

Open Data & Data Management: Issues and Challenges

from the viewpoint of a synthetic chemist

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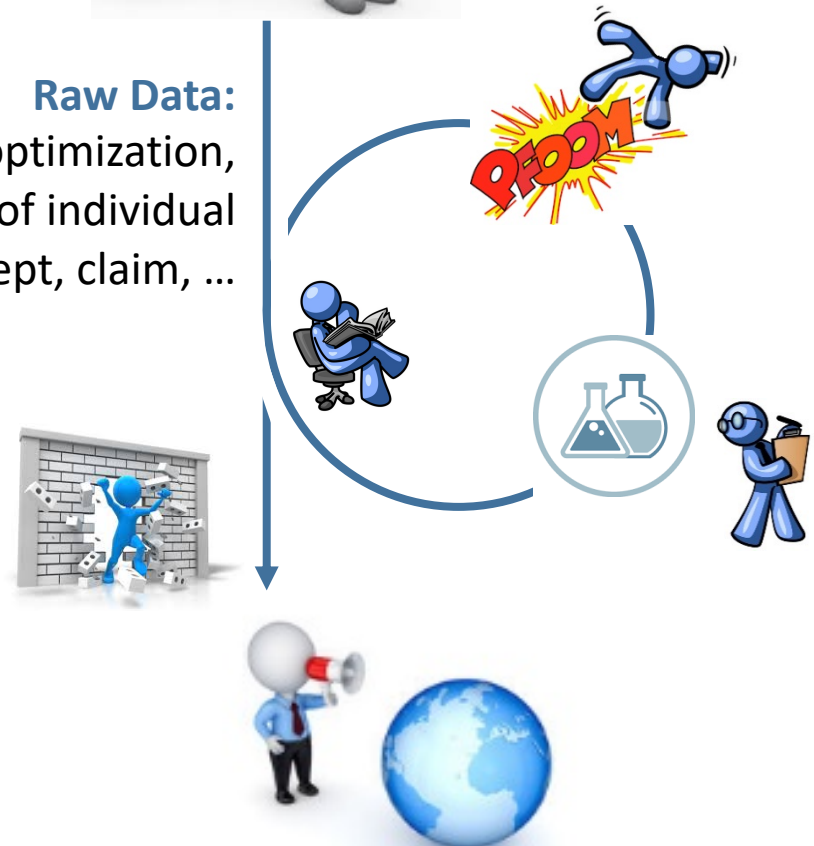
(Raw) Data \neq (Raw) Data



