

## Zoznam publikačnej činnosti

Ing. Roman Szücs, PhD.

### ADC Vedecké práce v zahraničných karentovaných časopisoch

ADC01 Masár, Marián (aut) [UKOPRCAL] (35%) - Hradski, Jasna (aut) [UKOPRCAL] (30%) - Schmid, Martin G. (aut) (5%) - Szücs, Roman (aut) [UKOPRCAL] (30%): Advantages and Pitfalls of Capillary Electrophoresis of Pharmaceutical Compounds and Their Enantiomers in Complex Samples: Comparison of Hydrodynamically Opened and Closed Systems

Lit.: 36 zázn.

In: International journal of molecular sciences. - Roč. 21, č. 18 (2020), s. [1-14], art. no. 6852. - ISSN (online) 1422-0067

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Indikátor časopisu:

IF (JCR) 2020=5,924

Kvartil Q:

wos-jcr -- Q1 [Biochemistry & molecular biology] -- 2020

wos-jcr -- Q2 [Chemistry, multidisciplinary] -- 2020

Ohlasy (8):

[n1] 2022 zz ~ Masci, M. - Zoani, C. - Nevigato, T. - Turrini, A. - Jasionowska, R. - Caproni, R. - Ratini, P.: Authenticity assessment of dairy products by capillary electrophoresis. In: Electrophoresis, Vol. 43, No. 1-2, 2022, s. 340-354 --SCOPUS

[n1] 2022 zz ~ Kocadal, K. - Alkas, F.B. - Battal, D. - Saygi, S.: A review on advances and perspectives of glyphosate determination: challenges and opportunities. In: Archives of Environmental Protection, Vol. 48, No. 3, 2022, s. 89-98 --SCOPUS

[n1] 2022 zz ~ Piestansky, J. - Cizmarova, I. - Matuskova, M. - Mikus, P.: Comparison of 1D a 2D ITP-MS performance parameters and application possibilities: Ultratrace determination of B vitamins in human urine. In: Electrophoresis, Vol. 43, No. 9-10, 2022, s. 998-1009 -- SCOPUS

[n1] 2022 zz ~ Suntornsuk, L. - Anurukvorakun, O.: Sensitivity enhancement in capillary electrophoresis and their applications for analyses of pharmaceutical and related biochemical substances. In: Electrophoresis, Vol. 43, No. 9-10, 2022, s.939-954 -- SCOPUS

[n1] 2022 zz ~ Stefanik, O. - Horniakova, A. - Cizmarova, I. - Matuskova, M. - Mikusova, V. - Mikus, P. - Piestansky, J.: Enhanced Sample Throughput Capillary Zone Electrophoresis with UV Detection in Hydrodynamically Closed System for Determination of Ibuprofen. In: Separations, Vol. 9, No. 5, 2022, Art. No. 118 -- SCOPUS

[n1] 2022 zz ~ Kavita Jyoti - Gupta, S. - Tejavath, K.K. - Verma, R.K.: Selective detection of diethanolamine utilizing an LMR/LSPR-based optical fiber sensor. In: Analyst, Vol. 147, No. 20, 2022, s. 4587-4597 -- SCOPUS

[n1] 2022 zz ~ Yu, R.B. - Quirino, J.P.: Pseudophase-to-solvent microextraction for in-line sample concentration of anionic analytes in capillary zone electrophoresis. In: Journal of Chromatography A, Vol. 1679, August, 2022, Art. No. 463383-- SCOPUS

[n1] 2022 sk ~ Cizmarova, I. - Matuskova, M. - Stefanik, O. - Horniakova, A. - Mikus, P. - Piestansky, J.: Determination of thiamine and pyridoxine in food supplements by a green ultrasensitive two-dimensional capillary electrophoresis hyphenated with mass spectrometry. In: Chemical Papers, Vol. 76, No. 10, 2022, s. 6235-6245 -- SCOPUS

ADC02 Masár, Marián (aut) [UKOPRCAL] (30%) - Hradski, Jasna (aut) [UKOPRCAL] (30%) - Nováková, Michaela (aut) (10%) - Szücs, Roman (aut) [UKOPRCAL] (15%) - Sabo, Martin (aut) [UKOMFKEF] (5%) - Matejčík, Štefan (aut) [UKOMFKEF] (10%): Online coupling of microchip electrophoresis with ion mobility spectrometry for direct analysis of complex liquid samples

Lit.: 41 zázn.

In: Sensors and Actuators B: Chemical. - č. 302 (2020), s. [1-8], Art. No. 127183. - ISSN (print) 0925-4005

*Registrované v:*

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SCIE Science Citation Index Expanded

*Indikátor časopisu:*

IF (JCR) 2020=7,460

*Kvartil Q:*

wos-jcr -- Q1 [Chemistry, analytical] -- 2020

wos-jcr -- Q1 [Electrochemistry] -- 2020

wos-jcr -- Q1 [Instruments & instrumentation] -- 2020

*Ohlasy (5):*

[o1] 2020 ~ Hartner, N.T. - Raddatz, C.-R. - Thoben, C. - Piendl, S.K. - Zimmermann, S. - Belder, D.: On-line coupling of chip-electrochromatography and ion mobility spectrometry. In: Analytical Chemistry, Vol. 92, No. 22, 2020, s. 15129-15136-- SCOPUS

[o1] 2020 ~ Vogel, M. - Engewald, W. - Dettmer-Wilde, K. - Schmitz, O.J. - Sperling, M. - Huber, C.G. - Regl, C. - Berger, T. - Piendl, S. - Belder, D. - Matysik, F.-M.: Trendbericht Analytische Chemie II: Trenntechniken und Elektroanalytik. In: Nachrichten aus der Chemie, Vol. 68, No. 10, 2020, s. 48-53 -- SCOPUS

[o1] 2020 ~ Theodoridis, K. - Stergiopoulos, F. - Bechtsis, D. - Nikolaidis, N. - Triantafyllidis, D. - Tsagaris, A. - Filelis, A. - Papaikonou, A.: An Innovative and Fully Automated System for Gel Electrophoresis. In: Computer Aided Chemical Engineering, Vol. 48. Amsterdam : Elsevier B.V., 2020, s. 847-852 -- SCOPUS

[n1] 2022 zz ~ Nabgan, W. - Jalil, A.A. - Nabgan, B. - Ikram, M. - Ali, M.W. Ankit kumar Lakshminarayana - P.,: A state of the art overview of carbon-based composites applications for detecting and eliminating pharmaceuticals containing wastewater. In: Chemosphere, Vol. 288, February, 2022, Art. No. 132535 -- SCOPUS

[n1] 2022 zz ~ Hu, W. - Meng, Q. - Lu, Y. - Xu, Y. - Nwadiuso, O.J. - Yu, J. - Liu, W. - Jing, G. - Li, W. - Liu, W.: Fourier Deconvolution Ion Mobility Spectrometry. In: Talanta, Vol. 241, May, 2022, Art. No. 123270 -- SCOPUS

ADC03 Masár, Marián (aut) [UKOPRCAL] (20%) - Hradski, Jasna (aut) [UKOPRCAL] (20%) - Vargová, Eva (aut) (15%) - Miškovčíková, Adriána (aut) [UKOPRCAL] (15%) - Božek, Peter (aut) [UKOPRCAL] (5%) - Ševčík, Juraj (aut) (5%) - Szűcs, Roman (aut) [UKOPRCAL] (20%): Determination of Carminic Acid in Foodstuffs and Pharmaceuticals by Microchip Electrophoresis with Photometric Detection [elektronický dokument]

Lit.: 29 zázn.

In: Separations [elektronický dokument]. - Roč. 7, č. 4 (2020), s. [1-13], art. no. 72 [online]. - ISSN (online) 2297-8739

*Registrované v:*

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*Indikátor časopisu:*

IF (JCR) 2020=2.777

*Kvartil Q:*

wos-jcr -- Q3 [Chemistry, analytical] -- 2020

*Ohlasy (5):*

[n1] 2021 zz ~ You, Y. - Xu, Z. - Zhong, Q. - Zhu, L. - Lin, S. - Li, Q. - Cao, Y. - Tao, Y. - Chen, S. - Wang, P.: Multivariate Statistical Analysis Uncovers Spectrum-Effect Relationship between HPLC Fingerprints and Antioxidant Activity of Saffron. In: Journal of Chemistry, Vol. 2021, November, 2021, art. no. 7352938 -- SCOPUS

[n1] 2022 zz ~ Bayer, G. - Shayganpour, A. - Zia, J. - Bayer, I.S.: Polyvinyl alcohol-based films plasticized with an edible sweetened gel enriched with antioxidant carminic acid. In: Journal of Food Engineering, Vol. 323, June, 2022, art. no.111000 -- SCI ; SCOPUS

[n1] 2022 zz ~ Alizadeh, M. - Demir, E. - Aydogdu, N. - Zare, N. - Karimi, F. - Kandomal, S.M. - Rokni, H. - Ghasemi, Y.: Recent advantages in electrochemical monitoring for the analysis of amaranth and carminic acid as food color. In: Food and Chemical Toxicology, Vol. 163, May, 2022, art. no. 112929 -- SCI ; SCOPUS

[n1] 2022 zz ~ Valdés, A. - Álvarez-Rivera, G. - Socas-Rodríguez, B. - Herrero, M. - Cifuentes, A.: Capillary electromigration methods for food analysis and Foodomics: Advances and applications in the period February 2019-February 2021. In: Electrophoresis, Vol. 43, No. 1-2, 2022, s. 37-56 -- SCI ; SCOPUS

[n1] 2022 zz ~ Kavieva, L. - Ziyatdinova, G.: Sensitive voltammetric quantification of carminic acid in candies using selenium dioxide nanoparticles based electrode. In: Food Chemistry, Vol. 386, August, 2022, art. no. 132851 -- SCI ; SCOPUS

ADC04 Hradski, Jasna (aut) [UKOPRCAL] (30%) - Ďuriš, Marta (aut) [UKOPRCAL] (25%) - Szücs, Roman (aut) [UKOPRCAL] (15%) - Moravský, Ladislav (aut) [UKOMFKEF] (5%) - Matejčík, Štefan (aut) [UKOMFKEF] (5%) - Masár, Marián (aut) [UKOPRCAL] (20%): Development of microchip isotachopheresis coupled with ion mobility spectrometry and evaluation of its potential for the analysis of food, biological and pharmaceutical samples [elektronický dokument]

Lit.: 32 zázn.

In: Molecules [elektronický dokument]. - Roč. 26, č. 20 (2021), s. [1-14], art. no. 6094 [online]. - ISSN (online) 1420-3049

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*Indikátor časopisu:*

IF (JCR) 2021=4.927

*Kvartil Q:*

wos-jcr -- Q2 [Biochemistry & molecular biology] -- 2021

wos-jcr -- Q2 [Chemistry, multidisciplinary] -- 2021

*Ohlasy (1):*

[n1] 2022 zz ~ Mala, Z. - Gebauer, P.: Recent progress in analytical capillary isotachopheresis (2018 - March 2022). In: Journal of Chromatography A, Vol. 1677, August, 2022, Art. No. 463337 -- SCOPUS

ADC05 Szücs, Roman (aut) [UKOPRCAL] (65%) - Brown, Roland (aut) (5%) - Brunelli, Claudio (aut) (5%) - Heaton, James C. (aut) (5%) - Hradski, Jasna (aut) [UKOPRCAL] (20%): Structure Driven Prediction of Chromatographic Retention Times: Applications to Pharmaceutical Analysis

Lit.: 39 zázn.

In: International Journal of Molecular Sciences. - Roč. 22, č. 8 (2021), s. [1-15], art. no. 3848. - ISSN (online) 1422-0067

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*Indikátor časopisu:*

IF (JCR) 2021=6,208

*Kvartil Q:*

wos-jcr -- Q1 [Biochemistry & molecular biology] -- 2021

wos-jcr -- Q2 [Chemistry, multidisciplinary] -- 2021

*Ohlasy (1):*

[n1] 2021 zz ~ Kensert, A. - Bouwmeester, R. - Efthymiadis, K. - Van Broeck, P. - Desmet, G. - Cabooter, D.: Graph Convolutional Networks for Improved Prediction and Interpretability of Chromatographic Retention Data. In: Analytical Chemistry, Vol. 93, No. 47, 2021, s. 15633-15641 -- SCOPUS

ADC06 Troška, Peter (aut) [UKOPRCAL] (30%) - Hradski, Jasna (aut) [UKOPRCAL] (25%) - Chropeňová, Lucia (aut) (5%) - Szücs, Roman (aut) [UKOPRCAL] (20%) - Masár, Marián (aut) [UKOPRCAL] (20%): Potential

of microchip electrophoresis in pharmaceutical analysis: Development of a universal method for frequently prescribed nonsteroidal anti-inflammatory drugs

Lit.: 19 záz.

In: Journal of Chromatography A. - č. 1654 (2021), s. [1-6], art. no. 462453. - ISSN (print) 0021-9673

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*Indikátor časopisu:*

IF (JCR) 2021=4.601

*Kvartil Q:*

wos-jcr -- Q2 [Biochemical research methods] -- 2021

wos-jcr -- Q1 [Chemistry, analytical] -- 2021

*Ohlasy (4):*

[n1] 2022 zz ~ Semail, N.-F. - Keyon, A.S.A. - Saad, B. - Kamaruzaman, S. - Zain, N.N.M. - Lim, V. - Miskam, M. - Abdullah, W.N.W. - Raoov, M. - Yahaya, N.: Induced sample via transient isotachopheresis mediated with sweeping in micellar electrokinetic chromatography for the dual-stacking strategy of non-steroidal anti-inflammatory drugs in environmental water samples. In: Journal of Chromatography A, Vol. 1685, December, 2022, Art. No. 463616 -- SCOPUS

[n1] 2022 zz ~ Alatawi, H. - Hogan, A. - Albalawi, I. - O'Sullivan-Carroll, E. - AElfri, S. - Wang, Y. - Moore, E.: Rapid determination of NSAIDs by capillary and microchip electrophoresis with capacitively coupled contactless conductivity detection in wastewater. In: Electrophoresis, Vol. 43, No. 20, 2022, s. 1944-1952 -- SCOPUS

[n1] 2022 zz ~ Mala, Z. - Gebauer, P.: Recent progress in analytical capillary isotachopheresis (2018 - March 2022). In: Journal of Chromatography A, Vol. 1677, August, 2022, Art. No. 463337 -- SCOPUS

[n1] 2022 zz ~ Kokosa, J.M. - Przyjazny, A.: Green microextraction methodologies for sample preparations. In: Green Analytical Chemistry, Vol. 3, 2022, Art. No. 100023 -- SCOPUS

## V2 Vedecký výstup publikačnej činnosti ako časť editovanej knihy alebo zborníka

V201 Szücs, Roman (aut) [UKOPRCAL] (50%) - Brunelli, Claudio (aut) (5%) - Lestremau, Francois (aut) (5%) - Hradski, Jasna (aut) [UKOPRCAL] (35%) - Hanna-Brown, Melissa (aut) (5%): Liquid chromatography in the pharmaceutical industry

Lit.: 30 záz.

In: Liquid Chromatography: Applications : volume 2. - Amsterdam : Elsevier, 2023. - S. 867-889. - ISBN 9780323983006

kapitola

## V3 Vedecký výstup publikačnej činnosti z časopisu

V301 de Villiers, André (aut) (20%) - Lauer, Henk (aut) (20%) - Szücs, Roman (aut) [UKOPRCAL] (20%) - Goodall, Stuart (aut) (20%) - Sandra, Pat (aut) (20%): Influence of frictional heating on temperature gradients in ultra-high-pressure liquid chromatography on 2.1 mm I.D. columns

Lit.: 22 záz.

In: Journal of Chromatography A. - Roč. 1113, č. 1-2 (2006), s. 84-91. - ISSN (print) 0021-9673

článok

*Registrované v:*

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*Indikátor časopisu:*

IF (JCR) 2006=3.554

*Kvartil Q:*

wos-jcr -- Q1 [Chemistry, analytical] -- 2006

*Ohlasy (28):*

- [n1] 2018 zz ~ Marchetti, N. - Maietti, A. - Pasti, L. - Cavazzini, A.: New Trends in Chiral High-Performance Liquid Chromatography-Tandem Mass Spectrometry. In: Comprehensive Analytical Chemistry, Vol. 79, 2018, s. 53-79 -- SCOPUS
- [n1] 2018 zz ~ Asnin, L.D. - Stepanova, M.V.: Van't Hoff analysis in chiral chromatography. In: Journal of Separation Science, Vol. 41, No. 6, 2018, s. 1319-1337 -- SCOPUS
- [n1] 2018 zz ~ Separovic, L. - Saviano, A.M. - Lourenco, F.R.: Using measurement uncertainty to assess the fitness for purpose of an HPLC analytical method in the pharmaceutical industry. In: Measurement: Journal of the International Measurement Confederation, Vol. 119, April, 2018, s. 41-45 -- SCOPUS
- [n1] 2018 zz ~ Wahab, M.F. - Weatherly, C.A. - Patil, R.A. - Armstrong, D.W.: Chiral liquid chromatography. In: Chiral Analysis: Advances in Spectroscopy, Chromatography and Emerging Methods: Second Edition. Amsterdam : Elsevier, 2018, S.507-564 -- SCOPUS
- [n1] 2018 zz ~ Makarov, A.A. - Mann, B.F. - Regalado, E.L. - Pirrone, G.F. - Sun, C. - Sun, S. - Nowak, T. - Wang, H. - Mangion, I.: Visualizing and studying frictional heating effects in reversed-phase liquid chromatography using infrared thermal imaging. In: Analytica Chimica Acta, Vol. 1018, August, 2018, s. 1-6 - - SCOPUS
- [n1] 2018 zz ~ Lambert, N. - Felinger, A.: The effect of the frictional heat on retention and efficiency in thermostated or insulated chromatographic columns packed with sub-2- $\mu\text{m}$  particles. In: Journal of Chromatography A, Vol. 1565, August, 2018, s. 89-95 -- SCOPUS
- [n1] 2018 zz ~ Vera, C.M. - Samuelsson, J. - Fornstedt, T. - Dennis, G.R. - Shalliker, R.A.: Protocol for the visualisation of axial temperature gradients in ultra high performance liquid chromatography using infrared cameras. In: Microchemical Journal, Vol. 141, September, 2018, s. 141-147 -- SCOPUS
- [n1] 2018 zz ~ Majors, R.E.: HPLC Column technology: The first 50 years. In: American Laboratory, Vol. 50, No. 8, 2018, s. 24-31 -- SCOPUS
- [n1] 2018 zz ~ Deridder, S. - Smits, W. - Benkahla, H. - Broeckhoven, K. - Desmet, G.: Numerical and analytical investigation of the possibilities to enhance the thermal conductivity of core-shell particle packed beds. In: Journal of Chromatography A, Vol. 1575, November, 2018, s. 26-33 -- SCOPUS
- [n1] 2019 zz ~ Dores-Sousa, J.L. - De Vos, J. - Eeltink, S.: Resolving power in liquid chromatography: A trade-off between efficiency and analysis time. In: Journal of Separation Science, Vol. 42, No. 1, 2019, s. 38-50 -- SCOPUS
- [n1] 2019 zz ~ Eeltink, S. - De, Vos J.: Liquid chromatography ? Ultra-high-pressure liquid chromatography. In: Encyclopedia of Analytical Science. Amsterdam : Elsevier, 2019, S. 261-269 -- SCOPUS
- [n1] 2019 zz ~ Kresge, G.A. - Wong, J.-M.T. - De Pra, M. - Steiner, F. - Grinias, J.P.: Using Superficially Porous Particles and Ultrahigh Pressure Liquid Chromatography in Pharmacopeial Monograph Modernization of Common Analgesics. In: Chromatographia, Vol. 82, No. 1, 2019, s. 465-475 -- SCOPUS
- [n1] 2019 zz ~ Vera, C.M. - Samuelsson, J. - Fornstedt, T. - Dennis, G.R. - Shalliker, R.A.: Visualisation of axial temperature gradients and heat transfer process of different solvent compositions in ultra high performance liquid chromatography using thermography. In: Microchemical Journal, Vol. 145, March, 2019, s. 927-935 -- SCOPUS
- [n1] 2019 zz ~ Wouters, S. - Dores-Sousa, J.L. - Liu, Y. - Pohl, C.A. - Eeltink, S.: Ultra-High-Pressure Ion Chromatography with Suppressed Conductivity Detection at 70 MPa Using Columns Packed with 2.5  $\mu\text{m}$  Anion-Exchange Particles. In: Analytical Chemistry, Vol. 91, No. 21, 2019, s. 13824-13830 -- SCOPUS
- [n1] 2020 zz ~ Broeckhoven, K. - Desmet, G.: Advances and Challenges in Extremely High-Pressure Liquid Chromatography in Current and Future Analytical Scale Column Formats. In: Analytical Chemistry, Vol. 92, No. 1, 2020, s. 554-560 -- SCOPUS
- [n1] 2020 zz ~ Felletti, S. - De Luca, C. - Lievore, G. - Pasti, L. - Chenet, T. - Mazzocanti, G. - Gasparrini, F. - Cavazzini, A. - Catani, M.: Investigation of mass transfer properties and kinetic performance of high-efficiency columns packed with C18 sub-2  $\mu\text{m}$  fully and superficially porous particles. In: Journal of Separation Science, Vol. 43, No. 9-10, 2020, s. 1737-1745 -- SCOPUS
- [n1] 2020 zz ~ Vanderheyden, Y. - Broeckhoven, K. - Desmet, G.: Alternative method to study the radial dispersion in liquid chromatography columns. Part II: Experimental. In: Journal of Chromatography A, Vol. 1618, May, 2020, Art. No. 460870-- SCOPUS
- [n1] 2020 zz ~ Bupp, C.R. - Wirth, M.J.: Making Sharper Peaks for Reverse-Phase Liquid Chromatography of Proteins. In: Annual Review of Analytical Chemistry, Vol. 13, June, 2020, s. 363-380 -- SCOPUS

- [n1] 2020 zz ~ Lesko, M. - Samuelsson, J. - Asberg, D. - Kaczmarek, K. - Fornstedt, T.: Evaluating the advantages of higher heat conductivity in a recently developed type of core-shell diamond stationary phase particle in UHPLC. In: Journal of Chromatography A, Vol. 1625, August, 2020, Art. No. 461076 -- SCOPUS
- [n1] 2021 zz ~ Tanacs, D. - Berkecz, R. - Misicka, A. - Tymecka, D. - Fulop, F. - Armstrong, D.W. - Ilisz, I. - Peter, A.: Enantioseparation of  $\alpha$ -amino acids by liquid chromatography using core-shell chiral stationary phases based on teicoplanin and teicoplanin aglycone. In: Journal of Chromatography A, Vol. 1653, September, 2021, Art. No. 462383 -- SCOPUS
- [n1] 2021 zz ~ Moussa, A. - Deridder, S. - Broeckhoven, K. - Desmet, G.: Computational fluid dynamics study of potential solutions to alleviate viscous heating band broadening in 2.1 millimeter liquid chromatography columns. In: Journal of Chromatography A, Vol. 1654, September, 2021, Art. No. 462452 -- SCOPUS
- [n1] 2021 zz ~ Baert, M. - Wicht, K. - Moussa, A. - Desmet, G. - Broeckhoven, K. - Lynen, F.: Implementations of temperature gradients in temperature-responsive liquid chromatography. In: Journal of Chromatography A, Vol. 1654, September, 2021, Art. No. 462425 -- SCOPUS
- [n1] 2021 zz ~ Rozing, G.: Micropillar array columns for advancing nanoflow HPLC. In: Microchemical Journal, Vol. 170, November, 2021, Art. No. 106629 -- SCOPUS
- [n1] 2022 zz ~ Moussa, A. - Deridder, S. - Broeckhoven, K. - Desmet, G.: Detailed computational fluid dynamics study of the parameters contributing to the viscous heating band broadening in liquid chromatography at pressures up to 2500 bar in 2.1 mm columns. In: Journal of Chromatography A, Vol. 1661, January, 2022, Art. No. 462683 -- SCOPUS
- [n1] 2022 zz ~ Ali, A. - Alharthi, S. - Al-Shaalan, N.H. - Santali, E.Y.: Development of Narrow-Bore C18 Column for Fast Separation of Peptides and Proteins in High-Performance Liquid Chromatography. In: Polymers, Vol. 14, No. 13, 2022, Art.No. 2576 -- SCOPUS
- [n1] 2022 zz ~ Anderson, K.W. - Hudgens, J.W.: Chromatography at -30°C for Reduced Back-Exchange, Reduced Carryover, and Improved Dynamic Range for Hydrogen-Deuterium Exchange Mass Spectrometry. In: Journal of the American Society for Mass Spectrometry, Vol. 33, No. 7, 2022, s. 1282-1292 -- SCOPUS
- [n1] 2022 zz ~ Berger, T.A.: The evolution and current state of instrumentation for analytical supercritical fluid chromatography. In: Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, Vol. 1211, November, 2022, Art. No. 123478 -- SCOPUS
- [n1] 2019 zz ~ Kaplitz, A.S. - Kresge, G.A. - Selover, B. - Horvat, L. - Franklin, E.G. - Godinho, J.M. - Grinias, K.M. - Foster, S.W. - Davis, J.J. - Grinias, J.P.: High-Throughput and Ultrafast Liquid Chromatography. In: Analytical Chemistry, Vol. 92, No. 1, 2019, s. 67-84 -- SCOPUS

V302 de Villiers, André (aut) (16.67%) - Lestremay, Francois (aut) (16.666%) - Szücs, Roman (aut) [UKOPRCAL] (16.666%) - Gélébart, Sylvie (aut) (16.666%) - David, Frank (aut) (16.666%) - Sandra, Pat (aut) [KAUT] (16.666%): Evaluation of ultraperformance liquid chromatography : Part I. Possibilities and limitations Lit.: 31 zázn.

