# *Do's* and *Don'ts* for writing impactful papers about scientific software

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PLOS COMPUTATIONAL BIOLOGY

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EDITORIAL

# Ten simple rules for writing a paper about scientific software

Joseph D. Romano, Jason H. Moore

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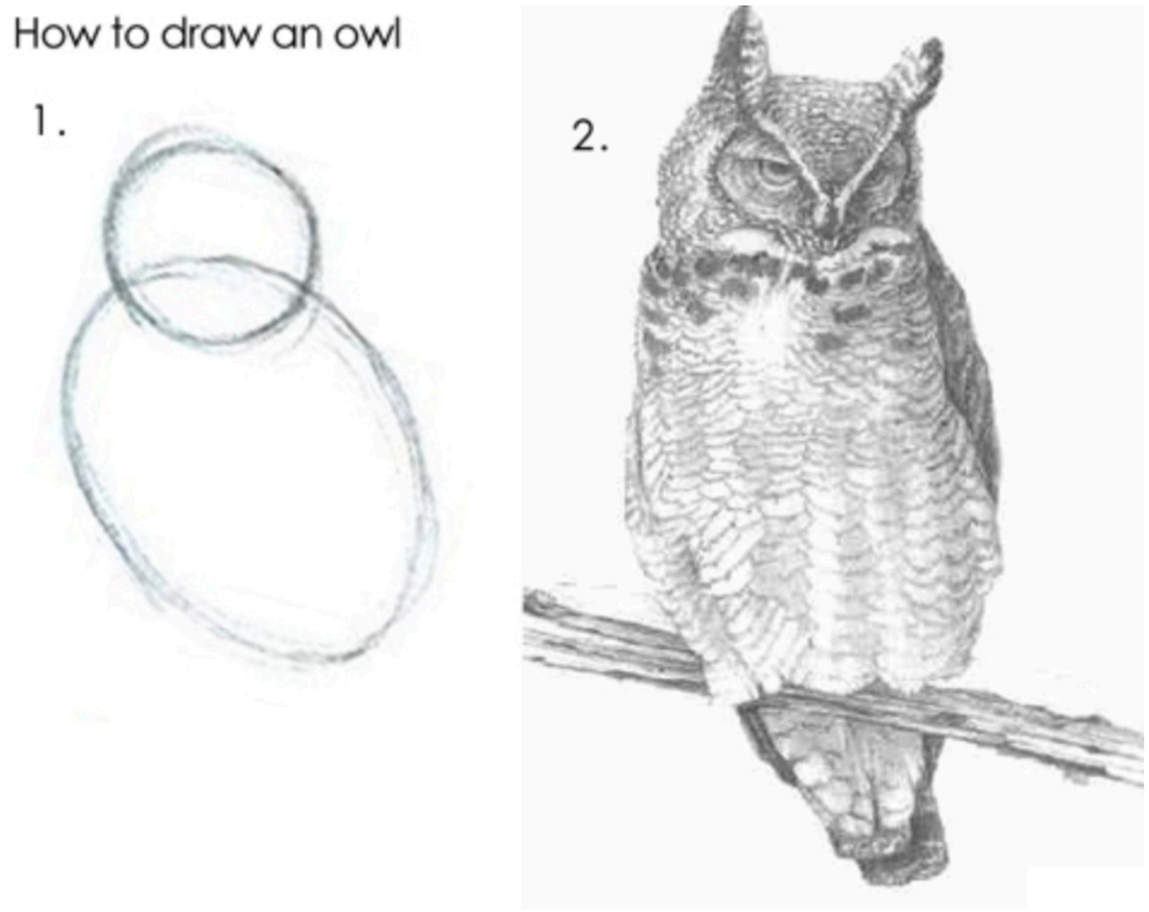
**Rules with a ‘*’ := Heavily opinionated!**

# Rule 1: Make sure your scientific software is *good* scientific software



# Rule 1: Make sure your scientific software is *good* scientific software

# Rule 2: Know the right publication venues

- Some journals offer specific publication types for software papers:
  - Bioinformatics - "Application Notes"
  - BMC Bioinformatics - "Software articles"
  - Journal of Open Source Software (JOSS) - all articles
  - PLOS Computational Biology - "Software articles"
- Pay attention to journal requirements!
  - E.g., page/word/figure limits are usually pretty restrictive
  - Some require evaluations using real (not synthetic) data!

