

The Molecular Chemometrics Principles #3: stand on shoulders

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Abstract

I have blogged about two Molecular Chemometrics principles so far:

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I have blogged about two Molecular Chemometrics principles so far:

- [McPrinciple #1: access to data](#)
- [McPrinciple #2: be clear in what you mean](#)

Peter's post [#solo10: Green Chain Reaction; where to store the data? DSR? IR? BioTorrent, OKF or ???](#) gives me enough basis to write up a third principle:

Molecular Chemometrics Principles #3: We make scientific progress if we build on past achievements.

Sounds logical, right? Practically, the way we share our cheminformatics knowledge makes this standing on shoulders pretty difficult. But there is one particular aspect I would like to ask your attention for: you can contribute by making clear what shoulders you would like to stand on. That is, where do you prefer to put your effort, and what message would you like to give to your user community.

In the aforelinked post, Peter asks where he should upload his data, and he suggest [BioTorrent](#) (see my review [BitTorrents for Science](#)), DSpace, and [CKAN](#). Now, his [Green Chain Reaction](#) is picked up (see [these few blog](#) posts), and the resulting data should be distributed as much as possible. The exact location does not really matter..

But...

By picking where you upload, you make a statement to your community: *"Look guys, we are distributing our data via Foo, because we believe those guys are doing good work! Perhaps you can support them too."*

This principle does not only apply to data, it applies to things too. For example, when [iChemLabs and RSC ChemSpider Announce Partnership](#) they do not just improve the user experience of ChemSpider (which I certainly won't object against), but they also imply *"Look dudes, your product is just not good enough and we do not want to help you improve it either"*. Of course, ChemSpider has every right, and for them to succeed it is crucial to make decisions like this. Fortunately, [ChemDoodle is GPL](#).

Every project with a user base has the opportunity to support shoulders, if they only visibly stand on them. By merely discussion the *Green Chain Reaction*, I show to support this social web experiment. You can too. Use these powers wisely. May the McPrinciples be with you.