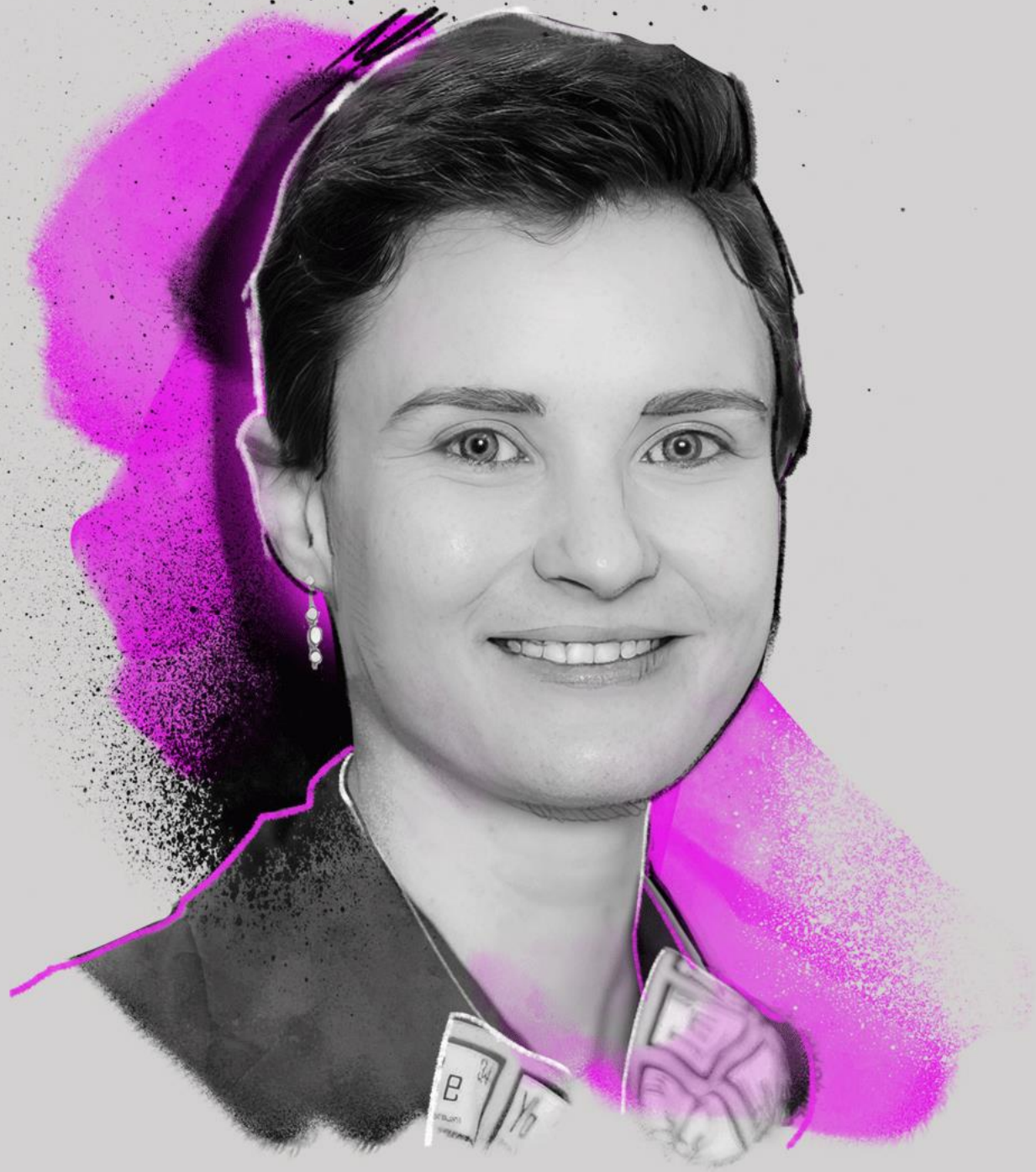


How not to waste a chemist's time: Chemical insights through great user experience

Nessa Carson

AstraZeneca

Associate Principal Scientist, Digital Champion

AstraZeneca

How not to waste a chemist's time

Chemical insights through great user experience

Nessa Carson
Early Chemical Development, Pharmaceutical Sciences, R&D, AstraZeneca, Macclesfield, UK

25 September 2024

Digital Transformation

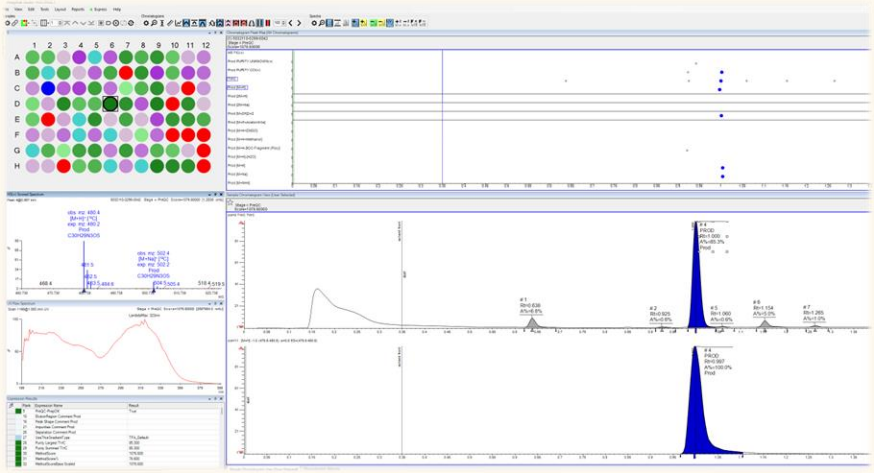
Digitalization is one of the most prominent issues for chemical industry (according to CEO's)

