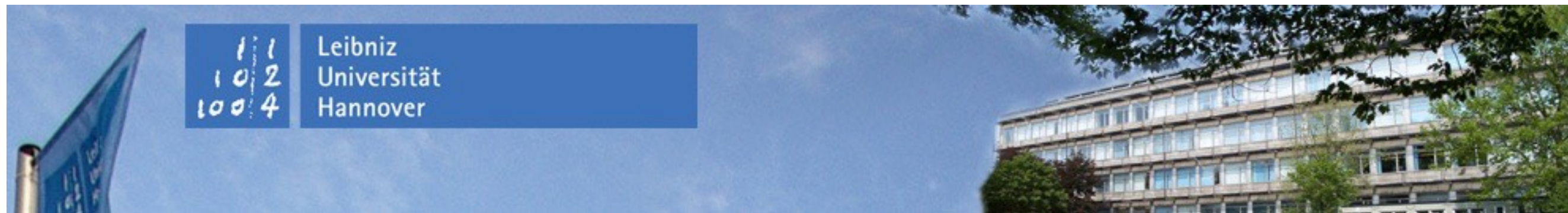


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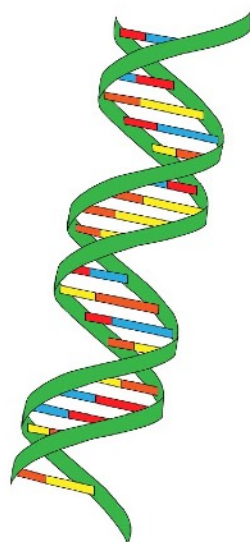
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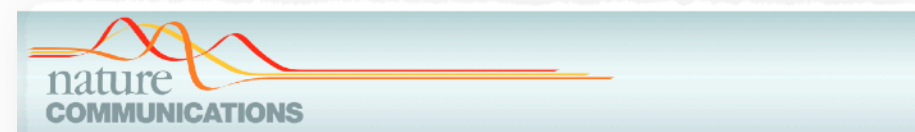
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- ✱ Ph.D. University of Durham UK, 1992
- ✱ Post-Doc Alberta, Canada and Norwich UK, 1995
- ✱ Lecturer University of Bristol, UK 1996
- ✱ Full Professor, University of Bristol, UK 2008
- ✱ Full Professor, Leibniz University of Hannover, 2013
- ✱ Editor in Chief, *RSC Advances*, 2018

✱ Research in the area of *Fungal Biotechnology* and *Natural Products Chemistry*



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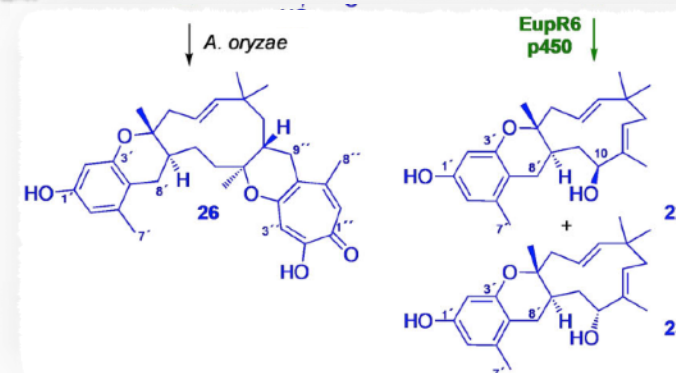


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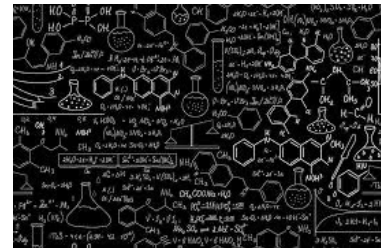
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Three previously unrecognised classes of biosynthetic enzymes revealed during the production of xenovulene A

Raissa Schor^{1,2}, Carsten Schotte^{1,2}, Daniel Wibberg³, Jörn Kalinowski³ & Russell J. Cox^{1,2}



Working Pattern



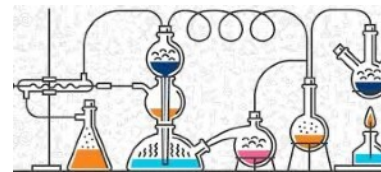
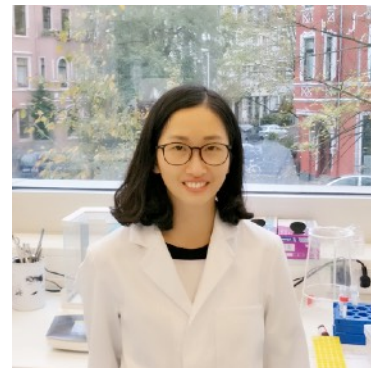
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Biosynthesis

Biosynthesis of 6-Hydroxymellein Requires a Collaborating Polyketide Synthase-like Enzyme

Lukas Kahlert, Miranda Villanueva, Russell J. Cox,* and Elizabeth J. Skellam*



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PAPER

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In vitro studies of maleidride-forming enzymes†

