Dear Editor,

We would like to submit a research article entitled “GCalignR: An R package for aligning Gas-Chromatography data” for consideration for publication in PLOS ONE.

Chemical signals are arguably the oldest and most fundamental means of animal communication and play a fundamental role in mate choice and kin selection. However, downstream analyses rely on the correct alignment of homologous substances, represented by peaks, across samples. Previously, we developed an algorithm for the alignment of gas-chromatography (GC) data that was successfully applied in a study of chemical communication in Antarctic fur seals *Arctocephalus gazella,* where we showed that mother-pup pairs and breeding colony membership are reflected in chemical signatures (Stoffel *et al.* 2015). This manuscript builds upon this previous work by implementing the alignment procedure together with a suite of related tools in form of an R package.

In this manuscript, we present the R package GCalignR, which can be used for the processing of GC data in studies that seek to unravel broad patterns of chemical similarity among individuals. The package also implements a suite of dynamic visualisation tools to facilitate inspection of the resulting alignments and can be integrated within a broader workflow in R to facilitate downstream multivariate analyses. We demonstrate an example workflow and show that the resulting alignments are relatively insensitive to realistic levels of randomly introduced noise, and also test the package on three pre-validated datasets to reveal generally rather low alignment error rates. We hope that GCalignR will help to simplify the processing of chemical datasets and contribute towards improved standardization and reproducibility.

We suggest the following editors to handle our manuscript:

Giorgio F Gilestro

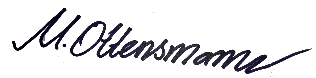
Imperial College London, United Kingdom

Expertise in open source software development

**Patrick J. O. Miller**  
University of Saint Andrews, United Kingdom

Focuses on communication and behavioural ecology of marine mammals

Sincerely,



Meinolf Ottensmann, MSc candidate