conferenceseries LLC Ltd
2142th Conference

September 2018 | Volume 09 | ISSN: 2157-7064
Journal of Chromatography & Separation Techniques
Open Access

Proceedings of

Joint Event on

8th World Congress on Chromatography

&

4th International Conference on

Polymer Science and Technology

September 13-14, 2018 | Prague, Czech Republic

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Keynote Forum
DAY 1

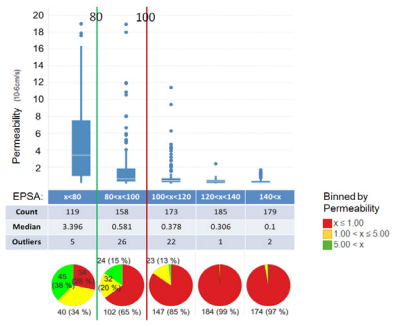
Gilles Goetz, J Chromatogr Sep Tech 2018, Volume: 09
DOI: 10.4172/2157-7064-C2-042

EPSA: a novel supercritical fluid chromatography technique enabling the design of permeable cyclic peptides

Gilles Goetz

Pfizer, USA

Applications of a new chromatographic method using SFC technology developed recently at Pfizer are described here. The EPSA method, as readout of polarity, correlates retention on a specific stationary phase with the exposed polarity of a molecule. Changes in retention can be interpreted by changes in polarity induced by the presence of intra-molecular hydrogen bonding (IMHB): indeed, IMHBs tend to impact molecular conformation, inducing hidden polarity that results in a decrease in analyte retention on the EPSA support. We demonstrate here the impact of this method on multiple beyond rule of five projects (NS5A, Oxytocin Receptor, CXCR7 Modulator, others). Given that conformational changes (induced and/or stabilized by the formation of IMHB) increases potential for membrane permeability, we show here that EPSA, and the EPSA prediction model, have significant impact in peptide drug design.



Biography

Gilles Goetz is a Principal Scientist at Pfizer in Groton, Connecticut, USA. He received his BSc (1991) and PhD (1995) at the University of Strasbourg in France. After his Post-doctoral studies at the University of Hawaii (1996-97) and of Neuchatel (CH) (1998-99) studying marine and fungal natural products, he joined Monsanto in 2000. There, he worked through mergers and acquisitions for Pharmacia and Pfizer successively in the natural product group, the HTS group (analytical support), and the purification group. In 2010, he transferred to the expert purification group at Pfizer Groton and in 2011 to the molecular properties group. He is a part of the team influencing medicinal chemistry design through insights into molecular properties such as polarity, lipophilicity, shape, and conformation that will impact molecular behaviors like solubility, permeability, and efflux. They develop and use mainly chromatographic techniques (EPSA) to assess those properties, and work towards predicting molecular behaviors.

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Karoly Heberger, J Chromatogr Sep Tech 2018, Volume: 09
DOI: 10.4172/2157-7064-C2-042

Separation selectivity of liquid chromatographic columns: a comparison by nonparametric methods

Károly Héberger

RCNS- Hungarian Academy of Sciences, Hungary

There are two legitimate aims for column selection: i) to determine similar ones to an existing one and ii) to find diverse (orthogonal) one(s) for optimal separation. Several different methods have already been elaborated to compare selectivity of chromatographic columns. All comparisons realize empirical approaches and based on measuring retention data of several well-chosen test compounds. Proper multivariate analyses can find similarities and differences in retention behavior of test compounds and stationary phases. As an illustration we adopted Wilson et al.'s data of 67 test compounds and 10 highly similar columns (C18-bonded silica stationary phases). The inherent characteristic groupings by physical properties were revealed with correct statistical tests and several independent methodologies. Generalized pair correlation method (GPCM)2 and sum of (absolute) ranking differences (SRD)3,4 unambiguously showed the same ranking pattern. The clustering by SRD is delivered to the reference. Therefore, all columns have been chosen as gold standard once and only once (comparison with one variable at a time). All lines of boxes correspond to an SRD ordering always with a different reference column (Figure 1). COVAT heatmaps show destroying the true pattern if the hydrophobic-subtraction model (HSM) evaluation is used. The ranking (clustering) pattern of chromatographic columns based on retention data (log k values) of 67 compounds and selectivity parameters of hydrophobic-subtraction model (HSM) provided various column groupings. Loss of information is inevitable for using the HSM data handling. Processing of retention data resulted in patterns that are consistent with differences in the columns' physicochemical parameters, whereas HSM results are deviating to a higher or lesser degree, depending on the particular chemometric approach. GPCM, SRD and COVAT procedures can be carried out on any data sets partially and on the whole to select the most similar and dissimilar columns, though our calculations were completed to the data set of Wilson et al.