- For *growth…*
- For *making the future happen…*
- For *sustainability…*

Transformative change

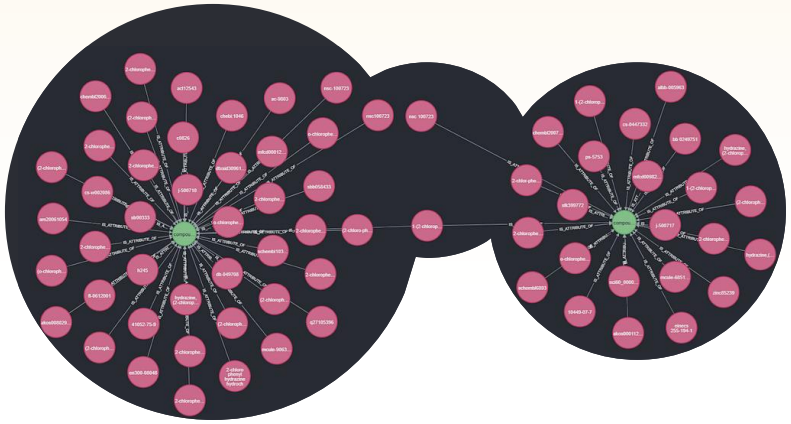
Smart sensors in the lab

Software to enable experimentation

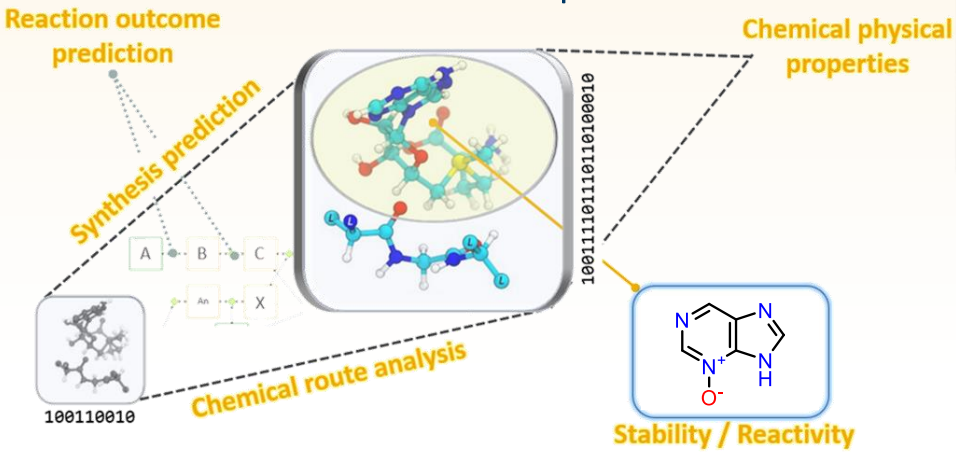


Autonomous robotics

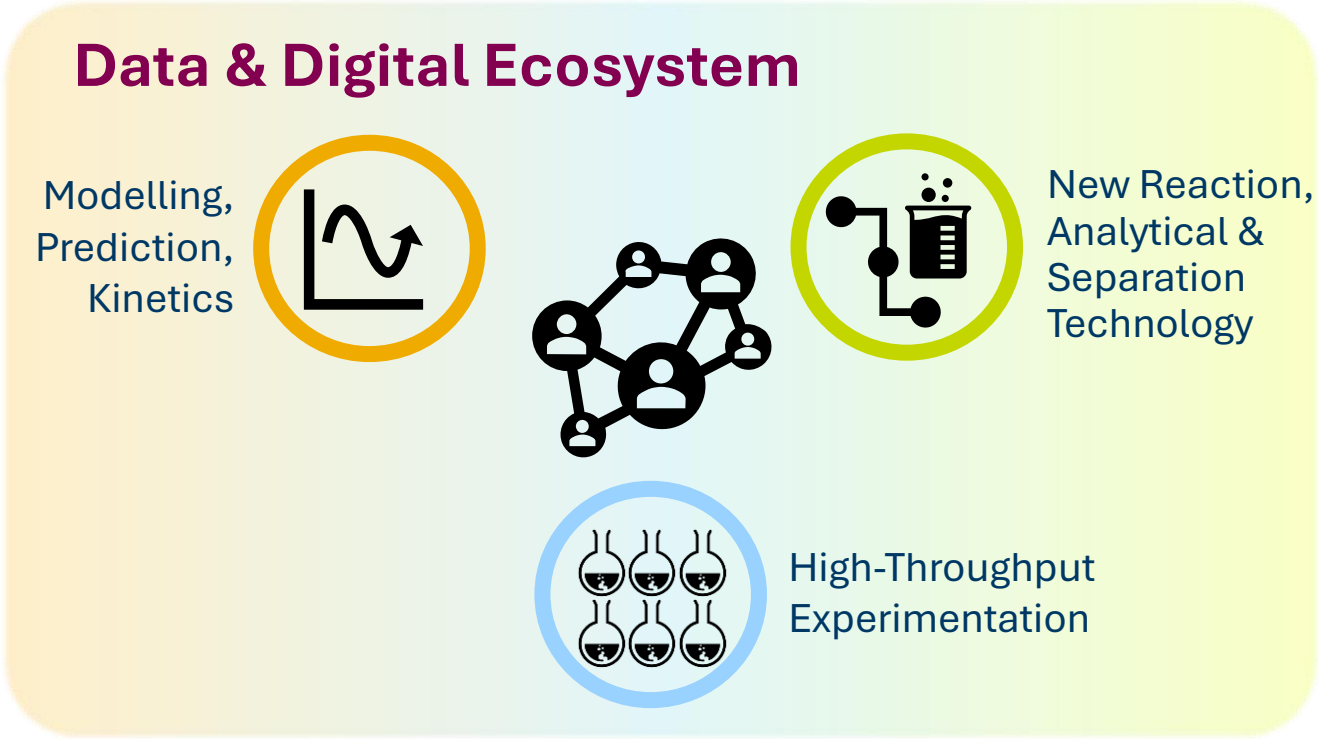
Big chemistry data



Accessible computation

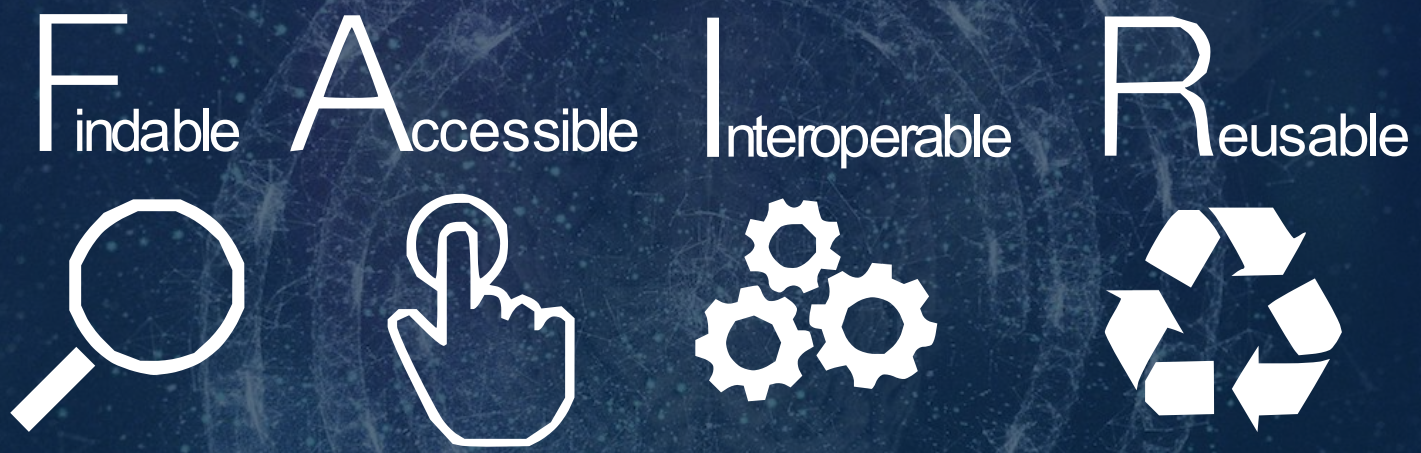


Data flow enables enabling technology



- Vast majority of chemistry workflows run on data science:
