WORKSHOP 2° EDIZIONE

Società Chimica Italiana
Sezione Abruzzo

UNIVERSITÀ DEGLI STUDI DE L'AQUILA

Ud'A
Università degli Studi "G. d'Annunzio"

UNIVERSITÀ DEGLI STUDI DI TERAMO

BOOK OF ABSTRACTS

12 – 13 Luglio 2022
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Cari Colleghi e Colleghe,

a nome del Comitato Scientifico ed Organizzatore sono lieto di invitarVi a partecipare alla 2° Edizione del Workshop "I Giovani e la Chimica in Abruzzo". L'evento è dedicato in particular modo ai giovani chimici in formazione (neo-laureati, borsisti, dottorandi, assegnisti) presso gli Atenei della regione Abruzzo e delle altre Università italiane. Le tematiche affrontate nel corso del workshop saranno multidisciplinari con interventi in forma di comunicazione orale che saranno incentrate in particular modo su aspetti di chimica farmaceutica, analisi farmaceutica, a chimica analitica, chemometria, chimica organica, chimica degli alimenti e tecnologia farmaceutica. Sono previsti anche interventi in forma di keynotes da parte di esperti del mondo accademico e rappresentanti di aziende. Il workshop con il suo carattere spiccatamente multidisciplinare rappresenta altresì un'occasione di confronto sullo stato di avanzamento delle varie attività di ricerca, per raccogliere nuovi spunti e suggerimenti e per avviare nuove collaborazioni scientifiche. Con la speranza di vederVi numerosi nella partecipazione al Workshop, rinnovo il benvenuto a tutti i Partecipanti

Prof. Francesco Epifano
Presidente Sezione Abruzzo della Società Chimica Italiana
Chairman

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COMUNICAZIONI ORALI

OC1

An easy way for the simultaneous hydrolysis, pre-concentration, and chemical stabilization of crocetin from saffron powder

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Crocetin is the main apocarotenoid extracted from *Crocus sativus*. The most of properties of saffron are ascribed to crocetin and its diester with gentiobiose, known as crocin-1 (Figure 1). It is nowadays well established to act as valuable and powerful nutraceutical, especially in the prevention and management of metabolic disorders in humans, myocardial dysfunctions, neurological disorders, and associated syndromes [1]. With the aim of its selective concentration by means of extractions from saffron powder aqueous solutions in the heterogeneous phase, we report herein that some synthetic clays, like zinc hydroxy chloride, magnesium aluminium hydroxy chloride, magnesium aluminium hydroxy acetate, and zinc aluminium chloride are not only able to selectively retain crocetin in the solid phase, but also to lead to its hydrolysis from its digentiobyosil ester (crocin) in nearly quantitative yield and to its chemical stabilization (e.g. oxidation) over time. This phenomenon was assessed by HPLC analyses after desorption of crocetin from the respective support, evaluating its degradation along a period of 30 days. The method we set up could represent a good mean to obtain pure crocetin from saffron powder, preserving in the meantime its chemical properties for a concrete exploitation for food, pharmaceutical, and cosmetic purposes.

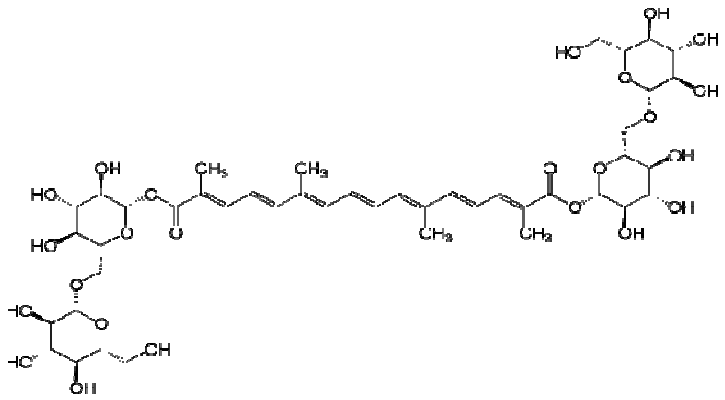

Figure 1: Chemical structure of crocin-1

[1] Moshiri, M.; Vahabzadeh, M.; Hosseinzadeh, H. *Drug Res.* **2015**, *65*, 287-295.

OC2

UV-Vis Spectroscopy and chemometrics for the detection of expired saffron

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Saffron production consists of several time-consuming phases; whether the cultivation conditions and harvesting stages can affect the final yield of the product and, together with the high costs, the propensity of producers to commit fraud, the drying and the storage conditions phases actually affect the commercial quality of the spice. Indeed storage induces oxidative or hydrolytic decomposition, whereas spice stability depends on relative humidity, temperature, and light exposure. In this context, the quality control is regulated by the ISO 3632-1 and 2, which allows saffron to be assigned to quality classes according to its moisture, quantity of extraneous material, and concentration of its secondary metabolites (picrocrocin, crocins, and safranal). Thus, the purpose of the work was to assess if, in the context of UV-Vis quality control of the spice, it is possible, by means of chemometrics, to differentiate between FRESH products (i.e., saffron produced and marketed within a year) COMPLIANT (product not yet expired) and legally EXPIRED products (produced over two years). Therefore, spectra were collected on 104 FRESH Umbrian samples between the years 2016 and 2020; exactly the same batches were reanalyzed in 2021 from the interval of 5 years (the 2016 samples) to the interval of 8 months (the 2020 samples).