In: Journal of Chromatography A. - Roč. 1127, č. 1-2 (2006), s. 60-69. - ISSN (print) 0021-9673  
článok

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*Indikátor časopisu:*

IF (JCR) 2006=3.554

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, analytical] – 2006

*Ohlasy (31):*

[n1] 2018 zz ~ Lv, H. - Shen, E. - Luo, L. - Xu, Y. - Pan, Y. - Wu, K. - Xing, Z. - Ye, F. - Zhang, Y.: An UPLC-MS/MS method for the determination of EA1045 in plasma and tissues and its application to pharmacokinetic and distribution studies in rats. In: Pharmazie, Vol. 73, No. 11, 2018, s. 630-634 -- SCOPUS

[n1] 2018 zz ~ Levin, S.: Solid-core or fully porous columns in ultra high-performance liquid chromatography- Which way to go for better efficiency of the separation?. In: Advances in Chromatography, Vol. 55. Boca Raton : CRC Press, 2018, S.185-204 -- SCOPUS

[n1] 2018 zz ~ Parr, M.K. - Schmidt, A.H.: Life cycle management of analytical methods. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 147, January, 2018, s. 506-517 -- SCOPUS

- [n1] 2018 zz ~ Rosado, T. - Soares, S. - Malaca, S. - Goncalves, J. - Barroso, M. - Gallardo, E.: The role of liquid chromatography in toxicological analysis. In: High-Performance Liquid Chromatography: Types, Parameters and Applications. New York : Nova Science Publishers, 2018, S. 1-120 -- SCOPUS
- [n1] 2018 zz ~ Vera, C.M. - Samuelsson, J. - Fornstedt, T. - Dennis, G.R. - Shalliker, R.A.: Protocol for the visualisation of axial temperature gradients in ultra high performance liquid chromatography using infrared cameras. In: Microchemical Journal, Vol. 141, September, 2018, s. 141-147 -- SCOPUS
- [n1] 2018 zz ~ Vanderlinden, K. - Desmet, G. - Bell, D.S. - Broeckhoven, K.: Detailed efficiency analysis of columns with a different packing quality and confirmation via total pore blocking. In: Journal of Chromatography A, Vol. 1581-1582, December, 2018, s. 55-62 -- SCOPUS
- [n1] 2019 zz ~ Dore-Sousa, J.L. - De Vos, J. - Eeltink, S.: Resolving power in liquid chromatography: A trade-off between efficiency and analysis time. In: Journal of Separation Science, Vol. 42, No. 1, 2019, s. 38-50 -- SCOPUS
- [n1] 2019 zz ~ Su, X.-J. - Hu, J. - Zhang, L. - Li, L.: Liquid chromatography-tandem mass spectrometric assay for AZD9291 in rat plasma. In: Latin American Journal of Pharmacy, Vol. 38, No. 4, 2019, s. 737-742 -- SCOPUS
- [n1] 2019 zz ~ Zhong, Y. - Wang, Q. - Wang, H. - Zhang, Q.: A quick method for the determination of neomangiferin in rat plasma by UPLC-MS/MS. In: Latin American Journal of Pharmacy, Vol. 38, No. 6, 2019, s. 1265-1270 -- SCOPUS
- [n1] 2019 zz ~ Memon, N. - Qureshi, T. - Bhangar, M.I. - Malik, M.I.: Recent trends in fast liquid chromatography for pharmaceutical analysis. In: Current Analytical Chemistry, Vol. 15, No. 4, 2019, s. 349-372 -- SCOPUS
- [n1] 2019 zz ~ Shimizu, H. - Toyoda, K. - Mawatari, K. - Terabe, S. - Kitamori, T.: Femtoliter Gradient Elution System for Liquid Chromatography Utilizing Extended Nanofluidics. In: Analytical Chemistry, Vol. 91, No. 4, 2019, s. 3009-3014 -- SCOPUS
- [n1] 2019 zz ~ Vera, C.M. - Samuelsson, J. - Fornstedt, T. - Dennis, G.R. - Shalliker, R.A.: Visualisation of axial temperature gradients and heat transfer process of different solvent compositions in ultra high performance liquid chromatography using thermography. In: Microchemical Journal, Vol. 145, March, 2019, s. 927-935 -- SCOPUS
- [n1] 2019 zz ~ Xuejing, D. - Wenyu, W. - Hong, W. - Zhengrong, Z. - Li, D. - Jun, F. - Ran, D. - Feng, L. - Yan, W. - Xiang, Z.: UHPLC-MS/MS analysis of sphingosine 1-phosphate in joint cavity dialysate and hemodialysis solution of adjuvant arthritis rats: Application to geniposide pharmacodynamic study. In: Biomedical Chromatography, Vol. 33, No. 7, 2019, Art. No. e4526 -- SCOPUS
- [n1] 2019 zz ~ Borovcova, L. - Havlicek, V. - Lemr, K.: Fast chromatographic separation. In: Chemické Listy, Vol. 113, No. 7, 2019, s. 407-414 -- SCOPUS
- [n1] 2019 zz ~ Jeong, S.-H. - Jang, J.-H. - Cho, H.-Y. - Lee, Y.-B.: Simultaneous determination of diethyl phthalate and its major metabolite, monoethyl phthalate, in rat plasma, urine, and various tissues collected from a toxicokinetic study by ultrahigh performance liquid chromatography-tandem mass spectrometry. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 173, September, 2019, s. 108-119 -- SCOPUS
- [n1] 2019 zz ~ Gouveia, F. - Bicker, J. - Goncalves, J. - Alves, G. - Falcão, A. - Fortuna, A.: Liquid chromatographic methods for the determination of direct oral anticoagulant drugs in biological samples: A critical review. In: Analytica Chimica Acta, Vol. 1076, October, 2019, s. 18-31 -- SCOPUS
- [n1] 2019 zz ~ Ali, F. - Malik, A.R. - Cheong, W.J. - Rehman, N.-U.: Demonstration of high separation efficiency for polystyrene-modified sub-1 μm particles originating from silica monolith under isocratic elution mode in liquid chromatography. In: Journal of Liquid Chromatography and Related Technologies, Vol. 42, No. 19-20, 2019, s. 662-672 -- SCOPUS
- [n1] 2020 zz ~ Wu, M.-Y. - Wang, B.-B. - Xue, H. - Kang, Y.-F. - Zhang, Y.-X. - Qiu, X.-J.: Development and validation of UPLC-MS/MS method for determination of brexpiprazole in rat plasma. In: Latin American Journal of Pharmacy, Vol. 39, No.8, 2020, s. 1605-1610 -- SCOPUS
- [n1] 2020 zz ~ Semwal, A. - Dogra, R. - Verma, K. - Bhatia, R.: Impact of uplc-ms in food and drug/metabolite analysis. In: Current Pharmaceutical Analysis, Vol. 17, No. 1, 2020, s. 10-30 -- SCOPUS
- [n1] 2020 zz ~ Broeckhoven, K. - Desmet, G.: Advances and Challenges in Extremely High-Pressure Liquid Chromatography in Current and Future Analytical Scale Column Formats. In: Analytical Chemistry, Vol. 92, No. 1, 2020, s. 554-560 -- SCOPUS
- [n1] 2020 zz ~ Bupp, C.R. - Wirth, M.J.: Making Sharper Peaks for Reverse-Phase Liquid Chromatography of Proteins. In: Annual Review of Analytical Chemistry, Vol. 13, June, 2020, s. 363-380 -- SCOPUS

- [n1] 2020 zz ~ Sharma, T. - Jain, A. - Saini, S. - Katare, O.P. - Singh, B.: Implementation of analytical quality-by-design and green analytical chemistry approaches for the development of robust and eco friendly UHPLC analytical method for quantification of chrysin. In: Separation Science Plus, Vol. 3, No. 9, 2020, s. 384-398 -- SCOPUS
- [n1] 2020 zz ~ Zhang, X. - Saini, A. - Hao, C. - Harner, T.: Passive air sampling and nontargeted analysis for screening POP-like chemicals in the atmosphere: Opportunities and challenges. In: TrAC - Trends in Analytical Chemistry, Vol. 132, November, 2020, Art. No. 116052 -- SCOPUS
- [n1] 2021 zz ~ Broeckhoven, K. - Desmet, G.: Methods to determine the kinetic performance limit of contemporary chromatographic techniques. In: Journal of Separation Science, Vol. 44, No. 1, 2021, s. 323-339 -- SCOPUS
- [n1] 2021 zz ~ Kilinska, K. - Zalewski, P.: Radiation sterilization of antibiotics in solid state. In: Current Analytical Chemistry, Vol. 17, No. 8, 2021, s. 1097-1103 -- SCOPUS
- [n1] 2021 zz ~ Hou, Z. - Broeckhoven, K. - Desmet, G. - Lynen, F.: Through-pore polymerization in polar high-performance liquid chromatography columns allowing scanning electron microscopy based imaging of the packing order. In: Journal of Chromatography A, Vol. 1638, February, 2021, Art. No. 461851 -- SCOPUS
- [n1] 2021 zz ~ Hakiem, A.F.A. - Hamdy, A.K. - Ali, H.R.H. - Gomaa, M. - Aboraia, A.S.: In depth investigation of the retention behavior of structurally related  $\hat{I}_t$ -blockers on RP-HPLC column: Quality by design and quantitative structure-property relationship complementary approaches for optimization and validation. In: Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, Vol. 1166, March, 2021, Art. No. 122549 -- SCOPUS
- [n1] 2021 zz ~ Witika, B.A. - Aucamp, M. - Mweetwa, L.L. - Makoni, P.A.: Application of fundamental techniques for physicochemical characterizations to understand post-formulation performance of pharmaceutical nanocrystalline materials. In: Crystals, Vol. 11, No. 3, 2021, Art. No. 310 -- SCOPUS
- [n1] 2022 zz ~ Veloz Martinez, I. - Ek, J.I. - Ahn, E.C. - Sustaita, A.O.: Molecularly imprinted polymers via reversible addition-fragmentation chain-transfer synthesis in sensing and environmental applications. In: RSC Advances, Vol. 12, No.15, 2022, s. 9186-9201 -- SCOPUS
- [n1] 2022 zz ~ Ren, J. - Lin, J. - Yu, L. - Yan, M.: Lysophosphatidylcholine: Potential Target for the Treatment of Chronic Pain. In: International Journal of Molecular Sciences, Vol. 23, No. 15, 2022, Art. No. 8274 -- SCOPUS
- [n1] 2022 zz ~ Ghosh, S. - AlKafaas, S.S. - Bornman, C. - Apollon, W. - Hussien, A.M. - Badawy, A.E. - Amer, M.H. - Kamel, M.B. - Mekawy, E.A. - Bedair, H.: The application of rapid test paper technology for pesticide detection in horticulture crops: a comprehensive review. In: Beni-Suef University Journal of Basic and Applied Sciences, Vol. 11, No. 1, 2022, Art. No. 73 -- SCOPUS

V303 Górecki, Tadeusz (aut) (25%) - Lynen, Frederic (aut) (25%) - Szücs, Roman (aut) [UKOPRCAL] (25%) - Sandra, Pat (aut) (25%): Universal Response in Liquid Chromatography Using Charged Aerosol Detection Lit.: 13 zázn.

In: Analytical Chemistry. - Roč. 78, č. 9 (2006), s. 3186-3192. - ISSN (print) 0003-2700  
článok

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*Ohlasy (53):*

[n1] 2018 zz ~ Poplawska, M. - Blazewicz, A. - Kaminski, K. - Bednarek, E. - Fijalek, Z. - Kozerski, L.: Application of high-performance liquid chromatography with charged aerosol detection (LC-CAD) for unified quantification of synthetic cannabinoids in herbal blends and comparison with quantitative NMR results. In: Forensic Toxicology, Vol. 36, No. 1, 2018, s. 122-140 -- SCOPUS

[n1] 2018 zz ~ Wahl, O. - Cleyhens, J. - Verbruggen, A.M. - Holzgrabe, U.: Impurity profiling of N,N'-ethylenebis-L-cysteine diethyl ester (Bicisate). In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 150, February, 2018, s. 132-136-- SCOPUS



[n1] 2018 zz ~ Lucci, P. - Moret, S. - Buchini, F. - Ferlat, G. - Conte, L.: Improved analysis of olive oils triacylglycerols by UHPLC-charged aerosol detection. In: *Journal of Food Composition and Analysis*, Vol. 66, March, 2018, s. 230-236 --SCOPUS

[n1] 2018 zz ~ Pinto, E.C. - Goncalves, M.D.S. - Cabral, L.M. - Armstrong, D.W. - de, Sousa V.P.: Development and validation of a stability-indicating HPLC method for topiramate using a mixed-mode column and charged aerosol detector. In: *Journal of Separation Science*, Vol. 41, No. 8, 2018, s. 1716-1725 -- SCOPUS

[n1] 2018 zz ~ Ohira, S.-I. - Kaneda, K. - Matsuzaki, T. - Mori, S. - Mori, M. - Toda, K.: Universal HPLC Detector for Hydrophilic Organic Compounds by Means of Total Organic Carbon Detection. In: *Analytical Chemistry*, Vol. 90, No. 11, 2018, s. 6461-6467 -- SCOPUS

[n1] 2018 zz ~ Klencsar, B. - Li, S. - Balcaen, L. - Vanhaecke, F.: High-performance liquid chromatography coupled to inductively coupled plasma - Mass spectrometry (HPLC-ICP-MS) for quantitative metabolite profiling of non-metal drugs. In: *TrAC - Trends in Analytical Chemistry*, Vol. 104, July, 2018, s. 118-134 -- SCOPUS

[n1] 2018 zz ~ Baker, T.R. - Regg, B.T.: A multi-detector chromatographic approach for characterization and quantitation of botanical constituents to enable in silico safety assessments. In: *Analytical and Bioanalytical Chemistry*, Vol. 410, No. 21, 2018, s. 5143-5154 -- SCOPUS

[n1] 2018 zz ~ Lie, A. - Pedersen, L.H.: Resolution and signal-to-noise in analysis of carbohydrate isomers by graphitised carbon chromatography with charged aerosol detection. In: *Journal of Chromatography A*, Vol. 1567, September, 2018, s.147-154 -- SCOPUS

[n1] 2018 zz ~ Eckardt, M. - Kubicova, M. - Simat, T.J.: Universal response quantification approach using a Corona Charged Aerosol Detector (CAD) - Application on linear and cyclic oligomers extractable from polycondensate plastics polyesters, polyamides and polyarylsulfones. In: *Journal of Chromatography A*, Vol. 1572, October, 2018, s. 187-202 -- SCOPUS

[n1] 2018 zz ~ Ferey, L. - Slabi, S.A. - Roy, C.-E. - Barthelemy, P. - Gaudin, K.: Chromatographic study of nucleoside-lipids by RP-UHPLC-DAD/CAD. In: *Analytical and Bioanalytical Chemistry*, Vol. 410, No. 29, 2018, s. 7711-7721 -- SCOPUS

[n1] 2018 zz ~ Schilling, K. - Pawellek, R. - Lovejoy, K. - Muellner, T. - Holzgrabe, U.: Influence of charged aerosol detector instrument settings on the ultra-high-performance liquid chromatography analysis of fatty acids in polysorbate 80. In: *Journal of Chromatography A*, Vol. 1576, November, 2018, s. 58-66 -- SCOPUS

[n1] 2018 zz ~ Li, P. - Sun, W. - Zuo, L. - Zhu, Z. - Zhao, T. - Wang, R. - Zhu, M. - Leng, X. - Qiu, X. - Bai, L. - Shan, G.: Fast simultaneous determination of main components and impurity sodium ion in PAMA injection by mixed-mode chromatography. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 161, November, 2018, s. 407-413 -- SCOPUS

[n1] 2019 zz ~ Takeda, H. - Takahashi, M. - Hara, T. - Izumi, Y. - Bamba, T.: Improved quantitation of lipid classes using supercritical fluid chromatography with a charged aerosol detector. In: *Journal of Lipid Research*, Vol. 60, No. 8, 2019, s. 1465-1474 -- SCOPUS

[n1] 2019 zz ~ Zhang, K. - Kurita, K.L. - Venkatramani, C. - Russell, D.: Seeking universal detectors for analytical characterizations. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 162, January, 2019, s. 192-204 -- SCOPUS

[n1] 2019 zz ~ Davies, S.R. - Kankaew, P. - Tarrant, G.J. - Donald, W.A. - Greaves, R.F.: Comprehensive certification of a testosterone calibration standard facilitating the investigation of charged aerosol detection for the quantification of impurities of related structure. In: *Metrologia*, Vol. 56, No. 2, 2019, Art. No. 024004 -- SCOPUS

[n1] 2019 zz ~ Bareford, L. - Peng, H. - Ali, A. - Kolwyck, D. - Dickens, J.: Development of a rapid and reliable analytical method for screening poloxamer 188 for use in cell culture process. In: *Biotechnology Progress*, Vol. 35, No. 3, 2019, Art. No. e2792 -- SCOPUS

[n1] 2019 zz ~ Bossmann, D. - Bartling, B. - de Vries, I. - Winkler, J. - Neumann, H. - Lammers, F. - Beutel, S. - Scheper, T.: Charged aerosol detector HPLC as a characterization and quantification application of biopharmaceutically relevant polysialic acid from *E. coli* K1. In: *Journal of Chromatography A*, Vol. 1599, August, 2019, s. 85-94 -- SCOPUS

[n1] 2019 zz ~ Haidar Ahmad, I.A. - Blasko, A. - Tam, J. - Variankaval, N. - Halsey, H.M. - Hartman, R. - Regalado, E.L.: Revealing the inner workings of the power function algorithm in Charged Aerosol Detection: A simple and effective approach to optimizing power function value for quantitative analysis. In: *Journal of Chromatography A*, Vol. 1603, October, 2019, s. 1-7 -- SCOPUS

[n1] 2019 zz ~ Dunn, P.J.H. - Malinovsky, D. - Achtar, E. - Clarkson, C. - Goenaga-Infante, H.: Systematic comparison of post-column isotope dilution using LC-CO-IRMS with qNMR for amino acid purity determination. In: *Analytical and Bioanalytical Chemistry*, Vol. 411, No. 27, 2019, s. 7207-7220 -- SCOPUS

[n1] 2019 zz ~ Ye, X.-Y. - Guo, Q. - Guo, B. - Tan, L. - Huang, Q. - Zhang, Y.-H. - Yang, D.-D. - Shi, H.-W.: Qualitative and quantitative analysis of cyclovirobuxine d and related substances by hplc-cad in the active pharmaceutical ingredient of huangyangning tablets. In: *Yaoxue Xuebao*, Vol. 54, No. 12, 2019, s. 2303-2307 - - SCOPUS

[n1] 2020 zz ~ Eckardt, M. - Kubicova, M. - Tong, D. - Simat, T.J.: Determination of color developers replacing bisphenol A in thermal paper receipts using diode array and Corona charged aerosol detection-A German market analysis 2018/2019. In: *Journal of Chromatography A*, Vol. 1609, January, 2020, Art. No. 460437 -- SCOPUS

[n1] 2020 zz ~ Sica, V.P. - Krivos, K.L. - Kiehl, D.E. - Pulliam, C.J. - Henry, I.D. - Baker, T.R.: The role of mass spectrometry and related techniques in the analysis of extractable and leachable chemicals. In: *Mass Spectrometry Reviews*, Vol. 39, No. 1-2, 2020, s. 212-226 -- SCOPUS

[n1] 2020 zz ~ Wang, R. - Liu, Y. - Zhou, H. - Chen, Y. - Wang, J. - Zhang, X. - Yu, R. - Liang, X.: Integration of micro-fractionation, high-performance liquid chromatography-ultraviolet detector-charged aerosol detector-mass spectrometry analysis and cellular dynamic mass redistribution assay to accelerate alkaloid drug discovery. In: *Journal of Chromatography A*, Vol. 1616, April, 2020, Art. No. 460779 -- SCOPUS

[n1] 2020 zz ~ Schilling, K. - Holzgrave, U.: Recent applications of the Charged Aerosol Detector for liquid chromatography in drug quality control. In: *Journal of Chromatography A*, Vol. 1619, May, 2020, Art. No. 460911 -- SCOPUS

[n1] 2020 zz ~ Wang, J. - Liu, G. - Zhu, B. - Tang, L.: Universal quantification method of degradation impurities in 16-membered macrolides using HPLC-CAD and study on source of the impurities. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 184, May, 2020, Art. No. 113170 -- SCOPUS

[n1] 2020 zz ~ Qiu, J. - Wright, E.J. - Thomas, K. - Li, A. - McCarron, P. - Beach, D.G.: Semiquantitation of paralytic shellfish toxins by hydrophilic interaction liquid chromatography-mass spectrometry using relative molar response factors. In: *Toxins*, Vol. 12, No. 6, 2020, Art. No. 398 -- SCOPUS

[n1] 2020 zz ~ Hashimoto, H. - Furutsuka, K. - Kawamura, K. - Ohkubo, T. - Ogawa, M. - Kurihara, Y. - Nengaki, N. - Zhang, M.-R.: Simultaneous measurements of the molar radioactivity, radiochemical purity and chemical impurity in the [11C]choline injection using radio-HPLC with a corona-charged aerosol detector. In: *Applied Radiation and Isotopes*, Vol. 162, August, 2020, Art. No. 109192 -- SCOPUS

[n1] 2020 zz ~ Kolderova, N. - Jurasek, B. - Kuchar, M. - Lindner, W. - Kohout, M.: Gradient supercritical fluid chromatography coupled to mass spectrometry with a gradient flow of make-up solvent for enantioseparation of cathinones. In: *Journal of Chromatography A*, Vol. 1625, August, 2020, Art. No. 461286 - - SCOPUS

