

# Molecular Chemometrics

Egon Willighagen 

Published December 12, 2006

## Citation

Willighagen, E. (2006). Molecular Chemometrics. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/frmbe-grb50>

## Keywords

Chemometrics, Cheminf

## Abstract

I just found out that a review article that I wrote earlier this year got printed: Molecular Chemometrics (DOI:10.1080/10408340600969601), with my personal view on the interplay between chemoinformatics and chemometrics.

## Copyright

Copyright © Egon Willighagen 2006. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

## chem-bla-ics

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 :)