

GCalignR: An R package for aligning Gas-Chromatography data

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11/1/2015

1 Abstract

Metabolomics approaches such as Gas-Chromatography (GC) are increasingly used by researchers in ecology and evolution to study the chemical basis of animal communication. However, the statistical analysis of patterns across individuals requires the alignment of chemical data, which is inherently noisy due to subtle, random and often unavoidable variation of the GC machine parameters (Pierce et al. 2005). We developed an R package, **GCalignR**, which provides easy-to-use function to align GC data in R and evaluate the quality of the alignment.

Key-words: GC-MS, chemical communication, olfactory communication, alignment

2 Introduction

2.1 Availability

The latest version of **GCalignR** can be downloaded from GitHub.

```
install.packages("devtools")  
devtools::install_github("mastoffel/GCalignR")
```

We welcome any contributions or feedback on the package.

2.2 Data accessibility

References

Pierce, Karisa M, Janiece L Hope, Kevin J Johnson, Bob W Wright, and Robert E Synovec. 2005. "Classification of Gasoline Data Obtained by Gas Chromatography Using a Piecewise Alignment Algorithm Combined with Feature Selection and Principal Component Analysis." *Journal of Chromatography A* 1096 (1). Elsevier: 101–10.