# Rule 2: Know the right publication venues

- However, it might be better to publish a "traditional" article in a non-computational journal
- Ask yourself: Who is my intended audience? What *kind* of impact do I want this software/paper to have?

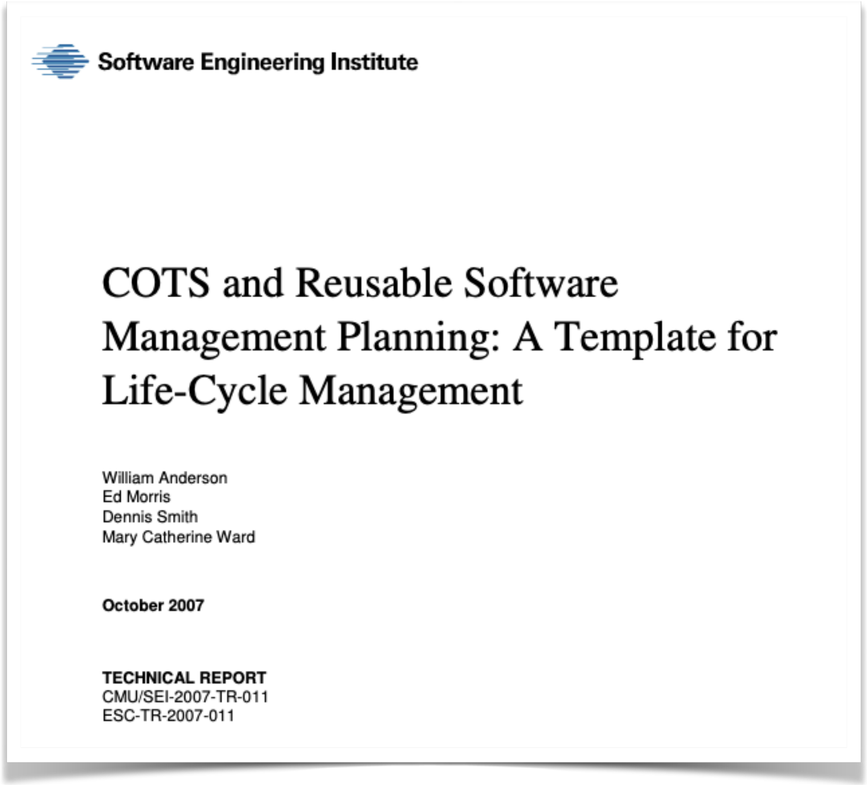
# Rule 3: Publish for users, not developers*

- Remember: source code and code documentation are often meant for developers rather than the average user
- Software papers are for your scientific audience; i.e., your desired users
- (Keep this in mind for Rule 6)

# Rule 3: Publish for users, not developers*

- Possible issues when publishing using a "conventional" article type:
  - Might need to be creative how you present your methods and results to fit the paper requirements
    - A good strategy is to present a handful of use-cases in Results
  - Reviewers might not know how to handle software papers
    - Contact an editor when in doubt!!!
    - Suggest reviewers with computational expertise if you have the option to do so
  - Write your paper at the appropriate level of technical detail for the "typical reader" of your journal

