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Use of solid–liquid distribution coefficients to determine retention properties of Porapak-Q resins Determination of optimal conditions to isolate alkyl-methoxypyrazines and beta-damascenone from wine

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Abstract

The solid–liquid distribution coefficients of different analytes – all of which are important aroma compounds – between hydroalcoholic solutions or wines and different sorbents have been determined by measuring the amount of analyte removed by a given mass of sorbent in equilibrium with a given volume of standard solution. These data have shown that the best extraction conditions for non-polar compounds from wine are the use of Porapak-Q resins and 6% (v/v) alcoholic solutions. Phase ratio, hold-up volumes and number of plates for Porapak-Q beds have been measured in different experiments. With all these data it has been possible to calculate breakthrough volumes in good agreement with experimental results. The Lövkvist–Jönsson model is more appropriate for estimating breakthrough volumes of a 2-cm Porapak-Q bed. The model estimates that a 5-cm bed is needed to achieve a quantitative recovery of 3-alkyl-2-methoxypyrazines and β-damascenone from 500 ml of wine (diluted to 1000 ml with water). Experimental results confirm the predictions of the model and show that in a single isolation step detection limits below 10 ng/l can be reached for these compounds using GC–MS detection.

Keywords: Solid-phase extraction; Wine; Breakthrough volume; Distribution coefficients; β-Damascenone; Alkyl-methoxypyrazine

1. Introduction

Solid phase axtraction (SPE) has become an important sample preparation technique for either matrix simplification or trace enrichment [1–9]. Its great advantages are its ability to be automated, the limited use of solvents, the elimination of problems related to emulsions, and the possibility of exploiting additional selectivity and efficiency effects. Due to its flexibility, SPE is a multivariate process whose optimization should be approached from a multivariate perspective. The optimization of a SPE procedure implies the selection of the most appropriate sorbent, the design of the SPE bed, the determination of the volume of sample to load, and of the nature and volumes of solvents to wash the column first and further elute the analyte [2,5,10,11].

The complexity of the optimization process makes

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it necessary to carry out an excessively large number of experiments, if the optimization is to be done properly and in a systematic way. Perhaps this explains why, in most cases, studies do not really explore all the existent possibilities to reach the optima and more often use a trial-and-error approach to find experimental conditions good enough to extract or enrich the compounds of interest. In any case, SPE method development is a tedious and time-consuming process. There is a logical interest, therefore, in the use of alternative approaches allowing for a simulation of the SPE process.

SPE theory, particularly applied to method development, has been thoroughly reviewed recently [6,10]. The most important parameter controlling the SPE process is the breakthrough volume, which is the volume that can be loaded onto a SPE bed providing a given ratio of outlet to inlet analyte concentration. Other authors use a definition based on mass instead of concentration [3,12,13]. According to this, the breakthrough level is the fraction of the total mass of analyte which has passed out of the column and has been lost. Breakthrough volumes can be determined experimentally in several ways using either on-line or off-line detection, but this is time consuming, particularly if off-line methods are used [11]. Because of this, several methods to estimate breakthrough volumes from solute properties have been considered, among them, the solvation parameter model has provided highly satisfactory results [14–16]. Alternatively, models based on the relationships between breakthrough volumes and the different operating parameters of SPE devices are useful [2,3,17,18], since they allow the estimation of breakthrough volumes provided that a few parameters from the SPE bed and from the analyte are known. Required bed parameters are N, number of plates, and V_M, hold-up or dead volume of the bed. The chromatographic retention factor of the analyte, k, is the most often used parameter to measure its retention properties. The two expressions most commonly used are as follows:

$$V_B = (1 + k)V_M\left(1 - \frac{2.3}{\sqrt{N}}\right) \quad (1)$$

$$V_B = \frac{1}{\sqrt{a_0 + \frac{a_1}{N} + \frac{a_2}{N^2}}}(1 + k)V_M \quad (2)$$

Eq. (1) gives the breakthrough volume at the 1% breakthrough level and applies to systems in which the conditions of linear chromatography apply and the plate number is large enough. Eq. (2) was proposed by Lövkvist and Jönsson and applies to systems with a small number of plates. The coefficients a_0, a_1 and a_2 are characteristic of the breakthrough level. The values for a_0, a_1 and a_2 can be found in Ref. [3]. There are several authors that have confirmed that this relationship holds in different cases [14,15,19–21]. Both models suggest that the chromatographic retention factor is the key parameter determining the breakthrough volume since, for a limited range of flow-rates and a specified sampling system, changes in the hold-up volume and plate number provide only a marginal change in breakthrough volumes [11], of course, provided that N and V_M are not very small.