  data management is critical at all times
- Data must be **FAIR** at all points
- Data collection must be:
  - **very fast** (automated)
  - user-friendly
  - also FAIR

My FAIR data



"Improving the FAIRness of digital resources will increase their reuse"

www.go-fair.org/fair-principles
Michel Dumontier, Maastricht University

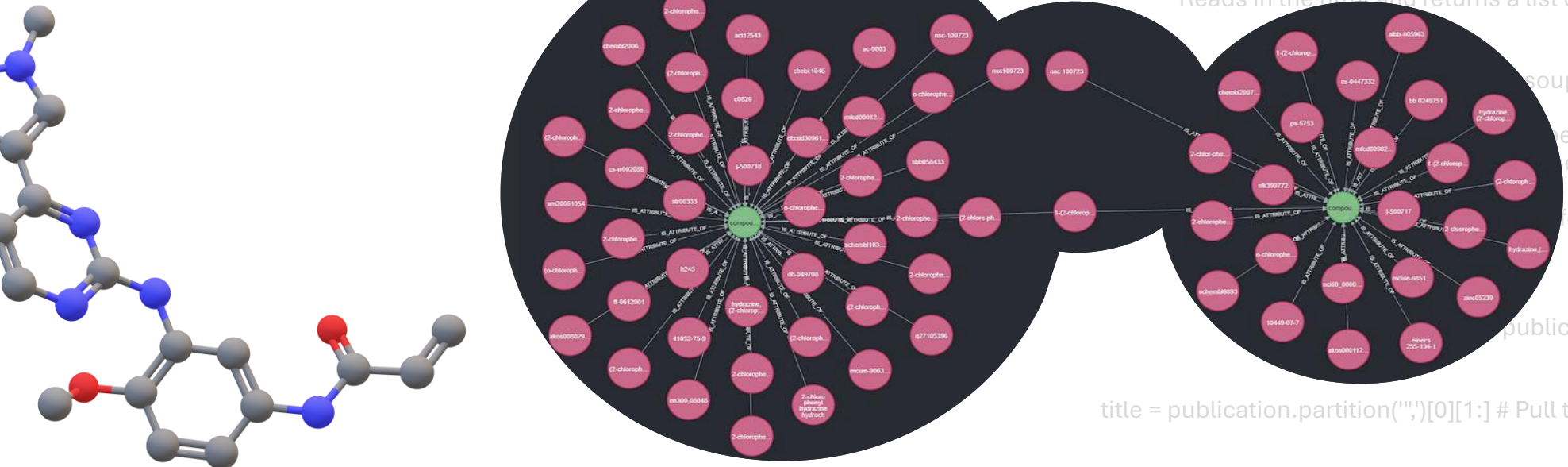
Data flow enables enabling technology

Data chemists want:

- Good data standards
- Incorporation of FAIR metadata

Lab chemists want:

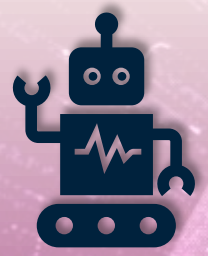
- Decrease in admin
- Incorporation of FAIR metadata



Chemical data, connected

It's starting to happen…

Self-driving labs

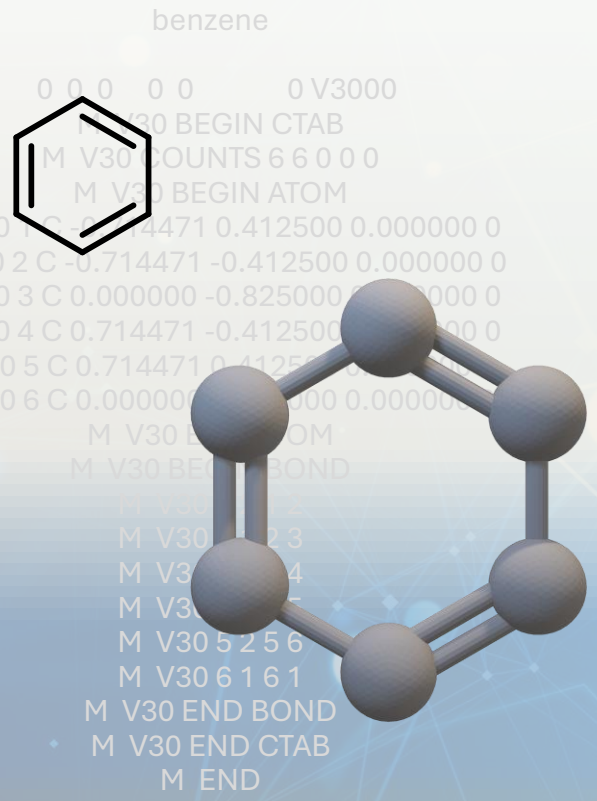


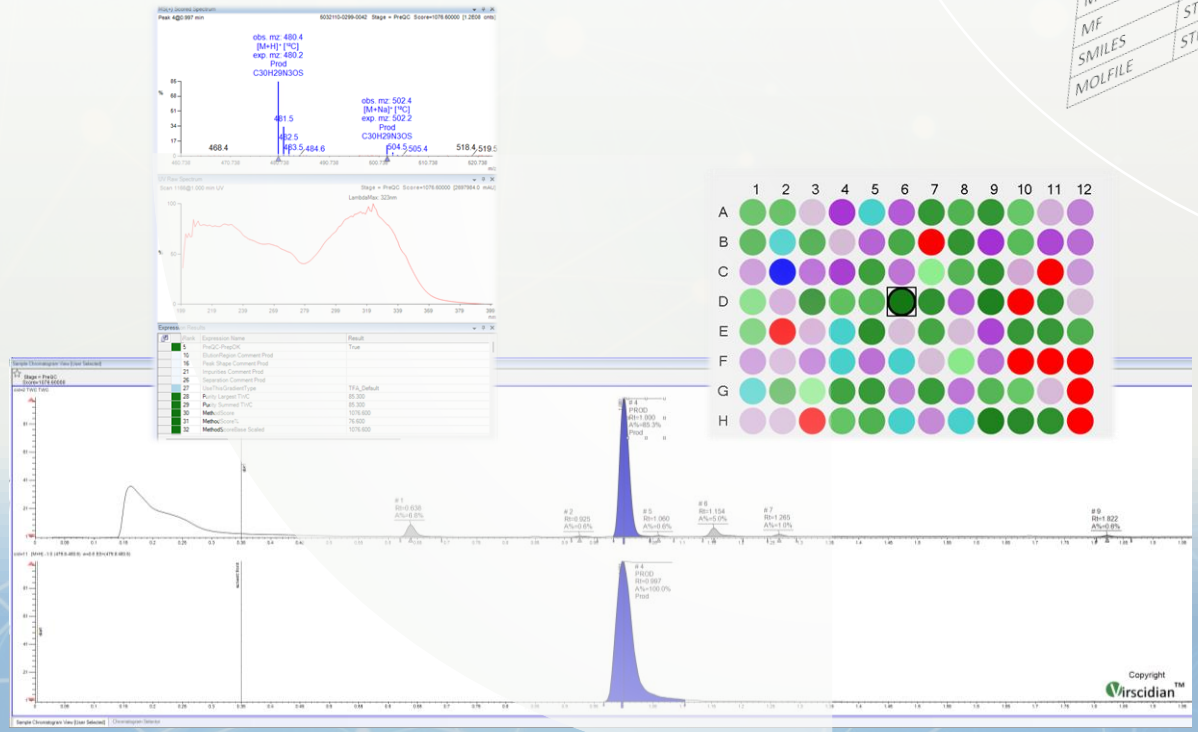
Reaction prediction

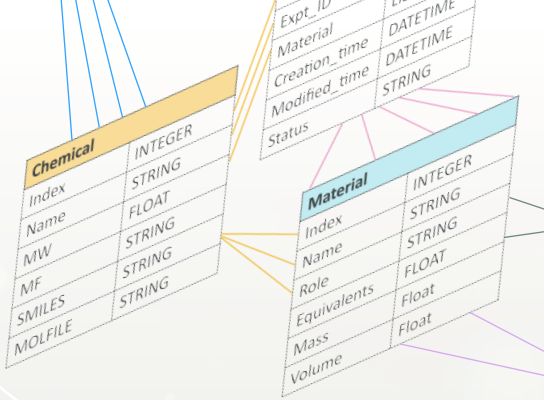
Smart instruments

DMTA acceleration

70% of digital transformations **fail**

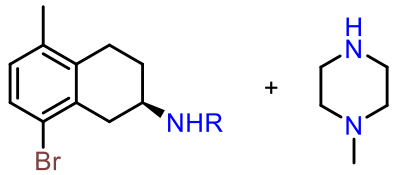


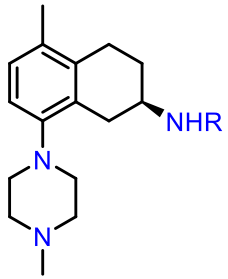


