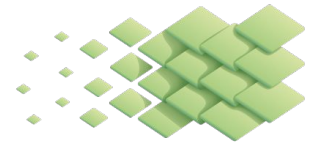


Roadmap for Data-driven biomaterial discovery

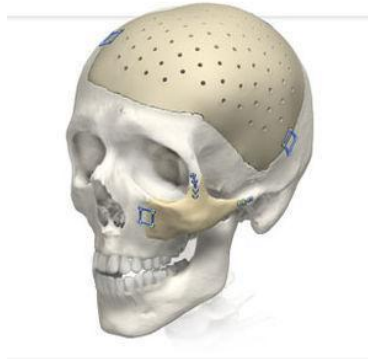
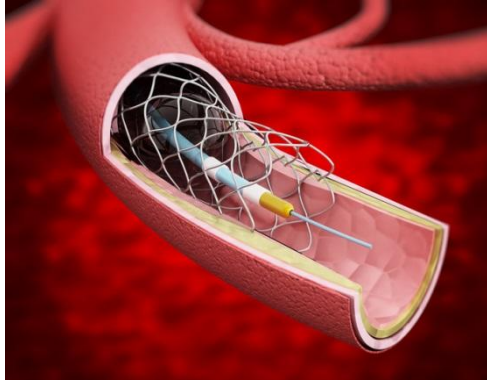
Aliaksei Vasilevich



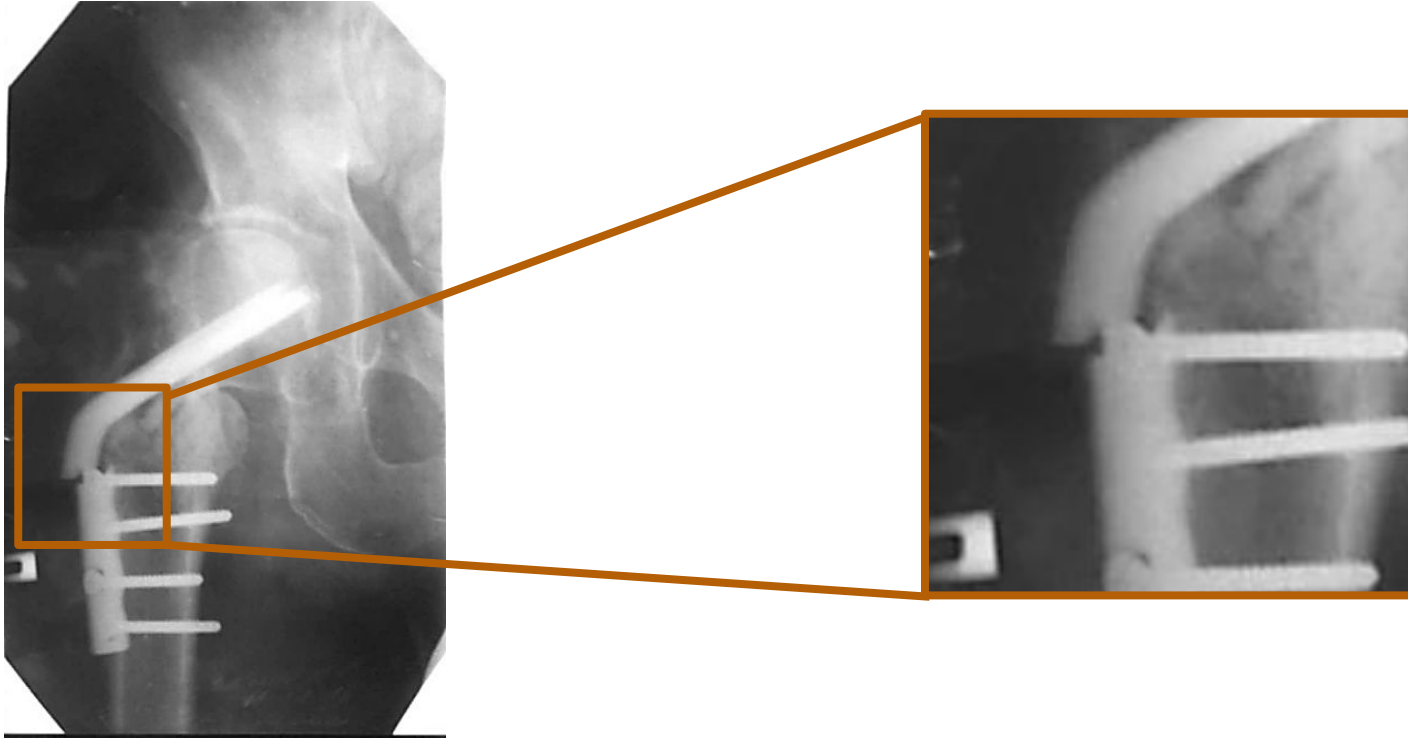
What are biomaterials?