Cite this: RSC Adv., 2021, 11, 14922

Sen Yin, Steffen Friedrich, Vjaceslavs Hrupins and Russell J. Cox*



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COMMUNICATION

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Evidence for enzyme catalysed intramolecular [4+2] Diels–Alder cyclization during the biosynthesis of pyrichalasin H†

Cite this: DOI: 10.1039/c9cc09590j

Received 10th December 2019
Accepted 6th January 2020

Verena Hantke,* Elizabeth J. Skellam and Russell J. Cox*

DOI: 10.1039/c9cc09590j



Mycological Progress (2020) 19:235–245
https://doi.org/10.1007/s11557-019-01552-9

ORIGINAL ARTICLE

Intragenomic polymorphisms in the ITS region of high-quality genomes of the Hypoxylaceae (Xylariales, Ascomycota)

Marc Stadler¹ · Christopher Lambert¹ · Daniel Wibberg² · Jörn Kalinowski² · Russell J. Cox³ · Miroslav Kolářik^{1,2,3,4} · Eric Kuhnert³



Science REPORTS

Cite as: S. Günther et al., Science 10.1126/science.abh7945 (2021).

X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease

Sebastian Günther^{1,†}, Patrick Y. A. Reinkens^{2,†}, Yaiza Fernández-García³, Julia Lieske⁴, Thomas J. Lane⁵, Helen M. Giann⁶, Faisal H. M. Koua⁷, Christiane Ehart⁸, Wiebke Ewert⁹, Dominik Oberthuer¹⁰, Olesandr Yefanov¹¹, Susanne Meier¹², Kristina Lorenzen¹³, Boris Krichel¹⁴, Janine Denise Kopicik¹⁵, Luca Gelisio¹⁶, Wolfgang Brehm¹⁷, Ilona Danilch¹⁸, Brandon Seychell¹⁹, Henry Gieseler²⁰, Brenna Norton Baker²¹, Beatriz Escudero-Pérez²², Martin Domaracký²³, Sofiane Saouane²⁴, Alexandra Tolstikova²⁵, Thomas A. White²⁶, Anna Hünle²⁷, Michael Gröschler²⁸, Holger Hoekenslein²⁹, Fabian Trost³⁰, Martina Galchenkova³¹, Yaroslav Gevorgov³², Chunfeng Li³³, Salah Awet³⁴, Arianna Peck³⁵, Miriam Barthelmeus³⁶, Frank Schillhauer³⁷, J. Louisa Xavier³⁸, Nadine Werner³⁹, Ilana Andjelob⁴⁰, Najesh Chhal⁴¹, Svea Falke⁴², Vasundara Srivastava⁴³, Bruno Alves Franco⁴⁴, Martin Schweitzer⁴⁵, Hésila Brogiero⁴⁶, Cromarte Rogers⁴⁷, Dijojo Vello⁴⁸, Joana J. Zalisova-Doyle⁴⁹, Jara Knoska⁵⁰, Gisel E. Peña-Murillo⁵¹, Aida Rahmani Mashhour⁵², Vincent Hennicke⁵³, Pontus Fischer⁵⁴, Johanna Hakampää⁵⁵, Jan Meyer⁵⁶, Philip Gribbon⁵⁷, Bernhard Ellinger⁵⁸, Maria Kuzikov⁵⁹, Markus Wolf⁶⁰, Andrea R. Beccari⁶¹, Gleb Bourenkov⁶², David von Stetten⁶³, Guillaume Pompidor⁶⁴, Isabel Bento⁶⁵, Saravanan Panneerselvam⁶⁶, Ivars Karpics⁶⁷, Thomas R. Schneider⁶⁸, Maria Marta Garcia-Alai⁶⁹, Stephan Niebling⁷⁰, Christian Günther⁷¹, Christina Schmidt⁷², Robin Schubert⁷³, Huijiong Han⁷⁴, Juliane Boger⁷⁵, Diana C. F. Monteiro⁷⁶, Liliina Zhang⁷⁷, Xinyuanyuan Sun⁷⁸, Jonathan Pieter Ziegler⁷⁹, Jan Wollenhaupt⁸⁰, Christian G. Veller⁸¹, Manfred S. Weiss⁸², Eike Christian Schulz⁸³, Pedram Mehrabi⁸⁴, Katarina Karalic⁸⁵, Aleksandra Usevic⁸⁶, Jure Loboda⁸⁷, Heonling Tidow⁸⁸, Ashwin Chari⁸⁹, Rolf Tilgner⁹⁰, Charlotte Uetrecht⁹¹, Russell Cox⁹², Andrea Zaliani⁹³, Tobias Beck⁹⁴, Matthias Rarey⁹⁵, Stephan Günther⁹⁶, Dusan Turk⁹⁷, Winfried Hinrichs⁹⁸, Henry N. Chapman⁹⁹, Arwen R. Pearson¹⁰⁰, Christian Betzel¹⁰¹, Alke Meents¹⁰²

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By: **Shelley, Matthew**; Pastore, Alessandro
UNIVERSE Volume: 7 Issue: 5 Article Number: 131 Published: MAY 2021
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Matthew Shelley * and Alessandro Pastore

