АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ

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ПРЕДЛАГА

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- Компютърна химия
- Медицинска химия
- Химия с маркетинг
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Магистърски програми:

- Медицинска химия
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- Компютърна химия
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Курсове за квалификация:

- Високоефективна течна хроматография

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- Неопределеност при химични изпитвания и изготвяне бюджет на неопределеността на резултати от химични анализи
- Вътрешно-лабораторно валидиране на процедурата на изпитване при химични анализи
- Пламъков атомно-абсорбционен спектрален анализ (FAAS), аналитични характеристики и приложения
- Електротермичен атомно-абсорбционен спектрален анализ (ETAAS), аналитични характеристики и приложения
- Оптико емисионен анализ с индуктивно свързана плазма (ICP-OES), аналитични характеристики и приложения
- Приложение на масспектрометричния анализ с индуктивно свързана плазма (ICP-MS)

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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ПРОГРАМА

08^{30} – 09^{00}	**Регистрация**
09^{00} – 09^{15}	**Откриване на семинара** *Проф. д-р Румен Младенов, Ректор на ПУ „Паисий Хилендарски“* *Андон Минков, Управител на АСМ2 ЕООД* *доц. д-р Веселин Кметов, Декан на ХФ при ПУ „Паисий Хилендарски“*
09^{15} – 10^{00}	**Пробоподготовка за постигане на поставените цели при следови анализ на метали във води и храни** *Mr. Valerio Rindone, Milestone Srl*
10^{00} – 10^{45}	**Анализ на остатъчни компоненти в замърсители с помощта на течна хроматография с масспектрометрия (LC/MS)** *Mr. Simonas Rudys, Thermo Fisher Scientific*
10^{45} – 11^{15}	**Кафе пауза**
11^{15} – 12^{00}	**Приложения при анализ на води с помощта на йонна хроматография – многовалентни йони и замърсители.** *Mr. Roman Repas, Thermo Fisher Scientific*
12^{00} – 12^{30}	**Предизвикателства при анализа на полярни пестициди** *Mr. Simonas Rudys, Thermo Fisher Scientific*
12^{30} – 13^{45}	**Обяд**
13^{45} – 14^{30}	**Анализ на приоритетни вещества - късоверижни полихлорирани алкани (SCCPs) и полибромирани диетилови етери (PBDEs) във водни екосистеми, чрез GC/MS/MS/NCI** *Г-жа Весела Генина, ИАОС, РЛ-Пловдив*
14^{30} – 15^{15}	**ICP-MS "fit for purpose" съгласуваност с регулативните изисквания** *Доц. д-р Веселин Кметов, ПУ „Паисий Хилендарски”*
15^{15} – 15^{30}	**Дискусия**
15^{30} – 17^{30}	**Постерна сесия**
16^{00} –	**Коктейл**

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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Организационен комитет:

Председател:

Доц. д-р Веселин Кметов – Декан на Химически факултет ПУ

Членове:

Д-р Христо Йорданов – ACM2
Доц. д-р Кирил Симитчиев – Химически факултет ПУ
Гл. ас. д-р Деяна Георгиева – Химически факултет ПУ
Гл. ас. д-р Евелина Върбанова – Химически факултет ПУ
Гл. ас. д-р Галя Тончева – Химически факултет ПУ

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Проф. д-р Илиан Иванов – Катедра ОХ
Проф. дхн Пламен Пенчев – Катедра АХКХ
Доц. д-р Петя Маринова – Катедра ОНХ с МОХ
Доц. д-р Виолета Стефанова – Зам. декан на ХФ
Доц. д-р Георги Патронов – Катедра ХТ

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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ЛЕКЦИИ

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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ACHIEVING THE TARGET IN TRACE METAL ANALYSIS FOR FOOD AND WATER SAMPLES UNDERSTANDING THE PROCESS OF MICROWAVE ASSISTED DIGESTION FOR METAL & TRACE METAL ANALYSIS IN FOOD AND WATER SAMPLES: THE FIRST STEP TO MAXIMIZE THE PERFORMANCES OF YOUR ELEMENTAL ANALYSER

Valerio Rindone,

Milestone Srl, Via Fatebenefratelli, 1-5, 24010, Sorisole, Italy,
v.rindone@milestonesrl.com

No matters your sample type, your throughput or your analysis instrument: sample preparation for metal determination is a fundamental step to ensure greater analysis quality, higher throughput and lower running costs. Today, digestion is a pivotal step in metals and trace metals analysis, which provides real benefits and a superior workflow for your laboratory. In order to achieve optimum results and the lowest possible detection limit, chemists must consider several factors. The presentation will provide a comprehensive description of all the parameters involved in a digestion step for food and water samples.

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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RESIDUE ANALYSIS BY LC/MS TECHNIQUES

Simonas Rudys

Technical Sales Manager
Emerging Markets EMEA
Chromatography and Mass Spectrometry
Thermo Fisher Scientific
simonas.rudys@thermofisher.com
Thermo Fisher Scientific, Czech Republic,
michal.godula@thermofisher.com

Food safety standards change and evolve, so what was once at the lower end of permissible residues analysis results today, may be at the upper end tomorrow. Innovative technologies help laboratories stay ahead of the curve. With the rapid developments in instrumental methods of chemical analysis, especially mass spectrometry techniques coupled to gas chromatography and liquid chromatography, laboratories have the capability to analyze several hundred compounds in a single sample. Effective sample preparation is a critical yet challenging step in residues analysis workflows. As the demand grows for more sensitive measurements of a larger number of compounds per analysis, historic large-scale extraction methods that can create a bottleneck in laboratory efficiency are being replaced by QuEChERS or automated sample preparation solutions such as the accelerated solvent extraction. Triple quadrupole mass spectrometry is considered the gold standard for screening and quantitation however, high-resolution accurate mass (HRAM) LC-MS/MS is growing in popularity, in part because it allows for retrospective analysis on additional analytes of interest and screening for unknown or unexpected compounds is possible. Comprehensive solutions which includes sample preparation, LC-MS system and software, column and method parameters to provide a start-to-finish workflow are always welcome in any laboratory.

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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ION CHROMATOGRAPHY NEW APPROACHES TO WATER ANALYSIS – NEW APPLICATIONS METAL SPECIATION, NEW CONTAMINANTS

Roman Repas, Thermo Fisher Scientific,

Im Steingrund 4-6, 63303 Dreieich, Germany
roman.repas@thermofisher.com

Municipal water authorities must treat water to provide their communities with safe drinking water. The most common chemical disinfectants are chlorine, chlorine dioxide, chloramine, and ozone. However, the disinfectants themselves can react with naturally occurring materials in the water to form unintended disinfection byproducts (DBPs), which may pose health risks. Chlorination of drinking water can produce haloacetic acids and chlorate. Similarly, chlorine dioxide treatment generates inorganic oxyhalides, DBPs, chlorite, and chlorates. Chlorate may also be generated in the presence of chloramine. Ozone reacts with natural sources of bromide, which may be found at various levels in water supplies, to produce bromate. To date, there are no practical methods for removing bromide or its bromate byproduct from water. Currently, the only solution to the problem is to limit bromate formation during the water treatment process. Limiting bromate formation requires careful monitoring of bromate concentration to ensure that it does not exceed safe drinking water standards.

