Roadmap for Data-driven biomaterial discovery

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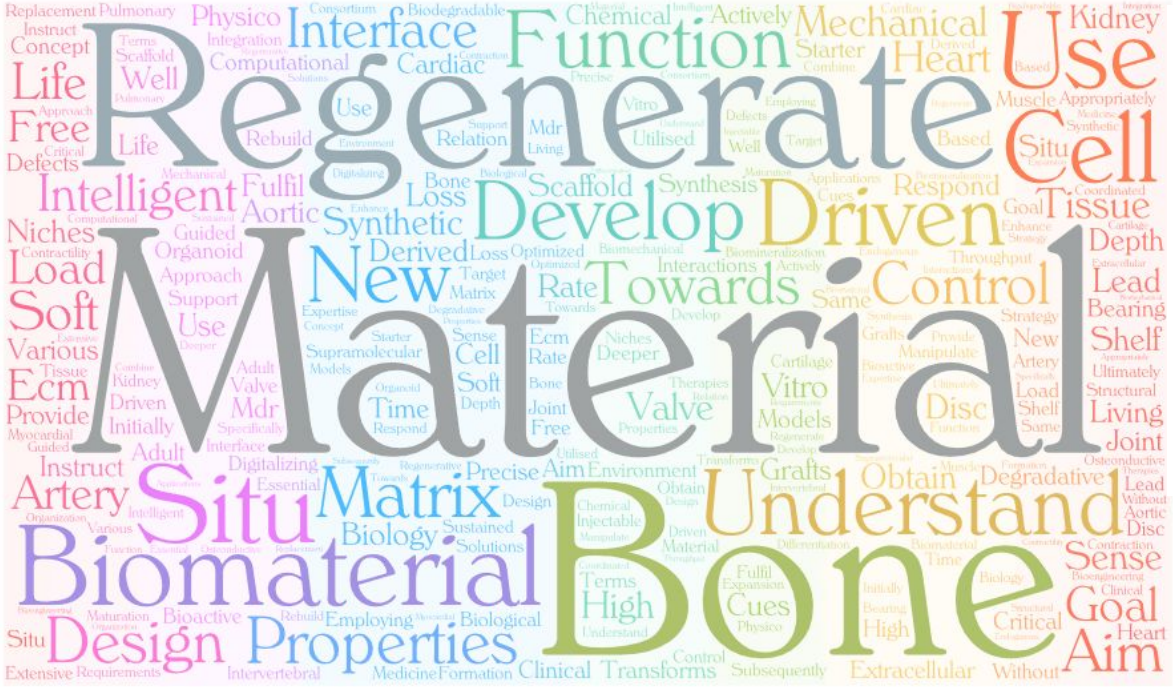
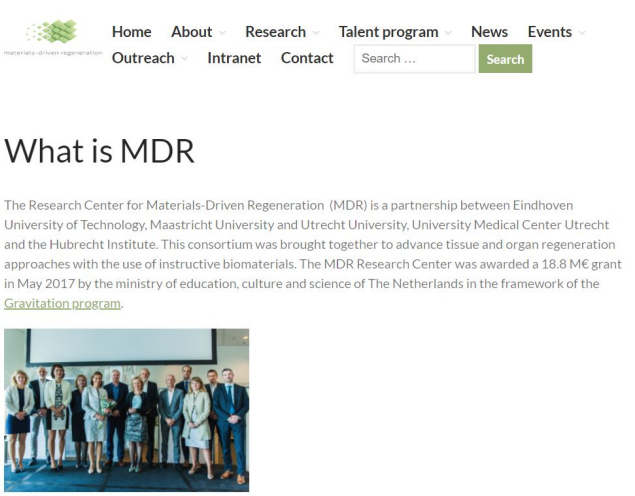
materials-driven regeneration

MDR-Research Center for Materials-Driven Regeneration

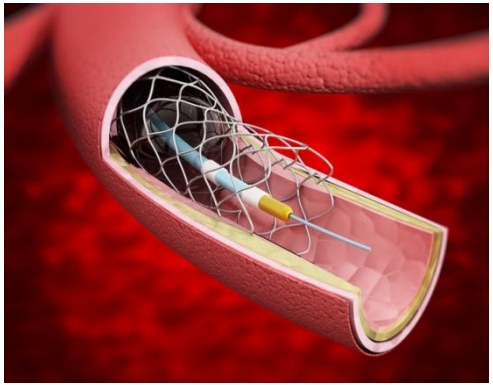


https://wordart.com/create

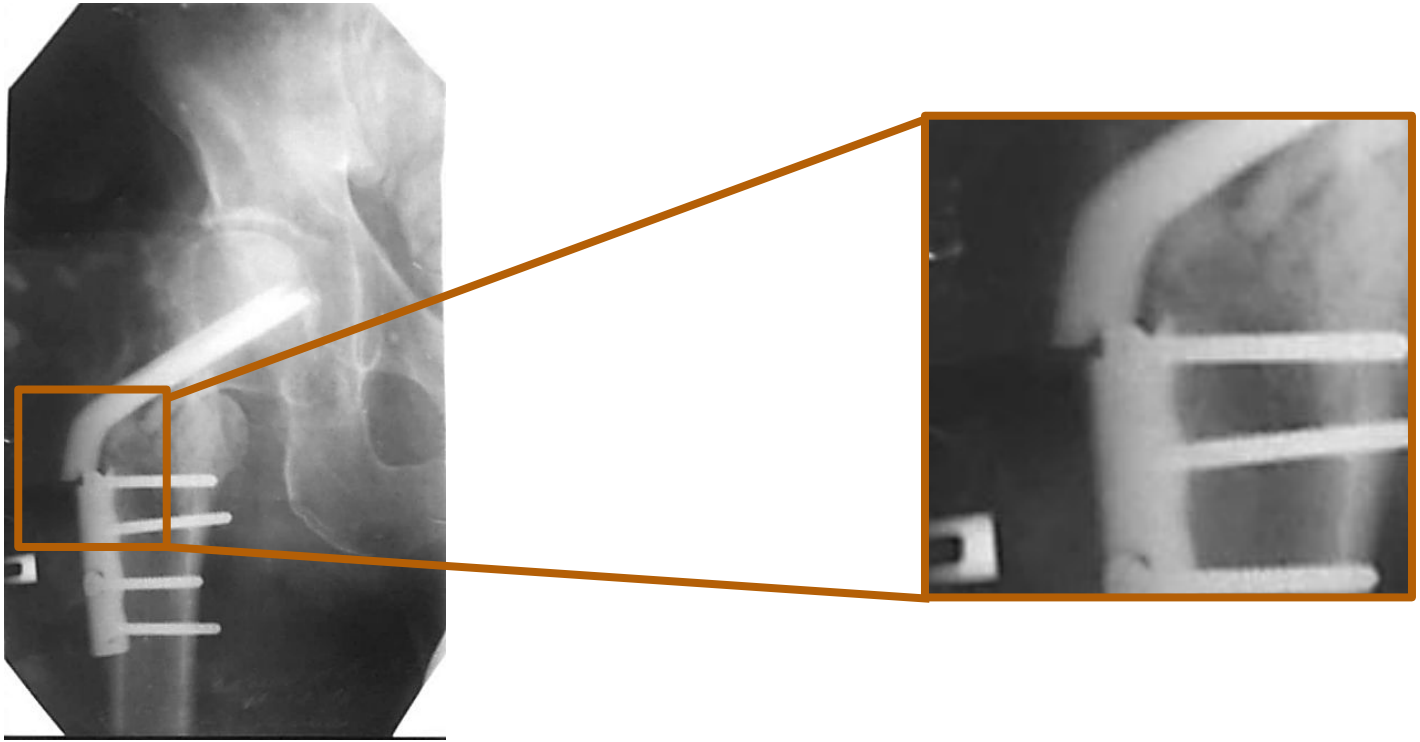


What are biomaterials?

