

Towards more rational techniques for the isolation of valuable essential oils from plants

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Attention is drawn to the use of new and clean alternative methods for the isolation of essential oils from plants. A critical overview is presented of conventional methods (based on either organic solvent extraction or distillation) and new alternatives (including microwave-assisted extraction (MAE) as well as supercritical CO₂ (SC-CO₂) extraction and subcritical water extraction). The advantages and disadvantages of each technique are reported and special emphasis is given to the use of continuous subcritical water extraction which emerges as clearly advantageous over conventional techniques (by avoiding the use of organic solvents and considerably shortening the extraction time, as well as increasing the efficiency) and recent techniques, such as MAE (by increasing the efficiency) and SC-CO₂ extraction (by avoiding the co-extraction of cuticular waxes and lipids and the need for a sample drying stage prior to extraction). ©1999 Published by Elsevier Science B.V. All rights reserved.

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1. Introduction

Essential oils are aromatic substances that are widely used in the perfume industries, in the pharmaceutical sector and in the food and human nutrition field. They are mixtures of more than 200 compounds [1], that can be grouped basically into two fractions, a volatile fraction, that constitutes 90–95% of the whole oil and contains monoterpenes and sesquiterpene

hydrocarbons and their oxygenated derivatives, along with aliphatic aldehydes, alcohols and esters, and a non-volatile residue, that constitutes from 5 to 10% of the whole oil and contains hydrocarbons, fatty acids, sterols, carotenoids, waxes, coumarins, psoralens and flavonoids. The terpene fraction, ranging from approximately 99% of the volatile fraction in grapefruit oil to 60% in bergamot oil, makes little contribution to the flavour or fragrance of the oil. Moreover, since terpenes are mostly unsaturated compounds, they are decomposed by heat, light and oxygen to produce undesirable compounds which can give off-flavours and off-aromas. The oxygenated fraction is highly odoriferous and is mainly responsible for the characteristic flavours.

The isolation, concentration and purification of essential oils have been important processes for many years, as a consequence of the widespread use of these compounds. The common methods used so far are mainly based on solvent extraction and steam distillation. The drawbacks linked to these techniques have led to the searching for new alternative extraction processes. Another important aspect in the essential oils industry is the enhancement of the quality of the oil. As essential oils used in the food and perfume industries are commonly isolated by cold pressing, they contain more than 95% of monoterpene hydrocarbons, mainly limonene. In this context, it is worth mentioning the process known as deterpenation or 'folding'. The industrial practice of folding is to remove some of the limonene along with other unstable terpenes and to concentrate the oxygenated fraction. This process is carried out in order to improve the oil stability, increase the solubility of the oil in low-proof alcohol, in food solvent and in water and to reduce storage and transportation costs. The commercial methods currently used for folding essential oils are fractional vacuum distillation [2], selective solvent extraction [3] and chromatographic separation [4]. All these methods have important drawbacks, such as low yields, formation of by-products (owing

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to the time of exposure to high temperatures) and the presence of toxic organic residues in the extracts. The implementation of new techniques is thus mandatory in this context.

The aim of this article is to pay attention to the use of new alternatives, such as supercritical CO₂ (SC-CO₂) extraction and especially subcritical water extraction, as effective methods for the isolation of high-quality essential oils. A critical discussion is given from conventional techniques (including discontinuous, continuous and hybrid approaches) through the use of SC-CO₂ and particularly focused on the promising field of subcritical water extraction. The advantages and drawbacks of each method are also considered.

2. Conventional techniques

Techniques for the extraction of essential oils have been traditionally based on the use of discontinuous, continuous and hybrid approaches. The discontinuous techniques include the use of either organic solvents (assisted by ultrasounds or not) or water, whilst steam distillation and vacuum distillation are continuous methods. Some methods involving both continuous and discontinuous approaches, such as distillation–extraction and Soxhlet extraction, have also been reported.

