Subject: Video tutorials on using Datawarrior Posted by Jo W on Mon, 29 Sep 2025 12:57:10 GMT

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Dear Datawarrior users

Recently, some Datawarrior tutorials on youtube have been appearing that are very clear and concise - they are very good.

Disclaimer: Please note I am not affiliated with this channel and don't know the person (Bruno) that has created them.

I am chemist and have been using Datawarrior for around 5 years now (almost everyday) and I have still learnt a lot from these videos.

Please have a look (in part so that the YouTube view numbers get higher and subscribe if possible to help the channel out – in my opinion there are not enough tutorials on Datawarrior)

The link to one is here:

Introduction to Core-Based SAR in DataWarrior – Part 7 https://www.youtube.com/watch?v=WKBvPe5CgOI

If you see this - thank you so much Bruno for your efforts – it is greatly appreciated – the low number of views so far are at variance with the quality of your work here.

What else does the DW community think we need tutorials on?

Some things I would like to see:

- Several tutorials on docking in Datawarrior (DW).
- Examples of using DWs very helpful version of the PDB database file for example they have cropped the proteins so the file sizes are much smaller and it is also much more straightforward to search for substructures than on the pdb site itself what else has been done and what have people found?
- The use of the docking feature in DW and how to export docked ligands out of DW.
- Docking when combined with evolutionary algorithms (EL).
- How to align conformers and use in SAR.
- The use of machine learning features in DW.
- Short videos on specific hacks, short cuts creative ideas for use specifically in DW
- How to create custom-made plugins for DW for example I am developing a plugin for searching pubchem but I dont have a coding background (I created it by using just chatgpt)and it works but I have come across some problems and its now a bit slow going trying to solve it...... Any other ideas for custom plugins or short tutorial videos?

Also check out Julio's work on DW and using EL's - his published papers are also accompanied with explanatory videos (great idea – I think it should be done with every paper published) plus he even uploaded the dwar files for you to try yourselves:

https://chemrxiv.org/engage/chemrxiv/article-details/670b9b2 112ff75c3a147b97b

Look forward to hearing the DW community views, suggestions etc

Thanks again Bruno and Julio for your efforts and of course the Datawarrior developers themselves for bringing into existence such a great piece of software

Subject: Re: Video tutorials on using Datawarrior Posted by Jo W on Mon, 29 Sep 2025 13:04:06 GMT

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Of course there are other videos on DW on YouTube - some from the datawarrior creators/colleagues and from other cheminformatics - I just highlighted the above as they are more recent and currently active

Subject: Re: Video tutorials on using Datawarrior Posted by Jo W on Tue, 30 Sep 2025 18:09:46 GMT

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The above link to Julio's paper does not include dwar files after all- but here is one that does and it also includes some videos which describe how to use certain functions in DW (I think it includes the use of EL from memory - as I dont have access to the video right now) see -

https://chemrxiv.org/engage/chemrxiv/article-details/674d8b6 a7be152b1d0a899d3