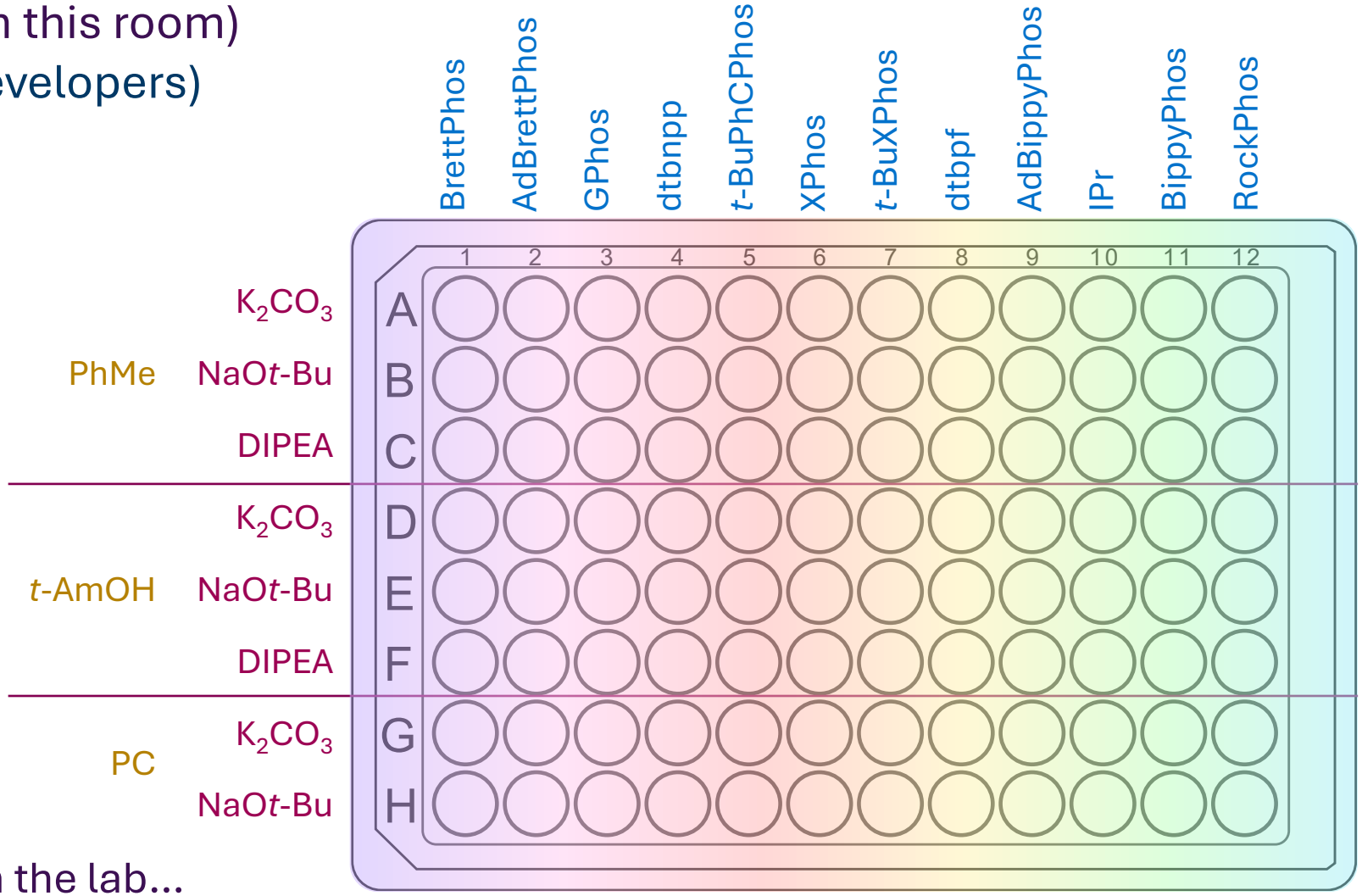


Everybody needs to think about UX

(or at least everybody in this room)
(ie: not just software developers)







This is what I used to do in the lab...

(these are not real data!)

Reaction scheme from P Yaseneva, P Hodgson, J Zakrzewski, S Falß, RE Meadows, AA Lapkin, "Continuous flow Buchwald–Hartwig amination of a pharmaceutical intermediate". *React. Chem. Eng.* **2016**, *1*, 229–238

