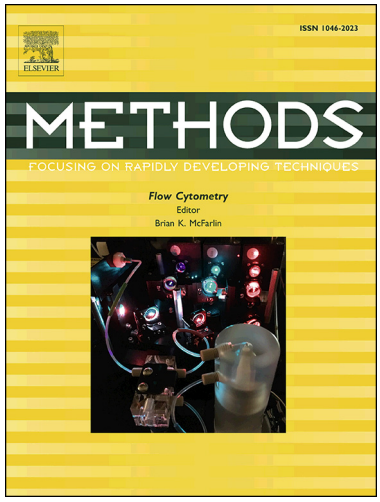
Accepted Manuscript



Predicting Ion Mobility-Mass Spectrometry Trends of Polymers using the Concept of Apparent Densities

Jean R.N. Haler, Denis Morsa, Philippe Lecomte, Christine Jérôme, Johann Far, Edwin De Pauw

PII: S1046-2023(17)30465-6
DOI: https://doi.org/10.1016/j.ymeth.2018.03.010
Reference: YMETH 4433

To appear in: *Methods*

Received Date: 29 January 2018
Revised Date: 14 March 2018
Accepted Date: 26 March 2018

Please cite this article as: J.R.N. Haler, D. Morsa, P. Lecomte, C. Jérôme, J. Far, E. De Pauw, Predicting Ion Mobility-Mass Spectrometry Trends of Polymers using the Concept of Apparent Densities, *Methods* (2018), doi: https://doi.org/10.1016/j.ymeth.2018.03.010

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.

ACCEPTED MANUSCRIPT

Predicting Ion Mobility-Mass Spectrometry Trends of Polymers using the Concept of Apparent Densities

Jean R. N. Haler[1], Denis Morsa[1], Philippe Lecomte[2], Christine Jérôme[2], Johann Far[1], Edwin De Pauw[1]*

[1]Mass Spectrometry Laboratory, University of Liège, MolSys Research unit, Quartier Agora, Allée du Six Aout 11, B-4000 Liège, Belgium

[2]Center for Education and Research on Macromolecules, University of Liège, CESAM Research unit, Quartier Agora, Allée du Six Aout 13, B-4000 Liège, Belgium

*Corresponding author email address: jean.haler@uliege.be

Keywords: Ion Mobility-Mass Spectrometry, Synthetic polymers, Gas phase structures, Apparent densities, Data fitting, Prediction

Declarations of interest: none

Abstract

Ion Mobility (IM) coupled to Mass Spectrometry (MS) has been used for several decades, bringing a fast separation dimension to the MS detection. IM-MS is a convenient tool for structural elucidation. The folding of macromolecules is often assessed with the support of computational chemistry. However, this strategy is strongly dependent on computational initial guesses. Here, we propose the analysis of the Collision Cross-Section (CCS) trends of synthetic homopolymers based on a fitting method which does not rely on computational chemistry *a prioris* of the three-dimensional structures. The CCS trends were evaluated as a function of the

Download English Version:

https://daneshyari.com/en/article/8340009

Download Persian Version:

https://daneshyari.com/article/8340009

Daneshyari.com