

# ICCS2025: back in Noordwijkerhout

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## Keywords

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## chem-bla-ics

This week the 13th [International Conference on Chemical Structures](#) took place (see also [this Scholia overview](#) or [this overview of the full ICCS history](#)). This is the conference I first [joined 20 years ago](#) as a PhD student [presenting a poster](#) (see [these past blog posts](#)). Of course, I am actually co-organizer nowadays (actually, co-treasurer). Organizing a meeting with just over 200 participants, and I like to thank [Gerard](#) and [Willem](#) in particular, but also [Pieter](#), [Marcus](#), [Frank](#), [Jenke](#), and Frans Koeman who has helped us during the past three events.

The meeting started, as usual, with the [CSA Trust Mike Lynch Award](#), this year awarded to Prof. [Val Gillet](#) (see also [this press release](#)).








[This time](#), there were the following themes, where the first was by far the most dominant theme:

- Artificial Intelligence, Machine Learning, and QSAR (five sessions)
- New Modalities and Large Chemical Data Sets (one session)
- Advanced Cheminformatics Techniques (two sessions)
- Integrative Structure-Based Drug Design (two sessions)

My contribution this time was a poster for the [VHP4Safety](#) project, but more about that later.

Like last time, I have been annotating speakers with identifier and accounts, if they provided those:

## Wednesday, June 4, 2025

8:30 – 10:00	<b>Advanced Cheminformatics Techniques 1</b> Chair: Egon Willighagen    , Maastricht University	Rotonde
8:30 – 9:00	<b>Transformers for molecular property prediction: Domain adaptation efficiently improves performance</b> Afnan Sultan  , Saarland University	
9:00 – 9:30	<b>Navigating Synthon Space: Property-Driven Molecular Optimization for Pharmacokinetics</b> Rafał Adam Bachorz, Simulations Plus	
9:30 – 10:00	<b>Scaffold Hopping with Generative Reinforcement Learning</b> Luke Rossen  , Eindhoven University of Technology	
10:00 – 10:30	BREAK	Atrium
10:30 – 12:30	<b>Advanced Cheminformatics Techniques 2</b> Chair: Greg Landrum	Rotonde
10:30 – 11:00	<b>Honey, I shrunk the database: Making multi-billion compound libraries as small as possible</b>  John Wilkinson Mayfield  , NextMove Software	
11:00	<b>Docking-based geometric graph models for kinase-ligand affinity</b>	

## chem-bla-ics

As you can see, it also includes PDFs, for both [talks](#) and [posters](#). At the time of writing, I collected PDFs of two presentations and five posters. Additions are still most welcome, ideally with DOI, so that they can be cited (doi:[10.5281/zenodo.15494630](https://doi.org/10.5281/zenodo.15494630), doi:[10.13140/RG.2.2.27441.90720](https://doi.org/10.13140/RG.2.2.27441.90720) doi:[10.5281/zenodo.15614295](https://doi.org/10.5281/zenodo.15614295), and doi:[10.13140/RG.2.2.36774.23365](https://doi.org/10.13140/RG.2.2.36774.23365))!

Finally, I like to remind everyone that there is again a [proceedings collection in the Journal of Cheminformatics](#), and presenters of oral and poster presentations are invited to submit their presented work to this collection.