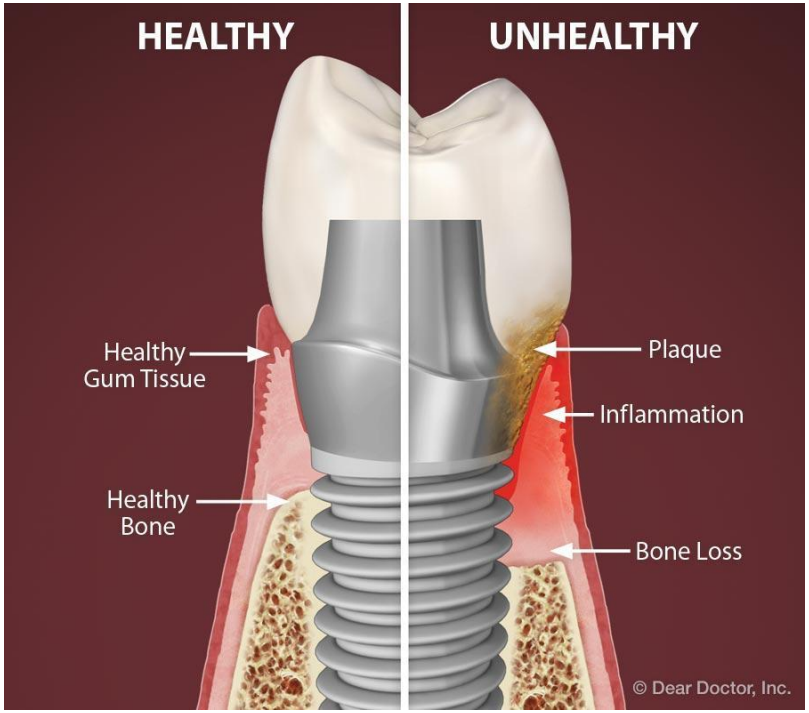
Biomaterials are used in implants



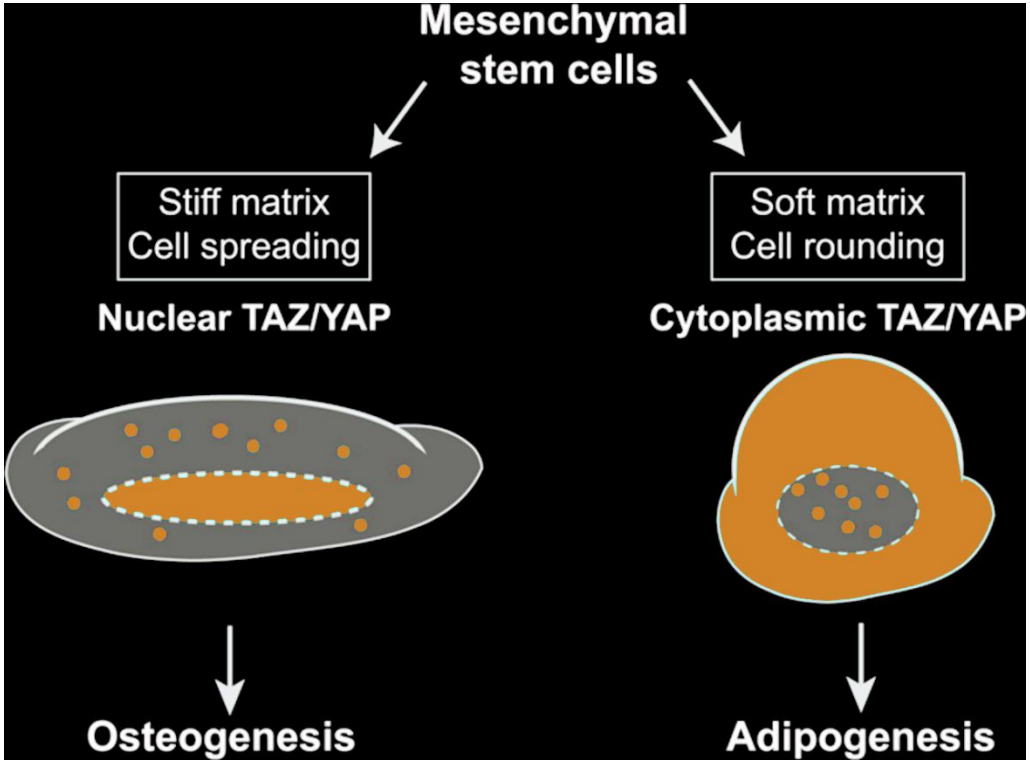
But implants can fail…



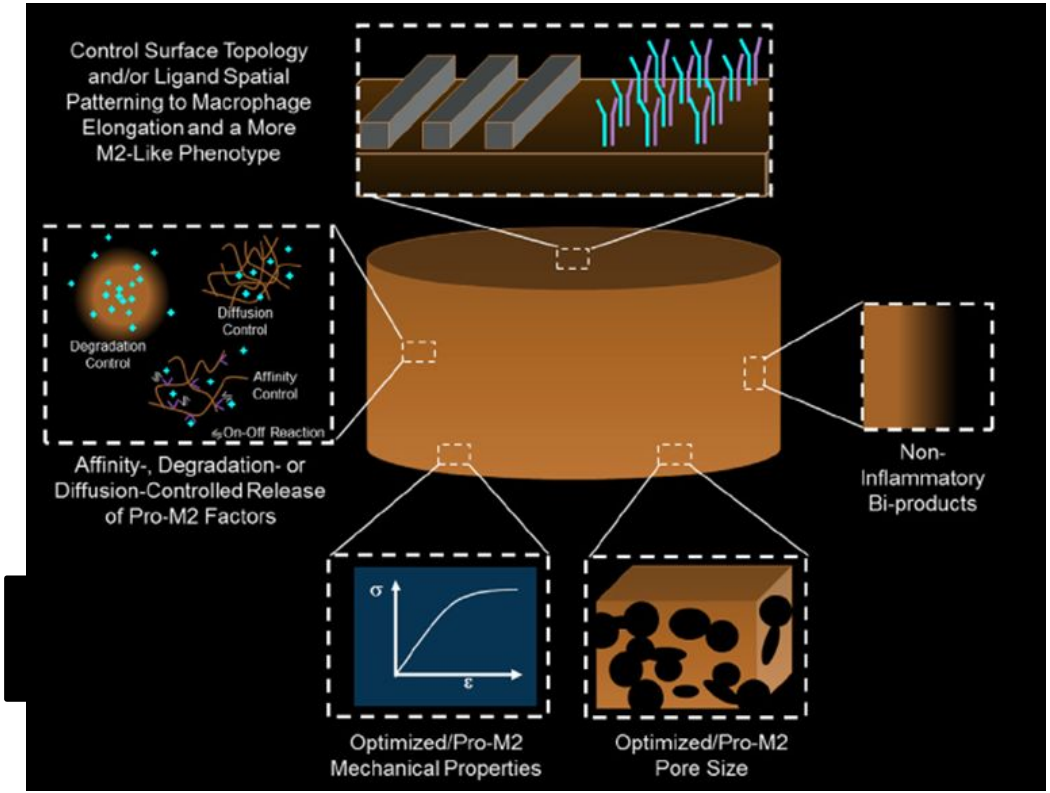
Dental implant failure example



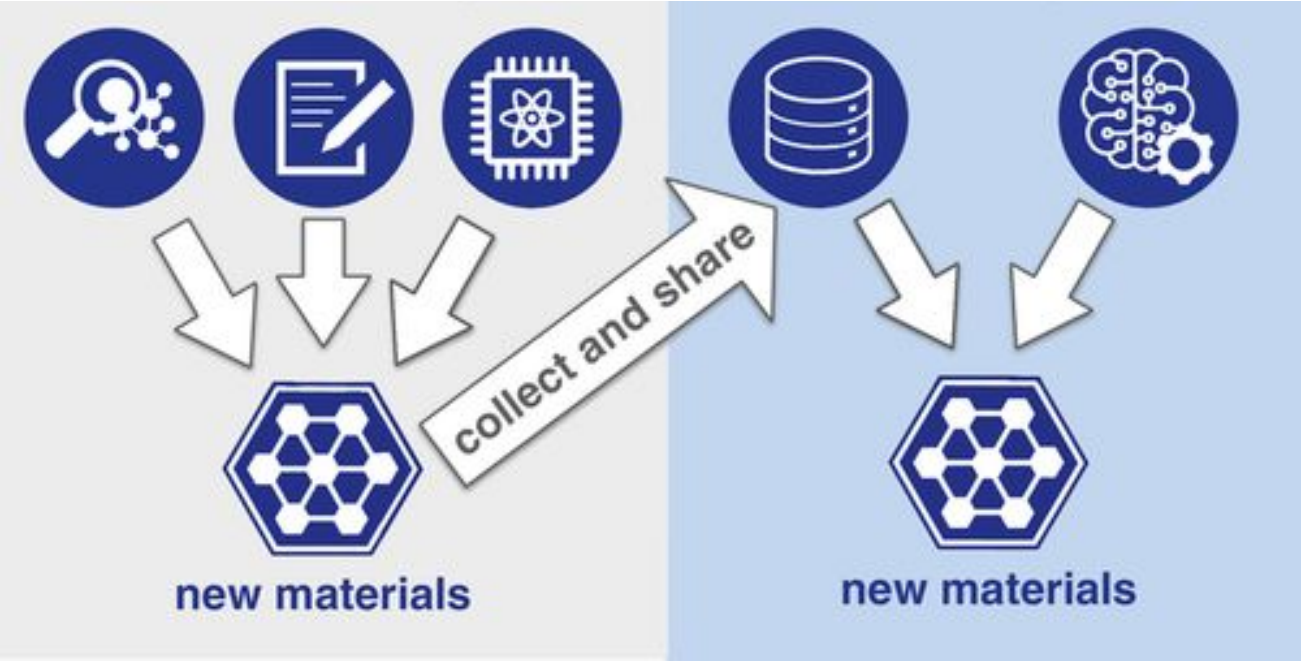
Biomaterials affect cells fate



Biomaterial composition