Dataset	Production Year	Aging	N samples
S2016(F)	1	1	18
S2017(F)	2	1	27
S2018(F)	3	1	28
S2019(F)	4	1	14
S2020(F)	5	1	15
S2016(AE)	1	2	18
S2017(AE)	2	3	27
S2018(AE)	3	4	28
S2019(AC)	4	5	14
S2020(AC)	5	6	15

Figure 1. Dataset of Fresh (F), Aged but Compliant (AC) Aged and Expired (AE) samples, factor columns, and number of samples

Anova- Simultaneous Component Analysis confirmed a significant effect of both the Production Year and Aging. The loading inspection confirmed the loss of the spice color power due to the crocins degradation [1]. SIMCA constructed on FRESH samples showed a sensitivity of 81% (6 samples erroneously refused over 32 in external validation), a specificity of 91% for the EXPIRED class and of 89% for the COMPLIANT class. The reported results are excellent, considering the model was built on a class consisting of samples produced over a 5-year period (variability recognized as significant at the exploratory stage). In conclusion, following the ISO regulation and with an appropriate

OC2

database, it is possible to evaluate the compliance and the freshness of the spice during its quality control.

[1] Cid-Perez, T. S.; Nevárez-Moorillón, G. V.; Ochoa-Velasco, C. E.; Navarro-Cruz, A. R.; Hernández-Carranza, P.; Avila-Sosa, R. *Molecules* **2021**, *26*, 6954.

OC3

Determination of derivatized short chain fatty acids in faeces by means of LC-MS/MS

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Short-chain fatty acids (SCFAs) are generated as end products, by the degradation and fermentation of indigestible carbohydrates by the gut microbiota, a process termed called saccharolytic fermentation [1]. They can act as signaling molecules as ligands of G-protein-coupled receptors and they are implicated in the increase of anorexic hormone production and energy expenditure [2]. Consequently, SCFA production was linked to preventing the progression of obesity and related complications [3]. Also gut microbiota-derived acetate is an important precursor for the synthesis of fatty acids and phospholipids in the liver. SCFAs are typically quantified by gas chromatography (GC), liquid chromatography (LC), nuclear magnetic resonance (NMR), and capillary electrophoresis (CE) [4]. These methods require derivatization using, for example, 2-nitrophenylhydrazin, 3-nitrophenylhydrazine, O-benzylhydroxylamine, or aniline. LC coupled with mass spectrometry (MS) with electrospray ionization (ESI) is now the most widely used analytical technique in metabolomics. Ion-exclusion and reversed-phase LC–MS with post-column neutralization, were used for the determination of SCFAs in the pig colon and blood. The complex instrument setup for these two methods, however, makes them unsuitable for routine analysis in most laboratories. On the other hand, LC-MS quantitation without the use of an isotopically-labeled internal standard (IS) for an analyte often makes the analysis questionable because of the notorious matrix effects in ESI [5], especially when no efficient clean-up is carried out for the quantification of these compounds. The aim of this work was to develop a new analytical method for SCFA based on 3-nitrophenylhydrazone (3NPH) derivatization followed by SPE clean-up to minimize matrix effect and improve extraction selectivity. The LC-MS/MS method was performed both in Multi Reaction Monitoring (MRM) for quantitative analysis and in precursor ion scan analysis (PIS) to achieve semi-targeted analysis for a wide number of SCFA compounds based on derivatization reactions, that could be used for putative identification and screening of SCFA compounds in biological samples.

[1] Koh, A.; De Vadder, F.; Kovatcheva-Datchary, P.; Backhed, F. *Cell* **2016**, *165*, 1332 - 1345.
[2] Cani, P.D.; Van Hul, M.; Lefort, C.; Depommier, C.; Rastelli, M.; Everard, A.. *Nat. Metab.* **2019**, *1*, 34 - 46.

OC3

[3] Kindt, A.; Liebisch, G.; Clavel, T.; Haller, D.; Hoermannsperger, G.; Yoon, H.; Kolmeder, D.; Sigruener, A.; Krautbauer, S.; Seeliger, C. *Nat. Commun*., **2018,** 9
[4] Primec, M.; Micetic-Turk, D.; Langerholc, T. *Anal. Biochem.* **2017**, *526*, 9 - 21.
[5] Vogeser, M.; Seger,C. *Clin. Chem.* **2010,** *56*, 1234 – 1244.

OC4

Extraction of carotenoids from pumpkins of different varieties by using innovative techniques

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Pumpkin is a vegetable belonging to Cucurbitaceae family that consist both wild and domesticated species, among which the most common and used worldwide are *Cucurbita maxima*, *C. pepo*, and *C. moschata*. Due to the presence of phytochemicals (carotenoids, fiber and tocopherols), pumpkin is considered functional and medicinal food [1]. The aim of this study was to select the best method, in terms of cost, time and yield, for the recovery of carotenoids from *C. moschata* pulp, applying two innovative extraction techniques (UAE, ultrasound-assisted extraction; MAE, microvawe-assisted extraction). The pulp, cut into thin slices and dehydrated, was grinded to obtain a fine and homogeneous powder, and then stored in the dark. For each extraction method, hexane/isopropanol (60:40, *v:v*) mixture and a 1:20 solid:liquid ratio were used according to the conditions reported in a previous paper [2] with slight modifications. As regards UAE, the sample was sonicated in a ultrasonic bath for 30 min at 45 °C; regarding MAE, the temperature was set at 45 °C, while the extraction time was 15 or 30 min. For a comparison, a conventional extraction technique, based on dynamic maceration (MAC) for 4h at room temperature with the same solvent, was also used.[2] Extraction yield, antioxidant activity by ABTS (2,2-azinobis(3-ethylbenzothiazoline-6-sulfonic acid) assay, and RP-HPLC-DAD chromatographic analysis of extracts were evaluated. The obtained results suggest that UAE is the most performing and efficient procedure for carotenoids extraction from pumpkin pulp in respect to the other methods (MAE and MAC). In addition to a main peak corresponding to *all-trans*-β-carotene, the chromatographic profiles of extracts highlighted the presence of other interesting bioactive compounds (violaxanthin, neoxanthin, antheraxanthin, lutein, but also mono- and diesterified structures). HPLC-MS analyses to confirm the identity of molecules, tentatively identified on the basis of UV spectrum and bibliographic data, are in progress.

