

ChemRxiv: The Preprint Server for the Chemistry Community

Darla Henderson, Ph.D.

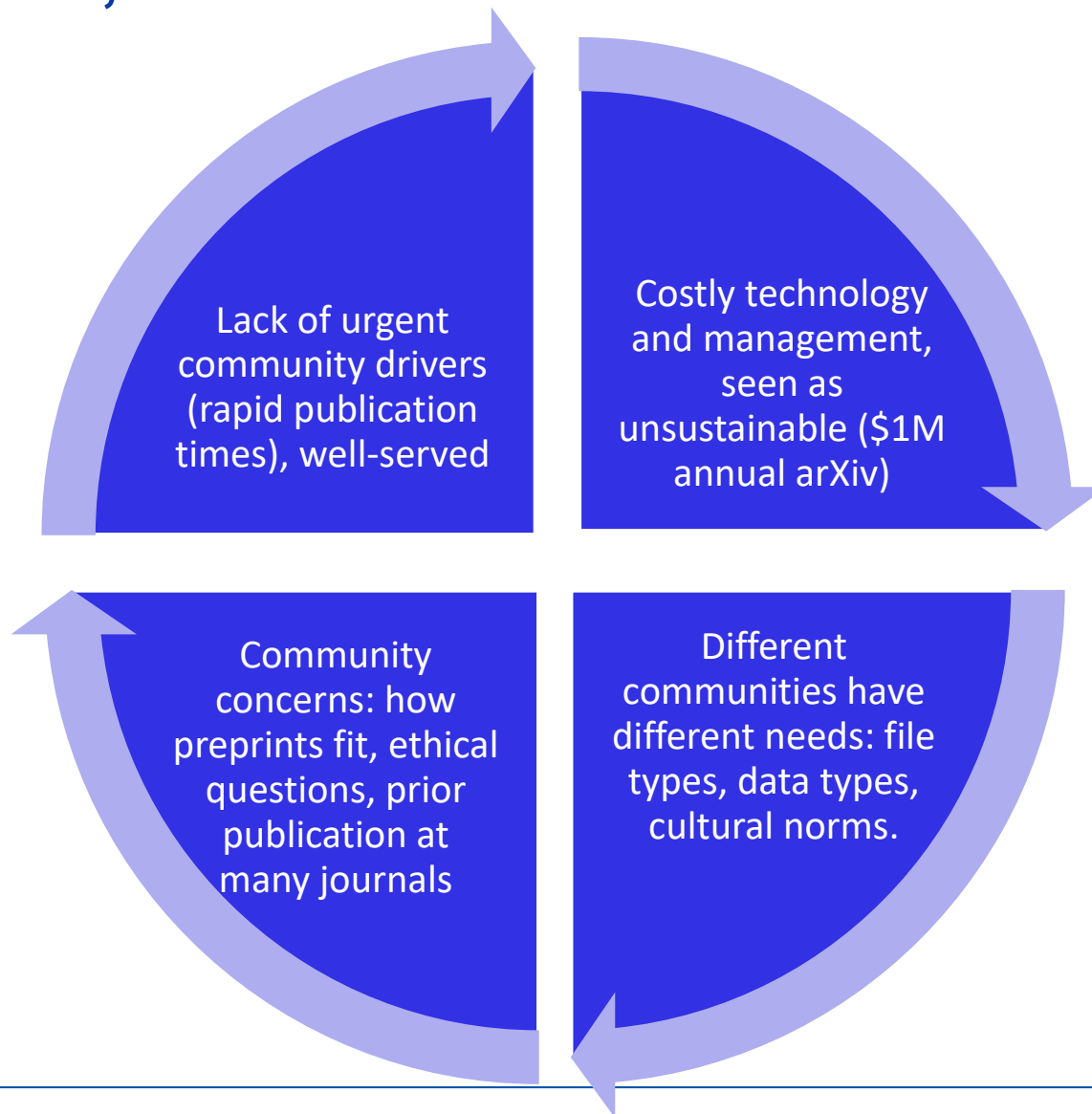
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Preprints and chemistry: precedent, unresolved issues



Preprint R&D Phase

Found our bearings:

- Re-invigorated research in preprints
- Logical piece of the chemistry communication cycle
- Clear that successful preprint servers are a community effort

Challenged existing assumptions

- Old: Community uninterested, chemistry journals publish rapidly.
- New: Many (not all) are now willing to experiment. Recognize additional benefits beyond improvements in time to publication

- Old: Preprints have unsustainable costs.
- New: Technology solutions make costs more manageable

Focused on the value we (and our partners) bring

E.g., Core assets ACS is known for:

- Quality and ethical peer review and publishing
- Streamlined simple submission, peer review, and publishing
- Community-led processes, practicing research scientists
- Strong discoverability - smart systems, global reach



LAURA KIESSLER



Engaged. Everywhere. Continuously. Ongoing. Integral.