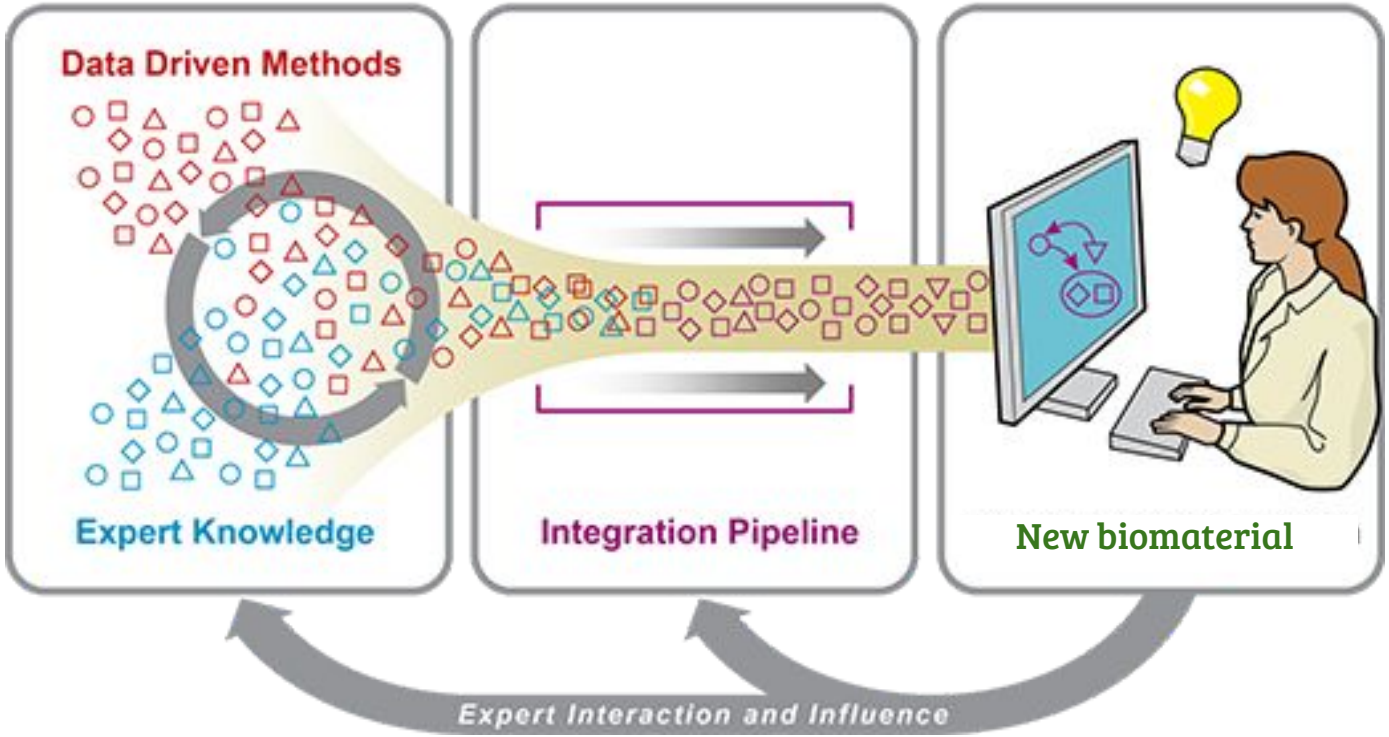


To discover the patterns we need to systematically collect more data



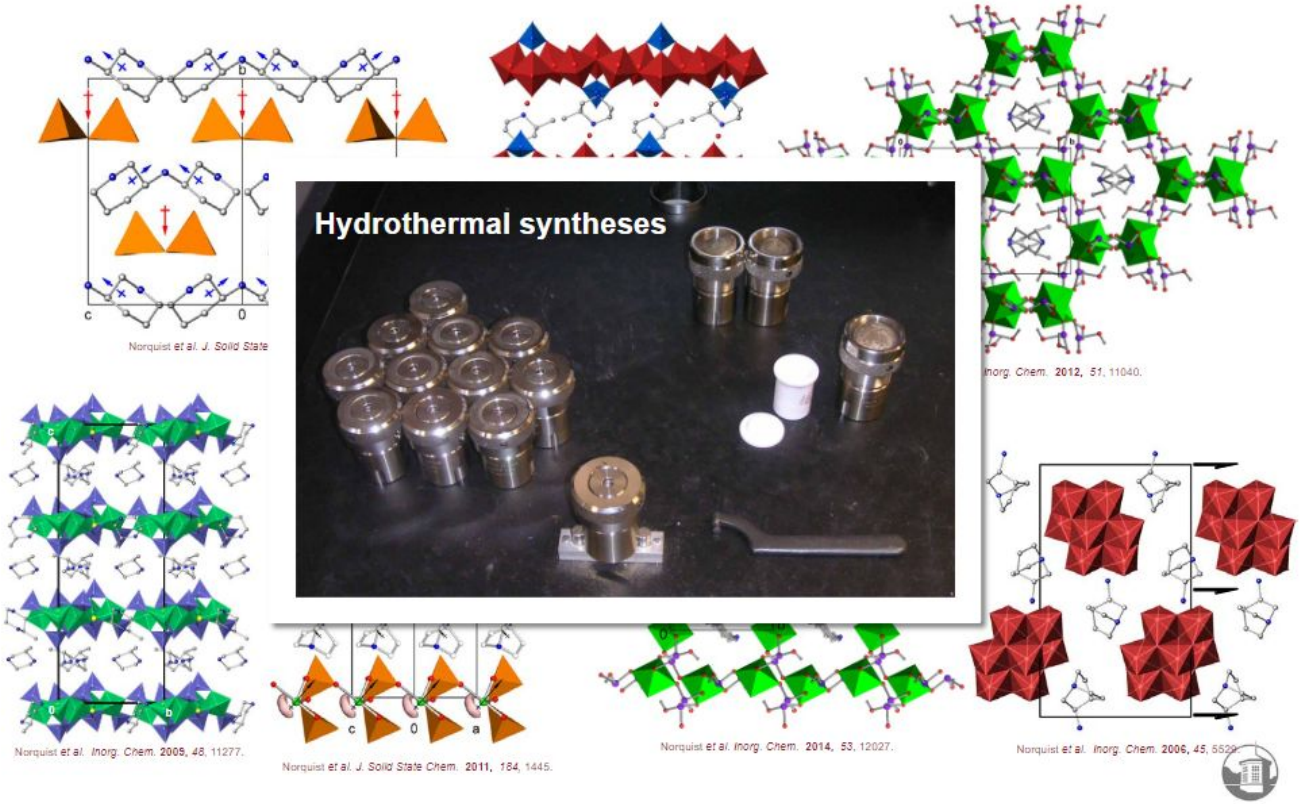
https://onlinelibrary.wiley.com/doi/full/10.1002/advs.201900808

Data-Driven Discovery uses the leverage of computers to crack large numbers

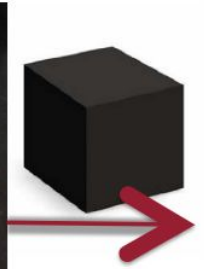


