Immediate Differentiation of Unusual Seed Oils by Easy Ambient Sonic-Spray Ionization Mass Spectrometry

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Abstract

We describe herein the immediate and low cost characterization of nine seed oils via TAGs profiles by EASI-MS.

Introduction

Here we show that EASI(+)-MS offers indeed a powerful immediate tool able to characterize and differentiate unusual seed oils obtained from *Jatropha curcas* (JC), *Bombacopsis glabra* (BG), *Capparis flexuosa* (CF), *Siparuna guianensis (SG), Moringa oleifera (MO), Hibiscus tiliaceus* (HT), *Virola bicuhyba* (VB), *Pouteria caimito* (PC) and *Syagrus coronate* (SC). The oils were found to display quite contrasting TAG profiles, which provide important information for their quality control and potential applications in biofuels and foods.

Results and Discussion

Oils were extracted by the Soxhlet method from 5g of ground seeds using 230 mL of ethyl ether heated at 65°C for 4 h. The crude samples (2 µL) were dropped on a paper surface and EASI-MS data were acquired in a single quadrupole for over 30 s, initially scanning over the range of *m/z* 200-1200. The EASI source in house-fabricated was operated with methanol flow rate of 20 µL min^{-1} and 3 L min^{-1} for the nebulizing gas (N_2).[1] Fig. 1 shows, as an example, the EASI(+)-MS distinct profiles of TAGs from *V. bicuhyba* and *S. coronata*.

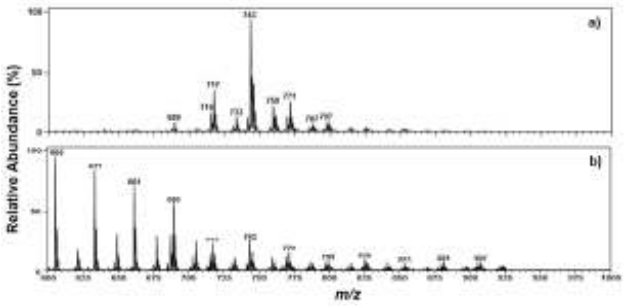

Figura 1. EASI(+)-MS analysis fingerprinting seed oils of a) *V. bicuhyba* and b) *S. coronata*.

Table 1 shows the TAG compositions revealed by such $[TAG + Na]^+$ profiles.

Table 1. $[TAG + Na]^+$ ions and relative abundance (%) detected via EASI(+)-MS for the oils.

[TAG+Na]⁺ m/z	TAG	CF	JC	HT	MO	BG	SG	PC	VB	SC
605	LaCaCa	-	-	-	-	-	-	-	-	**100**
633	LaLaCa	-	-	-	-	-	-	-	-	93.1
689	LaLaM	-	-	-	-	-	-	-	6.6	66.8
717	LaLaP	-	-	-	-	-	-	-	40.9	26.1
743	LaLaO	-	-	-	-	-	-	-	**100**	28.7
745	LaLaS	-	-	-	-	-	-	-	47.9	17.4
771	MMPo	-	-	-	-	-	-	-	33.3	17.6
773	MMP	-	-	-	-	-	-	-	10.2	5.5
799	MMO	-	-	-	-	-	-	-	9.9	10.2
825	PPoPo	-	-	-	-	-	-	-	5.8	11.4
829	PPP	5.7	-	-	-	-	-	-	-	-
853	PPL	43.6	-	55.1	-	80.8	48.3	30.8	-	6.3
855	PPO	55.4	8.2	12.9	-	**100**	53.4	53.3	-	-
877	PLL/POLn	32.6	41.4	**100**	-	-	35.6	12.8	-	-
879	PLO/PSLn	53.2	54.2	67.4	12.1	13.3	71.1	49.2	-	5.8
881	POO/PSL	**100**	43.4	18.6	24.9	32.4	**100**	**100**	-	9.1
883	PSO	33.0	13.8	-	10.1	75.0	40.8	26.8	-	-
901	LLL/OLLn	-	28.8	42.5	-	-	-	7.2	-	-
903	OLL/OOLn	-	94.7	46.5	-	-	12.6	9.9	-	-
905	OOL/SLL	25.4	**100**	37.8	-	12.4	35.1	34.9	-	7.5
907	OOO/SLO	45.1	94.6	-	**100**	27.9	57.7	55.3	-	8.5
909	SOO/SSL	25.5	44.9	-	44.4	38.4	50.7	31.3	-	-
911	SSO	-	-	-	9.5	15.6	17.7	7.5	-	-
935	ALO	-	10.1	9.1	18.1	-	-	-	-	-
937	SAL/AOO	-	9.5	-	19.0	12.5	10.4	-	-	-
939	SAO	11.4	5.25	-	-	-	-	-	-	-
965	AAL	-	-	-	11.0	-	-	-	-	-
967	AAO	-	-	-	6.0	-	-	-	-	-
969	AAS	-	-	-	-	-	-	-	-	-

Note that all oils display predominance of TAG composed by palmitic (P), oleic (O), stearic (S) and linoleic (L) acids. But two exceptions were found for the *V. bicuhyba* and *S. coronata* seed oils, which are composed mainly by TAG containing lauric acid (La). To evaluate the performance of the EASI-MS technique to discriminate the different types of vegetable oils in terms of their TAG profiles, PCA and HCA were applied.

Conclusions

EASI(+)-MS profiles of TAGs constituents provide immediate typification and differentiation of oils and can be obtained in a quite direct and rapid fashion.

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