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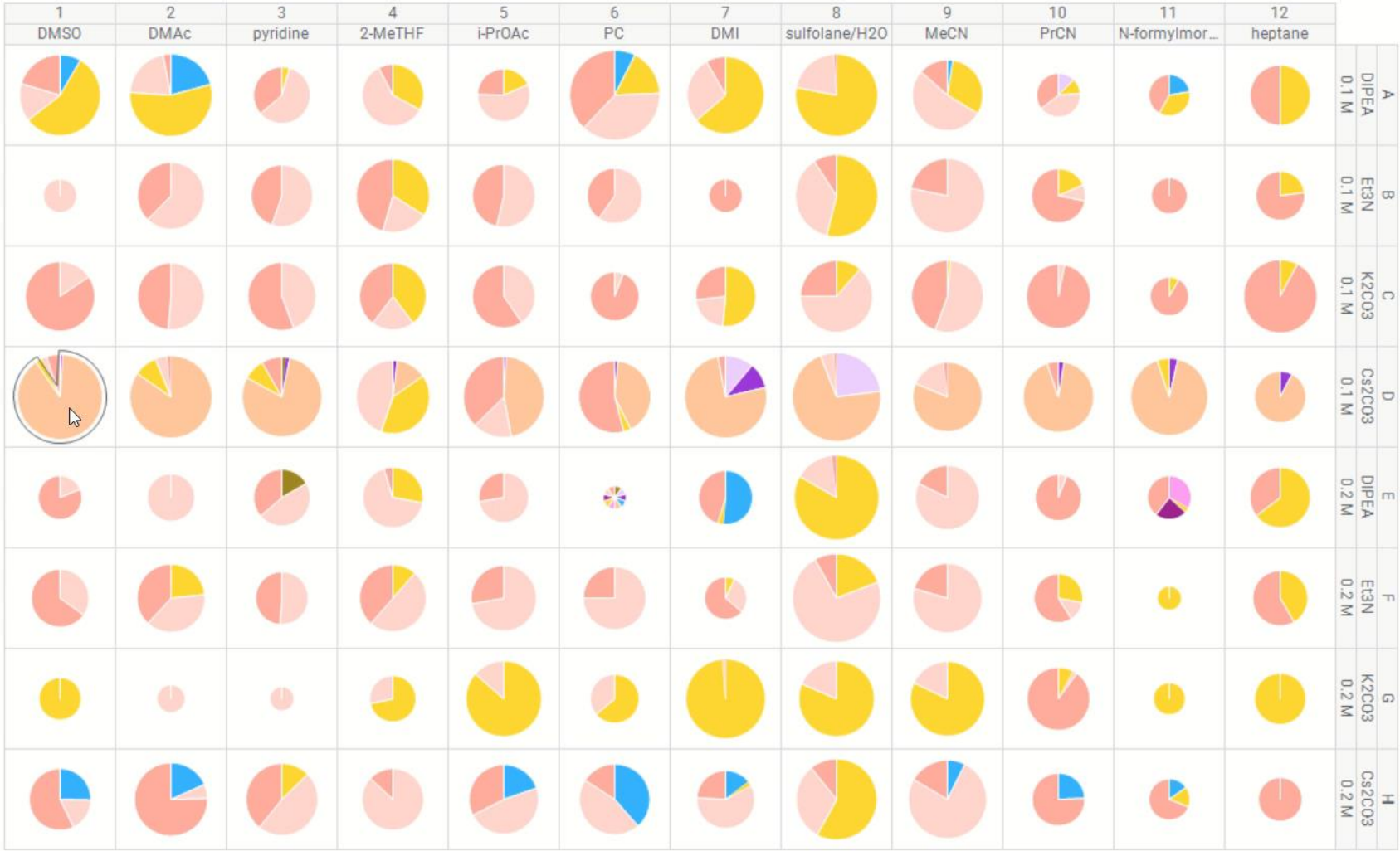


Data table:

Mocked data

Color by:

Component

- Aryl1OAryl1 Area %
- Aryl1OTf Area %
- Aryl2H Area %
- Aryl2OAryl2 Area %
- Aryl2OH Area %
- cyclized Area %
- dp Area %
- dp-CHO Area %
- Phenol Area %
- Triflate Area %

Sector size by:

Sum(Purity)

Size by:

Sum(Purity)

≥ 95.00

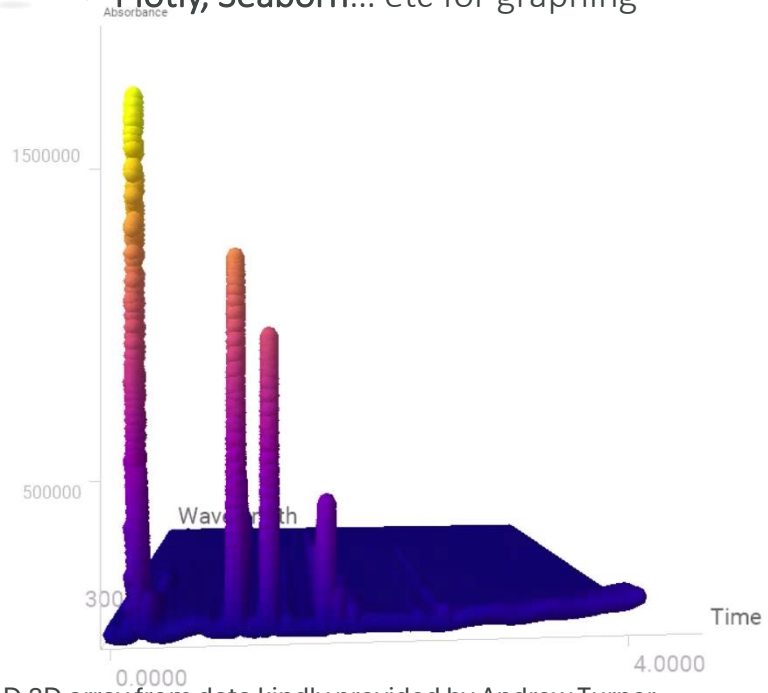
≤ 0.00

User-friendliness ➞ adoption

http://lawsofux.com

to interact

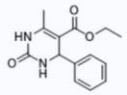
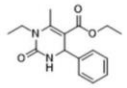
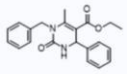
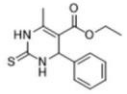
- Dash, Shiny, PySimpleGUI GUI's
- Plotly, Seaborn… etc for graphing