[1] Rico, X.; Gullón, B.; Alfonso, J.L.; Yáñez, R. *Food Res. Int.* **2020***, 132*, 109086.
[2] Rocchetti, G.; Blasi, F.; Montesano, D.; Ghisoni, S.; Marcotullio, M. C.; Sabatini, S.; Cossignani, L.; Lucini, L. *Food Res.Int.* **2019**, *115*, 319.

OC5

Fabric phase sorptive extraction (PSE) as an efficient sample preparation platform for the extraction of antidepressant drugs from biological fluids

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Antidepressants drugs (ADs) are the most widely prescription drugs to treat major depressive disorder (MDD). The wide increase in the use of antidepressant drugs is due to their role not only in the treatment of major depressive disorder, but also in the management of other related conditions such as anxiety, obsessive compulsive disorder, and nutrition and sleep disorders. Fabric phase sorptive extraction (FPSE), a recently introduced microextraction technique, has been herein applied to achieve a simple and rapid simultaneous extraction of seven common antidepressant drugs (ADs, venlafaxine, citalopram, paroxetine, fluoxetine, sertraline, amitriptyline, and clomipramine) from biological fluids (urine, saliva and whole blood) as well as from post–mortem samples (particularly whole blood and cerebrospinal liquor) collected during autopsies. By eliminating the protein precipitation step and reducing solvent consumption, this technique resulted in sample preparation compliant with Green Analytical Chemistry (GAC) principles. Among all tested FPSE membranes, the sol-gel Carbowax 20M coating on cellulose substrate showed optimal extraction efficiency for ADs. The analysis was carried by high-performance liquid chromatography coupled to photo diode array detector (HPLC-PDA). Ammonium acetate buffer and acetonitrile were used as mobile phases. The limit of detection (LOD) ranged from 0.04 to 0.06 μg/mL, whereas limit of quantification (LOQ) was 0.1 μg/mL. The established analytical method has been successfully applied for the bioanalysis of real samples obtained from volunteers as well as samples collected during various autopsies. Unequivocally, this test was the most decisive criterion for evaluating the efficacy of the analytical method and the extraction efficiency of FPSE.

OC6

Chemistry and mass-spectrometry applied to Gran Sasso National Laboratories RENOIR radiobiology experiment: mineralization and characterization of different sample matrices

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In addition to particle and sub-particle physics experiments, the Gran Sasso National Laboratories in Italy also host radiobiology experiments. The current RENOIR experiment uses the fruit fly *Drosophila melanogaster* as a model organism with the aim of understanding the effects of environmental background radiation on the metabolism of living organisms. RENOIR aims to study the biophysical mechanisms that trigger the different biological response observed in Drosophila reared in the above ground environment compared to the underground environment, where the cosmic ray flux is significantly reduced. One of the main objectives of RENOIR is a detailed characterization of the radiation field to which the biological system is exposed in both the above ground and underground laboratory through spectrometric and dosimetric characterization of the environments and the experimental set-up. An important contribution to the radiation background comes from the intrinsic radioactivity in the experimental set up components named caps, vials, and culture medium as well as from the biological system itself. The evaluation of the intrinsic ionizing radiation contribution by experimental set-up was carried out Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Different techniques of mineralization were adopted to solubilize materials involved in experimental set-up (cup, vials, and culture medium); intrinsic contribution of radioactivity was determined to evaluate possible use of materials; Specifically, we adopted thermal heating, microwave mineralization and ashing treatment. To determine total amount of impurities regards to natural radioactive elements (Th, U, K), so intrinsic contribution of radioactivity, High Resolution Inductively Coupled Plasma Mass Spectrometry was used to quantitative analysis of interested elements. Obtained results and relative considerations will discuss to describe radioactivity of our experimental environment

OC7

Miniaturised blood samples for cariprazine analysis: an analitical approach based on volumetric absorptive microsampling

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Pharmaco-toxicological analysis in the framework of therapeutic drug monitoring (TDM) requires the improvement of current sampling and bioanalysis procedures, with the aim of streamline experimental protocols and provide straight-forward and high-throughput automatable strategies [1]. In order to meet these requirements, in this study a miniaturised method based on volumetric absorptive microsampling (VAMS) was developed exploiting a polymeric tip able to collect an accurate volume of 10 µL of capillary whole blood, following a simple finger prick (Figure 1). VAMS technology provides for accurate whole blood sampling independently from haematocrit values for the generation of fixed-volume dried microsamples [2]. A feasible and reliable VAMS-HPLC-UV method was developed for the TDM of cariprazine (3-[4-[2-[4-(2,3-dichlorophenyl)piperazin-1-yl]ethyl]cyclohexyl]-1,1-dimethylurea), a third generation antipsychotic drug, obtaining satisfactory validation results on fortified blank samples in terms of linearity, precision and extraction yield. Thus, this method was applied to real samples within the TDM of patients treated with cariprazine, showing good agreement between the dataset obtained from VAMS samples and the one from a plasma procedure developed *ad hoc*. This innovative strategy is suitable for self- and home-sampling by patients themselves increasing their compliance, and allows storage, shipping and sample handling procedures at room conditions. The reliable results obtained within this study qualify the developed strategy as a promising tool with immediate applicability in clinical practice, with the aim of performing frequent and accurate TDM, to obtain personalised therapies in the future perspective of sound bioanalysis strategies for precision medicine.