2.1. Discontinuous conventional techniques

Organic solvent extraction has long been used for the isolation of essential oils from natural products. This technique uses either pure organic solvents or mixtures of them. An example of the former is the isolation of Australian tea essential oil by ethanol during 30 h with subsequent gas chromatography (GC)–mass spectrometry (MS) separation–detection [5]. Ethanol extraction has also been used prior to the determination of antioxidants in *Asteraceae* plants' essential oil by thin layer chromatography [6] and (by refluxing for 16 h) for that of vanillin and related phenolic components in vanilla by high performance liquid chromatography (HPLC)–ultraviolet (UV) [7]. Dichloromethane extraction prior to GC–MS has enabled both the isolation of terpenes from plant material [8] and the analysis of honeysuckle fragrance [9]. Methanol extraction has been reported for the isolation of poppy essential oil, with subsequent determination of opioids by HPLC–UV [10]. Extraction by organic solvent mixtures has also widely been used, in the pentane–dichloromethane extraction, for 2 days,

before the aroma analysis of guajava by GC–MS [11]. Also, sequential extraction with toluene, citric acid and benzene has been proposed as a step prior to the determination of vinblastine in rose essential oil by HPLC–UV [12].

Organic solvent extraction assisted by ultrasounds, also known as sonication, is another technique widely used for the isolation of essential oils from plants. Thus, sonication methods based on 30 and 20 min extraction with methanol–chloroform mixtures have been used for the isolation of white clove essential oil prior to detection of selenium compounds [13] and cyanogenic glucosides [14].

The use of organic solvent extraction (assisted or not by ultrasounds) has as its main shortcomings both the remaining of solvent residues in the extract, with the subsequent toxicological risk, and the long extraction time required in most cases for achieving efficient extractions. In addition, organic solvents have a low selectivity. Thus, apart from the desired substances, high molecular weight, non-volatile components, such as fatty oils, resins, waxes and colouring matters, are co-extracted. The infeasibility of automation of the technique is another important drawback to be taken into account.

Water extraction (under ambient conditions, without the application of an auxiliary energy source) has proved to be an effective technique for the isolation of essential oil from citrus as a step prior to GC–FID analysis [15]. The main shortcomings of this alternative lie again in its slowness (because an equilibrium must be established between the plant and extractant), its non-quantitative nature (because partitioning must be reached between the solid and liquid phases) and its infeasibility for automation.

Thus, discontinuous conventional techniques have the main and common drawbacks of requiring long extraction times, being unfeasible for automation and having both a non-quantitative nature and lack of selectivity, with the particular shortcoming of the presence of toxic solvent residues in the extract after liquid–liquid extraction.

2.2. Continuous conventional techniques

Steam distillation has been, together with solvent extraction, the most widely used conventional technique for the extraction of essential oils from plants. This technique has been applied extensively as a step prior to GC–MS for compositional studies of essential oils, such as in the case of calendula [16], valeriana [17], curcuma [18], marjoram [19], cinnamon [20] and of

rosemary, sage and lavender [21]. The evaluation of anti-microbial activity of essential oils has also been implemented widely by using steam distillation and GC-MS, as in the case of *Alpinia speciosa* [22], carrot [23] and wild plants growing in Argentina [24].

The use of this conventional technique has a major disadvantage (namely, the risk of losses of thermolabile compounds) and also two significant drawbacks (namely, the infeasibility for automation and the long time required for extraction).

An attempt to avoid thermolabile compound losses uses vacuum distillation, in which the conventional distillation process is performed at a reduced pressure, as in the extraction of Australian eucalyptus essential oil (as a step prior to the separation and determination of volatiles by GC-MS) [25]), but this still shows the two other drawbacks described before for conventional distillation.

2.3. Conventional hybrid (continuous-discontinuous) techniques

The simultaneous combination of steam distillation and solvent extraction, usually implemented by a Likens-Nickerson apparatus, has also been widely used for the isolation of essential oils whose composition was investigated by GC-MS, as in the case of pinus needle oil [26] and lavender [27], among others.

A combination of solvent extraction followed by hydrodistillation has been used for studying the chemical composition of essential oils as for that of the ginger flowers [28] and *Lauraceae* plants [29].

