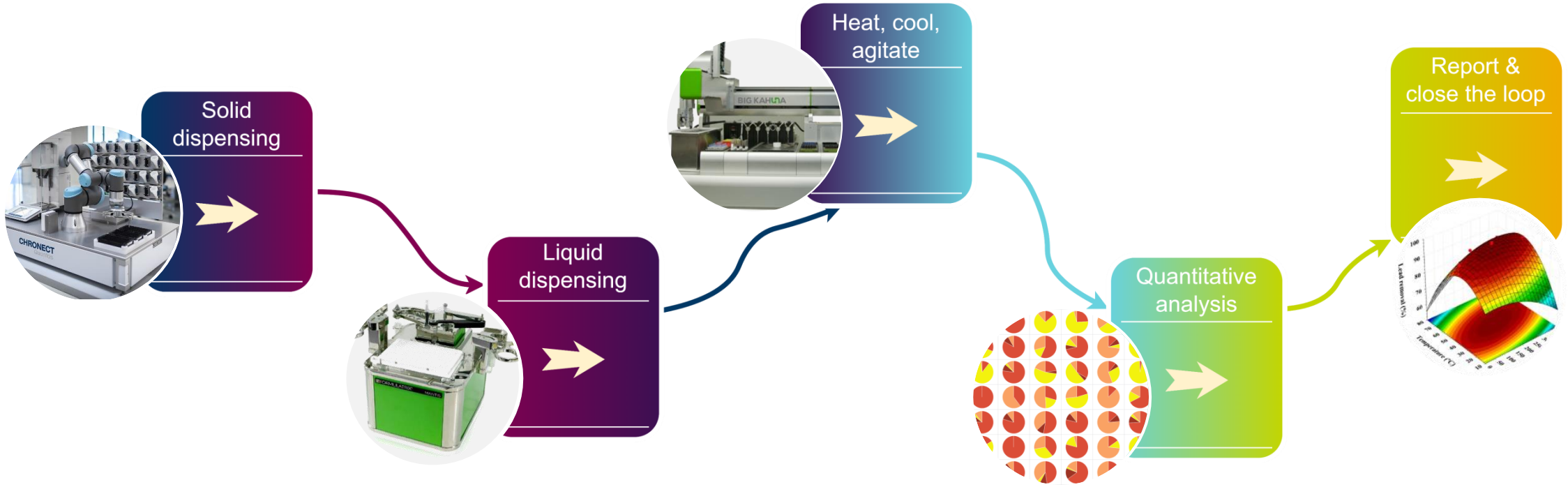
Data flow enables enabling technology

Data chemists want:

- Incorporation of FAIR metadata
- Good data standards

Automation chemists want:

- Decrease in admin

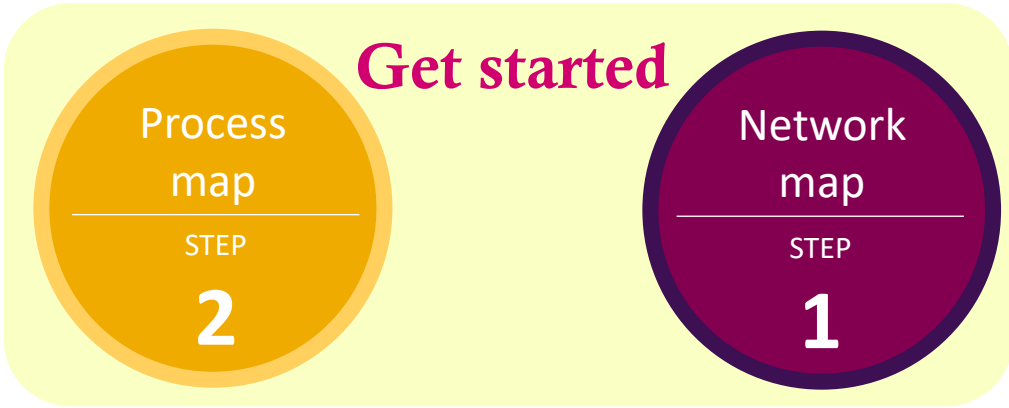


Perspective on the enabling impacts of HTE: Carson, N – Chem. Eur. J., **2020**, *26*, 3194–3196

So you've decided you want to automate your workflow

Do I need to code?