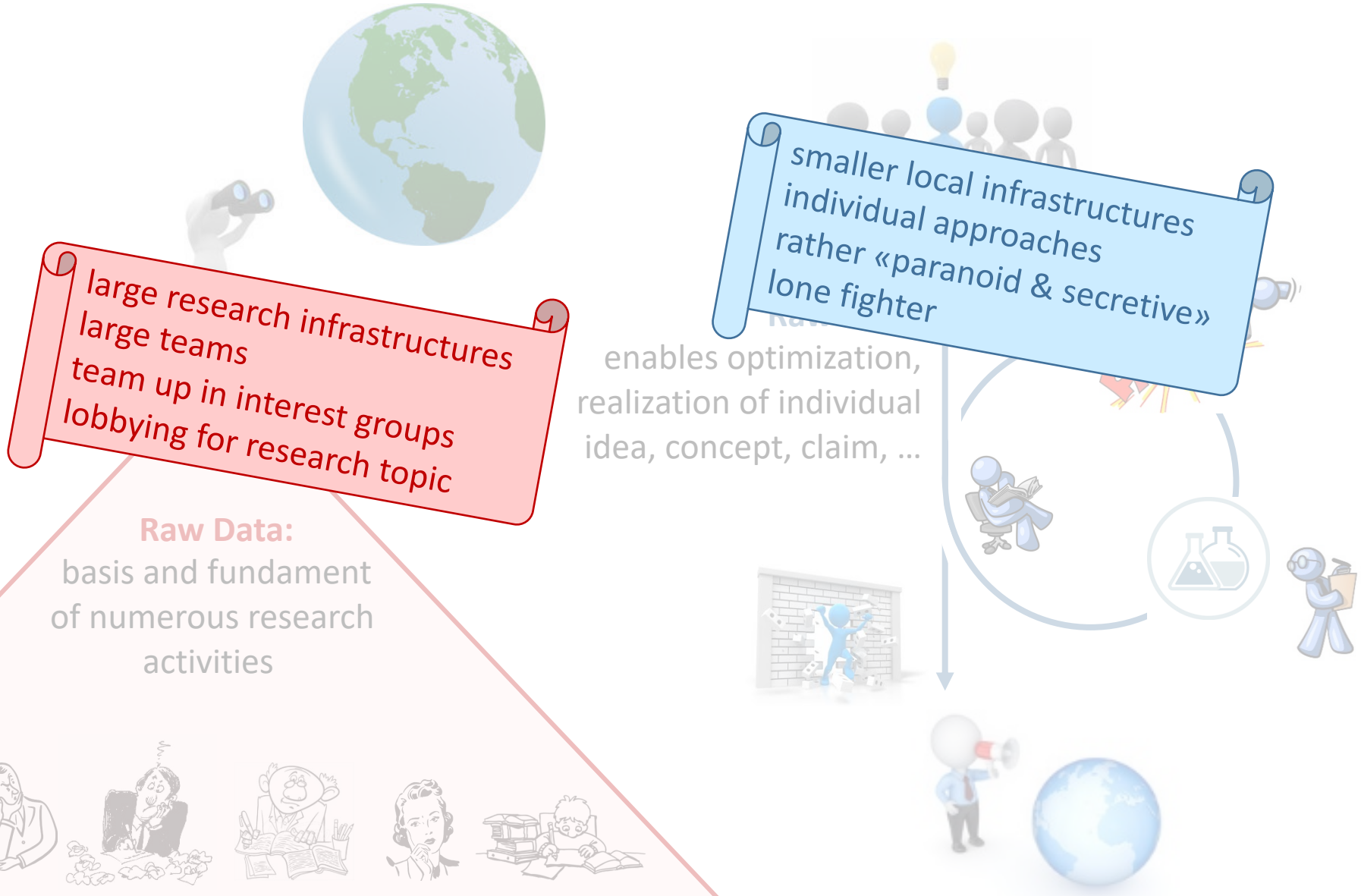
Raw Data:
basis and fundament
of numerous research
activities



Raw Data:
enables optimization,
realization of individual
idea, concept, claim, ...



(Raw) Data \neq (Raw) Data



Reality in a Chemistry Lab



Idea:

searching for:

- generous funding
- talented coworkers
- suitable collaborations



Experimental Investigation:

- compromise between ease of access & chance of success
- usually numerous failures before success
- creating loads of (never published) data paving the way to the (finally published) successful approach



Breakthrough & Success:

- protect IP by patenting
- publish in (specialized) journals
- increasing public awareness by highlights and news letters

Reality in a Chemistry Lab

Idea:

sharing with colleagues and reviewers is scary...
... often delayed proposal to guarantee advantage in international competition

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Experimental Investigation:

- idea & developments are IP of the PI and his institution
- lab journals cannot be public
- hide research target until success
- analytical data are not publishable
- making them publishable would require personnel

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Breakthrough & Success:

1. patents if applied & useful
2. publish as sexy & interesting as possible (with all data leading to success)
3. broad public awareness (balance between scientifically correct & appreciable by a broader public)

Breakthrough & Success:


- protect IP by patenting
- publish in (specialized) journals
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Reality in a Chemistry Lab



Idea:

chiral molecular
«geländer-type»
structures:
supported by 



Experimental Investigation:

- 2 PhD students (Michael Rickhaus & Rajesh Mannancherry)
- 6 years synthesis (sweat, tears, failures, frustrations, findings, successes...)
- ≈ 360'000 CHF (320 lab journal pages)
- ≈ 2'400 FIDs (NMR spectra)



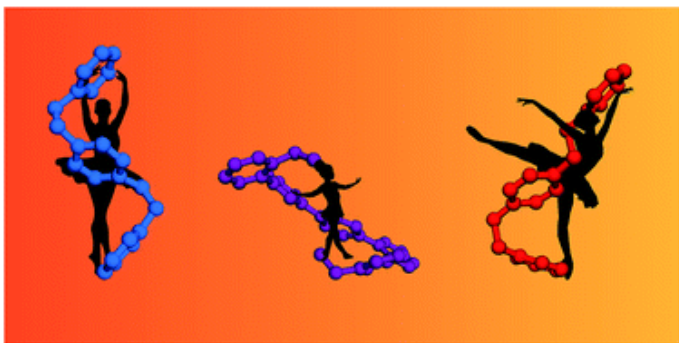
Breakthrough & Success:

- 6 publications, from which 4 in high impact journals
- 4 highlights and news letters

Reality in a Chemistry Lab

112 pages supporting information

as example the last publication:
«Molecular dynamic staircases:
all-carbon axial chiral “Geländer”
structures», R. Mannancherry, M.
Rickhaus, D. Häußinger, A.
Prescimone, M. Mayor,
Chem. Sci., **2018**, *9*, 5758-5766



8 pages publication

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Breakthrough & Success:

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- 4 highlights and news letters

Summary

very different situations between disciplines and research directions

no general applicable regulation possible

from a synthetic chemistry view point:

no raw data public available!

neither conceptual ideas nor intermediate results shared in public

achievements & findings are IP of the PI

complete data only public available after publication

Summary

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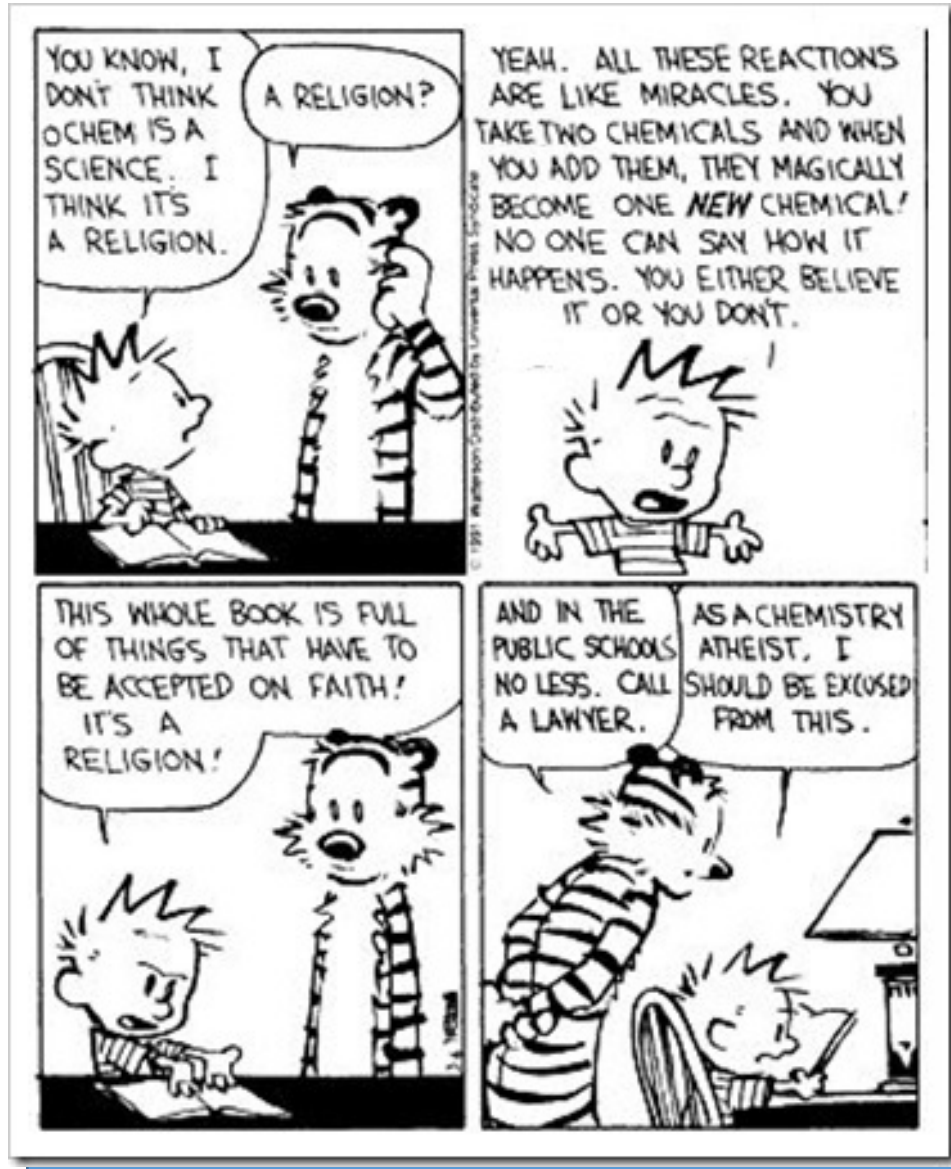
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Content of my DMP
submitted:
1.10.2017
accepted by SNF:
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Summary



en disciplines and

on possible

view point:

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inter

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