Example of DD research from Materials field

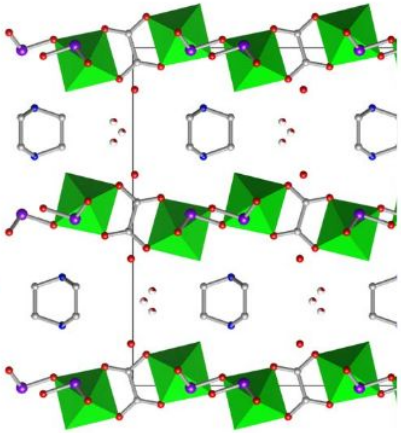
Amine-Templated Metal Oxides produced by hydrothermal synthesis



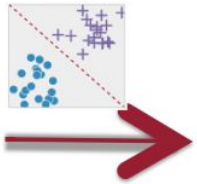
Can ML be used to predict synthesis outcome?



"chemistry"



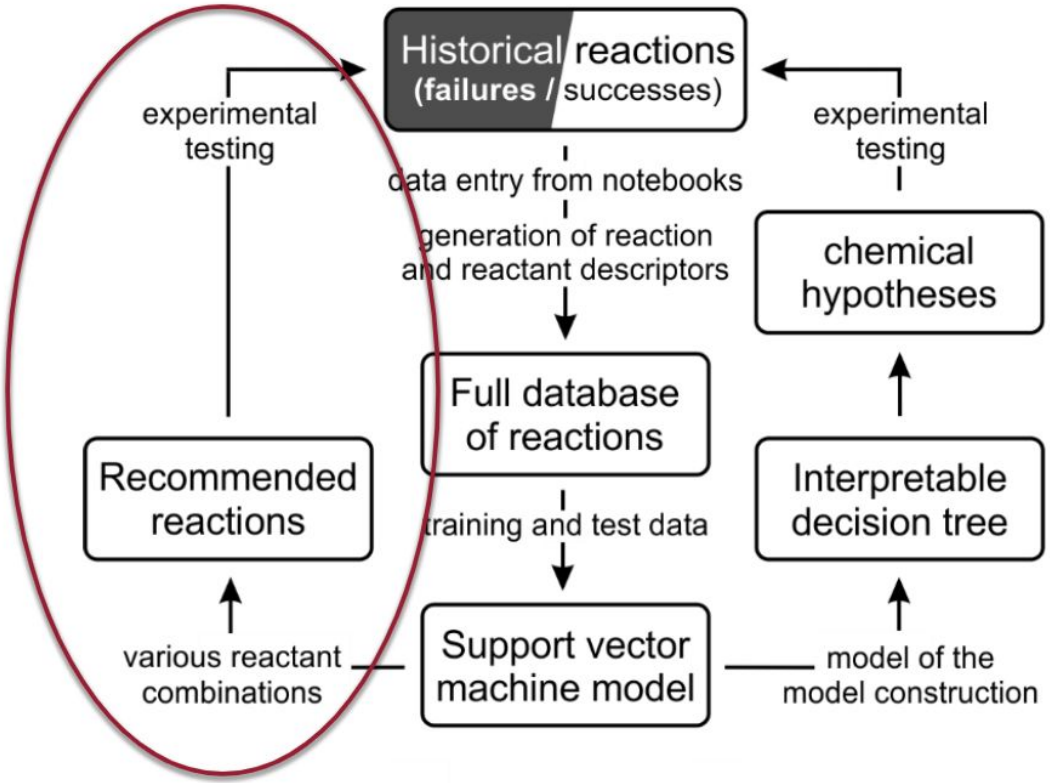
Inputs:
Concentration
pH
Time
Temperature
Etc.