[n1] 2020 zz ~ Dufour, A. - Thiebaut, D. - Loriau, M. - Ligiero, L. - Vial, J.: Corona charged aerosol detector non-uniform response factors of purified alcohol ethoxylated homologues using liquid chromatography. In: *Journal of Chromatography A*, Vol. 1627, September, 2020, Art. No. 461402 -- SCOPUS

[n1] 2020 zz ~ Patriarca, C. - Balderrama, A. - Moze, M. - Sjoberg, P.J.R. - Bergquist, J. - Tranvik, L.J. - Hawkes, J.A.: Investigating the Ionization of Dissolved Organic Matter by Electrospray. In: *Analytical Chemistry*, Vol. 92, No. 20, 2020, s. 14210-14218 -- SCOPUS

[n1] 2020 zz ~ Scholz, K. - Lipphardt, A. - Wienken, C.M. - Tiso, T. - Hayen, H.: Hyphenation of supercritical fluid chromatography with different detection methods for identification and quantification of liamocin biosurfactants. In: *Journal of Chromatography A*, Vol. 1631, November, 2020, Art. No. 461584 -- SCOPUS

[n1] 2020 zz ~ Garcia-Montoto, V. - Denti, P. - Malmquist, L.M.V. - Verdier, S. - Bouyssiere, B. - Christensen, J.H.: Hyphenating supercritical fluid chromatography and inductively coupled plasma mass spectrometry: A proof of concept. In: *Journal of Analytical Atomic Spectrometry*, Vol. 35, No. 12, 2020, s. 2852-2858 -- SCOPUS

[n1] 2021 zz ~ Knol, W.C. - Pirok, B.W.J. - Peters, R.A.H.: Detection challenges in quantitative polymer analysis by liquid chromatography. In: *Journal of Separation Science*, Vol. 44, No. 1, 2021, s. 63-87 -- SCOPUS

[n1] 2021 zz ~ Xu, F. - Wang, P. - Zhang, X. - Hou, T. - Qu, L. - Wang, C. - Wang, J. - Liu, Y. - Liang, X.: Identification and target-pathway deconvolution of FFA4 agonists with anti-diabetic activity from *Arnebia euchroma* (Royle) Johnst. In: *Pharmacological Research*, Vol. 163, January, 2021, Art. No. 105173 -- SCOPUS

[n1] 2021 zz ~ Mroczek, A. - Klimczak, U. - Kowalczyk, M.: Determination of saponins in leaves of four Swiss chard (*Beta vulgaris* L.) cultivars by UHPLC-CAD/QTOF-MS/MS. In: Polish Journal of Food and Nutrition Sciences, Vol. 71, No. 2, 2021, s. 147-159 -- SCOPUS

[n1] 2021 zz ~ Moldoveanu, S. - David, V.: Modern Sample Preparation for Chromatography. In: . Amsterdam : Elsevier, 2021, S. 1-679 -- SCOPUS

[n1] 2021 zz ~ Robards, K. - Ryan, D.: Principles and Practice of Modern Chromatographic Methods. In: . Amsterdam : Elsevier, 2021, S. 1-518 -- SCOPUS

[n1] 2021 zz ~ Liu, G. - Zhu, B. - Ren, X. - Wang, J.: Universal response method for the quantitative analysis of multi-components in josamycin and midecamycin using liquid chromatography coupled with charged aerosol detector. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 192, January, 2021, Art. No. 113679 -- SCOPUS

[n1] 2021 zz ~ Wu, H.H. - Garidel, P. - Michaela, B.: HP-beta-CD for the formulation of IgG and Ig-based biotherapeutics. In: International Journal of Pharmaceutics, Vol. 601, May, 2021, Art. No. 120531 -- SCOPUS

[n1] 2021 zz ~ Pawellek, R. - Holzgrabe, U.: Influence of the mobile phase composition on hyphenated ultraviolet and charged aerosol detection for the impurity profiling of vigabatrin. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 201, July, 2021, Art. No. 114110 -- SCOPUS

[n1] 2021 zz ~ Singh, G. - Lu, D. - Liu, C. - Hower, D.: Analytical challenges and recent advances in the identification and quantitation of extractables and leachables in pharmaceutical and medical products. In: TrAC - Trends in Analytical Chemistry, Vol. 141, August, 2021, Art. No. 116286 -- SCOPUS

[n1] 2021 zz ~ Scherer, B. - Matsysik, F.-M.: Investigations of polymer samples of polyamide 11 concerning the content of monomer, oligomers, and the oxidation stabilizer Irganox 1098 by utilizing inverse gradient HPLC in combination with a triple detection system (diode array detection/mass spectrometry/charged aerosol detection). In: Talanta Open, Vol. 3, August, 2021, Art. No. 100023 -- SCOPUS

[n1] 2021 zz ~ Causevic, A. - Olofsson, K. - Adlercreutz, P. - Grey, C.: Non-aqueous reversed phase liquid chromatography with charged aerosol detection for quantitative lipid analysis with improved accuracy. In: Journal of Chromatography A, Vol. 1652, August, 2021, Art. No. 462374 -- SCOPUS

[n1] 2021 zz ~ Infantes-Garcia, M.R. - Verkempinck, S.H.E. - Guevara-Zambrano, J.M. - Hendrickx, M.E. - Grauwet, T.: Development and validation of a rapid method to quantify neutral lipids by NP-HPLC-charged aerosol detector. In: Journal of Food Composition and Analysis, Vol. 102, September, 2021, Art. No. 104022 - - SCOPUS

[n1] 2021 zz ~ Pawellek, R. - Krmar, J. - Leistner, A. - Djajic, N. - Otasevic, B. - Protic, A. - Holzgrabe, U.: Charged aerosol detector response modeling for fatty acids based on experimental settings and molecular features: a machine learning approach. In: Journal of Cheminformatics, Vol. 13, No. 1, 2021, Art. No. 53 -- SCOPUS

[n1] 2021 zz ~ Pawellek, R. - Holzgrabe, U.: Performance of ion pairing chromatography and hydrophilic interaction liquid chromatography coupled to charged aerosol detection for the analysis of underivatized amino acids. In: Journal of Chromatography A, Vol. 1659, December, 2021, Art. No. 462613 -- SCOPUS

[n1] 2022 zz ~ Moldoveanu, S. - David, V.: Essentials in Modern HPLC Separations. In: . Amsterdam : Elsevier, 2022, S. 1-705 -- SCOPUS

[n1] 2022 zz ~ Langley, G.J. - Cancho-Gonzalez, S. - Herniman, J.M.: Different detectors used with SFC. In: Separation Science and Technology (New York), Vol. 14. Amsterdam : Elsevier, 2022, S. 299-324 -- SCOPUS

[n1] 2022 zz ~ Wang, C. - Chao, I. - Qin, Y. - Zhang, W. - Zhao, J. - Zhang, Q. - Li, S.: Comparison for quantification of eight components in *Alpinia officinarum* Hance by using high-performance liquid chromatography coupled with diode array detector and charged aerosol detector with individual and substitute reference compound. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 210, February, 2022, Art. No. 114545 -- SCOPUS

[n1] 2022 zz ~ Roslon, M. - Jaworska, M. - Anuszevska, E.L.: Determination of Glycerophospholipids in Biological Material Using High-Performance Liquid Chromatography with Charged Aerosol Detector HPLC-CAD-A New Approach for Isolation and Quantification. In: Molecules, Vol. 27, No. 10, 2022, Art. No. 3356 -- SCOPUS

[n1] 2022 zz ~ Hettiarachchi, K. - Streckfuss, E. - Sanzone, J.R. - Wang, J. - Hayes, M. - Kong, M. - Greshock, T.J.: Microscale Purification with Direct Charged Aerosol Detector Quantitation Using Selective Online One- or Two-Dimensional Liquid Chromatography. In: Analytical Chemistry, Vol. 94, No. 23, 2022, s. 8309-8316 -- SCOPUS

[n1] 2022 zz ~ Zheng, W. - Zhou, M. - Chai, R.-P. - Liang, H.-Z. - Zhang, J. - Zhao, Y. - Zheng, X.-H. - Jin, Y. - Guo, B.-L. - Ma, B.-P.: Quality analysis of hawthorn leaves (the leaves of *Crataegus pinnatifida* Bge. var

major N.E.Br) indifferent harvest time. In: *Phytochemical Analysis*, Vol. 33, No. 7, 2022, s. 1147-1155 -- SCOPUS

[n1] 2022 zz ~ Wei, J. - Zhao, X. - Wang, S. - Zhang, M. - Yao, W. - Yuan, Y.: Determination of related substances in egg yolk lecithin by HPLC-CAD and characterization of its profiling by HPLC-Q-TOF-MS. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 221, November, 2022, Art. No. 115079 -- SCOPUS

V304 Alzaga, Roberto (aut) (13%) - Ryan, Robert W. (aut) (13%) - Taylor-Worth, Karen (aut) (13%) - Lipczynski, Andrew M. (aut) (13%) - Szücs, Roman (aut) [UKOPRCAL] (35%) - Sandra, Pat (aut) (13%): A generic approach for the determination of residues of alkylating agents in active pharmaceutical ingredients by in situ derivatization headspace gas chromatography mass spectrometry  
Lit.: 34 zázn.

In: *Journal of Pharmaceutical and Biomedical Analysis*. - Roč. 45, č. 3 (2007), s. 472-479. - ISSN (print) 0731-7085

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wos-jcr – Q2 [pharmacology&pharmacy] -- 2007

*Ohlasy (15):*

[n1] 2018 zz ~ Uppala, R. - Arthanareeswari, M.: Determination of hydroxylamine genotoxic impurity by derivatization in penicillamine drug substance by GCHS-MS. In: *Materials Today: Proceedings*, Vol. 34, February, 2018, s. 506-509 -- SCOPUS

[n1] 2018 zz ~ Zacharis, C.K. - Vastardi, E.: Application of analytical quality by design principles for the determination of alkyl p-toluenesulfonates impurities in Aprepitant by HPLC. Validation using total-error concept. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 150, February, 2018, s. 152-161 -- SCOPUS

[n1] 2018 zz ~ Teasdale, A. - Elder, D.P.: Analytical control strategies for mutagenic impurities: Current challenges and future opportunities?. In: *TrAC - Trends in Analytical Chemistry*, Vol. 101, April, 2018, s. 66-84 -- SCOPUS

[n1] 2018 zz ~ Liu, X.-W. - Zhang, W.-P. - Han, H.-Y. - Sun, L. - Chen, D.-Y.: Trace determination of mutagenic alkyl toluenesulfonate impurities via derivatization headspace-GC/MS in an active pharmaceutical ingredient of a candidate drug. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 155, June, 2018, s. 104-108 -- SCOPUS

[n1] 2018 zz ~ Xie, W.-Q. - Gong, Y.-X. - Yu, K.-X.: Utilizing two detectors in the measurement of trichloroacetic acid in human urine by reaction headspace gas chromatography. In: *Biomedical Chromatography*, Vol. 32, No. 10, 2018, Art. No.e4288 -- SCOPUS

[n1] 2018 zz ~ Liu, X. - Li, C. - Han, H. - Zhang, W. - Chen, D.: Advances on genotoxic impurities of sulfonate esters in pharmaceuticals. In: *Chinese Journal of Chromatography (Se Pu)*, Vol. 36, No. 10, 2018, s. 952-961 -- SCOPUS

[n1] 2019 zz ~ Jin, B. - Guo, K. - Zhang, T. - Li, T. - Ma, C.: Simultaneous Determination of 15 Sulfonate Ester Impurities in Phentolamine Mesylate, Amlodipine Besylate, and Tosufloxacin Tosylate by LC-APCI-MS/MS. In: *Journal of Analytical Methods in Chemistry*, Vol. 2019, 2019, Art. No. 4059765 -- SCOPUS

[n1] 2019 zz ~ Li, M. - Gu, C. - Luo, L. - Zhou, J. - Liu, J. - Zheng, F.: Determination of trace methanesulfonates in drug matrix using derivatization and headspace single drop microextraction followed by high-performance liquid chromatography with ultraviolet detection. In: *Journal of Chromatography A*, Vol. 1591, April, 2019, s. 131-137 -- SCOPUS

[n1] 2019 zz ~ Liu, Z. - Fan, H. - Zhou, Y. - Qian, X. - Tu, J. - Chen, B. - Duan, G.: Development and validation of a sensitive method for alkyl sulfonate genotoxic impurities determination in drug substances using gas chromatography coupled to triple quadrupole mass spectrometry. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 168, May, 2019, s. 23-29 -- SCOPUS

- [n1] 2020 zz ~ Rodinkov, O.V. - Bugaichenko, A.S. - Moskvina, L.N.: Static Headspace Analysis and Its Current Status. In: Journal of Analytical Chemistry, Vol. 75, No. 1, 2020, s. 1-17 -- SCOPUS
- [n1] 2020 zz ~ Nomura, S. - Ito, Y. - Takegami, S. - Kitade, T.: Development of trace analysis for alkyl methanesulfonates in the delgocitinib drug substance using GC-FID and liquid-liquid extraction with ionic liquid. In: Open Chemistry, Vol.18, No. 1, 2020, s. 1020-1029 -- SCOPUS
- [n1] 2020 zz ~ Ahirrao, V.K. - Jadhav, R.A. - Rane, V.P. - Bhamare, H.R. - Yeole, R.D.: Time-dependent selected reaction monitoring-based GC-MS/MS method for estimation of genotoxic impurities in new antibacterial agent: alalevonadifloxacin mesylate. In: Journal of Analytical Science and Technology, Vol. 11, No. 1, 2020, Art. No. 22 -- SCOPUS
- [n1] 2021 zz ~ Teasdale, A.: Mutagenic Impurities: Strategies for Identification and Control. In: . New Jersey : Wiley, 2021, S. 1-524 -- SCOPUS
- [n1] 2022 zz ~ Wang, Y. - Feng, J. - Wu, S. - Shao, H. - Zhang, W. - Zhang, K. - Zhang, H. - Yang, Q.: Determination of Methyl Methanesulfonate and Ethyl Methylsulfonate in New Drug for the Treatment of Fatty Liver Using Derivatization Followed by High-Performance Liquid Chromatography with Ultraviolet Detection. In: Molecules, Vol. 27, No. 6, 2022, Art. No. 1950 -- SCOPUS
- [n1] 2022 zz ~ Maniavannan, M. - Ilayaraja, P. - Parthiban, P.: Trace-level analysis of genotoxic sulfonate ester impurities in teneligliptin by GC-MS. In: Journal of Applied Pharmaceutical Science, Vol. 12, No. 11, 2022, s. 052-060 -- SCOPUS

V305 Cabooter, Deirdre (aut) (16.67%) - Clicq, David (aut) (16.666%) - De Boever, Filip (aut) (16.666%) - Lestremau, Francois (aut) (16.666%) - Szücs, Roman (aut) [UKOPRCAL] (16.666%) - Desmet, gert (aut) (16.666%): A Variable Column Length Strategy To Expedite Method Development  
Lit.: 31 zázn.

In: Analytical Chemistry. - Roč. 83, č. 3 (2011), s. 966-975. - ISSN (print) 0003-2700  
článok

*Registrované v:*

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WOS CC Web of Science Core Collection

SCIE Science Citation Index Expanded

*Indikátor časopisu:*

IF (JCR) 2011=5.856

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, analytical] -- 2011

V306 Hutchinson, Joseph P. (aut) (12.5%) - Remenyi, Tomas (aut) (12.5%) - Nesterenko, Pavel (aut) (12.5%) - Farrell, William (aut) (12.5%) - Groeber, Elizabeth (aut) (12.5%) - Szücs, Roman (aut) [UKOPRCAL] (12.5%) - Dicinovski, Greg (aut) (12.5%) - Haddad, Paul R. (aut) (12.5%): Investigation of polar organic solvents compatible with Corona Charged Aerosol Detection and their use for the determination of sugars by hydrophilic interaction liquid chromatography  
Lit.: 39 zázn.

In: Analytica Chimica Acta. - č. 750 (2012), s. 199-206. - ISSN (print) 0003-2670

článok

*Registrované v:*

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WOS CC Web of Science Core Collection

SCIE Science Citation Index Expanded

*Indikátor časopisu:*

IF (JCR) 2012=4.387

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, analytical] -- 2012

*Ohlasy (19):*

[n1] 2018 zz ~ Souza, O.A. - Carneiro, R.L. - Vieira, T.H.M. - Funari, C.S. - Rinaldo, D.: Fingerprinting Cynara scolymus L. (Artichoke) by Means of a Green Statistically Developed HPLC-PAD Method. In: Food Analytical Methods, Vol. 11, No. 7, 2018, s. 1977-1985 -- SCOPUS

[n1] 2019 zz ~ Ikegami, T.: Hydrophilic interaction chromatography for the analysis of biopharmaceutical drugs and therapeutic peptides: A review based on the separation characteristics of the hydrophilic interaction chromatography phases. In: *Journal of Separation Science*, Vol. 42, No. 1, 2019, s. 130-213 -- SCOPUS

[n1] 2019 zz ~ Davies, S.R. - Kankaew, P. - Tarrant, G.J. - Donald, W.A. - Greaves, R.F.: Comprehensive certification of a testosterone calibration standard facilitating the investigation of charged aerosol detection for the quantification of impurities of related structure. In: *Metrologia*, Vol. 56, No. 2, 2019, Art. No. 024004 -- SCOPUS

[n1] 2019 zz ~ Haidar Ahmad, I.A. - Blasko, A. - Tam, J. - Variankaval, N. - Halsey, H.M. - Hartman, R. - Regalado, E.L.: Revealing the inner workings of the power function algorithm in Charged Aerosol Detection: A simple and effective approach to optimizing power function value for quantitative analysis. In: *Journal of Chromatography A*, Vol. 1603, October, 2019, s. 1-7 -- SCOPUS

[n1] 2019 zz ~ Pitsch, J. - Weghuber, J.: Hydrophilic interaction chromatography coupled with charged aerosol detection for simultaneous quantitation of carbohydrates, polyols and ions in food and beverages. In: *Molecules*, Vol. 24, No. 23, 2019, Art. No. 4333 -- SCOPUS

[n1] 2020 zz ~ Haidar Ahmad, I.A. - Stoll, D.R.: Profilerf - the newest innovation to quantify total fluorine content. In: *LC-GC North America*, Vol. 38, No. 12, 2020, s. 1-4 -- SCOPUS

[n1] 2020 zz ~ Haidar Ahmad, I.A. - Stoll, D.R.: Tips for liquid chromatography coupled with charged aerosol detection. In: *LC-GC North America*, Vol. 38, No. 12, 2020, s. 648-652 -- SCOPUS

[n1] 2020 zz ~ Maljuric, N. - Otasevic, B. - Golubovic, J. - Krmar, J. - Zecevic, M. - Protic, A.: A new strategy for development of eco-friendly RP-HPLC method using Corona Charged Aerosol Detector and its application for simultaneous analysis of risperidone and its related impurities. In: *Microchemical Journal*, Vol. 153, March, 2020, Art. No. 104394 -- SCOPUS

[n1] 2020 zz ~ Han, B. - Park, J.W. - Kang, M. - Kim, B. - Jeong, J.-S. - Kwon, O.-S. - Son, J.: Simultaneous analysis of monosaccharides using ultra high performance liquid chromatography-high resolution mass spectrometry without derivatization for validation of certified reference materials. In: *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, Vol. 1160, December, 2020, Art. No. 122370 -- SCOPUS

[n1] 2021 zz ~ Dajic, N. - Otasevic, B. - Malenovic, A. - Zecevic, M. - Holzgrabe, U. - Protic, A.: Corona Charged Aerosol Detector in studying retention and beta-cyclodextrin complex stability using RP-HPLC. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 193, January, 2021, Art. No. 113711 -- SCOPUS

[n1] 2021 zz ~ Feng, C. - Xue, L. - Lu, D. - Jin, Y. - Qiu, X. - Gonzalez, F.J. - Wang, G. - Zhou, Z.: Novel Strategy for Mining and Identification of Acylcarnitines Using Data-Independent-Acquisition-Based Retention Time Prediction Modeling and Pseudo-Characteristic Fragmentation Ion Matching. In: *Journal of Proteome Research*, Vol. 20, No. 3, 2021, s. 1602-1611 -- SCOPUS

[n1] 2021 zz ~ Borges, M.S. - Zanatta, A.C. - Souza, O.A. - Pelissari, J.H. - Camargo, J.G.S. - Carneiro, R.L. - Funari, C.S. - Bolzani, V.S. - Rinaldo, D.: A green and sustainable method for monitoring the chemical composition of soybean: an alternative for quality control. In: *Phytochemical Analysis*, Vol. 32, No. 4, 2021, s. 562-574 -- SCOPUS

[n1] 2021 zz ~ Park, N. - Walsh, M.K.: Microbial inhibitory properties of maltodextrin fatty acid esters against food-related microorganisms. In: *LWT*, Vol. 147, July, 2021, Art. No. 111664 -- SCOPUS

[n1] 2021 zz ~ Pawellek, R. - Holzgrabe, U.: Influence of the mobile phase composition on hyphenated ultraviolet and charged aerosol detection for the impurity profiling of vigabatrin. In: *Journal of Pharmaceutical and Biomedical Analysis*, Vol. 201, July, 2021, Art. No. 114110 -- SCOPUS

[n1] 2021 zz ~ Moravcova, D. - Cmelik, R. - Krenkova, J.: Separation of labeled isomeric oligosaccharides by hydrophilic interaction liquid chromatography - the role of organic solvent in manipulating separation selectivity of the amide stationary phase. In: *Journal of Chromatography A*, Vol. 1651, August, 2021, Art. No. 462303 -- SCOPUS

[n1] 2021 zz ~ Pawellek, R. - Krmar, J. - Leistner, A. - Djajic, N. - Otasevic, B. - Protic, A. - Holzgrabe, U.: Charged aerosol detector response modeling for fatty acids based on experimental settings and molecular features: a machine learning approach. In: *Journal of Cheminformatics*, Vol. 13, No. 1, 2021, Art. No. 53 -- SCOPUS

[n1] 2021 zz ~ Pawellek, R. - Holzgrabe, U.: Performance of ion pairing chromatography and hydrophilic interaction liquid chromatography coupled to charged aerosol detection for the analysis of underivatized amino acids. In: *Journal of Chromatography A*, Vol. 1659, December, 2021, Art. No. 462613 -- SCOPUS

[n1] 2022 zz ~ Wang, J. - Zhao, Y. - Yang, Y. - Chen, X. - Jin, Y. - Ke, Y.: Separation of minor steviol glycosides using hydrophilic interaction liquid chromatography (HILIC) and off-line two-dimensional

reversed-phase liquid chromatography/HILIC methods. In: Journal of Food Composition and Analysis, Vol. 112, September, 2022, Art. No. 104683 -- SCOPUS  
[n1] 2019 zz ~ Dong, M.W.: UHPLC: Perspectives, Performance, Practices, and Potential Issues. In: HPLC and UHPLC for Practicing Scientists. Hoboken : John Wiley & Sons, 2019, S. 118-145 -- SCOPUS

V307 Talebi, Mohammad (aut) [KAUT] (20%) - Schuster, Georg (aut) (20%) - Shellie, Robert A. (aut) (20%) - Szűcs, Roman (aut) [UKOPRCAL] (20%) - Haddad, Paul R. (aut) (20%): Performance comparison of partial least squares-related variable selection methods for quantitative structure retention relationships modelling of retention times in reversed-phase liquid chromatography

Lit.: 38 zázn.

