chem-bla-ics

American Chemical Society Fall 2023 meeting

Published September 9, 2023

Citation

Willighagen, E. (2023, September 9). American Chemical Society Fall 2023 meeting. *Chem-bla-ics*. https://doi.org/10.59350/zqtdm-66432

Keywords

Acs, Scholia, Wikidata, Acsfall2023, Conference

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About four weeks ago the Fall 2023 American Chemical Society meeting (#ACSFall2023). I have attended a few ACS meetings in person and even organized a symposium at the 2010 ACS meeting in Boston. This time too, I did not participate in person, tho visiting San Francisco again would have been nice. I gave two presentations (slides doi:10.5281/zenodo.8255394), but have not uploaded my slides of the first presentation to Zenodo yet.

The theme of the meeting was data, and this resulted in a wealth of presentations with cheminformatics. What is striking here is that a lot of work has not changed so much in 20 years, except for the scale. What I missed here was the large open data sets, but generally the level of open science was heartwarming! So many preprints mentions, GitHub repositories, and Zenodo deposits. The Blue Obelisk was truly ahead of its time, but it is a delight to see the field of chemistry catch up. I can now say a lot of about peer review, and why the field is not benefitting from all the experience that exists in the field because people publish in the wrong journals, but that is for another time.

I attended multiple sessions, which is a bit of a challenge, doing this remotely from Central European Summer Time (CEST). Of course, the Sunday started with the Chemical informatics (R)evolution: Towards Democratization and Open Science session, where I had my first talk, and later that day the Enhance your Data - Smart Ways to Metadata and Knowledge Graphs session, where I gave a second talk, about Bioschemas' `ChemicalSubstance` and `MolecularEntity`. Sadly, I had to leave that meeting early because it was getting too late.

There were so many interesting sessions, I could not attend everything. I also have to go back to all my notes and isolate things I want to follow up on, prominently open datasets.

More later.