# Rule 4: Have a long-term software management plan



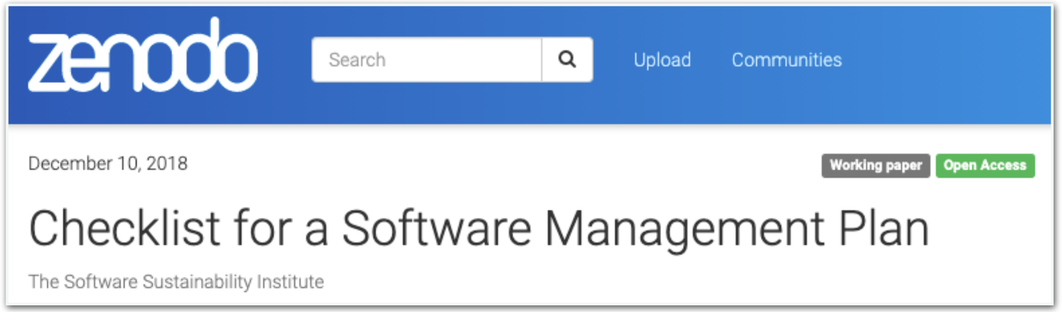
Software Engineering Institute

COTS and Reusable Software Management Planning: A Template for Life-Cycle Management

William Anderson
Ed Morris
Dennis Smith
Mary Catherine Ward

October 2007

TECHNICAL REPORT
CMU/SEI-2007-TR-011
ESC-TR-2007-011



zenodo Search Upload Communities

December 10, 2018 Working paper Open Access

Checklist for a Software Management Plan

The Software Sustainability Institute

https://doi.org/10.5281/zenodo.2159713

# Rule 4: Have a long-term software management plan

- Who is responsible for maintaining the software in the future?
- What is the cost of keeping the software (and related tools) online? Have you planned for continued funding?
- Who owns the IP behind the software?
- Will updates / bug fixes be provided?
- What will happen if dependencies go offline?
- When and how will you archive the software?

