Research dissemination: preprints, data repositories, and the traditional journal

October 9, 2017











Survey Drawing











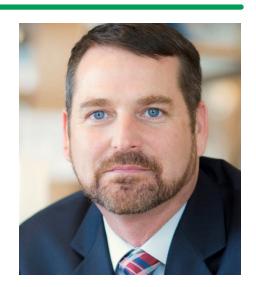
Announcements

• After today's presentation, please take the survey!

Our presenter today:

Gary Miller, PhD

- Professor, Rollins School of Public Health
- Asa Griggs Candler Professor of Environmental Health
- Doctoral training in Pharmacology & Toxicology
- Postdoctoral training in Molecular Neuroscience
- Director of the Emory HERCULES center, an NIEHS-funded center focused on the exposome, the environmental analogue to the genome.



- Serves as Director of Emory's CHEAR U2C Center and Emory's NIEHS-funded T32
 Training Grant in Environmental Health Sciences and Toxicology.
- A Georgia Research Alliance Distinguished Investigator and received the Achievement Award from the Society of Toxicology.
- Serves as Editor-in-Chief of Toxicological Sciences, the official journal of the Society of Toxicology.

Research dissemination: preprints, data repositories, and the traditional journal

Gary W. Miller, PhD
Associate Dean of Research
Rollins School of Public Health

Toxicological Sciences

SOT | Society of Toxicology

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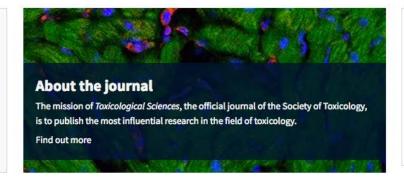
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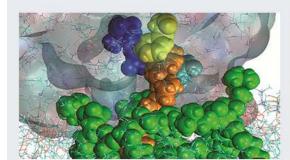
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Current Issue Volume 156, Issue 1 March 2017 Editor-in-Chief Gary W. Miller

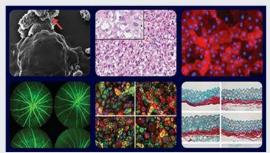






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Toxicology News

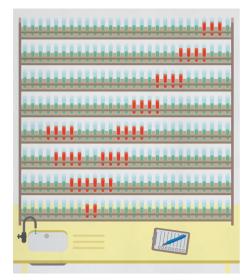
- SOT 2017 Annual Meeting Website Has Launched: See You in Baltimore!
- Nominate SOT Members for SOT Council and Elected Standing Committees by August 1
- Nominate a Worthy Candidate for the 2017 SOT Arnold J.

Policy: NIH plans to enhance reproducibility

Francis S. Collins & Lawrence A. Tabak

27 January 2014

Francis S. Collins and Lawrence A. Tabak discuss initiatives that the US National Institutes of Health is exploring to restore the self-correcting nature of preclinical research.



NIH plans to enhance reproducibility

Francis S. Collins and Lawrence A. Tabak discuss initiatives that the US National Institutes of Health is exploring to restore the self-correcting nature of preclinical research.

A growing chorus of concern, from scientists and laypeople, contends that the complex system for ensuring

shorter term, however, the checks and balances that once ensured scientific fidelity have been hobbled. This has compromised outnumbered by the hundreds of thousands published each year in good faith.

Instead, a complex array of other factors seems to have contributed to the lack of reproducibility. Factors include poor training of researchers in experimental design; increased emphasis on making provocative statements rather than presenting technical details; and publications that do not report basic elements of experimental design4 Crucial experimental design elements that are all too frequently ignored include blinding, randomization, replication, sample-size calculation and the effect of sex differences. And some scientists reputedly use a 'secret sauce' to make their experiments work and withhold details from publication or describe them only vaguely to retain a competitive edge5. What hope is there that other scientists will be able to build on such work to further biomedical progress?

Exacerbating this situation are the policies and attitudes of funding agencies, academic centres and scientific publishers. Funding agencies often uncritically encourage the overvaluation of research published in high-profile journals. Some academic centres also provide incentives for publications in such journals, including promotion and tenure, and in extreme circumstances, cash rewards.

Then there is the problem of what is not published. There are few venues for researchers to publish negative data or papers that point out scientific flaws in previously published work. Further compounding the problem is the difficulty of accessing unpublished data—and the failure of funding agencies to establish or enforce policies that insist on data access.

PRECLINICAL PROBLEMS

Reproducibility is potentially a problem in all scientific disciplines. However, human clinical trials seen to be less at risk because they are already governed by various regulations that stipulate rigorous design and independent oversight—including randomization, blinding, power estimates, pre-registration of outcome measures in standardized, public databases such as ClinicalTrials gov and oversight by institutional review boards and data safety monitoring boards. Furthermost the clinical trials community has taken important steps towards adopting standard reporting elements.