- Practicing chemists: >100 meetings and phone interviews, 50+ surveys with ACS Journal Editors, technical ACS Divisions
- Journal Editorial board meetings, visiting and talking with other journals outside ACS, engaging with societies (>500 practicing research editors around the globe, >1000 EAB members)
- With bioRxiv, arXiv, other societies, publishers, funding agencies, initiatives (ASAPbio) or interested parties in this space
- PR in August 2016 invites other participants to the table, opens door to broader feedback



Committed to Think Sustainably. From the Beginning.

- Don't assume it has to work the way it always has. Be willing to experiment. Collected broad responses to RFP
- Evaluated sustainability issues over a 5-10 year period, identified key costs that needed to scale and mapped out plans to address

Why chemistry authors care about preprints



ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

- **Broad engagement before publication** can improve manuscripts that are then submitted and published in journals.
- **Share urgent information, data, and new findings** with communities months before publication, may relax time pressures during peer review process
- Find others in similar areas for **collaborations** or discussions
- Document research results, provide scholarly credit for **grant reviewers, employers** prior to publication
- **In some cases, establish priority** of a discovery (providing a timestamp)
- **Attract attention** of journal editors, journalists to important work
- In some recently emerging cases, because their funders care
- **Speed up science** – rapid evaluation of controversial results

Why chemistry funders care about preprints

- **More rapid dissemination** of research advances they funded
- **Speeds up science**
- **Improves collaborations**
- **Improves grant assessment**, fellowship reviews, particularly for starting career scientists who have less time to build repertoire – better information than “manuscript submitted” or “paper in press”
- Gains research and researchers they funded **broad exposure** consistent with public access policies and goals
- **Does not preclude nor replace the importance of validation** through peer review and publication in authoritative journals, anticipate grant renewals will take this difference into consideration



54,000
members



>30,000
members

**Combined, ChemRxiv governance
today already represents
>234,000 member chemists**



ACS
Chemistry for Life

>150,000
members

Scholarly societies bring great value to governance of a preprint server

1. **Mission-led, skilled.** Missions, visions, and skillset center around engaging, educating, informing the community, organizing and advancing the fields they represent.
2. **Community-led, diverse.** Well-known for coordinating community-led governance and best practices, established infrastructure and experience, aware of diversity needs and biases and seek for representative status. Can reduce the signal to noise of a less focused service.
3. **Sustainability-centered.** Driven to focus on sustainability, experienced strategies ready
4. **Social change drivers.** Well-positioned for innovating, experimenting, and addressing community challenges – social, publishing, communication, and technological
5. **Non-profit** versus commercial can positively impact community perceptions, ease concerns, and allow creation of community-wide, community beneficial resources

TRUST

ChemRxiv Beta: Simple Two-Step Process to Submit

Step 1: One-time Sign up

Sign up to ChemRxiv

First name *

Last name *

Email *

Confirm email *

Password *

I agree to the [Terms & Conditions](#) *

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Authors can track the status and progress of their preprint

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DP Henderson

My data

Activity

+ Create a new item

61.24 kB 20 GB

search my data...



Actions

STATUS

TYPE

CREATED

SIZE



test file 1.docx



PREPRINT

18.8.2017
22:13

11.17 kB



Test File



PREPRINT

18.8.2017
20:50

25.03 kB



Test File 2



PREPRINT

18.8.2017
17:33

25.03 kB

Current handling time:
<24 business hours from submission to
posting

Dr. Marshall Brennan

Publishing Manager, ChemRxiv
@ChemRxiv



Applying the appropriate level of triage and helping ensure trust

Triage at ChemRxiv:

- Science (is this science? chemistry related?)
- Plagiarism or previous publication (iThenticate) – ChemRxiv focusing on content not already published to provide sustainable path forward for preprints and avoid community confusion
- Identify offensive, dangerous content for further checks or exclusion
- Proper subject categorization of content
- Ensure files are readable and viewable

Is Triage at ChemRxiv the same as peer review at a journal?

