ICCS2025: back in Noordwijkerhout

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Abstract
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

chem-bla-ics

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

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

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, doi:10.13140/RG.2.2.27441.90720 doi:10.5281/zenodo.15614295, and doi: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.