Two years of CiTO annotations

Egon Willighagen [1,*,orcid:0000-0001-7542-0286]

• Correspondance: egon.willighagen@maastrichtuniversity.nl

Abstract

Citations are an essential aspect of research communication and have become the basis of many metrics in the academic publishing world. Some see citation counts as a mark of scientific impact or even quality, but in reality the reasons for citing other work are manifold. Two years ago the *Journal of Cheminformatics* proposed a pilot for the adoption of annotating citations with their annotations. Basically, when you cite a source like a journal article or datasets, you also explain why specifically you cite that article. Particularly, the agreement and disagreement and reuse of methods and data is interesting. This article explores what happened after the launch of the pilot, gives examples of how people used the idea, and what needs to happen next.

Main text

Communiting new research findings is primarily done by written texts in the form of scholarly articles, books, and book chapters. To not having to repeat past research by themselves or others, authors cite research relevant [1]. However, the reasons why authors cite literature vary, which complicates how we use citations [2]. Typing citations is therefore of interest: it allows us to navigate literature more easily: it points us to essential research methods, data, and can warn us of research that cannot be reproduced, or others disagree with [2].

With the use of citations increasingly being picked up to help researchers with tools like scite.ai [2] en Connected Papers, having typed citations will help us explore literature. Therefore, the *Journal of Cheminformatics* started a pilot for the adoption of annotating citations with their annotations [3].

The Citation Typing Ontology Pilot

The pilot consists of a couple of components and the editorial explains some of them [3]. The Citation Typing Ontology was selected to express the intention [1], the intention is expressed a compact identifier wrapped in square brackets [4], and the *bibnotes* concept of the Springer Nature publishing platform was used as carrier. Authors are guided by a landing page consisting of a BioMedCentral Collection at https://www.biomedcentral.com/collections/cito and author guidelines explaining to authors how they can add the annotations with their favoriate editor at https://jcheminform.github.io/jcheminform-author-guidelines/cito.

Because the CiTO ontology has many terms for many different citation intentions, we made a selection of CiTO terms authors could use [5]: [cito:citesAsDatasource] to indicate to a source the provides data to back up a claim, [cito:usesDataFrom] to indicate that the authors reused data, [cito:usesMethodIn] when a method or protocol explain in that source is used, and a few more general intentions like [cito:discusses], [cito:extends], [cito:agreesWith], and [cito:disagreesWith]. The journal itself would adopt the following CiTO annotations: [cito:retracts], [cito:repliesTo], and [updates]. Fortunately, it has not been used yet, but the first would be used if an article with be retracted from the journal. The second would be used when an Letter to the Editor replies to an earlier published article, and [cito:updates] when an Correction was published.

Wikidata and Scholia

To track the uptake but also to demonstrate the impact, we extended Scholia to visualize citation intention data. Scholia is a graphical interface around the data stored in Wikidata [6] and includes citations from OpenCitations [7] and PubMed. Wikidata allows adding qualifier to statements which allowed us to define a data model for citations annoted with CiTO intention; the Wikidata property P3712 has been used for this, labeled *objective of project or action* (see Figure 1).

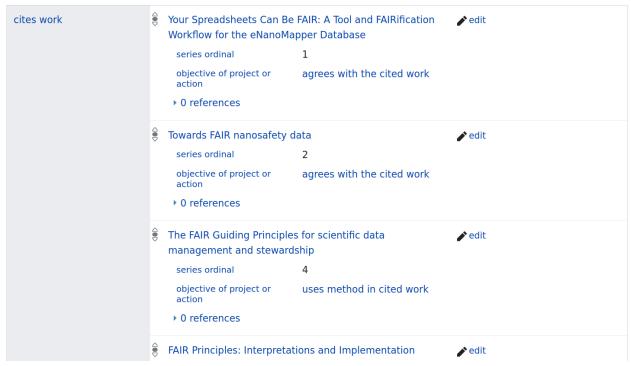


Figure 1: Screenshot of the citation statements for an article where the *objective of project or action* qualifier is used to annotate the citation with their CiTO intentions.