Department of Physics, University of York, York YO10 5DD, UK; alessandro.pastore@york.ac.uk
* Correspondence: mges501@york.ac.uk

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Biosynthesis
Biosynthesis of 6-Hydroxymellein Requires a Collaborating Polyketide Synthase-like Enzyme
Lukas Kahlert, Miranda Villanueva, Russell J. Cox,* and Elizabeth J. Skellam*

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International Edition: doi.org/10.1002/anie.202100969
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In vitro studies of maleidride-forming enzymes†
Sen Yin, Steffen Friedrich, Vjaceslavs Hrupins and Russell J. Cox*

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COMMUNICATION

Evidence for enzyme catalysed intramolecular [4+2] Diels–Alder cyclization during the biosynthesis of pyrichalasin H†
Verena Hantke,* Elizabeth J. Skellam and Russell J. Cox*

Mycological Progress (2020) 19:235–245
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Science REPORTS

X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease
Sebastian Günther^{1,†}, Patrick Y. A. Reinkens^{2,†}, Yaiza Fernández-García³, Julia Lieske⁴, Thomas J. Lane⁵, Helen M. Ginn⁶, Faisal H. M. Koua⁷, Christiane Ehart⁸, Wiebke Ewert⁹, Dominik Oberthuer¹⁰, Olesandr Yefanov¹¹, Susanne Meier¹², Kristina Lorenzen¹³, Boris Krichel¹⁴, Janine Denise Kopelke¹⁵, Luca Gelisio¹⁶, Wolfgang Brohm¹⁷, Ilona Danilch¹⁸, Brandon Seychell¹⁹, Henry Gieseler²⁰, Brenna Norton Baker²¹, Beatriz Escudero-Pérez²², Martin Domaracký²³, Sofiane Saouane²⁴, Alexandra Tolstikova²⁵, Thomas A. White²⁶, Anna Hillel²⁷, Michael Groesler²⁸, Holger Floeckstein²⁹, Fabian Trost³⁰, Martina Galchenkova³¹, Yaroslav Gevorgyan³², Chunfeng Li³³, Sarah Awot³⁴, Arianna Peck³⁵, Miriam Barthelmees³⁶, Frank Schützgen³⁷, J. Louisa Kayler³⁸, Nadine Werner³⁹, Ilana Andujar⁴⁰, Najesh Chahal⁴¹, Sven Falke⁴², Vasundhara Srinivasan⁴³, Bruno Alves Fraga⁴⁴, Martin Schwinzer⁴⁵, Hésila Brogiero⁴⁶, Cromarte Rogers⁴⁷, Diego Melo⁴⁸, Joanna J. Zaitseva-Doyle⁴⁹, Jaraž Koska⁵⁰, Gisel E. Peña-Murillo⁵¹, Aida Rahmani Mashhour⁵², Vincent Hennicke⁵³, Pontus Fischer⁵⁴, Johanna Hakampää⁵⁵, Jan Meyer⁵⁶, Philip Gribbon⁵⁷, Bernhard Ellinger⁵⁸, Maria Kuzikov⁵⁹, Markus Wolf⁶⁰, Andrea R. Beccari⁶¹, Gleb Bourenkov⁶², David von Stetten⁶³, Guillaume Pompidor⁶⁴, Isabel Bento⁶⁵, Saravanan Panneerselvam⁶⁶, Ivars Karpics⁶⁷, Thomas R. Schneider⁶⁸, Maria Marta Garcia-Alai⁶⁹, Stephan Niebling⁷⁰, Christian Günther⁷¹, Robin Schubert⁷², Huijiong Han⁷³, Juliana Boger⁷⁴, Diana C. F. Monteiro⁷⁵, Liliya Zhang⁷⁶, Xinyuanyuan Sun⁷⁷, Jonathan Pietzer Zelger⁷⁸, Jan Wollenhaupt⁷⁹, Christian G. Veller⁸⁰, Manfred S. Welke⁸¹, Rike Christlau Schultz⁸², Pedram Mehrabi⁸³, Katarina Karalica⁸⁴, Aleksandra Usenik⁸⁵, Jure Loboda⁸⁶, Heonil Tidov⁸⁷, Ashwin Chari⁸⁸, Rolf Tilgenfeld⁸⁹, Charlotte Uetrecht⁹⁰, Russell Cox⁹¹, Andrea Zaliani⁹², Tobias Beck⁹³, Matthias Rarey⁹⁴, Stephan Günther⁹⁵, Dusan Turk⁹⁶, Winfried Hinrichs⁹⁷, Henry N. Chapman⁹⁸, Arwen R. Pearson⁹⁹, Christian Betzel¹⁰⁰, Alke Meents¹⁰¹

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RSC Advances

PAPER



Cite this: *RSC Adv.*, 2021, 11, 14922

Received 17th March 2021
Accepted 15th April 2021

DOI: 10.1039/d1ra02118d
rsc.li/rsc-advances

In vitro studies of maleidride-forming enzymes†

Sen Yin, Steffen Friedrich, Vjaceslavs Hrupins and Russell J. Cox *

In vitro assays of enzymes involved in the biosynthesis of maleidrides from polyketides in fungi were performed. The results show that the enzymes are closely related to primary metabolism enzymes of the citric acid cycle in terms of stereochemical preferences, but with an expanded substrate selectivity. A key citrate synthase can react both saturated and unsaturated acyl CoA substrates to give solely *anti* substituted citrates. This undergoes *anti*-dehydration to afford an unsaturated precursor which is cyclised *in vitro* by ketosteroid-isomerase-like enzymes to give byssochlamic acid.

