

# **International**



Innovation in Knowledge Based and Intelligent Engineering Systems

#### INVITED SESSION SUMMARY

#### Title of Session:

Graph Generation: Theory and Applications

## Name, Title and Affiliation of Chair:

- Prof. Monica Bianchini Professor University of Siena, Department of Information Engineering and Mathematics
- Pietro Bongini, Ph.D. PostDoc Researcher University of Siena, Department of Information Engineering and Mathematics
- Niccolò Pancino, Ph.D. PostDoc Researcher University of Siena, Department of Information Engineering and Mathematics
- Caterina Graziani Ph.D. Candidate University of Siena, Department of Information Engineering and Mathematics
- Veronica Lachi Ph.D. Candidate University of Siena, Department of Information Engineering and Mathematics
- Elia G. Ceroni Ph.D. Student University of Siena, Department of Information Engineering and Mathematics

# Details of Session (including aim and scope):

Graph generation has gained increasing momentum and is leading to outstanding solutions in many applicative fields, particularly in the biomedical ambit. Graph generators can create graph structures for a wide variety of applications. In particular, molecular graph generation is fundamental to explore the space of possible molecules and to create possible new candidate drug structures. Our session intends to give space to theoretical works that analyze and explain the algorithms and models that are making this advancement possible, as well as the applicative works and the outstanding results that are being achieved. Space will be given to the most promising theories and techniques, from sequential methods to variational autoencoders, with a particular focus on methods based on artificial neural networks. Moreover, conditional and hierarchical graph generation will be highlighted as the two main directions currently under analysis by the research community.

# Main Contributing Researchers / Research Centres (tentative, if known at this stage):

University of Siena – Department of Information Engineering and Mathematics – Siena, IT University of Pisa – Department of Informatics – Pisa, IT University of Cambridge – Computer Laboratory – Cambridge, UK

Third sity of Cambridge – Computer Laboratory – Cambridge, ON

Toscana Life Sciences Foundation - Siena, IT

# Website URL of Call for Papers (if any):

## **Email & Contact Details:**

- monica.bianchini@unisi.it
- pietro.bongini@unisi.it
- niccolo.pancino@unisi.it
- caterina.graziani@student.unisi.it
- veronica.lachi@student.unisi.it
- elia.ceroni@student.unisi.it