In: Journal of Chromatography A. - č. 1424 (2015), s. 69-76. - ISSN (print) 0021-9673  
článok

*Registrované v:*

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WOS CC Web of Science Core Collection

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*Indikátor časopisu:*

IF (JCR) 2015=3.657

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, medicinal] -- 2015

wos-jcr – Q2 [Chemistry, multidisciplinary] -- 2015

*Ohlasy (19):*

[n1] 2018 zz ~ Parr, M.K. - Schmidt, A.H.: Life cycle management of analytical methods. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 147, January, 2018, s. 506-517 -- SCOPUS

[n1] 2018 zz ~ Hu, M. - Muller, E. - Schymanski, E.L. - Ruttkies, C. - Schulze, T. - Brack, W. - Krauss, M.: Performance of combined fragmentation and retention prediction for the identification of organic micropollutants by LC-HRMS. In: Analytical and Bioanalytical Chemistry, Vol. 410, No. 7, 2018, s. 1931-1941 -- SCOPUS

[n1] 2018 zz ~ Fouad, M.A. - Tolba, E.H. - El-Shal, M.A. - El, Kerdawy A.M.: QSRR modeling for the chromatographic retention behavior of some beta-lactam antibiotics using forward and firefly variable selection algorithms coupled with multiple linear regression. In: Journal of Chromatography A, Vol. 1549, May, 2018, s. 51-62 -- SCOPUS

[n1] 2018 zz ~ Larbi, H. - Didaoui, L. - Righezza, M.: Characterization of stationary phases based on monosubstituted benzene retention indices using correspondence factor analysis and linear solvation energy relationships in RPLC. In: Journal of the Iranian Chemical Society, Vol. 15, No. 10, 2018, s. 2295-2305 -- SCOPUS

[n1] 2018 zz ~ Noreldeen, H.A.A. - Liu, X. - Wang, X. - Fu, Y. - Li, Z. - Lu, X. - Zhao, C. - Xu, G.: Quantitative structure-retention relationships model for retention time prediction of veterinary drugs in food matrixes. In: International Journal of Mass Spectrometry, Vol. 434, November, 2018, s. 172-178 -- SCOPUS

[n1] 2020 zz ~ Buszewski, B. - Zuvella, P. - Sagandykova, G. - Walczak-skierska, J. - Pomastowski, P. - David, J. - Wong, M.W.: Mechanistic chromatographic column characterization for the analysis of flavonoids using quantitative structure-retention relationships based on density functional theory. In: International Journal of Molecular Sciences, Vol. 21, No. 6, 2020, Art. No. 2053 -- SCOPUS

[n1] 2020 zz ~ Du, J. - Chang, Y. - Zhang, X. - Hu, C.: Development of a method of analysis for profiling of the impurities in phenoxymethylpenicillin potassium based on the analytical quality by design concept combined with the degradation mechanism of penicillins. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 186, July, 2020, Art. No. 113309 -- SCOPUS

[n1] 2020 zz ~ Krmar, J. - Vukicevic, M. - Kovacevic, A. - Protic, A. - Zecevic, M. - Otasevic, B.: Performance comparison of nonlinear and linear regression algorithms coupled with different attribute selection methods for quantitative structure - retention relationships modelling in micellar liquid chromatography. In: Journal of Chromatography A, Vol. 1623, July, 2020, Art. No. 461146 -- SCOPUS

[n1] 2020 zz ~ Zhang, L. - Sun, J. - Zhou, X. - Nirere, A. - Wu, X. - Dai, R.: Classification detection of saccharin jujube based on hyperspectral imaging technology. In: Journal of Food Processing and Preservation, Vol. 44, No. 8, 2020, Art. No. e14591 -- SCOPUS

[n1] 2020 zz ~ Ibrahim, A.M. - Hendawy, H.A.M. - Hassan, W.S. - Shalaby, A. - ElMasry, M.S.: Determination of terazosin in the presence of prazosin: Different state-of-the-art machine learning algorithms with UV spectroscopy. In: Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, Vol. 236, August, 2020, Art. No. 118349 -- SCOPUS

[n1] 2020 zz ~ Huygens, B. - Efthymiadis, K. - Nowe, A. - Desmet, G.: Application of evolutionary algorithms to optimise one- and two-dimensional gradient chromatographic separations. In: Journal of Chromatography A, Vol. 1628, September, 2020, Art. No. 461435 -- SCOPUS

[n1] 2020 zz ~ Andries, J.P.M. - Goodarzi, M. - Heyden, Y.V.: Improvement of quantitative structure-retention relationship models for chromatographic retention prediction of peptides applying individual local partial least squares models. In: Talanta, Vol. 219, November, 2020, Art. No. 121266 -- SCOPUS

[n1] 2021 zz ~ Parinet, J.: Prediction of pesticide retention time in reversed-phase liquid chromatography using quantitative-structure retention relationship models: A comparative study of seven molecular descriptors datasets. In: Chemosphere, Vol. 275, July, 2021, Art. No. 130036 -- SCOPUS

[n1] 2022 zz ~ He, Q. - Li, H. - Jin, B. - Li, W. - Shao, B. - Zhang, L.: QSRR model for identification and screening of emerging pollutants based on artificial intelligence algorithms. In: Environmental Pollutants and Bioavailability, Vol.34, No. 1, 2022, s. 331-337 -- SCOPUS

[n1] 2022 zz ~ Si-Hung, L. - Izumi, Y. - Nakao, M. - Takahashi, M. - Bamba, T.: Investigation of supercritical fluid chromatography retention behaviors using quantitative structure-retention relationships. In: Analytica Chimica Acta, Vol.1197, March, 2022, Art. No. 339463 -- SCOPUS

[n1] 2022 zz ~ Klingberg, J. - Keen, B. - Cawley, A. - Pasin, D. - Fu, S.: Developments in high-resolution mass spectrometric analyses of new psychoactive substances. In: Archives of Toxicology, Vol. 96, No. 4, 2022, s. 949-967 -- SCOPUS

[n1] 2022 zz ~ Kamedulska, A. - Kubik, L. - Jacyna, J. - Struck-Lewicka, W. - Markuszewski, M.J. - Wiczling, P.: Toward the General Mechanistic Model of Liquid Chromatographic Retention. In: Analytical Chemistry, Vol. 94, No. 31, 2022, s.11070-11080 -- SCOPUS

[n1] 2022 zz ~ Jin, X. - Xiao, Z.-Y. - Xiao, D.-X. - Dong, A. - Nie, Q.-X. - Wang, Y.-N. - Wang, L.-F.: Quantitative inversion model of protein and fat content in milk based on hyperspectral techniques. In: International Dairy Journal, Vol.134, November, 2022, Art. No. 105467 -- SCOPUS

[n1] 2020 zz ~ Xia, Z. - Liu, W. - Zheng, F. - Huang, W. - Xing, Z. - Peng, W. - Tang, T. - Luo, J. - Yi, L. - Wang, Y.: VISSA-PLS-DA-Based Metabolomics Reveals a Multitargeted Mechanism of Traditional Chinese Medicine for Traumatic Brain Injury. In: ASN Neuro, Vol. 12, 2020, s. 1-12 -- SCOPUS

V308 Amos, Ruth I. J. (aut) [KAUT] (10.835%) - Tyteca, Eva (aut) (10.833%) - Talebi, Mohammad (aut) (10.833%) - Haddad, Paul R. (aut) (10.833%) - Szücs, Roman (aut) [UKOPRCAL] (35%) - Dolan, John W. (aut) (10.833%) - Pohl, Christopher A. (aut) (10.833%): Benchmarking of Computational Methods for Creation of Retention Models in Quantitative Structure-Retention Relationships Studies [elektronický dokument]

Lit.: 72 zázn.

In: Journal of Chemical Information and Modeling [elektronický dokument]. - Roč. 57, č. 11 (2017), s. 2754-2762 [print]. - ISSN (print) 1549-9596

článok

*Registrované v:*

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WOS CC Web of Science Core Collection

SCIE Science Citation Index Expanded

*Indikátor časopisu:*

IF (JCR) 2017=3.804

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, medicinal] -- 2017

wos-jcr – Q2 [Chemistry, multidisciplinary] -- 2017

*Ohlasy (7):*

[n1] 2018 zz ~ Zuvela, P. - David, J. - Wong, M.W.: Interpretation of ANN-based QSAR models for prediction of antioxidant activity of flavonoids. In: Journal of Computational Chemistry, Vol. 39, No. 16, 2018, s. 953-963 -- SCOPUS



[n1] 2018 zz ~ Noreldeen, H.A.A. - Liu, X. - Wang, X. - Fu, Y. - Li, Z. - Lu, X. - Zhao, C. - Xu, G.: Quantitative structure-retention relationships model for retention time prediction of veterinary drugs in food matrixes. In: International Journal of Mass Spectrometry, Vol. 434, November, 2018, s. 172-178 -- SCOPUS

[n1] 2020 zz ~ Pavlic, B. - Teslic, N. - Kojic, P. - Pezo, L.: Prediction of the GC-MS retention time for terpenoids detected in sage (*Salvia officinalis* L.) essential oil using QSRR approach. In: Journal of the Serbian Chemical Society, Vol.85, No. 1, 2020, s. 9-23 -- SCOPUS

[n1] 2020 zz ~ Poole, C.F.: Evaluation of the solvation parameter model as a quantitative structure-retention relationship model for gas and liquid chromatography. In: Journal of Chromatography A, Vol. 1626, August, 2020, Art. No. 461308 --SCOPUS

[n1] 2020 zz ~ Schulze, B. - Jeon, Y. - Kaserzon, S. - Heffernan, A.L. - Dewapriya, P. - O'Brien, J. - Gomez Ramos, M.J. - Ghorbani Gorji, S. - Mueller, J.F. - Thomas, K.V. - Samanipour, S.: An assessment of quality assurance/quality control efforts in high resolution mass spectrometry non-target workflows for analysis of environmental samples. In: TrAC - Trends in Analytical Chemistry, Vol. 133, December, 2020, Art. No. 116063 -- SCOPUS

[n1] 2021 zz ~ Bride, E. - Heinisch, S. - Bonnefille, B. - Guillemain, C. - Margoum, C.: Suspect screening of environmental contaminants by UHPLC-HRMS and transposable Quantitative Structure-Retention Relationship modelling. In: Journal of Hazardous Materials, Vol. 409, May, 2021, Art. No. 124652 -- SCOPUS

[n1] 2022 zz ~ Hu, Q. - Sun, Y. - Yuan, P. - Lei, H. - Zhong, H. - Wang, Y. - Tang, H.: Quantitative structure-retention relationship for reliable metabolite identification and quantification in metabolomics using ion-pair reversed-phase chromatography coupled with tandem mass spectrometry. In: Talanta, Vol. 238, February, 2022, Art. No. 123059 -- SCOPUS

V309 Park, Soo Hyun (aut) (12.5%) - Talebi, Mohammad (aut) (12.5%) - Amos, Ruth I. J. (aut) (12.5%) - Tyteca, Eva (aut) (12.5%) - Haddad, Paul R. (aut) [KAUT] (12.5%) - Szűcs, Roman (aut) [UKOPRCAL] (12.5%) - Pohl, Christopher A. (aut) (12.5%) - Dolan, John W. (aut) (12.5%): Towards a chromatographic similarity index to establish localised quantitative structure-retention relationships for retention prediction [elektronický dokument] : II Use of Tanimoto similarity index in ion chromatography  
Lit.: 56 zázn.

In: Journal of Chromatography A [elektronický dokument]. - č. 1523 (2017), s. 173-182 [print]. - ISSN (print) 0021-9673

článok

*Registrované v:*

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WOS CC Web of Science Core Collection

SCIE Science Citation Index Expanded

*Indikátor časopisu:*

IF (JCR) 2017=3.716

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, analytical] -- 2017

wos-jcr – Q1 [Biochemical research methods] -- 2017

*Ohlasy (4):*

[n1] 2018 zz ~ Parr, M.K. - Schmidt, A.H.: Life cycle management of analytical methods. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 147, January, 2018, s. 506-517 -- SCOPUS

[n1] 2018 zz ~ Larbi, H. - Didaoui, L. - Righezza, M.: Characterization of stationary phases based on monosubstituted benzene retention indices using correspondence factor analysis and linear solvation energy relationships in RPLC. In: Journal of the Iranian Chemical Society, Vol. 15, No. 10, 2018, s. 2295-2305 -- SCOPUS

[n1] 2018 zz ~ Noreldeen, H.A.A. - Liu, X. - Wang, X. - Fu, Y. - Li, Z. - Lu, X. - Zhao, C. - Xu, G.:

Quantitative structure-retention relationships model for retention time prediction of veterinary drugs in food matrixes. In: International Journal of Mass Spectrometry, Vol. 434, November, 2018, s. 172-178 -- SCOPUS

[n1] 2021 zz ~ Sagandykova, G. - Buszewski, B.: Perspectives and recent advances in quantitative structure-retention relationships for high performance liquid chromatography. How far are we?. In: TrAC - Trends in Analytical Chemistry, Vol.141, August, 2021, Art. No. 116294 -- SCOPUS

V310 Russo, Giacomo (aut) (20%) - Grumetto, Lucia (aut) (20%) - Szücs, Roman (aut) [UKOPRCAL] (20%) - Barbato, Francesco (aut) (20%) - Lynen, Frederic (aut) [KAUT] (20%): Determination of in Vitro and in Silico Indexes for the Modeling of Blood Brain Barrier Partitioning of Drugs via Micellar and Immobilized Artificial Membrane Liquid Chromatography [elektronický dokument]  
 Lit.: 42 zázn.  
 In: Journal of Medicinal Chemistry [elektronický dokument]. - Roč. 60, č. 9 (2017), s. 3739-3754 [print]. - ISSN (print) 0022-2623  
 článok  
*Registrované v:*  
 CCC Current Content Connect  
 SCO SCOPUS  
 WOS CC Web of Science Core Collection  
 SCIE Science Citation Index Expanded  
 OA Open access  
*Indikátor časopisu:*  
 IF (JCR) 2017=3.716  
*Kvartil Q:*  
 wos-jcr – Q1 [Chemistry, analytical] -- 2017  
 wos-jcr – Q1 [Biochemical research methods] -- 2017  
*Ohlasy (15):*  
 [n1] 2018 zz ~ Tsopelas, F. - Stergiopoulos, C. - Tsantili-Kakoulidou, A.: Immobilized artificial membrane chromatography: From medicinal chemistry to environmental sciences. In: ADMET and DMPK, Vol. 6, No. 3, 2018, s. 225-241 -- SCOPUS  
 [n1] 2018 zz ~ Sharma, B. - Luhach, K. - Kulkarni, G.T.: In vitro and in vivo models of BBB to evaluate brain targeting drug delivery. In: Brain Targeted Drug Delivery Systems: A Focus on Nanotechnology and Nanoparticulates. Amsterdam : Elsevier, 2018, S. 53-101 -- SCOPUS  
 [n1] 2018 zz ~ Ermondi, G. - Vallaro, M. - Caron, G.: Learning how to use IAM chromatography for predicting permeability. In: European Journal of Pharmaceutical Sciences, Vol. 114, March, 2018, s. 385-390 - - SCOPUS  
 [n1] 2019 zz ~ Caudana, F. - Ermondi, G. - Vallaro, M. - Shalaeva, M. - Caron, G.: Permeability prediction for zwitterions via chromatographic indexes and classification into 'certain' and 'uncertain'. In: Future Medicinal Chemistry, Vol. 11, No. 13, 2019, s. 1553-1563 -- SCOPUS  
 [n1] 2019 zz ~ Brusac, E. - Jelacic, M.-L. - Mornar, A.: Biomimetic chromatography- A approach in drug development [Biomimeticka kromatografija-novi pristup u razvoju lijekova]. In: Farmaceutski Glasnik, Vol. 75, No. 11, 2019, s. 793-817 --SCOPUS  
 [n1] 2019 zz ~ Chen, Y. - Wu, B. - Hao, Y. - Liu, Y. - Zhang, Z. - Tian, C. - Ning, X. - Guo, Y. - Liu, J. - Wang, X.: Structure-activity relationship studies of (E)-3,4-dihydroxystyryl alkyl sulfones as novel neuroprotective agents based on improved antioxidant, anti-inflammatory activities and BBB permeability. In: European Journal of Medicinal Chemistry, Vol. 171, June, 2019, s. 420-433 -- SCOPUS  
 [n1] 2019 zz ~ Ermondi, G. - Caron, G.: MLR, PLSR-BR Analysis and MBPLSR to Interpret Multivariate QSPR Models. The Case of a Micellar Liquid Chromatography Descriptor (log K<sub>WSDS</sub>). In: Molecular Informatics, Vol. 38, No. 8-9, 2019, Art. No.1800144 -- SCOPUS  
 [n1] 2020 zz ~ Valko, K.L.: Application of HPLC measurements for the determination of physicochemical and biomimetic properties to model in vivo drug distribution in support of early drug discovery. In: Handbook of Analytical Separations, Vol. 8. Amsterdam : Elsevier, 2020, S. 667-758 -- SCOPUS  
 [n1] 2020 zz ~ Lombardo, D. - Calandra, P. - Caccamo, M.T. - Magazu, S. - Pasqua, L. - Kiselev, M.A.: Interdisciplinary approaches to the study of biological membranes. In: AIMS Biophysics, Vol. 7, No. 4, 2020, s. 267-290 -- SCOPUS  
 [n1] 2020 zz ~ Ciura, K. - Dziomba, S.: Application of separation methods for in vitro prediction of blood-brain barrier permeability-The state of the art. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 177, January, 2020, Art. No. 112891 -- SCOPUS  
 [n1] 2020 zz ~ Ciura, K. - Ulenberg, S. - Kapica, H. - Kawczak, P. - Belka, M. - Baczek, T.: Assessment of blood-brain barrier permeability using micellar electrokinetic chromatography and P\_VSA-like descriptors. In: Microchemical Journal, Vol. 158, November, 2020, Art. No. 105236 -- SCOPUS

[n1] 2021 zz ~ Sagandykova, G. - Buszewski, B.: Perspectives and recent advances in quantitative structure-retention relationships for high performance liquid chromatography. How far are we?. In: TrAC - Trends in Analytical Chemistry, Vol.141, August, 2021, Art. No. 116294 -- SCOPUS

[n1] 2021 zz ~ Pastewska, M. - Bednarczyk-Cwynar, B. - Kovacevic, S. - Bulawska, N. - Ulenberg, S. - Georgiev, P. - Kapica, H. - Kawczak, P. - Baczek, T. - Sawicki, W. - Ciura, K.: Multivariate assessment of anticancer oleanane triterpenoids lipophilicity. In: Journal of Chromatography A, Vol. 1656, October, 2021, Art. No. 462552 -- SCOPUS

[n1] 2021 zz ~ Carrasco-Correa, E.J. - Ruiz-Allica, J. - Rodriguez-Fernandez, J.F. - Miro, M.: Human artificial membranes in (bio)analytical science: Potential for in vitro prediction of intestinal absorption-A review. In: TrAC - Trends in Analytical Chemistry, Vol. 145, December, 2021, Art. No. 116446 -- SCOPUS

[n1] 2022 zz ~ de Lange, E.C.M. - Hammarlund, Udenaes M.: Understanding the Blood-Brain Barrier and Beyond: Challenges and Opportunities for Novel CNS Therapeutics. In: Clinical Pharmacology and Therapeutics, Vol. 111, No. 4, 2022, s. 758-773-- SCOPUS

V311 Taraji, Maryam (aut) (14.29%) - Haddad, Paul R. (aut) [KAUT] (14.285%) - Amos, Ruth I. J. (aut) (14.285%) - Talebi, Mohammad (aut) (14.285%) - Szücs, Roman (aut) [UKOPRCAL] (14.285%) - Dolan, John W. (aut) (14.285%) - Pohl, Christopher A.(aut) (14.285%): Error measures in quantitative structure-retention relationships studies

Lit.: 29 zázn.

In: Journal of Chromatography A. - č. 1524 (2017), s. 298-302. - ISSN (print) 0021-9673  
článok

*Registrované v:*

CCC Current Content Connect

SCO SCOPUS

WOS CC Web of Science Core Collection

SCIE Science Citation Index Expanded

*Indikátor časopisu:*

IF (JCR) 2017=3.716

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, analytical] -- 2017

wos-jcr – Q1 [Biochemical research methods] -- 2017

*Ohlasy (21):*

[n1] 2018 zz ~ Chakraborty, A. - Roy, S. - Banerjee, R.: Characterization of performance-emission indices of a diesel engine using ANFIS operating in dual-fuel mode with LPG. In: Heat and Mass Transfer/Waerme- und Stoffuebertragung, Vol. 54, No. 9, 2018, s. 2725-2742 -- SCOPUS

[n1] 2018 zz ~ Noreldeen, H.A.A. - Liu, X. - Wang, X. - Fu, Y. - Li, Z. - Lu, X. - Zhao, C. - Xu, G.:

Quantitative structure-retention relationships model for retention time prediction of veterinary drugs in food matrixes. In: International Journal of Mass Spectrometry, Vol. 434, November, 2018, s. 172-178 -- SCOPUS

[n1] 2019 zz ~ Consonni, V. - Todeschini, R. - Ballabio, D. - Grisoni, F.: On the Misleading Use of QF32 for QSAR Model Comparison. In: Molecular Informatics, Vol. 38, No. 1, 2019, Art. No. 1800029 -- SCOPUS

[n1] 2019 zz ~ D'Atri, V. - Fekete, S. - Clarke, A. - Veuthey, J.-L. - Guillarme, D.: Recent Advances in Chromatography for Pharmaceutical Analysis. In: Analytical Chemistry, Vol. 91, No. 1, 2019, s. 210-239 -- SCOPUS

[n1] 2019 zz ~ Zuvela, P. - Skoczylas, M. - Jay Liu, J. - Baczek, T. - Kaliszan, R. - Wong, M.W. - Buszewski, B.: Column Characterization and Selection Systems in Reversed-Phase High-Performance Liquid Chromatography. In: Chemical Reviews, Vol. 119, No. 6, 2019, s. 3674-3729 -- SCOPUS

[n1] 2019 zz ~ Zhang, S. - Zhao, G. - Lang, K. - Su, B. - Chen, X. - Xi, X. - Zhang, H.: Integrated satellite, unmanned aerial vehicle (UAV) and ground inversion of the spad of winter wheat in the reviving stage. In: Sensors, Vol. 19, No. 7, 2019, Art. No. 1485 -- SCOPUS

[n1] 2019 zz ~ Liu, J.J. - Alipuly, A. - Baczek, T. - Wong, M.W. - Zuvela, P.: Quantitative structure-retention relationships with non-linear programming for prediction of chromatographic elution order. In: International Journal of Molecular Sciences, Vol. 20, No. 14, 2019, Art. No. 3443 -- SCOPUS

[n1] 2019 zz ~ Hu, C.-Q. - Zhang, X.: Current situation and the trend in impurity profiling of chemical drugs. In: Yaoxue Xuebao, Vol. 54, No. 12, 2019, s. 2214-2231 -- SCOPUS