Introduction

Alkyl citrates are a class of fungal secondary metabolites derived from a polyketide or fatty acid component and oxaloacetic acid. They include relatively simple monomeric compounds such as **1** and **2**, piliformic acid **3**,¹ oryzines A and B **4–5**,² sporothriolide **6**,³ CJ-13,981 **7** (ref. 4 and 5) and hexylitaconic acids⁶ known from *Aspergillus niger* (Fig. 1). More complex examples include compounds such as viridifungin A **8** (ref. 7) and squalestatin S1 **9** (ref. 8 and 9) which are potent inhibitors of squalene synthase. In many cases dehydration of the alkyl citrate affords a maleic anhydride as observed in **1** and **2**, and dimerisation of these monomers leads to the formation of compounds with large alicyclic rings known as heptadrides, octadrides and nonadrides.¹⁰ Collectively such compounds are known as maleidrides.¹¹ These include agnestadride A **10**,¹¹ zopfellein **11** (ref. 12 and 13) byssochlamic acid **12** (ref. 14) and the selective herbicide cornexistin **13**.^{15,16} These types of compounds are wide-spread in fungi (Fig. 1).¹⁷

To-date the main evidence for the biochemical reactions involved in the biosynthesis of alkyl citrates and maleidrides has come indirectly from *in vivo* genetic knockout or heterologous expression experiments. Thus, in the case of byssochlamic acid **12**, for example, we showed that co-expression in the host *Aspergillus oryzae* of genes encoding: a fungal highly-reducing polyketide synthase (hr-PKS); an $\alpha\beta$ -hydrolase; a citrate synthase-like protein (CS); and a homolog of 2-methylcitrate dehydratase (2MCDH) results in production of **1** and **2**. Likewise, Oikawa and coworkers expressed homologous genes from the phomoidride BGC from unidentified fungus ATCC 74256 and related genes from *Talaromyces stipitatus* and showed production of anhydride monomers related to **1** and **2**.¹⁸

OCI, BMWZ, Leibniz University of Hannover, Schneiderberg 38, 30167, Hannover, Germany. E-mail: russell.cox@oci.uni-hannover.de

† Electronic supplementary information (ESI) available. See DOI: 10.1039/d1ra02118d

14922 | *RSC Adv.*, 2021, 11, 14922–14931

These experiments suggest a series of events in which a polyketide synthase produces a linear acyl group attached to its acyl carrier protein (ACP) **14**. This must be released (*e.g.* **15**) and reacted with oxaloacetate to form a vinyl citrate **16** by the citrate synthase enzyme (Scheme 1). Dehydration by the 2MCDH enzyme would then provide the observed substituted maleic

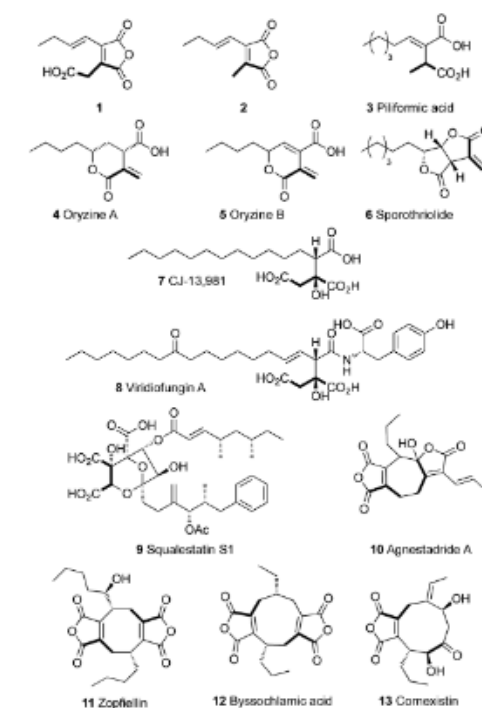


Fig. 1 Structures mentioned in the text. Bold bonds indicate atoms derived from oxaloacetate.

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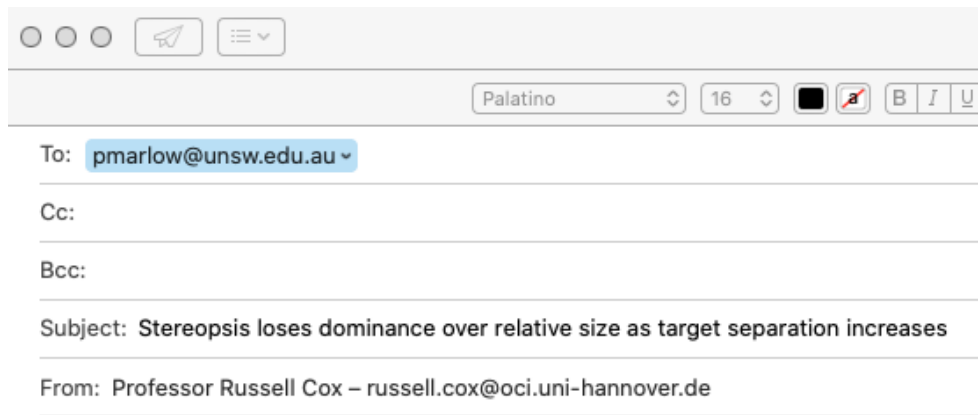
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Phillip Marlow[¶], Barbara J Gillam