Proceedings of the National Academy of Sciences of the United States of America

Revised standards for statistical evidence

Valen E. Johnson¹

Department of Statistics, Texas A&M University, College Station, TX 77843-3143

Edited by Adrian E. Raftery, University of Washington, Seattle, WA, and approved October 9, 2013 (received for review July 18, 2013)



THE WALL STREET JOURNAL.

THE SATURDAY ESSAY

The Breakdown in Biomedical Research

Contaminated samples, faulty studies and inadequate training have created a crisis in laboratories and industry, slowing the quest for new treatments and cures



ILLUSTRATION: DOUG CHAYKA

By RICHARD HARRIS
Updated April 7, 2017 2:05 p.m. ET

Open Mike

Helping connect you with the NIH perspective, and helping connect us with yours

Posted on March 28, 2017 by Mike Lauer

Following Up On Interim Research Products

The role of preprints — complete and public draft manuscripts which have not gone through the formal peer review, editing, or journal publishing process — continues to be a hot topic in the biological and medical sciences. In January, three major biomedical research funders — HHMI, the MRC, and the Wellcome Trust, changed their policies to allow preprints to be cited in their progress reports and applications.

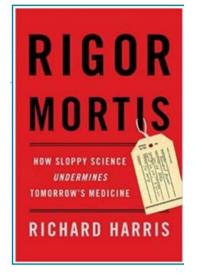


Dr. Michael Lauer is NIH's Deputy Director for Extramural Research, serving as the principal scientific leader and advisor to the NIH Director on the NIH extramural research program.



March 8-10, 2017; Washington, D.C. Reproducibility of Research: Issues and Proposed Remedies





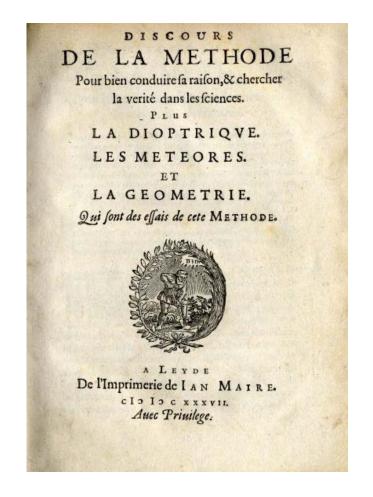
Retraction Watch

Tracking retractions as a window into the scientific process

"Failure is an essential part of science:" ...a new book on reproducibility

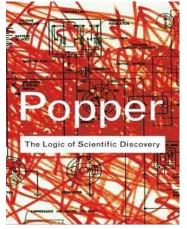
This is not a new topic

"Discourse on the Method of Rightly Conducting One's Reason and of Seeking Truth in the Sciences" Rene Descartes, 1637



Rigor, Reproducibility, and Method

- Popper (Logic of Scientific Discovery, 1934)
- Kuhn (Structure, 1962)
- Feyerabend (Against Method, 1975)



 How we define and use the scientific method has been the topic of debate for centuries. It is a never-ending struggle to seek the truth.

Improving Reproducibility in Toxicology @

Gary W. Miller X

Toxicol Sci (2014) 139 (1): 1-3. **DOI:** https://doi.org/10.1093/toxsci/kfu050

Published: 15 April 2014

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Issue Section: Editorial

Over the past few months there has been considerable discussion in scientific circles regarding reproducibility of data, or more specifically, the lack thereof (Nature, 2012, 2013). This is a very serious issue for science, including the discipline of toxicology. The director and deputy director of the National Institutes of Health (NIH) in the United States, Dr Francis Collins and Dr

Poland et al. Particle and Fibre Toxicology 2014, 11:42 http://www.particleandfibretoxicology.com/content/11/1/42



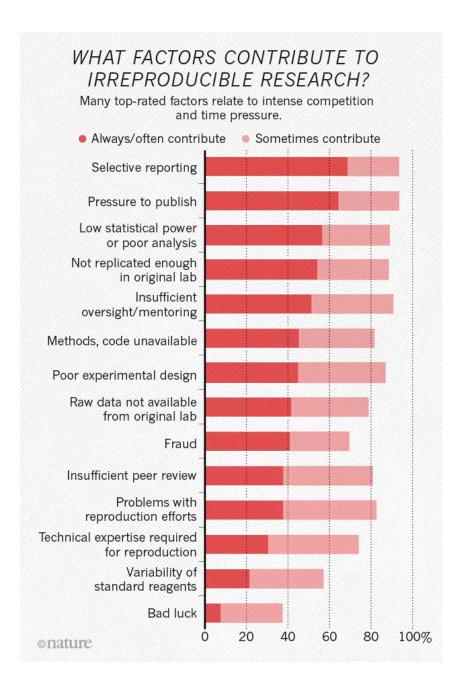
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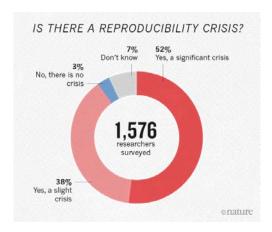
The elephant in the room: reproducibility in toxicology