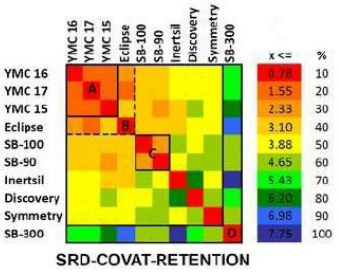

Figure 1. Heatmap plot of SRD analysis using primary retention data (67 test compounds) and comparison of one variable at a time.

Biography

Károly Héberger has completed his PhD, Cand. scient., DSc and t. Prof. In his early career, he investigated liquid phase oxidation (radical) processes and determined rate constants by kinetic ESR spectroscopy. Later, he studied quantitative structure activity (property) relationships like QSAR, QSPR and QSRR. Now, he deals with chemometrics such as multivariate data evaluation techniques, principal component analysis, stepwise linear regression, partial least squares regression, variable selection, model building and validation, pattern recognition (supervised and unsupervised), classification of food products, clustering, method comparison and ranking etc. His scientific results were presented in more than 160 papers (including book chapters) and has given more than 300 lectures (or posters) with h-index=34 and i-10 index=83 (Web of Science). The papers were cited above 3500 times.

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Hong Xue, J Chromatogr Sep Tech 2018, Volume: 09
DOI: 10.4172/2157-7064-C2-042

Dispersed mobile-phase countercurrent chromatography

Hong Xue

Hong Kong University of Science and Technology, Hong Kong

Countercurrent distribution based on liquid-liquid partition is a powerful separation method with minimal incurrence of loss of solutes, but its industrial application has been limited by cumbersome shifting of immiscible solvents. Although centrifugation has been employed to facilitate equilibration between phases, process scaling-up remains difficult. In this study, a dispersed mobile-phase countercurrent chromatography (DMCC) method has been developed to adapt the countercurrent distribution principle to a continuous column chromatography format. Continuous solute-exchange between two immiscible phases within a series of separation columns is achieved by mechanical dispersion of an influx of mobile phase into an upward stream of small droplets travelling through the columns filled with stationary phase. The diameter, length and number of columns and the number of stationary phases employed in the different columns can be varied to match the requisite scale and resolution of operation. Illustrations of DMCC were provided by examples of solute separations where the fractionated solutes could be collected either from the eluate of the series of columns or from drainage of the stationary phases in the individual columns at the end of a chromatographic run.

