chem-bla-ics

CiTO updates #1: first research paper in the Journal of Cheminformatics with CiTO annotation published

Egon Willighagen

Published November 1, 2020

Citation

Willighagen, E. (2020). CiTO updates #1: first research paper in the Journal of Cheminformatics with CiTO annotation published. In *chem-bla-ics*. chem-bla-ics. https://doi.org/10.59350/w03hn-k8p90

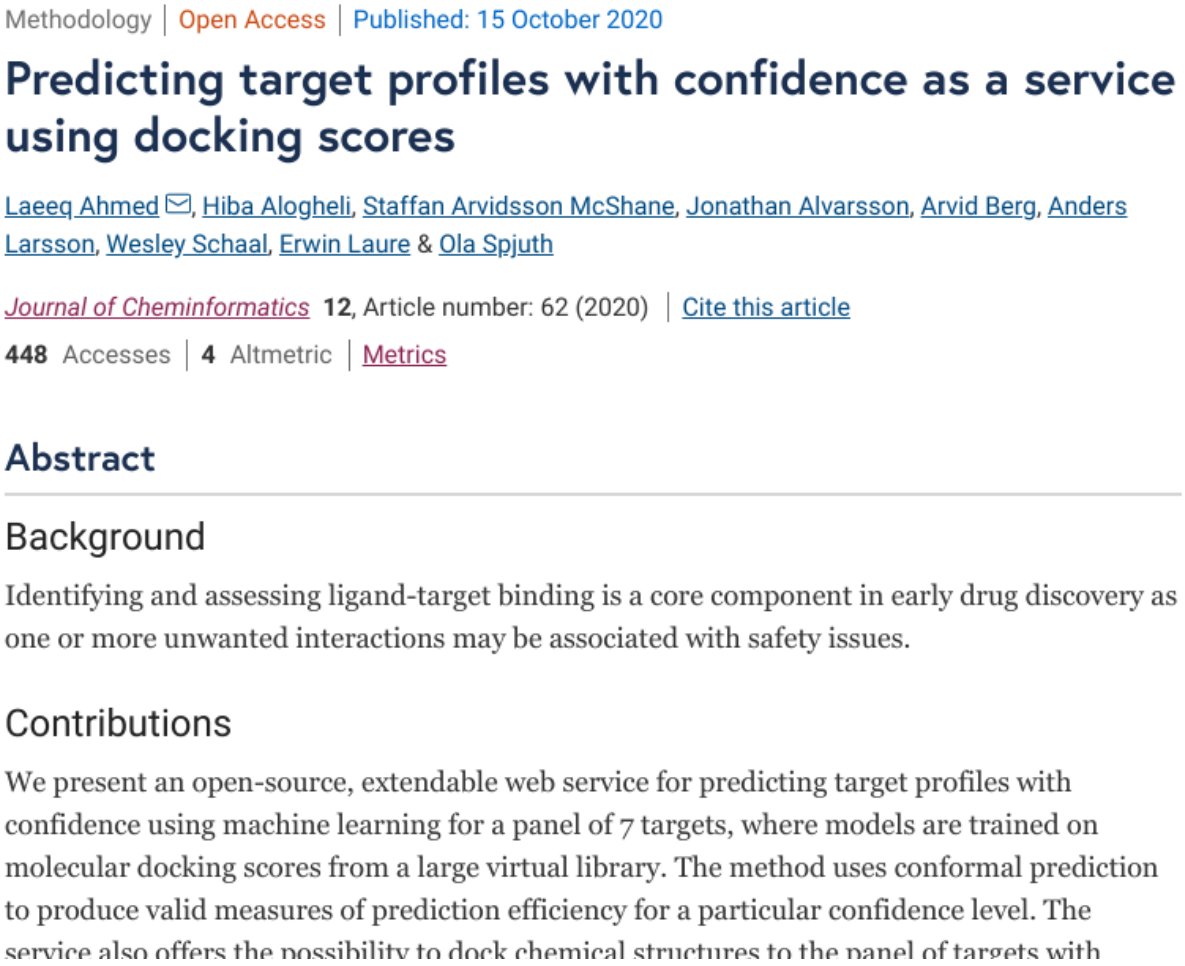
Keywords

Cito, Jcheminf

Abstract

After a time of exploration of technical needs, idea, plans, the Journal of Cheminformatics launched its Citation Typing Ontology (CiTO) Pilot this summer (doi:10.1186/s13321-020-00448-1). I am very excited about this, because the CiTO tells us why we are citing literature. We are a very long way away from publishing industry adoption, but we have to start somewhere.

After a time of exploration of technical needs, idea, plans, the Journal of Cheminformatics launched its Citation Typing Ontology (CiTO) Pilot this summer (doi:10.1186/s13321-020-00448-1). I am very excited about this, because the CiTO tells us why we are citing literature. We are a very long way away from publishing industry adoption, but we have to start somewhere. Laeeq Ahmed *et al.* published a few weeks ago the first research article with CiTO annotation of references ("Predicting target profiles with confidence as a service using docking scores")!



Methodology | Open Access | Published: 15 October 2020

Predicting target profiles with confidence as a service using docking scores

Laeeq Ahmed ✉, Hiba Alogheli, Staffan Arvidsson McShane, Jonathan Alvarsson, Arvid Berg, Anders Larsson, Wesley Schaal, Erwin Laure & Ola Spjuth

Journal of Cheminformatics **12**, Article number: 62 (2020) | Cite this article

448 Accesses | **4** Altmetric | Metrics

Abstract

Background

Identifying and assessing ligand-target binding is a core component in early drug discovery as one or more unwanted interactions may be associated with safety issues.

Contributions

We present an open-source, extendable web service for predicting target profiles with confidence using machine learning for a panel of 7 targets, where models are trained on molecular docking scores from a large virtual library. The method uses conformal prediction to produce valid measures of prediction efficiency for a particular confidence level. The service also offers the possibility to dock chemical structures to the panel of targets with

Of course, I also have to show a screenshot of what the annotation actually looks like, so here goes:

21. Capuccini M, Spark cheminformatics utils. https://github.com/mcapuccini/spark-cheminformatics. **[cito:usesMethodIn]** (2015–2020)

22. Alvarsson J, Eklund M, Andersson C, Carlsson L, Spjuth O, Wikberg JE (2014) Benchmarking study of parameter variation when using signature fingerprints together with support vector machines. J Chem Inf Model 54(11):3211–3217 **[cito:agreesWith]**

CAS PubMed Article Google Scholar

23. Cortes C, Vapnik V (1995) Support vector networks. Mach Learn 20(3):273–297 **[cito:citesAsAuthority]**

Google Scholar

Thanks for the authors for adding these annotations!