Lorentz Workshop 'Artificial Intelligence for Natural Product Drug Discovery' - Pre-final Programme

Monday	13:00-13:30	**Session 1: introduction to the workshop** *Workshop Organizers, Gilles van Wezel (IBL), Lorentz Center Team*
	13:30-14:15	**Tutorial lecture: omics-based natural product discovery** *Serina Robinson, Justin van der Hooft & Marnix Medema*
	14:15-15:00	**Tutorial lecture: computational drug design** *Gerard van Westen & Willem Jespers*
	15:00-15:30	**Online speed networking** 5 x 5 minutes (based on preferences supplied via Google Form)
	15:30-16:00	**Coffee break (on-site and on *Wonder*)**
	16:00-17:45	**Lecture session 2a: Advances in AI technology** *Chair: Gerard van Westen* 16:00-16:30 Daniel Reker, Duke University (online) *Machine Learning and Natural Products for Drug Delivery* 16:30-17:00 Francesca Grisoni, Eindhoven University of Technology *Chemical language models for de novo drug design* 17:00-17:30 Phillippe Schwaller, IBM Research (online) *Title TBD* 17:30-17:45 Alan Aspuru-Guzik, University of Toronto (online) *Self-driving labs for automated chemical synthesis*
	17:45-18:30	Welcome reception
Tuesday	09:00-10:30	**Lecture session 2b: advances in AI technology** *Chair: Gerard van Westen* 09:00-09:15 Hyun Uk Kim, Korea Advanced Institute of Science & Technology (online) *Genome-scale metabolic modeling and machine learning for drug discovery and development* 09:15-09:30 Marwin Segler, Microsoft Research (online) *Title TBD* 09:30-09:45 Janani Durairaj, University of Basel *Fast and interpretable representations of protein and compound structures* 09:45-10:00 break 10:00-10:15 Djork Arne Clevert, Bayer (online) *Representation learning for latent space chemistry* 10:15-10:30 Raphael Reher, Martin-Luther-University Halle-Wittenberg *Natural Product Discovery in the Age of AI*
	10:30-12:30	**Break-out groups part I (on-site only)** BG01: Chemical featurization technologies *Chairs: Egon Willighagen & David Meijer* BG02: Opportunities from new AI algorithms & models

		Chairs: Connor Coley (online) & Barbara Terlouw BG03: Deep learning: hype or hope? *Chairs: Andrea Volkamer (online) & Janani Durairaj* BG04: Visualizing and navigating chemical space *Chairs: Willem Jespers & Francesca Grisoni* *Online participants provide textual feedback online.*
	12:30-14:00	Lunch / interaction time
	14:00-15:30	**Break-out groups part II (continued, hybrid)** - BG01: Chemical featurization technologies - BG02: Opportunities from new AI algorithms & models - BG03: Deep learning: hype or hope? - BG04: Visualizing and navigating chemical space
	15:30-16:00	**Recapitulation session 2 (jr chairs)** ● bullet points on ResearchDrive
	16:00-17:45	**Lecture session 3: data and metadata standardization** *Chair: Roger Linington* 16:00-16:30 Michael Skinnider, University of British Columbia (online) *Predicting biological activities of genomically encoded natural products: a case study in data standardization* 16:30-17:00 Nadja Cech, University of North Carolina at Greensboro (online) *Optimizing dataset quality for untargeted mass spectrometry metabolomics of natural products* 17:00-17:30 Roger Linington, Simon Fraser University (online) *The dissemination fallacy: addressing the incompatibility between traditional publishing and modern data science*
Wednesday	09:00-10:30	**Lecture session 3 (continued)** *Chair: Marnix Medema* 09:00-09:15 Maria Sorokina, Friedrich Schiller University Jena *Collecting and standardizing natural products: The COCONUT project* 09:15-09:30 Kai Blin, Technical University of Denmark *Robust natural product databases* 09:30-09:45 Katherine Duncan, Strathclyde University *Practical applications of genomic and metabolomic data integration for microbial natural product discovery* 09:45-10:00 break 10:00-10:15 Justin van der Hooft, Wageningen University *FAIRification leads to PAIRification in omics studies* 10:15-10:30 Egon Willighagen, Maastricht University *Interoperability starts with resources, identifiers, and linking*
	10:30-12:30	**Break-out groups part I (on-site only)** BG05: Standards and ontologies for biological activities *Chairs: Joleen Masschelein & Allison Walker*

