

Accepted Manuscript

Unmixing of mixed oil using chemometrics

Zhao-Wen Zhan, Yan-Rong Zou, Jian-Ting Shi, Jia-Nan Sun, Ping'an Peng

PII: S0146-6380(15)00202-8

DOI: <http://dx.doi.org/10.1016/j.orggeochem.2015.11.006>

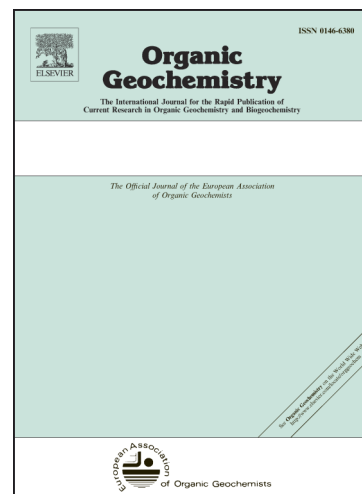
Reference: OG 3335

To appear in: *Organic Geochemistry*

Received Date: 4 June 2015

Revised Date: 12 October 2015

Accepted Date: 4 November 2015



Please cite this article as: Zhan, Z-W., Zou, Y-R., Shi, J-T., Sun, J-N., Peng, P., Unmixing of mixed oil using chemometrics, *Organic Geochemistry* (2015), doi: <http://dx.doi.org/10.1016/j.orggeochem.2015.11.006>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Unmixing of mixed oil using chemometrics

Zhao-Wen Zhan^{a,b}, Yan-Rong Zou^{a,*}, Jian-Ting Shi^{a,b}, Jia-Nan Sun^{a,b}, Ping'an Peng^a

^aState Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, 510640, China;

^bUniversity of Chinese Academy of Sciences, Beijing 10039, China.

Abstract:

In this study, chemometrics was used to unmix a set of oil samples that had been mixed in the laboratory using three end-member oils. It was shown that the concentrations of individual compounds in the mixed oil varied linearly with the fractional contribution of each end-member oil. However, biomarkers ratios in the mixed oils varied non-linearly with the amount of each end-member oil. This study demonstrates that concentrations and ratios of biomarkers yield different results when de-convoluting mixed oils. Concentrations of biomarkers are therefore more suitable than the biomarker ratios for unmixing mixed oils. Alternating least squares of biomarker concentrations (ALS-C) provides an excellent way to calculate the number, proportions, and compound compositions of the end-members in mixed oil samples. The ALS-C results are accurate, regardless of whether end-member oils are included in the sample set. The biomarker ratios of end-member oils cannot be

* Corresponding author. Tel.: +86 20 85290187; fax: +86 20 85290706.
E-mail address: zouyr@gig.ac.cn (Y.-R. Zou).

Download English Version:

<https://daneshyari.com/en/article/5161819>

Download Persian Version:

<https://daneshyari.com/article/5161819>

[Daneshyari.com](https://daneshyari.com)