In the presentation new ion chromatography water analysis methods will be discussed. Reagent Free Ion Chromatography (RFIC), high-efficiency anion exchange separation column with 4 micrometer particles size and suppressed conductivity detection is used for the analysis of oxyhalides and standard inorganic anions.

The combination of ion chromatography and mass spectrometry offers sensitive and rapid detection without the need for sample pretreatment for the analysis of haloacetic acids and bromate in drinking water by IC-MS/MS.

In water samples many trace elements are typically found in more than one chemical form, each of which with different chemical properties and behavior, such as toxicity. Through the combination of the ion chromatography system with the ICP-MS, sensitive, robust methods for the speciation analysis of trace levels of metals in natural waters have been developed. Examples of the speciation analysis of chromium and arsenic will be presented..

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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CHALLENGING APPLICATIONS - POLAR PESTICIDES STORY.

Simonas Rudys

Technical Sales Manager
Emerging Markets EMEA
Chromatography and Mass Spectrometry
Thermo Fisher Scientific
simonas.rudys@thermofisher.com

Using a combination of LC-MS and GC-MS it is common for laboratories to analyze hundreds of pesticides and metabolites. Still, difficult challenges remain, not least the analysis of the polar ionic pesticides. Historically, pesticides such as glyphosate, glufosinate, fosetyl, and alike were analyzed individually using specialist methods involving derivatization or ion pairing to overcome unwanted interactions during extraction and chromatographic separation. Consequently these frequently-used pesticides were infrequently tested because of the additional costs involved. To help bridge the gap Quick Polar Pesticides (QuPPe) method has been developed. The method is used by laboratories in Europe and has resulted in recent findings of residues of chlorate, perchlorate, phosphonic acid and glyphosate in food and beverages. There are more than 20 such pesticides and metabolites identified in the scope of the QuPPE method. Despite the controversy and uncertainties surrounding much of the information available, one obvious need is for more sensitive and robust methods to enable more cost-effective monitoring to provide more data underpin a more valid assessment of the frequency and levels of residues in the food supply. Developments in technology have enabled the use of suppressed ion chromatography coupled to mass spectrometer (IC-MS/MS) for more effective solution to polar pesticide residue analysis.

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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ANALYSIS OF PRIORITY SUBSTANCES - SHORT-CHAIN CHLORINATED PARAFFINS ($SCCP_s$) AND POLYBROMINATED DIPHENYL ETHERS ($PBDE_S$) IN AQUATIC ECOSYSTEMS THROUGH GC / MS / MS / NCI

Vesela. M. Genina[1]

Executive Environmental Agency, branch Plovdiv, 1 Perushtitsa Str., Plovdiv 4000, Bulgaria

E-mail: vgenina@abv.bg

Methods for the quantification of the sum of short chain chlorinated paraffins (SCCPs) by GC–ECNI-MS have been developed. These methods are appropriate to the special demands of environmental water and sediment analysis. The method is based on the integration of the signals for two selected m/z values (375 and 423) over the full retention range of the SCCPs. The calibration is performed using three synthetic mixtures representing the variety of SCCP-mixtures as found in environmental samples as well as in technical mixtures. Quantification is performed using a multiple linear regression calibration with two selected m/z value signals achieving an LOQ of 0.1 µg/l for water samples and LOQ of 300 µg/kg for sediment samples. The proposed quantification procedure for water and sediments samples was verified by independently prepared and differently composed SCCP-mixtures simulating a variety of sediment samples. For the analysis of the water and sediment samples a clean-up was applied comprising a column chromatographic clean-up. SCCPs are found world-wide in the environment, wildlife and humans. They are bioaccumulative in wildlife and humans, are persistent and transported globally in the environment, and toxic to aquatic organisms at low concentrations.

Methods for the quantification of Polybrominated diphenyl ethers (PBDEs) in water, sediments and biota by GC–MS-MS have been developed. Extraction of brominated diphenyl ethers with organic solvent was performed and the extract was cleaned. After concentration, the brominated diphenyl ethers were separated by capillary gas chromatography and mass spectrometry detection in the selected ion-monitoring mode using electron impact (EI). A calibration with an internal standard is used to determine the concentration in the sample. Quantification is performed using linear calibration achieving an LOQ of 0.014 µg/l for water samples, LOQ of 100 µg/kg for sediment samples and LOQ of 0,003 µg/kg for biota samples. PBDEs are a class of bioaccumulative halogenated compounds that have emerged as a major environmental pollutant. PBDEs are used as a flame-retardant and are found in consumer

goods such as electrical equipment, construction materials, coatings, textiles and polyurethane foam (furniture padding). Similar in structure to polychlorinated biphenyls (PCBs), PBDEs resist degradation in the environment. Less brominated PBDEs like tetra-, penta- and hexa- demonstrate high affinity for lipids and can accumulate in the bodies of animals and humans.

The methods allows for a standardized analysis according to the Water Framework Directive 2000/60/EC and Directive 2013/39/EU as regards priority substances in the field of water policy, especially in the case of trend monitoring of sediments.

Key words: water, sediment, biota, SCCPs, PBDEs

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ICP-MS "FIT FOR PURPOSE" COMPLIANCE WITH REGULATORY REQUIREMENTS

V. Kmetov, V. Stefanova, D. Georgieva, L. Kaynarova,
E. Varbanova, K. Simitchiev

University of Plovdiv "Paisii Hilendarski",
Department of Analytical Chemistry and Computer Chemistry

E-mail: kmetov@uni-plovdiv.bg

The lecture will show how important it is to select an appropriate approach to validate analytical tests by ICP-MS analysis of trace elements in food, water, and natural objects. Current regulations resulting from the new version of BDS EN ISO/IEC 17025 will be discussed. A model will be presented for the assessment of the dominant factors in constructing the uncertainty budget of the measurement results and their role in achieving compliance with the target uncertainty of a particular analytical task. Examples of "fit for purpose" ICP-MS testing will be demonstrated in light of the requirements of the Commission Regulation (EC) 1881 and the Water Framework Directive for water analysis.

A relatively new ability of ICP-MS for characterization of nanomaterials using single particle approach will be presented with a model for theoretical calculation of optimal dilution factor for aspiration of suspensions with different size nanoparticles.

Acknowledgements:
The authors would like to thank to the NSF Project DN19/9 2017-2020 (INISA)

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
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ПОСТЕРИ

ADSORPTION STUDIES ON THE POSSIBILITIES OF *HYPERICUM PERFORATUM L.* FOR THE REMOVAL OF Cu^{2+} IONS FROM AQUEOUS SOLUTIONS

Lidia Ivanova, Paunka Vassileva*, Albena Detcheva

Bulgarian Academy of Sciences, Institute of General and Inorganic Chemistry, Acad. Georgi Bonchev Str., Bl. 11, 1113, Sofia, Bulgaria. E-mail: pnovachka@svr.igic.bas.bg

The effective removal of toxic ions from wastewaters is a significant problem nowadays. On the other hand, the biosorption is a new technology that uses the metal binding capacities of various biological materials. Although copper is an essential element for humans, it can be very toxic at high concentrations and have to be removed from contaminated waters.

