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Title: Performance comparison of partial least squares-related variable selection methods for quantitative structure retention relationships modelling of retention times in reversed-phase liquid chromatography

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1 HIGHLIGHTS:

- 2 • The relative performance of six PLS-related variable selection methods was
3 compared in the context of QSRR.
- 4 • All methods demonstrated very small demands of computational time and effort.
- 5 • All models derived from selected subset of descriptors outperformed the reference
6 PLS model derived from all descriptors.
- 7 • Combining variable selection methods can further improve the overall
8 performance of the resulting model.
- 9 • The most commonly selected molecular descriptors were found relevant to the
10 retention mechanism of RPLC.

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12 **Performance comparison of partial least squares-related variable selection methods for**
13 **quantitative structure retention relationships modelling of retention times in reversed-**
14 **phase liquid chromatography**

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