

GCalignR: An R package for aligning Gas-Chromatography data

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Abstract

Chemical signals are among the most fundamental and oldest means of animal communication. The desire to unravel broader patterns of chemical communication in birds and mammals paved the way for two not entirely new techniques, gas-chromatography and mass-spectrometry, in the fields of ecology and evolution. Comparing chemical profiles or chromatograms across many individuals yields some major obstacles as even the newest GC machines have an inherent error when measuring the retention times of chemical substances. Here we present GCalignR, an R package for the alignment of chromatography peaks among samples prior to hypothesis testing using multivariate statistics. GCalignR is specifically designed to be used by non-chemists by providing easy to use functions to check and align gas-chromatography data based on retention times. In addition, the package implements heatmaps and other plots to evaluate and potentially adjust the peak alignment. We hope that GCalignR will provide a tool that fits into a common biologist's workflow in R and that the package will contribute to the standardization and reproducibility of studies on chemical communication.

Introduction

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Materials and methods

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Results

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Discussion 45

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Conclusion 52

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Supporting information 66

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References

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