In the present investigation the feasibility of using plant material based on *Hypericum perforatum L.* for the removal of Cu^{2+} ions from aqueous solutions was studied. Batch experiments were performed to evaluate the effect of contact time, of solution acidity, of sample amount, of temperature and initial ion concentration on Cu^{2+} adsorption. It was established that the adsorption equilibrium is attained within the first two minutes which suggests an excellent affinity of the investigated material towards Cu^{2+} ions in aqueous media. Optimum pH value was found to be about 4. Temperature and sample amount do not influence significantly the biosorption. FTIR and SEM analysis were also performed. It was proved that amide, ester and hydroxyl functional groups are responsible for the retention of Cu^{2+} ions and the complex formation between the investigated material and the metal ions is very fast. SEM analysis after metal loading revealed that the copper ions are distributed homogenously on the sorbent surface. Linear Langmuir, Freundlich and Dubinin-Radushkevich models were used to analyse equilibrium experimental data and it was established that Dubinin-Radushkevich isotherm most adequately described the adsorption process. The maximum adsorption capacity was calculated (20.67 mg g^{-1}) and this demonstrates the good potential of the investigated material as a sorbent. Hence we conclude that *Hypericum perforatum L.* could be used as effective biosorbent for the removal of copper ions from aqueous solutions.

Acknowledgements: This work is supported by the Bulgarian Ministry of Education and Science under the National Research Programme "Healthy Foods for a Strong Bio-Economy and Quality of Life" approved by DCM # 577 / 17.08.2018.

ANALYTICAL CHARACTERIZATION OF *HYPERICUM PERFORATUM L.* WITH RESPECT TO ITS POTENTIAL AS BIOSORBENT USING MODERN INSTRUMENTAL TECHNIQUES

Lidia Ivanova, Albena Detcheva*, Paunka Vassileva

Bulgarian Academy of Sciences, Institute of General and Inorganic Chemistry, Acad. Georgi Bonchev Str., Bl. 11, 1113, Sofia, Bulgaria

E-mail: albena@svr.igic.bas.bg

In the present study a material based on the medicinal plant *Hypericum perforatum L.* was investigated with respect to its adsorption properties towards metal ions. Instrumental methods such as XRD, TGA, FTIR, SEM and BET-analysis were used for its characterization. Particle size distribution, slurry pH and texture parameters of the investigated material were also determined. Granulometric analysis after sample pretreatment showed monomodal distribution with a maximum at about 100 μm and the slurry pH was found to be 4.6. XRD-patterns revealed the presence of one broad peak characteristic for amorphous phase (lignin, hemicelluloses and amorphous cellulose) and peaks indicating crystalline forms of cellulose 1a. Two main stages were clearly shown on the pyrolysis TGA curves - the first region was attributed to the extraction of adsorbed water from the sample and the second corresponds to the thermal decomposition of hemicelluloses, cellulose and part of the lignin. The final part of the graph above 400^{O}C can be assigned to the decomposition of the remaining lignin. The presence of numerous functional groups on the surface of the investigated material was registered by FTIR spectroscopy in the range of 4000–400 cm^{-1}. Among the active groups, carboxylic acid, carbonyl, amino and hydroxyl groups could play the major role in the adsorption process due to complex formation between the biosorbent and the metal ions. The data obtained from low-temperature nitrogen adsorption/desorption curves (BET-analysis) showed that the plant material is mesoporous with relatively small specific surface area. SEM analysis proved its porous heterogeneous structure, which is favourable for the adsorption of metal ions on different parts of the surface. Thus we suggest that the investigated material has good potential as biosorbent for purification of contaminated waters.

Acknowledgements: This work is supported by the Bulgarian Ministry of Education and Science under the National Research Programme "Healthy Foods for a Strong Bio-Economy and Quality of Life" approved by DCM # 577 / 17.08.2018.

CHEMICAL COMPOSITION OF LUPIN SEEDS (*LUPINUS ANGUSTIFOLIUS* L. CULTIVAR 'BOREGINE')

Zh. Petkova, P. Yanev, G. Antova, M. Angelova-Romova, I.Todorova

University of Plovdiv 'Paisii Hilendarski', Department of Chemical Technology, 24 Tzar Asen Street, 4000, Plovdiv, Bulgaria.
E-mail: zhanapetkova@uni-plovdiv.net

Chemical composition of lupin seeds (*Lupinus angustifolius* L. cultivar 'Boregine') has been examined. The seeds were with German origin but were introduced in Bulgaria. The plants were grown under identical meteorological and agro-ecological conditions and the seeds were collected in June 2017. The lupin seeds are rich in carbohydrates (57.1%) and proteins (23.9%), but possess low oil content (7.4%). The content of starch and dietary fibers is 24.1 and 10.1%, respectively. The individual composition of water soluble carbohydrates were determined by high performance liquid chromatography on a Agilent® LC 1220 instrument equipped with Zorbax Carbohydrate column and Zorbax Reliance Cartridge guard-column and refractive index detector. It was established that the only disaccharides in the seeds are sucrose (2341.4 mg/100g) and cellobiose (883.1 mg/100g), while the main monosaccharides are fructose (244.9 mg/100g) and glucose (221.6 mg/100g). The moisture of the seeds is found to be 7.7% and the ash is 3.9%. The content of the main nutrients in lupin seeds is relatively high which determines their satisfying energy value – 391 kcal/100g (1658 kJ/100g).

Acknowledgements: This work was supported by the Bulgaria National Science Fund (BNSF), Ministry of Education and Science, projects of junior basic researchers and postdocs – 2018 [grant number КР-06-М29/2, 01.12.2018].

APPLICATION OF 4-(2-PYRIDYLAZO) RESORCINOL FOR FLOTATION-SPECTROPHOTOMETRIC DETERMINATION OF IRON

Siyna Chobanova[1], Mariela Kalendarska[1], Ivelina Koicheva[1], Kiril Gavazov[2], Galya Toncheva[1]

[1] Faculty of Chemistry, Department of General and Inorganic Chemistry with Methodology of Chemical Education, University of Plovdiv "Paissii Hilendarski", 24 Tsar Assen St., Plovdiv 4000, Bulgaria, E-mail: galq_toncheva@mail.bg

[2]Faculty of Pharmacy, Department of Chemical Sciences, Medical University of Plovdiv, 120 Buxton Brothers St., Plovdiv 4004, Bulgaria

Liquid-liquid extraction systems for Fe(II) containing 4-(2-pyridylazo) resorcinol (PAR) were studied. Optimum conditions for flotation-spectrophotometric determination of iron based a 1:2 Fe^{II}-PAR complex were found to be as follows: flotation solvent (chloroform), shaking time (2 min), pH (4.5±0.5), concentration of PAR 2.0×10^{-4} mol L^{-1}), reducing agent (hydroxylamine hydrochloride), solvent for the floated compound dimethylsul-phoxide, DMSO), wavelength for spectrophotometric measurements (718 nm), and volumes of the organic solvents (5 mL of chloroform and 3 mL of DMSO). Calibration graphs were compared for different volumes of the aqueous phase – 10 mL and 40 mL; the corresponding linear ranges were 0.30–1.3 μg mL^{-1} and 0.25–1.0 μg mL^{-1}. Various ions which are often found together with iron in natural and industrial samples were used to test the selectivity of the proposed procedure.

KEY WORDS: Iron(II), Fe-PAR complex, Flotation, Spectrophotometry

ACKNOWLEDGEMENTS: This work was supported by the Plovdiv University Scientific Fund (Grant No SP19-009)

REMOVAL OF HEXAVALENT CHROMIUM USING MANGANESE FERRITE NANOPARTICLES

Nikolay Marinkov, Christina Tzvetkova, Paunka Vassileva*,

Galia Gentscheva, Daniela Kovacheva

Bulgarian Academy of Sciences, Institute of General and Inorganic Chemistry, Acad. Georgi Bonchev Str., Bl. 11, 1113, Sofia, Bulgaria.

