ECMC 2023

*Abstract*

# Quantitative relations among measurands of molecular isotopologues of halogenated pharmaceutics – stochastic dynamic mass spectrometric approach†

**Bojidarka Ivanova** [1,*]

[1] Lehrstuhl für Analytische Chemie, Institut für Umweltforschung, Fakultät für Chemie und Chemische Biologie, Universität Dortmund, Otto-Hahn-Straße 6, 44221 Dortmund, Nordrhein-Westfalen, Deutschland; bojidarka.ivanova@yahoo.com; b_ivanova@web.de
* Correspondence: bojidarka.ivanova@yahoo.com
† Presented at the title, place, and date.

**Abstract:** The paper serves two goals. Its first aim is to approach mass spectrometric measurands such as mass-to-charge and peak intensity variables of molecular isotopologies of halogenated pharmaceutics diclofenac (1) and loratadine (2) with respect to experimental conditions of measurements, involving collision energy and concentration of the presented formic acid; if any *via* our stochastic dynamic method and model equation [ $D_{SD}^{",tot} = \sum_{i}^{n} D_{SD}^{",i} = \sum_{i}^{n} 2.6388.10^{-17} \times \left(\overline{I_i^2} - \left(\overline{I_i}\right)^2\right)$]. In addition, the study tests its most recently derivative formulas [ $\overline{I^{TOT,q}} = \frac{1}{2} \times \frac{A_I^q}{A_D^q} \times D_{SD}^{",q}$ ] and [ $D_{SD,l}^{"} + D_{SD,m}^{"} = \left|r_{l,m}\right| \times \sqrt{\overline{I_{l,q}^2} - \left(\overline{I_{l,q}}\right)^2} \times \sqrt{\overline{I_{m,q}^2} - \left(\overline{I_{m,q}}\right)^2}$ ], connecting among measurands with respect to experimental conditions of measurements, particularly, accounting for collision energy values and concentration of formic acid. So far, the latter two formulas have been tested on only two molecular systems of labetalol and acetaminophen. Secondly, the first shown equation is used to determine 3D molecular and electronic structures of the analytes, mass spectrometrically. The task is carried out *via* its complementary application with the Arrhenius's equation. Those two domains constitute the fundamental background of the *analytical mass spectrometry* consisting in quantitative and 3D structural analysis of analytes, which are approaches only employing one and the same stochastic dynamic equation. There are used ultra-high resolution electrospray ionization mass spectrometric data in addition to high accuracy quantum chemical static methods as well as molecular dynamics. Tests of chemometrics are employed, as well.

**Keywords:** mass spectrometry; stochastic dynamics; isotopologies; diclofenac; loratadine.

**Supplementary Materials:**
**Author Contributions:** Conceptualization, B.I.; methodology, B.I.; software, B.I.; validation, B.I.; formal analysis, B.I.; investigation, B.I.; resources, B.I.; data curation, B.I.; writing—original draft preparation, B.I.; writing—review and editing, B.I.; visualization, B.I.; supervision, B.I.; project administration, B.I.; funding acquisition, B.I. All authors have read and agreed to the published version of the manuscript.
**Funding:** This research was funded by Deutsche Forschungsgemeinschaft [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:** Please refer to suggested Data Availability Statements in section "MDPI Research Data Policies" at https://www.mdpi.com/ethics.

**Acknowledgments:** The author is grateful to Deutscher Akademischer Austausch Dienst, the Alexander von Humboldt Stiftung, the Deutsche Forschungsgemeinschaft, the central instrumental laboratories for structural analysis at Dortmund University (Nordrhein-Westfalen, Germany) and analytical and computational laboratory clusters at the Institute of Environmental Research at the same University.
**Conflicts of Interest:** The author declares no conflict of interest.

**Citation:** Lastname, F.; Lastname, F.; Lastname, F. Title. *Med. Sci. Forum* **2023**, 2, x. https://doi.org/10.3390/xxxxx

Academic Editor: Firstname Lastname

Published: date