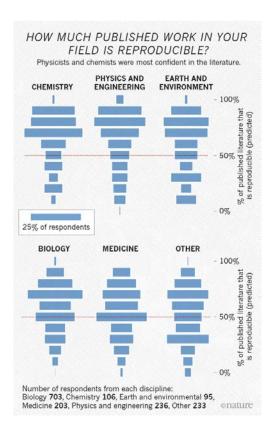
Craig A Poland^{1*}, Mark R Miller², Rodger Duffin³ and Flemming Cassee^{4,5}

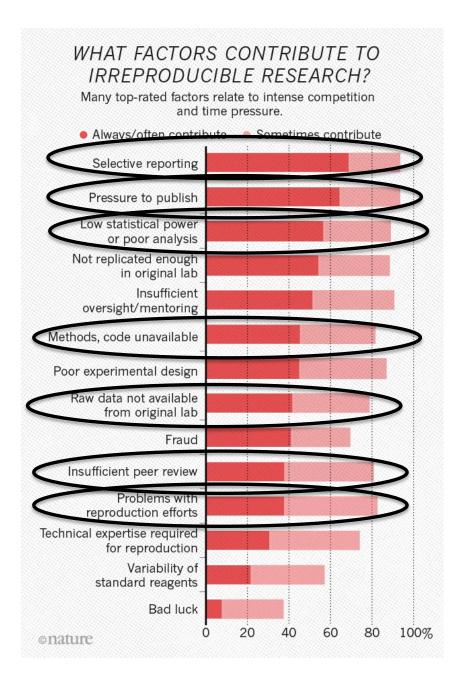
The issue of reproducibility of results in toxicology has long been a concern and, perhaps, at the back of many of our minds but not necessarily at the forefront of our thinking – 'the elephant in the room'. Are the results we have published literally *our* results or are they reproducible and truly part of a credible theory? In the excellent editorial by Gary Miller [1], Editor-in-Chief of the journal *Toxicological Sciences*, he discusses the issue of reproducibility in scientific manu-

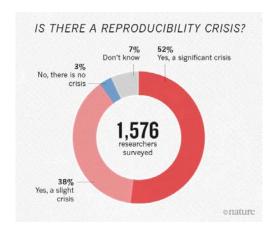
driven by the researcher, are heavily influenced by funding bodies, public opinion and political motivations. All will play a role in the distribution of a limited pool of research funds, and rightly expect progress in return for financial support. Yet a lack of reproducibility can destabilise research and undermine the confidence of stakeholders. An additional area of concern relating to reproducibility is when findings are translated into the 'real world' where acceptance and use of premature conclusions resulting