E-mail: pnovachka@svr.igic.bas.bg

Cr (VI) is considered to be a group “A” human carcinogen because of its mutagenic and carcinogenic properties. To protect human health, the adsorption is a simple and effective method for the Cr (VI) removal from aqueous solutions. Nano-sized ferrite particles gained an attraction as a new emerging class of inorganic compounds because of their applications in applied chemistry, biochemistry and targeted drug delivery. The paramount features about ferrite nanoparticles are that these compounds are non-toxic, biofriendly and exhibit strong antibacterial potential and magnetic capability.

The present study aimed to remove Cr (VI) from aqueous solutions by manganese ferrite nanoparticles. The use of $MnFe_2O_4$ offers an additional advantage due to the fact that after the chromium adsorption process a magnetic separation can be employed. The investigated material was obtained by solution combustion method. The starting reagents: $Mn(NO_3)_2.4H_2O$ and $Fe(NO_3)_3.9H_2O$ and citric acid were dissolved in deionized water and the resulting solution was heated on a magnetic stirrer. After the dehydration of the solution, it reaches its flash point and ignites releasing a large amount of heat. The final product was treated at 400°C for 2 hours in air. The analyses show that material is single phase $MnFe_2O_4$ with crystallite size of about 10 nm and specific surface area of $66 m^2 g^{-1}$. The effects of various experimental parameters, such as chromium concentration, contact time and acidity of initial solutions, were evaluated. The Cr (VI) adsorption was significantly affected by the pH value and the optimum pH range was found to be about 2.0. Pseudo-first order, pseudo-second order and intraparticle diffusion models were used to analyze kinetic data. Equilibrium experimental data were fitted to linear Langmuir and Freundlich models. The Freundlich isotherm was found to be the most adequate in describing the adsorption processes. The maximum adsorption capacity was calculated. The results indicated that nanosized $MnFe_2O_4$ is suitable adsorbent for removal Cr (VI) from contaminated aqueous solutions.

RAPID PROCEDURE FOR RHENIUM DETERMINATION IN CEMENTATION COPPER CONCENTRATE

Christina Tzvetkova[1], Tsvetan Vassilev[2]

Bulgarian Academy of Sciences, [1]Institute of General and Inorganic Chemistry,[2] Institute of Physical Chemistry "Rostislaw Kaischew", Acad. Georgi Bonchev Str., Bl. 11, 1113, Sofia, Bulgaria.
E-mail: hrisi@svr.igic.bas.bg

Asarel porphyry copper deposit is the main source for copper production in Bulgaria. The mined ores contain also a number of valuable minor components such as Au, Ag, Mo, Re, etc. During the enrichment processes they are concentrate in two final products - flotation and cementation copper concentrate. Determination of the Re content in these products is of importance due to the rising demand of raw material for Re production. Since Re is most likely in the form of ReS_2, a standard alkaline fusion of the concentrates with Na_2O_2 and Na_2CO_3 in nickel crucibles at T= 520^oC in a muffle furnace for 1 h followed by extraction of Re with water was applied. Determination of Re in aqueous extracts were performed according to the high selective catalytic spectrophotometric method with N'N-Dimethyldithiooxamide (DMDTO). The results show that flotation copper concentrate contains 1 g Re/t, while in the cementation concentrate the Re content reaches up to 135 g Re/t- the value with industrial importance.

In this study, the authors offer a rapid and energy-saving pretreatment procedure for determination of Re in cementation concentrate. The procedure involves two steps:1) thermal treatment of this product at T= 180^oC for 1 h; 2) 100% extraction of Re by water. It is known that cementation concentrate is obtained as a result of bacterial bioleaching of low grade sulfide ores ($CuFeS_2$) in sulfuric acid medium (pH=1.5-2.5) followed by cementation with iron turnings. At this process the sulfur is oxidized to soluble sulfate and Cu^{2+} pass into solution. It is possible that ReS_2 is also oxidized to water soluble perrhenate ions (ReO_4^-). The experiments for direct leaching of Re from cementation copper concentrate by water were carried out. The results showed that after soaking of concentrate in cold and hot water, 22 % and 44% respectively of Re was leached. The same experiment with hot water resulted in 44% extraction of Re. Pre- heat treatment of the concentrate at T=180^oC for 1 h leads to full oxidation of the rest ReS_2. In this case, all the Re pass into the aqueous solution.

ВРЪЗКА МЕЖДУ СПЕКТРАЛНОТО И СТРУКТУРНО ПОДОБИЕ: ТЪРСЕНЕ ПО ПИКОВЕ В ИЧ СПЕКТРИ

С. Цонева[1], С. Начкова[1], П. Пенчев[1]

[1]Химически факултет, ПУ „П. Хилендарски“, ул. „Цар Асен“ №24, 4000 Пловдив, България. E-mail: plamen@uni-plovdiv.net

Изследването на връзката между спектралното и структурното подобие е важно не само от теоретичен аспект, но има практическо значение при т.н. търсене по подобие в спектрални библиотеки. Досега изследвания са публикувани за мас-спектри, ИЧ спектри от К. Вармуца [1] и Раман спектри от нашата група [2]. При спектралното търсене на ИЧ спектри са използвани четири мерки за спектрално подобие, които работят с цяла спектрална крива [1]. В настоящето изследване са приложени две спектрални мерки, изчислявани с пиковете на ИЧ спектри. Пиковете в спектъра се отчитат с тяхното местоположения във вълново число и тяхната интензивност в абсорция. Методиката на изследване наподобява тази на Вармуца и съавтори [1], но двете спектрални са коефициент на Sørensen–Dice и скаларно произведение на пикове.

Резултатите показват, че с повишаване на толерансите по вълново число и абсорция до определена тяхна стойност структурното подобие на неизвестната структура с първи хит или с първите десет хита се повишава. След това структурното подобие намалява. Причина за това е, че чувствителността на разпознаване на структурите се повишава, но намалява селективността при библиотечното търсене. За двете мерки на спектрално сравнение оптималните стойности на толерансите са съответно ΔA = 0.2 a.u. и $\Delta\nu$ = 25 cm^{-1} и ΔA = 0.7 a.u. и $\Delta\nu$ = 25 cm^{-1}, като втората мярка дава по-добри резултати на структурното подобие на първия хит в хит-списъка - 0.702 срещу 0.676. По-голямата стойност на толеранса на ΔA за втората спектрална мярка се обяснява с нейната по-високата селективност, защото при скаларното произведение се отчита относителната интензивност на пиковете в спектрите.

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ОПРЕДЕЛЯНЕ НА ЖИВАК ЧРЕЗ MSIS-MP-AES: ОПТИМИЗАЦИЯ НА МЕТОДА НА СТУДЕНИТЕ ПАРИ ЧРЕЗ ЕКСПЕРИМЕНТАЛЕН ДИЗАЙН

В. Маркова[1,2], К. Симитчиев[1]

[1]ПУ „Паисий Хилендарски“, Катедра аналитична химия и компютърна химия, 4000, Пловдив, България,
E-mail: vzapryanova@uni-plovdiv.net

[2]Енергийна агенция Пловдив, Лаборатория за изпитване на твърди биогорива и компост, 4000, Пловдив, България

Методът на студените пари се използва рутинно в комбинация с атомно-спектрометричните техники за определяне на следи от живак. Този подход за разделяне и концентриране позволява съществено понижаване на границата на инструменталното откриване спрямо конвенционалната пулверизация на течни проби.