There are two approaches for determining retention factors. One of the proposed systems involves the use of HPLC to measure the chromatographic retention characteristics of the analyte by using a SPE cartridge as chromatographic column [2,4,16–18]. A second approach is the equilibrium method in which a given volume of sample solution with a known concentration of analyte is continuously circulated through the SPE bed until a steady state is reached [22–25]. The mass of analyte retained in the SPE bed is then measured by elution and analysis and related to the retention factor through the expression k = mass sorbed/(mass in a ''hold-up volume'' of liquid phase).

In this paper, we have used quite a similar approach, based also in equilibrium conditions. A known mass of sorbent is contacted and equilibrated in a glass vial with a given volume of solution containing known amounts of analytes. After the equilibrium is reached, the system is analyzed to determine the solid–liquid distribution coefficients of the analytes between the sample and the sorbent. The sorbent/liquid phase ratio of the SPE bed is separately determined and used to calculate the retention factor. This approach is less rigorous than the previous ones, but it can provide results accurate enough to model SPE systems with a not very large effort, since retention factors for several analytes and several sorbents can be determined in the same batch with a simple experimental design. The approach has been applied to the development of an optimal

isolation procedure on Porapak-Q resins of some important wine volatile compounds present at very low concentrations such as 3-alkyl-2-methoxypyrazines and β-damascenone.

2. Material and methods

2.1. Materials

The following solvents were used: absolute ethanol, ACS-quality from Riedel-de Häen (Seelze, Germany); dichloromethane, HPLC-quality from Fisher Scientific (Loughborough, UK); methanol, HPLC-grade from Lab-Scan (Dublin, Republic of Ireland); diethyl ether, P.A.-grade from Fluka (Buchs, Switzerland) and pentane, 95% pestipur from SDS (Peypen, France). Water was obtained from a Milli-Q purification system (Millipore, Bedford, MA, USA). The solid sorbents used were XAD-4 and Porapak-Q, purchased from Supelco-España (Madrid, Spain), octadecyl-functionalized silica gel (C_{18}) from Aldrich (Steinhein, Germany) and Carbograph 1 SPE from Alltech (Deerfiel, IL, USA). The following chemical standards were used: acetic acid from Panreac (Barcelona, Spain); sotolon, isoamyl alcohol, isovaleric acid, guaiacol, ethyl pentanoate, phenylethyl acetate and 3-isopropyl-, 3-isobutyl- and 3-*sec*.-butyl-2-methoxypyrazines from Aldrich-España (Madrid, Spain); furfural from Chemservice (West Chester, PA, USA) and β-phenylethanol from Fluka-España (Madrid, Spain); β-damascenone was a gift from Firmenich-España (Barcelona, Spain).

The wines used in the study were: (1) a young red wine made with grenache grapes (pH 3.2; 12.5%, v/v, alcohol); (2) a 4-year-old red wine (pH 3.3; 12.5%, v/v, alcohol) and (3) a young red table wine (pH 3.8; 13%, v/v, alcohol).

The internal standard solution was 2-octanol in ethanol (1000 μg/ml). The hydroalcoholic solutions were 12 or 6% (v/v) in ethanol, 5 g/l tartaric acid, pH adjusted to 3.2 with NaOH 1 *M* and containing 10 mg/l of the selected volatile compounds.

2.2. Determination of the distribution coefficients of solid–liquid systems

Solid sorbents were previously washed with methanol and dried under vacuum (25 mm until constant weight). An exact weight of the sorbent (between 0.45 and 0.50 g) was placed inside a 30- or 100-ml glass vial, together with a volume (between 10 and 50 ml) of hydroalcoholic solution or wine sample containing 10 mg/l of the selected compounds. The vials were shaken softly for 24 h. After this, 7.9 ml of the liquid were removed and added to a 15-ml centrifuge tube containing 3.3 g of $(NH_4)_2SO_4$ and 20 μl of the internal standard solution and 1 ml of dichloromethane. The tubes were closed, shaken gently for 45 min, centrifuged and the organic phases were analyzed by GC–FID. Relative areas were interpolated in calibration graphs, built by the analysis of hydroalcoholic solutions containing known amounts of volatile compounds. All the experiments were duplicated.

