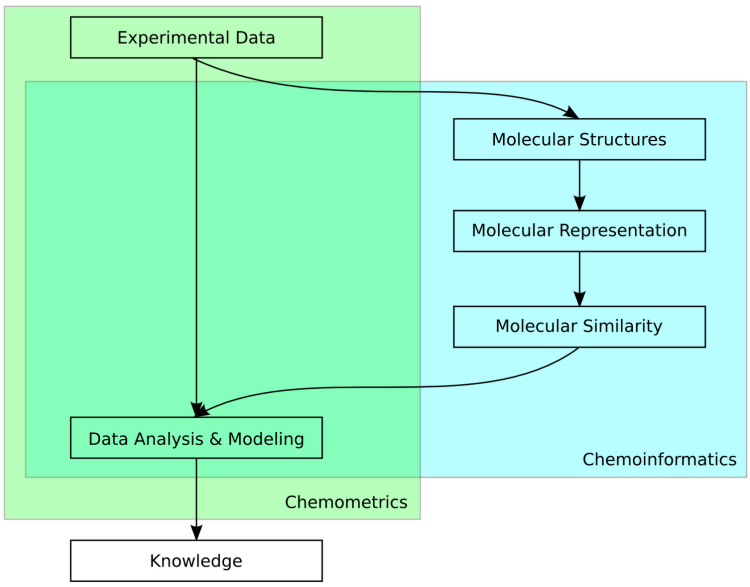
Writing up my PhD introduction chapter...

Egon Willighagen

Published February 4, 2007

Citation

Willighagen, E. (2007, February 4). Writing up my PhD introduction chapter. *Chem-bla-ics*. https://doi.org/10.59350/k9nar-6wt60



Copyright

chem-bla-ics

The last twelve months or so, I have been doing two jobs (excluding hobbies of mine, such as Chemical blogspace): my postdoc in the group of Christoph Steinbeck on computer aided structure elucidation, and finishing my PhD. The topic of my PhD is about the interplay between chemoinformatics and chemometrics: the first being strong in dealing with molecular structures, the latter strong in data analysis and mining, originally on experimental data. Really, I focused on a few existing problems, such as how to represent and analyze large libraries of crystal structures, the use of NMR spectra in QSAR studies, and two more practical problems regarding reproducibility of scientific results, which includes communication of data, and transferability of algorithms. Actually, I also studied fragment mining in QSAR for a set of transfactants, but that has not lead to firm results yet.

The below diagram shows how I see the interplay between both fields: