

Bojidarka Ivanova / Michael Spiteller

Mass spectrometric study of randomly acetylated cyclodextrins and their associates. A stochastic dynamic approach

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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 ($A^i = (m \cdot D_{SD}^i) / \{ -(\ln((k_B \cdot T)/m))^3 \cdot (2 \cdot T \cdot \Delta t \cdot k_B) \}$.) An approximation to A_i simplifies further our basic equation yielding to formula: $D'_{SD} \approx 1.3194 \cdot 10^{-17} \cdot (\langle I^2 \rangle - \langle I \rangle^2)$ is also tested. The experimental proof of these model equations is presented, as well.

TABLE OF CONTENT

		Page
	PREFACE	3
	ACKNOWLEDGMENTS	7
	ABBREVIATIONS	9
1.	INTRODUCTION	11
2.	EXPERIMENTAL	19
2.1.	Materials and methods	19
2.2.	Sample preparation for ESI- and APCI-MS measurements	19
2.3.	Determination of statistical parameters <i>accuracy</i> and <i>precision</i>	20
2.4.	Determination of statistical parameters <i>repeatability</i> and <i>reproducibility</i>	20
2.5.	Chemometrics	20
2.6.	Theory/computations	20
2.6.1.	Stochastic dynamic theory and model formulas	20
2.6.2.	Quantum chemical computations	26
2.7.	Experimental design	27
3.	RESULTS	29
3.1.	Figures of merit	29
3.2.	Mass spectrometric data	32
3.2.1.	Assignment of fragment ions of randomly acetylated Ac- β - and Ac- γ -cyclodextrins	32
3.2.1.1.	Fragment ions within low m/z -values	32
3.2.1.2.	Fragment ions within high m/z -values	37
3.2.1.2.1.	Self-associates of nonsubstituted cyclodextrins	37
3.2.1.2.2.	Self-associates of randomly acetylated cyclodextrins	39

3.2.2.	Determination of mass spectrometric diffusion parameters and correlative analysis with the quantum chemical diffusion data	42
3.2.3.	Temperature dependency of the stochastic dynamic diffusion parameters	47
3.2.4.	Functional relationship of the stochastic dynamic diffusion parameters and the statistical parameters within the framework of the empirical modification of the characteristic function diffusion	48
4.	DISCUSSION	53
	CONCLUSION	59
	REFERENCES	63
	APPENDIX A (Chemometrics)	73
	APPENDIX B (Experimental mass spectrometric data)	95
	APPENDIX C (Theoretical quantum chemical data)	113

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Conflicts of interest

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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 $\pm$)	Standard deviation
se(yEr $\pm$)	Standard error