2.3. Determination of phase ratios, holdup volumes and number of plates of the SPE systems

Phase ratio, Φ, and hold-up volumes, V_M, were directly measured by weighing the chromatographic beds before (m_0) and after (m_1) the addition of the necessary amount of mobile phase (whose density, ρ, was calculated) to form the bed. $m_1 = m_0 + V_M\rho$, then, $V_M = (m_1 - m_0)/\rho$. And the phase ratio, Φ, is then $\Phi = m_0/V_M$.

The hold-up volumes were estimated, in addition, directly from the breakthrough curves through the relationship $V_M = V_R/(1 + k)$.

The number of plates, *N*, was estimated from the breakthrough curves built in frontal elution experiments as described below. The graphic procedure for its determination is described in Ref. [2].

2.4. Determination of breakthrough volumes and breakthrough curves

An exact weight of the dried sorbent (around 0.60 g) was suspended in methanol and then placed inside a glass chromatographic column (1 cm I.D.). The bed ($L = 2$ cm) was then washed with 10 ml of a 12% ethanol solution and then 500 ml of the hydroalcoholic solution (12%) containing the selected compounds were loaded at a flow-rate of 1 ml/min.

The eluate of the column was recovered in fractions of 5 ml (first 100 ml), 10 ml (100–300 ml) or 20 ml (300–500 ml). Aliquots of 5 ml of these

fractions were then placed into 15-ml centrifuge tubes containing 2.1 g of $(NH_4)_2SO_4$, together with 20 μl of the internal standard solution and 1 ml of dichloromethane, and were extracted and analyzed by GC–FID. The breakthrough volumes were determined as the volumes at which a given percent of mass of analyte is eluted out of the column.

2.5. Isolation of methoxypyrazines and β-damascenone from wines

Samples of 1.5 g of dried Porapak-Q resins were packed in a glass chromatographic column (1 cm I.D.) to form a 5-cm high bed. The resins were conditioned first with 20 ml of methanol and later with 20 ml of a 6% (v/v) hydroalcoholic solution. Wine, spiked or not with 1 μg/l of methoxypyrazines and β-damascenone, was diluted with water 1:1, and 1 l of diluted wine was then loaded onto the column at 5 ml/min. After this, 50 ml of a 12% (v/v) hydroalcoholic solution were passed through to wash the system. Elution was carried out with 15 ml of diethylether–pentane (1:1). This volume was then concentrated in a microKuderna-Danish fitted with a three-ball Snyder column up to 1 ml, and later under nitrogen up to 100 μl. The extract has 5 μl of the internal standard added and was then analyzed by GC–MS. This experiment was carried out with six samples, the three wines spiked and non-spiked.

2.6. Gas chromatography–flame ionization detection conditions

Apparatus: Hewlett-Packard 5890 Series II fitted to a 7673 HP autosampler; analytical column: Carbowax 20 *M*, 50 m×0.32 mm and 0.5 μm film thickness from J&W (Folsom, CA, USA); the column was preceded by a 2 m×0.53 mm uncoated precolumn; temperature program: 40°C for 5 min, then raised at 5°C/min up to 190°; carrier gas: H_2 at 3 ml/min; splitless injection: splitless time=20 s, split flow=30 ml/min; injection volume: 3 μl.

2.7. Gas chromatography–mass spectrometry conditions

Apparatus: Star 3400CX gas chromatograph fitted to a Saturn 5 electronic impact mass spectrometer from Varian; analytical column: DB-WAX, 60 m× 0.32 mm and 0.5-μm film thickness from J&W (Folsom, CA, USA) preceded by a 2 m×0.53 mm uncoated precolumn; carrier gas: He at 1 ml/min; temperature program: 40°C for 5 min, then raised to 200°C at 2°C/min; transfer line temperature: 220°C; injection was made with a 1093 autosampler from Varian; injector: SPI (septum-equipped programmable injector). Conditions: initial temperature= 30°C for 6 s, then raised to 190°C at 200°C/min; injection volume: 1 μl; mass spectrometry: mass range=m/z 35–200; filament current: 19 μA.