This data in Wikidata can then be accessed via Scholia and Scholia tells use some overall statisticss of the number of annotations, which we reported on about a year ago too [8]. Since last year and written down on August 25, the number of annotations and the number of annotated citations have almost doubled (from 377 to 603 and from 304 to 494, respectively). The first number is higher because one citation can have more than one citation intention. To continue, the current number of citations are citing 387 articles in 141 different scholarly journals, and they are found in 98 articles in 48 different journals (see Figure 2) [9].

Citation Typing Ontology Intentions

Page with general info about CiTO annotation in Wikidata.

Table of Contents

- Statistics
- · Number of articles with CiTO-annotated citations by year
- Use of the various CiTO intentions
- · Journals and how many CiTO different intentions they use

Statistics

		Search	n:
Count	$\uparrow \downarrow$	Description	$\uparrow \downarrow$
603		Total number of annotations	
494		Total number of annotated citations	
387		Total number of articles receiving annotated citations	
141		Number of cited venues with annotated citations	
98		Total number of articles providing annotated citations	
48		Number of citing venues with annotated citations	
10		Number of article with explicit CiTO annotation	
1		Number of journals with explicit CiTO annotation	
Wikidata Query Service			cito-index: statistics.sparql

Figure 2: XXXX.

It must be noted that the *Journal of Cheminformatics* is only one possible source, but is still the only journal that uses CiTO annotation explicitly in the articles itself. And with 335 annotated citations in 32 articles it also is the major source of CiTO annotations in Wikidata at the time of writing. However, CiTO intention annotations in Wikidata can come from other sources too and be added both manually and automatically using the tools around Wikidata. When all annotation is combined, Scholia shows us that [cito:citesAsAuthority] is the most used intention, with 226 annotated citations (out of 603) in 38 articles. [cito:usesMethodIn] follows with 102 annotated citations.

Adoption by Journal of Cheminformatics authors

Table 1: Journal of Cheminformatics articles in the first year of the pilot.

Type	Article	Intentions	%CiTO
Editorial	Adoption of the Citation Typing	cito:citesAsAuthority,	42%
	Ontology by the Journal of	cito:citesForInformation,	
	Cheminformatics [3]	cito:usesMethodIn	
Methodology	Predicting target profiles with	cito:agreesWith, cito:extends,	47%
30	confidence as a service using docking	cito:citesAsAuthority,	
	scores [10]	cito:citesAsDataSource,	
		cito:usesMethodIn	

Type	Article	Intentions	%CiTO
Research article	Too sweet: cheminformatics for	cito:citeAsAuthority,	
	deglycosylation in natural products	cito:citesForInformation,	
	[11]	cito:usesDataFrom,	
		cito:usesMethodIn	
Educational	A ligand-based computational drug	cito:agreesWith,	98%
	repurposing pipeline using KNIME	cito:citesAsAuthority,	
	and Programmatic Data Access: case	cito:citesAsDataSource, cito:discusses,	
	studies for rare diseases and	cito:usesDataFrom,	
	COVID-19 [12]	cito:usesMethodIn	
Database	COCONUT online: Collection of	cito:citesForInformation,	41%
	Open Natural Products database [13]	cito:usesDataFrom,	
		cito:usesMethodIn	
Editorial	What is the role of cheminformatics	cito:agreesWith,	91%
	in a pandemic? [14]	cito:citesAsAuthority,	
		cito:citesAsDataSource,	
		cito:citesForInformation,	
		cito:citesAsPotentialSolution	
Research article	Empowering large chemical	cito:citesAsAuthority,	100%
	knowledge bases for exposomics:	cito:citesAsDataSource,	
	PubChemLite meets MetFrag [15]	cito:citesAsMetadataDocument,	
		cito:discusses, cito:extends,	
		cito:usesDataFrom,	
		cito:usesMethodIn	
Software	IDSM ChemWebRDF: SPARQLing	cito:citesAsAuthority,	97%
	small-molecule datasets [16]	cito:citesAsRelated,	
		cito:usesDataFrom,	
		cito:usesMethodIn	
Letter to the	FAIR chemical structures in the	cito:citesAsAuthority, cito:documents	100%
Editor	Journal of Cheminformatics [17]	• /	
Letter	Reply to "FAIR chemical structure in	cito:agreesWith,	100%
Response	the Journal of Cheminformatics" [18]	cito:citesAsAuthority,	
	. 1	cito:citesAsDataSource,	
		cito:obtainsBackgroundFrom,	
		cito:repliesTo	

Table 2: *Journal of Cheminformatics* articles in the second year of the pilot. The * indicates that the percentage is based on CiTO intends different from cito:cites.