В настоящата работа бе проучено определянето на живак по метода на студените пари в комбинация с атомно-емисионната спектрометрия с микровълнова плазма (MP-AES). Процесът на редукция на живак бе проведен в поточен режим чрез използването на търговски достъпна реакционна камера - Multimode Sample Introduction System (MSIS®) [1]. Приложен бе централно-композиционен план за моделиране на експеримента, при който бяха оптимизирани i) концентрацията на редуциращия агент ($SnCl_2$), ii) киселинността на средата (HCl), при която се провежда реакцията и iii) обемната скорост на потока на проба, внасян в MSIS камерата. Установено бе, че концентрацията на редуциращия агент и киселинността на средата имат съществено влияние, като не бе наблюдавано взаимодействие между отделните фактори.

[1] Agilent Technologies, Flexible sample introduction with the Multimode Sample Introduction System, Technical overview 5991-6453EN, 2016

Благодарности: Фирма Т.Е.А.М. ООД за предоставения демонстрационен спектрометър на Agilent 4200 MP-AES в Химически Факултет на Пловдивски Университет „Паисий Хилендарски“; ФНИ Проект ДН19/9 2017-2020 (INISA)

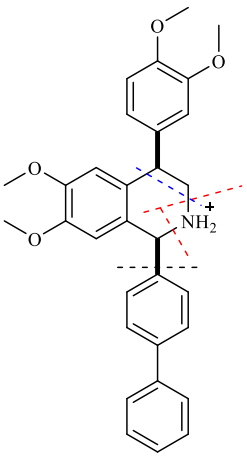
MS ANALYSIS OF SYNTHETIC DERIVATIVES OF NATURAL COMPOUNDS USING HIGH RESOLUTION MASS SPECTROMETRY (HRMS)

S. Manolov[1], D. Bojilov[1], I. Ivanov[1, 2]

[1]University of Plovdiv, Department of Organic chemistry, 4000, Plovdiv, Bulgaria. E-mail: ivanov@uni-plovdiv.bg

[2]University of Plovdiv, branch-Smolyan, 32 "Dicho Petrov"Str., Smolyan, 4700, Bulgaria

The *Amaryllidaceae* alkaloids represent a large (over 300 alkaloids have been isolated) and still expanding group of biogenetically related isoquinoline alkaloids that are found exclusively in plants belonging to this family. *Cherylline* is a naturally occurring optically active, 4-aryl-1,2,3,4- tetrahydroisoquinoline alkaloid, isolated from *Crinum Powelli*, *Amaryllidaceae* plant. We have successfully obtained *Cherylline* derivatives applying simple reduction of 1,4-disubstituted 3,4-dihydroisoquinoline derivatives using sodium borohydride. We have found that the reduction of 1,4-disubstituted 3,4-dihydroisoquinoline leads to formation of two compounds. Using HRMS analysis was found that both compounds have equal mass and element composition so they are diastereoisomers. The diastereoisomers were successfully separated by preparative column chromatography and 2:1 (cis:trans) ratio is determined.



Scheme 1. HRMS fragmentation of synthetic *Cherylline* derivatives

In this study we report MS spectral pattern of diastereoisomers, obtained under ESI conditions using QExactive Quadrupole-Orbitrap Mass Spectrometer.

СЪСТАВ НА ЕТЕРИЧНОТО МАСЛО ОТ БЕЗСМЪРТНИЧЕ (*HELICHRYSUM ITALICUM*)

Д. Божилов[1], С. Даньо[1], С. Манолов[1], И. Динчева[3], Ил. Иванов[1, 2]

[1] *Пловдивски Университет „Паисий Хилендарски", Катедра Органична химия,ул. Цар Асен, 24, 4000 Пловдив, България, E-mail: dagnon@uni-plovdiv.bg*

[2] *Пловдивски Университет „Паисий Хилендарски", Филиал-Смолян, ул. „Дичо Петров", Смолян 4700, България*

[3]*АгроБиоИнститут, Селскостопанска академия, бул. „Драган Цанков" 1164 София, България*

Helichrysum italicum е медицинско растение и се среща в района на Средиземно море – о. Корсика и Кордоба (Южна Испания). В България е наричано безсмъртниче. През последните години *H. italicum* се използва все повече за медицински цели и в козметиката. Поради тази причина вече се култивира в България и се използва за получаване на етерично масло. Етеричното масло, получено от *H. italicum*, събирано от района на с. Турия, Южна България, беше получено чрез хидродестилация и анализирано с GC-FID и GC-MS. За целта на изследването растителният материал е събиран по време на бутонизация и пълен цъфтеж. Надземната част (листата и цветовете) от безсмъртниче бяха използвани за анализ на химичния състав, при което добивът на етеричното масло при бутонизация и пълен цъфтеж е съответно 0,5 % и 0,4 %. В състава му бяха идентифицирани 40 съединения, които представляват 89,25 – 95,63 % от общия състав. Етеричното масло е богато на сескитерпени, което представлява 37,15 – 50,26 % от общия състав на маслото. Най-ниско е съдържанието на кислород-съдържащите сескитерпени (3,06 – 11,01 %). Основните компоненти на етеричното масло изолирано от *H. italicum* са *α*-куркумен, *γ*-куркумен (12,46 – 25,76 %), нерилацетат (12,02 – 20,6 %), *α*-пинен (5,59 – 19,52 %), *α*-копаен (5,42 – 6,23 %), D-лимонен (4,45 %), *α*-бергамотен, *β*-кариофилен (3,07 – 4,86 %), *β*-еудесмен (3,07 – 5,57 %), *δ*-аморфен (3,47 %), неролидол (4,54 – 4,86 %).

СРАВНЕНИЕ/ОЦЕНКА НА РАЗПРЕДЕЛЕНИЕТО ПО РАЗМЕРИ НА СРЕБЪРНИ НАНОЧАСТИЦИ ЧРЕЗ ДВА КАЛИБРАЦИОННИ ПОДХОДА

Л. Кайнарова, Д. Георгиева, В. Стаева, Г. Тенева, В. Стефанова

Пловдивски университет „П. Хилендарски“, Катедра аналитична химия и компютърна химия, Пловдив, ул. Цар Асен 24
E-mail: stefanova@uni-plovdiv.net

В настоящото изследване е направено сравнение на две калибрационни стратегии при охарактеризиране размерите на AgNPs чрез SP-ICP-MS метода: по референтни материали със сертифициран размер на частиците и по йонни стандарти, с отчитане на транспортната ефективност. Калибрацията по йонни стандарти дава възможност да се оцени приносът на неопределеността на регистрираните сигнали върху определяне на размерите на наночастиците. Установено е, че кубичната зависимост на диаметъра от масата на частицата се отразява в несиметричност на интервалната оценка, която нараства в посока на по-малките размери. С намаляване на диаметъра на частицата се разширява и неопределеността, а несиметричността на интервалната оценка е по-ясно изразена. Разделителната способност на SP-ICP-MS метода при анализ на суспензии от AgNPs силно зависи от размерите на частиците, като за диаметри <20 nm тя драстично намалява.