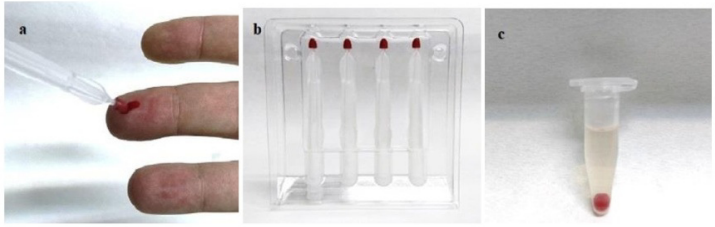

Figure 1. VAMS sampling by finger prick (a), VAMS sample drying (b) and VAMS tip extraction (c)

OC7

[1] Bernieh, D.; Lawson, G.; Tanna, S. *J. Pharm. Biomed. Anal.* **2017**, *142*, 232-243.
[2] Protti, M.; Mandrioli, R.; Mercolini, L. *Anal. Chim. Acta* **2019**, *1046*, 32-47.

OC8

Reference introduction study for calibration of thermal desorber – gas chromatography

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Thermal desorption (TD) combined with gas chromatography (GC) was originally developed for offline air monitoring. In the meantime, more and more applications arose in the pharmaceutical field where conventional approaches like headspace – GC are not usable. A nice example is the determination of residual solvents in solid drug carriers like mesoporous silica, gelatine and albumin [1, 2].For the latter applications, proper reference introduction prior to calibration is not so evident. Indeed, the analysis of solid samples using liquid reference solutions is problematic since the procedures for calibration and sample analysis are not the same. In practice, often offline liquid calibration (OLC) is performed and results are accepted, even if they are inaccurate since assumptions in terms of complete adsorption and desorption are not fulfilled.Although the issues related to the common OLC technique are known among users, no in-depth investigation about possible causes has been carried out. Such research has been realised here and explanations for the observed phenomena are given so that a better insight has been achieved and possible solutions could be elaborated. With a TD tube containing only quartz filters, a relative loss of more than 80% was noticed for some solvents due to tube manipulation processes. Enclosing a bed of mesoporous silica as alternative sorbent limited the losses to about 25% when samples were immediately analysed, and even better results were obtained when tubes were stored for several hours so that proper adsorption could take place. An additional sweep gas during injection boosted the transfer of analytes with recoveries above 95%. However, one could still not be sure that complete desorption had been accomplished. So, an additional injector was installed on the apparatus to allow direct injection of reference compounds in the primary desorption gas stream of the TD, which is referred to as inline liquid calibration (ILC). This sorbent free, independent calibration tool avoids the drawbacks of other approaches.

[1] Khayyat, L.; Essawy, A.; Sorour, J.; Soffar A. *Peer J.*, **2017**, *5*, e3041.
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OC9

Organocatalyzed Michael addition to nitroalkenes *via* masked acetaldehyde

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We recently reported a novel and safer reaction protocol for the enantioselective enamine-catalysed addition of acetaldehyde to nitroalkenes; this protocol makes use of a safe acetaldehyde precursor to access important intermediates to Active Pharmaceutical Ingredients (APIs), and allows the use of fewer equivalents of acetaldehyde and lower catalyst loadings compared to previous reports. The use of acetaldehyde dimethyl acetal in the aminocatalytic enantioselective addition to nitroalkenes avoided the use of free acetaldehyde, which is toxic, very reactive and has a low boiling point [1].

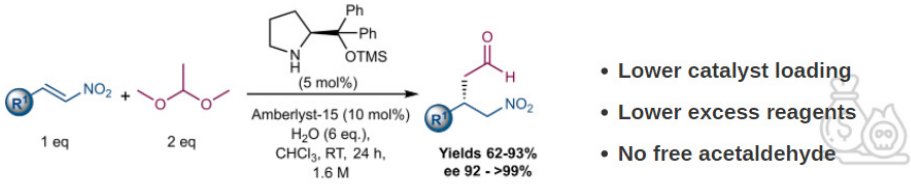

Figure 1. Enantioselective Michael addition of masked acetaldehyde to nitroalkenes.

However, a limitation of the report is the use of chloroform, a class 2 solvent. To overcome this hurdle, we decided to explore the possibility to carry out the reaction in water, using especially designed organocatalysts. Furthermore, to optimize the reaction conditions, Design of Experiment (DoE) was used [2].

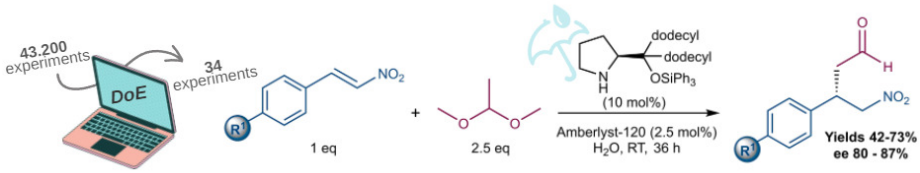

Figure 2. Enantioselective Michael addition of masked acetaldehyde to nitroalkenes in water.