Type	Article	Intentions	%CiTO
Research article	DECIMER 1.0: deep learning for		
	chemical image recognition using		
	transformers [19]		
Research article	DrugEx v2: de novo design of drug		
	molecules by Pareto-based		
	multi-objective reinforcement learning		
	in polypharmacology[20]		
Database	PSnpBind: a database of mutated		
	binding site protein-ligand complexes		
	constructed using a multithreaded		
	virtual screening workflow [21]		
Editorial	Diversifying cheminformatics [22]		

Type	Article	Intentions	%CiTO
Data Note	DECIMER - hand-drawn molecule images dataset [23]	cito:agreesWith, cito:cites, cito:citesAsAuthority, cito:extends, cito:usesDataFrom, cito:usesMethodIn	41% (*)

Technological innovation

Markdown template...

To make life easier for authors, and following a Twitter discussion in Spring 2021, we developed a Markdown template with native CiTO support. Here, the author merely indicates the CiTO type when they cite the article. This is using a method introduced by Krewinkel et al. [24].

The manuscript can then easily be saved as a Word file to enable submission to the journal. The *Journal of Cheminformatics* template is available from our GitHub repository, and authors and editors should feel free to adapt it to their own journal needs.

Discussion

Formatting issues

Citation level intention annotation: only Markdown

What is next?

With X articles published in the CiTO Collection, the adoption is not as high as one would have hoped. Nevertheless, the pilot is triggering interest with both authors and publishing platforms. The Scholia use case shows how the information can be used downstream. Further uptake of this idea of typed citations depends on the combined willingness of journal editors, authors, publishers and indexing services alike. The rise of services like scite.ai shows that the research community needs this kind of information.

Availability of data and materials Text for this section.

Competing interests Text for this section.

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References

- 1. Shotton D (2010) CiTO, the citation typing ontology. Journal of Biomedical Semantics 1:S6+. https://doi.org/10.1186/2041-1480-1-s1-s6 [cito:agreesWith] [cito:citesAsAuthority] [cito:usesMethodIn]
- 2. Nicholson JM (2021) Smart(er) citations. Matter 4:756–758. https://doi.org/10.1016/j.matt.2021.02.007 [cito:agreesWith] [cito:citesAsAuthority]