No. Most journals conduct the same checks as triage above. However, at ChemRxiv, no assessment is made of the accuracy, completeness, or import of the science.

ChemRxiv: Preservation, integrity, user features

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10-step Synthesis of 20-nor-Salvinorin A by Dynamic Strategic Bond Analysis

17.08.2017, 15:38 by Jeremy Roach, Yusuke Sasano, Cullen Schmid, Saheem Zaidi, Vsevolod Katritch, Raymond Stevens, Laura Bohn, [Ryan Shenvi](#)

Salvinorin A (SalA) is a plant metabolite that agonizes the human *kappa*-opioid receptor (κ -OR) with high affinity and high selectivity over *mu*- and *delta*-opioid receptors. Its therapeutic potential has stimulated extensive semi-synthetic studies and total synthesis campaigns. However, structural modification of SalA has been complicated by its instability, and efficient total synthesis has been frustrated by its dense, complex architecture. Treatment of strategic bonds in SalA as dynamic and dependent on structural perturbation enabled the identification of an efficient retrosynthetic pathway. Here we show that deletion of C20 simultaneously stabilizes the SalA skeleton, simplifies its synthesis and retains its high affinity and selectivity for the κ -OR. The resulting 10-step synthesis now opens the SalA scaffold to deep-seated property modification.

TOPIC

2273 views | 341 downloads | 0 citations

ChemRxiv™

CATEGORIES

• Chemistry

KEYWORD(S)

Salvinorin A

Kappa Opioid Receptor Agonist

Total Synthesis

Natural Products

retrosynthesis planning software

Preservation and Integrity

- Preprints assigned DOI
- EVERY preprint version is time/date stamped, viewable
- Preprints cannot be taken down by authors, however, may be removed by ChemRxiv in cases of ethical, safety, privacy, or copyright issues
- ChemRxiv establishes links between preprints and later published articles


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- Open API compatible – full documentation, Open API Swagger specifications available
 - Will support OAuth 2.0 Authorization Framework (specific tokens coming soon)

Date/time stamp
and citable DOI

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and Altmetrics

10-step Synthesis of 20-nor-Salvinorin A by Dynamic Strategic Bond Analysis

Version 2  19.08.2017, 18:27 by Jeremy Roach, Yusuke S
Version 2 19.08.2017, 18:27 by David Stevens, Laura Bohn, Ryan
Version 1 17.08.2017, 15:38

Salvinorin A (Salv) is a plant metabolite that agonize
(κ -OR) with high affinity and high selectivity over *mu*- and *delta*-opioid receptors. Its

-  Picked up by 1 news outlets
-  Blogged by 2
-  Tweeted by 45
-  On 1 Facebook pages

[See more details](#) | [Close this](#)

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Predicting the Mechanical Properties of Zeolite Frameworks by Machine Learning

29.08.2017, 10:19 by Jack D. Evans, François-xavier Coudert

We show here that machine learning is a powerful new tool for predicting the elastic response of zeolites. We built our machine learning approach relying on geometric features only, which are related to local geometry, structure and porosity of a zeolite, to predict bulk and shear moduli of zeolites with an accuracy exceeding that of force field approaches. The development of this model has illustrated clear correlations between characteristic features of a zeolite and elastic moduli providing exceptional insight into

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[Predicting the Mechanical Properties of Zeolite Frameworks by Machine Learning](#)
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Abstract: Two-dimensional nanomaterials such as carbon nanotubes rely on strong and directional covalent connections that stabilize their high aspect ratio shapes from further. This requirement has prohibited making isolated long, thin nanotubes by stacking molecular nanomaterials as their conventional stacking interaction are generally too weak. Here we report high aspect ratio (1-100), hexagonal nanotubes of stacked, nanoscale, nanotubes, which are formed by polymerization of the corresponding unfunctionalized nanotubes and formation of their relative connections that are two orders of magnitude stronger than the initial nanotubes, as revealed by radiative electron microscopy. Nanotube formation enhances the isolation time, which otherwise rapidly hydrolyzes, and is controlled and oriented upon addition of bases and acids. As also proven by tracking a chemical process or monitoring ultraviolet spectra, also related nanotube assembly, allowing their concentration to be coupled to electron yield, and, over assembly, they can be fixed permanently by crosslinking their protein surface. As this paper, whether the nanoscale chemical liquid crystals, nanoscale nanotubes are easily accessible through a simple design and provide a means to rational synthesis structures that mirror the morphology and topology of carbon nanotubes and biological ...