Soxhlet extraction with ethanol during 10 h has been used for the determination of glucosides in green vanilla beans prior to HPLC-UV separation-detection [30]. This leaching technique, although one of the most widely used, has hardly been applied for the isolation of essential oils, as a consequence of its slowness, its infeasibility for automation and especially because of the losses of volatiles and decomposition of thermolabile compounds caused by the high temperature to which the extract is continuously subjected.

3. New techniques

Microwave-assisted extraction (MAE) together with both SC-CO₂ and continuous subcritical water extraction (CSWE) are considered here as recent alternatives for the isolation of highly valuable essential oils. The studies already made, as well as future

trends arising from them (particularly in the case of CSWE), are discussed.

3.1. MAE

MAE [31] is a simple technique that provides a novel way of extracting soluble products into a fluid, from a wide range of materials, helped by microwave energy. The technique can be applied to both liquid phase extraction (when a liquid is used as solvent) and gas phase extraction (when a gas acts as extractant). The extraction process in liquid phase extraction (used for the isolation of essential oils from plants) is based on a basic physical principle, namely the different ability to absorb microwave energy depending on the chemical nature of the species being subjected to microwave irradiation. The parameter generally used as a measure of this physical property is the dielectric constant. Thus, liquid phase extraction assisted by microwaves is based on the fact that it is possible to immerse the matrix to be extracted into a solvent that is characterised both by a low dielectric constant and a relative transparency to microwaves. The first applications of the technique dealt with the extraction of essential oils from plant products [32]. The kinetics of the microwave extraction of rosemary leaves in hexane, ethanol or hexane-ethanol mixtures, as well as the influence of factors such as the source of the leaf, the microwave energy, duration of irradiation and sample load, on the rate of extraction of the compounds have been reported [33]. In more recent research, MAE has been coupled with liquid chromatography for the determination of herbicides in plant tissue [34].

3.2. SC-CO₂ extraction

Supercritical fluid extraction (SFE) is a relatively recent extraction technique based on the enhanced solvating power of fluids above their critical point [35,36]. Its usefulness for sample extraction is due to the combination of gas-like mass transfer properties and liquid-like solvating characteristics with diffusion coefficients greater than those of a liquid. The majority of analytical SFEs have been focused on the use of CO₂ because of its preferred critical properties, low toxicity and chemical inertness. SC-CO₂ extraction has also been used recently for the extraction of essential oils from plants, in an attempt to avoid the drawbacks linked to conventional techniques. Such is the case with the extraction of volatile oil in camomile flower heads [37]. The effects of the extraction time and extraction conditions have been studied for the

extraction of volatile compounds from lavandin and thyme [38] and from lavender and rosemary [39,40]. The composition of the essential oil extracted by SFE has been analysed in most of the cases by GC-MS coupling. Thus, many methods for identifying and quantitating flavour and fragrance compounds, such as those from rose [41], rosemary [42], peppermint [43], camomile [44], cardamon [45], strawberry [46] and guajava [47], have been described. The use of supercritical fluid chromatography coupled to MS has been proposed as a separation-detection system for the analysis of thyme essential oil isolated by CO₂ extraction [48]. The on-line coupling of the extraction and separation-determination steps (by SC-CO₂ extraction and GC-FID, respectively) has been proposed successfully for the analysis of herbs [49] and for vetiver essential oil [50].

SC-CO₂ extraction is also a suitable technique for enhancing the quality of essential oils obtained by conventional extraction methods, by means of fractionation and deterpenation. Thus, the separation of citrus oils into different classes of substances by SC-CO₂ has been widely investigated. Temelli et al. reported a method for the extraction of terpene hydrocarbons from cold-pressed Valencia orange oil with SC-CO₂, using both static and dynamic flow approaches [51]. Another paper has reported the SC-CO₂ extraction of terpenes from cold-pressed orange oil in a temperature range from 40 to 70°C and pressures from 83 to 124 bar [52]. The deterpenation and psoralens elimination of lemon peel oil by extraction with SC-CO₂ has also been reported [53]. The procedure included the increase of CO₂ density in successive steps. More recently, a method for the deterpenation of the citrus essential oils with SC-CO₂, using adsorption on silica gel to enhance the selectivity of the separation between the hydrocarbons and the oxygenated compounds, has been reported [54].

