

# Subset selection: mind the complexity

Egon Willighagen 

Published December 23, 2005

## Citation

Willighagen, E. (2005). Subset selection: mind the complexity. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/52me2-0wm09>

## Keywords

Cheminf

## Abstract

In a recent JCIM article, Schuffenhauer compares a few subset selection methods, and notes that some of them reduce the average complexity of the molecules. They put this in relation to other research that states that lead compounds with high complexity have higher activities. Recommended reading material for the holidays.

## Copyright

Copyright © Egon Willighagen 2005. 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

In a recent [JCI](#) article, Schuffenhauer [compares](#) a few subset selection methods, and notes that some of them reduce the average complexity of the molecules. They put this in relation to other research that states that lead compounds with high complexity have higher activities. Recommended reading material for the holidays.