School of Psychology, University of New South Wales, Sydney 2052, NSW, Australia;

e-mail: pmarlow@unsw.edu.au

Received 8 June 2011, in revised form 13 December 2011

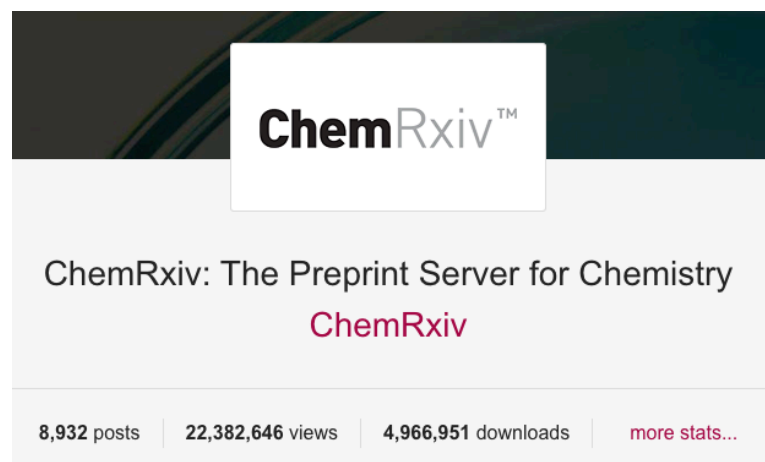