- Options: Python, VBA, MATLAB, KNIME, no-code…



- Mundane tasks: we use everyday solutions with simple interfaces
- Upskilling general users increases quickness of these wins

- **Software** is relatively easy to find business justification for
  People overemphasize hardware costs
  and underemphasize time costs *(the sunk costs fallacy)*

A network map

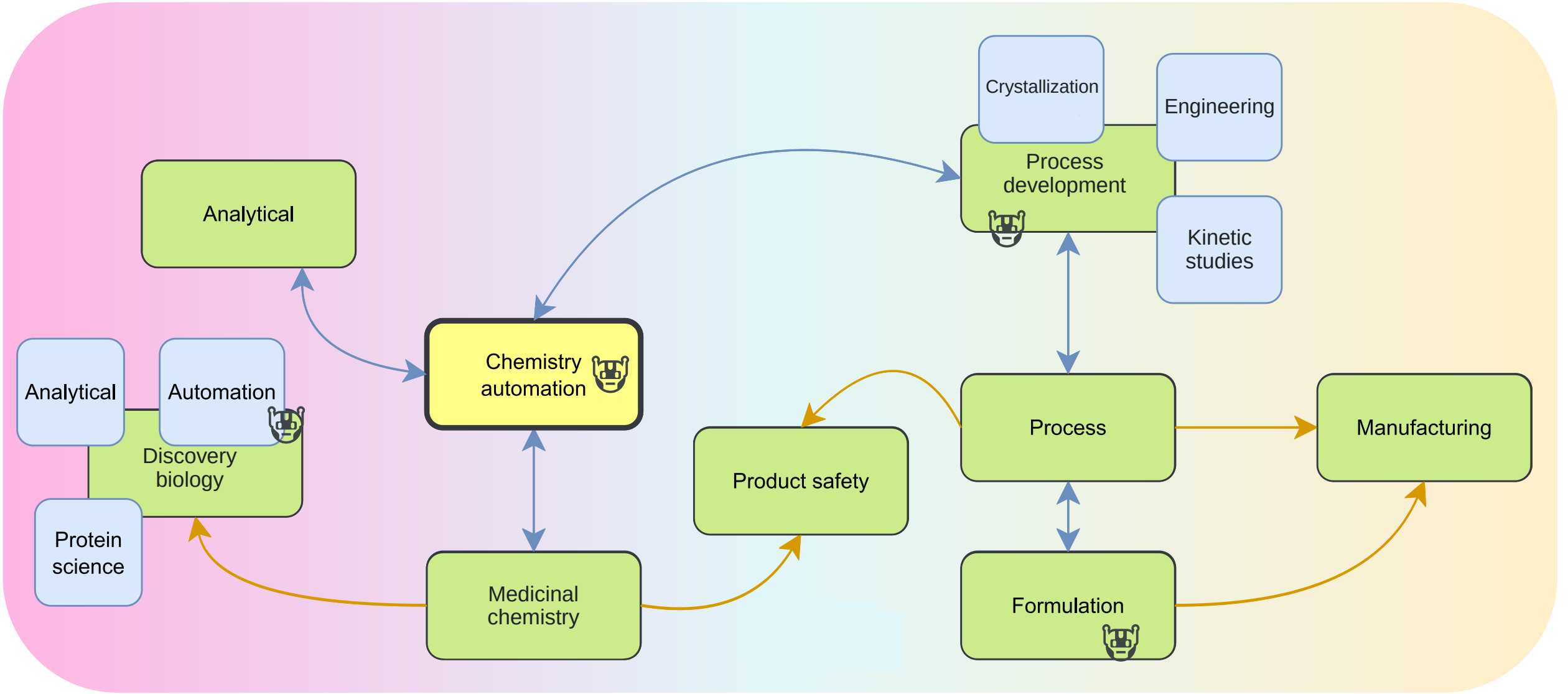
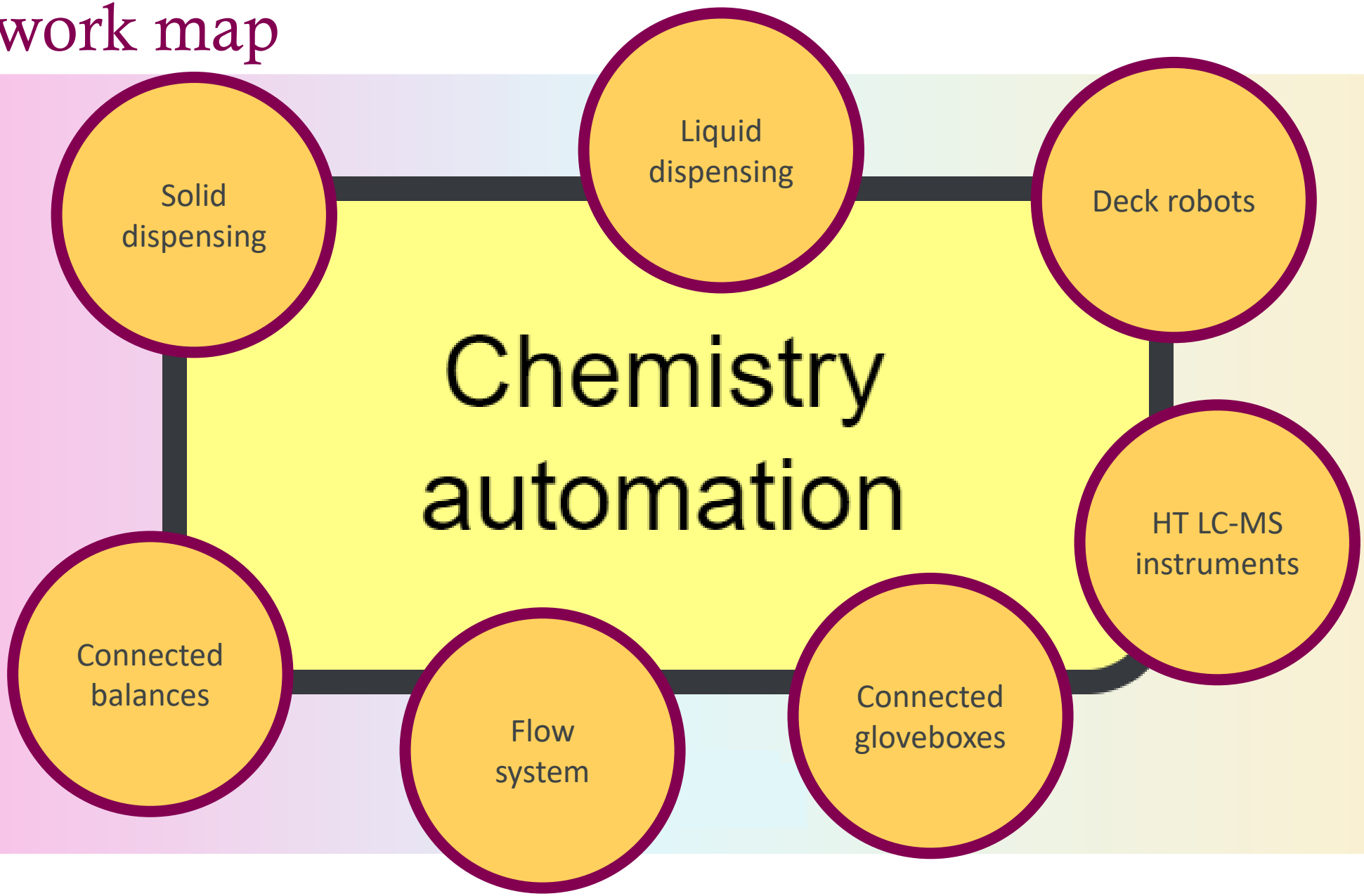


