

# Making Science FAIR

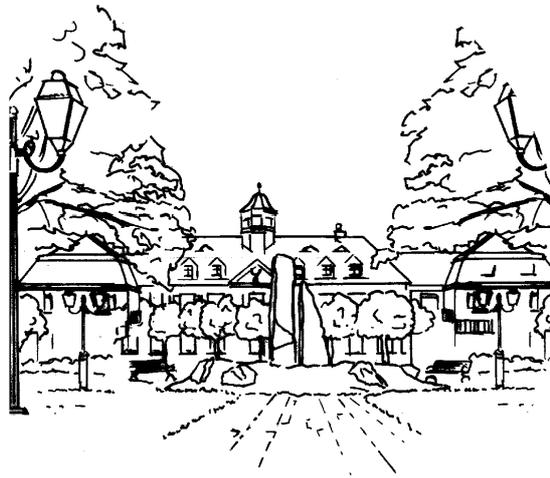


## Beilstein Open Science Symposium 2018

8 - 10 October, 2018  
Hotel Jagdschloss Niederwald  
Rüdesheim, Germany



BEILSTEIN SYMPOSIUM



8 - 10 October, 2018  
Hotel Jagdschloss Niederwald  
Rüdesheim, Germany

## The Beilstein-Institut and Open Science

The non-profit Beilstein-Institut is one of the most respected organizations in the communication and dissemination of high-quality information in chemistry. Since 1951, when the foundation was established by the Max Planck Society, we have been fulfilling our mission to support the scientific community by providing high-quality information that is essential for research.

Our role has evolved over the years: from the production of the Beilstein Handbook and Database, to being one of the first open access journal publishers in chemistry, to host of interdisciplinary symposia and supporter of open data initiatives. We believe that free access to scientific research results, giving everyone in the world an equal chance to read and reuse experimental findings and data, is the best way to advance science.

Open Science is a new approach to scientific research. It is based on cooperation and uses new ways to disseminate information and broaden knowledge through digital technologies and new collaborative tools. It aims to make the primary outputs of publicly funded research results – publications (open access) and the research data (open data) – publicly accessible in digital format with no or minimal restriction.

The Beilstein-Institut supports open science and makes the results of its projects freely available to the scientific community as open access publications. This is an essential contribution to the foundation's mission to advance the chemical and related sciences. All journal articles, conference proceedings and videos are open access to allow the worldwide, unhindered sharing and exchange of ideas. This allows scientists, students, educators and the public the opportunity to inform themselves of the latest developments in research and to build on these ideas to further advance scientific knowledge.

Our two platinum open access journals, the *Beilstein Journal of Organic Chemistry* and the *Beilstein Journal of Nanotechnology*, which we fully fund, have no fees for authors or readers. Both journals are produced and managed by the Beilstein Editorial Office team, who work together with a global scientific network of experts that are responsible for the peer review. In 2015, the Beilstein Journals were awarded the DOAJ Seal which recognizes the exceptionally high level of publishing standards and best practices adhering to these journals.

An essential prerequisite for open science data is reporting guidelines and technical standards that provide the framework for the exchange of data from one laboratory to another without technical and textual barriers.

The Beilstein-Institut runs two data standards projects: STRENDA which is concerned with the reporting of enzymology data and MIRAGE with the reporting of glycomics experimental results. Both of which are now widely accepted and acknowledged by the scientific community.

The direct interaction and the exchange of thoughts and ideas between scientists are supported by a program of regularly hosted symposia. These international meetings are organized by the Beilstein-Institut and cover a variety of topics ranging from organic chemistry and biochemistry to nanotechnology and open science as well as interdisciplinary meetings on contemporary topics.

The Beilstein-Institut has been hosting symposia since 1988. Each meeting is always an interesting event with an open result: the Beilstein-Institut provides the framework and the lively and intense exchange of thoughts and ideas of the participants turn it into a memorable and lasting experience. The number of participants is usually limited to around 50 and the program is designed specifically to allow sufficient time for discussions. In some ways the talks can be seen as providing a catalyst for these discussions which often go on into the night and have led to subsequent cooperation projects. The resulting exchange between researchers is the underlying goal of the meeting and gives the Beilstein Symposium their unique character.

Regularly updated information about our symposia is available at [www.beilstein-symposia.org](http://www.beilstein-symposia.org).

Upcoming symposia in 2018:

**[Beilstein Nanotechnology Symposium 2018](#)**

*Molecular Mechanisms in Tribology*

2 – 4 October 2018, Potsdam, Germany

Scientific Program:

Roland Bennewitz and Astrid de Wijn

**[Beilstein Organic Chemistry Symposium 2018](#)**

*Mechanochemistry: Microscopic and Macroscopic Aspects*

13 – 15 November, 2018, Rüdesheim, Germany

Scientific Program:

José G. Hernández

# Book of Abstracts

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## Overview

A new science eco-system is in the making: Open Science. It will impact the way research is carried out and reported, in particular focussing on improving the way research data is stored and shared. Open Science aims to make research and development more effective by improving the communication of scientific knowledge through free access to research results, by encouraging researchers to share their data, and ensuring that data are complete, comprehensive and transparent.

The lack of a framework for structured and standardized data reporting and the largely outdated infrastructure for reporting and publishing scientific research results means that the ability to validate, verify and reuse data is insufficient to allow data-driven research and development. A good way forward is to adopt the FAIR principles that aim to make data Findable, Accessible, Interoperable and Reusable.

However, achieving these goals requires not only investment in hardware and personnel (data scientists) but also cultural changes for researchers to be more open to sharing results – perhaps prior to publishing as a journal article.

This symposium addresses the interfaces between the laboratory and the new infrastructures currently being set up. In chemistry, biochemistry and neighbouring areas, funding agencies and national and supranational bodies are mandating the sharing and depositing of data. The digitization of chemistry is picking up speed as new technologies are diffusing into the lab allowing devices to be interconnected, data automatically recorded, and experiments to be automated. The impact of open science on science research will be critically reviewed and the development of highly interconnected, collaborative research in data driven laboratories of the future will be discussed.

Enjoy the Symposium!