3.3. CSWE

CSWE, a technique based on the use of water as an extractant in a dynamic mode, at temperatures between 100 and 374°C (critical point of water, 221 bar and 374°C) and a pressure high enough to maintain the liquid state, is emerging as a powerful alternative for solid sample extraction [55]. The most outstanding feature of this leaching agent is the easy manipulation of its dielectric constant (ϵ). In fact, this parameter can be changed within a wide range just by changing the temperature under moderate pres-

sure. Thus, at ambient temperature and pressure, water has a dielectric constant of ca. 80, making it an extremely polar solvent. This parameter is drastically lowered by raising the temperature under moderate pressure. For example, subcritical water at 250°C and a pressure over 40 bar has $\epsilon = 27$, which is similar to that of ethanol and allows for the leaching of low-polarity compounds. Thus, subcritical water has been used widely to extract pollutants within a wide range of polarities from environmental samples [56-61]. Coupling CSWE with an immunoassay has been reported to provide a fast and efficient determination of pesticides [62] and of PAHs from soil [63]. Also, CSWE has been shown to be an effective alternative for the accelerated leaching of iron from soil [64]. The use of this technique in the field of essential oil isolation is recent and very promising. Thus, subcritical water under pressure, between 125 and 175°C, has been shown to extract rapidly the oxygenated fragrance and flavour compounds from rosemary, whilst the monoterpenes are extracted slowly and only very small amounts of the sesquiterpenes, waxes and lipids are removed. The extraction rate of the process is determined by the partition of the compounds between the plant material and the water and not by the rate of diffusion of the compounds out of the plant material. From the experiments reported in this paper, it can also be inferred that the composition and quality of the oil can be adjusted by controlling the amount of water relative to the mass of plant material [65]. Similar trends are observed for the isolation of marjoram essential oil with water at 50 bar, 150°C and 2 ml/min. An in-depth study of the variables affecting the extraction process was carried out in this case. The temperature was found to be the key variable. Its influence was studied between 100 and 175°C and a value of 150°C was the optimum because it provided the best quality essential oil (in terms of the amount of oxygenated compounds) [66]. In both cases, the analysis of the compounds was performed by GC-FID or GC-MS for determination and identification, respectively. CSWE, at 20 bar, 150°C and 2 ml/min, has been used recently for the isolation of essential oil from clove buds [67], by a procedure similar to that followed in the papers cited above. An additional rinsing step of the coil was mandatory in order to sweep out precipitated compounds. The subsequent separation-determination of the compounds was performed by GC-FID. Kinetic curves for the three major compounds in the oil (namely, caryophyllene, eugenol and eugenyl acetate) were determined, from which the fact that the extraction rate of the process was con-

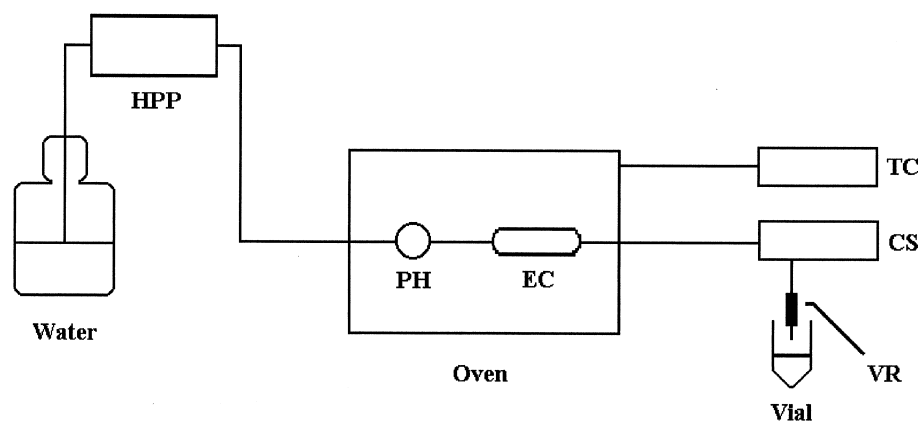


Fig. 1. Schematic diagram of a continuous water extractor. HPP, high-pressure pump; PH, pre-heater; EC, extraction chamber; TC, temperature controller; CS, cooling system; VR, variable restrictor. A three-way valve and on-off valve are included in the dynamics system before and after the oven for static-dynamic performance.

trolled by partitioning between the water and the plant matrix was inferred.

