#### **Workshop Title:**

The first international workshop on AI for Pharmaceutical Discovery and Development (AIP-D2 2023)

#### Organizers:

#### Chair:

- Rui Zhang, PhD (contact), Division Chief and Associate Professor, University of Minnesota, Minneapolis, MN, US. <a href="mailto:realizable-re
- Fei Wang, PhD, Associate Professor, Weill Cornell University. NYC, NY, USA. few2001@med.cornell.edu
- Chang Su, PhD, Assistant Professor, Temple University, Philadelphia, PA, USA. <a href="mailto:su.chang@temple.edu">su.chang@temple.edu</a>
- You Chen, PhD, Assistant Professor, Vanderbilt University, Nashville, TN, USA, you.chen@vumc.org

#### **Workshop Description:**

Given the high attrition rates, substantial costs and slow pace of new drug discovery and development, repurposing of 'old' drugs to treat both common and rare diseases is increasingly becoming an attractive proposition because it involves the use of de-risked compounds, with potentially lower overall development costs and shorter development timelines. Various data-driven and experimental approaches have been suggested for the identification of repurposable drug candidates; however, there are also major technological and regulatory challenges that need to be addressed.

As another important aspect of pharmaceutical research, drug-drug interactions (DDI) occur when the presence of another drug modifies the effect of one drug. DDIs are broadly classified into pharmacodynamic (PD: effect vs. time) and pharmacokinetic (PK: concentration vs. time). The investigation of DDIs, focusing on PK, PD, and their relationships, can support the discovery and development of new drugs in the pharmaceutical industry. Developing advanced data mining, machine learning, and natural language processing methods and applying them to Spontaneous reports (e.g., FAERS), electronic health records, and the literature can generate and prioritize DDI hypotheses, which can support large pragmatic randomized trials to confirm actual DDIs.

The goal of this workshop is to provide a unique platform to bring together researchers and practitioners in healthcare informatics working with drug discovery and development, and facilitate close interaction among students, scholars, and industry professionals on drug repurposing challenges worldwide. This will be a half-day workshop that consists of invited speakers, podium talks, and poster presentations.

We will invite papers and short abstracts on novel Al approaches, works in progress, comparative analyses of tools, and original state-of-the-art work in Al methods for drug repurposing and DDIs. Selected papers will be presented as podium talks, and other interesting submissions and abstracts will be showcased as poster presentations.

#### Audience:

Target audience includes both health AI researchers, basic and translational researchers, and pharma industry. Anyone interested in AI-based drug repurposing and DDI approaches is welcome. Researchers and students working on health AI projects and others interested in learning about and sharing drug repurposing and DDI resources are strongly encouraged to attend. The anticipated number of attendees is around 30-50.

### Publicity:

To attract attendees, we will advertise the workshop widely, including: (1) sending emails using community mailing lists such as AMIA Working Group mailing list; (2) creating a dedicated web site for the workshop, (3) contacting individuals through personal connections of organizers and committee members, (4) leveraging social media such as LinkedIn and Twitter, and (5) contacting training programs in computer science, information science, and biomedical informatics to attract additional students and trainees.

#### **Workshop Structure**:

This will be a half-day workshop (3 hours). We will allocate about 30 minutes for an invited keynote presentation, 2 hours of podium talks of accepted papers and poster presentation, and 30 mins for panel discussion and open Q&A session.

## Reviewing:

We will accept both full paper and poster submissions of original research in health NLP. All submissions will be submitted and handled through EasyChair. A program committee (PC) will be formed consisting of members from the steering committee and other researchers with relevant experience. All submitted papers will undergo a peer review process conducted by at least 2 reviewers from the PC. All accepted submissions will be presented at the workshop and published in the IEEE ICHI 2023 Proceedings (including being archived in IEEE Xplore Digital Library). We also propose to invite selected papers to publish an extended version of their work in a special issue. (We will start negotiating with the journal after proposal acceptance).

#### Call for Papers:

Tentative call

# The First international Workshop on Al for Drug Repurposing (AIDR 2023) at ICHI

# **Call for Participation**

Al for drug repurposing have received significant attention in the medical domain and have demonstrated numerous successful uses in healthcare applications. The 2023 AIDR workshop will provide a unique platform for close interactions among students, scholars, and industry professionals who are interested in drug repurposing using innovative AI methods. We are calling for papers and abstracts about original research and works in progress in methods, tools, and applications.

#### **Topics of interest**

- Real-world evidence based computational drug repurposing
- Drug repurposing based on network medicine and knowledge graph
- Molecular structure generation
- Integrative modeling of multi-modal biomedical data for drug repurposing
- Drug interaction and drug combination therapy prediction.

#### Schedule-at-a-Glance

- **Keynote**, 0.5 hour
- Paper/poster presentation, 2 hours
- Panel discussion, 0.5 hour

#### **Submission and Review**

Anyone who is interested in drug repurposing is invited to submit his or her work to the AIDR 2023. We accept both full paper submissions (8 pages) and poster submissions (2 pages). All papers will be submitted and handled through EasyChair at URL, with peer review by domain experts.

#### More information

• For more information, please visit URL.

#### **Important Dates**

- Deadline for all submissions: March 1st, 2023
- Notification of decisions: March 21st, 2023
- Notification of workshop paper acceptance: March 21st, 2023
- Camera ready workshop papers due: March 30th, 2023
- Workshop date: June 10th, 2023