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## Scientific Committee

**Martin G. Hicks and Carsten Kettner**

Beilstein-Institut, Frankfurt  
mhicks@beilstein-institut.de  
ckettner@beilstein-institut.de

## Registration

All participants must be registered to have access to the conference area.

Participants can ask the organizers for a confirmation of the payment of the conference registration fee.

Insurance of participants against accidents, sickness, cancellation, theft, property damage or loss is not covered. Participants are advised to take out adequate personal insurance (see also „Liability and Insurance“).

Participants are responsible for settling their hotel bills directly with the hotel on departure.

The total price for participants staying at the Hotel Jagdschloss Niederwald is 558 EUR and includes both accommodation for four nights and the conference package that covers lunches, dinners and coffee breaks as well as admits access to the conference room.

**Participants not staying at the Hotel Jagdschloss Niederwald are requested to register with the hotel for booking and paying the conference package, i.e. 291 EUR per person.**

Extras, such as drinks, telephone calls etc. are **not** included in the price.

## Conference Venue

The conference, lunches and dinners will take place at the conference hotel, i.e.:

Hotel Jagdschloss Niederwald  
Jagdschloss Niederwald 1  
65385 Rüdesheim  
Germany

T +49 (0)6722 - 7106 0  
F +49 (0)6722 - 7106 666

[www.niederwald.de](http://www.niederwald.de)  
[jagdschloss@niederwald.de](mailto:jagdschloss@niederwald.de)



The hotel offers wireless internet access free of charge. The hotel accepts MasterCard, Visa and EC-Cash (Maestro-Cards).

## The Symposium

The symposium will be held from 8 to 10 October, 2018, with the 7th and the 10th (after lunch) for travelling.

The setting and the limited number of participants (max. 50 persons) provide a very convivial atmosphere for the ready exchange of thoughts and ideas.

The scientific program will take place over two and a half days and will

start at 9.00 am on Monday, the 8th, and

end around noon (ca. 1.00 pm) on Wednesday, the 10th.

If you wish to extend your stay, please contact the hotel directly.

For the length of the individual talks, please refer to the program. Speakers should allow sufficient time for discussion at the end of their talks (e.g. a 40 min slot includes 30 min talk + 10 min for questions). We will have an LCD projector connected to a Windows PC available.

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## Presentations of Posters

**Poster Exhibition: Monday, 8th October, 17.00, Room “Maximilian”**

### Location of the posters

The Poster exhibition will be placed close to the conference room. Your poster board will be marked with your poster number which is the same in the abstract book.

### Poster mounting

Please mount your poster on the 7th October from 6 pm or on the 8th latest by 8.30 am. Your poster will be on display throughout the Symposium. You are asked to remove all poster materials from the board at the end of the meeting otherwise it will be taken down on time and disposed by the organizers. The organizers cannot take any responsibility for this material.

### Poster Material

The size of your poster board is 120 x 90 cm (height x width). Hanging material for the poster boards will be provided on-site.

### Presentations

The oral poster presentations will take place as indicated in the scientific program. The presentations should not exceed 5 min. You will have 1 min in addition for questions.

Please make sure that you are using the power point template sent out and that you have delivered your final presentation to the organizers in time.

We will have an LCD projector connected to a Windows PC available.

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## Liability and Insurance

The Beilstein-Institut will not be liable for any accident, theft or damage to property, nor for any delays or modification in the program due to unforeseen circumstances.

Participants and accompanying persons are advised to arrange personal travel and health insurance.

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## Scientific Program

**Sunday, 7th October**

19.30 Welcome reception

20.00 Dinner

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**Monday, 8th October**

09.00	Opening and Introductory Remarks	Martin G. Hicks
	<i>Session Chair: Antony J. Williams</i>	
09.20	<a href="#">Open, FAIR and GO FAIR</a>	Erik Schultes
10.00	<a href="#">Brokering Trust – How Open Science Will Change Academia to the Better</a>	Kim Daasbjerg
10.40	<i>Coffee Break</i>	
11.00	<a href="#">FAIR in the Community: How Can We Implement the Principles at the Disciplinary Level?</a>	Simon J. Coles
11.40	<a href="#">Changing the Research Culture to Increase Openness</a>	Timothy Errington
12.20	<i>Lunch</i>	
	<i>Session Chair: Christoph Steinbeck</i>	
13.30	<a href="#">“I Like Not Fair Terms and a Villain's Mind” Incentives for Openness in Biomedical Research</a>	Matthew H. Todd
14.10	<a href="#">Opening Science in a Data-driven World – Challenges and Opportunities</a>	Rok Roškar
14.50	<i>Tea Break</i>	
15.10	<a href="#">Making Research Outputs FAIR: A Funder Perspective</a>	David R. O. Carr
15.50	<a href="#">Delivering Transparency in Research Data from the US EPA National Center for Computational Toxicology via Web-based Dashboards</a>	Antony J. Williams
16.30	<a href="#">Oral Poster Presentations</a> Poster #1 - 4	<a href="#">C. Kramer</a> ; <a href="#">H. Brinken</a> ; <a href="#">M. Linne</a> , <a href="#">J. Colomb</a>
17.00	Poster Session	
19.30	<i>Dinner</i>	

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**Tuesday, 9th October***Session Chair: Richard Kidd*

- 09.00 [Open Science at the Royal Society](#) Stuart Taylor
- 09.40 [Bringing Intelligence into Chemistry](#) Dobrila D. Rudnicki
- 10.20 *Coffee Break*
- 10.40 [An Open Standard for Automation and Programming in Organic Synthesis](#) Lee Cronin
- 11.20 [dokieli: A Researcher-centric Decentralised Application for Publishing, Annotation, and Social Interactions](#) Sarven Capadisli
- 12.00 [ChemScanner\(-DB\): an Initiative to Collect Chemistry Data by a Community Effort](#) Nicole Jung
- 12.40 *Lunch*

*Session Chair: Elizabeth Marincola*

- 14.00 [The SGC \(Structural Genomics Consortium\) Open Access Network](#) Stefan Knapp
- 14.40 [Data Management in Chemistry](#) Dørte Solle
- 15.20 Panel Discussion
- 16.00 *Tea Break*
- 16.20 [On the Road to Reproducible Research: Data Stewardship in Practice](#) Marta Teperek
- 17.00 [Who Will Own the Operating System of Science? - Or: How Adopting Open Data and Open Source Practices Has Become a Core Challenge of Research Infrastructure Development](#) Lambert Heller
- 19.30 *Dinner*

