

Artificial Intelligence for Natural Product Drug Discovery

27 September -1 October 2021, Lorentz Center @Oort / Hybrid

Scientific

Short description of the aims for the virtual meeting

The main aims of the workshop included:

- 1) *Exchange of ideas and improved communication between the fields of omics-based natural product discovery and computational drug design*
- 2) *Discuss advances in machine learning methodologies and how they could be applied to the connect and integrate approaches from the two fields to achieve new synergies.*

Short summary of key moments (key debates, breakthroughs, etc.)

The breakout sessions were a highlight of this workshop as they enabled targeted group discussions and resulted in more active interactions between on-site and online workshop participants. Several key breakthroughs came from brainstorming sessions. One memorable brainstorming session tackled the bottleneck of 'lack of high-quality training data' by identifying key incentives or so-called 'carrots' to promote database contributions from the scientific community to amass quantities of training data necessary for AI methods. Other specific discussion points included methods of chemical featurization, algorithmic design, data and metadata standardization, biological activity prediction, and how to connect heterogeneous types of data (including omics data and 3D structural data) to predict natural product functions and mechanisms of action.

Outcome(s)

The final day of the workshop included a 24-hour writing marathon with continuous work on a group manuscript through the combined effort of participants around the world. This was absolutely a highlight! In a very limited amount of time, a full draft with >10,000 words was written jointly by dozens of scientists around the globe. Another outcome was the interface between two disciplines resulting in knowledge transfer. There was a significant educational outcome from this workshop since participants learned from each other about new topics outside their own research fields.

Organization

Preparation

The organizing committee included five researchers (Medema, Robinson, Linington, van Westen, Hirsch) under the leadership of Prof. Medema. In total the organizing committee met virtually ~20 times over a period of 8 months prior to the conference. In addition email and Google Documents were used extensively to develop the provisional program, identify delegates to invite to the workshop, and assign moderators and session chairs.

One challenge faced by the organizing committee was that, even with considerable effort from the organizing team, it was difficult to create a delegate list that had perfectly equal representation of both genders. In several cases, invited speakers could not attend but nominated other lab members of the opposite gender. This created some complications given the small number of participants. The hybrid format was helpful with this issue, because it provided some flexibility to increase participant numbers, and to offer opportunities to a broad diversity of participants.

Duration of the workshop and time management

The workshop lasted from Monday until Friday (27 Sept - 1 Oct). The schedule was split between time for small group discussions and short talks followed by ample time for questions and plenary discussions.

Platform(s) used before and during the workshop

During the workshop, we mainly used MS Teams to facilitate the hybrid presentations and discussions. We also used Google Forms, Docs, and Spreadsheets for the purpose of organizing the 'speed dating' and the 'writing marathon schedule.' For the follow-up, we used Google docs to organize the writing marathon (see next section).

Short- and long-term plans for follow-up

As mentioned above, workshop participants from around the world contributed to a collaborative manuscript targeted for submission to Nature Reviews Drug Discovery. After several rounds of editing by workshop participants following the workshop, we as organizers are now compiling the different sections of the manuscript for submission to a scientific journal in December.

In the long-term, we have built a strong network of researchers bridging the scientific disciplines of natural products and drug discovery which we anticipate will result in multiple collaborations. We look forward to further strengthening these connections at future meetups and workshops as well as through publications.

Lessons learned for future virtual events

The hybrid format worked remarkably well apart from a few technological glitches. One major takeaway from this event was that the schedule was a bit too tightly packed and it would have been wise to build in more time for coffee breaks and unstructured social interactions (as Anna of the Lorentz Center had wisely advised us).

With only one laptop and camera, we also had to pay close attention to where the camera was pointing during the discussion sections to make sure that the online participants were fully involved in the process. Having a split screen or a second camera to allow simultaneous views of the presenter and the audience would have been useful.

Lorentz Center (virtual) Support

Comments/points for improvement for the Lorentz Center team.

We would recommend always connecting the workshop laptop on-site with an ethernet cable as the WiFi can be unreliable.

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Roger Linington (Vancouver, Canada)

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