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2018_03_Sun_Ch... .pdf (22.14 MB)

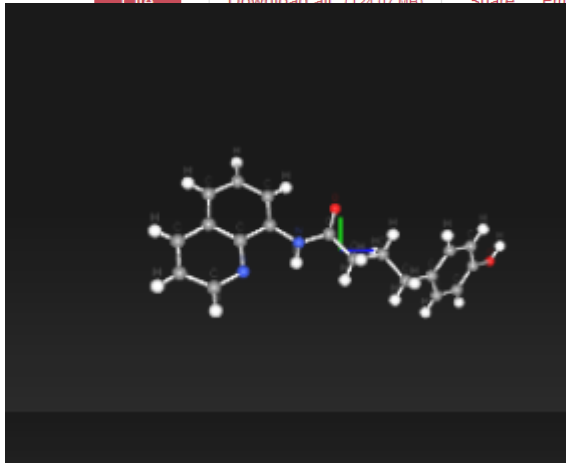
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Supplementary Vi... .mp4 (12.25 MB)

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assembl

Ch Chavez, At
Bedzyk, Mon



12
benzene example

C	0.00000	1.40272	0.00000
H	0.00000	2.49029	0.00000
C	-1.21479	0.70136	0.00000
H	-2.15666	1.24515	0.00000
C	-1.21479	-0.70136	0.00000
H	-2.15666	-1.24515	0.00000
C	0.00000	-1.40272	0.00000
H	0.00000	-2.49029	0.00000
C	1.21479	-0.70136	0.00000
H	2.15666	-1.24515	0.00000
C	1.21479	0.70136	0.00000
H	2.15666	1.24515	0.00000