Подходът за калибрация по йонни стандарти при охарактеризиране на разпределението по размери на Ag наноколоиди е верифициран чрез анализ на три референтни материала с размери съответно: 40±4, 60±8 и 100±8 nm. Направените статистически оценки за разпределението по размери чрез калибрация по йонни стандарти са сравнени с експериментално получените при конвенционална калибрация по референтен материал.

Наред с известните предимства, които предлага калибрирането по йонни стандарти при SP-ICP-MS метода като: възможност за анализ на различни НЧ без необходимост от идентичен РМ и гъвкав избор на работен диапазон от калибрационни стандарти, в съответствие с присъстващите в конкретна проба наночастици, проведеното изследване показва, че този подход позволява по-надеждна оценка на аналитичните характеристики на метода.

Благодарности: Проект за финансиране на научни изследвания DN19/9 2017-2020 (INISA)

ОПТИМИЗАЦИЯ НА ИНСТРУМЕНТАЛНИТЕ УСЛОВИЯ И ИЗБОР НА КАЛИБРАЦИОННА СТРАТЕГИЯ ПРИ ОПРЕДЕЛЯНЕ НА ХРОМ ЧРЕЗ MP-AES СЛЕД ЕКСТРАКЦИЯ ПРИ ТЕМПЕРАТУРА НА КОАГУЛАЦИЯ

Мария Качарова, Евелина Върбанова, Кирил Симитчиев

Пловдивски университет „П. Хилендарски“, Катедра аналитична химия и компютърна химия, Пловдив, ул. Цар Асен 24
E-mail: k.simitchiev@uni-plovdiv.net

Целта на настоящото изследване бе да се оптимизират условията за инструментално определяне на Cr чрез атомно-емисионна спектрометрия с микровълнова плазма (MP-AES) след провеждане на екстракция при температура на коагулация като метод за разделяне и концентриране на целевия елемент. Приложен бе експериментален дизайн (централно-композиционен план) за определяне на оптималните стойности на обемната скорост на потока на пробата и на пулверизиращия газ.

След процедурата на екстракция хромът се изолира в краен разтвор, съдържащ 4% w/w Triton X-114 и 3 mol/L HNO_3. При инструменталната регистрация на аналита в този разтвор бе наблюдавано 30% повишение на сигнал спрямо стандарти, приготвени в 1% v/v HNO_3. Проучена бе възможността за корекция на неспектралното матрично влияние чрез метода на вътрешния стандарт. В качеството на кандидати за вътрешни стандарти бяха тествани Ni, V, Mo, Rh, Ga, за които бе доказано, че не пораждат спектрални пречения върху аналитичните линии на хром. Намерен бе вътрешен стандарт, който успешно коригира неспектралното пречене и инструменталния дрейф на чувствителността.

Благодарности: Фирма Т.Е.А.М. ООД за предоставения демонстрационен спектрометър на Agilent 4200 MP-AES в Химически Факултет на Пловдивски Университет „Паисий Хилендарски“.

DATA PROCESSING FOR CHEMICAL SUBSTANCES AND NANOMATERIALS

Gergana Tancheva[1], Nikolay Kochev[1, 2], Nina Jeliazkova[2], Vesselina Paskaleva[1]

[1] Department of Analytical Chemistry and Computer Chemistry, University of Plovdiv, 24 Tzar Assen Str., 4000 Plovdiv, Bulgaria

[2] Ideaconsult Ltd, 4 A. Kanchev str., Sofia 1000, Bulgaria,

Engineered nanomaterials production requires thorough study of their properties especially those related to human health and environmental exposure. Chemical substance analysis includes generation of large data sets derived from different sources and consequent statistical processing, QSAR modelling, data curation and merging into large databases. The principle data model utilized in popular chemical databases supports chemical structures and properties as well as facilities linking the latter. However, this approach is too restrictive for many challenging cases such as nanomaterials and industrial chemicals, which may have complex compositions. We present a substance data model, implemented in Ambit chemoinformatics platform applied for processing large data collections from EU Nanosafety Cluster (NSC). The data is integrated with the help of eNanoMapper public database hosting nanomaterials characterization data, biological and toxicological information. The database provides various functionalities for searching and exploring information and export in several standard formats. The data model supports experimental data for all endpoints of regulatory interest and is successfully used to handle chemical substances and safety data from ECHA dossiers. The eNanoMapper data model has also been successfully used in European Observatory for Nanomaterials. On top of the substance data model we process the data from NSC ongoing projects predominantly stored as custom spreadsheet templates, currently encompassing over 1500 Excel files.

We have developed a dedicated software application NMDataParser (https://github.com/enanomapper/nmdataparser) applied to nanomaterial data and metadata from NSC. NMDataParser is a fully configurable software tool that maps the spreadsheet data onto the substance data model via JSON configuration files. The substance data model is used by various EU projects, helping to identify and, where possible, resolve a range of data quality and completeness issues.

Acknowledgment: Plovdiv University Scientific Fund (project MU19-HF-003)

MELTING POINT PREDICTION USING GROUP CONTRIBUTION METHOD. MP-NOTEBOOK PRESENTATION.

V. Paskaleva, N. Kochev, O. Pukalov

University of Plovdiv, Department of Analytical Chemistry and Computer Chemistry, 4000, Plovdiv, Bulgaria.

E-mail: vesselina.paskaleva@uni-plovdiv.net, nick@uni-plovdiv.net, oggy@uni-plovdiv.net

The methods for quantitative structure-property relationship (QSPR) are recommended for regulatory usage together with the experimental protocols for particular endpoints. The melting point (MP) of a molecule is one of the physicochemical properties required from REACH (Registration, Evaluation, Authorisation and Restriction of Chemical Regulation). MP value (experimental or computed) plays important role in determining other properties such as vapor pressure, liquid viscosity, boiling point and etc. Computer prediction of the melting point is a great challenge. In this work, we present a group contribution model for predicting MP of organic compounds developed with the help of in-house developed open-source software Ambit-GCM [1]. The modeling workflow includes: data manipulation and representation, descriptor and fingerprint calculation, model building, model validation, result output and storage. Typically, such a workflow is accomplished by a number of different software tools and sometimes it hinders the reproducibility of published model results due to version differences, commercial software usage etc. One of the emerging software solutions for such issues are so called “Electronic Notebooks”. The notebook is a combination of text, data and code chunks, assembling tools from different software packages making easy to trace the steps of a particular modeling workflow. We present the first prototype of MP-Notebook for building and validation of QSPR models for melting points of organic compounds.

Acknowledgement: Plovdiv University Scientific Fund (project MU19-HF-003).

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МИКРОБНА МУТАГЕННОСТ. ПРОУЧВАТЕЛЕН АНАЛИЗ НА КОМПЮТЪРНИ ПОДХОДИ ЗА КЛАСИФИКАЦИЯ.

J. Statieva, V. Paskaleva

University of Plovdiv, Department of Analytical Chemistry and Computer Chemistry, 4000, Plovdiv, Bulgaria.