The experimental set-up to develop CSWE is very simple, as can be seen in Fig. 1. It consists of a water reservoir, a high-pressure pump, an extractor with a stainless steel cylindrical extraction chamber which is closed with screws at either end that permit the circulation of the leaching fluid through them. This chamber, together with a stainless steel pre-heater, is located in an oven designed to work up to 300°C. A cooler system is used to cool the fluid from the oven. Finally, a variable restrictor allows the desired pressure to be maintained into the dynamic system.

Very recently, subcritical water extraction has also been shown to be a promising technique for the determination of lemon oil, removing approximately 96% of the monoterpenes (mainly limonene) [68]. A simple change in the extractor shown in Fig. 1 (namely, in line connection of a three-way valve and off-on valve in the dynamic system, before and after the oven, respectively) allows for its hybrid static-dynamic performance. The modified approach has been used for isolation of laurel essential oil. The joint use of both extraction modes makes feasible shorter extraction times, a better quality of the oil produced, higher selectivity (as the composition of the extracts can be manipulated), cheaper cost and cleaner features as compared with both conventional and new extraction alternatives [69].

4. Comparison of techniques

A critical comparison between conventional and recent techniques, in terms of advantages and drawbacks of each, is summarised in Table 1.

4.1. MAE versus conventional techniques

The comparison between MAE and conventional techniques, such as Soxhlet extraction, has been reported for the isolation of fresh peppermint essential oil [32]. Soxhlet extraction was carried out for 6 h and microwave treatment consisted of a single irradiation period of 20 s, using hexane in both cases. From the study, the specificity of the MAE technique was demonstrated, as the microwave-treated plants retained the structural characteristics of their leaf surfaces, while most of the morphological characteristics of the leaves were removed by the Soxhlet extraction. The yield was greater for the Soxhlet extraction, but the quality of the MAE extract, as evidenced from the absence of chlorophyll, was far superior, thus avoiding the need for further purification of the essential oil, a step which was required when the Soxhlet was applied. Moreover, MAE offers other advantages over conventional techniques, such as a reduced energy consumption, smaller volumes of chemical solvents, use of less toxic solvents and a smaller quantity of waste products.

4.2. SC-CO₂ extraction versus conventional techniques

SC-CO₂ and hydrodistillation have been widely compared as techniques for the isolation of essential oils. Such is the case with Mexican spices [70], rosemary [71], savory, peppermint and dragonhead [72], Australian sandalwood [73] and coriander [74]. Comparisons between SC-CO₂ extraction, steam distillation and Soxhlet, as well as with steam distillation and solvent extraction, have been reported for the lavender, basil, clove and ginger [75] and for the iris essential oil [76]. SC-CO₂ extraction and sonication have also been compared as extraction methods for the determination of natural antioxidants in rosemary [77]. From all these studies, it can be inferred that the use of SC-CO₂ extraction for isolation of essential oils offers several significant advantages versus conventional techniques. The extractions are fast and they can be performed at lower temperatures (thus avoiding both losses and degradation of volatile and thermolabile compounds). The technique is also feasible for automation, allowing for coupling with chromatographies and, hence, the analysis of extracted substances whose concentration in plants is low. Moreover, as the solvent strength of supercritical fluids is proportional to their density, a selective extraction can be obtained using either a pressure or temperature gradient. Finally, solvent-free extracts can be obtained after the depressurisation stage. For these reasons, the application of SC-CO₂ extraction versus conventional techniques for the isolation of essential oils from herbaceous matrices has been considered very promising in principle. Unfortunately, some difficulties exist, because SC-CO₂ shows a high affinity not only for essential oil components but also for many other classes of low-polarity compounds included in