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**Wednesday, 10th October**

*Session Chair: Simon J. Coles*

09.00	<a href="#"><u>Open Science Publishing in Africa</u></a>	Elizabeth Marincola
09.40	<a href="#"><u>eLife – Learning How Improvements in Publishing can Support Open Science</u></a>	Mark Patterson
10.20	<i>Coffee Break</i>	
10.40	<a href="#"><u>Open Data Sharing at PLOS: Four Years of Experience and Next Steps</u></a>	Leonie A. Mueck
11.20	<a href="#"><u>UCL Open: A New University Press Megajournal Publishing Model</u></a>	Ian Caswell
12.00	<a href="#"><u>Open Access and Beyond: SciPost</u></a>	Jean-Sébastien Caux
12.40	Closing Remarks	Martin G. Hicks
13.00	<i>Lunch</i>	

## List of Posters

The poster presentation includes a short (5 min) oral presentation on Monday, 8th October, and the poster session afterwards. The posters will be displayed throughout the entire symposium from Monday, the 8th, to Wednesday, the 10th October.

### Monday, 8th October

- |                    |  |                |
|--------------------|--|----------------|
| <a href="#">#1</a> | RDMO – Research Data Management Organiser  | Claudia Kramer |
| <a href="#">#2</a> | Fit for Open Science?! FOSTERING Learning Opportunities for Researchers                          | Helene Brinken |
| <a href="#">#3</a> | The GO FAIR Initiative: Getting Scientific Data Ready for the Internet of FAIR Data and Services | Monika Linne   |
| <a href="#">#4</a> | Using Open Science Principles in Open Science Advocacy: the RDM Case                             | Julien Colomb  |

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# Abstracts

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**Monday****09.20**

## **Open, FAIR and GO FAIR**

**Erik Schultes**GO FAIR International Support and Coordination Office  
Leiden, The Netherlands

The 15 FAIR Principles [1] have found unusually rapid uptake among a broad spectrum of stakeholders, from research scientists who make data, to publishers who distribute data, to science funders who track impact of data. Erik will describe the FAIR Principles and how they apply in the case of both Open and Closed data. This will include example implementations from chemistry and related fields. This discussion will be presented in the context of the International GO FAIR Initiative [2]. GO FAIR is a voluntary community of stakeholders creating the minimal standards and working implementations that drive convergence toward a new data infrastructure called the Internet of FAIR Data and Services (IFDS).

### References

[1] Wilkinson, M. D. et al. (2016) The FAIR Guiding Principles for scientific data management and stewardship. *Sci. Data* **3**:160018 doi:10.1038/sdata.2016.18.  
<https://www.nature.com/articles/sdata201618>

[2] <https://www.go-fair.org>

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**Monday**

## **Brokering Trust – How Open Science Will Change Academia to the Better**

**10.00****Kim Daasbjerg**

Aarhus University  
Interdisciplinary Nanoscience Center (iNANO)  
Aarhus, Denmark

The In 2016, Aarhus University and 18 manufacturing companies joined forces in finding new classes of smart polymer materials and technologies – and they share the results with the world free of charge. The open collaboration resembles a knowledge based community that translates the manufacturing sector's need for new smart materials (e.g. sustainable materials) into basic research projects. The members actively share data, equipment, knowledge, and results with each other and the rest of the world. The companies are offered a risk-free platform to explore the value proposition of basic research to industrial innovation.

The open science community takes legal measures to ensure that the direct output of the projects can not be patented – such as concepts for new materials and technologies. However, anyone is free to protect the specific applications of the results for e.g. product development. Although at a very early stage, the open science initiative already shows promise to yield long-term financial benefits for both academia and industry. These benefits seem to be closely linked to the trust that arises between partners in a no-fee, open, and informal collaborative set-up. The openness on research results – both positive and negative – raise the quality and value of the research data produced. The transparency is high, since projects are discussed early on from the initial idea phase to create a better foundation for identifying the best suited research approaches and partners.

Several Scandinavian, German, and French universities now contribute actively to the open science platform and the concept is penetrating other research fields such as catalysis, machine learning, and life science. At Aarhus University a knowledge center for open science was established in 2017 to create a qualified basis for decision-makers via research and evaluation of these specific open science initiatives as well as similar initiatives worldwide.

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What works? What does not work? The hope is that the knowledge collected can form the basis for future changes to the incentive structures and researcher assessment at the universities. In the long run the open collaboration model might even pave the way for changes to the University Act.

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**Monday****11.00**

## **FAIR in the Community: How Can We Implement the Principles at the Disciplinary Level?**

**Simon J. Coles**University of Southampton  
Department of Chemistry  
Southampton, United Kingdom

Over the last year or so the FAIR principles have become truly widespread, and the message is now going far beyond the community of ‘concerned enthusiasts’ and reaching out to everyday, practising researchers. There is also substantial interest with other stakeholders e.g. funders and publishers, to the point that significant initiatives are underway and are gaining traction across the board.

However, when discussing FAIR practice with a broad range of members of the chemistry community, it becomes clear that there are widely varying extents to which FAIR principles are practiced, understood or likely to be adopted. For a researcher the concept of FAIR can often be easily sold, but for most it is difficult to see how it may be implemented.

The time is therefore right for bodies that represent and guide the chemistry discipline from a ground up basis to be involved in providing some guidance. This talk will outline how work between IUPAC’s Committee on Publications and Cheminformatics Data Standards and the EU-sponsored GO FAIR initiative is aiming to provide the community with guidance, examples and a framework by which FAIR practice can be understood and defined. In the first instance the GO FAIR Chemistry Implementation Network (ChIN) aims to create a culture based on FAIR principles and examples of approaches to providing support and guidance will be presented. The ChIN will go on to leverage existing initiatives and perform a gap analysis to provide a framework defining chemistry standards and infrastructure. The talk will also discuss how the ChIN fits into the complex Open Data landscape with organisations such as the Research Data Alliance and CODATA. .