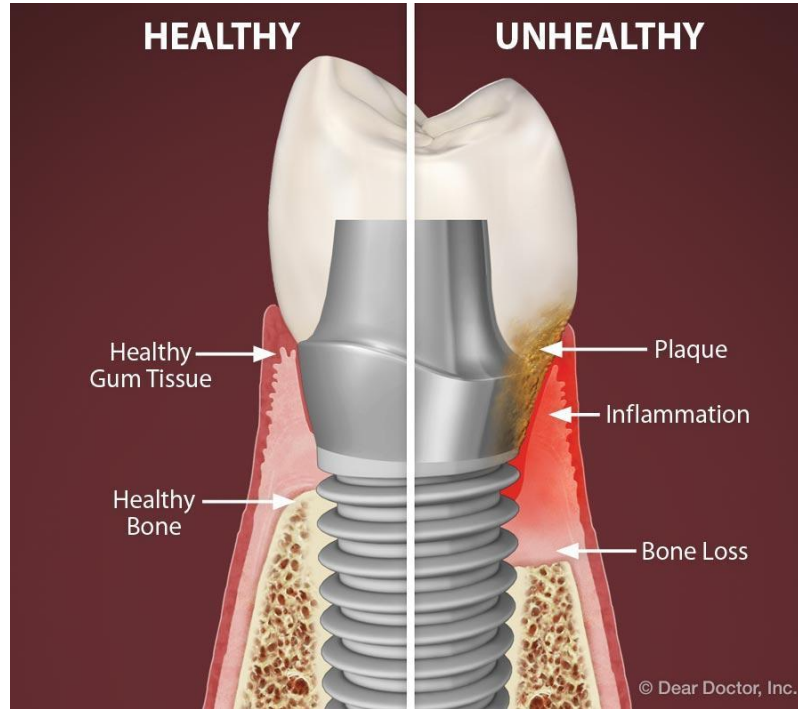
Biomaterials are used in implants



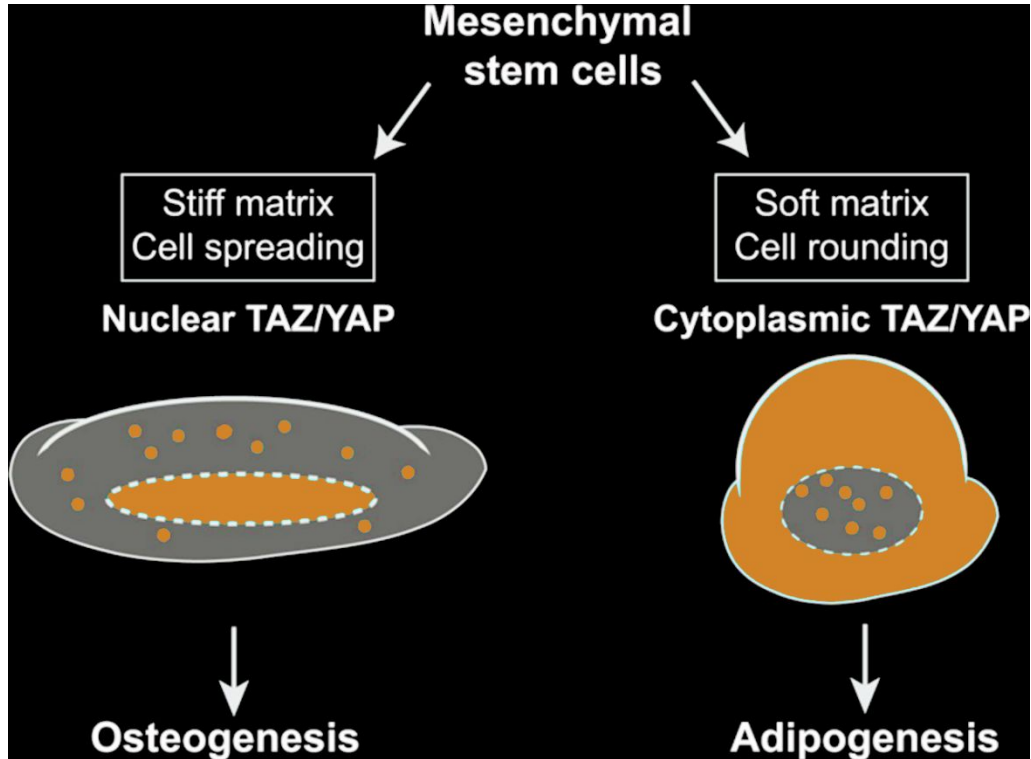
But implants can fail...



