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MASS SPECTROMETRIC STUDY OF RANDOMLY ACETYLATED CYCLODEXTRINS AND THEIR ASSOCIATES — A STOCHASTIC DYNAMIC APPROACH

By Bojidarka Ivanova*, Michael Spiteller

PREFACE

A work on nonsubstituted cyclodextrins does illustrate persuasively the applicability of our innovative stochastic dynamic formulas connecting among measurable outcome *intensity*, analyte concentration in solution, the *temperature* and molecular properties to quantify and determine 3D structurally analytes. They bridge the gap between theory and experiment, in developing highly selective, sensitive, accurate and precise methods for quantification and exact 3D structural analytes by *mass spectrometry*. In this work, we will explore the same theoretical framework considering significantly more complex macromolecular objects of randomly acetylated derivatives of β- and γ-cyclodextrins as well as their noncovalent bond interacting self-associates (*m/z* 1400–1900.) The relationship between statistical parameter A_i of the SineSqr fitting of experimental relationship $(I-\langle I\rangle)^2 = f(t)$ and diffusion parameter is tested ($A^i = (m.D^i_{SD})/\{-(\ln((k_B.T)/m)^3.(2.T.\Delta t.k_B)\}$.) An approximation to A_i simplifies further our basic equation yielding to formula: $D'_{SD} \approx 1.3194.10^{-17}.(\langle I^2\rangle - \langle I\rangle^2)$ is also tested. The experimental proof of these model equations is presented, as well.

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The contribution was carefully carried out. Nevertheless, authors and publisher do not warrant the information to be free of errors. It is being published in English aiming at a widest access to the scientific information. English is not native language of the authors; thus, stylistic rough edges might occur. The authors hope for understanding of the reader.

Conflicts of interest

Michael Spiteller has received research grant (255/22-1, DFG); Bojidarka Ivanova has received research grant (255/22-1, DFG).

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Keywords:

Mass spectrometry; diffusion; quantum chemistry; stochastic dynamics; acetylated cyclodextrins

ABBREVIATIONS

ANOVA	Analysis of variance
APCI	Atmospheric pressure chemical ionization (mass spectrometric method)
BO	Born-Oppenheimer
CB	Carbohydrates
CD	Cyclodextrins
CID	Collision induced dissociation (mass spectrometry)
CM	Concentration of the analyte in solution
DFT	Density functional theory
D_{QC}	Quantum chemical diffusion parameter
D_{SD}	Stochastic dynamic diffusion parameter
ESI	Electrospray ionization
GS	Ground state
I	Intensity (mass spectrometric outcome)
ICR	Ion cyclotron resonance
LM	Local minimum
LMW	Low-molecular weight (analytes)
MALDI	Matrix-assisted laser desorption/ionization (mass spectrometry)
MD	Molecular dynamics
MS	Mass spectrometry
PES	Potential energy surface
RT	Retention time
SD	Stochastic dynamics
sd(yEr±)	Standard deviation
se(yEr±)	Standard error