- [n1] 2020 zz ~ Marlot, L. - Batteau, M. - Faure, K.: Classification of biphasic solvent systems according to Abraham descriptors for countercurrent chromatography. In: Journal of Chromatography A, Vol. 1617, April, 2020, Art. No. 460820 --SCOPUS
- [n1] 2020 zz ~ Ser, C.T. - Zuvela, P. - Wong, M.W.: Prediction of corrosion inhibition efficiency of pyridines and quinolines on an iron surface using machine learning-powered quantitative structure-property relationships. In: Applied Surface Science, Vol. 512, May, 2020, Art. No. 145612 -- SCOPUS
- [n1] 2020 zz ~ Zuvela, P. - Liu, J.J. - Wong, M.W. - Baczek, T.: Prediction of Chromatographic Elution Order of Analytical Mixtures Based on Quantitative Structure-Retention Relationships and Multi-Objective Optimization. In: Molecules, Vol.25, No. 13, 2020, Art. No. 3085 -- SCOPUS
- [n1] 2021 zz ~ Ciura, K. - Fedorowicz, J. - Saczewski, J. - Kapica, H. - Pastewska, M. - Sawicki, W.: Interaction between antifungal isoxazolo[3,4-b]pyridin 3(1h)-one derivatives and human serum proteins analyzed with biomimetic chromatography and QSAR approach. In: Processes, Vol. 9, No. 3, 2021, Art. No. 512 -- SCOPUS
- [n1] 2021 zz ~ Bride, E. - Heinisch, S. - Bonnefille, B. - Guillemain, C. - Margoum, C.: Suspect screening of environmental contaminants by UHPLC-HRMS and transposable Quantitative Structure-Retention Relationship modelling. In: Journal of Hazardous Materials, Vol. 409, May, 2021, Art. No. 124652 -- SCOPUS
- [n1] 2021 zz ~ Sagandykova, G. - Buszewski, B.: Perspectives and recent advances in quantitative structure-retention relationships for high performance liquid chromatography. How far are we?. In: TrAC - Trends in Analytical Chemistry, Vol.141, August, 2021, Art. No. 116294 -- SCOPUS
- [n1] 2021 zz ~ Zhang, N. - Li, P.-C. - Liu, H. - Huang, T.-C. - Liu, H. - Kong, Y. - Dong, Z.-C. - Yuan, Y.-H. - Zhao, L.-L. - Li, J.-H.: Water and nitrogen in-situ imaging detection in live corn leaves using near-infrared camera and interference filter. In: Plant Methods, Vol. 17, No. 1, 2021, Art. No. 117 -- SCOPUS
- [n1] 2022 zz ~ Moldoveanu, S. - David, V.: Essentials in Modern HPLC Separations. In: . Amsterdam : Elsevier, 2022, S. 1-705 -- SCOPUS
- [n1] 2022 zz ~ Sun, Z. - Wang, Y.: A Deep Fuzzy Clustering Network for Gearbox Health Assessment. In: 2022 Global Reliability and Prognostics and Health Management Conference, PHM-Yantai, China, 2022. New Jersey : Institute of Electrical and Electronics Engineers Inc., S. 1-4 -- SCOPUS
- [n1] 2022 zz ~ Liapikos, T. - Zisi, C. - Kodra, D. - Kademoglou, K. - Diamantidou, D. - Begou, O. - Pappalouisi, A. - Theodoridis, G.: Quantitative structure retention relationship (QSRR) modelling for Analytes' retention prediction in LC-HRMS by applying different Machine Learning algorithms and evaluating their performance. In: Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, Vol. 1191, February, 2022, Art. No. 123132 -- SCOPUS
- [n1] 2022 zz ~ Krmar, J. - Dzical, M. - Stojkovic, J. - Protic, A. - Otasevic, B.: Gradient Boosted Tree model: A fast track tool for predicting the Atmospheric Pressure Chemical Ionization-Mass Spectrometry signal of antipsychotics based on molecular features and experimental settings. In: Chemometrics and Intelligent Laboratory Systems, Vol. 224, May, 2022, Art. No. 104554 -- SCOPUS
- [n1] 2022 zz ~ Cravero, F. - Diaz, M.F. - Ponzoni, I.: Polymer informatics for QSPR prediction of tensile mechanical properties. Case study: Strength at break. In: Journal of Chemical Physics, Vol. 156, No. 20, 2022, Art. No. 204903 -- SCOPUS
- [n1] 2022 zz ~ Sun, M.-M. - Li, Q.-S. - Zhou, K. - Han, X.-L.: Modal Identification Technologies for High-Rise Buildings under Non-Stationary Excitations. In: International Journal of Structural Stability and Dynamics, Vol. 22, No. 9, 2022, Art. No. 2250104 -- SCOPUS

V312 Taraji, Maryam (aut) (11.67%) - Haddad, Paul R. (aut) (11.666%) - Amos, Ruth I. J. (aut) [KAUT] (11.666%) - Talebi, Mohammad (aut) (11.666%) - Szücs, Roman (aut) [UKOPRCAL] (30%) - Dolan, John W. (aut) (11.666%) - Pohl, Christopher A. (aut) [KAUT] (11.666%): Rapid Method Development in Hydrophilic Interaction Liquid Chromatography for Pharmaceutical Analysis Using a Combination of Quantitative Structure Retention Relationships and Design of Experiments [elektronický dokument]  
Lit.: 59 zázn.  
In: Analytical Chemistry [elektronický dokument]. - Roč. 89, č. 3 (2017), s. 1870-1878 [print]. - ISSN (print) 0003-2700

článok

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SCIE Science Citation Index Expanded

*Indikátor časopisu:*

IF (JCR) 2017=6.024

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, analytical] -- 2017

*Ohlasy (23):*

[n1] 2018 zz ~ Yin, H. - Zou, L. - Sheng, Y. - Bai, X. - Liu, Q. - Yan, B.: Rapid HPLC analytical method development for Herbal medicine formulae based on retention rules acquired from the constituting herbs. In: Analytical Sciences, Vol. 34, No. 2, 2018, s. 207-214 -- SCOPUS

[n1] 2018 zz ~ Parsazadeh, N. - Yousefi, F. - Ghaedi, M. - Dashtian, K. - Borousan, F.: Preparation and characterization of monoliths HKUST-1 MOF: Via straightforward conversion of Cu(OH)<sub>2</sub>-based monoliths and its application for wastewater treatment: Artificial neural network and central composite design modeling. In: New Journal of Chemistry, Vol. 42, No. 12, 2018, s. 10327-10336 -- SCOPUS

[n1] 2018 zz ~ Sahu, P.K. - Ramiseti, N.R. - Cecchi, T. - Swain, S. - Patro, C.S. - Panda, J.: An overview of experimental designs in HPLC method development and validation. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 147, January, 2018, s. 590-611 -- SCOPUS

[n1] 2018 zz ~ Miller, T.H. - Bury, N.R. - Owen, S.F. - MacRae, J.I. - Barron, L.P.: A review of the pharmaceutical exposome in aquatic fauna. In: Environmental Pollution, Vol. 239, August, 2018, s. 129-146 -- SCOPUS

[n1] 2018 zz ~ Arase, S. - Kimura, S. - Ikegami, T.: Method optimization of hydrophilic interaction chromatography separation of nucleotides using design of experiment approaches I: Comparison of several zwitterionic columns. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 158, September, 2018, s. 307-316 -- SCOPUS

[n1] 2018 zz ~ Noreldeen, H.A.A. - Liu, X. - Wang, X. - Fu, Y. - Li, Z. - Lu, X. - Zhao, C. - Xu, G.: Quantitative structure-retention relationships model for retention time prediction of veterinary drugs in food matrixes. In: International Journal of Mass Spectrometry, Vol. 434, November, 2018, s. 172-178 -- SCOPUS

[n1] 2019 zz ~ Takayama, T. - Mizuno, H. - Toyo'Oka, T. - Todoroki, K.: Introducing an experimental design approach for efficient optimization of chiral derivatization conditions for D- and L-glyceric acids. In: Analytical Sciences, Vol. 35, No. 9, 2019, s. 1053-1056 -- SCOPUS

[n1] 2019 zz ~ Borousan, F. - Yousefi, F. - Ghaedi, M.: Removal of Malachite Green Dye Using IRMOF-3-MWCNT-OH-Pd-NPs as a Novel Adsorbent: Kinetic, Isotherm, and Thermodynamic Studies. In: Journal of Chemical and Engineering Data, Vol. 64, No.11, 2019, s. 4801-4814 -- SCOPUS

[n1] 2020 zz ~ Kaliszan, R.: Recent advances in quantitative structure-retention relationships. In: Handbook of Analytical Separations, Vol. 8. Amsterdam : Elsevier, 2020, S. 587-632 -- SCOPUS

[n1] 2020 zz ~ Buszewski, B. - Zuvela, P. - Sagandykova, G. - Walczak-skierska, J. - Pomastowski, P. - David, J. - Wong, M.W.: Mechanistic chromatographic column characterization for the analysis of flavonoids using quantitative structure-retention relationships based on density functional theory. In: International Journal of Molecular Sciences, Vol. 21, No. 6, 2020, Art. No. 2053 -- SCOPUS

[n1] 2020 zz ~ Taniguchi, A. - Tamura, S. - Ikegami, T.: The relationship between polymer structures on silica particles and the separation characteristics of the corresponding columns for hydrophilic interaction chromatography. In: Journal of Chromatography A, Vol. 1618, May, 2020, Art. No. 460837 -- SCOPUS

[n1] 2020 zz ~ Li, L. - Tan, D. - Liu, S. - Jiao, R. - Yang, X. - Li, F. - Wu, H. - Huang, W.: Optimization of Factor Combinations for Stem Cell Differentiations on a Design-of-Experiment Microfluidic Chip. In: Analytical Chemistry, Vol. 92, No. 20, 2020, s. 14228-14235 -- SCOPUS

[n1] 2021 zz ~ Araujo, A.S. - Andrade, D.F. - Babos, D.V. - Castro, J.P. - Garcia, J.A. - Speranca, M.A. - Gamela, R.R. - Machado, R.C. - Costa, V.C. - Guedes, W.N. - Pereira-Filho, E.R. - Pereira, F.M.V.: Key information related to quality by design (QbD) applications in analytical methods development. In: Brazilian Journal of Analytical Chemistry, Vol. 8, No. 30, 2021, s. 14-28 -- SCOPUS

[n1] 2021 zz ~ Ge, Z. - Zhang, K. - Chen, D.D.Y. - Yan, B.: Data-driven development of liquid chromatography-mass spectrometry methods for combined sample matrices. In: Talanta, Vol. 224, March, 2021, Art. No. 121880 -- SCOPUS

[n1] 2021 zz ~ Besenhard, M.O. - Tsatse, A. - Mazzei, L. - Sorensen, E.: Recent advances in modelling and control of liquid chromatography. In: Current Opinion in Chemical Engineering, Vol. 32, June, 2021, Art. No. 100685 -- SCOPUS

[n1] 2021 zz ~ Sagandykova, G. - Buszewski, B.: Perspectives and recent advances in quantitative structure-retention relationships for high performance liquid chromatography. How far are we?. In: TrAC - Trends in Analytical Chemistry, Vol.141, August, 2021, Art. No. 116294 -- SCOPUS

[n1] 2021 zz ~ Yang, Q. - Ji, H. - Fan, X. - Zhang, Z. - Lu, H.: Retention time prediction in hydrophilic interaction liquid chromatography with graph neural network and transfer learning. In: Journal of Chromatography A, Vol. 1656, October,2021, Art. No. 462536 -- SCOPUS

[n1] 2021 zz ~ Dinh, N.P. - Shamshir, A. - Hulaj, G. - Jonsson, T.: Validated modernized assay for foscarnet in pharmaceutical formulations using suppressed ion chromatography developed through a quality by design approach. In: Separations, Vol. 8, No. 11, 2021, Art. No. 209 -- SCOPUS

[n1] 2022 zz ~ Beck, T.I.H. - Toussaint, B. - Surget, E. - Herrenknecht, C. - Boudy, V. - Jaccoulet, E.: Investigation of hydrophilic interaction liquid chromatography coupled with charged aerosol detector for the analysis of tromethamine. In: Talanta, Vol. 238, February, 2022, Art. No. 123050 -- SCOPUS

[n1] 2022 zz ~ Van Laethem, T. - Kumari, P. - Hubert, P. - Fillet, M. - Sacre, P.-Y. - Hubert, C.: A pharmaceutical-related molecules dataset for reversed-phase chromatography retention time prediction built on combining pH and gradient time conditions. In: Data in Brief, Vol. 42, June, 2022, Art. No. 108017 -- SCOPUS

[n1] 2022 zz ~ Latrous, L.: Optimization and Validation in Liquid Chromatography Using Design of Experiments. In: Chemistry Africa, Vol. 5, No. 3, 2022, s. 437-458 -- SCOPUS

[n1] 2022 zz ~ Kumar, P. - Kumar, A. - Lal, S. - Singh, D. - Lotfi, S. - Ahmadi, S.: CORAL: Quantitative Structure Retention Relationship (QSRR) of flavors and fragrances compounds studied on the stationary phase methyl silicone OV-101 column in gas chromatography using correlation intensity index and consensus modelling. In: Journal of Molecular Structure, Vol. 1265, October, 2022, Art. No. 133437 -- SCOPUS

[n1] 2022 zz ~ Van Laethem, T. - Kumari, P. - Boulanger, B. - Hubert, P. - Fillet, M. - Sacre, P.-Y. - Hubert, C.: User-Driven Strategy for In Silico Screening of Reversed-Phase Liquid Chromatography Conditions for Known Pharmaceutical-Related Small Molecules. In: Molecules, Vol. 27, No. 23, 2022, Art. No. 8306 -- SCOPUS

V313 Taraji, Maryam (aut) (14.29%) - Haddad, Paul R. (aut) [KAUT] (14.285%) - Amos, Ruth I. J. (aut) (14.285%) - Talebi, Mohammad (aut) (14.285%) - Szücs, Roman (aut) [UKOPRCAL] (14.285%) - Dolan, John W. (aut) (14.285%) - Pohl, Christopher A.(aut) (14.285%): Prediction of retention in hydrophilic interaction liquid chromatography using solute molecular descriptors based on chemical structures [elektronický dokument] Lit.: 61 zázn.

In: Journal of Chromatography A [elektronický dokument]. - č. 1486 (2017), s. 59-67 [print]. - ISSN (print) 0021-9673

článok

*Registrované v:*

CCC Current Content Connect

SCO SCOPUS

WOS CC Web of Science Core Collection

SCIE Science Citation Index Expanded

*Indikátor časopisu:*

IF (JCR) 2017=3.716

*Kvartil Q:*

wos-jcr – Q1 [Chemistry, analytical] -- 2017

wos-jcr – Q1 [Biochemical research methods] -- 2017

*Ohlasy (26):*

[n1] 2018 zz ~ Parr, M.K. - Schmidt, A.H.: Life cycle management of analytical methods. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 147, January, 2018, s. 506-517 -- SCOPUS

[n1] 2018 zz ~ Blazenovic, I. - Kind, T. - Ji, J. - Fiehn, O.: Software tools and approaches for compound identification of LC-MS/MS data in metabolomics. In: Metabolites, Vol. 8, No. 2, 2018, Art. No. 31 -- SCOPUS

[n1] 2018 zz ~ Miller, T.H. - Bury, N.R. - Owen, S.F. - MacRae, J.I. - Barron, L.P.: A review of the pharmaceutical exposome in aquatic fauna. In: Environmental Pollution, Vol. 239, August, 2018, s. 129-146 -- SCOPUS

[n1] 2018 zz ~ Yadrova, A.A. - Shafigulin, R.V. - Bulanova, A.V. - Golov, A.A. - Belousova, Z.P.: Studying the Sorption of Certain Benzimidazoles on Octadecyl Silica Gel from Water-Acetonitrile Solutions via Liquid Chromatography. In: Russian Journal of Physical Chemistry A, Vol. 92, No. 8, 2018, s. 1572-1582 -- SCOPUS

[n1] 2018 zz ~ Noreldeen, H.A.A. - Liu, X. - Wang, X. - Fu, Y. - Li, Z. - Lu, X. - Zhao, C. - Xu, G.: Quantitative structure-retention relationships model for retention time prediction of veterinary drugs in food matrixes. In: International Journal of Mass Spectrometry, Vol. 434, November, 2018, s. 172-178 -- SCOPUS

[n1] 2019 zz ~ D'Atri, V. - Fekete, S. - Clarke, A. - Veuthey, J.-L. - Guillarme, D.: Recent Advances in Chromatography for Pharmaceutical Analysis. In: Analytical Chemistry, Vol. 91, No. 1, 2019, s. 210-239 -- SCOPUS

[n1] 2019 zz ~ Hu, C.-Q. - Zhang, X.: Current situation and the trend in impurity profiling of chemical drugs. In: Yaoxue Xuebao, Vol. 54, No. 12, 2019, s. 2214-2231 -- SCOPUS

[n1] 2020 zz ~ Fu, X. - Cebo, M. - Ikegami, T. - Lammerhofer, M.: Retention characteristics of poly(N-(1H-tetrazole-5-yl)-methacrylamide)-bonded stationary phase in hydrophilic interaction chromatography. In: Journal of Chromatography A, Vol.1609, January, 2020, Art. No. 460500 -- SCOPUS

[n1] 2020 zz ~ Skoczylas, M. - Bocian, S. - Buszewski, B.: Quantitative structure - retention relationships of amino acids on the amino acid- and peptide-silica stationary phases for liquid chromatography. In: Journal of Chromatography A, Vol.1609, January, 2020, Art. No. 460514 -- SCOPUS

[n1] 2020 zz ~ Dimic, D. - Milanovic, Z. - Jovanovic, G. - Sretenovic, D. - Milenkovic, D. - Markovic, Z. - Dimitric, Markovic J.: Comparative antiradical activity and molecular Docking/Dynamics analysis of octopamine and norepinephrine: the role of OH groups. In: Computational Biology and Chemistry, Vol. 84, February, 2020, Art. No. 107170 -- SCOPUS

[n1] 2020 zz ~ Roca, L.S. - Schoemaker, S.E. - Pirok, B.W.J. - Gargano, A.F.G. - Schoenmakers, P.J.: Accurate modelling of the retention behaviour of peptides in gradient-elution hydrophilic interaction liquid chromatography. In: Journal of Chromatography A, Vol. 1614, March, 2020, Art. No. 460650 -- SCOPUS

[n1] 2020 zz ~ Wang, X. - Cho, J.-H. - Poudel, S. - Li, Y. - Jones, D.R. - Shaw, T.I. - Tan, H. - Xie, B. - Peng, J.: JUMPm: A tool for large-scale identification of metabolites in untargeted metabolomics. In: Metabolites, Vol. 10, No. 5, 2020, Art. No. 190 -- SCOPUS

[n1] 2020 zz ~ Bonini, P. - Kind, T. - Tsugawa, H. - Barupal, D.K. - Fiehn, O.: Retip: Retention Time Prediction for Compound Annotation in Untargeted Metabolomics. In: Analytical Chemistry, Vol. 92, No. 11, 2020, s. 7515-7522 -- SCOPUS

[n1] 2020 zz ~ Krmar, J. - Vukicevic, M. - Kovacevic, A. - Protic, A. - Zecevic, M. - Otasevic, B.: Performance comparison of nonlinear and linear regression algorithms coupled with different attribute selection methods for quantitative structure - retention relationships modelling in micellar liquid chromatography. In: Journal of Chromatography A, Vol. 1623, July, 2020, Art. No. 461146 -- SCOPUS

[n1] 2020 zz ~ Huygens, B. - Efthymiadis, K. - Nowe, A. - Desmet, G.: Application of evolutionary algorithms to optimise one- and two-dimensional gradient chromatographic separations. In: Journal of Chromatography A, Vol. 1628, September, 2020, Art. No. 461435 -- SCOPUS

[n1] 2021 zz ~ Yashin Yakov, I. - Yashin, Alexander Ya.: 30th anniversary of hydrophilic interaction chromatography. In: Sorbtsionnye i Khromatograficheskie Protssesy, Vol. 21, No. 5, 2021, s. 708-716 -- SCOPUS

[n1] 2021 zz ~ Miyamoto, K. - Mizuno, H. - Sugiyama, E. - Toyo'oka, T. - Todoroki, K.: Machine learning guided prediction of liquid chromatography-mass spectrometry ionization efficiency for genotoxic impurities in pharmaceutical products. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 194, February, 2021, Art. No. 113781 -- SCOPUS

[n1] 2021 zz ~ Shi, P. - Li, M. - Fu, X. - Xia, B. - Zhou, Y.: Study on the separation mechanism of solid-substrate electrospray ionization mass spectrometry. In: Journal of Separation Science, Vol. 44, No. 5, 2021, s. 1026-1035 -- SCOPUS

[n1] 2021 zz ~ Bride, E. - Heinisch, S. - Bonnefille, B. - Guillemain, C. - Margoum, C.: Suspect screening of environmental contaminants by UHPLC-HRMS and transposable Quantitative Structure-Retention Relationship modelling. In: Journal of Hazardous Materials, Vol. 409, May, 2021, Art. No. 124652 -- SCOPUS

[n1] 2021 sk ~ Ranusova, P. - Nemecek, P. - Lehotay, J. - Cizmarik, J.: QSRR modelling aimed on the HPLC retention prediction of dimethylamino- and pyrrolidino-substituted esters of alkoxyphenylcarbamic acid. In: Chemical Papers, Vol. 75, No.6, 2021, s. 2525-2535 -- SCOPUS

- [n1] 2021 zz ~ Besenhard, M.O. - Tsatse, A. - Mazzei, L. - Sorensen, E.: Recent advances in modelling and control of liquid chromatography. In: Current Opinion in Chemical Engineering, Vol. 32, June, 2021, Art. No. 100685 -- SCOPUS
- [n1] 2021 zz ~ Yang, Q. - Ji, H. - Fan, X. - Zhang, Z. - Lu, H.: Retention time prediction in hydrophilic interaction liquid chromatography with graph neural network and transfer learning. In: Journal of Chromatography A, Vol. 1656, October, 2021, Art. No. 462536 -- SCOPUS
- [n1] 2022 zz ~ Moldoveanu, S. - David, V.: Essentials in Modern HPLC Separations. In: . Amsterdam : Elsevier, 2022, S. 1-705 -- SCOPUS
- [n1] 2022 zz ~ Tian, Z. - Liu, F. - Li, D. - Fernie, A.R. - Chen, W.: Strategies for structure elucidation of small molecules based on LC-MS/MS data from complex biological samples. In: Computational and Structural Biotechnology Journal, Vol.20, January, 2022, s. 5085-5097 -- SCOPUS
- [n1] 2022 zz ~ Liapikos, T. - Zisi, C. - Kodra, D. - Kademoglou, K. - Diamantidou, D. - Begou, O. - Pappalouisi, A. - Theodoridis, G.: Quantitative structure retention relationship (QSRR) modelling for Analytes' retention prediction in LC-HRMS by applying different Machine Learning algorithms and evaluating their performance. In: Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, Vol. 1191, February, 2022, Art. No. 123132 -- SCOPUS
- [n1] 2022 zz ~ Borkar, M.R. - Coutinho, E.C.: Amalgamation of comparative protein modeling with quantitative structure-retention relationship for prediction of the chromatographic behavior of peptides. In: Journal of Chromatography A, Vol.1669, April, 2022, Art. No. 462967 -- SCOPUS