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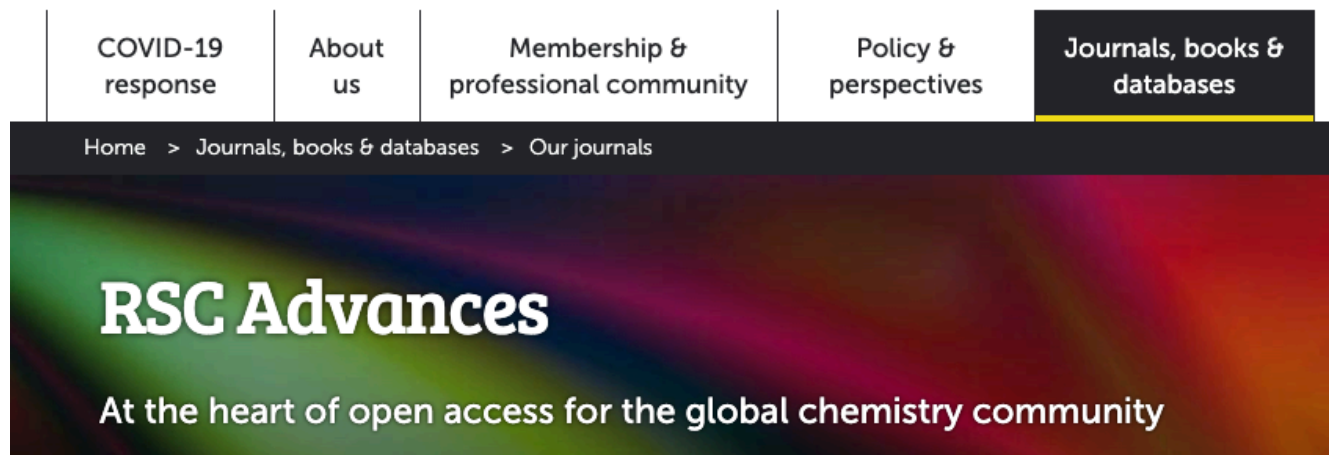
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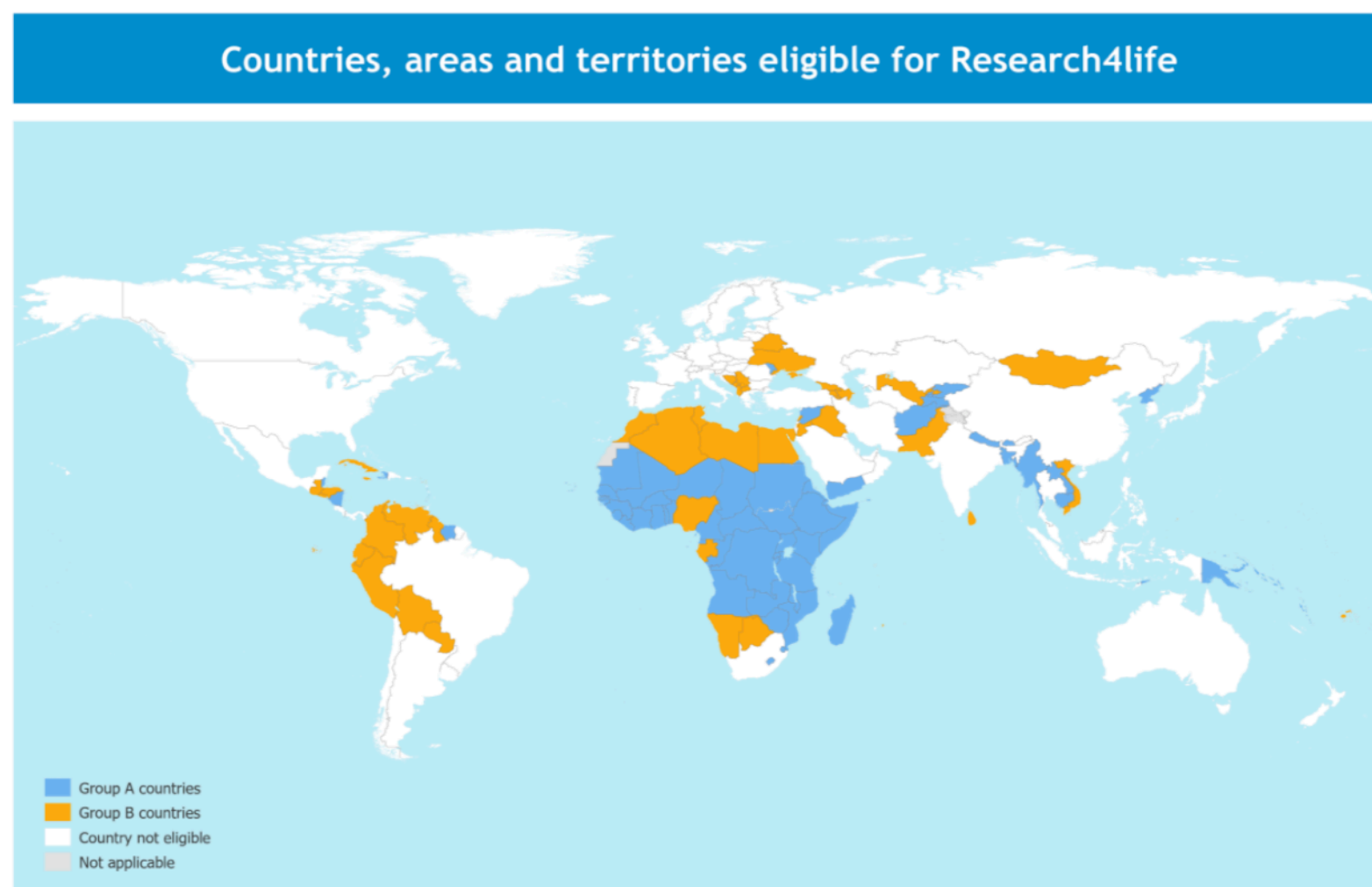