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**Monday**

## **Changing the Research Culture to Increase Openness**

**11.40****Timothy Errington**

Center for Open Science (COS),  
Charlottesville, VA, United States of America

Scientific communication can be improved to increase efficiency in the accumulation of knowledge. One urgent need is to increase the openness of research data. This requires changes to the present research culture that attend to the drivers of human behavior and the barriers to behavior change. Current efforts have mostly focused on studying the issues to know what to change, providing training to know how to change, and inculcating the values to believe it should be done. While these approaches might be necessary they are not sufficient.

This presentation will discuss additions to this strategy that include shifting the incentives to embrace change and utilizing technology to enable change.

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**Monday**

## **“I Like Not Fair Terms and a Villain's Mind” Incentives for Openness in Biomedical Research**

**13.30****Matthew H. Todd**University College London  
London, United Kingdom

It is a truth universally acknowledged that the FAIR open sharing of data improves the efficiency of scientific research. In the area of biomedical science and pharmaceutical innovation it might be said to be lifesaving.

Some FAIR is simple. Some is not. This talk will outline areas where our FAIR efforts have succeeded, those where we have failed and those where the problems are currently intractable. The examples will focus on our work in *Open Source Malaria* [1], and related efforts in other diseases [2-4].

What distinguishes drug discovery and development from other fields is the apparent incompatibility of open science with traditional economics. If we have no secrecy, there is no obvious path to a traditional return on investment. Do we necessarily have to compromise on our principles of openness, or obfuscate FAIRness, if we are to permit the usual ownership of intellectual property? If this happens, do we fatally compromise the delicate incentive structure for pursuing FAIRness?

### References

- [1] A. E. Williamson, et al. (2016) Open Source Drug Discovery: Highly Potent Antimalarial Compounds Derived from the Tres Cantos Arylpyrroles. *ACS Cent. Sci.* **2**:687–701 (10.1021/acscentsci.6b00086).
- [2] M. Woelfle, P. Olliaro and M.H. Todd (2011) Open Science is a Research Accelerator. *Nature Chem.* **3**:745–748 (10.1038/nchem.1149).

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- [3] M. Balasegaram, P. Kolb, J. McKew, J. Menon, P. Olliaro, T. Sablinski, Z. Thomas, M.H. Todd, E. Torreele and J. Wilbanks (2017) An Open Source Pharma Roadmap. *PLoS Med.*, **14**(4): e1002276 (10.1371/journal.pmed.1002276).
- [4] W. Lim, et al. (2018) Addressing the Most Neglected Diseases through an Open Research Model: the Discovery of Fenarimols as Novel Drug Candidates for Eumycetoma, *PLoS NTD* **12**(4): e0006437 (10.1371/journal.pntd.0006437).

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**Monday**

## Opening Science in a Data-driven World – Challenges and Opportunities

**14.10****Rok Roškar**ETH Zurich  
Swiss Data Science Center (SDSC)  
Zurich, Switzerland

Benefits of open science are numerous and various. The most obvious are transparency and verifiability. They are attributes that science requires from researchers who make a scientific claim public. Today, with the increasing volume and complexity of data, sharing scientific results in the form of an article is not sufficient to verify the validity of this claim. Open science in general promotes incentives, tools and best practices to share scientific results beyond the traditional publication format. In the light of the “reproducibility crisis” in various fields, it has become obvious to many scientists that transparency is one way to alleviate the risk of erroneous – or fraudulent – conclusions. Providing researchers with the skills and tools to properly document their studies will ultimately foster trust and excellence in science.

Researchers must be able to trust published research even when the data is not made public. There is therefore a critical need for tools enabling a trusted, verifiable science at all times.

In this context, I will discuss Renku, a platform developed by the Swiss Data Science Center that seeks to enable reusable, reproducible and shareable science.

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**Monday**

## **Making Research Outputs FAIR: A Funder Perspective**

**15.10****David R. O. Carr**Wellcome Trust  
London, United Kingdom

The Wellcome Trust is a global foundation dedicated to improving health for all by helping great ideas to thrive. Wellcome believes passionately that the outputs of the research we fund should be made available with as few restrictions as possible, and in ways that ensure these outputs can be accessed and used to maximise the resulting benefits to health and society. Over the last two decades, we have been a prominent champion and advocate for open access to research publications and research data sharing.

In 2017, Wellcome formally established an in-house Open Research team to act as a focal point for its work to maximise the value of research outputs. We also updated our long-standing policy on data management and sharing into a broader [policy on data, software and materials management and sharing](#). This new policy extends our long-standing approach on research data to cover other important research outputs – requiring those we fund to take a holistic view of their outputs and specify through an outputs management plan how they will seek to maximise their value.

In this talk, I will discuss Wellcome's experience in implementing our outputs sharing policy and how we are working as a funder to address some of the wider technical, cultural and professional barriers which constrain the sharing of data and other research outputs. I will introduce some of our current activities – including the establishment of the [Wellcome Open Research](#) publishing platform, the launch of our new [Open Research Fund](#), and work we are doing with others to help ensure efforts to share research outputs are given due recognition in funding decisions. I will also outline how we are working to support our researchers in making their research outputs FAIR, and monitor the extent to which our outputs fulfil the FAIR criteria.

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Monday

## Delivering Transparency in Research Data from the US EPA National Center for Computational Toxicology via Web-based Dashboards

15.50

**Antony J. Williams**

US Environmental Protection Agency  
National Center for Computational Toxicology  
Triangle Research Park, NC, United States of America

The U.S. Environmental Protection Agency (EPA) Computational Toxicology Program integrates advances in biology, chemistry, and computer science to help prioritize chemicals for further research based on potential human health risks. This involves computational and data-driven approaches that integrate chemistry, exposure and biological data. The National Center for Computational Toxicology (NCCT) has measured, assembled and delivered an enormous quantity and diversity of data for the environmental sciences, including high-throughput *in vitro* screening data, *in vivo* and functional use data, exposure models and chemical databases with associated properties. We have delivered these data via a number of publicly accessible websites, so-called dashboards, to provide transparent access to the outputs of the center. Since the inception of our research, software projects technologies have changed dramatically, as have the expectations regarding the methods by which to access data. Our informatics efforts provide access to millions of dollars of high-throughput screening data available in open, downloadable formats, via web services and through a rich web interface. Similarly, we provide access to experimental and predicted data associated with ~760,000 substances to serve the environmental chemistry community, as well as open source code for predictive models. This presentation will provide an overview of the efforts of NCCT to provide transparent access to our research and data via our publications (and accompanying supplementary data), via our Open Data policies, and through our databases, software tools and web services.