- 3. Willighagen E (2020) Adoption of the citation typing ontology by the journal of cheminformatics. Journal of Cheminformatics 12:47, s13321-020-00448-1. https://doi.org/10.1186/s13321-020-00448-1 [cito:discusses] [cito:citesForInformation]
- 4. Wimalaratne SM, Juty N, Kunze J, et al (2018) Uniform resolution of compact identifiers for biomedical data. Scientific Data 5:180029. https://doi.org/10.1038/sdata.2018.29 [cito:usesMethodIn]
- 5. (2020) Citation Typing Ontology (CiTO) Pilot
- 6. Nielsen FÅ, Mietchen D, Willighagen E (2017) Scholia, scientometrics and wikidata. In: Blomqvist E, Hose K, Paulheim H, et al (eds) The semantic web: ESWC 2017 satellite events. Springer International Publishing, Cham, pp 237–259 [cito:usesMethodIn]
- 7. Peroni S, Shotton D (2020) OpenCitations, an infrastructure organization for open scholarship. Quantitative Science Studies 1:428–444. https://doi.org/10.1162/qss_a_00023
- 8. E. W (2021) Typed Citations in the Journal of Cheminformatics. On Physical Sciences [cito:citesAsDataSource]
- 9. (2022) Citation Typing Ontology Intentions Scholia. https://scholia.toolforge.org/cito/. Accessed 26 Aug 2022 [cito:citesAsDataSource]
- 10. Ahmed L, Alogheli H, McShane SA, et al (2020) Predicting target profiles with confidence as a service using docking scores. Journal of Cheminformatics 12:62. https://doi.org/10.1186/s13321-020-00464-1 [cito:citesForInformation]
- 11. Schaub J, Zielesny A, Steinbeck C, Sorokina M (2020) Too sweet: Cheminformatics for deglycosylation in natural products. Journal of Cheminformatics 12:67. https://doi.org/10.1186/s13321-020-00467-y [cito:citesForInformation]
- 12. Tuerkova A, Zdrazil B (2020) A ligand-based computational drug repurposing pipeline using KNIME and programmatic data access: Case studies for rare diseases and COVID-19. Journal of Cheminformatics 12:71. https://doi.org/10.1186/s13321-020-00474-z [cito:citesForInformation]
- 13. Sorokina M, Merseburger P, Rajan K, et al (2021) COCONUT online: Collection of open natural products database. Journal of Cheminformatics 13:2. https://doi.org/10.1186/s13321-020-00478-9 [cito:citesForInformation]
- 14. Guha R, Willighagen E, Zdrazil B, Jeliazkova N (2021) What is the role of cheminformatics in a pandemic? Journal of Cheminformatics 13:16, s13321-021-00491-6. https://doi.org/10.1186/s13321-021-00491-6 [cito:citesForInformation]
- 15. Schymanski EL, Kondić T, Neumann S, et al (2021) Empowering large chemical knowledge bases for exposomics: PubChemLite meets MetFrag. Journal of Cheminformatics 13:19. https://doi.org/10.118 6/s13321-021-00489-0 [cito:citesForInformation]
- 16. Galgonek J, Vondrášek J (2021) IDSM ChemWebRDF: SPARQLing small-molecule datasets. Journal of Cheminformatics 13:38. https://doi.org/10.1186/s13321-021-00515-1 [cito:citesForInformation]
- 17. Schymanski EL, Bolton EE (2021) FAIR chemical structures in the journal of cheminformatics. Journal of Cheminformatics 13:50. https://doi.org/10.1186/s13321-021-00520-4 [cito:citesForInformation]
- 18. Guha R, Jeliazkova N, Willighagen E, Zdrazil B (2021) Reply to "FAIR chemical structure in the journal of cheminformatics." Journal of Cheminformatics 13:49. https://doi.org/10.1186/s13321-021-00521-3 [cito:citesForInformation]
- 19. Rajan K, Zielesny A, Steinbeck C (2021) DECIMER 1.0: Deep learning for chemical image recognition using transformers. Journal of Cheminformatics 13:61. https://doi.org/10.1186/s13321-021-00538-8 [cito:citesForInformation]
- 20. Liu X, Ye K, Vlijmen HWT van, et al (2021) DrugEx v2: De novo design of drug molecules by pareto-based multi-objective reinforcement learning in polypharmacology. Journal of Cheminformatics 13:85. https://doi.org/10.1186/s13321-021-00561-9 [cito:citesForInformation]

- 21. Ammar A, Cavill R, Evelo C, Willighagen E (2022) PSnpBind: A database of mutated binding site protein-ligand complexes constructed using a multithreaded virtual screening workflow. Journal of Cheminformatics 14:8. https://doi.org/10.1186/s13321-021-00573-5 [cito:citesForInformation]
- 22. Zdrazil B, Guha R (2022) Diversifying cheminformatics. Journal of Cheminformatics 14:25, s13321-022-00597-5. https://doi.org/10.1186/s13321-022-00597-5 [cito:citesForInformation]
- 23. Brinkhaus HO, Zielesny A, Steinbeck C, Rajan K (2022) DECIMER—hand-drawn molecule images dataset. Journal of Cheminformatics 14:36. https://doi.org/10.1186/s13321-022-00620-9 [cito:citesForInformation]
- 24. Krewinkel A, Winkler R (2017) Formatting open science: Agilely creating multiple document formats for academic manuscripts with pandoc scholar. PeerJ Computer Science 3:e112. https://doi.org/10.7717/peerj-cs.112 [cito:usesMethodIn]
- 25. MacKenzie C (2022) Add cito panel to work aspect with ask query. In: GitHub. https://github.c om/WDscholia/scholia/commit/0af60cf7732bc8664d828cbe51f233aa63201df9. Accessed 26 Aug 2022 [cito:citesAsEvidence]