		BG06: Database interoperability *Chairs: Kai Blin & Maria Sorokina* BG07: Data sharing: incentives & enabling technologies *Chairs: Justin van der Hooft & Doris van Bergeijk* BG08: Creating and leveraging 'gold-standard' data sets *Chairs: Rebecca Goss & Tristan de Rond* *Online participants provide textual feedback online.*
	12:30-14:00	Lunch / interaction time
	14:00-15:30	**Break-out groups part II (continued, hybrid)** - BG05: Standards and ontologies for biological activities - BG06: Database interoperability - BG07: Data sharing: incentives & enabling technologies - BG08: Creating and leveraging 'gold-standard' data sets
	15:30-16:00	**Recapitulation session 3 (jr chairs)** ● bullet points on ResearchDrive
	16:00-17:30	**Lecture session 4: predicting biological activities and mechanisms of action** *Chair: Serina Robinson* 16:00-16:30 Anna K. H. Hirsch, Helmholtz Institute for Pharmaceutical Sciences (online) *Virtual screening affords bioactive hit compounds for target-based anti-infective drug discovery* 16:30-17:00 Andrea Volkamer, Charité University Hospital (online) *In silico tools to support risk assessment of small molecules* 17:00-17:30 Maureen Hillenmeyer, Hexagon Bio (online) *Discovering novel oncology and anti-infective medicines from genomic data*
	18:30-23:00	Workshop dinner & social event (Koetshuis 'De Burcht')
Thursday	09:00-10:30	**Lecture session 4 (continued)** *Chair: Anna Hirsch* 09:00-09:15 Allison Walker, Vanderbilt University (online) *A machine learning bioinformatics tool for predicting natural product bioactivity* 09:15-09:30 Albert Hofstetter, ETH Zürich *Machine learning and molecular dynamics simulations* 09:30-09:45 Olga Kalinina, Helmholtz Institute for Pharmaceutical Research (online) *Graph neural networks for predicting drug-target interactions* 09:45-10:00 break 10:00-10:15 Nadine Ziemert, Eberhard Karls University Tübingen (online) *Using AI to predict antibiotic-producing strains based on primary metabolism* 10:15-10:30 Doris van Bergeijk, Leiden University *Who, where, which and why? Using ecology and genomics to unlock the Streptomyces treasure trove*
	10:30-12:30	**Break-out groups part I (on-site only)** BG09: Integration of heterogeneous data (genome, metabolome, structure, docking, biological screening)

		Chairs: Neha Garg & Katherine Duncan BG10: Algorithmic innovations for activity prediction: connecting top-down to bottom-up approaches *Chairs: Satria Kautsar & Raphael Reher* BG11: Community benchmarks for prediction algorithms *Chairs: Albert Hofstetter & Marina Gorostiola Gonzalez* BG12: Predicting biological activities from sequence data *Chairs: Chris Dejong & Friederike Biermann* *Online participants provide textual feedback online.*
	12:30-14:00	Lunch / interaction time
	14:00-15:30	**Break-out groups part II (continued, hybrid)** - BG09: Integration of heterogeneous data (genome, metabolome, structure, docking, biological screening) - BG10: Algorithmic innovations for activity prediction: connecting top-down to bottom-up approaches - BG11: Community benchmarks for prediction algorithms - BG12: Predicting biological activities from sequence data
	15:30-16:00	**Recapitulation session 4 (jr chairs)** ● bullet points on ResearchDrive
	16:00	**Start of 24h writing marathon** - Scientific position paper - Educational materials
Friday	09:00-11:30	**Parallel writing / drafting sessions** - Scientific position paper - Educational materials In the meantime: - Opportunities to discuss collaborations
	11:30-12:00	**Recapitulation and post-workshop planning**
	12:00-13:00	Lunch
	13:00-13:45	**Final Keynote Lecture** 13:00-13:45 Jim Collins, Massachusetts Institute of Technology (online) *Harnessing deep learning for antibiotic discovery and synthetic biology*
	13:45-14:00	**Closing, presenting current writing state**
	16:00	**End of 24h writing marathon**