DAD 3D array from data kindly provided by Andrew Turner

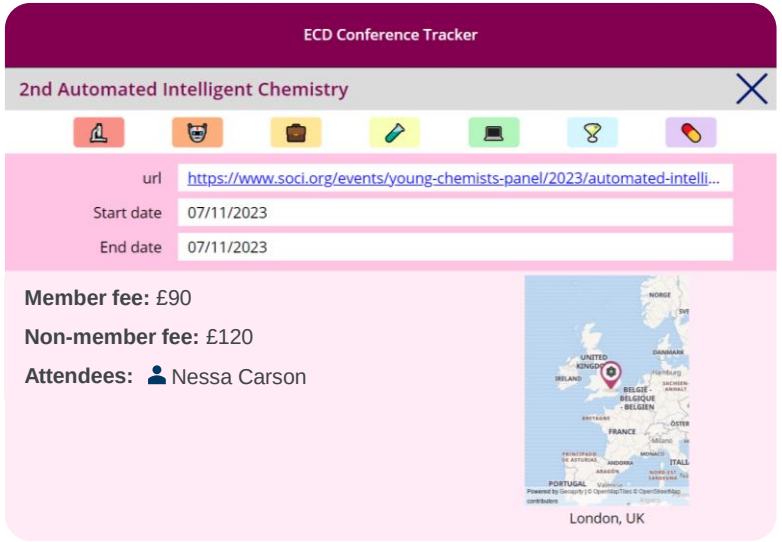
to analyse

TIBCO Spotfire

Entry	Product SMILES	Method	Temperature / °C	Time / min	Yield / %
1		A	120	10	92
2		A	120	10	18
3		A	120	10	43
4		B	120	10	56
5		D	120	10	41

to understand

Power Apps



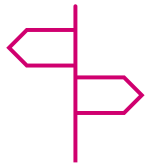
Library data table adapted with permission from N Carson, "Data visualization for high-throughput experimentation". In "The Power of High-Throughput Experimentation: General Topics and Enabling Technologies for Synthesis and Catalysis (Volume 1)".

User-friendliness ➞ adoption

Your users are worried about change.

Project-specific Factors

Type of change



Positive changes perceived ~15% more favorably

Probability of success

Willingness to consider change plateaus at ~60% certainty of success

Individual Factors

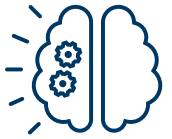
Connection to emotion

~20% more averse when change impacts friends (vs. strangers)