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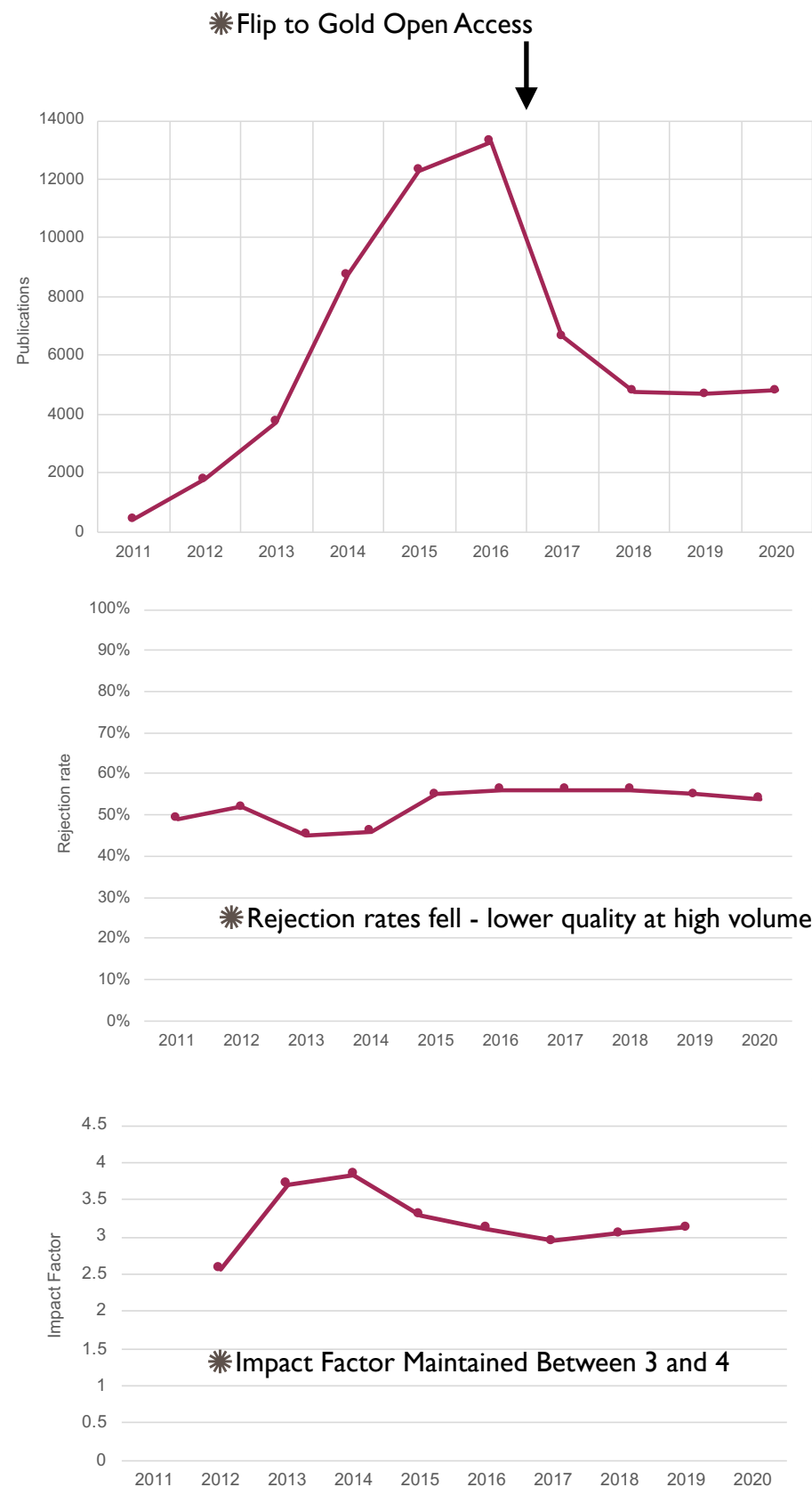
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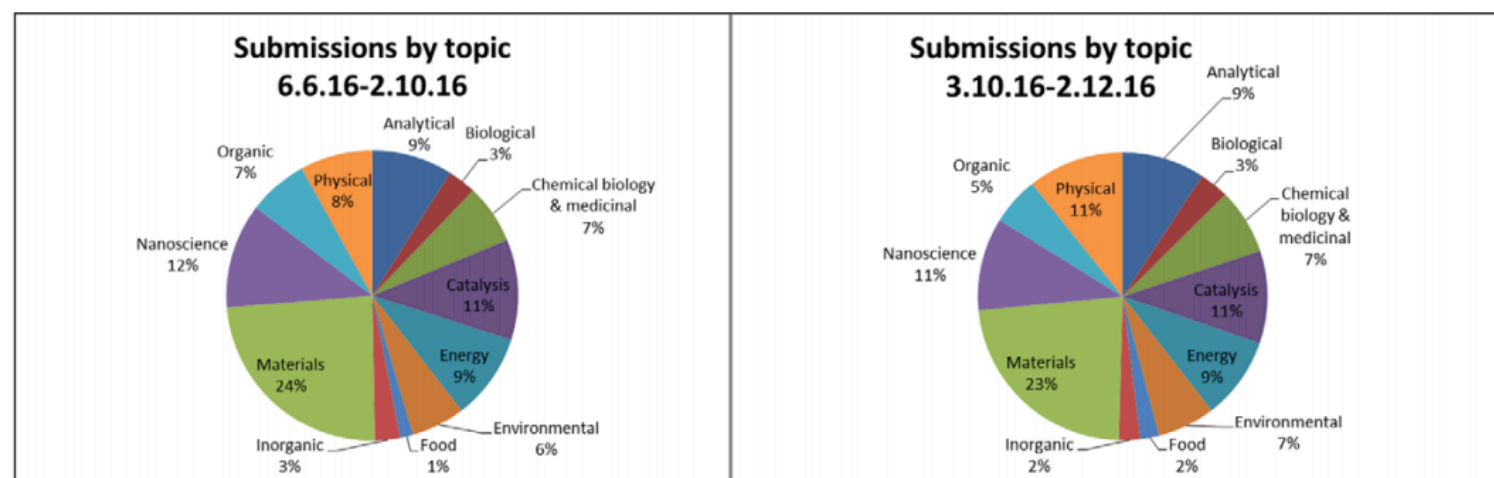