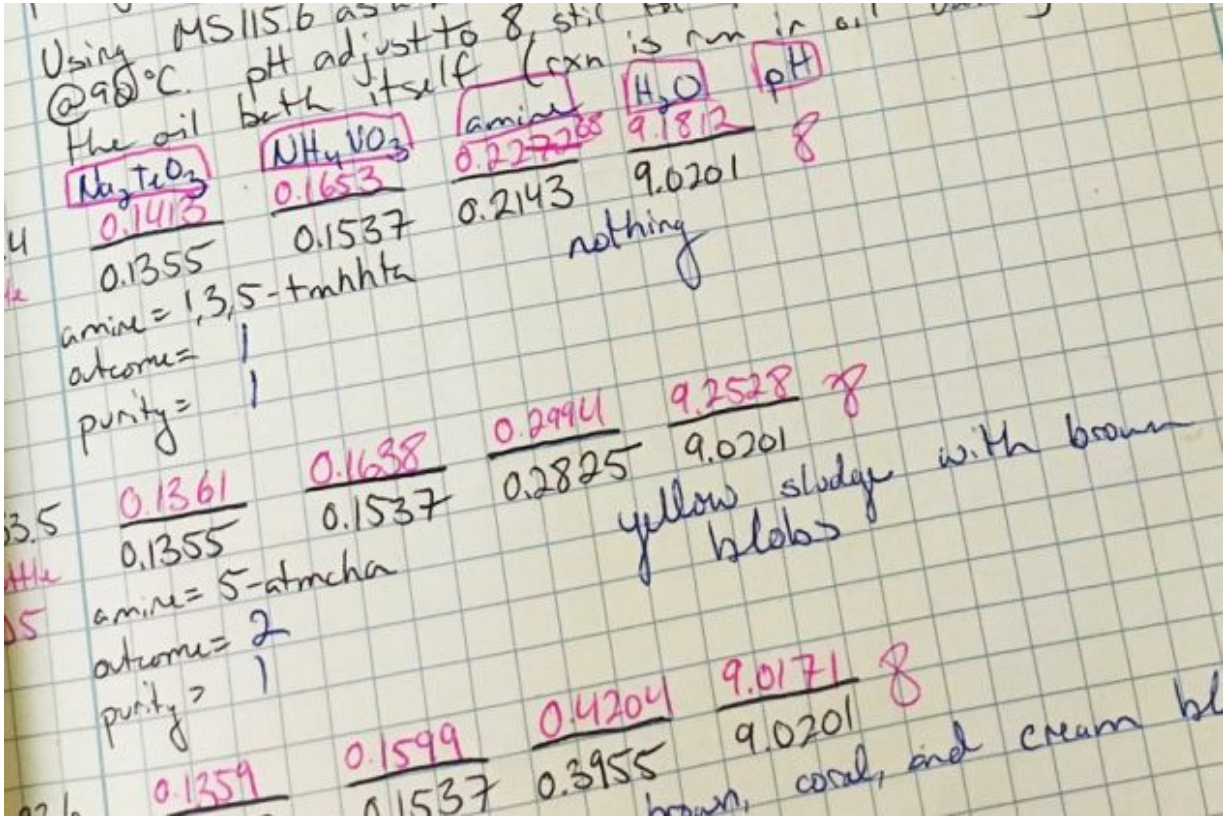
"machine learning"

Outputs:
Big crystal
Small crystal
Something bad ("tar")
No reaction

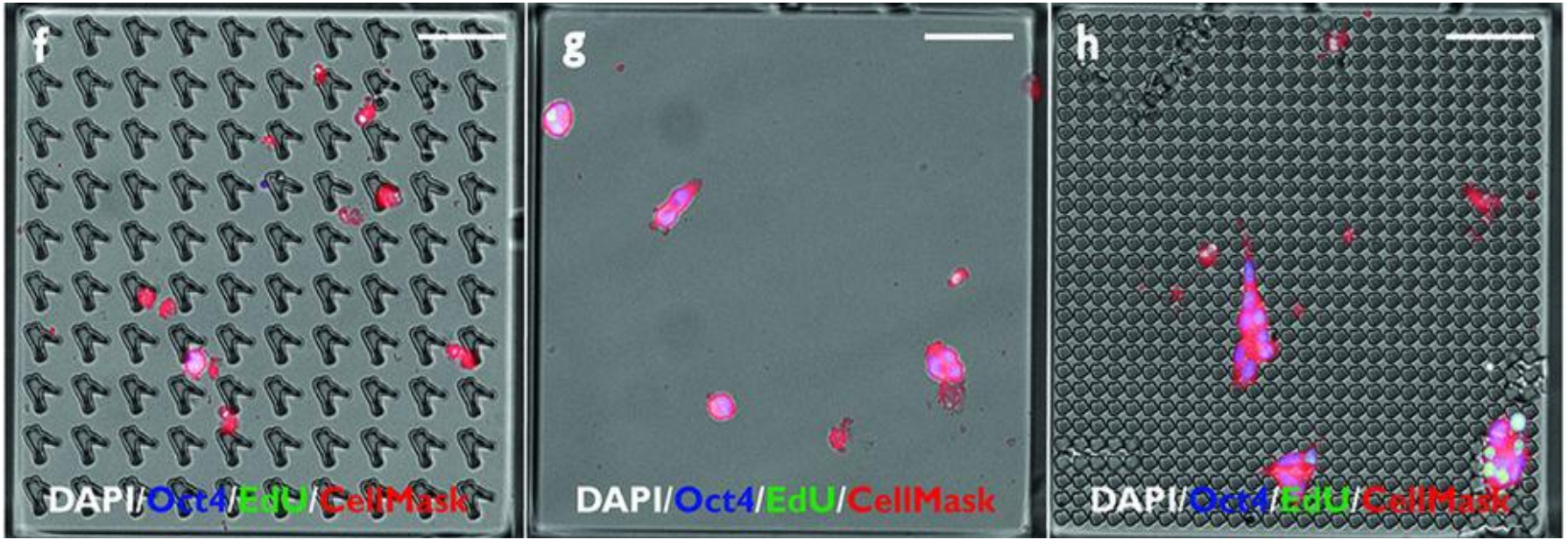
Combining ML and experiments to produce accurate model



