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Artificial intelligence for natural product drug discovery

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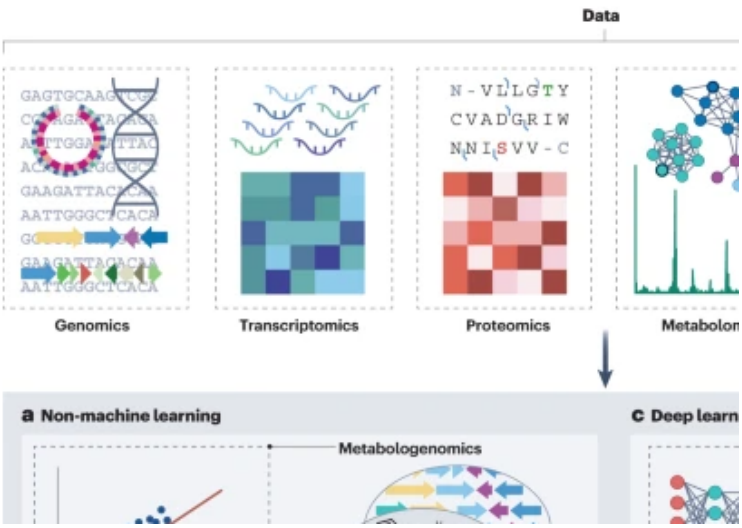
Keywords

Cheminf, Natprod

Fig. 1: Applications of artificial intelligence in natu



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Two weeks ago the write up of a week-long scientific discussions around artificial intelligence for natural product drug discovery in Leiden at the Lorentz Center got published (doi:10.1038/s41573-023-00774-7, free PDF).

Part of the copyrighted Figure 1 from the article. I hope this counts as fair use.

Sadly, the meetings was still during the (partial) lockdown, and I think my contribution could have been more extensive. But I am happy I got to pitch the idea of using Wikidata in this area too, taking advantage of the work done by the LOTUS (doi:10.7554/eLife.70780) team earlier.

And this is key to me: you cannot do statistics, chemometrics, machine learning, or artificial intelligence without good quality linked data. Happy reading!