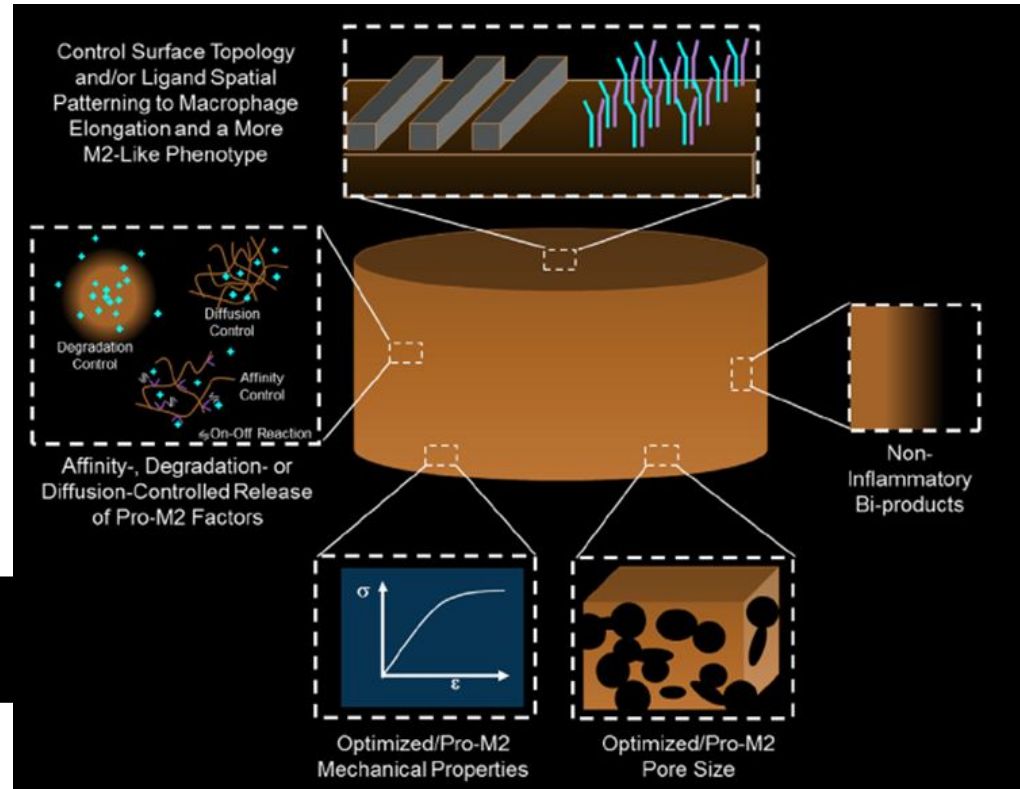
Dental implant failure example



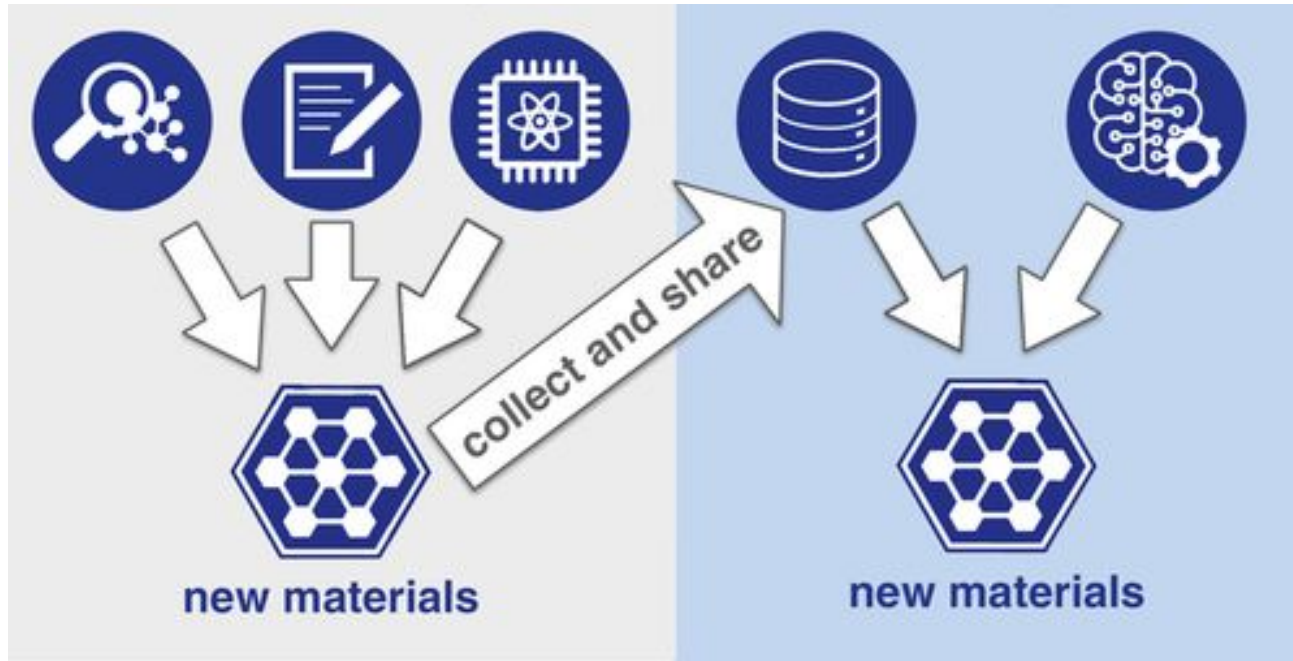
Biomaterials affect cells fate



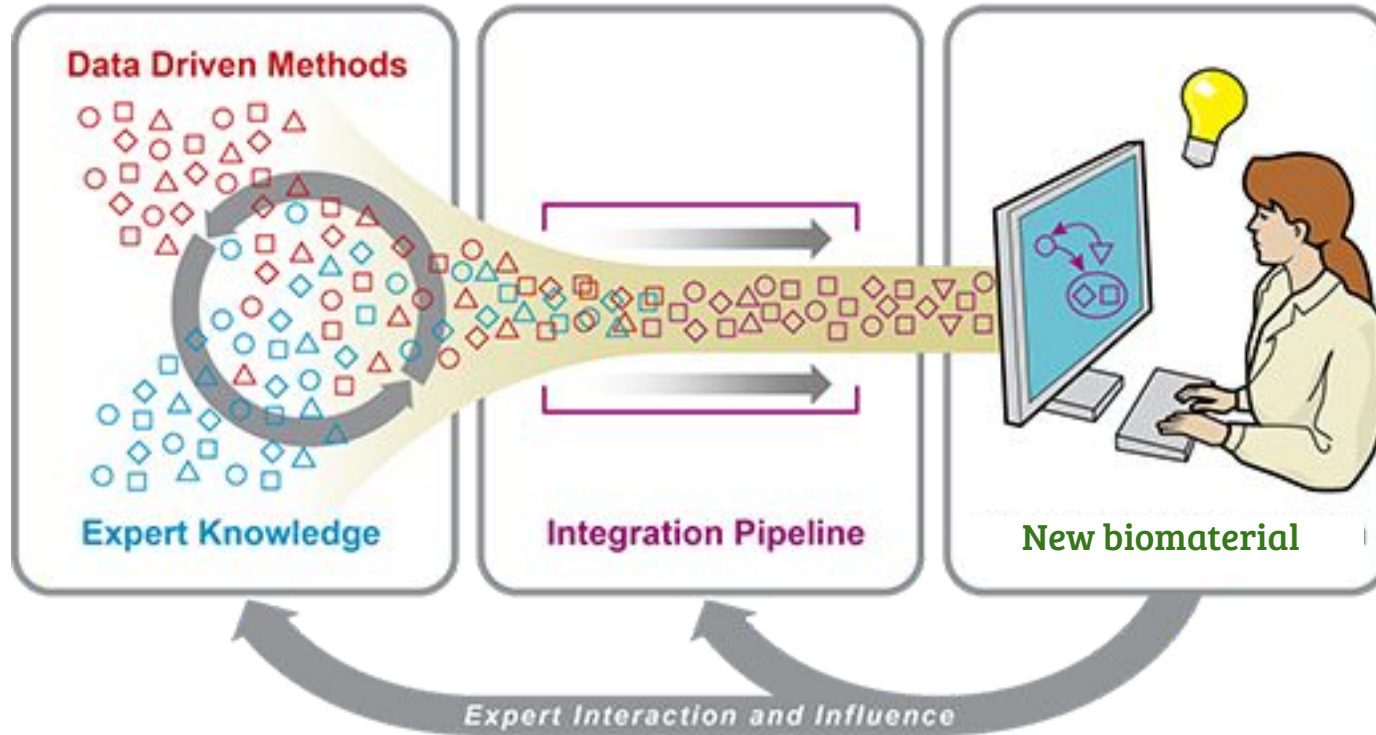
Biomaterial composition



To discover the patterns we need to systematically collect more data



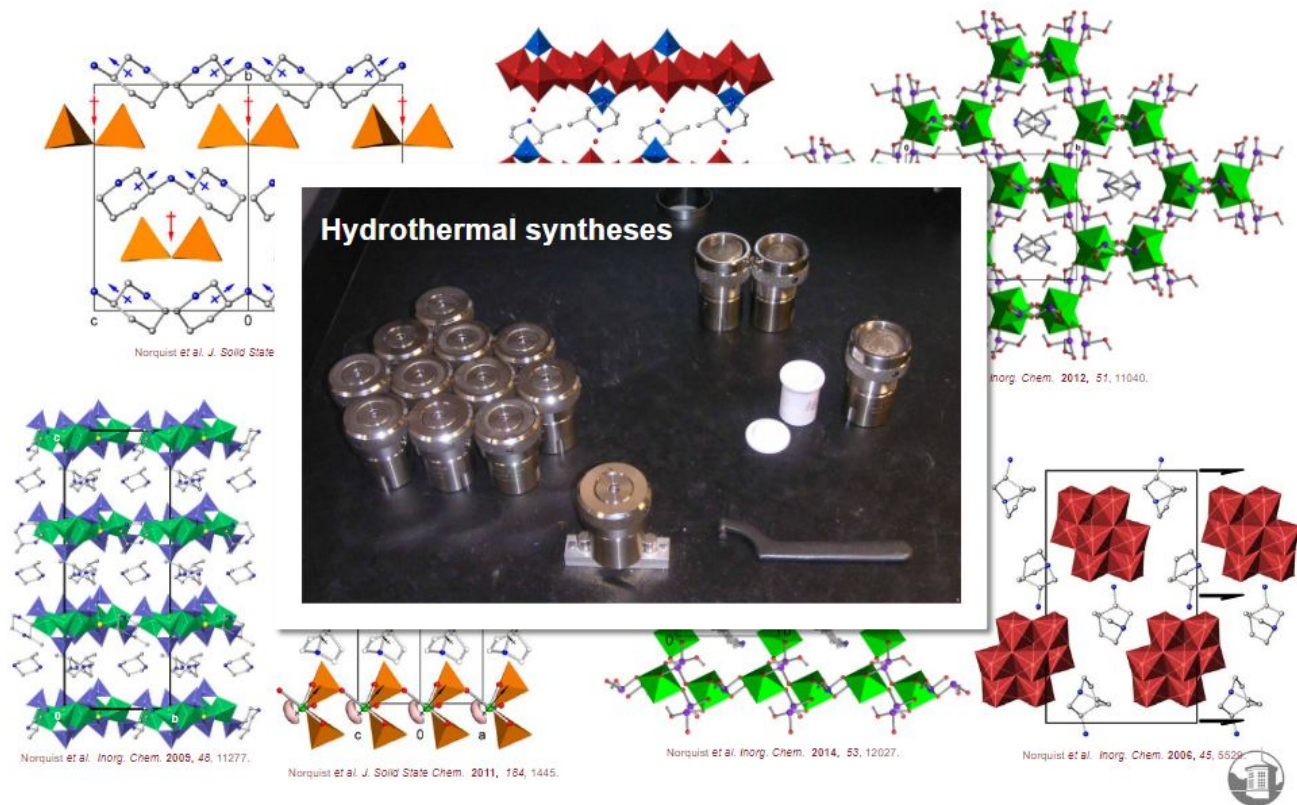
Data-Driven Discovery uses the leverage of computers to crack large numbers



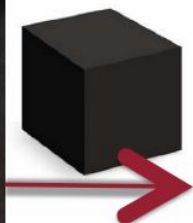
Example of DD research from Materials field



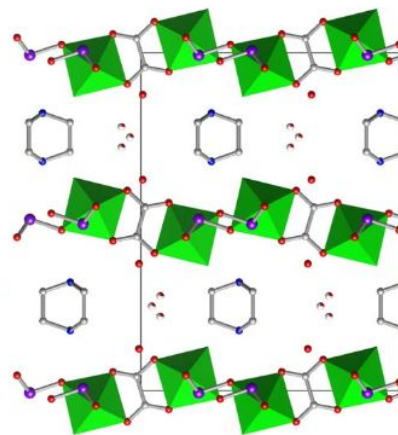
Amine-Templated Metal Oxides produced by hydrothermal synthesis



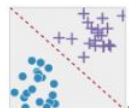
Can ML be used to predict synthesis outcome?