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OC10

Optimization of chlorogenic acid extraction from potato by-products

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Annually, 1300 million tonnes of waste are generated from the agricultural sector and this number is expected to rise due to an increase in demand for agricultural products [1]. The disposal of these by-products represents a cost and has a negative impact on the environment. Instead, these materials are considered a widely available and low-cost source of value-added compounds, the recovery of which therefore represents a promising opportunity [2]. In this frame, this work investigated the isolation of chlorogenic acid (5-CQA) from potato sprouts by Ultrasound-Assisted Extraction (UAE), and the optimization of the extraction conditions. 5-CQA is widely known for several health benefits due to its antioxidant, anti-inflammatory, anti-carcinogenic, and anti-obesity properties [3]. The optimization of the extraction was carried out through an experimental design approach to evaluate the effect of solvent composition, solid/solvent ratio, and extraction time on 5-CQA extraction yield. Potato sprouts were first ground and mixed, then eleven experiments were carried out using the solvent composition (EtOH:H_2O, 0.1% acetic acid) and the other extraction conditions provided by the software. The qualitative and quantitative determination of the extracts was performed by HPLC analysis, applying the conditions reported in a previous paper [4]. The results clearly evidenced significant differences in the recovery of 5-CQA, its isomers and caffeic acid. In particular, it was found that the best extraction conditions were: UAE for 5 minutes at room temperature, using 70% ethanol in water and a solid/liquid ratio of 1:10. Finally, the effect of the substitution of acetic acid in the hydroalcoholic mixture with citric acid or ascorbic acid was studied, with the aim of evaluating the possible protective effect on the inhibition of enzymatic browning. According to our results, ascorbic acid was the most efficient in extracting 5-CQA and related compounds from fresh potato sprouts.

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[2] Panzella L.; Moccia F.; Nasti R.; Marzorati S.; Verotta L.; Napolitano A. *Front. Nutri.* **2020**, *7*, 60.
[3] Lu, H.; Tian, Z.; Cui, Y.; Liu, Z.; Ma, X., *Compr. Revi. Food Sci. Food Chem.* **2020**, *19*, 3130.
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OC11

A comparative study on phytochemical fingerprint of two diverse *Phaseolus vulgaris* var. Tondino del Tavo and Cannellino bioextracts

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Common bean extracts (*Phaseolus vulgaris*) showed beneficial effects on metabolic disease and anti-obesity activity [1]. This effect is confirmed by many different preclinical studies in rat model [2]. In this study, two different Italian variety of bean, Tondino del Tavo and Cannellino Bio, have been analysed for their phenolic content by HPLC-PDA after the separation of diverse fractions through a well-established extraction procedure (Figure 1). Each extract has been evaluated for its antioxidant activity and enzyme inhibitory activity to determine their potential biological profile. The extracts characterized by the highest phenolic content (0.79 and 1.1 µg/mg of 3-hydroxy benzoic acid for hexane extract of Tondino del Tavo and Cannellino Bio respectively; 0.30 µg/mg *p*-coumaric acid for hexane extract of Tondino del Tavo) show the best antioxidant activity. Finally, the decoction extracts have been tested for their anti-inflammatory activity through zymosan-induced edema formation assay. Further investigations need to be conducted to define the feasible biological effects and phytochemical profile of Tondino del Tavo and Cannellino Bio extracts. Our extraction procedure may be useful to determine their protein content and the overall phenolic profile.

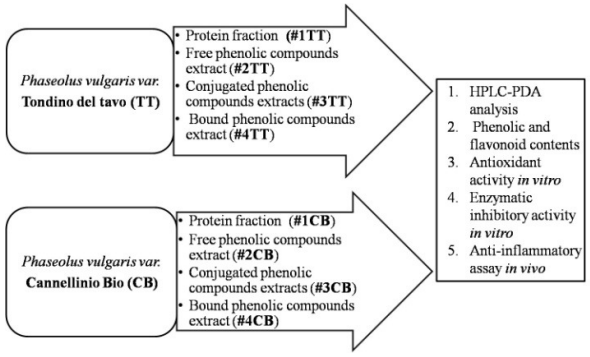

Figure 1. Workflow of the extraction procedure.

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OC12

Design of targeted polymeric nanoparticles for human breast cancer cell line

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Polymeric nanoparticles (NPs) are drug-delivery systems produced to improve the pharmacokinetic of drugs, reach specific sites, reduce the toxicity of the drug and increase permeation through biological membranes. In this project the copolymer poly (ethylene glycol) methylether-block-poly (lactic-co-glycolic) (mPLGA-PEG) was used for the realization of NPs due to its biodegradability, bioeliminability and low toxicity [1]. In particular, PLGA-PEG polymeric nanoparticles have been loaded with carnosic acid and covalently linked with Trastuzumab (TMAB) in order to target them towards the HER2-positive breast cancer cells. TMAB is a monoclonal antibody that has a double role:allows NPs to be targetted and causes inhibition of HER-2 cells, improving the life of patients. Carnosic acid, on the other hand, is a diterpene consisting of 20 carbon atoms,which enhances Trastuzumab inhibition of survival and cooperatively inhibits with this antibody, migration in ERBB2+ breast cancer cells. Furthermore, carnosic acid is highly used for its antimicrobial, anti-inflammatory.It is highly used for its antimicrobial, anti-inflammatory and antioxidant activity. Due to this latter activity it tends to easily degrade to different analogues and for this reason we added to the preparation alpha tocopherol, a co-oxidant, in order to prevent the excessive oxidation of carnosic acid. The nanoparticles were prepared according to the solvent emulsification-evaporation technique. The sample was then purified by three centrifuge cycles for 1 hour at 9000 rpm in order to get rid of the non-embedded drugs. Dynamic Laser Light Scattering (DLS)analyzes revealed the presenceof a single population of NPs, with dimensions between 200 and 250 nm, while the value of the Z potential was negative. Functionalization with TMAB was performed by covalent coupling by incubating the NPs for 3 hours in a refrigerator in the presence of EDC and NHS as well. The TMAB-functionalized NPs were then purified by centrifugation. The morphology of the NPs was accessed by Transmission Electron Microscope (TEM). Finally, all the samples were subjected to freeze-drying. Carnosic acid was quantified by HPLC and the calculated percentage entrapment efficiency was equal to 12.1% and 5% for NPs in the absence and in the presence of TMAB, respectively. The samples were used for *in vitro*analyses on different cell lines demonstrated to be selectively effective. In terms of survival, carnosic acid and TMAB NPs demonstrated to be more effective on SKBR-3 cell lines, whereas in terms of cytotoxicity demonstrated to be more effective on MDA-MB-361 cells lines.