# Rule 5: Safeguard against "link rot"

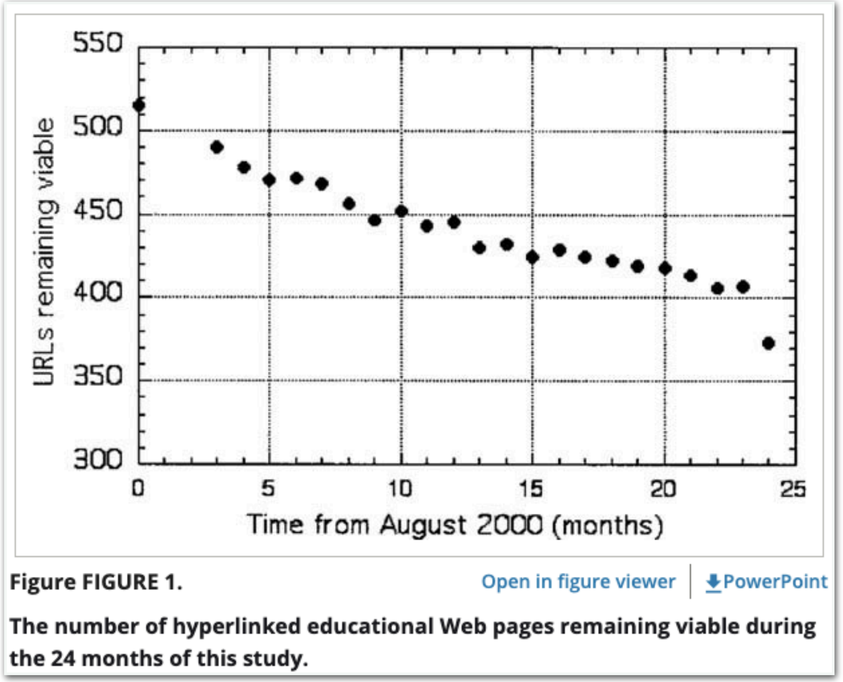



**Figure FIGURE 1.** Open in figure viewer | PowerPoint

**The number of hyperlinked educational Web pages remaining viable during the 24 months of this study.**

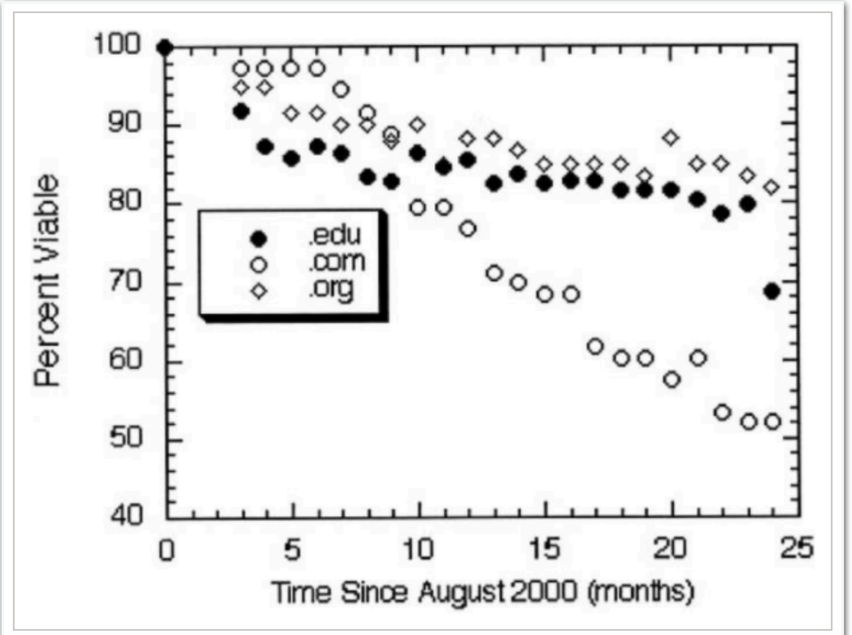



**Figure FIGURE 2.** Open in figure viewer | PowerPoint

**The loss of distributed resources in the .edu, .com, and .org domains over the 24 months of this study.**

Markwell and Brooks (2006); https://doi.org/10.1002/bmb.2003.494031010165

# Rule 5: Safeguard against "link rot"

- The average URL lifespan is 9.3 years (and decreasing)
- Consider non-institutional web pages
  - Affiliations change
  - Changes in organizational structure wreak havoc on websites
- Use Zenodo and/or FigShare to assign permanent DOIs to (versioned!) software and data
- Try to have semantically meaningful URLs
  - E.g., compare:

`http://<domain>/protein/BRCA1` `http://<domain>/540/65df7.php?id=18427`

# Rule 6: Know the difference between documentation and research results*

- Don't put code documentation in a software paper!
  Documentation changes when software changes!
  - Any time you put code in a paper, you are making a long-term commitment to syntax and semantics
- Only include example code in the paper if it's absolutely critical. Appendices might be OK, but do this sparingly.
- However, include a prominent link to (versioned!) documentation in the paper
- It's not a bad idea to have your documentation directly support results presented in the paper

