Screening and Classification of Hydrogenated Vegetable Oils using a Combination of SFC-FID, SFC-MS and GCxGC-MS.

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Sample	Class	Rep 1	Rep 2	Rep 3	Average	Standard Deviation
HVO 1	Polar	N.D.	N.D.	N.D.	N.D.	-
	Saturates	100.0%	100.0%	100.0%	100.0%	0.0%
	Aromatic	N.D.	N.D.	N.D.	N.D.	-
HVO 2	Polar	N.D.	N.D.	N.D.	N.D.	-
	Saturates	100.0%	100.0%	100.0%	100.0%	0.0%
	Aromatic	N.D.	N.D.	N.D.	N.D.	-
HVO 3	Polar	1.1%	1.2%	1.3%	1.2%	0.1%
	Saturates	98.5%	98.5%	98.3%	98.4%	0.1%
	Aromatic	0.4%	0.3%	0.5%	0.4%	0.1%
HVO 4	Polar	N.D.	N.D.	N.D.	N.D.	-
	Saturates	96.7%	96.9%	96.4%	96.7%	0.3%
	Aromatic	3.3%	3.1%	3.6%	3.3%	0.3%
HVO 5	Polar	<0.1%	<0.1%	<0.1%	<0.1%	<0.1%
	Saturates	99.9%	99.8%	99.8%	99.8%	<0.1%
	Aromatic	0.1%	0.2%	0.1%	0.1%	<0.1%
HVO 6	Polar	1.5%	1.5%	1.5%	1.5%	<0.1%
	Saturates	96.2%	96.3%	96.1%	96.2%	0.1%
	Aromatic	2.3%	2.2%	2.4%	2.3%	0.1%
HVO 7	Polar	0.3%	0.2%	0.2%	0.2%	<0.1%
	Saturates	98.2%	98.1%	98.3%	98.2%	0.1%
	Aromatic	1.6%	1.7%	1.5%	1.6%	0.1%

Table S1: SFC-FID Composition make-up for each of the undiluted HVOs analysed in triplicate.

N.D. – Not detected.

Sampla	Class	Ron 1	Ron 2	Ron 3	Avorago	Standard Deviation
HVO 1	iso-alkane	80.8%	80.8%	80 5%	80 7%	0.2%
	n alkane	10.2%	10.2%	10.5%	10.3%	0.2%
HVO 2	<i>iso</i> alkane	81.6%	81.3%	81.5%	81.5%	0.2%
	monocyclo alkana	0.2%	0.1%	0 10/	0.1%	0.270
	n alkana	18 20/2	18 60/	18 /0/	18 /0/	0.078
HVO 3	<i>n</i> -aikaite	0.6%	0.4%	0.5%	0.5%	0.276
	aldahyda	0.070	0.470	0.370	0.370	0.170
		0.170	0.170	0.170	0.170	<0.1%
		0.0%	0.0%	0.0%	0.0%	<0.1%
		0.1%	0.1%	0.1%	0.1%	<0.1%
	<i>iso-</i> aikane	1.9%	2.0%	2.1%	2.0%	0.1%
	mono-aromatic	<0.1%	0.1%	<0.1%	<0.1%	<0.1%
	<i>monocyclo</i> -alkane	1.4%	2.1%	1.9%	1.8%	0.4%
	<i>n</i> -alkane	95.9%	95.2%	95.3%	95.5%	0.4%
HVO 4	<i>bi-</i> and <i>tricyclo-</i> alkane	16.1%	16.1%	17.0%	16.4%	0.5%
	iso-alkane	51.2%	50.0%	50.2%	50.5%	0.7%
	<i>mono</i> -aromatic	1.0%	1.0%	1.1%	1.0%	0.1%
	<i>monocyclo</i> -alkane	13.4%	14.4%	14.1%	13.9%	0.5%
	<i>n</i> -alkane	18.2%	18.5%	17.6%	18.1%	0.5%
	polycyclo-alkanes	<0.1%	0.1%	0.1%	0.1%	<0.1%
HVO 5	iso-alkane	17.2%	17.1%	17.5%	17.3%	0.2%
	monocyclo-alkane	0.6%	0.7%	0.7%	0.7%	0.1%
	<i>n</i> -alkane	82.1%	82.2%	81.8%	82.0%	0.2%
HVO 6	<i>bi-</i> and <i>tricyclo-</i> alkane	0.8%	0.9%	0.9%	0.8%	0.1%
	diaromatic	<0.1%	<0.1%	<0.1%	<0.1%	<0.1%
	FAME	0.4%	0.4%	0.4%	0.4%	<0.1%
	iso-alkane	76.8%	76.3%	76.5%	76.6%	0.3%
	mono-aromatic	0.7%	0.8%	0.9%	0.8%	0.1%
	monocyclo-alkane	3.5%	3.5%	3.2%	3.4%	0.2%
	n-alkane	17.8%	18.1%	18.1%	18.0%	0.2%
HVO 7	<i>bi-</i> and <i>tricyclo-</i> alkane	0.1%	<0.1%	0.1%	<0.1%	<0.1%
	FAME	0.1%	0.1%	0.1%	0.1%	<0.1%
	<i>iso</i> -alkane	76.6%	77.0%	76.9%	76.9%	0.2%
	mono-aromatic	0.2%	0.2%	0.2%	0.2%	<0.1%
	monocyclo-alkane	0.9%	0.7%	0.8%	0.8%	0.1%
	<i>n</i> -alkane	22.1%	21.9%	22.0%	22.0%	0.1%

Table S2: GCxGC-MS Composition make-up for each of the diluted HVOs analysed in triplicate.



Figure S1: SFC-FID analysis of HVO 4, showing saturates and aromatics elution windows.



Figure S2: Reconstructed ion current chromatogram (RICC) of the negative ion ESI SFC-MS for HVO 5.