[1] Kumari, A.; Yadav, S. K.; Yadav, S. C. *Colloids Surf. B Biointerfaces* **2010**, *75*, 1 – 18.

OC13

Determination of anions in postmortem samples for forensic evaluation

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Ion chromatography (IC) is an analytical technique for the determination of inorganic and organic anions and cations. In the present study, a new method with IC was developed for separation and quantification of ten anions (fluoride, chloride, bromate, chlorite, nitrite, bromide, chlorate, nitrate, phosphate and sulfate) in postmortem samples, in particular drowning water, pleuric liquid and gastroduodenal content. The analytical method is simple, fast, accurate and selective for the separation and quantification of ten anions. This first application for forensic purposes showed interesting preliminary results. We observed an inverse relationship between the concentration of the target analytes (fluoride, chloride) and the time of death. The concentration of target anions decreases with increasing post mortem interval regardless of cause of death. This first application of ion chromatography for forensic purposes showed interesting preliminary results, as a support method for forensic investigation on PMI. Future integration with new samples to increase the significance of our observations and develop a chemometrics model that includes other factors.

OC14

Enantioseparation of two anti-inflammatory chiral sulfoxides with cellulose-based chiral stationary phases under polar organic conditions

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In the present study, two nitrooxyethyl sulfoxides (**1** and **2**, Figure 1) acting as cyclooxygenase-2 (COX-2) inhibiting/NO donors, along with their metabolites, hydroxyethyl derivatives (**3** and **4**) have been successfully enantioresolved with two cellulose *tris*(3,5-dichlorophenylcarbamate)-based chiral stationary phases (CSPs), one with a coated (CSP 1) and the other (CSP 2) with an immobilized chiral selector [1].

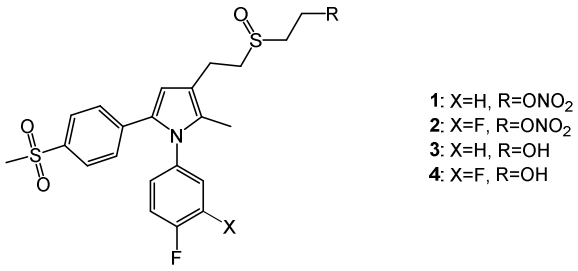

Figure 1

The immobilized selector in CSP 2 produced comparable-to-better performances than the coated version in CSP 1 (with α and R_S values up to 1.94 and 6.32, respectively) under polar-organic conditions with an ethanol/2-propanol (80:20, v/v) containing mobile phase. Electronic circular dichroism studies coupled to *ab initio* time-dependent density functional theory simulations allowed to define the enantiomer elution order (EEO) of three out of four compounds. For the two hydroxyethyl derivatives **3** and **4**, the same EEO [(*S*)<(*R*)] was obtained with both CSPs, while for the compounds containing the $-ONO_2$ group (**1** and **2**) a different elution order was found depending on the coated or immobilized nature of the chiral selector [that is, (*S*)<(*R*) with CSP 1 and (*R*)<(*S*) with CSP 2]. A molecular modelling study based on docking simulations allowed the explanation at a molecular level of the enantioseparation mechanism of compounds 3 and 4 on both CSPs.

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OC15

Determination of quinolizidine alkaloids in *Lupinus albus* L. by means of HPLC-MS/MS

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Bioactive compounds in plant matrices are widely studied for their important role in modulating metabolic processes and prevention of several chronic diseases in human health, due to their therapeutic properties. Among them, alkaloids are known to cause a wide variety of both negative and positive physiological effects in humans and animals. Quinolizidine alkaloids (C_5NC_4 skeleton) are L-lysine derived compounds, having one or more nitrogen atoms usually contained in a heterocyclic ring system, which can be divided in bicyclic, tricyclic, and tetracyclic alkaloids [1]. These compounds are especially found in plants belonging to the *Lupinus* L. genus (Fabaceae family), in which they impart the bitter taste and act as a defense mechanism against pathogens and herbivorous animals. There are almost 70 different quinolizidine alkaloids found in various lupin species, which levels and combinations vary according to botanical and geographic origin, but also to soil composition and climate; they can cause symptoms of poisoning in humans, affecting the nervous, circulatory and digestive systems. There are few methods in the literature about the quantification of alkaloids in this specific food matrix; most of them reported the using of gas chromatography coupled to mass spectrometry (GC-MS). In recent years, there has been an increase in the development of methods by liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) to detect alkaloid compounds in various matrices, both food and biological [2]. In this work, a sensitive method involving the use of LC-MS/MS was developed in multiple reaction monitoring (MRM) mode, with the aim of the simultaneous quantification and determination of twelve different alkaloids. The analysis was conducted on different commercial forms of white lupin (*L. albus* L.), through the development of an efficient extraction procedure followed by a suitable clean-up step, performed by Solid Phase Extraction, in order to decrease the amount of interfering compounds and to obtain reliable recoveries The presented analytical method was validated following FDA guidelines, which demonstrated the reliability and robustness of the procedure.