- V314 Amos, Ruth I. J. (aut) [KAUT] (20%) - Haddad, Paul R. (aut) (20%) - Szücs, Roman (aut) [UKOPRCAL] (20%) - Dolan, John W. (aut) (20%) - Pohl, Christopher A. (aut) (20%): Molecular modeling and prediction accuracy in Quantitative Structure-Retention Relationship calculations for chromatography [elektronický dokument]  
Lit.: 88 zázn.  
In: Trends in Analytical Chemistry [elektronický dokument]. - č. 105 (2018), s. 352-359 [print]. - ISSN (print) 0165-9936  
článok  
*Registrované v:*  
CCC Current Content Connect  
SCO SCOPUS  
WOS CC Web of Science Core Collection  
*Indikátor časopisu:*  
IF (JCR) 2018=8.428  
*Kvartil Q:*  
wos-jcr -- Q1 [Chemistry, analytical] -- 2018  
*Ohlasy (26):*  
[n1] 2019 zz ~ Ramezani, A.M. - Yousefinejad, S. - Shahsavari, A. - Mohajeri, A. - Absalan, G.: Quantitative structure-retention relationship for chromatographic behaviour of anthraquinone derivatives through considering organic modifier features in micellar liquid chromatography. In: Journal of Chromatography A, Vol. 1599, August, 2019, s. 46-54 -- SCOPUS
- [n1] 2019 zz ~ Karadzic Banjac, M.Z. - Kovacevic, S.Z. - Tepic Horecki, A.N. - Sumic, Z.M. - Vakula, A.S. - Podunavac-Kuzmanovic, S.O. - Jevric, L.R.: Toward consistent discrimination of common bean (*Phaseolus vulgaris* L.) based on grain coat color, phytochemical composition, and antioxidant activity. In: Journal of Food Processing and Preservation, Vol. 43, No. 12, 2019, Art. No. e14246 -- SCOPUS
- [n1] 2019 zz ~ Hu, C.-Q. - Zhang, X.: Current situation and the trend in impurity profiling of chemical drugs. In: Yaoxue Xuebao, Vol. 54, No. 12, 2019, s. 2214-2231 -- SCOPUS
- [n1] 2020 zz ~ Watanabe, N. - Murata, M. - Ogawa, T. - Vavricka, C.J. - Kondo, A. - Ogino, C. - Araki, M.: Exploration and Evaluation of Machine Learning-Based Models for Predicting Enzymatic Reactions. In: Journal of Chemical Information and Modeling, Vol. 60, No. 3, 2020, s. 1833-1843 -- SCOPUS
- [n1] 2020 zz ~ Abba, S.I. - Usman, A.G. - Isik, S.: Simulation for response surface in the HPLC optimization method development using artificial intelligence models: A data-driven approach. In: Chemometrics and Intelligent Laboratory Systems, Vol. 201, June, 2020, Art. No. 104007 -- SCOPUS
- [n1] 2020 zz ~ Tsopelas, F. - Dianas, P. - Pappa, A. - Tsantili-Kakoulidou, A.: Biopartitioning micellar chromatography under different conditions: Insight into the retention mechanism and the potential to model biological processes. In: Journal of Chromatography A, Vol. 1621, June, 2020, Art. No. 461027 -- SCOPUS



- [n1] 2020 zz ~ Kianpour, M. - Mohammadinasab, E. - Isfahani, T.M.: Comparison between genetic algorithm-multiple linear regression and back-propagation-artificial neural network methods for predicting the LD50 of organo (phosphate and thiophosphate) compounds. In: Journal of the Chinese Chemical Society, Vol. 67, No. 8, 2020, s. 1356-1366 -- SCOPUS
- [n1] 2020 zz ~ Zhu, Q.-F. - An, N. - Feng, Y.-Q.: In-Depth Annotation Strategy of Saturated Hydroxy Fatty Acids Based on Their Chromatographic Retention Behaviors and MS Fragmentation Patterns. In: Analytical Chemistry, Vol. 92, No. 21, 2020, s. 14528-14535 -- SCOPUS
- [n1] 2020 zz ~ Kadlecova, Z. - Kalikova, K. - Ansoerge, M. - Gilar, M. - Tesarova, E.: The effect of particle and ligand types on retention and peak shape in liquid chromatography. In: Microchemical Journal, Vol. 159, December, 2020, Art. No.105466 -- SCOPUS
- [n1] 2021 zz ~ He, M. - Zhou, Y.: How to identify "Material basis-Quality markers" more accurately in Chinese herbal medicines from modern chromatography-mass spectrometry data-sets: Opportunities and challenges of chemometric tools. In: Chinese Herbal Medicines, Vol. 13, No. 1, 2021, s. 2-16 -- SCOPUS
- [n1] 2021 zz ~ Keshavarz, M.H. - Shirazi, Z. - Rezayat, M.A.: Prediction of Retention Time of Morphine and Its Derivatives Without Using Computer-Encoded Complex Descriptors. In: Chromatographia, Vol. 84, No. 1, 2021, s. 87-96 -- SCOPUS
- [n1] 2021 zz ~ Paritala, J. - Peraman, R. - Kondreddy, V.K. - Subrahmanyam, C.V.S. - Ravichandiran, V.: Quantitative structure retention relationship (QSRR) approach for assessment of chromatographic behavior of antiviral drugs in the development of liquid chromatographic method. In: Journal of Liquid Chromatography and Related Technologies, Vol. 44, No. 13-14, 2021, s. 637-648 -- SCOPUS
- [n1] 2021 zz ~ Renslow, R.S. - Metz, T.O. - Nielson, F.F. - Colby, S.M. - Thomas, D.G.: Exploring the impacts of conformer selection methods on ion mobility collision cross section predictions. In: Analytical Chemistry, Vol. 93, No. 8, 2021, s. 3830-3838 -- SCOPUS
- [n1] 2021 zz ~ Gritti, F.: Perspective on the Future Approaches to Predict Retention in Liquid Chromatography. In: Analytical Chemistry, Vol. 93, No. 14, 2021, s. 5653-5664 -- SCOPUS
- [n1] 2021 zz ~ Sagandykova, G. - Buszewski, B.: Perspectives and recent advances in quantitative structure-retention relationships for high performance liquid chromatography. How far are we?. In: TrAC - Trends in Analytical Chemistry, Vol.141, August, 2021, Art. No. 116294 -- SCOPUS
- [n1] 2021 zz ~ Angeles, L.F. - Halwatura, L.M. - Antle, J.P. - Simpson, S. - Jaraula, C.M.B. - Aga, D.S.: In Silico Supported Nontarget Analysis of Contaminants of Emerging Concern: Increasing Confidence in Unknown Identification in Wastewater and Surface Waters. In: ACS ES and T Water, Vol. 1, No. 8, 2021, s. 1765-1775 -- SCOPUS
- [n1] 2021 zz ~ Ulenberg, S. - Baczek, T.: Comparison of quantum mechanics protocols during the evaluation of quantitative structure-retention relationships supported by genetic-algorithm multiple linear regression. In: Journal of Chromatography Open, Vol. 1, November, 2021, Art. No. 100019 -- SCOPUS
- [n1] 2022 zz ~ Biancolillo, A. - D'Archivio, A.A.: Transfer of gas chromatographic retention data among poly(siloxane) columns by quantitative structure-retention relationships based on molecular descriptors of both solutes and stationary phases. In: Journal of Chromatography A, Vol. 1663, January, 2022, Art. No. 462758 -- SCOPUS
- [n1] 2022 zz ~ Liapikos, T. - Zisi, C. - Kodra, D. - Kademoglou, K. - Diamantidou, D. - Begou, O. - Pappa-Louisi, A. - Theodoridis, G.: Quantitative structure retention relationship (QSRR) modelling for Analytes' retention prediction in LC-HRMS by applying different Machine Learning algorithms and evaluating their performance. In: Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, Vol. 1191, February, 2022, Art. No. 123132 -- SCOPUS
- [n1] 2022 zz ~ Sepehri, B. - Ghavami, R. - Farahbakhsh, S. - Ahmadi, R.: Machine learning-based quantitative structure-retention relationship models for predicting the retention indices of volatile organic pollutants. In: International Journal of Environmental Science and Technology, Vol. 19, No. 3, 2022, s. 1457-1466 -- SCOPUS
- [n1] 2022 zz ~ De Gauquier, P. - Vanommeslaeghe, K. - Heyden, Y.V. - Mangelings, D.: Modelling approaches for chiral chromatography on polysaccharide-based and macrocyclic antibiotic chiral selectors: A review. In: Analytica Chimica Acta, Vol.1198, March, 2022, Art. No. 338861 -- SCOPUS
- [n1] 2022 zz ~ Osipenko, S. - Nikolaev, E. - Kostyukevich, Y.: Retention Time Prediction with Message-Passing Neural Networks. In: Separations, Vol. 9, No. 10, 2022, Art. No. 291 -- SCOPUS
- [n1] 2022 zz ~ Kumar, P. - Kumar, A. - Lal, S. - Singh, D. - Lotfi, S. - Ahmadi, S.: CORAL: Quantitative Structure Retention Relationship (QSRR) of flavors and fragrances compounds studied on the stationary phase

methyl silicone OV-101 column in gas chromatography using correlation intensity index and consensus modelling. In: Journal of Molecular Structure, Vol. 1265, October, 2022, Art. No. 133437 -- SCOPUS  
 [n1] 2022 zz ~ Rocco, K. - Margoum, C. - Richard, L. - Coquery, M.: Enhanced database creation with in silico workflows for suspect screening of unknown tebuconazole transformation products in environmental samples by UHPLC-HRMS. In: Journal of Hazardous Materials, Vol. 440, October, 2022, Art. No. 129706 -- SCOPUS  
 [n1] 2022 zz ~ Ribar, D. - Rijavec, T. - Kralj, Cigic I.: An exploration into the use of Hansen solubility parameters for modelling reversed-phase chromatographic separations. In: Journal of Analytical Science and Technology, Vol. 13, No. 1, 2022, Art. No. 12 -- SCOPUS  
 [n1] 2022 zz ~ Gritti, F. - Trebel, N. - Holtzel, A. - Tallarek, U.: Prediction of surface excess adsorption and retention factors in reversed-phase liquid chromatography from molecular dynamics simulations. In: Journal of Chromatography A, Vol. 1685, December, 2022, Art. No. 463627 -- SCOPUS

V315 Russo, Giacomo (aut) (20%) - Grumetto, Lucia (aut) (20%) - Szücs, Roman (aut) [UKOPRCAL] (20%) - Barbato, Francesco (aut) (20%) - Lynen, Frederic (aut) [KAUT] (20%): Screening therapeutics according to their uptake across the blood-brain barrier [elektronický dokument] : A high throughput method based on immobilized artificial membrane liquid chromatography-diode-array-detection coupled to electrospray-time-of-flight mass spectrometry  
 Lit.: 64 zázn.  
 In: European Journal of Pharmaceutics and Biopharmaceutics [elektronický dokument]. - č. 127 (2018), s. 72-84 [print]. - ISSN (print) 0939-6411  
 článok  
 Registrované v:  
 CCC Current Content Connect  
 SCO SCOPUS  
 WOS CC Web of Science Core Collection  
 SCIE Science Citation Index Expanded  
 Indikátor časopisu:  
 IF (JCR) 2018=4.708  
 Kvartil Q:  
 wos-jcr -- Q1 [Pharmacology & pharmacy] -- 2018  
 Ohlasy (9):  
 [n1] 2019 zz ~ Brusac, E. - Jelicic, M.-L. - Mornar, A.: Biomimetic chromatography- A approach in drug development [Biomimeticka kromatografija-novi pristup u razvoju lijekova]. In: Farmaceutski Glasnik, Vol. 75, No. 11, 2019, s. 793-817 --SCOPUS  
 [n1] 2019 zz ~ Zhang, H. - Wu, Z.-Y. - Yang, Y.-Y. - Yang, F.-Q. - Li, S.-P.: Recent applications of immobilized biomaterials in herbal analysis. In: Journal of Chromatography A, Vol. 1603, October, 2019, s. 216-230 -- SCOPUS  
 [n1] 2020 zz ~ Ciura, K. - Dziomba, S.: Application of separation methods for in vitro prediction of blood-brain barrier permeability-The state of the art. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 177, January, 2020, Art.No. 112891 -- SCOPUS  
 [n1] 2020 zz ~ Janicka, M. - Sztanke, M. - Sztanke, K.: Predicting the blood-brain barrier permeability of new drug-like compounds via HPLC with various stationary phases. In: Molecules, Vol. 25, No. 3, 2020, Art. No. 487 -- SCOPUS  
 [n1] 2020 zz ~ Godyn, J. - Gucwa, D. - Kobrlova, T. - Novak, M. - Soukup, O. - Malawska, B. - Bajda, M.: Novel application of capillary electrophoresis with a liposome coated capillary for prediction of blood-brain barrier permeability. In: Talanta, Vol. 217, September, 2020, Art. No. 121023 -- SCOPUS  
 [n1] 2021 zz ~ Stepnik, K.: Biomimetic chromatographic studies combined with the computational approach to investigate the ability of triterpenoid saponins of plant origin to cross the blood-brain barrier. In: International Journal of Molecular Sciences, Vol. 22, No. 7, 2021, Art. No. 3573 -- SCOPUS  
 [n1] 2021 zz ~ Carrasco-Correa, E.J. - Ruiz-Allica, J. - Rodriguez-Fernandez, J.F. - Miro, M.: Human artificial membranes in (bio)analytical science: Potential for in vitro prediction of intestinal absorption-A review. In: TrAC - Trends in Analytical Chemistry, Vol. 145, December, 2021, Art. No. 116446 -- SCOPUS  
 [n1] 2022 zz ~ Janicka, M. - Sliwinska, A.: Quantitative Retention (Structure)-Activity Relationships in Predicting the Pharmaceutical and Toxic Properties of Potential Pesticides. In: Molecules, Vol. 27, No. 11, 2022, Art. No. 3599 -- SCOPUS

[n1] 2022 zz ~ Janicka, M. - Sliwinska, A. - Sztanke, M. - Sztanke, K.: Combined Micellar Liquid Chromatography Technique and QSARs Modeling in Predicting the Blood-Brain Barrier Permeation of Heterocyclic Drug-like Compounds. In: International Journal of Molecular Sciences, Vol. 23, No. 24, 2022, Art. No. 15887 -- SCOPUS

- V316 Taraji, Maryam (aut) (14.29%) - Haddad, Paul R. (aut) [KAUT] (14.285%) - Amos, Ruth I. J. (aut) (14.285%) - Talebi, Mohammad (aut) (14.285%) - Szücs, Roman (aut) [UKOPRCAL] (14.285%) - Dolan, John W. (aut) (14.285%) - Pohl, Christopher A.(aut) (14.285%): Chemometric-assisted method development in hydrophilic interaction liquid chromatography: A review [elektronický dokument]  
Lit.: 257 zázn.  
In: Analytica Chimica Acta [elektronický dokument]. - č. 1000 (2018), s. 20-40 [print]. - ISSN (print) 0003-2670  
článok  
*Registrované v:*  
CCC Current Content Connect  
SCO SCOPUS  
WOS CC Web of Science Core Collection  
SCIE Science Citation Index Expanded  
*Indikátor časopisu:*  
IF (JCR) 2018=5.256  
*Kvartil Q:*  
wos-jcr -- Q1 [Chemistry, analytical] -- 2018  
*Ohlasy (58):*  
[n1] 2018 zz ~ Kalikova, K. - Voborna, M. - Tesarova, E.: Chromatographic behavior of new deazapurine ribonucleosides in hydrophilic interaction liquid chromatography. In: Electrophoresis, Vol. 39, No. 16, 2018, s. 2144-2151 -- SCOPUS  
[n1] 2018 zz ~ Marrubini, G. - Appelblad, P. - Maietta, M. - Papetti, A.: Hydrophilic interaction chromatography in food matrices analysis: An updated review. In: Food Chemistry, Vol. 257, August, 2018, s. 53-66 -- SCOPUS  
[n1] 2019 zz ~ Hu, Y. - Cai, T. - Zhang, H. - Chen, J. - Li, Z. - Qiu, H.: Poly(itaconic acid)-grafted silica stationary phase prepared in deep eutectic solvents and its unique performance in hydrophilic interaction chromatography. In: Talanta, Vol. 191, January, 2019, s. 265-271 -- SCOPUS  
[n1] 2019 zz ~ Srata, L. - Farres, S. - Fethi, F.: Engine oil authentication using near infrared spectroscopy and chemometrics methods. In: Vibrational Spectroscopy, Vol. 100, January, 2019, s. 99-106 -- SCOPUS  
[n1] 2019 zz ~ Ikegami, T.: Hydrophilic interaction chromatography for the analysis of biopharmaceutical drugs and therapeutic peptides: A review based on the separation characteristics of the hydrophilic interaction chromatography phases. In: Journal of Separation Science, Vol. 42, No. 1, 2019, s. 130-213 -- SCOPUS  
[n1] 2019 zz ~ D'Atri, V. - Fekete, S. - Clarke, A. - Veuthey, J.-L. - Guilleme, D.: Recent Advances in Chromatography for Pharmaceutical Analysis. In: Analytical Chemistry, Vol. 91, No. 1, 2019, s. 210-239 -- SCOPUS  
[n1] 2019 zz ~ Bi, X. - Tian, W. - Wang, Y. - Cao, W. - Fan, S. - Wang, M. - Niu, L.: Modulated Preparation of Capillary Monolithic HILIC Column by Target-Analogues of Matrine and Oxymatrine and Applied for Extracted Analysis of Sophorae flavescens radix. In: Chemistry Select, Vol. 4, No. 1, 2019, s. 413-416 -- SCOPUS  
[n1] 2019 zz ~ Jacyna, J. - Kordalewska, M. - Markuszewski, M.J.: Design of Experiments in metabolomics-related studies: An overview. In: Journal of Pharmaceutical and Biomedical Analysis, Vol. 164, February, 2019, s. 598-606 -- SCOPUS  
[n1] 2019 zz ~ Racz, N. - Nagy, J. - Jiang, W. - Veress, T.: Modeling Retention Behavior on Analysis of Hallucinogenic Mushrooms Using Hydrophilic Interaction Liquid Chromatography. In: Journal of Chromatographic Science, Vol. 57, No. 3, 2019, s. 230-237 -- SCOPUS  
[n1] 2019 zz ~ Chen, L. - Gao, J. - Wu, Q. - Li, H. - Dong, S. - Shi, X. - Zhao, L.: Preparation and performance of a novel multi-mode COF-300aSiO<sub>2</sub> chromatographic stationary phase. In: European Polymer Journal, Vol. 116, July, 2019, s. 9-19-- SCOPUS  
[n1] 2019 zz ~ Fu, D. - Liu, Y. - Shen, A. - Xiao, Y. - Yu, L. - Liang, X.: Preparation of glutathione-functionalized zwitterionic silica material for efficient enrichment of sialylated N-glycopeptides. In: Analytical and Bioanalytical Chemistry, Vol. 411, No. 18, 2019, s. 4131-4140 -- SCOPUS

[n1] 2019 zz ~ Cai, T. - Zhang, H. - Chen, J. - Li, Z. - Qiu, H.: Polyethyleneimine-functionalized carbon dots and their precursor co-immobilized on silica for hydrophilic interaction chromatography. In: *Journal of Chromatography A*, Vol. 1597, July, 2019, s. 142-148 -- SCOPUS

[n1] 2019 zz ~ Garcia, P.G. - Zimmermann, B.H. - Carrazzone, C.: Hydrophilic interaction liquid chromatography coupled to mass spectrometry and multivariate analysis of the de novo pyrimidine pathway metabolites. In: *Biomolecules*, Vol. 9, No.8, 2019, Art. No. 328 -- SCOPUS

[n1] 2019 zz ~ Ma, Z.-H. - Wei, X.-Y. - Gao, H.-L. - Liu, G.-H. - Liu, Z.-Q. - Liu, F.-J. - Zong, Z.-M.: Selective and effective separation of five condensed arenes from a high-temperature coal tar by extraction combined with high pressure preparative chromatography. In: *Journal of Chromatography A*, Vol. 1603, October, 2019, s. 160-164 -- SCOPUS

[n1] 2019 zz ~ Subirats, X. - Abraham, M.H. - Roses, M.: Characterization of hydrophilic interaction liquid chromatography retention by a linear free energy relationship. Comparison to reversed- and normal-phase retentions. In: *Analytica Chimica Acta*, Vol. 1092, December, 2019, s. 132-143 -- SCOPUS

[n1] 2020 zz ~ Si, T. - Song, X. - Wang, L. - Guo, Y. - Liang, X. - Wang, S.: Preparation and evaluation of hydrophobically associating polyacrylamide coated silica composite as high performance liquid chromatographic stationary phase. In: *Microchemical Journal*, Vol. 152, January, 2020, Art. No. 104330 -- SCOPUS

[n1] 2020 zz ~ Kaliszan, R.: Recent advances in quantitative structure-retention relationships. In: *Handbook of Analytical Separations*, Vol. 8. Amsterdam : Elsevier, 2020, S. 587-632 -- SCOPUS

[n1] 2020 zz ~ Hu, Y. - Cai, T. - Zhang, H. - Chen, J. - Li, Z. - Zhao, L. - Li, Z. - Qiu, H.: Two copolymer-grafted silica stationary phases prepared by surface thiol-ene click reaction in deep eutectic solvents for hydrophilic interaction chromatography. In: *Journal of Chromatography A*, Vol. 1609, January, 2020, Art. No. 460446 -- SCOPUS

[n1] 2020 zz ~ Cao, Y. - Chai, C. - Chang, A. - Xu, X. - Song, Q. - Liu, W. - Li, J. - Song, Y. - Tu, P.: Optimal collision energy is an eligible molecular descriptor to boost structural annotation: An application for chlorogenic acid derivatives-focused chemical profiling. In: *Journal of Chromatography A*, Vol. 1609, January, 2020, Art. No. 460515 -- SCOPUS

[n1] 2020 zz ~ Si, T. - Ma, J. - Lu, X. - Wang, L. - Liang, X. - Wang, S.: Core-Shell Metal-Organic Frameworks as the Stationary Phase for Hydrophilic Interaction Liquid Chromatography. In: *ACS Applied Nano Materials*, Vol. 3, No. 1, 2020, s.351-356 -- SCOPUS

[n1] 2020 zz ~ Qing, G. - Yan, J. - He, X. - Li, X. - Liang, X.: Recent advances in hydrophilic interaction liquid interaction chromatography materials for glycopeptide enrichment and glycan separation. In: *TrAC - Trends in Analytical Chemistry*, Vol. 124, March, 2020, Art. No. 115570 -- SCOPUS

[n1] 2020 zz ~ Li, R. - Sun, W. - Xiao, X. - Chen, B. - Wei, Y.: Retention of stevioside polar compounds on a sulfonic acid-functionalized stationary phase. In: *Journal of Chromatography A*, Vol. 1620, June, 2020, Art. No. 460978 -- SCOPUS

[n1] 2020 zz ~ Si, T. - Wang, L. - Lu, X. - Liang, X. - Wang, S. - Guo, Y.: An alternative approach for the preparation of a core-shell bimetallic central metal-organic framework as a hydrophilic interaction liquid chromatography stationary phase. In: *Analyst*, Vol. 145, No. 11, 2020, s. 3851-3856 -- SCOPUS

[n1] 2020 zz ~ Murakami, H. - Omiya, M. - Miki, Y. - Umemura, T. - Esaka, Y. - Inoue, Y. - Teshima, N.: Evaluation of the adsorption properties of nucleobase-modified sorbents for a solid-phase extraction of water-soluble compounds. In: *Talanta*, Vol. 217, September, 2020, Art. No. 121052 -- SCOPUS

[n1] 2020 zz ~ Kulsing, C. - Nolvachai, Y. - Marriott, P.J.: Concepts, selectivity options and experimental design approaches in multidimensional and comprehensive two-dimensional gas chromatography. In: *TrAC - Trends in Analytical Chemistry*, Vol. 130, September, 2020, Art. No. 115995 -- SCOPUS

[n1] 2020 zz ~ Vasconez, J. - Pero-Gascon, R. - Gimenez, E. - Benavente, F.: Comparison of capillary electrophoresis and zwitterionic-hydrophilic interaction capillary liquid chromatography with ultraviolet and mass spectrometry detection for the analysis of microRNA biomarkers. In: *Talanta*, Vol. 219, November, 2020, Art. No. 121263 -- SCOPUS

[n1] 2020 zz ~ Andries, J.P.M. - Goodarzi, M. - Heyden, Y.V.: Improvement of quantitative structure-retention relationship models for chromatographic retention prediction of peptides applying individual local partial least squares models. In: *Talanta*, Vol. 219, November, 2020, Art. No. 121266 -- SCOPUS

[n1] 2020 zz ~ Zhang, X. - Wang, G. - Xue, H. - Zhang, J. - Wang, Q. - Zhang, Z. - Zhang, B.: Metabolite Profile of Xylem Sap in Cotton Seedlings Is Changed by K Deficiency. In: *Frontiers in Plant Science*, Vol. 11, December, 2020, Art. No.592591 -- SCOPUS