*This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.*

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Poster

No. 1

## RDMO – Research Data Management Organiser

H. Enke<sup>2</sup>, J. Klar<sup>2</sup>, **Claudia Kramer**<sup>1</sup>, J. Ludwig<sup>4</sup>,  
O. Michaelis<sup>2</sup>, H. Neuroth<sup>3</sup>, J. Straka<sup>3</sup>, F. Tristram<sup>1</sup>,  
K. Wedlich<sup>1</sup>

<sup>1</sup> Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen

<sup>2</sup> Leibniz Institute for Astrophysics, Potsdam (AIP)

<sup>3</sup> University of Applied Science, Potsdam (FHP)

<sup>4</sup> DINI/nestor Working Group “Research Data”  
Germany

The Research Data Management Organiser (RDMO) is a software designed to support scientists in data management issues and advises during and after a research project. The RDMO enables scientists to meet the requirements of several funders like the European Union (Horizon 2020) with respect to the generation of data management plans (DMP). It organizes all tasks with respect to FAIR data management and accommodates the relevant stakeholders. Users can access the collected information in various forms during the work on the research project and they may keep it up to date while the project evolves. RDMO features an API which can be used for further processing of the collected information by other software tools and allows for an integration into existing workflows, local environments and existing administrative IT infrastructures. The RDMO software includes a workflow providing a digital questionnaire guiding scientists through the recommended procedure. The questionnaire can be enhanced by connecting it to discipline specific information like recommending systems for electronic lab notebooks, research data repositories (e.g. Chemotion) and metadata, or institute specific regulations. The questions of the interview, the controlled vocabularies used as options for the answers, and the templates for the different output formats can be customized using a convenient web interface and exported and shared with other RDMO instances using XML files. Special consideration is given to the installation of RDMO by institutions and universities and its adaptation for discipline-specific or institutional needs. The software is open source and publicly available on GitHub [1].

[1] <https://github.com/rdmorganiser/rdmo>

Poster

## Fit for Open Science?! FOSTERing Learning Opportunities for Researchers

No. 2

**Helene Brinken**

Georg August University Göttingen  
State and University Library, Knowledge Commons  
Göttingen, Germany

Offering various training opportunities, the EU-funded project FOSTER Plus (2017-2019) supports researchers to put Open Science (OS) into practice. On the FOSTER portal, users can find training materials, advanced-level and discipline-specific courses and other resources that build capacity for a change in scientific culture.

The project developed new OS online courses (<https://www.fosteropenscience.eu/toolkit>) addressing key topics that provide focused, practical and, where relevant, discipline specific examples to try and answer some of the burning questions researchers may have about applying OS in their daily workflows. The courses include interactive content to ensure training is engaging and that capability can be assessed for issue of a badge upon completion.

The developed courses developed include:

- What is OS?
- Best practices
- Ethics & data protection
- Open access publishing
- Open peer review
- Managing & sharing research data
- Open source software & workflows
- OS & innovation
- Sharing preprints
- Licensing

In addition to these stand-alone courses, there are learning pathways through the content to help researchers to hone their skills in specific areas, e.g. the responsible data sharer ([www.fosteropenscience.eu/badges](http://www.fosteropenscience.eu/badges)).

We are reusing and reshaping training content deposited within the FOSTER portal during the first project phase (20-2016) and working with our discipline specific partners representing the arts and humanities, social sciences, and life sciences to provide relevant examples. All content is openly licensed and easy to download.

Apart from creating new courses, FOSTER follows a train the trainer approach to multiply training forces. The project provides trainings, infrastructure and materials, e.g. the OS training handbook, to support and equip future trainers, with methods, instructions, and exemplary training outlines. The FOSTER portal is a hub for people who want to learn about OS as well as for people delivering OS training.

This project has received funding from the European Union's Horizon2020 research and innovation programme under grant agreement No.741839.

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Poster

No. 3

## The GO FAIR Initiative: Getting Scientific Data Ready for the Internet of FAIR Data and Sciences

**Monike Linne**ZBS - Leibniz Information Centre for Economics  
Hamburg, Germany

GO FAIR is a bottom-up international approach for the practical implementation of the European Open Science Cloud (EOSC) as part of a global Internet of FAIR Data & Services (IFDS). At a practical level, this takes place on the basis of three interactive processes which constitute the pillars of GO FAIR: GO CHANGE, GO TRAIN and GO BUILD. GO CHANGE refers to socio-cultural change in the broader scientific system. As a part of this change research data – not just article publications – are recognized as a significant output of research and become a vehicle for reputation gain within academia. The GO TRAIN process refers to the development of training curricula focused on FAIR Data Stewardship as well as the development of certification schemes for competencies in FAIR Data Stewardship. GO BUILD is a process that involves designing and building the technical standards, best practices and infrastructure components needed to create the IFDS.

Organized in GO FAIR Implementation Networks, early movers can commence with crucial activities in these three pillars. Implementation Networks are constituted of individuals, institutions and organizations who are committed to defining and creating materials and tools as elements of the IFDS. In one way or another, their efforts contribute to making unlinked research data **findable, accessible, interoperable and reusable (FAIR)**. At any time, Implementation Networks can be joined or launched and as such, the GO FAIR consortium is entirely open, inclusive and stakeholder-driven.

GO FAIR provides coordination and international guidance, e.g. to prevent silo formation of data services, undue competition between different initiatives and to counteract a continuing fragmentation of the research data landscape. Apart from that, it is regarded as critical that within each participating Implementation Network, country or organization, optimal 'freedom to operate' must be safeguarded.