3. Results and discussion

3.1. Measurement of solid–liquid distribution coefficients

Preliminary experiments showed that solid–liquid distribution coefficients, *K*, can be measured just by contacting a known mass of sorbent with a volume of solution containing a known concentration of analytes. After equilibration time, the solution is analyzed to determine the remaining amount of analytes in the liquid solution. The requirements that the system must meet is that the resins must be completely dry to ensure an accurate mass weighting, equilibration time is achieved and the amount of analyte extracted by the resin is between 5 and 95% to ensure a more accurate measurement. This last requisite can make it necessary to essay different masses of sorbent or volumes of solution if the analytes behave differently. However, the concentration and number of analytes in the contacted solutions do not seem to be critical. In fact, consistent *K*-values have been found by essaying solutions containing a different number of analytes (1–20) present at different concentrations (0.1–20 μg/ml).

This approach has several advantages. First, it is possible to estimate the ability of a sorbent to extract compounds from a given solution, a previous optimization of the elution conditions or the dimensions of the SPE system not being necessary. Secondly, it is easy to carry out a comparative study between several sorbents. Third, a quite large number of

analytes can be tested simultaneously and, fourth, the determination of *K* can be made in a matrix similar to the real one.

3.2. Optimization of extraction conditions

Table 1 gives the *K*-values of a selected group of odorants measured in different systems. The three first columns give data exclusively from Porapak-Q resins in three different chemical environments: a 12% (v/v) hydroalcoholic solution, a 6% (v/v) hydroalcoholic solution and a wine diluted with water to adjust its alcoholic degree to 6%. These data clearly show that there are different behaviors with regards to the effect of the chemical environment on the solid–liquid distribution coefficients. A decrease of the alcoholic degree does not make *K* increase in the case of the most polar compounds, such as sotolon or acetic acid. On the contrary, in the case of not-very polar compounds, such as isovaleric acid or guaiacol, a decrease of the alcoholic degree brings about an increment of *K* by a factor two, and in the case of non-polar compounds by factors between 5 and 10. The conclusions of the study are that wines should not be diluted if polar compounds are the analytical targets, but that a 1:1 dilution with water is highly convenient if the analytes are non-polar compounds. In this case, not only the retention ability of the resins is improved but, the extract will contain less amounts of polar compounds, which are the major source of interference in the analysis of volatile compounds from alcoholic beverages. The third column of data in the table gives the values of *K* for the same analytes in a 6% (v/v) wine. A comparison of these figures with those obtained from hydroalcoholic solutions shows that the *K*-values obtained in a diluted wine are closer to those obtained in a 12% (v/v) hydroalcoholic solution than to those obtained in a 6% hydroalcoholic solution. The reasons for this are the presence in wine of compounds other than ethanol with an effect on both, the solubility of analytes in the liquid phase, and on the behavior of the resins.

The last four columns of data in the table give the solid–liquid distribution coefficients of the selected analytes between a wine and different sorbents. Data clearly show that Porapak-Q is the best sorbent of all those present in the table to extract non-polar compounds from wine, while Amberlite XAD-4 resins gives maximum *K*-values for polar compounds. The C_{18} sorbent has far smaller *K*-values, but it seems to have special affinity towards some non-polar compounds such as β-damascenone, which could be exploited to develop selective isolation strategies for this compound. Finally, the carbon-based sorbent showed a poor behavior perhaps due to its high affinity to some polyphenols of wine. In fact, wines equilibrated with this sorbent were decolored, which indicates that it is not a convenient sorbent to extract volatile compounds from wine.

Table 1
Solid–liquid distribution coefficients of a selected group of analytes in hydroalcoholic solutions or wine and several sorbents

Compound	Porapak-Q			XAD-4	Carbograph	C_{18}
	12% wine	6% wine	6% wine[a]	6% wine[a]	6% wine[a]	6% wine[a]
Acetic acid	7	8	8			
Sotolon	13	15	14	54	13	14
Furfural	17	32	25	61	7	6
Isoamyl alcohol	43	70	55	130	12	13
Isovaleric acid	56	94	52	123	5	5
β-Phenylethanol	128	257	116	202	4	9
Guaiacol	138	275	169	269	8	8
Ethyl pentanoate	1105	9633	5689	4920	66	129
Phenylethyl acetate	2230	21 128	2742	749	10	87
3-Isobutyl-2-methoxypyrazine	2120	18 650	1934	860	31	288
β-Damascenone	3048	≫ 30 000	3731	603	3	622

[a] Wine diluted with water to a final 6% (v/v) alcoholic degree.