E-mail: danny.statieva@gmail.com, vesselina.paskaleva@uni-plovdiv.net

Информацията за мутагенните свойства на веществата е важна характеристика включена в тексикологичната информация необходима при регистриране на съединения изискуема по регламента REACH. Също така Международният съвет за хармонизиране на техническите изисквания за лекарствени продукти за хуманна употреба (ICH) изисква информация за канцерогенните и мутагенни свойства при „Оценка на опасността“ (Hazard Assessment) на примесите във фармацевтичните продукти. При липса на налични експериментални данни, ICH препоръчва да бъдат използвани (Q)SAR методи за предсказване на микробната мутагенност [1]. Това обуславя нуждата от качествени модели с висока предсказателна способност на микробна мутагенност. (Q)SAR методите намират приложение и за приоритизиране на химичните субстанции при извършване на токсикологичните анализи, което минимизира употребата на тестови животни [2].

В настоящата работа представяме извършения проучвателен анализ на компютърните подходи за класифициране на химичните съединения спрямо микробната им мутагенност. Извършеният анализ включва подготовка и описание на работните извадки, построяване, валидиране и тестване на множество модели, анализ на резултатите и избор на модели за последваща оптимизация.

Литература:

[1] ICH Harmonised tripartite guideline. M7: Assessment and control of DNA reactive (mutagenic) impurities in pharmaceuticals to limit potential carcinogenic risk. Step 4 version dated 23 June 2014.

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ИЗБОР НА ПОДХОДЯЩИ ВЪТРЕШНИ СТАНДАРТИ ЗА КОРЕКЦИЯ НА НЕСПЕКТРАЛНИ МАТРИЧНИ ПРЕЧЕНИЯ ПРИ ICP-OES АНАЛИЗ НА МИКРОЕЛЕМЕНТИ В МАТРИЦИ ОТ МЕТАЛУРГИЧНО ПРОИЗВОДСТВО НА ОЛОВО И ЦИНК

N. Sotirova, V. Stefanova

University of Plovdiv "Paisii Hilendarski"; Department of Analytical Chemistry and Computer Chemistry, 4000 Plovdiv Bulgaria. E-mail:stefanova@uni-plovdiv.net

Осигуряването на перманентния мониторинг и контрол на технологичните процеси в цветната металургия поставя сериозни аналитични предизвикателства, защото изследваните обекти са с богат и разнообразен минерален състав. Методът на вътрешна стандартизация има потенциал да коригира матричните влияния, но при проби със сложен матричен състав, изборът на адекватен IS, отговарящ на всички изисквания е много труден и изисква задълбочени проучвания.

Целта на настоящото изследване е да се проведе систематично изследване на потенциални кандидати за вътрешни стандарти при определяне на As, Sb и In с ICP-OES в цинкови и оловни кекове и велц окиси от металургичното производство. За целта след пълен полуколичествен анализ на материалите са избрани осем елемента - Ga, Ir, Pd, Pt, Y, Re, Rh, Sc и двадесет и четири спектрални линии, които са съгласувани с аналитичните линии по отношение на: излъчваща форма, близост в спектъра и потенциал на възбуждане.

Проучени са: спектрални пречения от матрицата върху линиите на IS; пречения върху аналитите, породени от IS и между-елементни пречения от самите IS.

Най-сериозни спектрални пречения предизвикват макро елементите в пробите- Fe, Mn, Cu, Al. От направените експерименти се установи, че 13 от избраните линиите са ниско чувствителни или запречени от матрицата. При това три от тестваните елементи (Re, Sc и Ga) се оказаха неподходящи като IS, както и 3 спектрални линии на Ir.

От 24 спектрални линии за осем елемента подходящи кандидати за вътрешна стандартизация остават 5 линии на четири елемента- Rh, Pd, Pt, Ir.

Благодарности: Проект за финансиране на научни изследвания DN19/9 2017-2020 (INISA)

SEPARATION OF Ag^+ AND AgNPs BY MSPE COMBINED SP-ICP-MS ANALYSIS

E. Varbanova, D. Georgieva, V. Stefanova

University of Plovdiv, Department of analytical chemistry and computer chemistry, Plovdiv, Bulgaria

E-mail: evarbanova@uni-plovdiv.net

This study represents the further development of an established procedure for solid phase extraction of Ag^+ with magnetic nanoparticles ($MnFe_2O_4@SiO_2$) in order to separate ions from silver nanoparticles (AgNPs). The efficiency of separation is evaluated by single particle-ICP-MS analysis.

In a typical procedure, Ag^+ are quantitatively retained on the surface of magnetic particles under optimal conditions and then re-extracted in 1 mol/L nitric acid thus allowing very selective separation of silver from typical metals prior to instrumental analysis. In the current work, we studied the behavior of silver nanoparticles in the same extraction system. It was found that both Ag^+ and AgNPs are gathered by the sorbent. In such case, Ag^+ and AgNPs could not be analyzed separately after dissolution.

A slight modification of the procedure by the addition of non-ionic surfactant to the water phase leads to minimal extraction of AgNPs. Probably this effect is due to modification and encapsulation of the NPs surface and thus preventing them from retention of Ag^0. In addition it was established that the surfactant does not affect the extraction of silver ions.

The modified procedure allows separation and simultaneous determination of two silver species – Ag^+ and Ag^0 (AgNPs). The ions are retained on magnetic nanoparticles, separated for few minutes by external magnet and then re-extracted in acidic medium, while the AgNPs remain in the water phase and are directly measured by SP-ICP-MS.

The reduction of background signal due to the ionic silver after extraction allows the quantification of smaller AgNPs. After matrix separation, the eluted Ag^+ could be concentrated which allows decreasing the method detection limit.

Acknowledgements: The authors are grateful for the financial support from NSF Project DN19/9 2017-2020 (INISA).

СТАТИСТИЧЕСКИ ПОДХОДИ ЗА СЪПОСТАВКА НА РЕЗУЛТАТИТЕ, ПОЛУЧЕНИ ЧРЕЗ MP-AES И ICP-MS, ПРИ АНАЛИЗ НА МАГНЕЗИЙ, КАЛИЙ И НАТРИЙ В СЛАДКОВОДНИ И МОРСКИ ВОДОРАСЛИ

С. Чобанова[1], И. Койчева[2], M. Alonso[3], С. Симитчиева[1], А. Христозова[1], П. Цонева[1], Ю. Дренска[1], Р. Димова[1], Г. Тодорова[1], Г. Тончева[1,*], Л. Кайнарова[1,#], Е. Върбанова[1,#], К. Симитчиев[1,#]

[1]ПУ „Паисий Хилендарски“, Химически Факултет, Пловдив, България;[*]Катедра обща и неорганична химия с методика на обучението по химия; [#]Катедра аналитична химия и компютърна химия, E-mail: k.simitchiev@uni-plovdiv.net

[2]ПУ „Паисий Хилендарски“, Биологически Факултет, Пловдив, България;

[3]University of Alicante, Faculty of Science, Alicante, Spain

В настоящата работа бе проучена възможността за едновременен анализ чрез масспектрометрията с индуктивно свързана плазма (ICP-MS) на набор от следови (Ni, Cu, Zn, Mn, As, Pb, Hg) и есенциални (Na, K, Mg) елементи в проби водорасли. Получените резултати от ICP-MS за изследваните алкални и алкалоземни елементи бяха сравнени с концентрациите, определени чрез алтернативен анализ с атомно-емисионна спектрометрия с микровълнова плазма (MP-AES). Съпоставката на данните за съдържанието на Na, K и Mg, получени чрез двете инструментални техники бе извършена чрез използването на различни статистически подходи: i) регресионен анализ, ii) метод на Bland-Altman [1] и iii) модифициран от нас вариант на метода на Bland-Altman. Установено бе, че изводите от регресионния анализ могат да бъдат съществено повлияни от размаха на концентрациите на целевите елементи в изследваните проби. Методът, предложен от Bland и Altman [1] е подходяща алтернатива, в случаите когато разликите между резултатите от двете инструментални техники не зависят от концентрацията на аналита. Предложеният модифициран вариант на метода на Bland-Altman може да бъде използван при наличието на пропорционална зависимост на разликите между съпоставяните резултати и съдържанието на аналита в изследваните пробите.