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Poster

## Using Open Science Principles in Open Science Advocacy: the RDM Case

No. 4

**Julien Colomb**

University of Jena  
Department of Informatics  
Jena, Germany

The eeFDM project that aims at developing components for an effective and efficient research data management (RDM) was funded by the BMBF in 2017. As for most RDM projects, a significant amount of energy is put into outreach and teaching initiatives. We planned the creation of promotional and informative videos in order to raise the awareness researchers on the most important aspects of RDM. To ensure the efficacy of the videos, we have been analysing RDM outreach activities. Using the principles of open science and data management, we started by writing a data management plan and developing a strategy to work in the open.

On the one hand, we have been using existing technologies (R - RStudio, rmarkdown, blogdown- Github, zenodo, netify, dpmtool, dat, googlesheets, email) to collectively gather and list material, strategies and best arguments used for RDM promotion and teaching. On the other hand, we have been presenting the data and its analysis on a website, available both on the web and on dat (<https://rdmpromotion.rbind.io>, [dat:rdmpromotion.hasbase.io](https://rdmpromotion.hasbase.io)). While the technological part was relatively easy and fast to set-up, building an online community is a tough enterprise. We have been reaching out to existing communities or RDM specialists hoping they will contribute to and make use of our tool.

A preliminary analysis of the information gathered so far showed a discrepancy between the topics brought forward by data stewards and managers (data storage, safety, citation, and FAIRness) versus researchers (data preparation for analysis). We have therefore focused our efforts on showing the advantages of good RDM for data analysis and efficient research processes. The artistic framework of our videos is a mashup of clips that entered the public domain. The most recent version of the produced video will be screened during the oral presentation: *Better research in less time* \*

\* slogan modified from Lowndes et al., DOI:10.1038/s41559-017-0160

Tuesday

09.00

## Open Science at the Royal Society

**Stuart Taylor**The Royal Society  
London, United Kingdom

The Royal Society is the national academy of science for the UK. It is a self-governing Fellowship of the UK's and the Commonwealth's most distinguished scientists and elects Fellows and Foreign Members from all over the world based on the excellence of their science. The Society's mission, as set out in its founding charters of the 1660s, is to recognise, promote and support excellence in science and to support the development and use of science for the benefit of humanity. We have been publishing since 1665 when the world's first science journal, *Philosophical Transactions*, was launched.

We introduced open access on all our journals in 2006 and now almost half our articles are published with immediate open access under CC-BY licence. In 2015, we held a four day symposium 'The Future of Scholarly Scientific Communication' as part of our celebrations of 350 years of the science journal. The symposium brought together all stakeholders (scientists, universities, funders, learned societies, librarians, publishers) to explore the rapidly changing landscape and to look forward to future developments. As a result of this conference, and in synergy with the work of our Science Policy Centre, we decided to accelerate our implementation of open science principles in our journals.

Since 2015, we have introduced a more strictly enforced data sharing policy, ORCID iD requirement for authors, open peer review on four of our journals, Registered Reports, Accountable Replication Policy, support for preprints, and made data availability statements and author contribution statements mandatory for all articles.

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Tuesday

09.40

## Bringing Intelligence into Chemistry

**Dobriła D. Rudnicki**

National Institutes of Health  
National Center for Advancing Translational Sciences (NCATS)  
Bethesda, MA, United States of America

While our understanding of the molecular basis of disease has improved exponentially in the last 30 years, a major roadblock to timely translation is our inability to efficiently identify new areas of biologically active small-molecule chemical space. Recent innovations in automated chemical synthesis technologies, high-throughput biological screening, automation engineering, and machine learning/AI indicate that now is the time to converge these technologies and advance our understanding of the relationship between chemical and biological space. In response to this progress and input from the scientific community and other stakeholders, NCATS has recently proposed the development of 'A Specialized Platform for Innovative Research Exploration' (**NCATS ASPIRE**, [ncats.nih.gov/aspire](https://ncats.nih.gov/aspire)) to aid in the discovery and development of novel, safe, and effective treatments, while at the same time making the process faster and more cost-effective. The platform will utilize currently available knowledge to develop innovative algorithms and predict and synthesize novel structures capable of interacting with specific targets; enable small-scale synthesis of the predicted molecules; and incorporate in-line, rapid biological testing of the molecules. Results from immediate assessment of bioactivity will be fed back into chemical prediction algorithms to enable ongoing, user-independent optimization of compounds and remote exploration of novel chemical space.

**NCATS ASPIRE** will complement current NIH efforts in unexplored therapeutic space such as the NIH Common Fund 'Illuminating the Druggable Genome' ([commonfund.nih.gov/idg](https://commonfund.nih.gov/idg)) program and, as a BD2K program ([commonfund.nih.gov/bd2k](https://commonfund.nih.gov/bd2k)), integrate FAIR principles. If successful, such an ambitious, concerted, and highly collaborative effort will revolutionize chemical genomics and drug discovery and development, bringing the promise of science to patients ([ncats.nih.gov/heal](https://ncats.nih.gov/heal)).

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Tuesday

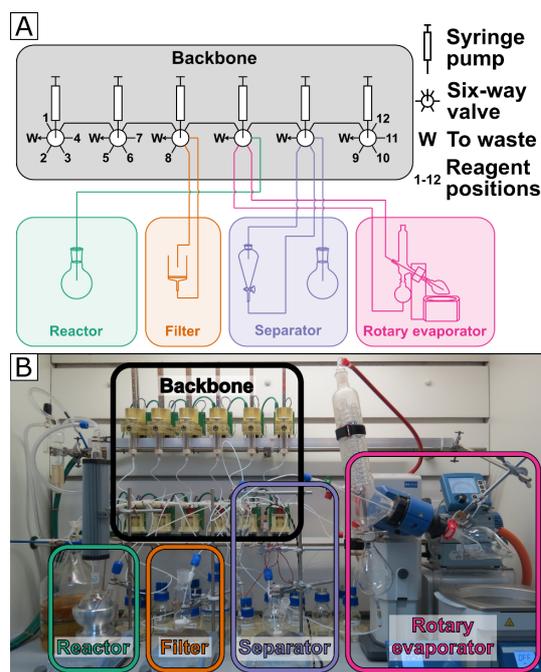
## An Open Standard for Automation and Programming in Organic Synthesis

