chem-bla-ics

# Reusing data: two new papers

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My research is about the interaction of (machine) representation and the impact on the success of data analysis (matchine learning, chemometrics, AI, etc). See the posts about molecular chemometrics. This got me into FAIR: making data interoperable and being able to (really) reuse data is the starting point of doing research.

So, when I get the chance to see something where I worked on to make more FAIR actually being used, I love to push the boundaries of FAIR a bit extra. The study of representation of molecules and molecular systems is not quite a popular science, but I find it important. Two new papers got recently published to which I contributed from this perspective.

The first paper by Anna Niarakis *et al.* is about using the SARS-CoV-2/COVID-19 knowledge base we have collected of the past 4 years (doi:10.3389/fimmu.2023.1282859). For me, this started with a WikiPathways with early knowledge about the virus proteins. I think in this and earlier papers, we improved our open science and bioinformatics and are actually more ready for a next pandemic, which inevitably will come.

The second paper by Alfaro Serrano *et al.* is about how access to data remains key to many things, and this, obviously, includes the Sustainable Development Goals (SDGs) (doi:10.1039/D3SU00148B). When it comes down to the face/off of FAIR versus Open, I think Open has more impact, hands-down.

About the latter, I recently wrote up ten simple actions you can take to make your nanosafety research output more FAIR (doi:10.5281/zenodo.10533126).