“chemistry”



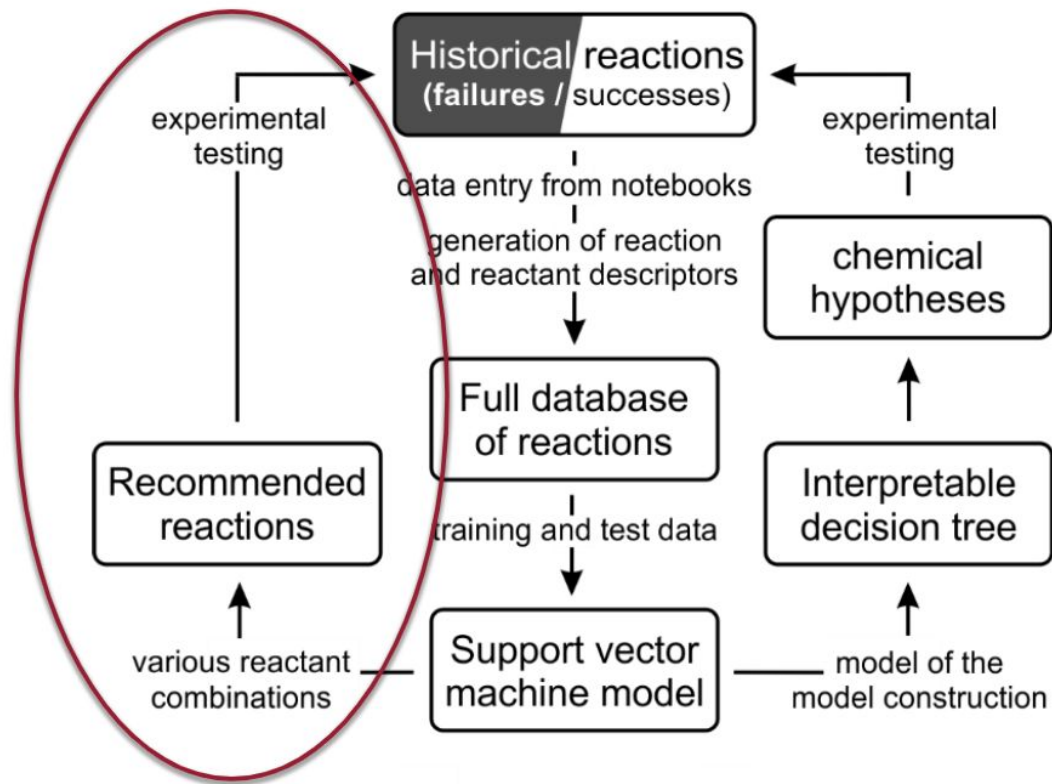
Inputs:
Concentration
pH
Time
Temperature
Etc.



“machine learning”