10.40

**Lee Cronin**

 University of Glasgow  
 School of Chemistry  
 Glasgow, United Kingdom

Much of chemical synthesis must be done manually as automation is limited to single classes of reactions, or work-flows. To address this, we developed an abstraction of organic synthesis which allows a universal connection between the conceptual steps and automation of the process [1-2].



```

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**Figure 1.** Left: Our Chemputer platform. Right: Code to run a Grignard reaction.

These steps were implemented in a modular robotic platform, running a chemical programming language which formalizes and controls the assembly of the molecules, see Figure 1.

We validated and demonstrated the concept by making three pharmaceutical compounds and doing over ten different classes of reactions without any physical intervention. Execution was demonstrated by the fully autonomous synthesis of the pharmaceuticals, Nytol, Rufinamide, and Sildenafil, with yields and purities of products and intermediates comparable or better to those achieved manually. The syntheses are captured as digital code that can be transferred flexibly between platform instances with no modification, published and versioned, thereby greatly enhancing reproducibility and reliable access to complex molecules.

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Tuesday

11.20

## **dokieli: A Researcher-centric Decentralized Application for Publishing, Annotation, and Social Interactions**

**Sarven Capadisli**

Technische Informationsbibliothek (TIB)  
German National Library of Science and Technology  
Hannover, Germany

In this talk we look into the mechanisms that are involved in the creation of a researcher and Web-centric scholarly application that is inherently decentralised, interoperable, and social. dokieli (<https://dokie.li/>) is a tooling that is designed to be socially-aware and aims at improving the write aspect of the read-write Linked Data Web for common scholarly functions such as authoring, publishing, annotations, and notifications about social activities. We discuss dokieli's underlying principles and how they are implemented: autonomy and freedom of expression, decentralisation and interoperability, universal access, reusability, as well as respecting users' security and privacy.

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Tuesday

12.00

## ChemScanner(-DB): an Initiative to Collect Chemistry Data by a Community Effort

**Nicole Jung**

Karlsruhe Institute of Technology (KIT)  
Institute of Organic Chemistry  
Eggenstein-Leopoldshafen, Germany

Currently, scientists have almost no influence on the visibility and findability of research data after the publication of scientific work. The process of scientific reuse of information is almost completely dependent on the workflow of journals and databases. Repositories for research data offer a very good alternative to disclose research data but unfortunately, the known repositories are rarely used and their content grows only slowly. Part of the Chemotion projects during the last months was the development of ChemScanner, a software that can be used for the extraction of information from (embedded) CDX or CDXML files in e.g. MS Word documents.

The software can deal with several challenges of common chemical drawings and offers a diverse library of abbreviations to translate even rarely used reagents and chemicals. ChemScanner is not OpenSource but the software and the access to the source code can be requested from the Stefan Bräse group at the KIT. Academic collaborators and contributors are welcome.

The next step for the establishment and use of ChemScanner is its installation to build an open chemistry database for reactions hosted at the KIT in Karlsruhe. Publications (manuscripts and Supporting Information) can be uploaded via a simple drag and drop procedure and the content is analyzed automatically. The obtained data is disclosed to the public and can be accessed by an Open Access model.

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Tuesday

14.00

## The SGC (Structural Genomics Consortium) Open Access Network

**Stefan Knapp**

Goethe-University Frankfurt  
Institute of Pharmaceutical Chemistry  
Frankfurt am Main, Germany

The SGC has a long history providing unencumbered data and reagents to the research community. Established in 2004 as a charity in the UK (University of Oxford) and Canada (University of Toronto), the initial mandate of the SGC was to provide high resolution crystal structures of proteins relevant to human health. Since this initial phase, the SGC diversified considerably both geographically (new sites have now been established at the Karolinska Institute in Stockholm, the Universities of North Carolina (USA) Sao Paulo (Brazil) and Frankfurt (Germany) as well in its main research output which includes now also development of chemical probes, disease relevant primary cell assay systems and more recently also drug development efforts.

The SGC is a public private partnership currently supported by 9 pharmaceutical companies and diverse public funding agencies. One of the founding principles of the SGC is to make generated data and reagents immediately and unrestricted available to the research community. This has been achieved using not only open access publishing but also by depositing data into databases and other web-based resources usually even before publication in peer reviewed journals. Since last year, SGC scientists also post all manuscript on a pre-print server (<https://www.biorxiv.org/>) and encourage our collaborators to do the same. Importantly, the SGC also make all reagents generated during research projects available. This ensures that data can be easily reproduced by other scientists. Before release of key reagents such as chemical probes two advisory boards review the quality of chemical tools characterized for instance by selectivity, chemical stability, cellular activity. In addition, probe characterization data are submitted to a web based portal (<http://www.chemicalprobes.org/>) for community feedback.

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Tuesday

14.40

## Data Management in Chemistry

**Dørte Solle**Leibniz University Hannover  
Institute of Technical Chemistry  
Hannover, Germany

Knowledge about chemical reactions and processes is usually gained from data created during practical experiments. Some of these experiments are based on standard analytical methods and routine measurements. However, most experiments require individual protocols, e.g. for the synthesis of target products, detection of different analytes or for specific product purification. Usually, each individual experiment has to be performed several times under various conditions in order to establish a new validated and optimized protocol. This is a very elaborate and time-consuming process, of which only the final protocol might be worth for publication. As modern analytical technologies and instruments, e.g. spectroscopy or imaging techniques, are increasingly used for monitoring of chemical processes, huge amounts of data from different sources are generated within one single experiment.

In order to handle and evaluate the collected data, scientists have to store and structure the data according to various criteria and in a reproducible manner. Since scientific data is usually supposed to be shared and compared to the data generated by other scientists, there is a need for the standardization of data processing. Up until now, there are only very few standards and databases that can be used for the storage and processing of chemical data, such as chemical structures or NMR data. In this talk, the state of the art and challenges of chemical data management are presented and options, that might lead to a smart chemical laboratory, are discussed.

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Tuesday

16.20

## On the Road to Reproducible Research: Data Stewardship in Practice

**Marta Teperek**

Delft University of Technology  
Library  
Delft, The Netherlands

Research reproducibility crisis has been a hot topic of many recent discussions. But who owns the problem? And how could it be solved? In her presentation, Marta will talk about good data stewardship and open science as key components of research integrity and research reproducibility. She will speak about some of the reasons which lead to reproducibility crisis, and suggest some possible actions to be taken by research institutions.