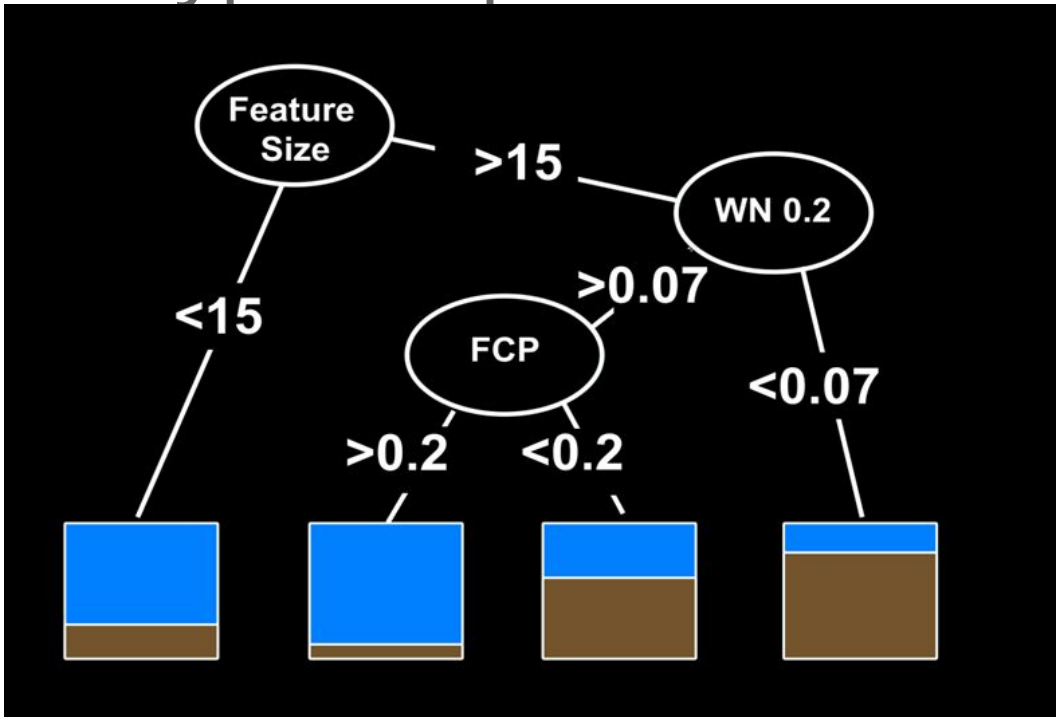
Dark reactions



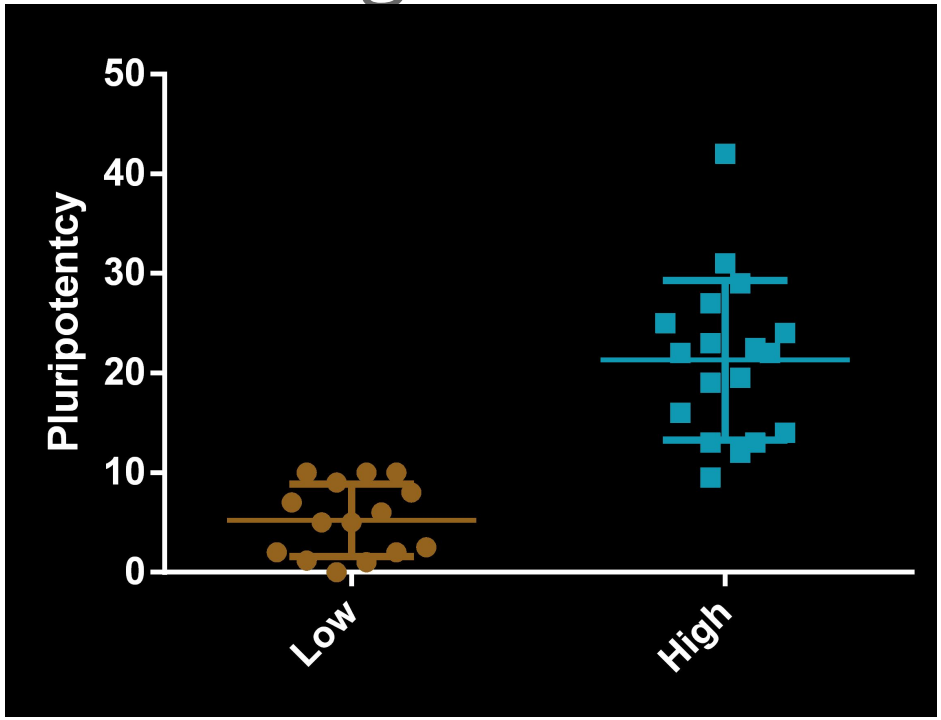
Example from our research. Design substrate that supports stem cells.



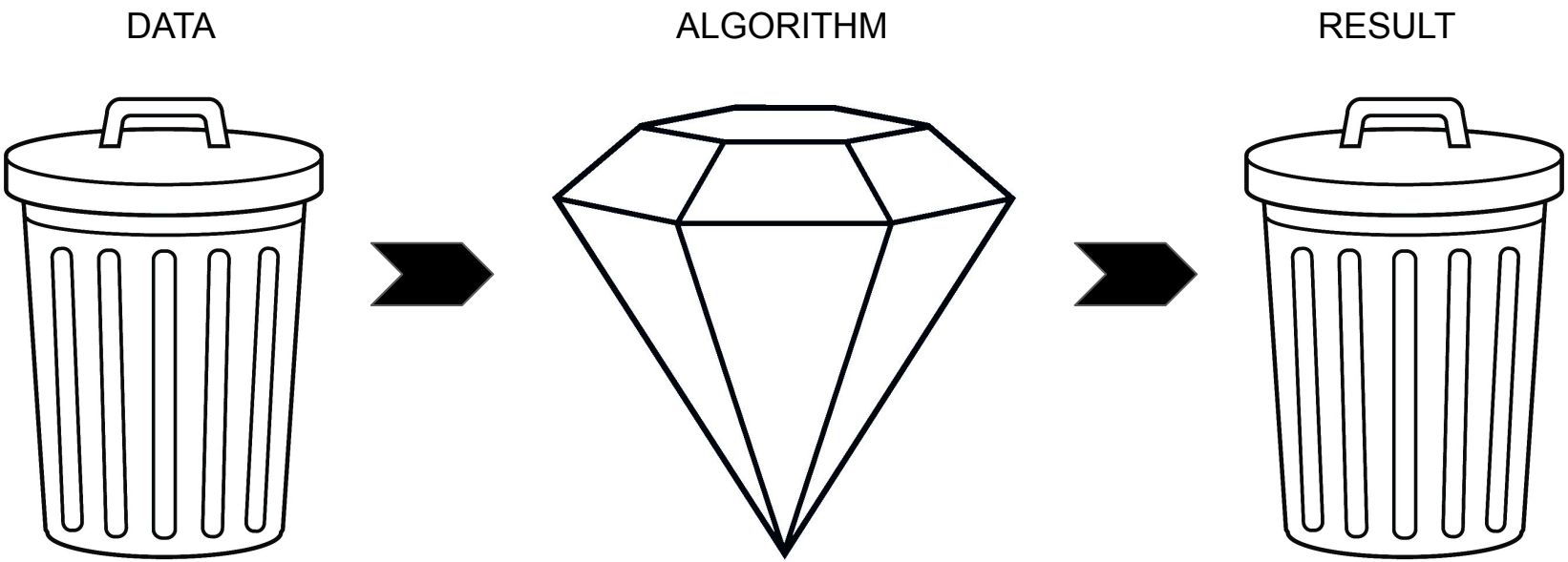
Algorithm finds relation between design and phenotypic response