[1] J. Bland, D. Altman, *Int. J. Nurs. Stud.*, **47** (2010) 931-936

As AND Sb DETERMINATION IN HUMAN URINE BY HG-MSIS-MP-AES MODIFIED BY MAGNETIC NANOPARTICLES

M. Kiryakova, D. Stoitsov, E. Varbanova, K. Simitchiev, V.Kmetov,

Department of Analytical Chemistry and Computer Chemistry,
University of Plovdiv "Paisii Hilendarski",
24 str."Tzar Assen", Plovdiv 4000, Bulgaria

E-mail: kiryakova@uni-plovdiv.net

The urine is a great source of trace element biomarkers, but it is a complex matrix - with high salt and carbon content. One of the main advantages of hydride generation (HG) for trace elements analysis is that the analyte could be separated from the matrix as a volatile hydride and loaded in the plasma source as a gas.

In the present study the potential of HG with nitrogen microwave plasma atomic emission spectrometry (MP-AES) and Multi Mode Sample Introduction System (MSIS)®, for determination of trace level of As and Sb in human urine was evaluate. To improve the analytical procedure we propose an innovative approach based on the modification of the HG by means of adding silica coated ($MnFe_2O_4$) magnetic nanoparticles (MNPs) into $NaBH_4$.The possibilities of a simple dilute-and-shoot sample preparation method for human urines and various dilution factors have been studied. The combination of nanoparticles and alcohol has a synergistic effect and improves the signal to noise ratio. Urine samples tent to foam in HG reactor, but the presence of MNPs visually suppresses the foaming and contributes to smoother and uniform reaction in MSIS. This results in stabilizing plasma conditions and improves precision of the both - background and spectral lines signals. The proposed innovative approach expands the capabilities of MSIS-MP-AES for analysis of As and Sb in urine samples with LODs up to 0.85 ppb and 0.25 ppb respectively. Recoveries (R %), obtained for spiked urine sample solutions were in the range 95%-102% for both elements.

Acknowledgements: The authors would like to thank T.E.A.M. Ltd. and Agilent technologies for kindly providing Agilent 4200 MP-AES instrumentation to the Department of Analytical chemistry and Computer chemistry in University of Plovdiv "P. Hilendarski" and NSF Project DN19/9 2017-2020 (INISA)

COMPARISON OF TWO PROCEDURES FOR MICROWAVE-ASSISTED DIGESTION FOR ICP-MS DETERMINATION OF Mn, Ni, Zn, Pb, Fe AND Sr IN *GINKGO BILOBA* SEEDS

G. Kirova[1,2], D. Davcheva[2,3] , T. Tomova[1,2], D. Tsvetkova[1], V. Kmetov[1,4]

[1]Technological Center for Emergency Medicine, Plovdiv

[2]Medical University – Plovdiv, Department of Chemical Sciences

[3]Medical University – Plovdiv, Department of Clinical Laboratory

[4]University of Plovdiv "Paisii Hilendarski"

E-mail: gergana_kiro@mail.bg

Before being analysed by ICP-MS solid samples should be dissolved to representative solutions by an appropriate procedure, which is an important part of the reliability of the overall analytical process. The green chemistry tendencies aim less harmful procedures with minimal reagent consumption. Hence the microwave digestion (MW) in closed vessels using minimum acid solutions under high pressure and temperatures is an effective option. In the following study, two procedures for microwave-assisted acid-digestion of *Ginkgo biloba* seeds with Anton Paar, Multiwave GO were compared. For the mineralization of 0.100 g of sample 2 mL of HNO_3 and 1 mL of H_2O_2 as an auxiliary oxidant were used, as in the second experiment only HNO_3 was added. After mineralization the samples were analysed by measuring the ion signals of ^{55}Mn, ^{60}Ni, ^{66}Zn, ^{208}Pb, ^{56}Fe and ^{88}Sr by ICP-MS (Thermo Fisher Scientific, iCAPQ) in KED mode, using ^{103}Rh as internal standard. Reference material NCS DC 73348 was analysed for evaluating the accuracy of the digestion process. The results showed the microwave-assisted acid digestion can be carried out under mild conditions, using only HNO_3 as oxidizing agent. No significant differences in IS stability were noted, with recoveries from 94.2 % to 97.2 % for both batches of samples. Significant contamination with Sn in samples prepared with H_2O_2 was found, as well as lower recoveries for Mn, Zn, Pb, Fe and Sr in the CRM, compared with samples treated only with HNO_3. There is also a higher risk of explosion in closed vessels with H_2O_2, hence MW assisted acid digestion with HNO_3 only should be preferred for such kind of plant samples.

OPEN ENVIRONMENTAL MONITORING NETWORK - PROOF OF CONCEPT

G. Dimitrov[1], S. Tenev[1], I. Kostova[1], V. Paskaleva[1], O. Pukalov[1], S. Tsoneva[1], L. Kaynarova[1], G. Patronov[1], V. Delchev[1], P. Penchev[1], N. Kochev[1], A. Terziyski[1,2]

[1]Affiliation 1 (University of Plovdiv, Department of Analytical Chemistry and Computer Chemistry, 4000, Plovdiv, Bulgaria)

[2]Affiliation 2 (Bulgarian Academy of Sciences, Institute of Information and Communication Technologies, 1113, Sofia, Bulgaria)

E-mail: atanas@uni-plovdiv.net

We present a proof of concept about an open environmental monitoring network. The network is aimed to evenly cover mainly the territory of Bulgaria, but also to include measurements from the neighbor Balkan countries. The network is built over multiple self-designed and self-made ground-based measuring stations (GBMS). Each station consists of a box, supported with two valves for better and controlled ventilation. The sensors set is built within the box. For avoiding infrared heat (mainly from the sun) the box itself will be covered by reflectors based on TiO_2, Caolin, SiO_2 and commercial Yellow GRX 86 pigment. Each GBMS include sensors for measuring ambient temperature, atmospheric pressure, relative humidity, particulate matter (size of 2.5 and 10 μm) and gamma radiation. A measure is performed each fifth minute and report is send to the server. The data is collected and is publicly available without any license restrictions on the web site www.meter.ac. The open environmental monitoring network offers a flexible interface to the users for browsing the data and derive their own conclusions. The current proof of concept network maintains over 30 ground-based measuring stations located in different parts of Bulgaria for more than half year.

Acknowledgements: Plovdiv University Scientific Fund (project FP19-HF001).

СЪДЪРЖАНИЕ

АКТУАЛНИ РЕГУЛАТИВНИ ИЗИСКВАНИЯ КЪМ ХИМИЧНИЯ АНАЛИЗ И МОДЕРНИ ИНСТРУМЕНТАЛНИ ТЕХНОЛОГИИ ЗА ТЯХНОТО ПОКРИВАНЕ
12 Юни 2019, ПЛОВДИВ


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