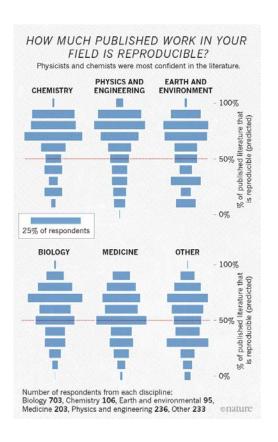






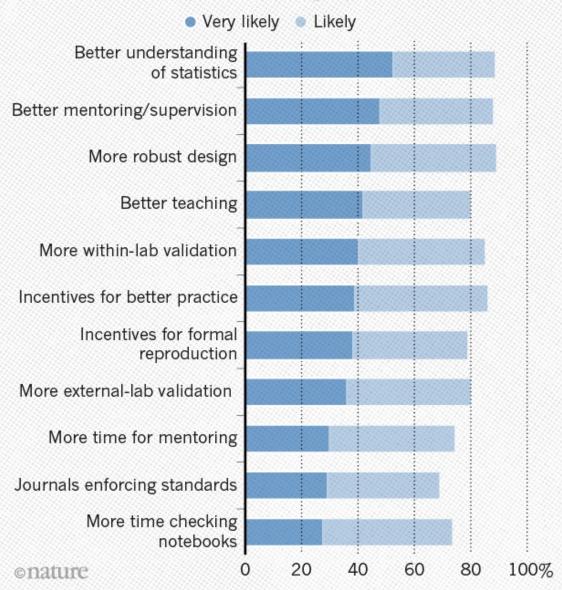






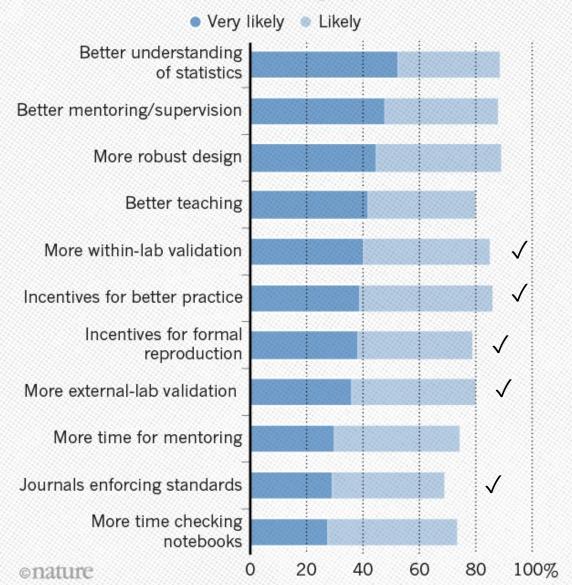
WHAT FACTORS COULD BOOST REPRODUCIBILITY?

Respondents were positive about most proposed improvements but emphasized training in particular.



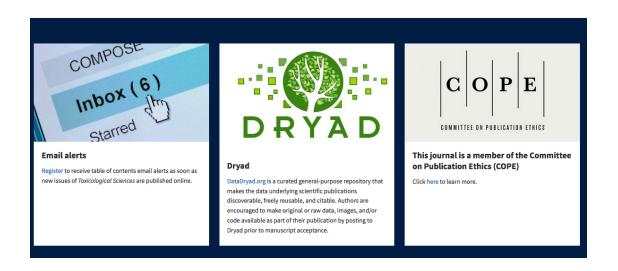
WHAT FACTORS COULD BOOST REPRODUCIBILITY?

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Beyond the NIH requirements

Use of data repositories, providing a venue for deposition of large data sets, code, and even methods



"There is no idea, however ancient or absurd, that is not capable of improving our knowledge." -Paul Feyerabend











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Schwarzfeld MD, Broad GR, Sperling FAH (2015) Data from: Molecular phylogeny of the diverse parasitoid wasp genus Ophion Fabricius (Hymenoptera: Ichneumonidae: Ophioninae). Systematic Entomology http://dx.doi.org/10.5061/dryad.49g98

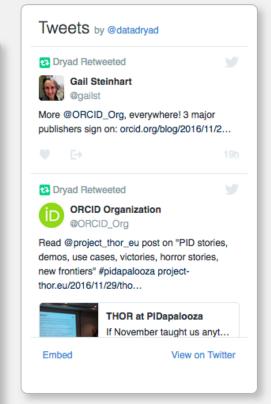
Pekcan-Hekim Z, Hellén N, Härkönen L, Nilsson PA, Nurminen L, Horppila J (2016) Data from: Bridge under troubled water: turbulence and niche partitioning in fish foraging. Ecology and Evolution http://dx.doi.org/10.5061/dryad.3q7c9

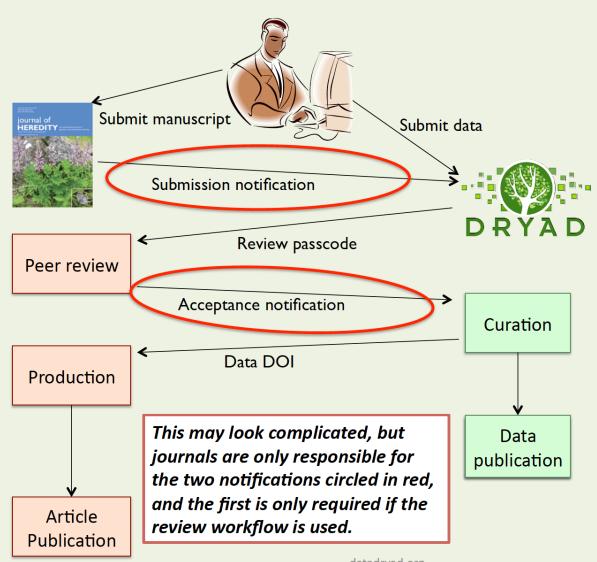
Lehnert S, Devlin R, Pitcher T, Semeniuk C, Heath D (2016) Data from: Redder isn't always better: cost of carotenoids in Chinook salmon eggs. Behavioral Ecology http://dx.doi.org/10.5061/dryad.2bp67

Douhard M, Pigeon G, Festa-Bianchet M, Coltmann DW, Guillemette S, Pelletier F (2016) Data from: Environmental and evolutionary effects on horn growth of male bighorn sheep. Oikos http://dx.doi.org/10.5061/dryad.m5648

Staats E, Agosta S, Vonesh J (2016) Data from: Predator diversity reduces habitat colonization by mosquitoes and midges. Biology Letters http://dx.doi.org/10.5061/dryad.2f452

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Mosedale M, Kim Y, Brock W, Roth S, Wiltshire T, Eaddy JS, Keele G, Corty R, Xie Y, Valdar W, Watkins P

