

# Subset selection: mind the complexity

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Published December 23, 2005

## Citation

Willighagen, E. (2005, December 23). Subset selection: mind the complexity. *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.

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## chem-bla-ics

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