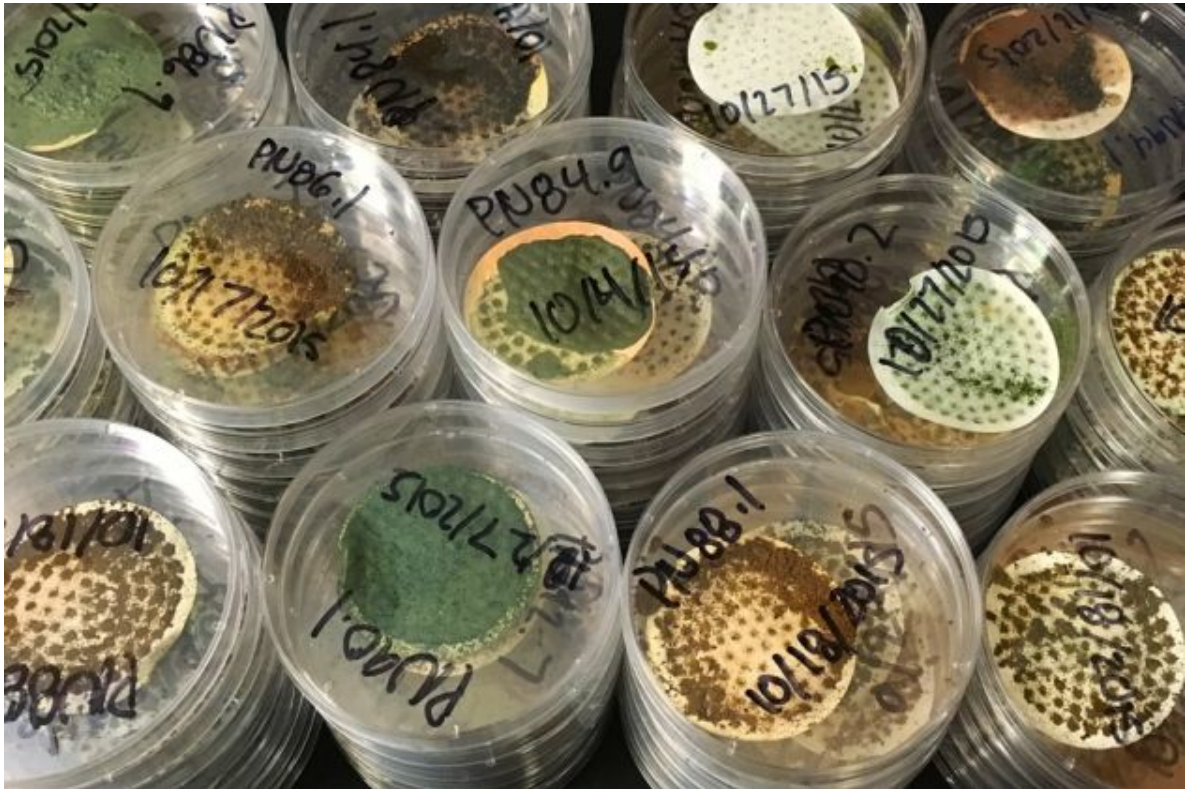
Algorithm predicts phenotypic response based on the design



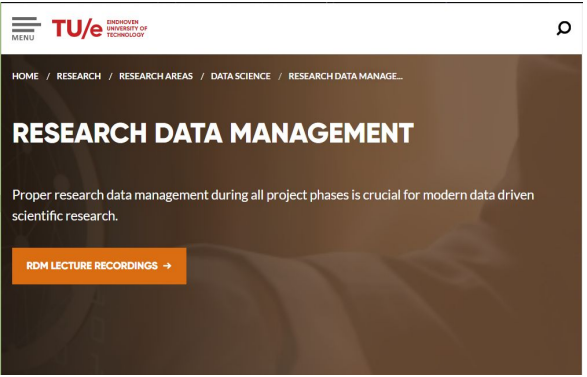
DD approach has its limitations

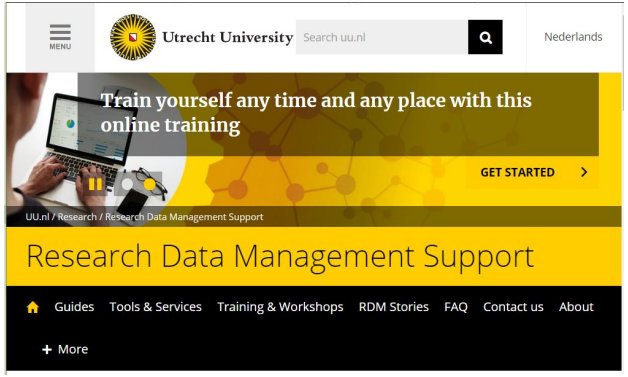


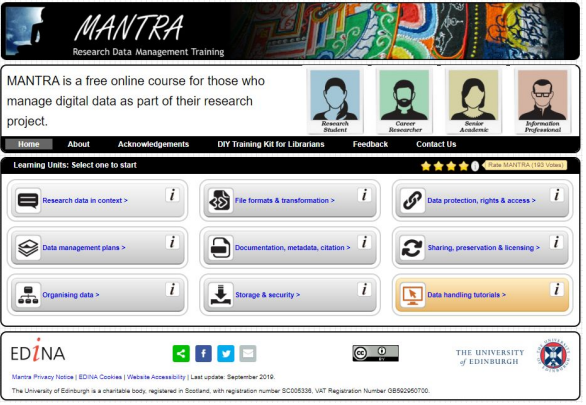
DATA is most important but it should be properly managed