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

Combining ML and experiments to produce accurate model

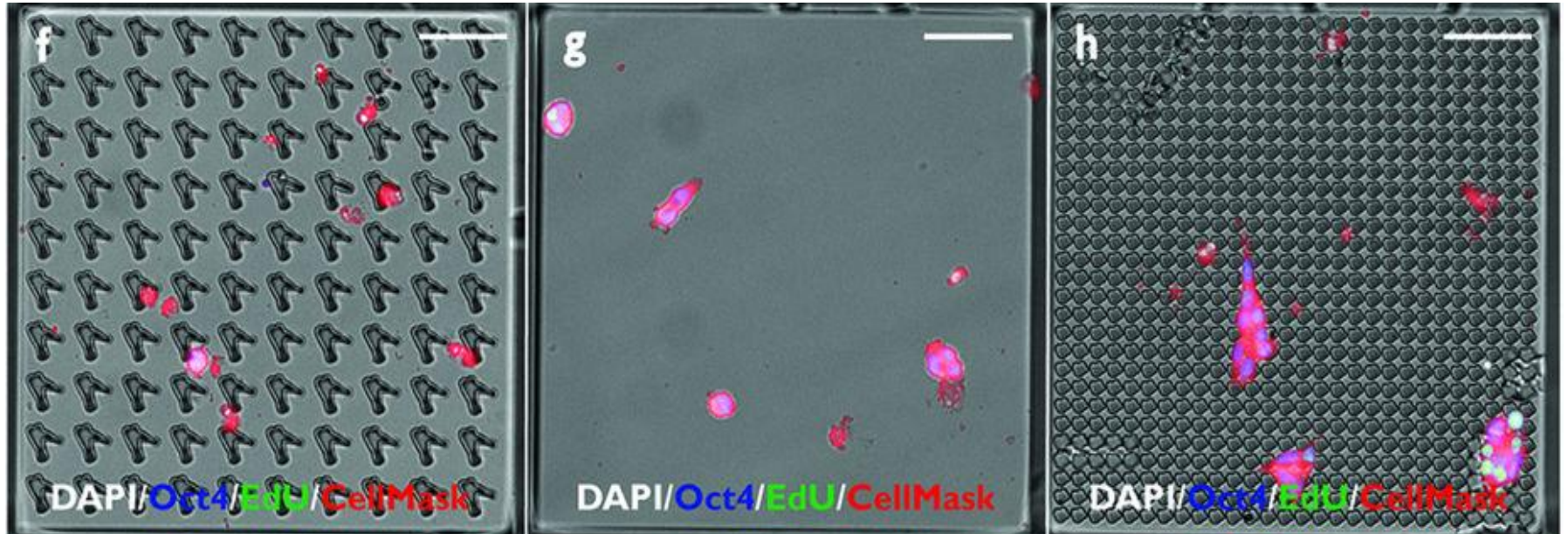


Dark reactions

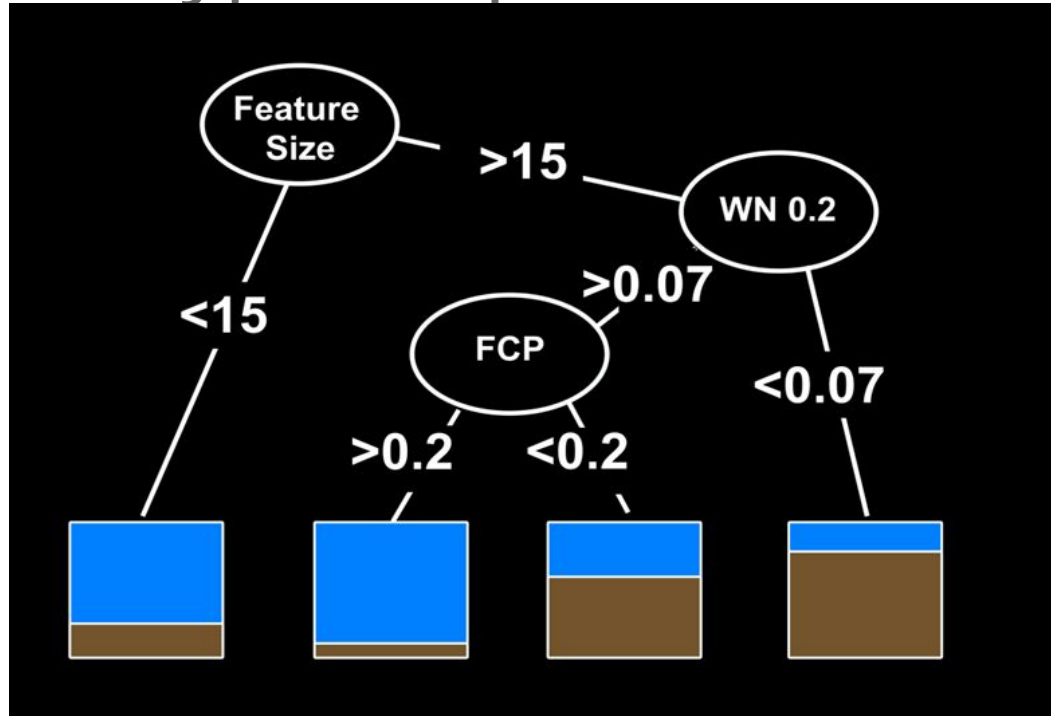
Using MS115.6 as a ...
 @90°C. pH adjust to 8, still ...
 the oil bath itself (rxn is run in oil bath)

	Na_2TeO_3	NH_4VO_3	amine	H_2O	pH
4	<u>0.1413</u>	<u>0.1653</u>	<u>0.227268</u>	<u>9.1812</u>	8
	0.1355	0.1537	0.2143	9.0201	nothing
	amine = 1,3,5-trmhta				
	outcome = 1				
	purity = 1				
3.5	<u>0.1361</u>	<u>0.1638</u>	<u>0.2994</u>	<u>9.2528</u>	8
4.5	0.1355	0.1537	0.2825	9.0201	yellow sludge with brown blobs
	amine = 5-atmcha				
	outcome = 2				
	purity = 1				
2.1	<u>0.1359</u>	<u>0.1599</u>	<u>0.4204</u>	<u>9.0171</u>	8
	0.1537	0.3955	9.0201		brown, coral, and cream bl

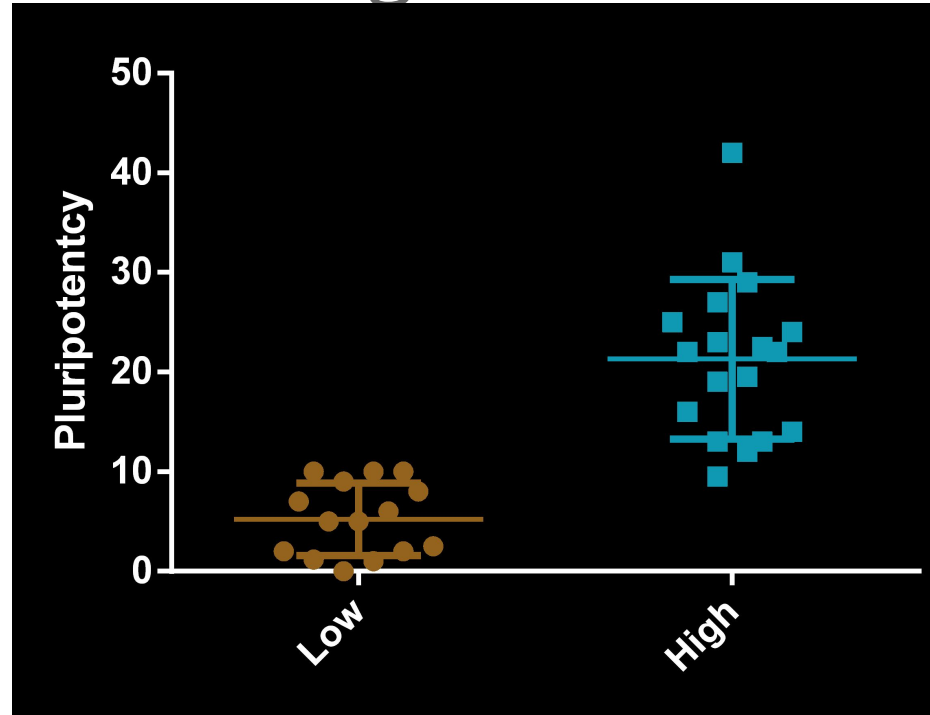
Example from our research. Design substrate that supports stem cells.



