*medical sciences forum*

MDPI

*Abstract*

# Stochastic Dynamics Mass Spectrometric 3D Structural Analysis of N-Glycans of Fetal Bovine Serum—An Experimental and Theoretical Study †

**Bojidarka Ivanova * and Michael Spiteller**

Institute of Environmental Research, Dortmund University of Technology, 44227 Dortmund, Germany
* Correspondence: b_ivanova@web.de
† Presented at the 8th International Electronic Conference on Medicinal Chemistry, 1–30 November 2022; Available online: https://ecmc2022.sciforum.net/.

**Abstract:** This study addresses the problem of performing mass spectrometric (MS), 3D molecular and electronic structural analyses of glycans mixtures from fetal bovine serum. This undertaking is unexpectedly difficult, due to: random variation of non-template-driven glycosylation and fucosylation processes; a lack of regioselective derivatization for mixtures of polydisperse glycans towards length and skeletal modifications; isomers of oligomers and polymers, including linear and branching molecular structures, respectively. These factors significantly increase the difficulty in glycan structural analysis using mass spectrometry. Furthermore, MS phenomena of carbohydrates include reactions of intramolecular rearrangement and cyclization, proton and charge transfer effects, noncovalently bound self-associations, alkali metal ion adducts, and multiply charged species under the tandem MS/MS operation mode. However, this study presents a plausible solution to the problem. It employs our innovative stochastic dynamic MS model formula $D''_{SD} = 2.6388.10^{-17}$. ($<I^2>-<I>^2$) that is capable of accurately quantifying the fluctuations and temporal behavior of measurable variable intensity (I) of analyte peaks. It has been shown that it can accurately and directly quantify analyte concentrations in solution and determine 3D molecular and electronic structures. This latter task is less straightforward. It employs the Arrhenius model equation within the framework of his transition state theory and the power capability of quantum chemical methods. The validity of the latter statements is examined, herein. This study, first, comes to grips with MS collision-induced dissociation phenomena of mixtures of 2-aminobenzamide-derivatized glycans. It utilizes ab initio and DFT static, molecular dynamics, molecular mechanics, and chemometrics.

**Keywords:** mass spectrometry; stochastic dynamics; glycans; structural analysis

check for updates

**Citation:** Ivanova, B.; Spiteller, M. Stochastic Dynamics Mass Spectrometric 3D Structural Analysis of N-Glycans of Fetal Bovine Serum—An Experimental and Theoretical Study. *Med. Sci. Forum* **2022**, *14*, 2. https://doi.org/10.3390/ECMC2022-12870

Academic Editor: Maria Emília Sousa

Published: 12 August 2022



**Supplementary Materials:** The poster can be downloaded at: https://www.mdpi.com/article/10.3390/ECMC2022-12870/s1.

**Author Contributions:** Conceptualization, B.I. and M.S.; methodology, B.I. and M.S.; formal analysis, B.I.; investigation, B.I.; writing—original draft preparation, B.I.; writing—review and editing, B.I.; visualization, B.I.; project administration, M.S. and B.I.; funding acquisition, B.I. and M.S. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by [Deutsche Forschungsgemeinschaft; Funder Id: http://dx.doi.org/10.13039/501100001659] grant number [255-22-1].

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** M. S. has received a research grant (DFG, Funder Id: http://dx.doi.org/10.13039/501100001659; grant 255/22-1); B. I. has received a research grant (DFG 255/22-1).