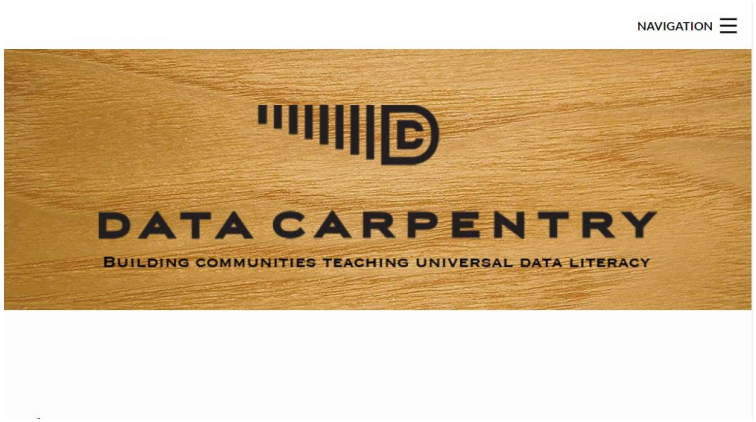


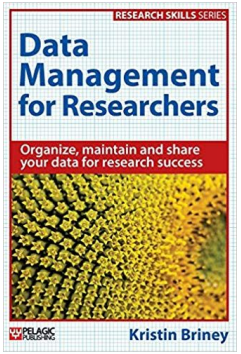
Practical Recommendations: Training



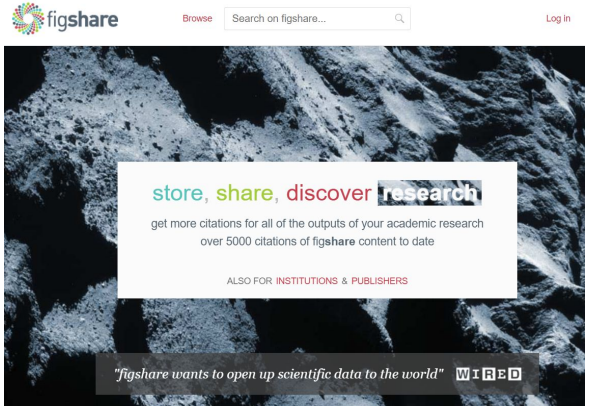


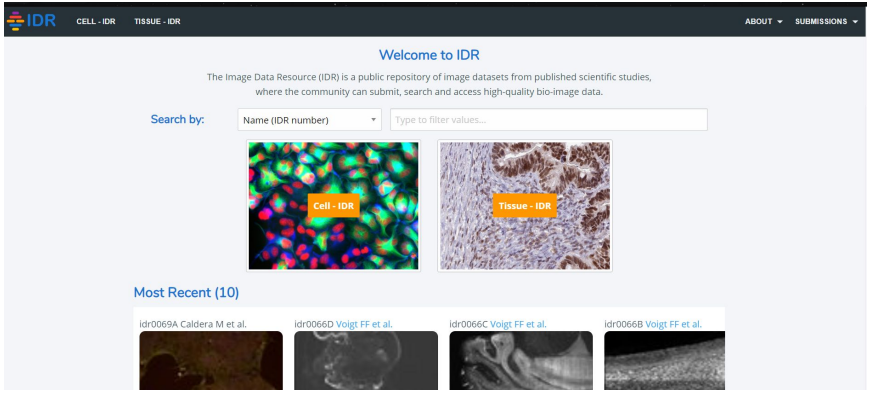


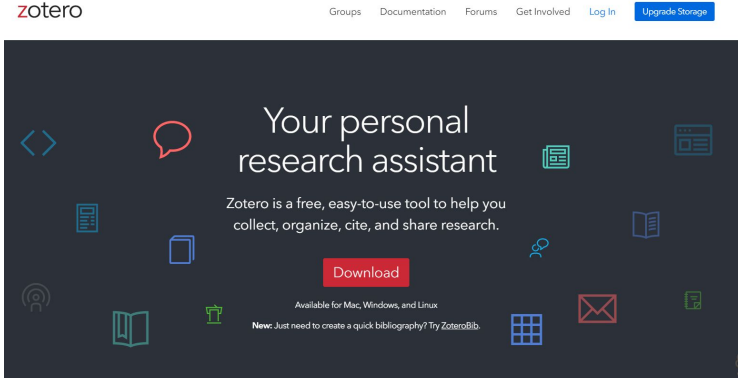


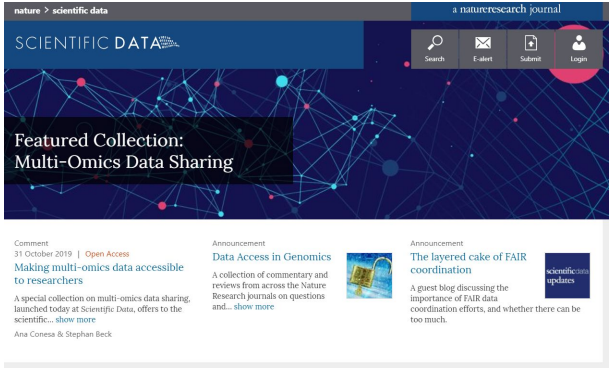


Practical: Open access Data storage

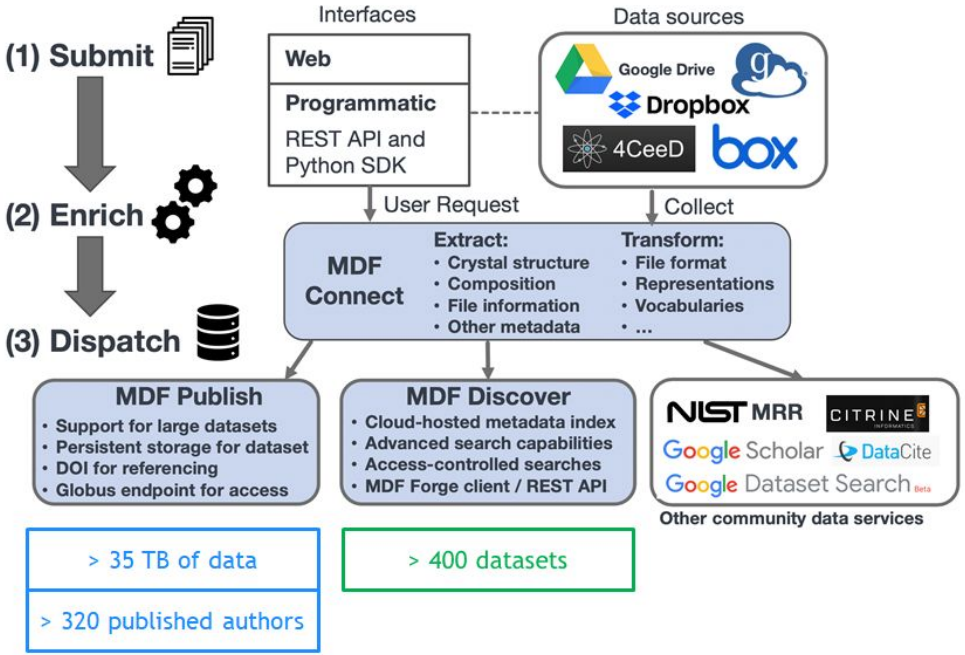








Practical: DATA exploration



- **Connect:** Extract domain-relevant metadata / transform the data
- **Publish:** Built to handle big data (many TB, millions of files), provides persistent identifier for data, distributed storage enabled
- **Discover:** Programmatic search index to aggregate and retrieve data across hundreds of indexed data sources

https://www.materialsdatafacility.org

CHiMaD NIST

Get in touch!

We are collecting case studies for data-driven discovery in biomaterial research.