Algorithm finds relation between design and phenotypic response

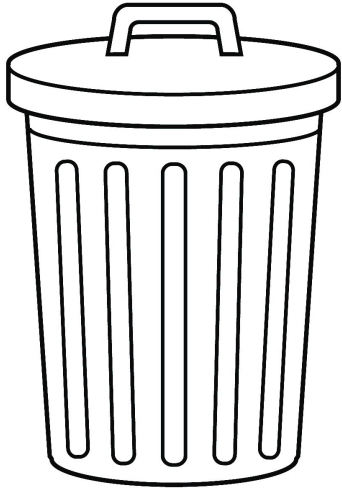


Algorithm predicts phenotypic response based on the design

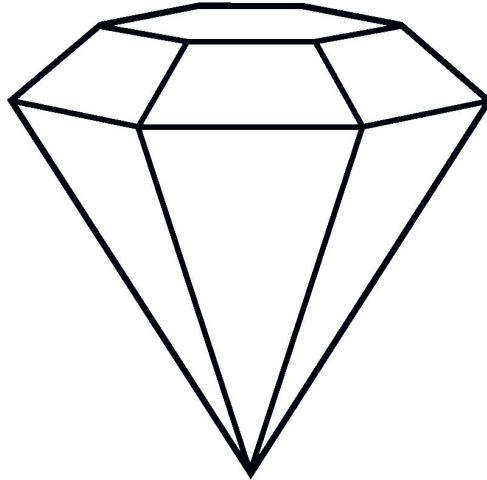


DD approach has its limitations

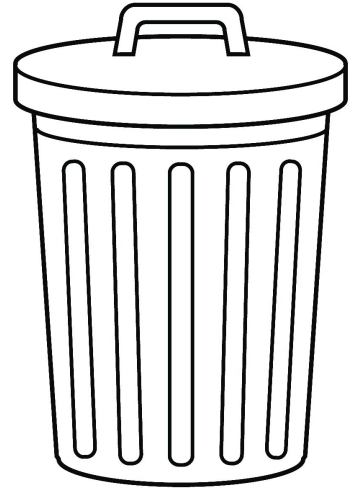
DATA



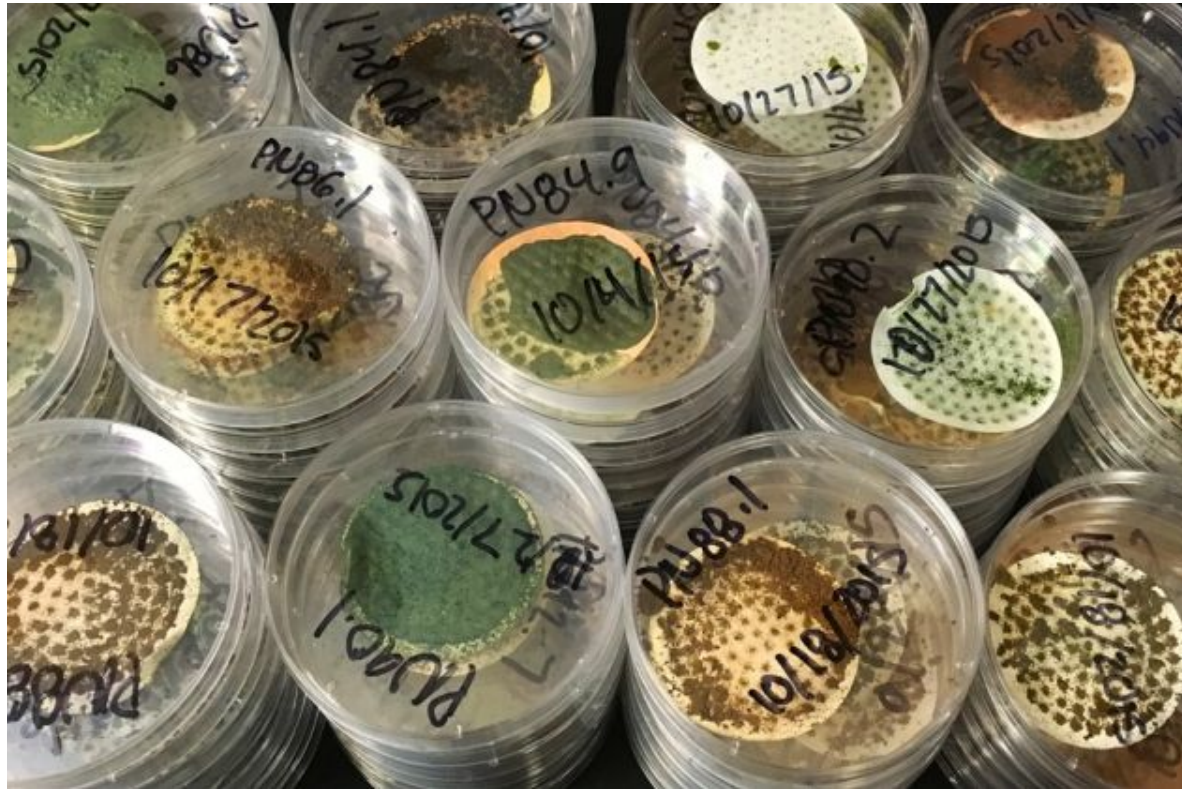
ALGORITHM



RESULT



DATA is most important but it should be properly managed



Practical Recommendations: Training

TU/e Eindhoven University of Technology

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RESEARCH DATA MANAGEMENT

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Research Data Management

Maastricht University is committed to making research data Findable, Accessible, Interoperable and Reusable (FAIR).

MANTRA Research Data Management Training

MANTRA is a free online course for those who manage digital data as part of their research project.