# Rule 7: Use modern tooling



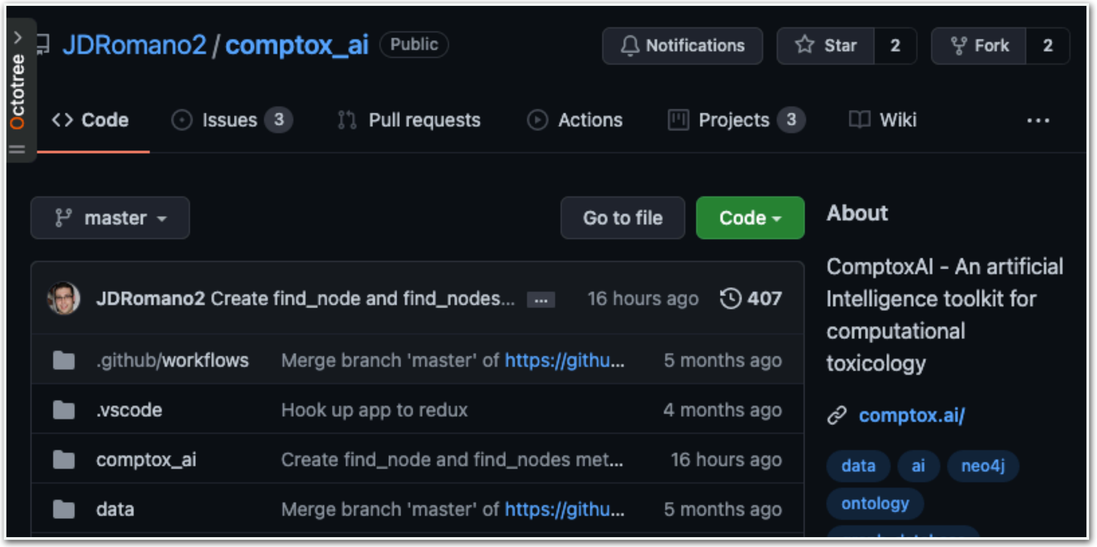


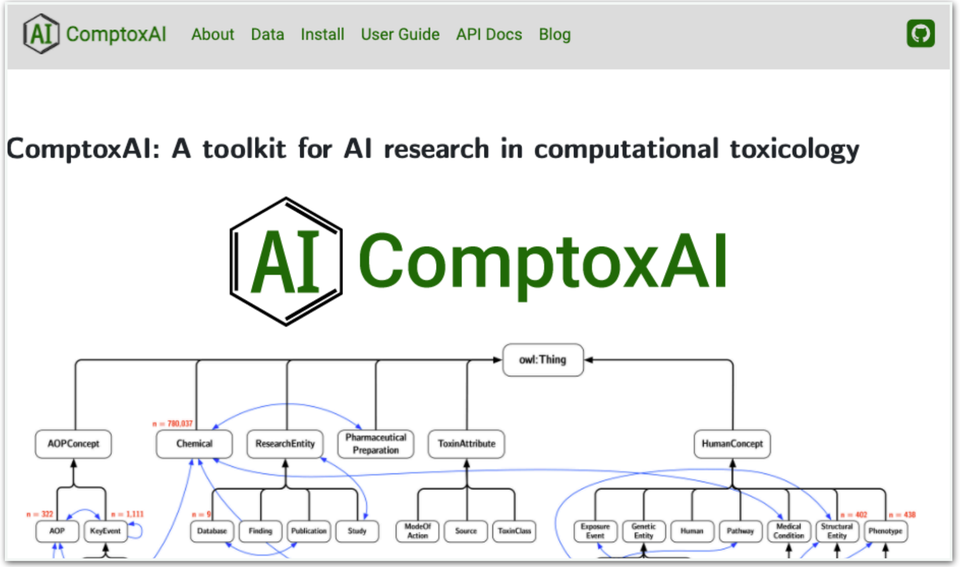
- Use a well-maintained, modern programming language
- Publish your software one one or more packaging index
- Distribute as both raw source code and pre-compiled / pre-packaged versions
- Provide detailed documentation (web-based, auto-generated documentation is great!) and instructions/examples
- Provide contribution instructions and ways to report bugs & ask for help

# Rule 8: Be consistent

- Across your software ecosystem, try to maintain consistent:
  - Spelling
  - Punctuation
  - Capitalization
  - Logos
- Apply version control, especially to code documentation
- Establish a consistent naming scheme if the software is part of a larger body of computational research
- Don't force acronyms - keep them simple or avoid them entirely****

# Rule 8: Be consistent



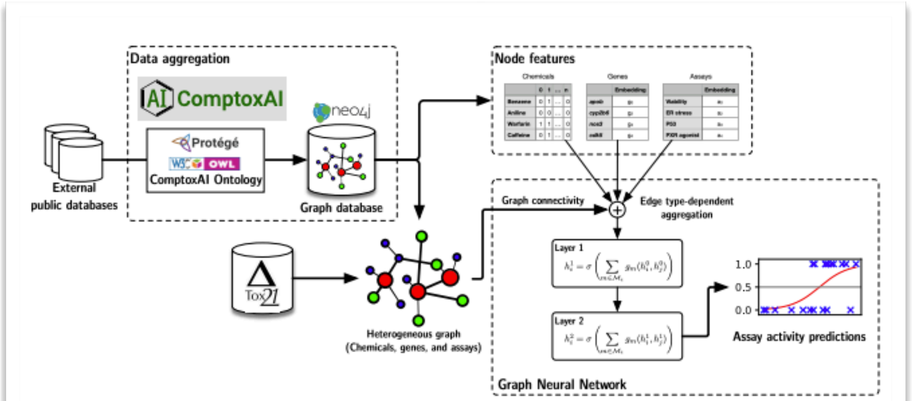




Fig. 1. Overview of the graph machine learning approach used in this study. We build a toxicology-focused graph database (named ComptoxAI) using data aggregated from diverse public databases, and extract a subgraph for QSAR analysis containing chemicals, assays, and genes. We then train and evaluate a graph neural network that predicts whether or not a chemical activates specific toxicology-focused assays from the Tox21 database.

