Reviewer's report

Title: Extraction of pure components from overlapped signals in gas chromatography-mass spectrometry (GC-MS)

Version: 1 Date: 29 June 2009

Reviewer: Jörg Rahnenführer

Reviewer's report:

The manuscript reviews methods for identifying the pure signals from co-eluting components when complex mixtures of chemicals are analyzed by GC-MS (gas chromatography–mass spectrometry). GC-MS is a powerful method for analyzing complex mixtures of products and has become important for a broad spectrum of applications. Co-elution of several components resulting in overlapping signals represents one major challenge in the statistical and computational analysis of GC-MS data.

The review is well-arranged and fosters comprehension of both principles as well as advantages and disadvantages of the different algorithmic approaches. First the nature of GC-MS data is introduced and the problem of signal overlap is formalized. Then methods are explained, classified into empirical methods, eigenvalue analysis, regression methods, and library comparison. The overview is up-to-date in a fast moving field.

The following extensive discussion is valuable for researchers faced with the problem of algorithm choice. First, reasons for experimental imperfections are given. Then, for all type of algorithms typical drawbacks are adequately discussed, pointing out especially the large number of parameters to be fitted for empirical methods and the lack of successful evaluations for matrix based methods. The manuscript ends by expressing the hope that the progress in computing capabilities in general will help to develop new methods that overcome all of the difficulties presented before.

The review is clearly presented, lists the most important representatives for tackling the problem at hand and has a particular strength in critically discussing remaining problems. Only English language should be checked before publication, the use of articles (e.g. on page 11, in line 10 a missing “the”, in line 12 a redundant “the”), repeated words (“an an” on page 16, “their their” on page 18), and the use of singular and plural (e.g. Discussion, line 5).

Level of interest: An article of importance in its field

Quality of written English: Acceptable

Statistical review: Yes, and I have assessed the statistics in my report.
Declaration of competing interests:
I declare that I have no competing interests.