[n1] 2021 zz ~ He, M. - Zhou, Y.: How to identify "Material basis-Quality markers" more accurately in Chinese herbal medicines from modern chromatography-mass spectrometry data-sets: Opportunities and challenges of chemometric tools. In: Chinese Herbal Medicines, Vol. 13, No. 1, 2021, s. 2-16 -- SCOPUS

[n1] 2021 zz ~ den Uijl, M.J. - Schoenmakers, P.J. - Pirok, B.W.J. - van, Bommel M.R.: Recent applications of retention modelling in liquid chromatography. In: Journal of Separation Science, Vol. 44, No. 1, 2021, s. 88-114 -- SCOPUS

[n1] 2021 zz ~ Robards, K. - Ryan, D.: Principles and Practice of Modern Chromatographic Methods. In: Amsterdam : Elsevier, 2021, S. 1-518 -- SCOPUS

[n1] 2021 zz ~ Si, T. - Liang, X. - Lu, X. - Wang, L. - Wang, S. - Guo, Y.: 2D metal-organic framework nanosheets-assembled core-shell composite material as stationary phase for hydrophilic interaction liquid chromatography. In: Talanta, Vol.222, January, 2021, Art. No. 121603 -- SCOPUS

[n1] 2021 zz ~ Si, T. - Lu, X. - Zhang, H. - Liang, X. - Wang, S. - Guo, Y.: A new strategy for the preparation of core-shell MOF/Polymer composite material as the mixed-mode stationary phase for hydrophilic interaction/ reversed-phase chromatography. In: Analytica Chimica Acta, Vol. 1143, January, 2021, s. 181-188 -- SCOPUS

[n1] 2021 zz ~ Kensert, A. - Collaerts, G. - Efthymiadis, K. - Desmet, G. - Cabooter, D.: Deep Q-learning for the selection of optimal isocratic scouting runs in liquid chromatography. In: Journal of Chromatography A, Vol. 1638, February, 2021, Art. No. 461900 -- SCOPUS

[n1] 2021 zz ~ Wang, X. - Shan, Y. - Wei, X. - Li, W. - E, L. - Jiang, Y.: Determination of Nucleotides in Infant Formula by Ultra-high Performance Liquid Chromatography. In: Shipin Kexue/Food Science, Vol. 42, No. 4, 2021, s. 254-262 --SCOPUS

[n1] 2021 zz ~ Si, T. - Wang, S. - Zhang, H. - Wang, L. - Lu, X. - Liang, X. - Guo, Y.: Design and evaluation of novel MOF-polymer core-shell composite as mixed-mode stationary phase for high performance liquid chromatography. In: Microchimica Acta, Vol. 188, No. 3, 2021, Art. No. 76 -- SCOPUS

[n1] 2021 zz ~ Li, J.-H. - Wei, X.-Y. - Zhao, H.-F. - Yan, W.-W. - Teng, D.-G. - Ma, Z.-H. - Gao, H.-S. - Zong, Z.-M.: Effective Separation of Condensed Arenes from High-Temperature Coal Tar and Insight into Related Intermolecular Interactions - In: Energy and Fuels, Vol. 35, No. 5, 2021 ; s. 4267-4272 ;SCOPUS

[n1] 2021 zz ~ Liu, H. - Jin, P. - Jiang, M. - Duan, Y. - Zhu, G. - Yu, H. - Qiu, H.: Performance evaluation of silica microspheres functionalized by different amine-ligands for hydrophilic interaction chromatography. In: Journal of Chromatography A, Vol. 1640, March, 2021, Art. No. 461967 -- SCOPUS

[n1] 2021 zz ~ Lu, J. - Liang, K. - Chen, Y. - Zhao, C. - Wang, X. - An, R.: Identification and determination of chemical constituents from Yinchen Qingjin granules by ultra high-performance liquid chromatography coupled with linear ion trap-Orbitrap mass spectrometry. In: Journal of Separation Science, Vol. 44, No. 7, 2021, s. 1324-1344 -- SCOPUS

[n1] 2021 zz ~ Gritti, F.: Perspective on the Future Approaches to Predict Retention in Liquid Chromatography. In: Analytical Chemistry, Vol. 93, No. 14, 2021, s. 5653-5664 -- SCOPUS

[n1] 2021 zz ~ Dugheri, S. - Mucci, N. - Mini, E. - Squillaci, D. - Marrubini, G. - Bartolucci, G. - Bucletti, E. - Cappelli, G. - Trevisani, L. - Arcangeli, G.: Characterization and separation of platinum-based antineoplastic drugs by zwitterionic hydrophilic interaction liquid chromatography (Hilic)-tandem mass spectrometry, and its application in surface wipe sampling. In: Separations, Vol. 8, No. 5, 2021, Art. No. 69 -- SCOPUS

[n1] 2021 zz ~ Besenhard, M.O. - Tsatse, A. - Mazzei, L. - Sorensen, E.: Recent advances in modelling and control of liquid chromatography. In: Current Opinion in Chemical Engineering, Vol. 32, June, 2021, Art. No. 100685 -- SCOPUS

[n1] 2021 zz ~ Sagandykova, G. - Buszewski, B.: Perspectives and recent advances in quantitative structure-retention relationships for high performance liquid chromatography. How far are we?. In: TrAC - Trends in Analytical Chemistry, Vol.141, August, 2021, Art. No. 116294 -- SCOPUS

[n1] 2021 zz ~ Bo, W. - Chen, L. - Qin, D. - Geng, S. - Li, J. - Mei, H. - Li, B. - Liang, G.: Application of quantitative structure-activity relationship to food-derived peptides: Methods, situations, challenges and prospects. In: Trends in Food Science and Technology, Vol. 114, August, 2021, s. 176-188 -- SCOPUS

[n1] 2021 zz ~ Angeles, L.F. - Halwatura, L.M. - Antle, J.P. - Simpson, S. - Jaraula, C.M.B. - Aga, D.S.: In Silico Supported Nontarget Analysis of Contaminants of Emerging Concern: Increasing Confidence in Unknown Identification in Wastewater and Surface Waters. In: ACS ES and T Water, Vol. 1, No. 8, 2021, s. 1765-1775 -- SCOPUS

[n1] 2021 zz ~ Li, Z. - Li, S. - Zhang, F. - Geng, H. - Yang, B.: A hydrolytically stable amide polar stationary phase for hydrophilic interaction chromatography. In: Talanta, Vol. 231, August, 2021, Art. No. 122340 -- SCOPUS

[n1] 2021 zz ~ Si, T. - Lu, X. - Zhang, H. - Liang, X. - Wang, S. - Guo, Y.: Fabrication of two-dimensional metal-organic framework nanosheets/PDA composites as mixed-mode stationary phase for chromatographic separation. In: *Microchimica Acta*, Vol. 188, No. 10, 2021, Art. No. 360 -- SCOPUS

[n1] 2021 zz ~ Yang, Q. - Ji, H. - Fan, X. - Zhang, Z. - Lu, H.: Retention time prediction in hydrophilic interaction liquid chromatography with graph neural network and transfer learning. In: *Journal of Chromatography A*, Vol. 1656, October, 2021, Art. No. 462536 -- SCOPUS

[n1] 2021 zz ~ Chen, T. - Yang, X. - Wang, S. - Song, G. - Zhou, H. - Shen, W. - Gao, L.: A new ionic liquid bridged periodic mesoporous organosilicas stationary phase for per aqueous liquid chromatography and its application in the detection of biogenic amines. In: *Talanta*, Vol. 235, December, 2021, Art. No. 122795 -- SCOPUS

[n1] 2022 zz ~ Balli, O.I. - Uversky, V.N. - Durdagi, S. - Coskuner-Weber, O.: Challenges and limitations in the studies of glycoproteins: A computational chemist's perspective. In: *Proteins: Structure, Function and Bioinformatics*, Vol. 90, No. 2, 2022, s. 322-339 -- SCOPUS

[n1] 2022 zz ~ Si-Hung, L. - Izumi, Y. - Nakao, M. - Takahashi, M. - Bamba, T.: Investigation of supercritical fluid chromatography retention behaviors using quantitative structure-retention relationships. In: *Analytica Chimica Acta*, Vol. 1197, March, 2022, Art. No. 339463 -- SCOPUS

[n1] 2022 zz ~ Si, T. - Lu, X. - Zhang, H. - Wang, S. - Liang, X. - Guo, Y.: Metal-organic framework-based core-shell composites for chromatographic stationary phases. In: *TrAC - Trends in Analytical Chemistry*, Vol. 149, April, 2022, Art. No. 116545 -- SCOPUS

[n1] 2022 zz ~ Si, T. - Wang, L. - Zhang, H. - Lu, X. - Liang, X. - Wang, S. - Guo, Y.: Core-shell MOFs-based composites of defect-functionalized for mixed-mode chromatographic separation. In: *Journal of Chromatography A*, Vol. 1671, May, 2022, Art. No. 463011 -- SCOPUS

[n1] 2022 zz ~ Wu, Y. - Gao, S. - Cui, J. - Zhang, B. - Zhu, Z. - Song, Q. - Zeng, X. - Liang, Y. - Yu, Z.: QuEChERS-based extraction and two-dimensional liquid chromatography-high resolution mass spectrometry for the determination of long chain chlorinated paraffins in sediments. In: *Journal of Chromatography A*, Vol. 1684, November, 2022, Art. No. 463585 -- SCOPUS

[n1] 2022 zz ~ Xin, M. - You, S. - Wu, J. - Xu, Y. - Li, C. - Zhu, B. - Shen, J. - Chen, Z. - Dang, L. - Dan, W. - Zhang, X. - Sun, S.: Evaluation of absorbent cotton for glycopeptide enrichment. In: *Analytical and Bioanalytical Chemistry*, Vol. 414, No. 29-30, 2022, s. 8245-8253 -- SCOPUS

[n1] 2022 zz ~ Peng, S. - Chen, H. - Yin, J.: Research progress of chromatography-mass spectrometry in detection of genotoxic impurities. In: *Drug Evaluation Research*, Vol. 45, No. 12, 2022, s. 2583-2590 -- SCOPUS

[n1] 2022 zz ~ Gritti, F. - Trebel, N. - Holtzel, A. - Tallarek, U.: Prediction of surface excess adsorption and retention factors in reversed-phase liquid chromatography from molecular dynamics simulations. In: *Journal of Chromatography A*, Vol. 1685, December, 2022, Art. No. 463627 -- SCOPUS

[n1] 2022 zz ~ Liu, Z. - Xu, M. - Zhang, W. - Miao, X. - Wang, P.G. - Li, S. - Yang, S.: Recent development in hydrophilic interaction liquid chromatography stationary materials for glycopeptide analysis. In: *Analytical Methods*, Vol. 247, No. 116, 2022, s. 4437-4448 -- SCOPUS

V317 Wen, Yabin (aut) (9.17%) - Talebi, Mohammad (aut) (9.166%) - Amos, Ruth I. J. (aut) (9.166%) - Szücs, Roman (aut) [UKOPRCAL] (45%) - Dolan, John W. (aut) (9.166%) - Pohl, Christopher A. (aut) (9.166%) - Haddad, Paul R. (aut) [KAUT] (9.166%): Retention prediction in reversed phase high performance liquid chromatography using quantitative structure-retention relationships applied to the Hydrophobic Subtraction Model

Lit.: 38 zázn.

In: *Journal of Chromatography A*. - č. 1541 (2018), s. 1-11. - ISSN (print) 0021-9673

[International Symposium on Electro- and Liquid Phase-Separation Techniques. 24, Sopot, 10.09.2017 - 13.09.2017]

článok z podujatia konferenčný príspevok

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SCIE Science Citation Index Expanded

CPCI-S Conference Proceedings Citation Index - Science

*Indikátor časopisu:*

IF (JCR) 2018=3.858

*Kvartil Q:*

wos-jcr -- Q1 [Biochemical research methods] -- 2018

wos-jcr -- Q1 [Chemistry, analytical] -- 2018

*Ohlasy (27):*

[n1] 2018 zz ~ Sousa, P.F.M. - de Waard, A. - Aberg, K.M.: Elucidation of chromatographic peak shifts in complex samples using a chemometrical approach. In: Analytical and Bioanalytical Chemistry, Vol. 410, No. 21, 2018, s. 5229-5235 -- SCOPUS

[n1] 2018 zz ~ Poole, C.F.: Chromatographic test methods for characterizing alkylsiloxane-bonded silica columns for reversed-phase liquid chromatography. In: Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, Vol. 1092, August, 2018, s. 207-219 -- SCOPUS

[n1] 2018 zz ~ Ren, X. - Zhang, K. - Gao, D. - Fu, Q. - Zeng, J. - Zhou, D. - Wang, L. - Xia, Z.: Mixed-mode liquid chromatography with a stationary phase co-functionalized with ionic liquid embedded C18 and an aryl sulfonate group. In: Journal of Chromatography A, Vol. 1564, August, 2018, s. 137-144 -- SCOPUS

[n1] 2018 zz ~ Larbi, H. - Didaoui, L. - Righezza, M.: Characterization of stationary phases based on monosubstituted benzene retention indices using correspondence factor analysis and linear solvation energy relationships in RPLC. In: Journal of the Iranian Chemical Society, Vol. 15, No. 10, 2018, s. 2295-2305 -- SCOPUS

[n1] 2018 zz ~ Kubik, A. - Kaliszan, R. - Wiczling, P.: Analysis of Isocratic-Chromatographic-Retention Data using Bayesian Multilevel Modeling. In: Analytical Chemistry, Vol. 90, No. 22, 2018, s. 13670-13679 -- SCOPUS

[n1] 2019 zz ~ Huang, Y. - Xiao, H. - Liu, Y. - Gan, J. - Yan, Q.: Column selection approach for related substances determination of progesterone by high-performance liquid chromatography. In: Chemical Biology and Drug Design, Vol. 93, No. 1, 2019, s. 29-37 -- SCOPUS

[n1] 2019 zz ~ Poole, C.F.: Reversed-phase liquid chromatography system constant database over an extended mobile phase composition range for 25 siloxane-bonded silica-based columns. In: Journal of Chromatography A, Vol. 1600, August, 2019, s.112-126 -- SCOPUS

[n1] 2019 zz ~ Hu, C.-Q. - Zhang, X.: Current situation and the trend in impurity profiling of chemical drugs. In: Yaoxue Xuebao, Vol. 54, No. 12, 2019, s. 2214-2231 -- SCOPUS

[n1] 2019 zz ~ Bennett, R. - Haidar Ahmad, I.A. - Dasilva, J. - Figus, M. - Hullen, K. - Tsay, F.-R. - Makarov, A.A. - Mann, B.F. - Regalado, E.L.: Mapping the Separation Landscape of Pharmaceuticals: Rapid and Efficient Scale-Up of Preparative Purifications Enabled by Computer-Assisted Chromatographic Method Development. In: Organic Process Research and Development, Vol. 23, No. 12, 2019, s. 2678-2684 -- SCOPUS

[n1] 2020 zz ~ Kaliszan, R.: Recent advances in quantitative structure-retention relationships. In: Handbook of Analytical Separations, Vol. 8. Amsterdam : Elsevier, 2020, S. 587-632 -- SCOPUS

[n1] 2020 zz ~ Skoczylas, M. - Bocian, S. - Buszewski, B.: Quantitative structure - retention relationships of amino acids on the amino acid- and peptide-silica stationary phases for liquid chromatography. In: Journal of Chromatography A, Vol.1609, January, 2020, Art. No. 460514 -- SCOPUS

[n1] 2020 zz ~ Luo, Q. - Ren, X. - Wei, S. - Zheng, Y. - Gao, D. - Fu, Q. - Xia, Z. - Wang, L.: Preparation and evaluation of a molybdenum disulfide quantum dots embedded C18 mixed-mode chromatographic stationary phase. In: Analytical and Bioanalytical Chemistry, Vol. 412, No. 6, 2020, s. 1365-1374 -- SCOPUS

[n1] 2020 zz ~ Stoll, D.R.: Selectivity in reversed-phase liquid chromatography: 20 years of the hydrophobic subtraction model. In: LC-GC North America, Vol. 38, No. 4, 2020, s. 205-210 -- SCOPUS

[n1] 2020 zz ~ Poole, C.F.: Evaluation of the solvation parameter model as a quantitative structure-retention relationship model for gas and liquid chromatography. In: Journal of Chromatography A, Vol. 1626, August, 2020, Art. No. 461308 --SCOPUS

[n1] 2020 zz ~ Passarin, P.B.S. - Lourenco, F.R.: Modeling an in silico platform to predict chromatographic profiles of UV filters using ChromSimulator. In: Microchemical Journal, Vol. 157, September, 2020, Art. No. 105002 -- SCOPUS

[n1] 2020 zz ~ Kulsing, C. - Nolvachai, Y. - Marriott, P.J.: Concepts, selectivity options and experimental design approaches in multidimensional and comprehensive two-dimensional gas chromatography. In: TrAC - Trends in Analytical Chemistry, Vol. 130, September, 2020, Art. No. 115995 -- SCOPUS

- [n1] 2020 zz ~ Haidar Ahmad, I.A. - Shchurik, V. - Nowak, T. - Mann, B.F. - Regalado, E.L.: Introducing Multifactorial Peak Crossover in Analytical and Preparative Chromatography via Computer-Assisted Modeling. In: Analytical Chemistry, Vol.92, No. 19, 2020, s. 13443-13451 -- SCOPUS
- [n1] 2020 zz ~ Zhou, J. - Ren, X. - Luo, Q. - Gao, D. - Fu, Q. - Zhou, D. - Zu, F. - Xia, Z. - Wang, L.: Ionic liquid functionalized beta-cyclodextrin and C18 mixed-mode stationary phase with achiral and chiral separation functions. In: Journal of Chromatography A, Vol. 1634, December, 2020, Art. No. 461674 -- SCOPUS
- [n1] 2021 zz ~ Paritala, J. - Peraman, R. - Kondreddy, V.K. - Subrahmanyam, C.V.S. - Ravichandiran, V.: Quantitative structure retention relationship (QSRR) approach for assessment of chromatographic behavior of antiviral drugs in the development of liquid chromatographic method. In: Journal of Liquid Chromatography and Related Technologies, Vol. 44, No. 13-14, 2021, s. 637-648 -- SCOPUS
- [n1] 2021 zz ~ Stoll, D.R. - Dahlseid, T.A. - Rutan, S.C. - Taylor, T. - Serret, J.M.: Improvements in the predictive accuracy of the hydrophobic subtraction model of reversed-phase selectivity. In: Journal of Chromatography A, Vol. 1636, January, 2021, Art. No. 461682 -- SCOPUS
- [n1] 2021 zz ~ Kensert, A. - Collaerts, G. - Efthymiadis, K. - Desmet, G. - Cabooter, D.: Deep Q-learning for the selection of optimal isocratic scouting runs in liquid chromatography. In: Journal of Chromatography A, Vol. 1638, February, 2021, Art. No. 461900 -- SCOPUS
- [n1] 2021 zz ~ Kyei Barffour, I. - Acheampong, D.O.: Prospect of reprogramming replication licensing for cancer drug development. In: Biomedicine and Pharmacotherapy, Vol. 136, April, 2021, Art. No. 111190 -- SCOPUS
- [n1] 2021 zz ~ Bride, E. - Heinisch, S. - Bonnefille, B. - Guillemain, C. - Margoum, C.: Suspect screening of environmental contaminants by UHPLC-HRMS and transposable Quantitative Structure-Retention Relationship modelling. In: Journal of Hazardous Materials, Vol. 409, May, 2021, Art. No. 124652 -- SCOPUS
- [n1] 2021 zz ~ Wiczling, P. - Kamedulska, A. - Kubik, L.: Application of Bayesian Multilevel Modeling in the Quantitative Structure-Retention Relationship Studies of Heterogeneous Compounds. In: Analytical Chemistry, Vol. 93, No. 18, 2021, s.6961-6971 -- SCOPUS
- [n1] 2021 zz ~ Sagandykova, G. - Buszewski, B.: Perspectives and recent advances in quantitative structure-retention relationships for high performance liquid chromatography. How far are we?. In: TrAC - Trends in Analytical Chemistry, Vol.141, August, 2021, Art. No. 116294 -- SCOPUS
- [n1] 2022 zz ~ Tian, Z. - Liu, F. - Li, D. - Fernie, A.R. - Chen, W.: Strategies for structure elucidation of small molecules based on LC-MS/MS data from complex biological samples. In: Computational and Structural Biotechnology Journal, Vol.20, January, 2022, s. 5085-5097 -- SCOPUS
- [n1] 2022 zz ~ Kumar, P. - Kumar, A. - Lal, S. - Singh, D. - Lotfi, S. - Ahmadi, S.: CORAL: Quantitative Structure Retention Relationship (QSRR) of flavors and fragrances compounds studied on the stationary phase methyl silicone OV-101 column in gas chromatography using correlation intensity index and consensus modelling. In: Journal of Molecular Structure, Vol. 1265, October, 2022, Art. No. 133437 -- SCOPUS

V318 Wen, Yabin (aut) (10%) - Amos, Ruth I. J. (aut) (10%) - Talebi, Mohammad (aut) (10%) - Szücs, Roman (aut) [UKOPRCAL] (40%) - Dolan, John W. (aut) (10%) - Pohl, Christopher A. (aut) (10%) - Haddad, Paul R. (aut) [KAUT] (10%): Retention Index Prediction Using Quantitative Structure Retention Relationships for Improving Structure Identification in Nontargeted Metabolomics [elektronický dokument]  
Lit.: 40 zázn.