Diagram created using diagrams.net

A network map



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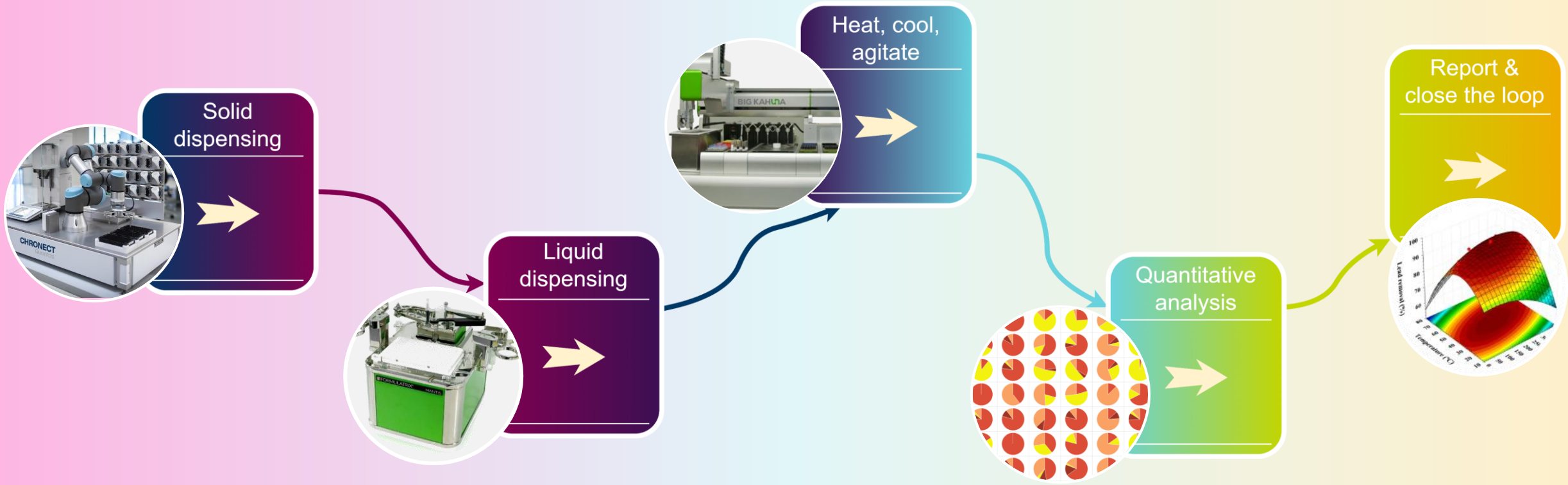
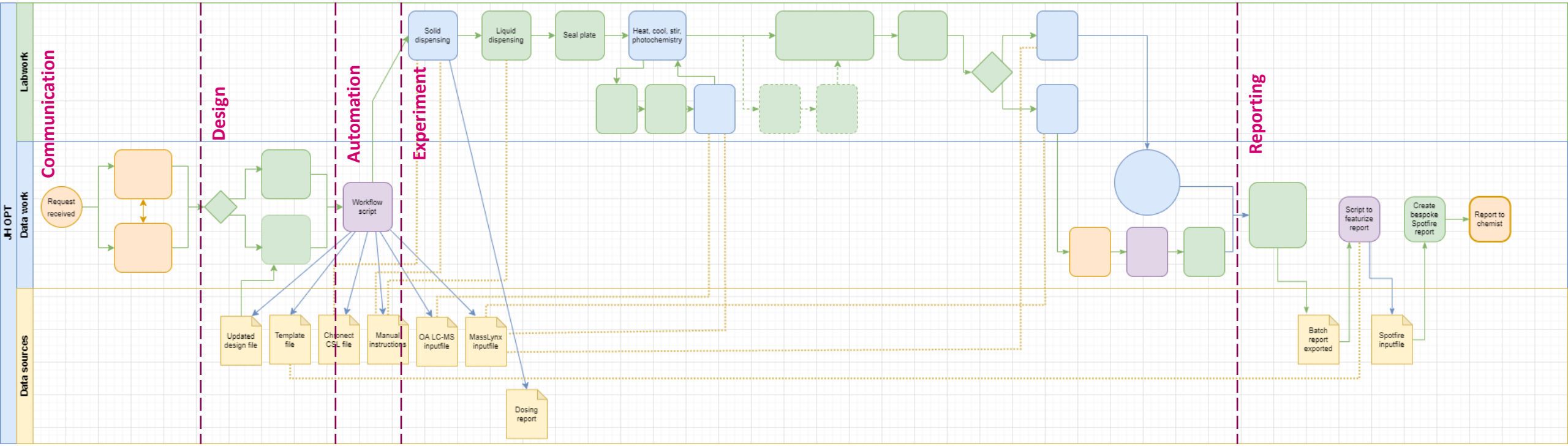
The bones of the reaction optimization workflow