[a]The full graph database for ComptoxAI can be found at `https://comptox.ai`, and will be described in a separate, upcoming publication.

# Rule 9: Plan for follow-ups

- It's not just for padding CVs or increasing citation counts!
- Follow-up papers describe major scientific changes to software (e.g., new algorithms) or datasets (e.g., new data types, overhauled database structure, etc.)
- Demonstrate that the authors rigorously follow the scientific process, and that the project is iterative and builds on previous work

# Rule 9: Plan for follow-ups

Journal Article

**DrugBank**: a knowledgebase for drugs, drug actions and drug targets

David S. Wishart, Craig Knox, An Chi Guo, Dean Cheng, Savita Shrivastava ...

*Nucleic Acids Research*, Volume 36, Issue suppl_1, 1 January 2008, Pages D901–D906, https://doi.org/10.1093/nar/gkm958

**Published:** 29 November 2007

Journal Article

**DrugBank** 3.0: a comprehensive resource for 'Omics' research on drugs

Craig Knox, Vivian Law, Timothy Jewison, Philip Liu, Son Ly ...

*Nucleic Acids Research*, Volume 39, Issue suppl_1, 1 January 2011, Pages D1035–D1041, https://doi.org/10.1093/nar/gkq1126

**Published:** 08 November 2010

...Craig Knox; Vivian Law; Timothy Jewison; Philip Liu; Son Ly; Alex Frolkis; Allison Pon; Kelly Banco; Christine Mak; Vanessa Neveu; Yannick Djoumbou; Roman Eisner; An Chi Guo; David S. Wishart Table 1. Comparison between the coverage in **DrugBank** 1.0, 2.0 and **DrugBank** 3.0 Category 1.0 2.0...

Journal Article

**DrugBank** 4.0: shedding new light on drug metabolism

Vivian Law, Craig Knox, Yannick Djoumbou, Tim Jewison, An Chi Guo ...

*Nucleic Acids Research*, Volume 42, Issue D1, 1 January 2014, Pages D1091–D1097, https://doi.org/10.1093/nar/gkt1068

**Published:** 06 November 2013

...Vivian Law; Craig Knox; Yannick Djoumbou; Tim Jewison; An Chi Guo; Yifeng Liu; Adam Maciejewski; David Arndt; Michael Wilson; Vanessa Neveu; Alexandra Tang; Geraldine Gabriel; Carol Ly; Sakina Adamjee; Zerihun T. Dame; Beomsoo Han; You Zhou; David S. Wishart **DrugBank's** experimental drug data set...

Journal Article

**DrugBank** 5.0: a major update to the **DrugBank** database for 2018

David S Wishart, Yannick D Feunang, An C Guo, Elvis J Lo, Ana Marcu ...

*Nucleic Acids Research*, Volume 46, Issue D1, 4 January 2018, Pages D1074–D1082, https://doi.org/10.1093/nar/gkx1037