In: Analytical Chemistry [elektronický dokument]. - Roč. 90, č. 15 (2018), s. 9434-9440 [print]. - ISSN (print) 0003-2700

článok

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*Indikátor časopisu:*

IF (JCR) 2018=6.350

*Kvartil Q:*

wos-jcr -- Q1 [Chemistry, analytical] -- 2018



*Ohlasy (16):*

- [n1] 2019 zz ~ Gika, H. - Virgiliou, C. - Theodoridis, G. - Plumb, R.S. - Wilson, I.D.: Untargeted LC/MS-based metabolic phenotyping (metabonomics/metabolomics): The state of the art. In: *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, Vol. 1117, June, 2019, s. 136-147 -- SCOPUS
- [n1] 2019 zz ~ Domingo-Almenara, X. - Guijas, C. - Billings, E. - Montenegro-Burke, J.R. - Uritboonthai, W. - Aisporna, A.E. - Chen, E. - Benton, H.P. - Siuzdak, G.: The METLIN small molecule dataset for machine learning-based retention time prediction. In: *Nature Communications*, Vol. 10, No. 1, 2019, Art. No. 5811 -- SCOPUS
- [n1] 2019 zz ~ Bennett, R. - Haidar Ahmad, I.A. - Dasilva, J. - Figus, M. - Hullen, K. - Tsay, F.-R. - Makarov, A.A. - Mann, B.F. - Regalado, E.L.: Mapping the Separation Landscape of Pharmaceuticals: Rapid and Efficient Scale-Up of Preparative Purifications Enabled by Computer-Assisted Chromatographic Method Development. In: *Organic Process Research and Development*, Vol. 23, No. 12, 2019, s. 2678-2684 -- SCOPUS
- [n1] 2020 zz ~ Buszewski, B. - Zuvela, P. - Sagandykova, G. - Walczak-skierska, J. - Pomastowski, P. - David, J. - Wong, M.W.: Mechanistic chromatographic column characterization for the analysis of flavonoids using quantitative structure-retention relationships based on density functional theory. In: *International Journal of Molecular Sciences*, Vol. 21, No. 6, 2020, Art. No. 2053 -- SCOPUS
- [n1] 2020 zz ~ Bonini, P. - Kind, T. - Tsugawa, H. - Barupal, D.K. - Fiehn, O.: Retip: Retention Time Prediction for Compound Annotation in Untargeted Metabolomics. In: *Analytical Chemistry*, Vol. 92, No. 11, 2020, s. 7515-7522 -- SCOPUS
- [n1] 2020 zz ~ Guo, Z. - Zhu, Z. - Huang, S. - Wang, J.: Non-targeted screening of pesticides for food analysis using liquid chromatography high-resolution mass spectrometry-a review. In: *Food Additives and Contaminants - Part A Chemistry, Analysis, Control, Exposure and Risk Assessment*, Vol. 37, No. 7, 2020, s. 1180-1201 -- SCOPUS
- [n1] 2020 zz ~ Haidar Ahmad, I.A. - Shchurik, V. - Nowak, T. - Mann, B.F. - Regalado, E.L.: Introducing Multifactorial Peak Crossover in Analytical and Preparative Chromatography via Computer-Assisted Modeling. In: *Analytical Chemistry*, Vol.92, No. 19, 2020, s. 13443-13451 -- SCOPUS
- [n1] 2020 zz ~ Guo, Z. - Huang, S. - Wang, J. - Feng, Y.-L.: Recent advances in non-targeted screening analysis using liquid chromatography - high resolution mass spectrometry to explore new biomarkers for human exposure. In: *Talanta*, Vol.219, November, 2020, Art. No. 121339 -- SCOPUS
- [n1] 2020 zz ~ Osipenko, S. - Bashkirova, I. - Sosnin, S. - Kovaleva, O. - Fedorov, M. - Nikolaev, E. - Kostyukevich, Y.: Machine learning to predict retention time of small molecules in nano-HPLC. In: *Analytical and Bioanalytical Chemistry*, Vol. 412, No. 28, 2020, s. 7767-7776 -- SCOPUS
- [n1] 2020 zz ~ Meshref, S. - Li, Y. - Feng, Y.-L.: Prediction of liquid chromatographic retention time using quantitative structure-retention relationships to assist non-targeted identification of unknown metabolites of phthalates in human urine with high-resolution mass spectrometry. In: *Journal of Chromatography A*, Vol. 1634, December, 2020, Art. No. 461691 -- SCOPUS
- [n1] 2021 zz ~ Kensert, A. - Collaerts, G. - Efthymiadis, K. - Desmet, G. - Cabooter, D.: Deep Q-learning for the selection of optimal isocratic scouting runs in liquid chromatography. In: *Journal of Chromatography A*, Vol. 1638, February, 2021, Art. No. 461900 -- SCOPUS
- [n1] 2021 zz ~ Fisher, C.M. - Croley, T.R. - Knolhoff, A.M.: Data processing strategies for non-targeted analysis of foods using liquid chromatography/high-resolution mass spectrometry. In: *TrAC - Trends in Analytical Chemistry*, Vol. 136, March, 2021, Art. No. 116188 -- SCOPUS
- [n1] 2021 zz ~ Gritti, F.: Perspective on the Future Approaches to Predict Retention in Liquid Chromatography. In: *Analytical Chemistry*, Vol. 93, No. 14, 2021, s. 5653-5664 -- SCOPUS
- [n1] 2022 zz ~ Tian, Z. - Liu, F. - Li, D. - Fernie, A.R. - Chen, W.: Strategies for structure elucidation of small molecules based on LC-MS/MS data from complex biological samples. In: *Computational and Structural Biotechnology Journal*, Vol.20, January, 2022, s. 5085-5097 -- SCOPUS
- [n1] 2022 zz ~ Biancolillo, A. - D'Archivio, A.A.: Transfer of gas chromatographic retention data among poly(siloxane) columns by quantitative structure-retention relationships based on molecular descriptors of both solutes and stationary phases. In: *Journal of Chromatography A*, Vol. 1663, January, 2022, Art. No. 462758 -- SCOPUS
- [n1] 2022 zz ~ de Cripán, S.M. - Cereto-Massague, A. - Herrero, P. - Barcaru, A. - Canela, N. - Domingo-Almenara, X.: Machine Learning-Based Retention Time Prediction of Trimethylsilyl Derivatives of Metabolites. In: *Biomedicine*, Vol. 10, No.4, 2022, Art. No. 879 -- SCOPUS

- V319 Wen, Yabin (aut) (10%) - Amos, Ruth I. J. (aut) (10%) - Talebi, Mohammad (aut) (10%) - Szücs, Roman (aut) [UKOPRCAL] (40%) - Dolan, John W. (aut) (10%) - Pohl, Christopher A. (aut) (10%) - Haddad, Paul R. (aut) [KAUT] (10%): Retention prediction using quantitative structure-retention relationships combined with the hydrophobic subtraction model in reversed-phase liquid chromatography  
Lit.: 22 zázn.  
In: Electrophoresis. - Roč. 40, č. 18-19 (2019), s. 2415-2419. - ISSN (print) 0173-0835  
článok  
*Registrované v:*  
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*Indikátor časopisu:*  
IF (JCR) 2019=3.081  
*Kvartil Q:*  
wos-jcr -- Q2 [Biochemical research methods] -- 2019  
wos-jcr -- Q2 [Chemistry, analytical] -- 2019  
*Ohlasy (3):*  
[n1] 2020 zz ~ Biancolillo, A. - Maggi, M.A. - Bassi, S. - Marini, F. - D'Archivio, A.A.: . In: Molecules, Vol. 25, No. 6, 2020, Art. No. 1262 --SCOPUS  
[n1] 2020 zz ~ Poole, C.F.: Evaluation of the solvation parameter model as a quantitative structure-retention relationship model for gas and liquid chromatography. In: Journal of Chromatography A, Vol. 1626, August, 2020, Art. No. 461308 --SCOPUS  
[n1] 2022 zz ~ Fedorova, E.S. - Matyushin, D.D. - Plyushchenko, I.V. - Stavrianidi, A.N. - Buryak, A.K.: Deep learning for retention time prediction in reversed-phase liquid chromatography. In: Journal of Chromatography A, Vol. 1664, February, 2022, Art. No. 462792 -- SCOPUS
- V320 Baert, Mathijs (aut) (16.67%) - Wicht, Kristina (aut) (16.666%) - Hou, Zhanyao (aut) (16.666%) - Szücs, Roman (aut) [UKOPRCAL] (16.666%) - Du Prez, Filip (aut) (16.666%) - Lynen, Frederic (aut) [KAUT] (16.666%): Exploration of the Selectivity and Retention Behavior of Alternative Polyacrylamides in Temperature Responsive Liquid Chromatography  
Lit.: 46 zázn.  
In: Analytical Chemistry. - Roč. 92, č. 14 (2020), s. 9815-9822. - ISSN (print) 0003-2700  
článok  
*Registrované v:*  
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*Indikátor časopisu:*  
IF (JCR) 2020=6.986  
*Kvartil Q:*  
wos-jcr -- Q1 [Chemistry, analytical] -- 2020  
*Ohlasy (4):*  
[n1] 2022 zz ~ Guo, D. - Zhou, X. - Muhammad, N. - Huang, S. - Zhu, Y.: An overview of poly (amide-amine) dendrimers functionalized chromatographic separation materials. In: Journal of Chromatography A, Vol. 1669, April, 2022, Art. No. 462960-- SCOPUS  
[n1] 2022 zz ~ Liu, H. - Prachyathipsakul, T. - Koyasseril-Yehiya, T.M. - Le, S.P. - Thayumanavan, S.: Molecular bases for temperature sensitivity in supramolecular assemblies and their applications as thermoresponsive soft materials. In: Materials Horizons, Vol. 9, No. 1, 2022, s. 164-193 -- SCOPUS  
[n1] 2021 zz ~ Fan, F. - Lu, X. - Wang, L. - Liang, X. - Guo, Y.: Hydrogel Coating with Temperature Response Retention Behavior and Its Application in Selective Separation of Liquid Chromatography. In: Analytical Chemistry, Vol. 93, No. 48,2021, s. 16017-16024 -- SCOPUS  
[n1] 2021 zz ~ Kasza, G. - Stumphauer, T. - Bisztran, M. - Szarka, G. - Hegedus, I. - Nagy, E. - Ivan, B.: Thermoresponsive poly(N,n-diethylacrylamide-co-glycidyl methacrylate) copolymers and its catalytically

active alpha-chymotrypsin bioconjugate with enhanced enzyme stability. In: Polymers, Vol. 13, No. 6, 2021, Art. No. 987 -- SCOPUS

- V321 Haddad, Paul R. (aut) [KAUT] (24.5% [1,2 AH]) - Taraji, Maryam (aut) (10.5% [0,5 AH]) - Szűcs, Roman (aut) [UKOPRCAL] (65% [3,2 AH]): Prediction of Analyte Retention Time in Liquid Chromatography  
Lit.: 200 záz. n.  
In: Analytical Chemistry. - Roč. 93, č. 1 (2021), s. 228-256. - ISSN (print) 0003-2700  
článok  
*Registrované v:*  
CCC Current Content Connect  
SCO SCOPUS  
WOS CC Web of Science Core Collection  
SCIE Science Citation Index Expanded  
*Indikátor časopisu:*  
IF (JCR) 2021=8.008  
*Kvartil Q:*  
wos-jcr -- Q1 [Chemistry, analytical] -- 2021  
*Ohlasy (35):*  
[n1] 2021 zz ~ Workman, J.: The 2021 winners of the lifetime achievement and emerging leader in chromatography awards. In: LC-GC North America, Vol. 39, No. 2, 2021, s. 84-95 -- SCOPUS  
[n1] 2021 zz ~ Vaskevicius, M. - Kapociute-Dzikiene, J. - Slepikas, L.: Prediction of chromatography conditions for purification in organic synthesis using deep learning. In: Molecules, Vol. 26, No. 9, 2021, Art. No. 2474 -- SCOPUS  
[n1] 2021 zz ~ Robards, K. - Ryan, D.: Principles and Practice of Modern Chromatographic Methods. In: . Amsterdam : Elsevier, 2021, S. 1-518 -- SCOPUS  
[n1] 2021 zz ~ Workman, J.: A lifetime of contributions for advancing research in separation science: paul haddad, the winner of the 2021 lifetime achievement in chromatography award. In: LC-GC North America, Vol. 39, No. 3, 2021, s. 146-148-- SCOPUS  
[n1] 2021 zz ~ Gritti, F.: Perspective on the Future Approaches to Predict Retention in Liquid Chromatography. In: Analytical Chemistry, Vol. 93, No. 14, 2021, s. 5653-5664 -- SCOPUS  
[n1] 2021 zz ~ Wiczling, P. - Kamedulska, A. - Kubik, L.: Application of Bayesian Multilevel Modeling in the Quantitative Structure-Retention Relationship Studies of Heterogeneous Compounds. In: Analytical Chemistry, Vol. 93, No. 18, 2021, s.6961-6971 -- SCOPUS  
[n1] 2021 zz ~ Lin, Z. - Tai, H.-C. - Zhu, G. - Fabiano, A. - Borges-Munoz, A. - Ye, Y.K. - He, B.L.: Evaluation of a polysaccharide-based chiral reversed-phase liquid chromatography screen strategy in pharmaceutical analysis. In: Journal of Chromatography A, Vol. 1645, May, 2021, Art. No. 462085 -- SCOPUS  
[n1] 2021 zz ~ Besenhard, M.O. - Tsaatse, A. - Mazzei, L. - Sorensen, E.: Recent advances in modelling and control of liquid chromatography. In: Current Opinion in Chemical Engineering, Vol. 32, June, 2021, Art. No. 100685 -- SCOPUS  
[n1] 2021 zz ~ Angeles, L.F. - Halwatura, L.M. - Antle, J.P. - Simpson, S. - Jaraula, C.M.B. - Aga, D.S.: In Silico Supported Nontarget Analysis of Contaminants of Emerging Concern: Increasing Confidence in Unknown Identification in Wastewater and Surface Waters. In: ACS ES and T Water, Vol. 1, No. 8, 2021, s. 1765-1775 -- SCOPUS  
[n1] 2021 zz ~ Aalizadeh, R. - Alygizakis, N.A. - Schymanski, E.L. - Krauss, M. - Schulze, T. - Ibanez, M. - McEachran, A.D. - Chao, A. - Williams, A.J. - Gago-Ferrero, P. - Covaci, A. - Moschet, C. - Young, T.M. - Hollender, J. - Slobodnik, J. - Thomaidis, N.S.: Development and Application of Liquid Chromatographic Retention Time Indices in HRMS-Based Suspect and Nontarget Screening. In: Analytical Chemistry, Vol. 93, No. 33, 2021, s. 11601-11611 -- SCOPUS  
[n1] 2021 zz ~ Huang, R. - Zhu, W. - Xu, Z. - Chen, J. - Jiang, B. - Chen, H. - Chen, W.: Accurate Retention Time Prediction Based on Monolinked Peptide Information to Confidently Identify Cross-Linked Peptides. In: Journal of the American Society for Mass Spectrometry, Vol. 32, No. 9, 2021, s. 2410-2416 -- SCOPUS  
[n1] 2021 zz ~ Yang, Q. - Ji, H. - Fan, X. - Zhang, Z. - Lu, H.: Retention time prediction in hydrophilic interaction liquid chromatography with graph neural network and transfer learning. In: Journal of Chromatography A, Vol. 1656, October, 2021, Art. No. 462536 -- SCOPUS

[n1] 2021 zz ~ Ju, R. - Liu, X. - Zheng, F. - Lu, X. - Xu, G. - Lin, X.: Deep Neural Network Pretrained by Weighted Autoencoders and Transfer Learning for Retention Time Prediction of Small Molecules. In: Analytical Chemistry, Vol. 93, No. 47, 2021, s. 15651-15658 -- SCOPUS

[n1] 2021 zz ~ Kensert, A. - Bouwmeester, R. - Efthymiadis, K. - Van Broeck, P. - Desmet, G. - Cabooter, D.: Graph Convolutional Networks for Improved Prediction and Interpretability of Chromatographic Retention Data. In: Analytical Chemistry, Vol. 93, No. 47, 2021, s. 15633-15641 -- SCOPUS

[n1] 2021 zz ~ Kawai, T. - Matsumori, N. - Otsuka, K.: Recent advances in microscale separation techniques for lipidome analysis. In: Analyst, Vol. 146, No. 24, 2021, s. 7398-7410 -- SCOPUS

[n1] 2022 zz ~ Moldoveanu, S. - David, V.: Essentials in Modern HPLC Separations. In: . Amsterdam : Elsevier, 2022, S. 1-705 -- SCOPUS

[n1] 2022 zz ~ Tian, Z. - Liu, F. - Li, D. - Fernie, A.R. - Chen, W.: Strategies for structure elucidation of small molecules based on LC-MS/MS data from complex biological samples. In: Computational and Structural Biotechnology Journal, Vol.20, January, 2022, s. 5085-5097 -- SCOPUS

[n1] 2022 zz ~ Biancolillo, A. - D'Archivio, A.A.: Transfer of gas chromatographic retention data among poly(siloxane) columns by quantitative structure-retention relationships based on molecular descriptors of both solutes and stationary phases. In: Journal of Chromatography A, Vol. 1663, January, 2022, Art. No. 462758 -- SCOPUS

[n1] 2022 zz ~ Hu, Q. - Sun, Y. - Yuan, P. - Lei, H. - Zhong, H. - Wang, Y. - Tang, H.: Quantitative structure-retention relationship for reliable metabolite identification and quantification in metabolomics using ion-pair reversed-phase chromatography coupled with tandem mass spectrometry. In: Talanta, Vol. 238, February, 2022, Art. No. 123059 -- SCOPUS

[n1] 2022 zz ~ Fedorova, E.S. - Matyushin, D.D. - Plyushchenko, I.V. - Stavrianidi, A.N. - Buryak, A.K.: Deep learning for retention time prediction in reversed-phase liquid chromatography. In: Journal of Chromatography A, Vol. 1664, February, 2022, Art. No. 462792 -- SCOPUS

[n1] 2022 zz ~ Liapikos, T. - Zisi, C. - Kodra, D. - Kademoglou, K. - Diamantidou, D. - Begou, O. - Pappalouisi, A. - Theodoridis, G.: Quantitative structure retention relationship (QSRR) modelling for Analytes' retention prediction in LC-HRMS by applying different Machine Learning algorithms and evaluating their performance. In: Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, Vol. 1191, February, 2022, Art. No. 123132 -- SCOPUS

[n1] 2022 zz ~ Si-Hung, L. - Izumi, Y. - Nakao, M. - Takahashi, M. - Bamba, T.: Investigation of supercritical fluid chromatography retention behaviors using quantitative structure-retention relationships. In: Analytica Chimica Acta, Vol.1197, March, 2022, Art. No. 339463 -- SCOPUS

[n1] 2022 zz ~ Wang, C. - Tang, R. - Pan, L. - Wu, W. - Ma, S. - Wei, Y. - Ou, J.: Preparation of core-shell microporous organic polymer-coated silica microspheres for chromatographic separation and N-glycopeptides enrichment. In: Journal of Separation Science, Vol. 45, No. 8, 2022, s. 1458-1468 -- SCOPUS

[n1] 2022 zz ~ Caldeweyher, E. - Bauer, C. - Tehrani, A.S.: An open-source framework for fast-yet-accurate calculation of quantum mechanical features. In: Physical Chemistry Chemical Physics, Vol. 24, No. 17, 2022, s. 10599-10610 -- SCOPUS

[n1] 2022 zz ~ Kamedulska, A. - Kubik, L. - Wiczling, P.: Statistical analysis of isocratic chromatographic data using Bayesian modeling. In: Analytical and Bioanalytical Chemistry, Vol. 414, No. 11, 2022, s. 3471-3481 -- SCOPUS

[n1] 2022 zz ~ Zhong, P. - Wei, X. - Li, X. - Wei, X. - Wu, S. - Huang, W. - Koidis, A. - Xu, Z. - Lei, H.: Untargeted metabolomics by liquid chromatography-mass spectrometry for food authentication: A review. In: Comprehensive Reviews in Food Science and Food Safety, Vol. 21, No. 3, 2022, s. 2455-2488 -- SCOPUS

[n1] 2022 zz ~ Svrkota, B. - Krmar, J. - Protic, A. - Zecevic, M. - Otasevic, B.: Optimization of chromatographic separation of aripiprazole and impurities: Quantitative structure-retention relationship approach. In: Journal of the Serbian Chemical Society, Vol. 87, No. 5, 2022, s. 615-628 -- SCOPUS

[n1] 2022 zz ~ Wu, Y. - Zhang, N. - Luo, K. - Liu, Y. - Bai, Z. - Tang, S.: Recent advances of innovative and high-efficiency stationary phases for chromatographic separations. In: TrAC - Trends in Analytical Chemistry, Vol. 153, August, 2022, Art. No. 116647 -- SCOPUS

[n1] 2022 zz ~ Zhao, J.-H. - Hu, L.-X. - He, L.-X. - Wang, Y.-Q. - Liu, J. - Zhao, J.-L. - Liu, Y.-S. - Ying, G.-G.: Rapid target and non-target screening method for determination of emerging organic chemicals in fish. In: Journal of Chromatography A, Vol. 1676, August, 2022, Art. No. 463185 -- SCOPUS

[n1] 2022 zz ~ Kamedulska, A. - Kubik, L. - Jacyna, J. - Struck-Lewicka, W. - Markuszewski, M.J. - Wiczling, P.: Toward the General Mechanistic Model of Liquid Chromatographic Retention. In: Analytical Chemistry, Vol. 94, No. 31, 2022, s.11070-11080 -- SCOPUS

[n1] 2022 zz ~ Gong, X. - Liu, W. - Cao, Y. - Wang, R. - Liang, N. - Cao, L. - Li, J. - Tu, P. - Song, Y.: Integrated strategy for widely targeted metabolome characterization of Peucedani Radix. In: Journal of Chromatography A, Vol. 1678, August, 2022, Art. No. 463360 -- SCOPUS

[n1] 2022 zz ~ Osipenko, S. - Nikolaev, E. - Kostyukevich, Y.: Retention Time Prediction with Message-Passing Neural Networks. In: Separations, Vol. 9, No. 10, 2022, Art. No. 291 -- SCOPUS

[n1] 2022 zz ~ Ribar, D. - Rijavec, T. - Kralj, Cigic I.: An exploration into the use of Hansen solubility parameters for modelling reversed-phase chromatographic separations. In: Journal of Analytical Science and Technology, Vol. 13, No. 1, 2022, Art. No. 12 -- SCOPUS

[n1] 2022 zz ~ Van Laethem, T. - Kumari, P. - Boulanger, B. - Hubert, P. - Fillet, M. - Sacre, P.-Y. - Hubert, C.: User-Driven Strategy for In Silico Screening of Reversed-Phase Liquid Chromatography Conditions for Known Pharmaceutical-Related Small Molecules. In: Molecules, Vol. 27, No. 23, 2022, Art. No. 8306 -- SCOPUS

[n1] 2022 zz ~ Gritti, F. - Trebel, N. - Holtzel, A. - Tallarek, U.: Prediction of surface excess adsorption and retention factors in reversed-phase liquid chromatography from molecular dynamics simulations. In: Journal of Chromatography A, Vol. 1685, December, 2022, Art. No. 463627 -- SCOPUS

V322 Žabenský, Branislav (aut) [UKOPRCAL] (25%) - Bodor, Róbert (aut) [UKOPRCAL] (30%) - Makata, Dávid (aut) (5%) - Szücs, Roman (aut) [UKOPRCAL] (25%) - Masár, Marián (aut) [KAUT] [UKOPRCAL] (15%): Trace determination of perchlorate in drinking water by capillary zone electrophoresis with isotachopheresis sample cleanup and conductivity detection  
Lit.: 57 zázn.  
In: Journal of Separation Science. - Roč. 45, č. 17 (2022), s. 3339-3347. - ISSN (print) 1615-9306  
článok  
*Registrované v:*  
SCO SCOPUS  
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IF (JCR) 2022=3.1  
*Kvartil Q:*  
wos-jcr -- Q2 [Chemistry, analytical] -- 2022

V323 Szücs, Roman (aut) [UKOPRCAL] (50%) - Brown, Roland (aut) (5%) - Brunelli, Claudio (aut) (5%) - Hradski, Jasna (aut) [UKOPRCAL] (30%) - Masár, Marián (aut) [KAUT] [UKOPRCAL] (10%): Impact of structural similarity on the accuracy of retention time prediction  
Lit.: 31 zázn.  
In: Journal of Chromatography A. - Roč. 1707 (2023), s. [1-8], art. no. 464317. - ISSN (print) 0021-9673  
článok  
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IF (JCR) 2022=4.1  
*Kvartil Q:*  
wos-jcr -- Q2 [Biochemical research methods] -- 2022

#### Štatistika kategórií (Záznamov spolu: 50):

ADC Vedecké práce v zahraničných karentovaných časopisoch (6)  
AFD Publikované príspevky na domácich vedeckých konferenciách (1)  
AFE Abstrakty pozvaných príspevkov zo zahraničných konferencií (1)  
AFG Abstrakty príspevkov zo zahraničných vedeckých konferencií (2)  
BFA Abstrakty odborných prác zo zahraničných podujatí (konferencie, ...) (1)  
V2 Vedecký výstup publikačnej činnosti ako časť editovanej knihy alebo zborníka (1)  
V3 Vedecký výstup publikačnej činnosti z časopisu (27)

O2 Odborný výstup publikačnej činnosti ako časť knižnej publikácie alebo zborníka (11)

**Štatistika ohlasov (463):**

[o1] Citácie v zahraničných publikáciách registrované v citačných indexoch (3)

[n1] Citácia v publikácii registrovaná v citačných indexoch (460)

Spracovala: Butková

8. 1. 2024