

cdk2024 #4: Chemistry Development Kit User Group Meeting - Day 1

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Abstract

As part of our Dutch Research Council (NWO) Open Science grant, we organized a Chemistry Development Kit User Group Meeting (#CDK25UGM), of which yesterday was the “conference” day, and today a hackathon.

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chem-bla-ics

As part of our [Dutch Research Council \(NWO\) Open Science grant](#), we organized a [Chemistry Development Kit User Group Meeting \(#CDK25UGM\)](#), of which yesterday was the “conference” day, and today a hackathon.

I opened the session with a few slides welcoming everyone at Maastricht University (and our [Dept of Translational Genomics](#), and explaining the NWO grant. [John Mayfield \(NextMove\)](#) spoke about “What’s New” in the Chemistry Development Kit 2.10, e.g. explaining more about the new (much faster) [AtomContainer](#), SMIRKS, and more.

After lunch, [Jonas Schaub \(Friedrich Schiller University Jena\)](#) showed various projects where the CDK is used, titled “Scaffolds, Functional Groups, Aglycones: Algorithmic Substructure Identification with CDK” (see doi:[10.1186/s13321-023-00762-4](#), doi:[10.1186/s13321-022-00656-x](#), and doi:[10.1186/s13321-020-00467-y](#)). [Lyudvika Radeva \(Ideacon Ltd, University of Plovdiv\)](#) showed what SYBYL Line Notation (SLN) is and how this is implemented in [Ambit](#) (see doi:[10.1002/minf.202100027](#)). [Sonja Herres-Pawlis \(RWTH Aachen University\)](#) updated us with “News from the InChI: making the InChI FAIR and including inorganics”, e.g. showing how they worked out how the InChI is going to handle organometallics, where the bonds and the stereochemistry as aspects that were not handled by the current InChI.

After the afternoon coffee break, [Zhixu Ni \(TU Dresden\)](#) showed his work on lipid maps characterization and identification. We previously met a few times at [EpiLipidNET COST action](#) meetings, and it was great to see his continued research on representation of lipids and lipid classes in his hit “A Fuzzy Solution for Lipid Structures Using CXSMILES”.

Finally, [Matthias Mailänder \(Lablicate GmbH\)](#) gave a “Live demo of where [OpenChrom](#) uses the CDK”, and [Yajie Ding \(University of Groningen\)](#) told her about her glycoscience research. There, cheminformatics can also greatly help and the CDK may provide them with solutions.

This really doesn’t do justice to all the discussions, examples, use cases, etc. But it gives you an idea. We had 11 people in the room, and were joined online by an additional 6 people.