the vegetable matrix, such as cuticular waxes, fatty acids, colouring matters and resins. Except for cuticular waxes, the content of these unwanted compounds can be controlled by choosing appropriate extraction conditions. In a single stage extraction, the co-extraction of cuticular waxes is unavoidable, because they are soluble in SC-CO₂ and thus favourably extracted. Nevertheless, it is possible to obtain pure essential oils with SC-CO₂ extraction, adopting a more sophisticated process scheme first proposed by Stahl et al. [78] and then successfully applied to the isolation of rosemary essential oil [71]. It consists of a fractional separation, applied following the extraction stage and performed within two separation vessels in series, operated and located downstream from the extractor. In this way, the essential oil is obtained in two steps, thus making the selective elimination possible of non-polar compounds, such as cuticular waxes. Another drawback linked to the use of SC-CO₂ extraction is the high purchase and maintenance cost required for this equipment.

4.3. CSWE versus conventional techniques and SC-CO₂ extraction

The research reported so far on the use of subcritical water for the continuous extraction of essential oils compares this technique with hydrodistillation [65–67], with CO₂-SFE [65,67] and with Soxhlet extraction [67]. From these studies, the use of superheated water as an extractant reveals several important advantages versus hydrodistillation. Thus, the extraction time required is lower and the quality of the oil produced by CSWE is much better, because of the high content of oxygenated compounds (the more odoriferous and hence, the more valuable) and the low content of terpenes. Therefore, the reproduction of the

Table 1
Comparison between conventional and recent techniques for the isolation of essential oils from plants

Aspect	Conventional techniques	Recent techniques
Extraction time	Long (–)	Short (+)
Efficiency	Good (+)	Worst/better (–/+) ^a
Quality of the extract	Bad	Good
Presence of toxic residues in the extract	Yes (–)	No (+)
Feasibility for automation	No (–)	Yes (+)
Extraction conditions	Drastic (–)	Milder (+)
Selectivity	No (–)	No/yes (–/+) ^b
Cost	Medium (–)	Medium/low (–/+) ^b

^aMAE-SC-CO₂ extraction and CSWE.

^bSC-CO₂ extraction and CSWE.

Table 2
Comparison between SC-CO₂ and subcritical water extraction for the isolation of essential oils from plants

Aspect	SC-CO ₂ extraction	CSWE
Drying stage	Yes (-)	No (+)
Co-extraction of cuticular waxes	Yes (-)	No (+)
Acquisition cost	High (-)	Medium (+)
Maintenance cost	High (-)	Low (+)
Extraction conditions	Mild (+)	Medium (-)
Pre-concentration effect	Yes (+)	No (-)
Environmentally clean character	Yes (+)	Yes (+)

natural aroma of the essential oil is better for the CSWE oil. The efficiency provided by CSWE is also better (about five times in the case of marjoram essential oil [66]) than that provided by hydrodistillation. Finally, the methods based on the use of subcritical water are economically advantageous over hydrodistillation, owing to the fact that the high amount of water required for CSWE (about 10 times more) is overwhelmingly compensated by the energy cost required for steam distillation, that surpasses that required by CSWE about 20 times [65]. This last feature is a key to the potential future implementation of this technique as a real alternative to hydrodistillation techniques.

The comparison of CSWE with SC-CO₂ extraction has also been reported [65,67] and, although the final yield of one of the major compounds (caryophyllene) in clove essential oil was shown to be less with CSWE, this technique in general is clearly advantageous versus SC-CO₂ extraction. The advantages and drawbacks of both techniques are compared in Table 2. The two main shortcomings of the application of subcritical water for the isolation of essential oils from plants can be easily overcome: first, the reactive nature of water under these conditions, that can damage the extractor, is precluded by using ultrapure and degasified water for performing the extraction. The most important drawback of CSWE for the isolation of essential oil from plants, the relatively high temperature required, makes it mandatory to perform a preliminary study of the thermal stability of the extracted compounds. In spite of these negative aspects derived from CSWE, the technique has been demonstrated to be advantageous compared to SC-CO₂ extraction, as can be inferred from Table 2, where the techniques are compared critically. Thus, there is no co-extraction of cuticular waxes in a single extraction stage, thus avoiding the use of the sophisticated system required