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OC16

Chemometric approaches in hyperspectral imaging

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Hyperspectral imaging is a powerful not destructive technique that gathers the chemical and the spatial information of a sample in a cube of data. It finds application in many sectors: food, biotechnology, forensic science, pharmaceutical, remote sensing as it can detect chemicals in a sample, but also where and how specific compounds are distributed. The hypercube can be investigated with chemometric approaches such as classification and spectral unmixing methods. The first aims to assign a class label to every pixel (e.g. case study in Figure 1.A), the second describes each pixel as a linear mixture of pure spectra characteristic of those unknown individual sources [1] (e.g. case study in Figure 1.B). However, some situations may be borderline for the use of both methods, which is the case in a mixture of two or more components for which only some compositions of the mixture are observed, and data distribution shows clear clusters (Figure 1.C). This is what spectroscopists often face in analysing biomedical images v[2, 3].

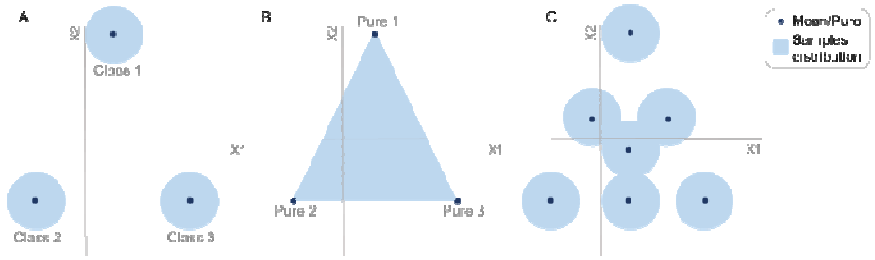

Figure 1. Normalized scores in PCA space

Here we present a series of simulations of hyperspectral image of three pure components facing different situations. Advantages and disadvantages of K-means and Multivariate Curve Resolution–Alternating Least Squares (MCR–ALS) approaches are evaluated in this work, in relation to the structure of the data, analysed in both the spectral and spatial mode to find a general application framework for classification and spectral unmixing methods. Results showed that MCR identified the three components in all the simulated datasets belonging to the cases in Figure 1.B and 1.C, including noisy simulations, and the results were highly depended of the added type of noise. K-means succeeded in classifying the data in the situation of Figure 1.A and 1.C. Of course, the classification technique for scenarios such as 1.B, in which the discrete samples are missed by varying the concentration profiles, was not efficient in terms of analysis time and results obtained. The presence of mixed pixels is one limitation because it can result in a misclassification problem. This work is a preliminary work and future development

OC16

on real datasets of biological tissue aims to investigate pure pixels in challenging scenarios.

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OC17

Biochar / transition metal dichalcogenides-based nanocomposites for electroanalytical purposes

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In the field of electrochemical (bio)sensors, nanomaterials (NMs) are gaining attention due to their peculiar properties that can offer new electroanalytical opportunities. Biochar (BH) is a carbonaceous material derived from carbon-rich biomasses, like agricultural or industrial waste. Properly produced and treated BH can possess useful electrochemical features and it is starting to be employed as an alternative NMs. In this framework, BH is particularly prone to form nanocomposites (NCs) since its ability to accommodate other nanomaterials, thanks to its porosity, large surface area, and ability to form networks [1]. Among NMs, transition metal dichalcogenides (TMDs) have been recently used in some works for (bio)sensing applications, showing large available surface area, structural versatility, and unique mechanical, optical, electrical and catalytic properties [2]. The main electroanalytical limitation of TMDs is their semiconductor characteristics that often hide useful features. In this presentation, NCs of BH and Group VI TMDs (i.e., MoS_2, WS_2, $MoSe_2$ and WSe_2) have been explored for the first time deepening the electroanalytical potentialities. To reduce the BH and TMDs dimensions a liquid phase exfoliation (LPE) conducted in water in presence of sodium cholate has been strategically used. NCs have been formed with BH and the four different TMDs, and after optimization of the NMs amounts, the electrochemical features and performances have been studied. Surprisingly, the electron transfer capacity of the BH was not affected by the presence of the TMDs, on the contrary, for selenides, it resulted improved. This demonstrates that BH is an excellent highly conductive support and, more interesting, maximizes the catalytic features of the TMDs, improving the electroanalytical performances. The BH-TMDs' potentiality has been demonstrated towards four different analytes of biological and agri-food interest i.e. dopamine (DP), serotonin (5-HT), quercetin (QR) and rutin (RT). Improved performances for the NCs, compared to commercial electrodes and the single NMs, were obtained. Limits of detections ≤ 0.2 μM were obtained for all the analytes. The most performing BH-TMD combinations have been selected and used for the contemporary determination of the neurotransmitters DP and 5-HT, and the flavonols 'isomers' (aglycone and glycone) QR and RT. Real samples analysis, with satisfactory recoveries, was obtained for cerebrospinal synthetic fluid and drugs for DP and 5-HT (recoveries 90-112%; RSD<6%, n=3), and analyzing food supplements for QR and RT (recoveries 90-102%; RSD<6%, n=3). Summing up, the proposed BH-TMDs NCs represents a cost-effective and

OC17

sustainable material particularly captivating for (bio)sensors development for electroanalytical applications.

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[2] Rojas, D. Della Pelle, F.; Del Carlo, M.; Compagnone, D.; Escarpa, A. *Electrochem Commun.* **2020**, *115*, 106718.