Table 2
Properties of Porapak-Q beds

	Porapak-Q
Mesh size	80/100
Particle diameter (d_p, mm)	0.18
Phase ratio (Φ, g of sorbent per ml of mobile phase)	0.94
Hold-up volume per cm of bed (ml)[a]	0.34
Hold-up volume per cm of bed (ml)[b]	0.35±0.03
Plate height (H, mm)	2.0±0.2
Plates per cm of bed (N/l, plates/cm)	5.0±0.5
Permeability coefficient (ϵ)	0.43
Interparticle mobile-phase velocity (u, mm/s)	0.5

[a] Determined as volume of liquid in the bed.
[b] Calculated from breakthrough curves.

3.3. Properties of Porapak-Q beds

Solid–liquid distribution coefficients corrected with the phase ratio, Φ, can be used to calculate the analyte chromatographic retention factors, k. In this work we have determined the phase ratio of the system Porapak-Q/synthetic wine by measuring the amount of liquid in the chromatographic bed, as it is detailed in Section 2. Once the k-values are known, they can be used, in turn, to calculate retention volumes and breakthrough volumes but, these calculations require a previous knowledge of the bed hold-up volumes and of the chromatographic efficiency of the sorbent beds. Both figures have been determined by the study of breakthrough curves of different analytes, as it is shown in Refs. [3,10,11]. In addition, the hold-up volume was also directly measured as the amount of liquid taken by the bed, in the same experiment in which phase ratio was calculated. As data in Table 2 show, there is a good agreement between hold-up volumes determined by the two different methods. Plate heights determined for different compounds were also similar (RSD= 10%) and, as it is shown in the table, a bed of Porapak-Q resins can provide up to five plates per cm at low flow-rates (1 ml/min). No attempt was made to measure the efficiency of the beds at higher flow-rates. A plate height of 2 mm is well below the figures obtained for cartridges packed with silica-based sorbents [16], which is in agreement with the higher particle size of Porapak-Q resins. This indicates that although retention properties of this sorbent are very good its physical properties are far from being optimal from the point of view of the chromatographic efficiency in these SPE experiments.

3.4. Comparison between measured and calculated V_B-values

Table 3 gives the measured retention and breakthrough volumes of several analytes and the calcu-

Table 3
Measured and calculated breakthrough volumes[a] for a 2-cm bed of Porapak-Q resins loaded with a 12% hydroalcoholic solution[b]

Compound	Measured			Calculated		
	V_R	V_B (1% level)	V_B (10% level)	Gaussian model (1% level)	Lövkvist–Jönsson model (1% level)	Lövkvist–Jönsson model (10% level)
Acetic acid	5	1	2	0	1	1
Sotolon	12	6	11	2	6	8
Furfural	11	5	9	3	7	11
Isoamyl alcohol	32	13	29	8	17	26
Isovaleric acid	40	17	36	10	23	34
β-phenylethanol	89	41	83	22	51	77
Guaiacol	92	42	86	24	55	83
Ethyl pentanoate	>500	410	>500	190	439	659
Phenylethyl acetate	>500	>500	>500	383	886	1329
Isobutyl-2-methoxypyrazine	>500	>500	>500	364	842	1264
β-Damascenone	>500	>500	>500	524	1211	1817

[a] Given in term of mass, except those estimated with the Gaussian model, which are in concentration terms.
[b] All data in ml.

