

My favourite chemistry things

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Yeah, it's my turn. Standing on the shoulders of [ChemJobber](#), [Azmanam](#), and [ScienceBase](#), here's list of things I like about chemistry. To put things into perspective first, a bit, I note that ChemJobber and Azmanam focused on wet-lab chemistry, and David on fancy molecules. Now, I am a theoretical chemist, and was thinking on what to orient the things I like, and on how general to make them. This meme is not easy, you now. But here goes:

1. chemical graph theory

Chemical graph theory is one of the common theoretical models chemists work with to make sense of chemical properties. I like it because the graph theory is fairly straightforward, but chemistry adds enough color (literally!) to create a nice complexity that kept the cheminformatics field going strong for more than 50 years now :) For example, how to adapt the theory to [deal with mutli-atom bonds](#) :)

2. rare nuclei in the NMRShiftDB

The [NMRShiftDB](#) is an Open Data repository for annotated NMR spectra. The fun here is to add NMR spectra of [rare nuclei](#) . Don't you just love a molecule with NMR shifts for all atoms?

3. metabolomics

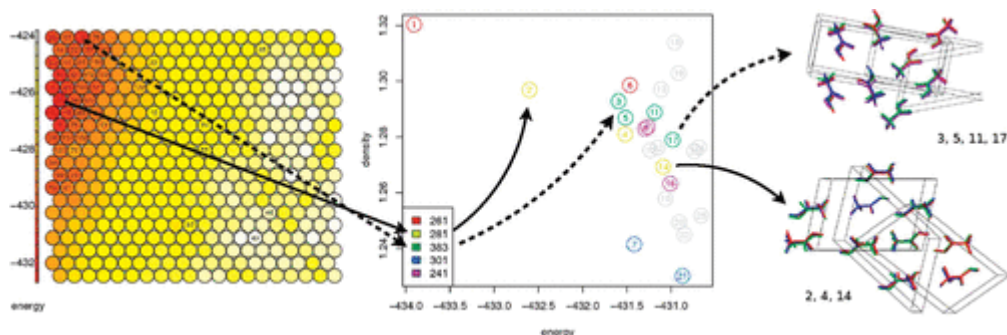
Metabolomics is the research field that studies the small molecules of life. Plant metabolomics is particularly fun. Tens of thousands of molecules, and a lot of metabolite identification to be done, and much more. Lot's of cool stuff to do here, and I am trying to secure funding for it. This is [what I blogged about metabolomics before](#). What about his nice [secondary metabolite](#) (source: [Wikipedia](#), [CC0](#)):

4. hexavalent carbon

Atom types is another theoretical model for chemistry. [Atom typing](#) is one of the underlying technologies of [force fields](#), which are used in many, many fields in chemistry. Now, force fields typically take only a subset of atom types. New atom types, consequently, need to be added. One such new atom type was the [hexavalent carbon](#). Rare, very rare, but just the amount of complexity I like about chemistry.

5. self-organizing maps

Kohonen maps, or [self-organizing maps](#) (SOM), are a machine learning method that have interesting visualization features. They have numerous applications, and also in chemistry. The group where I did my PhD developed a supervised SOM, which I used them to classify crystal structures (doi:[10.1021/cg060872y](#)). Another of my favorites is the [reaction classification by Aires-de-Sousa et al.](#) using unsupervised SOMs.



6. the Maillard reaction

People who know me personally, know that I like tasting things. That also makes me have to worry about overweight. Taste is to a large extent governed by cooking, and the [Maillard reaction](#) plays an important role here. If you like to learn more about the chemistry of cooking, checkout these [two blogs](#).

7. Cb

Cb is a new element on the world wide web. Well, not so new anymore, and the full name is likely more familiar: [Chemical blogspace](#). This social web application brings together blogging chemists world wide. Oh, and this meme is picked up nicely:

Popular posts this week

[My Favorite Things about Chemistry](#)



  [linked to by 7](#) posted to [Chemjobber](#) on Fri 7th 1

Because sometimes the facts about chemical emp aren't very fun. But this is!My Favorite Things about CJ)1. A chromatography column that works well.2. trove of literature, filled with truth, (a few) lies and idiosyncrasie

[The Haystacks Favorite Chemistry Things](#)



  [linked to by 5](#) posted to [C&ENtral Science](#) on M

Chemjobber got our creative juices flowing this Mor when he came up with a list of his favorite things al and called on us (and others) to come up with our c already answered the call. Here's our top ten, with...

[A Few of My Favorite \(Chemistry\) Things](#)



  [linked to by 5](#) posted to [Chemistry Blog](#) on Fri 7t

To carry on with Chemiobber's Favorite Things list

8. chemical abstracts

No, not the database, but the nice graphical article abstracts in chemistry journals. [ChemFeeds](#) gets it all together. BTW, there remains very much to be done about improving publishing chemistry. [I blogged about that repeatedly](#).

9. organometallics

[Organometallics](#) is, like metabolomics, a really interesting area, with lots of complexities (pun intended :). Actually, I am not even aware of a organometallics/metabolomics mashup. Anyone with some nice pointers? I have not blogged about it much, and [the one time](#) I did was in relation to chemical graph theory.

10. sparkling fire

Burning things. Nothing more to say about that, I guess. Well, perhaps. Chemists like burning things; others might too, but chemists at least. Blowing up things too. When I was a student, I had a very friendly colleague who liked blowing up things and made TNT himself and took that to university too (stabilized, mind you :). Cool!

Anyway, while googling for something to spice up this tenth item, I ran into this book: [Caveman Chemistry: 28 Projects, from the Creation of Fire to the Production of Plastics](#). The [prologue](#) nicely writes up that you need to sparkle some fire in education to get the students enlightened:

I teach chemistry at Hampden-Sydney College, a small liberal-arts college in central Virginia. The students here, by and large, do not come equipped with insatiable curiosity about my discipline and experience has convinced me that the profession of professing has more to do with motivation than with explanation; a student who is not curious will resist even the most valiant attempts at compulsory education; conversely, inquiring minds want to know. A great deal of my time, then, has been spent devising tricks, gimmicks, schemes and plots for leading stubborn horses to water, knowing full well that I can't make them think.

Now, that leaves me with tagging a few further blogs to tag to continue the meme. The meme is spreading fast, so I hope I do not tag someone who already is tagged. [Jean-Claude](#), [Peter](#), [Noel](#), [Rich](#), [Antony](#), would you mind letting us know your ten favourite chemistry things?