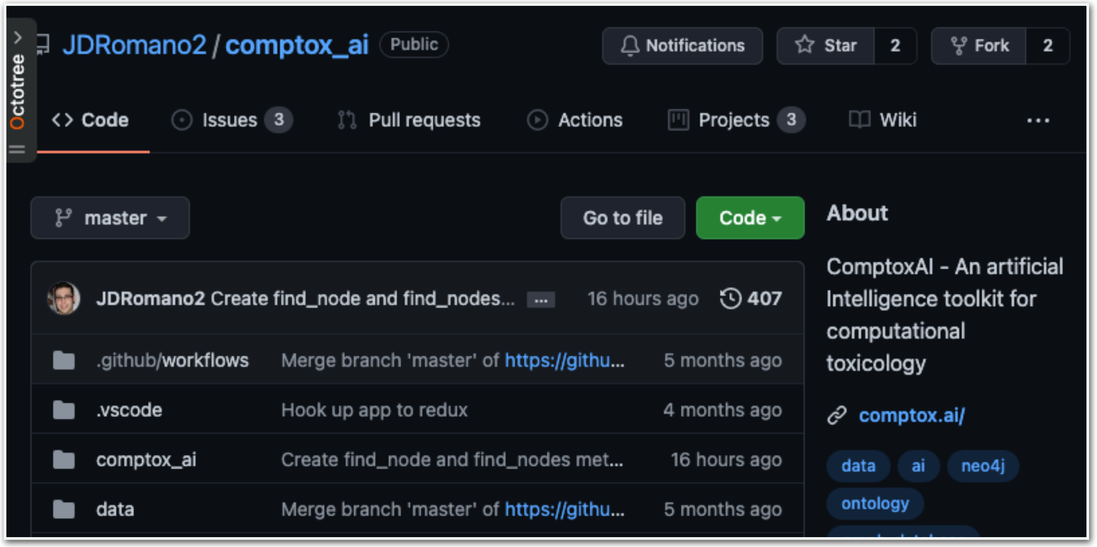
**Published:** 08 November 2017

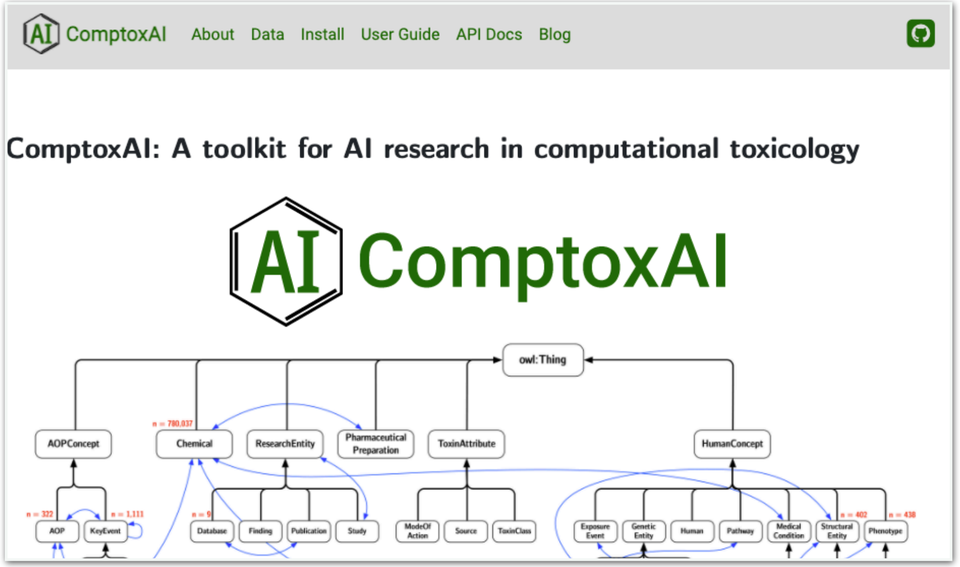
... journals.permissions@oup.com Abstract **DrugBank** ( www.drugbank.ca ) is a web-enabled database containing comprehensive molecular information about drugs, their mechanisms, their interactions and their targets. First described in 2006, **DrugBank** has continued to evolve over the past 12 years in response to marked...

