

Berlin, October 17th, 2023

Call for Papers:

## Workshop: The building blocks of (nearly) everything: Using Computational Chemistry to study R&D dynamics

Event Date: February 15th-16th, 2024

Location: ESMT Berlin, Schlossplatz 1, 10178 Berlin, Germany, [www.esmt.org](http://www.esmt.org)

Organizers: Arianna Martinelli (Sant'Anna), Elisa Giuliani (University of Pisa), Stefan Wagner (ESMT Berlin)

### Background:

Chemical compounds, often not found in nature, underpin a range of consumer goods from pharmaceuticals and cosmetics to industrial solvents, fertilizers, and pesticides. Despite their prevalence, knowledge gaps persist in our understanding of the R&D trajectories that give rise to such synthetic compounds, and their subsequent societal and environmental impacts.

This workshop spotlights the innovative application of computational chemistry in dissecting R&D dynamics, particularly emphasizing the use of chemical compound information in the pharma and chemistry domains. The focus is on understanding how computational methods can be synergized with traditional data sources like patents to provide deeper insights into R&D activities.

### Topics of Interest:

- New data sets exploiting information on chemical compounds and their characteristics
- Measuring technical changes across chemical sectors with tools from computational chemistry.
- Assessing regulatory and policy interventions using computational insights.

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- New indicators and methodologies for sustainable chemistry and material sciences.

Submission Guidelines:

Authors are invited to submit either full papers or extended abstracts.

**All submissions should be sent to Stefan Wagner at [stefan.wagner@esmt.org](mailto:stefan.wagner@esmt.org) by November 15th, 2023.**

Participants will be notified about the acceptance of their papers in early December 2023.

Participation without presentation is possible and encouraged for scholars interested in the workshop theme. Please reach out to Stefan Wagner to enquire about the availability of slots.

Travel Grants:

A select number of presenters will be eligible for (partial) travel cost reimbursement upon request. Please indicate whether you are requesting a travel grant in your submission.

Benefits of Participation:

- Engage in cross-disciplinary discussions, bridging computational chemistry, economics, and innovation studies.
- Explore emerging methods that leverage computational chemistry for empirical social sciences.
- Share and receive feedback on the latest research advancements in the field.

Don't miss this unique opportunity to contribute to an evolving interdisciplinary dialogue that has the potential to shape the future of industrial innovation and regulation.

**Join us in February 2024 at ESMT Berlin!**

Arianna, Elisa and Stefan