## Accepted Manuscript

How to Run Molecular Dynamics Simulations on Electrospray Droplets and Gas Phase Proteins: Basic Guidelines and Selected Applications

Lars Konermann, Haidy Metwally, Robert G. McAllister, Vlad Popa

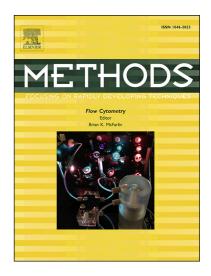
PII: S1046-2023(17)30464-4

DOI: https://doi.org/10.1016/j.ymeth.2018.04.010

Reference: YMETH 4447

To appear in: *Methods* 

Received Date: 24 January 2018 Revised Date: 10 April 2018 Accepted Date: 12 April 2018



Please cite this article as: L. Konermann, H. Metwally, R.G. McAllister, V. Popa, How to Run Molecular Dynamics Simulations on Electrospray Droplets and Gas Phase Proteins: Basic Guidelines and Selected Applications, *Methods* (2018), doi: https://doi.org/10.1016/j.ymeth.2018.04.010

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**

### **Invited Contribution**

for

"MS-based Methods to Study Macromolecular Higher Order Structure and Interactions"

Edited by Igor A. Kaltashov

How to Run Molecular Dynamics Simulations On Electrospray Droplets and Gas Phase Proteins: Basic Guidelines and Selected Applications

Lars Konermann,\* Haidy Metwally, Robert G. McAllister, Vlad Popa

Department of Chemistry, The University of Western Ontario, London,
Ontario,

N6A 5B7, Canada

\* corresponding author, konerman@uwo.ca

**Keywords:** protein conformation; charged droplet; charged residue model; ion mobility spectrometry; Gromacs

#### Download English Version:

# https://daneshyari.com/en/article/8340007

Download Persian Version:

https://daneshyari.com/article/8340007

<u>Daneshyari.com</u>