She will also talk about the Data Stewardship Programme: a case study example from Delft University of Technology about an institutional approach to supporting open science and reproducible research

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Tuesday

## Who Will Own the Operating System of Science? - Or: How Adopting Open Data and Open Source Practices Has Become a Core Challenge of Research Infrastructure Development

17.00

**Lambert Heller**

Technische Informationsbibliothek (TIB)  
German National Library of Science and Technology  
Open Science Lab  
Hannover, Germany

While business models based on academic content subscription are increasingly challenged by governments and funders, a new competition is on: Elsevier, but also other big players like Holtzbrinck, Wiley, Clarivate etc., each try to grow their own version of a “single operating system of science”, a platform of interlocking tools covering all steps of the research life cycle. If that’s true, what does that mean for Open Science? – I’ll assume here that Open Science means to make sure that research stays open – accountable and approachable towards the general public, open towards new approaches and findings, and open towards new generations of researchers doing unexpected and disruptive things.

Therefore, we – as stakeholders of tax-payer-funded research infrastructures, e.g. as research libraries – have to take care that the operating system(s) of science stays open. With the example of VIVO, an institutional research information system, I’ll show how a worldwide community of research institutions came up with an open-source and open-data answer to the daily administrative challenge of aggregating, reporting and assessing researcher profiles and metadata about their research outcomes. It’s a powerful example of how adopting open practices has become key to serving communities with infrastructure solutions that are open to new developments (e.g. taking into account unusual new research products), local adaptations, and that allow to stay independent and to be economically sustainable at the time.

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Wednesday

09.00

## Open Science Publishing in Africa

**Elizabeth Marincola**

The African Academy of Sciences  
Science Communication & Advocacy  
Nairobi, Kenya

Scientists everywhere in the world experience similar frustrations in disseminating the results of their research: delays of months or more; access constraints; bias resulting from opaque peer review; incomplete availability of data, and perhaps most damaging, the tyranny of the Impact Factor, which induces scientists to chase acceptance in a succession of journals, hoping to publish in the one with the highest possible IF – exacerbating the delay problem. African scientists are subject to all these barriers, with amplified effects resulting from the status of many as relatively unknown, often from unknown institutions. This submits scientists in Africa and other developing countries to an uneven playing field. African science can thrive best as it can anywhere in the world: by giving researchers themselves the tools with which to pursue and communicate their research.

To this end, the African Academy of Sciences has engaged F1000 to offer *AAS Open Research*, an open, transparent, dynamic, immediate and peer-reviewed publishing platform. AAS OR publishes research immediately, after it passes ethical and technical checks, from any scientist whose credibility is established by association with the Academy or its funding arm, the Alliance for Accelerating Excellence in Science in Africa (AESA). Output includes standard research articles as well as methods, study protocols, software tools, case reports, research notes, etc., and is peer reviewed by experts following publication.

All versions, and the reviews themselves, are transparent, offering credit and exposure not just to authors but also to reviewers. Work is fully indexed after it passes peer review. Innovative approaches such as *AAS Open Research* promise to enable scientists in Africa not just to catch up with the Global North, but to lead the world in scientific communication by returning control from publishers and editors to where it belongs: scientists themselves.

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Wednesday

09.40

## ***eLife* – Learning How Improvements in Publishing Can Support Open Science**

**Mark Patterson**eLife  
Cambridge, United Kingdom

*eLife* was launched by biomedical research funders to improve the way journals function in research communication. Our work focuses on three areas: publishing a high-quality open-access journal; creating open infrastructure to support more effective publishing; and promoting behavioural change through advocacy and outreach. The overarching purpose of *eLife* is to support a shift towards open science practices. We do this by experimentation and sharing what we build and learn.

This talk will focus on recent experiments in peer review, progress on software development and our engagement with the early-career community.

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Wednesday

10.40

## Open Data Sharing at PLOS: Four Years of Experience and Next Steps

**Leonie A. Mueck**Public Library of Science (PLOS)  
PLOS ONE  
Cambridge, United Kingdom

Since March 2014, all PLOS journals require that the minimal dataset necessary to replicate published results is made openly available [1]. Given the number of research articles *PLOS ONE* publishes and the breadth of our scope, we had to devise strategies of how to implement such policies at scale [2]. Recent analysis of our data availability statements suggests that, while the vast majority of researchers formally complies with our policy, encouraging scientific communities to fully embrace the philosophy of open data sharing may require more work [3].

As we are discussing with the communities what open and FAIR data sharing means for specific disciplines, including chemistry and materials science, we are actively thinking about which new policies would enhance replicability and reproducibility at PLOS.

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**Wednesday****11.20**

## ***UCL Open: A New University Press Megajournal Publishing Model***

**Ian Caswell**

University College London  
UCL Press  
London, United Kingdom

UCL Press believe that the future of academic and scholarly pursuit is best served by an open science/open scholarship agenda, towards a fully open access environment, where knowledge should be accessible to all, regardless of location or financial means. Founded as the UK's first open access university press, UCL Press aims to stimulate disruptive thinking to challenge prevailing scholarly publishing models across and beyond the university, and to transform the way new knowledge is shared.

Building on its foundation, the press is currently developing a new university press open access megajournal model that will champion the open science agenda, due for launch later in the year. This talk will highlight the motivation, model, and considerations, for a university press to undertake such an innovative and bold direction in academic and scientific publishing.

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**Wednesday****12.00**

## **Open Access and Beyond: SciPost**

**Jean-Sébastien Caux**

University of Amsterdam  
Institute of Physics  
Amsterdam, The Netherlands

This talk will present SciPost, a not-for-profit publishing initiative conceived, implemented and run by professional scientists. SciPost implements the so-called Genuine Open Access principles, which generalize FAIR ones. Currently active in the general field of physics (but looking forward to expansion in other disciplines), SciPost leverages the idea of openness to enforce top scientific quality while solving the accessibility problem without compromise. Importantly, SciPost also implements a cost-slashing, institutions-backed consortial business model not relying on subscription fees or article processing charges.

This talk will summarize operations since the launch of the portal in 2016, share experiences gained, and provide perspectives for future developments in the reform of scientific publishing

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