Perspective on the enabling impacts of HTE: Carson, N – Chem. Eur. J., **2020**, *26*, 3194–3196

Chronect Quantos robot: Axel Semrau; Mantis robot: Formulatrix; Big Kahuna: Unchained Labs; Pie charts: above ref; Ligand space surface plot: Sci. Rep. **2018**, *8*, 13456,

Mapping a workflow



1. Include every elementary step but imagine the data flow were ideal
2. Minimize manual script initiation
3. Automate all possible data manipulation
4. Anticipate deviations from “standard” behaviour

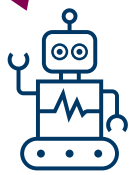
Diagram publicly-available from Syngenta

The prototype model

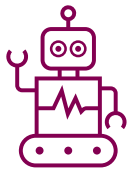
- MVP model: fully working prototype can still have easily-coded add-ons
- **Standard schema**: easier to add new systems and features

- Connect to other systems, eg: Teams bots
- Beyond HTE: what do other groups need?
  FAIR data? Excel manipulation? pdfs merging?

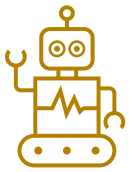
I want to add capabilities for my new liquid handler



I want conditions & descriptors accessible alongside results



I want my data table to have structures associated already

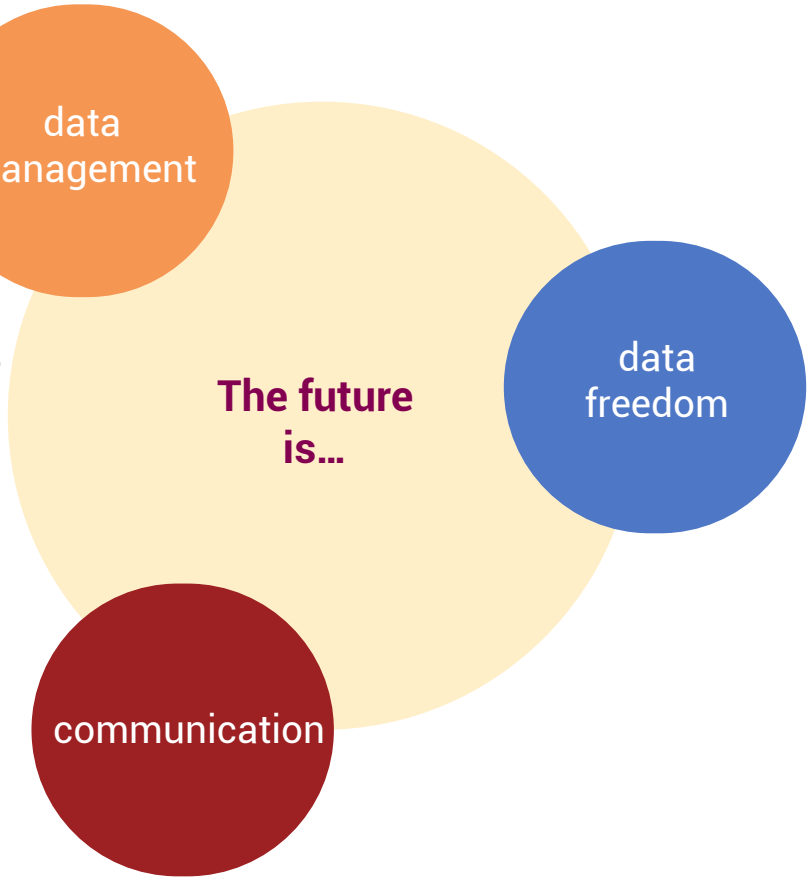


Now it's time for the software pros to step in!