Date Published: December 20, 2016

DOI: http://dx.doi.org/10.5061/dryad.ch4p5

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Subfunctionalization of Paralogous Aryl Hydrocarbon Receptors from the Frog Xenopus Laevis: Distinct Target Genes and Differential Responses to Specific Agonists in a Single Cell Type

Scott H. Freeburg, Eric Engelbrecht, and Wade H. Powell

Dryad in the UK and USA—Prospective and Retrospective Data Publication Kursheed Khan and Andrew Weeks

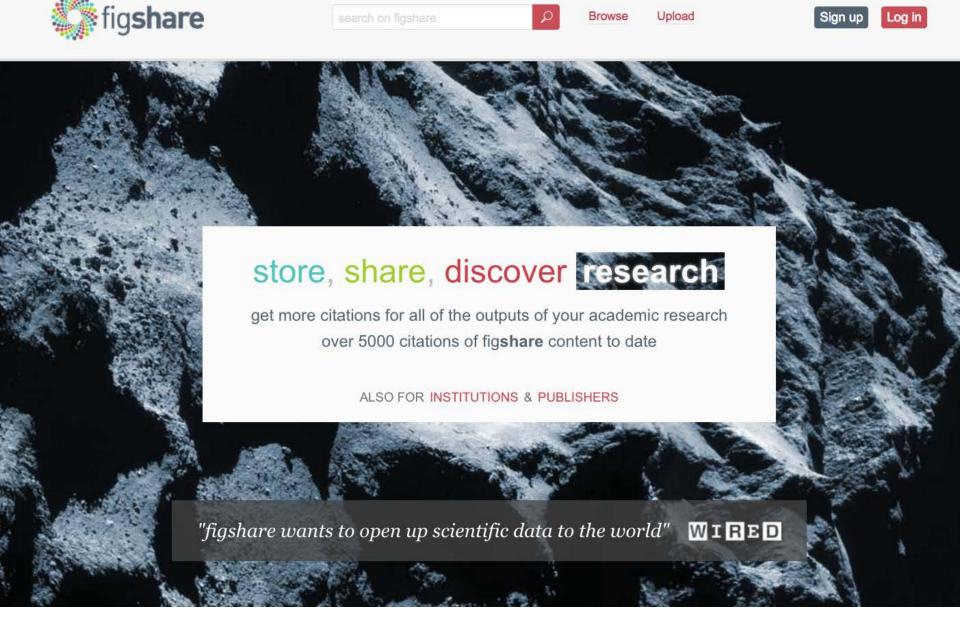
Editor's Highlight: Neonatal Activation of the Xenobiotic–Sensors PXR and CAR Results in Acute and Persistent Down–regulation of PPARα–Signaling in Mouse Liver Cindy Yanfei Li, Sunny Lihua Cheng, Theo K. Bammler and Julia Yue Cui

Identification of the Additional Mitochondrial Liabilities of 2-Hydroxyflutamide When Compared With its Parent Compound, Flutamide in HepG2 Cells

Amy L. Ball, Laleh Kamalian, Ana Alfirevic, Jonathan J. Lyon and Amy E. Chadwick

Vesicular Monoamine Transporter 2 (VMAT2) Level Regulates MPTP Vulnerability and Clearance of Excess Dopamine in Mouse Striatal Terminals

Kelly M. Lohr, Merry Chen, Carlie A. Hoffman, et. al





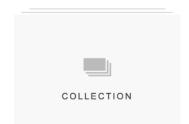
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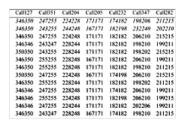
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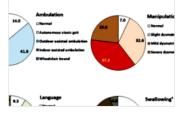
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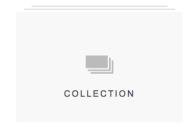
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Structural Evidence for the Dopamine-First Mechanism of Norcoclaurine Synthase

Version 2 V Published on 09 Oct 2017 - 08:49

Norcoclaurine synthase (NCS) is a Pictet-Spenglerase that catalyzes the first key step in plant benzylisoquinoline alkaloid metabolism, a compound family that includes bioactive natural products such as morphine. The enzyme has also shown great potential as a biocatalyst for the formation of chiral isoquinolines. Here we present new high-resolution X-ray crystallography data describing *Thalictrum flavum* NCS bound to a mechanism-inspired ligand. The structure supports two key features of the NCS "dopamine-first" mechanism: the binding of dopamine catechol to Lys-122 and the position of the carbonyl substrate binding site at the active site entrance. The catalytically vital residue Glu-110 occupies a previously unobserved ligand-bound conformation that may be catalytically significant. The potential roles of inhibitory binding and alternative amino acid conformations in the mechanism have also been revealed. This work significantly advances our understanding of the NCS mechanism and will aid future efforts to engineer the substrate scope and catalytic properties of this useful biocatalyst.