Table 4
Solid–liquid distribution coefficients between Porapak-Q and wine diluted 1:1 with water and estimated breakthrough volumes (in ml) for SPE beds of different size

Compound	*K*	Bed length (cm)					
		1	2	3	4	5	10
3-Isobutyl-2-methoxypyrazine	1934±57	295	780	1324	1895	2482	5512
3-Isopropyl-2-methoxypyrazine	1148±43	175	463	786	1125	1474	3273
3-*sec*.-Butyl-2-methoxypyrazine	2004±52	305	808	1372	1964	2572	5711
β-Damascenone	3731±109	569	1504	2553	3655	4788	10 631

lated values using the previously measured solid–liquid distribution coefficients, dead volume and plate number. Two different approaches have been considered to calculate breakthrough volumes. The first one is based in the gaussian model, and the second one, uses the equation proposed by Lövkvist and Jönsson. A small part of the differences observed between the measured and the calculated V_B with the gaussian model are due to the fact that this last model estimates V_B in concentration terms, while the table gives V_B in terms of mass. However, differences between both V_B values are small and, therefore, it can be said that results given by the gaussian model show a poor fit to experimental data. On the contrary, results clearly show that the Lövkvist–Jönsson model is more appropriate for predicting breakthrough volumes in this kind of SPE beds with only ten theoretical plates, in agreement with results from other groups [3,14,15,19–21].

The degree of agreement between measured and calculated values can be considered satisfactory, as the high linear regression coefficients between both sets of data show (r^2 is in both cases higher than 0.997). However, calculated breakthrough volumes at the 1% level are slightly higher than measured ones, while the opposite is observed at the 10% level. There is no clear reason for this, except perhaps some bias introduced in the graphic measurement of breakthrough volumes in term of mass.

3.5. Development of a method to isolate alkyl-methoxypyrazines and β-damascenone from wine

According to the previous experimental results, it seems feasible the use of solid–liquid distribution coefficients, together with some sorbent properties such as those shown in Table 2, to model and optimize SPE systems. Here we will show an application of the method to the isolation of alkyl-methoxypyrazines and β-damascenone from wine. The three different alkyl-methoxypyrazines that can be found in wines and β-damascenone are very important odorants that can be present at very low concentrations and that can be odor-active at concentrations as small as 2–20 ng/l [26]. As it is shown in Table 1, Porapak-Q is the best sorbent of all those considered in that table and the best extraction conditions are reached for 6% alcoholic solutions. Solid–liquid distribution coefficients for the four compounds can be seen in Table 4 and vary from 1000 to 3000 in wine diluted 1:1 with water. Table 4 also shows the results of the simulation made with the Lövkvist–Jönsson equation taking as input the average *K*-values shown in Table 4, and phase ratio, hold-up volume and plate number data

Table 5
Recoveries and estimated detection limits of a method based on the isolation of analytes from 500 ml of wine in a 5-cm SPE (Porapak-Q) bed[a]

	Recovery (%)	Detection limits (ng/l)
3-Isobutyl-2-methoxypyrazine	104±3	6
3-Isopropyl-2-methoxypyrazine	102±2	4
3-*sec*.-Butyl-2-methoxypyrazine	99±2	2
β-Damascenone	101±2	6

[a] GC–MS analysis.