Some hard-won advice…

The road less travelled

- Custom, niche middleware development
- A go-between is required: lots of medium/shallow domain knowledge
- Variable time commitment
- Most chemists are not (currently) trained in data science



Smoothing the path to change

1. Automatic data collection
2. Find a broad network, fast
3. Be clear on your applicability domain
4. Make things easy for your users
5. Repeatedly assess and demonstrate value
6. Be liberal with including people
7. Choose your language to smooth change

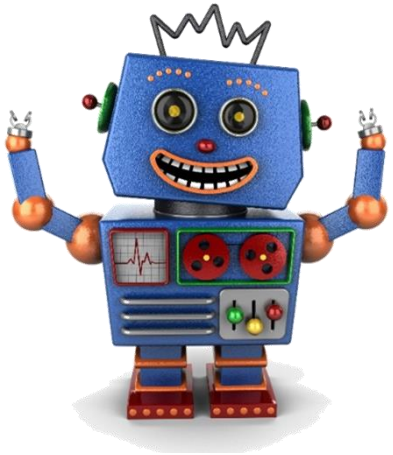


Image by Badboo, dreamstime.com

Acknowledgements

AstraZeneca Early Chemical Development

AstraZeneca Global High-Throughput Experimentation

References

- Handy Python packages:

PySimpleGUI

pyinstaller

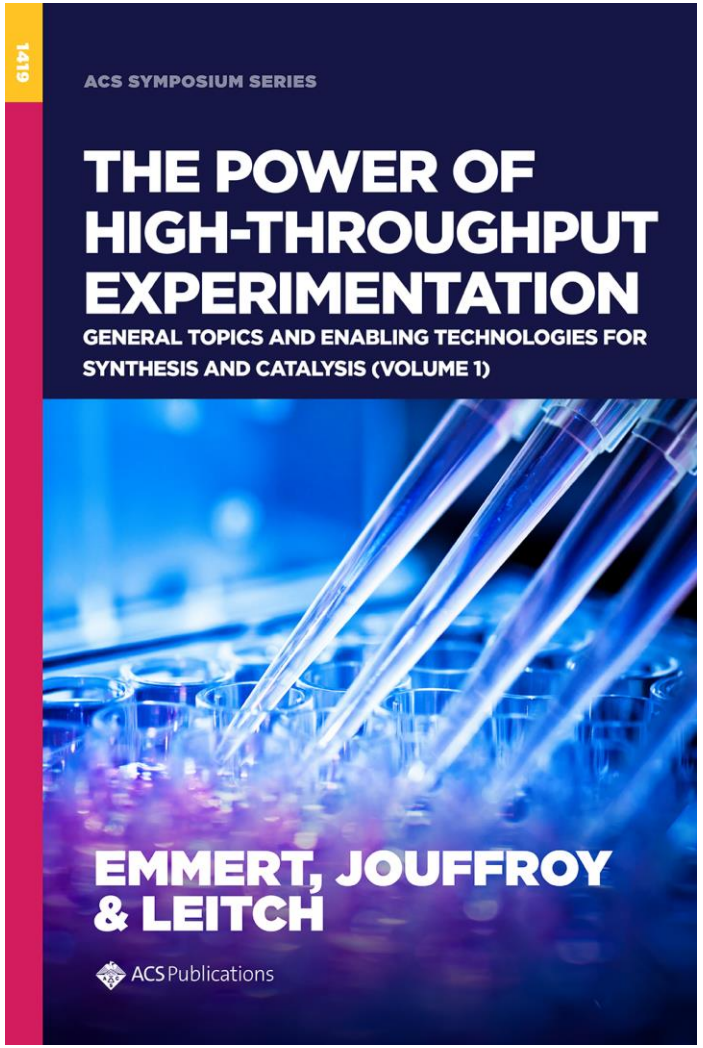
Dash/plotly

OpenPyXL

pandas

- Selected coding and HTE resources: https://supersciencegrl.co.uk/links/

References



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