CITE THIS COLLECTION

Lichman, Benjamin R.; Sula, Altin; Pesnot, Thomas; Hailes, Helen C.; Ward, John M.; H. Keep, Nicholas (2017): Structural Evidence for the Dopamine-First Mechanism of Norcoclaurine Synthase. ACS Publications.

https://doi.org/10.1021/acs.biochem.7b00769

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READ THE PEER-REVIEWED ARTICLE:

Structural Evidence for the Dopamine-First Mechanism of Norcoclaurine Synthase



AUTHORS

Benjamin R. Lichman Altin Sula Thomas Pesnot Helen C. Hailes John M. Ward Nicholas H. Keep

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Volume 95 Issue 40 | p. 22 | News of The Week Issue Date: October 9, 2017 | Web Date: October 5, 2017

Publishers taking legal action against ResearchGate to limit unlicensed paper sharing on networking site



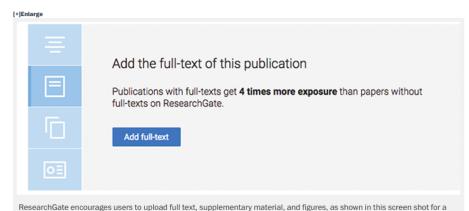
Credit: ResearchGate

Separate suit against pirate site Sci-Hub by the American Chemical Society appears likely to succeed

By Jyllian Kemsley & Andrea Widener

C&EN story referenced on the site.

. . . .



Several scientific publishers, including the American Chemical Society, are expanding their legal actions against sites that facilitate sharing of scientific articles in violation of copyright law.

The publishers are preparing to issue what could be millions of notices to the scientific networking site **ResearchGate** asking it to remove copyrighted material. ACS and Elsevier have

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doi: 10.1093/toxsci/kfu237 EDITORIAL

EDITORIAL

Data Sharing in Toxicology: Beyond Show and Tell

Gary W. Miller¹

EDITORIAL

Making Data Accessible: The Dryad Experience

Gary W. Miller¹

Editor-in-Chief, Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, Georgia 30322 and ¹For correspondence. E-mail: gary.miller@toxicology.org

EDITORIAL

More than Manuscripts: Reproducibility, Rigor, and Research Productivity in the Big Data Era

Lance A. Waller¹ and Gary W. Miller²

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ASM Media Advisory: ASM No Longer Supports Impact Factors for its Journals

Washington, DC - July 11, 2016 - The editors-in-chief of ASM journals and ASM leadership have decided to no longer advertise the impact factors of ASM journals on the journals' websites. This decision was made in order to avoid contributing to a distorted value system that inappropriately emphasizes high IFs. High-IF journals limit the number of accepted articles to create a perception of exclusivity, and individuals receive disproportionate rewards for articles in high IF journals, while science as a whole suffers from a distorted values system and delayed communication of research.

It is the hope of ASM journal editors-in-chief and ASM leadership to move away from this system and the undue focus on journal IF, which detracts from the advancement of scientific research, by removing IFs from ASM journal websites. In doing so, ASM hopes to make a statement of principle that other journals will follow.



NATURE | NEWS





Journal impact factors 'no longer credible'

The measure of scholarly impact is now being manipulated so much that it has ceased to be meaningful, editorial claims

Beat it, impact factor! Publishing elite turns against controversial metric

Senior staff at leading journals want to end inappropriate use of the measure.

THE IMPACT FACTOR'S LONG TAIL

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Journal impact factors are influenced heavily by a small number of highly cited papers. For all journals analysed, most papers published in 2013-14 garnered many fewer citations than indicated by the impact factor