Figure 5. Submissions by scientific topic before and after the journal transitioned to OA

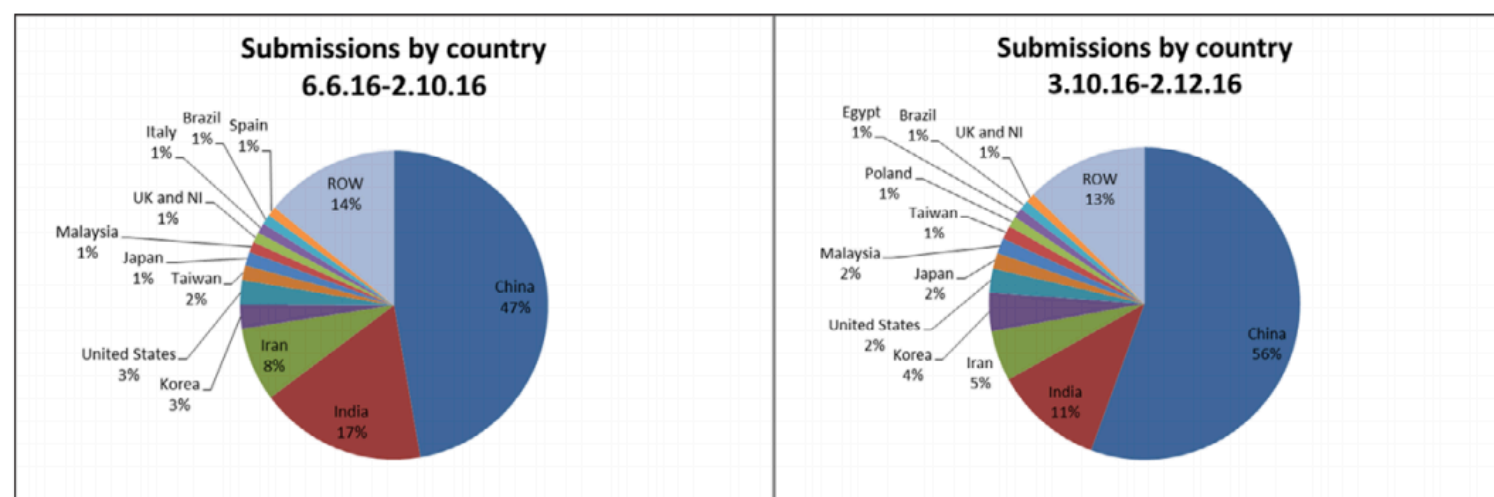


Figure 6. Submissions by country before and after the journal transitioned to OA. (The 'rest of the world' [ROW] section is made up of 71 countries and 50 countries, respectively)

* E. K. Wilson and J. Humphrey, *Insights*, 2017, **30(1)**, 38 - 46.

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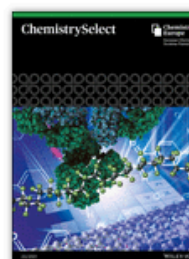
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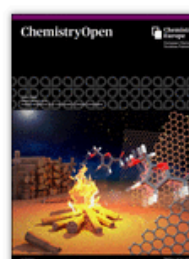
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Is there a gender gap in chemical sciences scholarly communication?†

A. E. Day, P. Corbett and J. Boyle

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Advantages of Open Access Model

- ✳ Fast and Free Access for all readers
- ✳ Maintains Peer Review
- ✳ Maintains High Quality PDF
- ✳ Simplified System
- ✳ Compatibility with Past and Present
- ✳ More Reads, Downloads and Citations
- ✳ APCs can be used to support under-represented groups
- ✳ Clears the way for other 'Open' Innovations - Open Peer Review etc

Disadvantages of Open Access Model

- ✳ Funding Model Confused
- ✳ Author Pays / Library pays for author
- ✳ Funding Model Varies Internationally
- ✳ Funding Model Varies by Journal (even within a single publisher)
- ✳ APCs vary widely - ca 1000 Euro to ca 10,000 Euro



✳ They are out to get you!

☆ Megan Taylor

Junk - o...hannover.de 18:09

MT

Information about special issue on
To: Russell Cox,
Reply-To: Megan Taylor

Hello Dr. Schor Raissa,

On the behalf of "**Austin Child & Adolescent Psychiatry**", this is a cordial invitation to publish your research work in our Journal upcoming Issue (Volume 5).

We are focused on publishing quality research articles, in-order to spread the research and development results to the world.

If you are interested in submission, please submit before June 15, 2021.

Please feel free to ask for more information about our journal.

I am looking forward to hearing from you.

**Best Regards,
Megan Taylor
Editorial Assistant
Journal of Child & Adolescent Psychiatry**

Publications - Where are we now ?



✱ Old Model: The Living Dead



✱ Hybrid Model:
Functional but Imperfect



✱ Gold Open Access: The Future



- ✱ Transition - *Movement of Budgets from Subscriptions to APCs*
- ✱ The transition itself is Painful - Worse than Either Full Model
- ✱ Scientists are Caught Between the Funders and the Publishers
- ✱ Nobody is Really Enjoying This !

Reccomendations - What Can We Do ?

Readers, Researchers, Teachers and Students

- ✳ No Change....

Scientists

- ✳ Select and Support Society Journals
- ✳ Select and Support Open Access
- ✳ Prioritise Reviewing and Editorial Work - *Cui Bono ?*

Funders

- ✳ Continue to Support and Push for Wider Open Access
- ✳ Accelerate Plan S
- ✳ Financial Support During the Transition

Publishers

- ✳ Only Start New Open Access Journals
- ✳ Flip More Journals - there is little to lose and much to gain
- ✳ More Deals with Funders and Libraries



- ✳ Gold Open Access: The Future

Libraries

- ✳ Keep Pushing the Publishers
Militant Action Where Needed !
- ✳ Simplify and Publicise the OA Payment Options

Personal !
^

Open Access in Chemistry - A Scientist's View

Thanks

- ✱ Janna Neumann, LU - Hannover
- ✱ Agnieszka Wenninger, FU Berlin
- ✱ Cox Group and Funders
- ✱ Royal Society of Chemistry



Institut für Organische Chemie