Biography

Hong Xue has obtained her MD from the Shanghai Second Military Medical University in 1983, PhD from the Institute of Medical Sciences and Department of Biochemistry, University of Toronto in 1992, and carried out Post-doctoral studies at the Department of Genetics, University of Glasgow before joining the Department of Biochemistry, Hong Kong University of Science & Technology (HKUST). Currently, she is the Director of Applied Genomics Center of HKUST, and Professor of Life Science at Hong Kong University of Science and Technology. Her group research focuses on genomics, bioinformatics and evolution biology to decipher the mechanisms of human complex diseases, in particular, schizophrenia. The group is also interested in translational research on novel therapeutics and diagnostics for complex neuropsychiatric disorders including anxiety, depression and neurodegenerative disorders, with a focus on GABAA receptors as the drug targets. In order to effectively isolate active components from medicinal herbs, her group has recently developed a novel chromatographic method designated as Disbursed Mobile-Phase Countercurrent Chromatography (DMCC). In 2003, she and her team discovered the association between schizophrenia and a segment of the GABRB2 gene encoding the β2 subunit of GABAA receptors, the positive selection of genotypes and haplotypes in this segment, determinant role of this segment in the alternate splicing of the β2 subunit protein, and the differential modulation of the GABA-induced membrane current by the long and short forms. These discoveries represent therefore the first instance where a schizophrenia-susceptibility gene has been linked to protein processing and further to electrophysiological response of neurons, thereby opening the door toward understanding the mechanism of schizophrenia etiology leading from gene to neuronal phenotype.

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Keynote Forum
DAY 2

Joanna Fiedor, J Chromatogr Sep Tech 2018, Volume: 09
DOI: 10.4172/2157-7064-C2-042

Chromatographic purification of photosynthetic water-soluble and membrane proteins for spectrometric analysis

Joanna Fiedor

AGH-University of Science and Technology, Poland

Purple non-sulphur phototrophic bacteria constitute a unique group of "photosynthetic" organisms capable of adjusting their metabolism in response to the alteration of environmental growth conditions. In the presence of light and absence of oxygen, bacterial cells develop extensive system of intracytoplasmic membranes, hosting entire "photosynthetic machinery". It comprises different types of pigment-protein complexes involved in capturing and extremely effective conversion of light energy into chemical energy. Recently, purple bacteria have been gaining considerable attention due to their increasing potential in a range of scientific and industrial applications. In the present study two species of anoxygenically grown phototrophic bacteria were used. Following the isolation of their membranes, the components of the photosynthetic apparatus were separated and purified by the application of weak anion exchange chromatography. This chromatographic technique is characterized by relative simplicity, vast availability as well as high effectivenes of structure's separation. Hence, it proved to be one of the most useful methods for isolation and purification of membrane as well as water-soluble proteins. Application of ion-chromatography resulted in preparation of a series of photosynthetic (pigment-) protein structures of adequate purity for spectrometric analysis. Here, total reflection X-ray fluorescence spectrometry (TXRF), one of the well-established spectroscopic techniques applied for the precise elemental profiling of organic and inorganic samples, was used to perform comprehensive examination of the elements present in bacterial proteins.

Biography

Joanna Fiedor has received her PhD degree in Biochemistry from the Jagiellonian University, Kraków, Poland. During 1997-1999, she visited the Ludwig-Maximilians University (LMU) in Munich, Germany, and in 2002 the Kwansei Gakuin University, Sanda, Japan. Currently, she is an Assistant Professor at the AGH-University of Science and Technology, Kraków, Poland. Her research interests are focused on: natural biocompounds (carotenoids) in relation to human health, and biotechnological applications of phototrophic microorganisms.

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Vakhtang Barbakadze, J Chromatogr Sep Tech 2018, Volume: 09
DOI: 10.4172/2157-7064-C2-042

Biopolymer from Medicinal Plants its Synthetic Monomer and their Anticancer Efficacy