by SC-CO₂ extraction for obtaining pure essential oils. Moreover, plant material often needs to be dried to make extraction by carbon dioxide effective, as water is not very soluble in it and tends to mask the desired compounds. Thus, the drying stage represents an additional cost and the risks of losing volatile aroma compounds that are absent in subcritical water extraction. The equipment for CSWE is clearly cheaper than that required for SC-CO₂ extraction (as the pressures involved are much lower). The use of water also allows for a substantial saving in the maintenance cost, as the price of CO₂ of supercritical grade is prohibitive.

The comparison of CSWE with Soxhlet extraction has also been considered [67]. The final yields obtained for the three major compounds of clove essential oil are slightly lower by Soxhlet extraction for 24 h with dichloromethane than those provided by CSWE at 2 ml/min, 150°C, 20 bar and only 100 min of extraction. Thus, CSWE is a quicker technique and avoids the presence of toxic organic residues in the extract. Moreover, the nature of the extracted components from SWE can be manipulated just by raising the temperature under a pressure high enough to maintain the liquid state, allowing for a high selectivity and a wide range of species to be extracted.

Thus, CSWE has emerged as a promising and powerful alternative to both conventional (hydrodistillation and solvent extraction) and new techniques (SC-CO₂ extraction), showing significant and decisive advantages over all of them.

5. Conclusions

The need for the implementation of more rational techniques for obtaining high-quality essential oils is an important task since the use of these products in industry is massive and the techniques used so far are clearly environmentally aggressive, slow and not suitable both for thermolabile and volatile compounds (organic solvent extraction, Soxhlet and hydrodistillation) or expensive and non-selective (SC-CO₂ extraction). Moreover, most of them (such as organic solvent extraction and hydrodistillation) are difficult or impossible to manipulate in order to obtain a product with the desired characteristics. In this context, CSWE appears as a promising method that still needs to be developed and studied in-depth, but which will probably be implemented in the near future for industrial essential oil production, as a conse-

quence of the significant and numerous advantages it shows over alternatives.

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book reviews

Handbook of chemometrics and qualimetrics

Handbook of Chemometrics and Qualimetrics: Part A, by D.L. Massart, B.G.M. Vandeginste, L.M.C. Buydens, S. DeJong, P.J. Lewi and J. Smeyers-Verbeke, Data Handling in Science and Technology 20A, xvii+867 pages, Elsevier, Amsterdam, 1997, Price \$273; ISBN 0-444-89724-0

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The Handbook of Chemometrics and Qualimetrics: Part A is a well-written text with information content applicable to both novice and experienced users of chemometrics. Essentially, the Handbook is a tutorial on applied statistics for chem-

ists. Many of the familiar chemometrics methods for pattern recognition, regression, and validation are not extensively covered. This is left to the myriad of other chemometrics texts. Instead, statistical methods, many familiar in name only to most chemists, are chosen and presented in an easy to understand manner.

One nice feature of the text is that every chapter is relatively self-contained; someone with a little knowledge in chemometrics can pick up the Handbook and begin reading from the chapter that is of interest without stumbling over nomenclature or convention. Each chapter contains basic background information that is essential to under-

stand a particular subject, and discussion regarding the intricacies of the state of the art. The examples are left general enough that the nuts and bolts of the statistical method being presented are not lost in the details of the chemistry and the ability to translate the subject to numerous other applications is evident. Every chapter concludes with a succinct list of key references.

The first two chapters serve as an introduction. The first puts chemometrics into context, discussing the utility and potential applications of chemometrics as well as providing a brief historical overview of the maturation of the field. Chapter 2 presents a basic tutorial on statistical nomenclature, definitions, data visualization, and propagation of errors. This chapter is the assumed