Lorentz workshop: AI-driven Nanoparticle Design for Drug Delivery

Day 1 (Feb 2nd) – Foundations and Framing (11:00–18:30)

- 11:00 – 11:30: Registration
- 11:30 – 12:00: Welcome and Icebreaker activity
- 12:00 – 13:00: Lunch
- 13:00 – 13:15: Overview of the workshop structure
- 13:15 – 14:00: **Prof. Willem Mulder (TU/e, NL)**
  Nanomedicine-based immunotherapy – How can AI facilitate clinical translation?
- 14:00 – 14:45: **Dr. Lotte Krabbenborg (Radboud University, NL)**
  Resistance or Warm Welcome: The societal adoption of new technologies in society
- 14:45 – 15:05: Coffee break
- 15:05 – 15:50: **Dr. Michal Ozery-Flato (IBM, Israel)**
  Accelerating Drug Design and Delivery with AI Foundation Models
- 15:50– 16:00: Group assignment
- 16:00-17:00: Discussion of Topic 1
- 17:00 – 18:30: Lorentz Center Welcome Reception

Day 2 (Feb 3rd) – Challenges & Opportunities (09:30–20:00)

- 09:30 – 11:00: **Yosi Shamay (Technion, Israel)**
  AI for Drug Delivery: Principles, Limitations, and Infinite Possibilities
- 11:00 – 11:15: Coffee Break
- 11:15 – 12:00: **Prof. Avi Schroeder (Technion, Israel)**
  Designing brain-targeted drug delivery systems for treating Parkinson's Disease
- 12:00-13:00: lunch
- 13:00 – 13:45: **Prof. Daniel Heller (Memorial Sloan Kettering Cancer Center, USA)**
  Quantitative Structure-Nanoparticle Assembly Prediction for Nanomedicine Development
- 13:45 – 14:00: Coffee break
- 14:00 – 14:45: **Prof. Christine Allen (U Toronto, Canada)**
- 14:45 – 15:30: Team discussion
- 15:30 – 16:00: Plenary synthesis – Prepare team presentations for Day 3
- 16:00 – 16:15: Coffee break
- 16:15 – 17:00: Research pitch (1 min max/ workshop participants)
- 18:00 – 20:00: Workshop Dinner

Day 3 (Feb 4th) – AI in Practice (09:30–17:00)

- 09:30 – 10:30: Group presentations (5 min presentation + 5 min Q&A, 6 groups total)
- 10:30-11:15: Poster session I
- 11:15-12:00: **Prof. Gerard van Westen (Leiden University, NL)**
  AlphaFold Meets De Novo Drug Design - Structural Protein Information in Multitarget Molecular Generative Models
- 12:00 – 13:30: Lunch

- 13:30 – 14:15: **Dr. Selma Pereira Lopes (Johnson & Johnson, NL)**
  AI in Pharma: Opportunities, Challenges, and Learnings in Drug Development
- 14:15 – 14:45: Coffee break
- 14:45 – 15:45: *AI 101 – terminology & hands-on demonstrations (non-AI experts) [**led by Adam Gromley- via Zoom**]*
  in parallel
  How to bridge the gap between AI experts and the outside world (AI experts)
- 15:45 – 16:15: Feedback on AI expert discussion with the non-AI experts (AI experts present their discussion summary and open to discussion with the whole audience)
- 16:15-17:00: Poster Session II (optional)

Day 4 (Feb 5th) – Co-design (09:30–16:45)

Morning Focus: Co-creating solutions with AI

- 10:00 – 11:00: Team discussion: Topic 2
- 11:00 – 11:15: Coffee break
- 11:15 – 12:00: Team discussion: Topic 2
- 12:00 – 13:00 : lunch
- 13:00 – 13:45: Keynote –**Prof. Willie Peijnenburg (RIVM & Leiden University, NL)**
  Shaping the future of AI-enabled nanoparticle design: reflections and priorities from an environmental regulatory scientist
- 13:45 – 14:00: Coffee break
- 14:00 – 14:45: **Dr. Philip Nickel (TU/e, NL)**
  Ethics via Trust: Reflections on AI Models in the Social Context of Drug Delivery Research
- 14:45 – 15:00: Coffee break
- 15:00 – 15:45: Panel discussion: AI and ethics in nanomedicine
  - **Dr. Philip Nickel**
  - **Prof. Willie Peijnenburg**
- 15:45 – 16:45: Group breakout discussion (prepare for presentation on Topic 2)

Day 5 (Feb 6th) – Roadmapping and Next Steps (09:30–12:00)

- 09:30 – 10:30: Group presentations (5 min presentation + 5 min Q&A, 6 groups total)
- 10:30 – 10:45: Coffee break
- 10:45 – 11:30: Brainstorm on the key points of our message to the outer world
- 11:30-12:00: Planning proposals & post-workshop collaboration
- Final remarks, commitments, and goodbye