NATURE

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SCIENCE

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Impact factor: 3.1

PLoS ONE

40 50

Number of citations

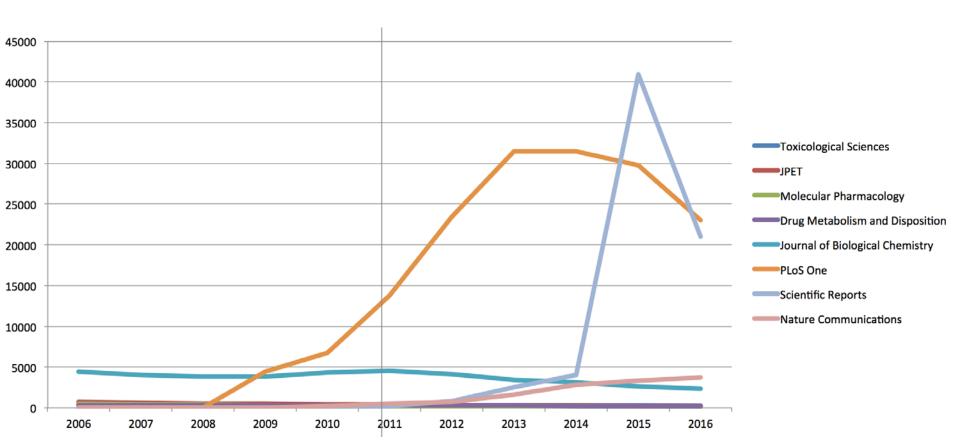
npact factor: 34.7

One way to increase IF

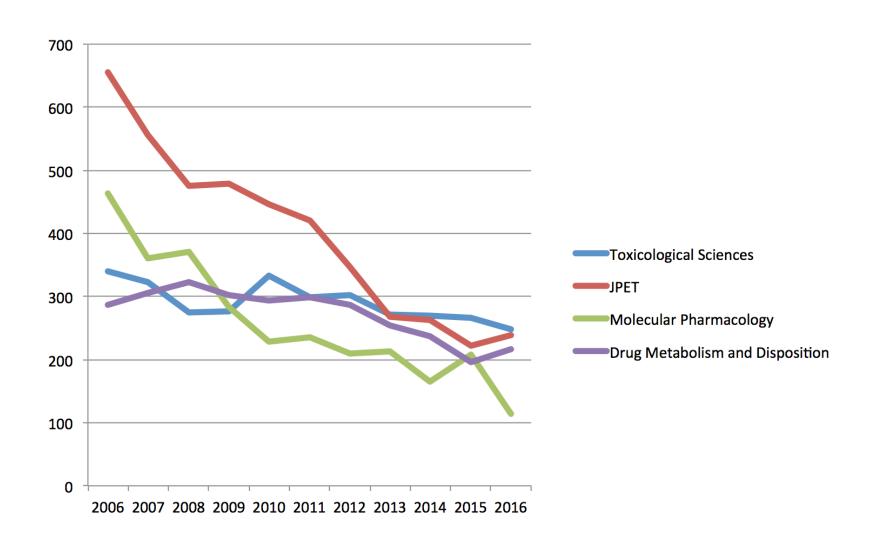
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By PHIL DAVIS | OCT 2, 2017 | 2 COMMENTS

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Microbiology is a growing field, nevertheless, a shrinking proportion of papers are being published in society-sponsored journals, a recent analysis of PubMed records reveals.

An editorial, "Support Science by Publishing in Scientific Society Journals," was published recently in the journal, *mBio*, by Pat Schloss, chair of the journals board for the American Society for Microbiology (ASM), Arturo Casadevall, Editor in Chief of *mBio* (an ASM journal), and Mark Johnston, the Editor in Chief of *Genetics*, from the Genetics Society of America (GSA).







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American Journal of Gastroenterology Supplements

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BDJ Team

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A new National Institutes of Health policy encourages researchers to include in their grant proposals preprints, which are early, unedited versions of papers that later appear in journals like these.

Sergei25/shutterstock

NIH enables investigators to include draft preprints in grant proposals

By **Jocelyn Kaiser** | Mar. 24, 2017, 5:45 PM

Researchers should feel free to include preprints, or draft manuscripts that haven't yet been gone through peer review, as part of their applications when they seek funding from the Bethesda, Maryland-based National Institutes of Health (NIH), the agency **announced today**.

arXiv.org, 1992

A rotating black hole in the Galactic Center

```
Heino Falcke (1)
Peter L. Biermann (1)
Wolfgang J. Duschl (2)
Peter G. Mezger (1)
```

Accepted for publication in A&A: December 4, 1992

Abstract

Recent observations of Sgr A* give strong constraints for possible models of the physical nature of Sgr A* and suggest the presence of a massive black hole with $M \leq 2 \cdot 10^6 M_{\odot}$ surrounded by an accretion disk which we estimate to radiate at a luminosity of $< 7 \cdot 10^5 L_{\odot}$. We therefore calculate





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Cell Biology Microbiology Education

Clinical Trials Molecular Biology Synthetic Biology

Developmental Biology Neuroscience Systems Biology

Zoology

Classification: Biological sciences, Pharmacology

Synaptic vesicle glycoprotein 2C (SV2C) modulates dopamine release and is disrupted in Parkinson's disease

Amy R. Dunn¹, Kristen A. Stout¹, Minagi Ozawa¹, Kelly M. Lohr¹, Alison I. Bernstein¹, Yingjie Li^{1,2}, Minzheng Wang¹, Carmelo Sgobio³, Namratha Sastry³, Huaibin Cai³, W. Michael Caudle^{1,2}, and Gary W. Miller*^{1,2}

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The synaptic vesicle glycoprotein 2 (SV2) family of proteins are involved in synaptic function throughout the brain. The whitevesty expressed SV2A has been widely implicated in

Disrupted vesicle function may represent a common pathway to degeneration and identifying novel mediators of