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- File formats & transformation
- Data protection, rights & access
- Data management plans
- Documentation, metadata, citation
- Sharing, preservation & licensing
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BUILDING COMMUNITIES TEACHING UNIVERSAL DATA LITERACY

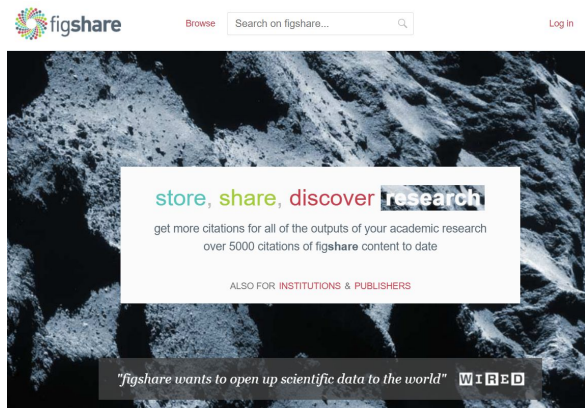
RESEARCH SKILLS SERIES

Data Management for Researchers

Organize, maintain and share your data for research success

Kristin Briney

Practical: Open access Data storage




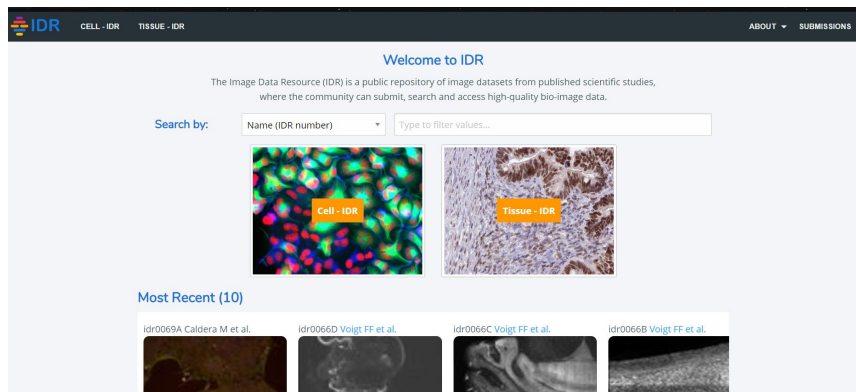
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Welcome to IDR

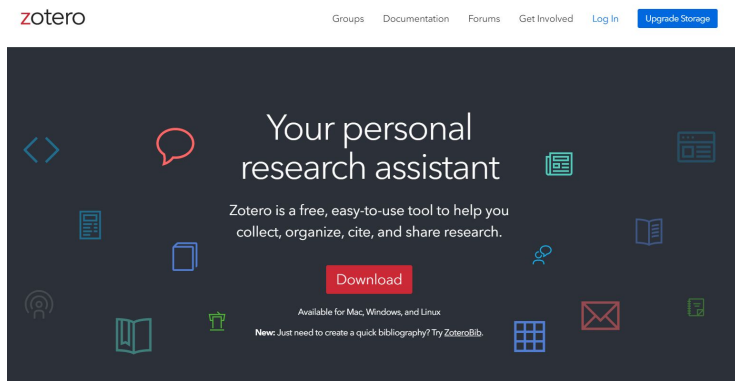
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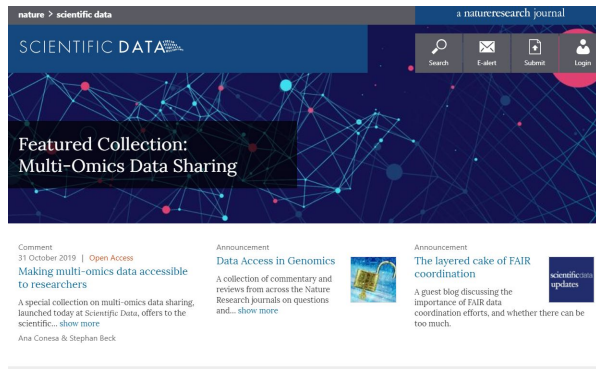
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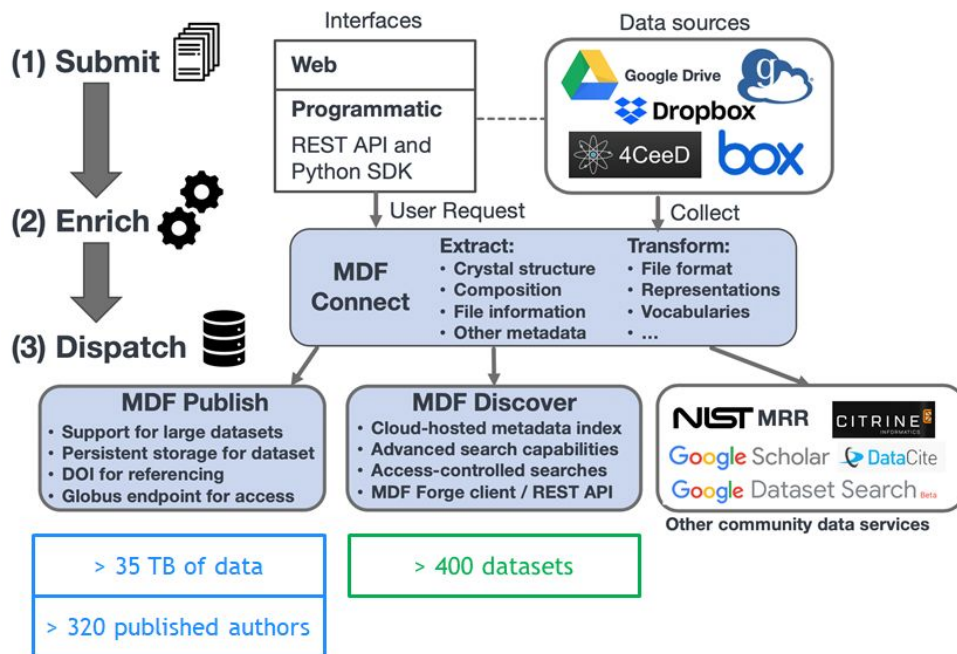
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scientific data updates

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>

Get in touch!

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