OC18

Improve the industrial process understanding through chemometrics

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The great part of the consumers expect products to always have the same quality properties values/ranges, such as taste, aspect, performance, and so on. In order to satisfy the consumer expectation the industries have a huge interest to strictly control own production line and applying real time monitoring. To achieve this aim, several process sensors (temperature, pressure, flux) are installed along the plant, however nowadays, in order to have a better control several companies are also implementing in chemical sensors (such as on-line spectroscopic sensor) to complement the classical process sensors. This work will illustrate as chemometrics is an invaluable tool to extract information from the diverse sensors data and hence furnishing a better understanding of and improved tools to monitor and control the industrial process. The pesto production in Barilla Company has been considered as a case of study. The basil, i.e. the raw material, that has a major influence on the quality, is controlled through off-line laboratory analysis and by a vision system that acquire in real-time RGB image of the basil passing on conveyor belt. In addition, an on-line near infrared (NIR) probe acquire in real-time the spectra of the intermediate of production, a mix of basil oil and salt. Finally, off-line laboratory analysis are used to control the final pesto quality. In particular, the focus has been on developing real time predictions of the final quality. To achieve this aim different multiblock methods have been evaluated to combine NIR and Imaging data in regression and classification models.

OC19

The impact of increasing structural rigidity on benzenesulfonamide small molecules in *V. cholerae* carbonic anhydrases inhibition: design, synthesis, computational and enzymatic studies

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Antimicrobial resistance (AMR) is a serious threat to the global Public Health, increased by COVD pandemics [1] and accounting for more than 30,000 deaths per year [2]. Moreover, in the geographical areas with low hygienic conditions and limited access to safe drinking water and food, every illness could be fatal, such as the difficult-to-treat drug-resistant infections, *i.e.* those from *Vibrio cholerae,* a Gram-negative bacterial species. Recently, the scientific community focused its efforts on the study of carbonic anhydrases (CAs), ubiquitary metalloenzymes catalyzing the hydration of carbon dioxide, as pharmacological targets and their modulation. In bacteria, these enzymes play relevant roles in the regulation of physio-pathological pathways [3], *i.e.* in *V. cholerae* the two CA isoforms (*Vch*αCA and *Vch*βCA) could be involved in the hydrogen carbonate-mediated expression of ToxT, a virulence-related transcription factor [4]. Hence, the development of *Vch*CAs inhibitors could represent a valuable strategy to treat cholera. Encouraged by the previous findings on benzenesulfonamide-bearing *Vch*CAs inhibitors [5], a large library of small molecules (Figure 1) was designed and synthesized exploiting a progressive increase in structural rigidity. In fact, the three series of derivatives are characterized by the presence of an amino, amide, and cyclic urea spacer in both para- and meta- positions with respect to the sulfonamide function.

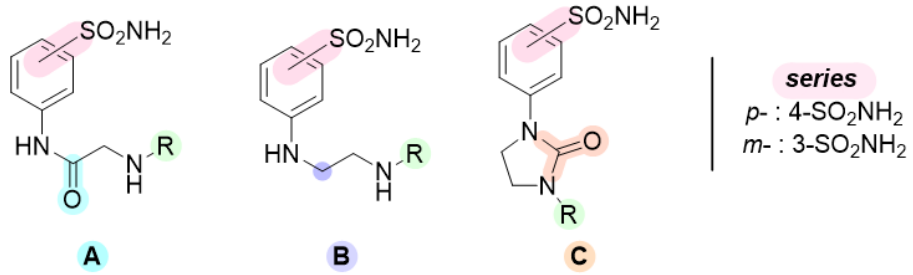

Figure 1. General structures of the three series of derivatives.

Then, the ability of these compounds to inhibit the bacterial and human CAs was assessed through a specific stopped flow-based inhibition assay, revealing a nano/micromolar activity for all the compounds on *Vch*CAs and, in some cases, a good selectivity. In the end, a computational study rationalized their binding pose and key interactions with the enzymes. While the 3D structure of *Vch*βCA, hCAs I and II are available, a homology model of the α isoform of *V. cholerae* was required to perform

OC19

the study.

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OC20

Targeting ESKAPE pathogens with novel cinnamic acid-based antimicrobials

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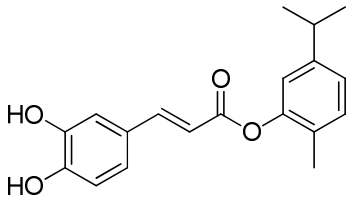
Bacteria develop several mechanisms of antimicrobial resistance (AMR), limiting the capacity to treat some infections, especially infections caused by ESKAPE pathogens [1]. In this work, the synthesis of novel cinnamic acid-based antimicrobials (**DM1-11**), as novel antibacterial drugs for the treatment of ESKAPE- related skin infections, has been reported [2]. Cinnamic acids were conjugated to carvacrol, a natural monoterpene, known for its antimicrobial properties, to treat complex skin infections [3]. **DM1-11** were investigated to select the best candidate to treat cutaneous infections caused by EKAPE pathogens. To evaluate their antimicrobial, antibiofilm, and wound-healing properties many assays were performed. Results revealed that **DM2**, bearing a catechol group on the aromatic ring of the cinnamic portion of the molecule, showed significant antibacterial activity against *S. aureus* and contrasted the biofilm-mediated *S. epidermidis* infection at low concentrations. Wound-healing assays showed that wound closure in 48 h was observed in **DM2**-treated keratinocytes with a better healing pattern at all concentrations tested. Cytotoxicity studies, determined on both human fibroblasts and keratinocytes cell lines, revealed that **DM2** did not show cytotoxicity at all tested concentrations. Taking together these data, **DM2** could be a safe wound healing topical agent for the treatment of skin wound infections caused by *S. aureus* and *S. epidermidis*.



DM2

Figure 1. Chemical structure of DM2.

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