

chem-bla-ics

Molecular Chemometrics

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I just found out that a review article that I wrote earlier this year got printed: *Molecular Chemometrics* (DOI:[10.1080/10408340600969601](https://doi.org/10.1080/10408340600969601)), with my personal view on the interplay between chemoinformatics and chemometrics. The review discusses interesting developments in the last five years, and was fun writing (reading too, I think :). It has four major topics:

- *molecular representation* (with 'molecular descriptors' and 'beyond the molecule')
- *chemical space, similarity and diversity*
- *activity and property modeling* (with 'dimension reduction' and 'model validation')
- *library searching*, which mostly focuses on semantic web developments

Comments most welcome; just leave them below this blog item, or blog about the article yourself :)