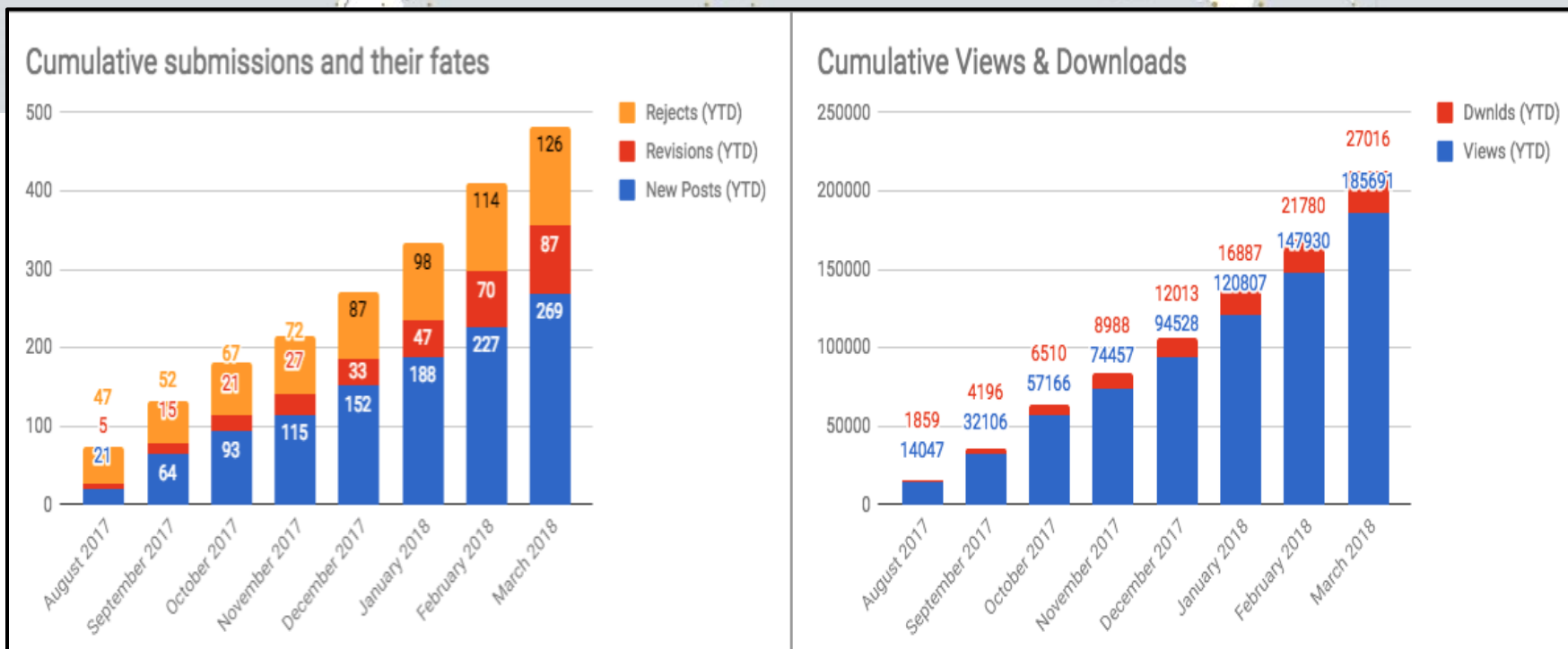
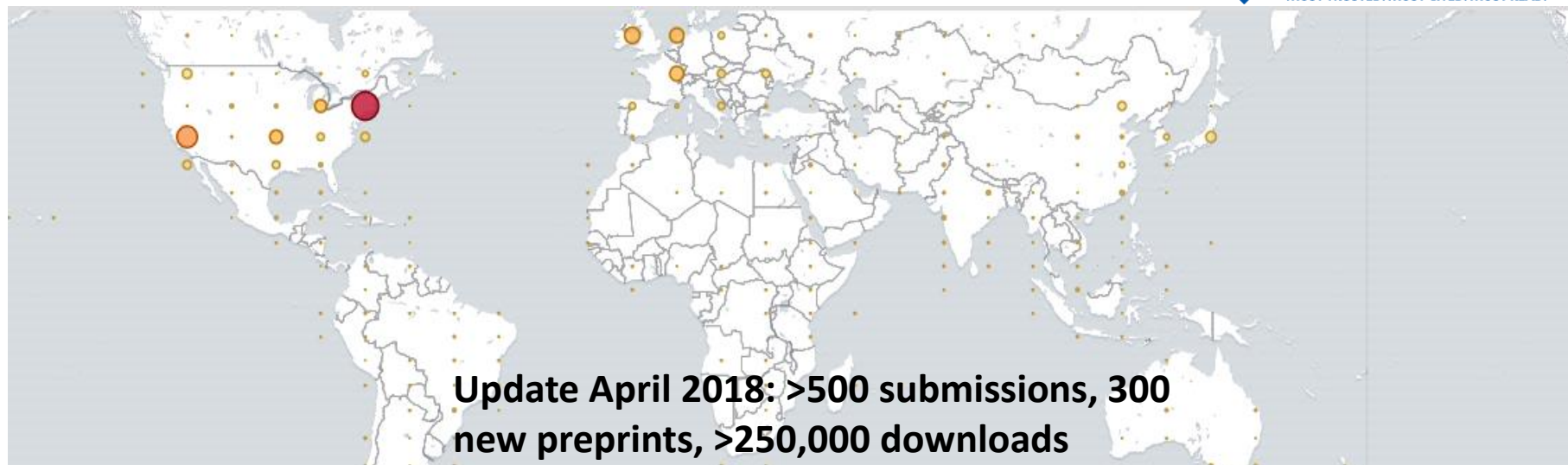
<https://chemrxiv.org/>

Source: <http://calistry.org/calculate/xyzviewer>

Roadmap for ChemRxiv

- Key Items for 2018:
 - Integration of iThenticate software to auto-run and deposit report to Publishing Manager dashboard
 - Inclusion of best fit categorization for chemistry
 - One-click transfer to/from journal submission sites
 - Continued evaluation and pass-through of information collected
 - Community development: specific sub-disciplines of chemistry
 - Data, metadata development opportunities

Geographic diversity of users growing



How can preprint servers be a successful, sustainable piece of the scholarly communication cycle?

- **Successful** →
 - partner, collaborate
 - engage broadly
 - care about preservation, integrity, leading to greater trust and growing adoption
 - address ethics (COPE)
- **Sustainable** →
 - explore new technology solutions
 - audit processes
 - automation, AI in future
- **Part of the Communication Cycle** → “do what needs to be done at the right time”
 - involve experts in the communication cycle, look ahead to future opportunities
 - bring existing resources and best practices from publishing where appropriate
 - integrate depositions to/from preprint servers/journals, seek efficiencies for all

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