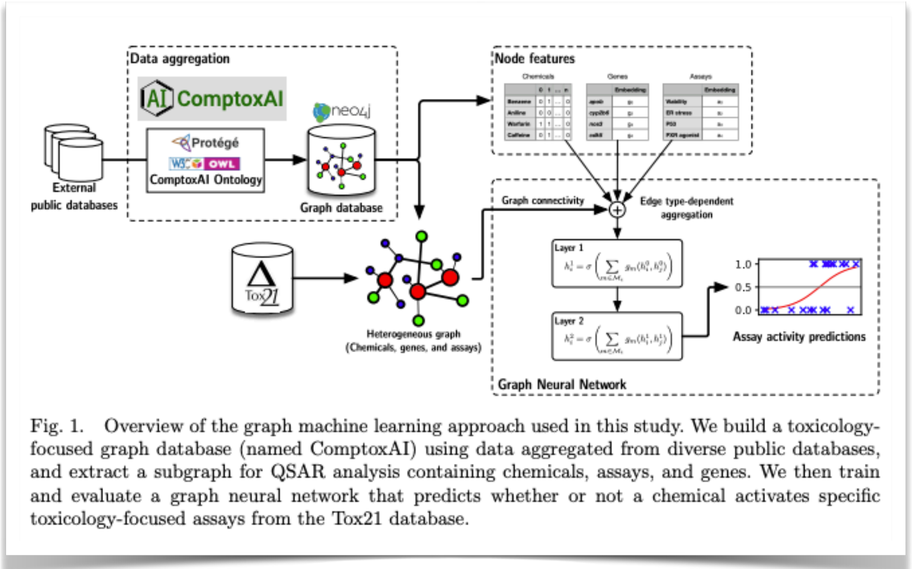
# Rule 9: Plan for follow-ups

- When **not** to write a follow-up paper:
  - Bug fixes or minor feature additions/changes
  - Adding/editing/removing relatively few data elements
  - Overhauled website in the absence of major features being added
  - New directions for the software if those directions haven't yet been implemented
  - New visualizations* or other ease-of-use tools

# Rule 10: Prioritize visibility and availability

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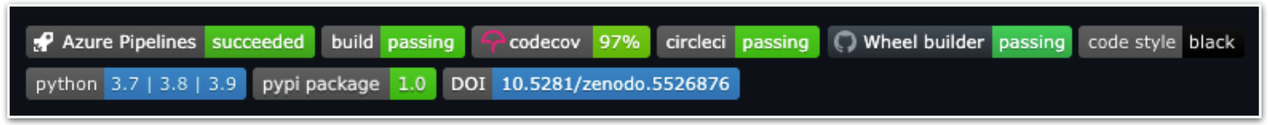
[a]The full graph database for ComptoxAI can be found at `https://comptox.ai`, and will be described in a separate, upcoming publication.

# Rule 10: Prioritize visibility and availability

- Search engine optimization isn't just for businesses!
- Links, links, and more links
- Social media (especially Twitter) is a great way to spread the word

# Rule 10: Prioritize visibility and availability

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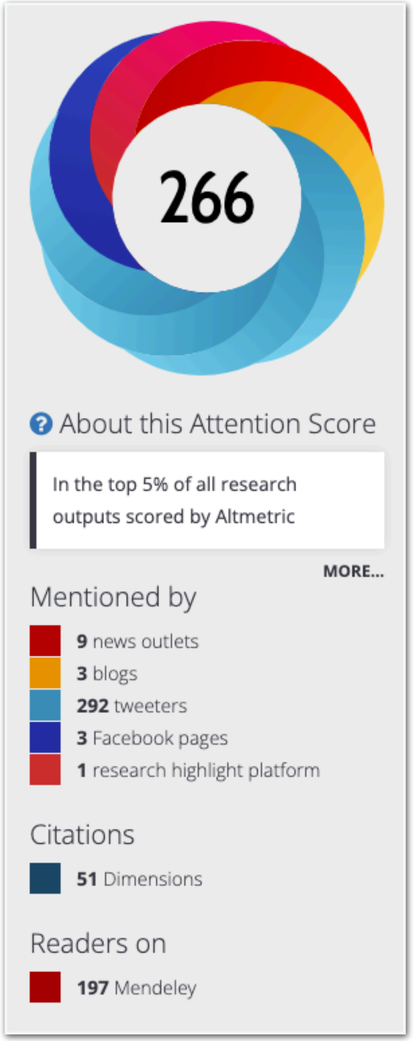
Polubriaginof FCG, Vanguri R, Quinnies K, et al. Disease Heritability Inferred from Familial Relationships Reported in Medical Records. *Cell*. 2018;173(7):1692-1704.e11. doi:10.1016/j.cell.2018.04.032



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