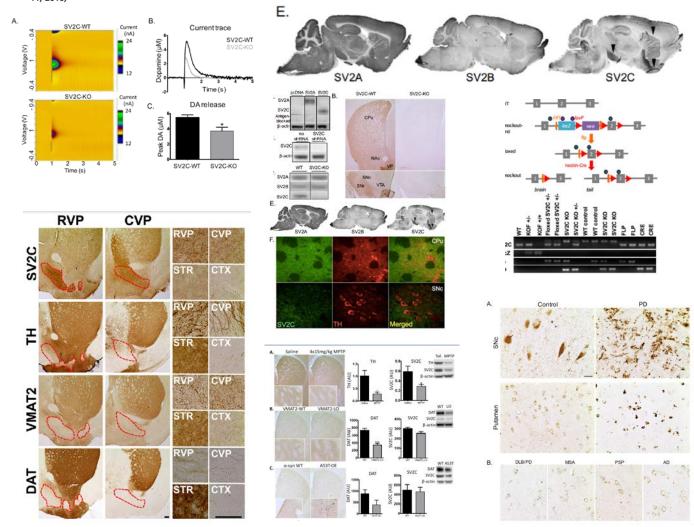
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Synaptic vesicle glycoprotein 2C (SV2C) modulates dopamine release and is disrupted in Parkinson disease

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Abstract

The synaptic vesicle glycoprotein 2 (SV2) family of proteins are involved in synaptic function throughout the brain. The ubiquitously expressed SV2A has been widely

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Editorial

EDITORIAL

Preprints in Toxicology

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Imagine attending a national meeting with the expectation of 50–100 people showing up to your presentation, and looking up

field of physics in 1991. This service called arXiv (pronounced "archive") was originally dedicated to papers in high-energy



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EDITORIAL

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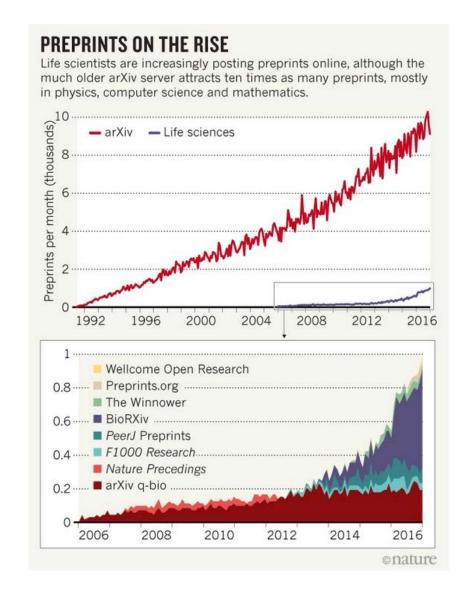






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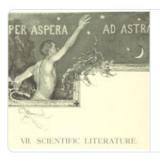
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- Sheldon: For a man whose last observation was our universe may be the surface of a multidimensional supercooled liquid, you're still awake seems like quite the sophomore slump.
- Leonard: You worked out all the math.
- Sheldon: Oh, I did more than work out all the math. I wrote a paper.
- Leonard: You wrote a paper on my idea?
- Sheldon: I wrote a paper on our idea.
- Leonard: When did my idea become our idea?
- Sheldon: When I mixed it with Sheldony goodness and cooked it in the Easy-Bake oven of my mind.
- Leonard: This is good. Our idea is really good.
- Sheldon: Well, the lightbulb in this oven is ridiculously bright.
- Leonard: You know, if no one's thought of this, yet, this could be a big deal.
- Sheldon: Only way we'll know for sure is if we post it online to the pre-print server. I have it ready to go, but I wasn't gonna do it without you.
- Leonard: Wow, it's all happening so fast. Should we just sleep on it?
- Sheldon: We could, but we always run the risk of someone else beating us to the punch.
- Leonard: You're sure it's good?
- Sheldon: My name is right on there with yours. That is
 a surefire mark of quality. That might as well say directed
 by Joss Whedon.
- Leonard: Okay, partner, let's do it.
- Sheldon: Come on. Click the mouse with me.
- Leonard: One, two three.
- Together: Click.
- Leonard: Well, we did it.
- Sheldon: Yes, we did, my friend.



Guest Post: Emory's Gary Miller, "The Literature of Science"



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Emory Professor and journal Editor in Chief Gary Miller offers a long term view of the scholarly literature and offers thoughts on the important values worth preserving in the shift from print to d...

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EDITORIAL

The Literature of Science

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Pouring through the stacks of journals during my early scientific training, I was awestruck. Reading scientific papers from 50 to 100 years ago instilled a sense of reverence. I could peruse the scientific literature for hours, not even looking for topics within my discipline. The writing was rich. The contributions were ob-

making the output seem more abstract and distancing the current creators of scientific knowledge from the archives of scientific literature. Does an interactive PDF convey the findings as well as the weathered and tattered pages of history? I am no Luddite, but at times I deliberately eschew technology because