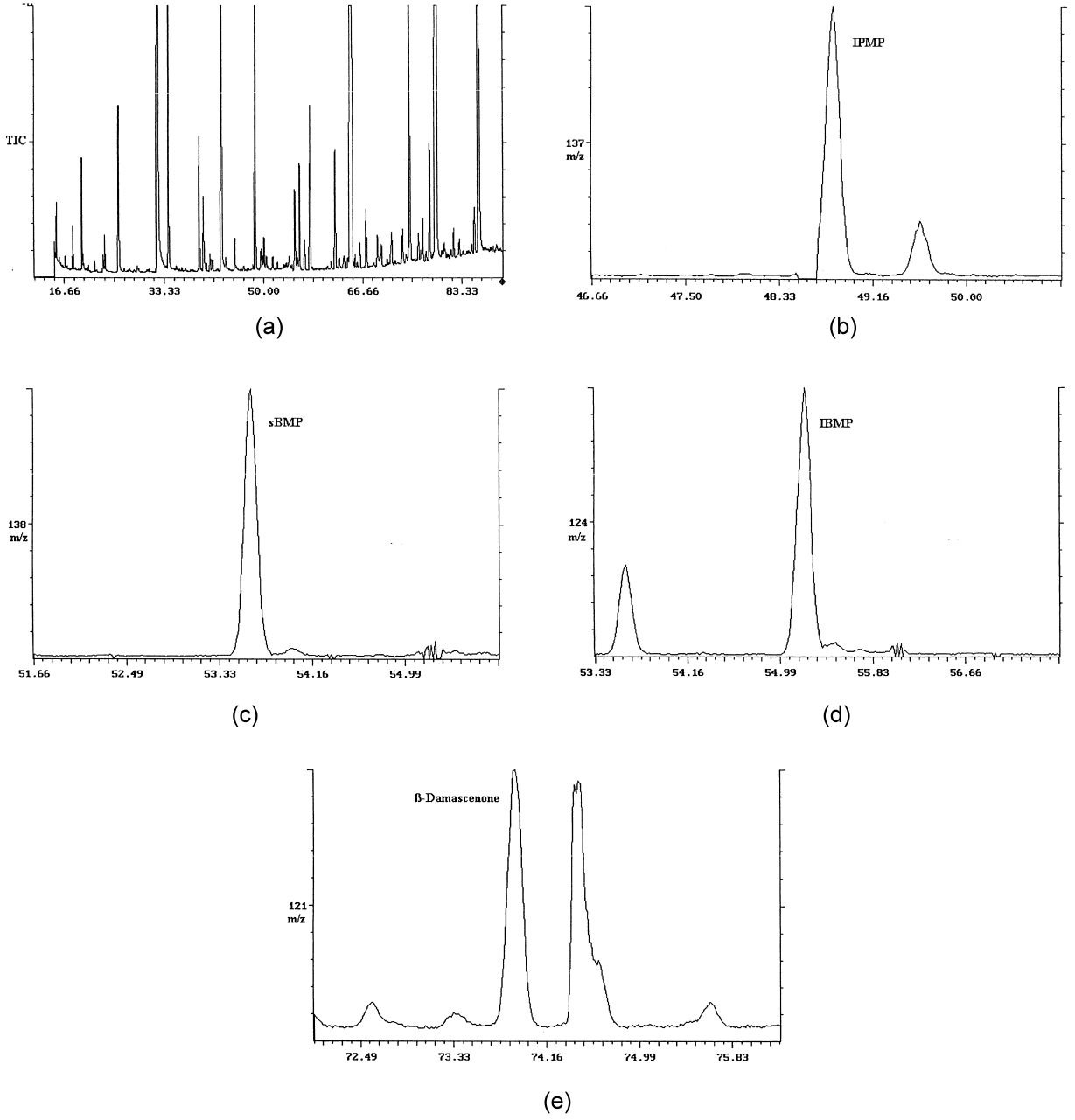

Fig. 1. GC–MS analysis of a Porapak-Q extract from 500 ml of wine spiked with 1 μg/l analytes: (a) reconstructed ion chromatogram; (b) mass peak of 3-isopropyl-2-methoxypyrazine; (c) mass peak of 3-*sec*.-butyl-2-methoxypyrazine; (d) mass peak of 3-isobutyl-2-methoxypyrazine; (e) mass peak of β-damascenone.

from Table 2. The concentration factor that should be reached in the isolation step is around 5000 because the instrument detection limit has been estimated as 25 μg/l and the desirable detection limit is around 5 ng/l. Therefore, if 0.1 ml is fixed as the minimum volume at which an extract can be

concentrated, an initial volume of 500 ml of wine should be processed. According to this, a 4-cm bed must be selected, but safer conditions will be achieved by using a 5-cm bed to extract 500 ml of wine diluted to 1000 ml with water. The extra loading capacity introduced by that additional 1 cm of bed should allow for including a wash step and for increasing the sample flow-rate. Recovery results for this approach are shown in Table 5, which corroborates that breakthrough volumes have not been reached and that elution has been complete. Fig. 1 shows the reconstructed ion chromatogram and the corresponding ionic peaks for the four analytes. It can be seen that, in spite of the complexity of the chromatogram, the ionic peaks are gaussian and are well separated from other potential interferences. The method detection limits with ion trap MS detection are in all cases below 10 ng/l and, therefore, can be considered satisfactory.

4. Conclusions

It can be concluded that solid–liquid distribution coefficients can be used to calculate retention properties of SPE beds, which can be advantageously exploited to model SPE systems. In short beds of Porapak-Q resins, the Lövkvist–Jönsson model is more appropriate than the gaussian-based model. Of all the sorbents tested, Porapak-Q is the best to extract some important non-polar odorants from wine. A 5-cm long bed is enough to extract quantitatively alkyl-methoxypyrazines and β-damascenone from 500 ml of wine as the model had predicted.

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