Vakhtang Barbakadze

Tbilisi State Medical University, Georgia

The caffeic acid-derived biopolymers from medicinal plants comfrey and bugloss were isolated which represent a new class of natural polyethers. According to ^{13}C-, ^{1}H-NMR, APT, 2D heteronuclear $^{1}H/^{13}C$ HSQC, 1D NOE and 2D DOSY experiments the polyoxyethylene chain is the backbone of the polymer molecule. 3,4-Dihydroxyphenyl and carboxyl groups are regular substituents at two carbon atoms in the chain. The repeating unit of this regular polymer is 3-(3,4-dihydroxyphenyl)-glyceric acid residue. Thus, the structure of natural polymer was found to be poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene] or poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDPGA). Then basic monomeric moiety of this polymer 3-(3,4-dihydroxyphenyl)glyceric acid was synthesized via Sharpless asymmetric dihydroxylation of trans-caffeic acid derivatives using a potassium osmium catalyst. Besides, methylated PDPGA was obtained via ring opening polymerization of 2-methoxycarbonyl-3-(3,4-dimethoxyphenyl)oxirane using a cationic initiator. PDPGA is endowed with intriguing pharmacological activities as immunomodulatary (anticomplementary), antioxidant, anti-inflammatory, burn and wound healing and anticancer properties. PDPGA and its synthetic monomer exerted anticancer activity *in vitro* and *in vivo* against androgen-dependent and androgen -independent human prostate cancer (PCA) cells via targeting androgen receptor, cell cycle arrest and apoptosis without any toxicity, together with a strong decrease in prostate specific antigen level in plasma. However anticancer efficacy of PDPGA against human PCA cells is more effective than its synthetic monomer. Methylated PDPGA did not show any activity against PCA. Overall, this study identifies PDPGA as a potent agent against PCA without any toxicity, and supports its clinical application.

Biography

Vakhtang Barbakadze has completed his Ph.D and D.Sci. in 1978 and 1999 from Institute of Organic Chemistry, Moscow, Russia and Institute of Biochemistry and Biotechnology, Tbilisi, Georgia, respectively. He is the head of Department of plant biopolymers and chemical modification of natural compounds at the Tbilisi State Medical University Institute of Pharmacochemistry. 1996 and 2002 he has been a visiting scientist at Utrecht University, The Netherlands, by University Scholarship and The Netherlands organization for scientific research (NWO) Scholarship Scientific Program, respectively. He has published more than 96 papers in reputed journals..

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Miroslav Ryska, J Chromatogr Sep Tech 2018, Volume: 09
DOI: 10.4172/2157-7064-C2-042

The Use of Isotopiocally Labeled Internal Standards in Quantitative LC/MS – The Way of The Full Compensation of Negative Impact of "Matrix Effect"

Miroslav Ryska

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The source of the "Matrix effect" as a consequence of analyte ions suppression or ions enhancement must be sought in the presence of unknown impurities from matrix. They are participating in the complex ionization process in parallel or competing ion-molecular reactions. Not only impurities from extracts but impurities adsorbed in the ion source and/or in the analytical system may play an important role. These adsorbed substances cannot be fully removed from the system by any cleaning procedure.

To fully compensate for the negative impact of the "Matrix effect", use of isotopically labeled internal standards (isotope dilution technique) proved to be the only effective technique. This applies especially to LC/MS/MS determination of drugs and their metabolites in complex extracts of biological matrices. The isotope dilution technique is successful regardless of the method of purification, the ionization technique (APCI or ESI) and the type of the equipment used. The isotope dilution technique proved to be 100% effective for the compensation of matrix effect influences in 181 analytical methods developed and validated. The strict requirements of EMA guidelines to investigate different plasma sources for the assessment of the matrix effect in the analytical method validation are discussed.

Biography

Miroslav Ryska (1938) holds an undergraduate degree from Charles University, along with an M.S. in Physical Chemistry from Moscow State University and a PhD. from the Institute of Macromolecular Chemistry of Czechoslovak Academy of Sciences. From 1961 to 1978 he worked at the Institute of Macromolecular Chemistry of the Czechoslovak Academy of Sciences. In 1978 - 1997 he worked as a researcher in the field of MS and its application in research of metabolism and pharmacokinetics of drugs at the Research Institute for Pharmacy and Biochemistry in Prague. He has written more than 100 publications mainly on the topic of mass spectrometry, trace analyses, analyses of drugs, metabolites and quantitative analysis. In the 1990's Mr. Ryska acted as an Editor of two international journals, The Journal of Mass Spectrometry and Rapid Communication in Mass Spectrometry. He founded Quinta-Analytica s.r.o.in 1997.

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