Complexity of circumstances

Confidence in context predicts ~50% of attitude towards change

Level of agency

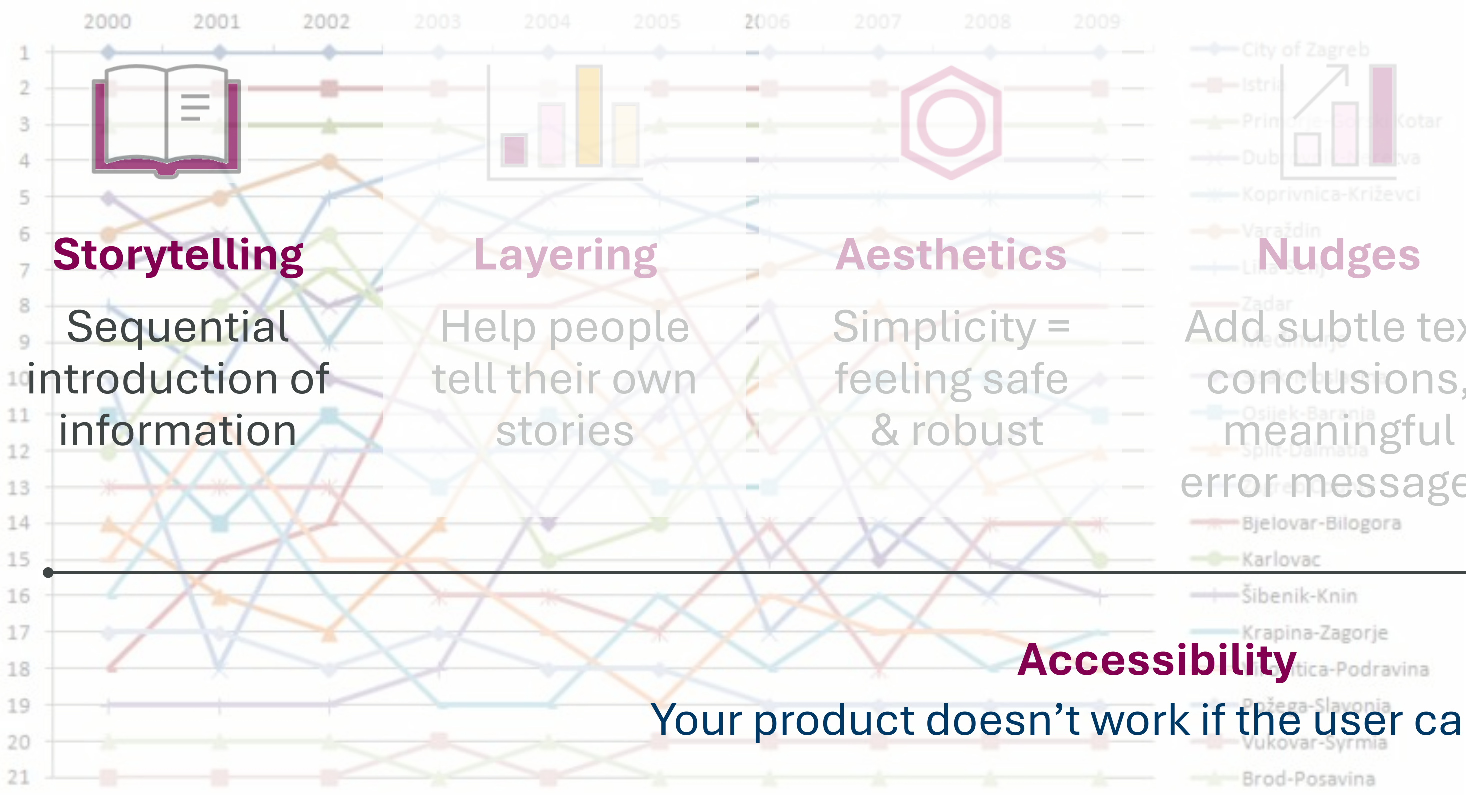


2x more likely to view change as negative when lack agency

Change aversion guidelines: Boston Consulting Group, https://www.bcg.com/publications/2023/how-change-aversion-can-derail-transformation

The *secret*: consider **cognitive load**

- Scientists must often deal with cognitively-complex information
- This hurts our heads. Yes, even if we are very clever.



Storytelling

Sequential introduction of information

Layering

Help people tell their own stories

Aesthetics

Simplicity = feeling safe & robust

Nudges

Add subtle text conclusions, meaningful error messages

Fa

Stick to common, trusted icons and layout

7

The **number of items** most people can **hold in their heads** simultaneously

Emphasis

Help them reach where you are

Accessibility

Your product doesn't work if the user can't work it

Acknowledgements

AZ Early Chemical Development

AZ Pharmaceutical Sciences

Christof Jäger

Per-Ola Norrby

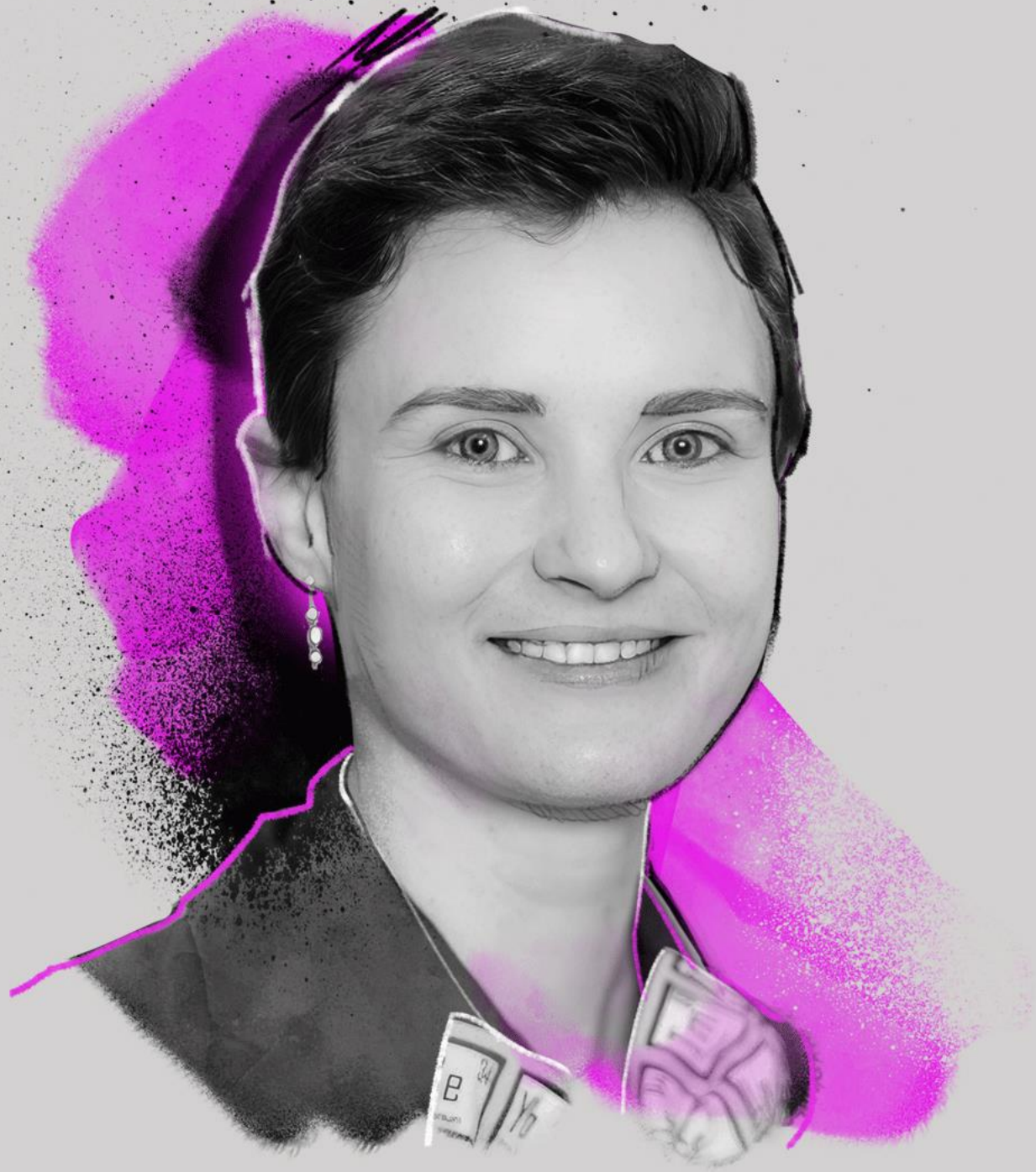
Selected chemistry & coding resources:
https://supersciencegrl.co.uk/links/

Automated Synthesis Forum 2024

11-12 Nov 2024

Oxford, UK

https://automatedsynthesisforum.com/



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