

Supplementary information for manuscript:

LC-Orbitrap-HRMS determination of two novel plastochromanol homologues

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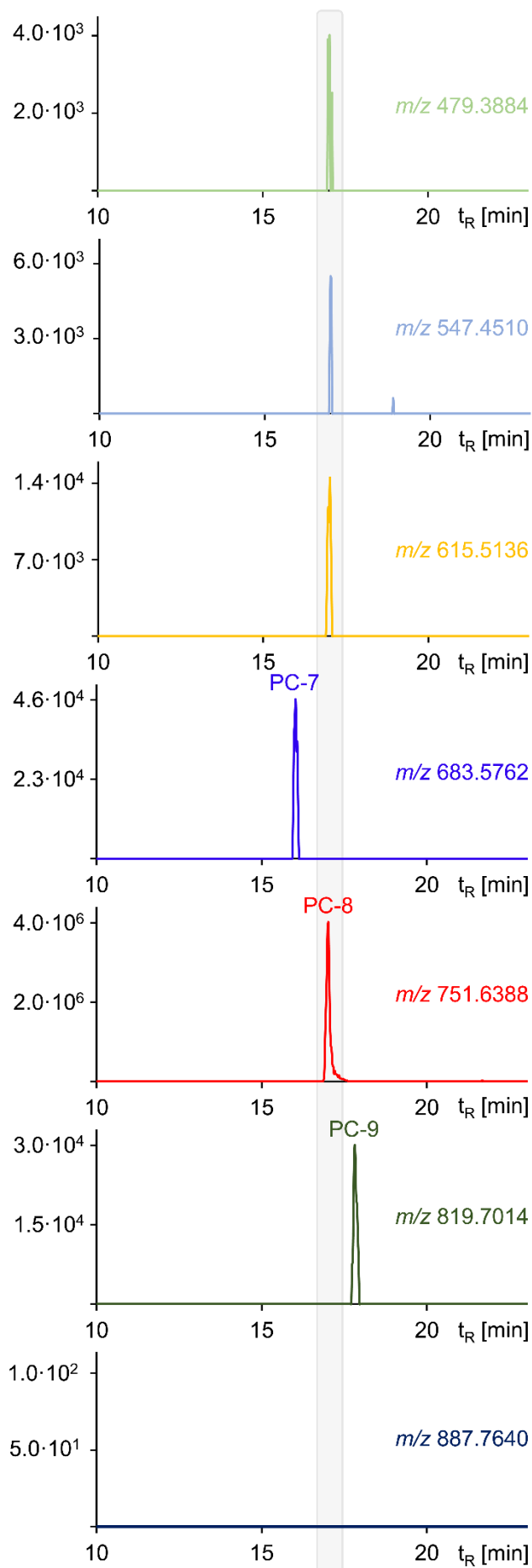


Fig. S1 LC-Orbitrap-HRMS chromatograms after extraction of the ion traces of the quasi-molecular ions $[M+H]^+$ of PC-4 (m/z 479.3884), PC-5 (m/z 547.4510), PC-6 (m/z 615.5136), PC-7 (m/z 683.5762), PC-8 (m/z 751.6388), PC-9 (m/z 819.7014), PC-10 (m/z 887.7640) of the saponified flaxseed oil 1.

SI Table S1 Isotope patterns of the $[M+H]^+$ ion determined by LC-Orbitrap-HRMS (APCI+ mode) of plastochoymanol-7 (PC-7) , plastochoymanol-8 (PC-8), and plastochoymanol-9 (PC-9) in different samples along with the relative deviations from the theoretical value (deviation) and their ratio. The peak area of the monoisotopic peak was set at 100% reference, respectively.

Sample	PC-7			PC-8			PC-9		
	Measured value [m/z]	Deviation [ppm]	(Area) Ratio	Measured value [m/z]	Deviation [ppm]	(Area) Ratio	Measured value [m/z]	Deviation [ppm]	(Area) Ratio
Flaxseed oil 1 A	683.5755 ^a	1.8	(460441) 100%	751.6382 ^d	1.5	(45466617) 100%	819.7009 ^h	1.2	(310057) 100%
	684.5781 ^b	2.9	42.2%	752.6415 ^e	1.6	58.3%	820.7041 ⁱ	1.4	65.8%
	685.5844 ^c	1.4	9.2%	753.6447 ^f	1.8	16.6%	821.7075 ^j	1.4	9.8%
				754.6479 ^g	2.0	2.9%			
Flaxseed oil 1 B	683.5753 ^a	2.1	(235130) 100%	751.6377 ^d	2.2	(25119196) 100%	819.7001 ^h	2.2	(157177) 100%
	684.5774 ^b	3.9	12.3%	752.6411 ^e	2.1	56.7%	820.7035 ⁱ	2.2	34.8%
	685.5812 ^c	3.2	2.6%	753.6441 ^f	2.6	16.4%	821.7075 ^j	1.4	4.1%
				754.6472 ^g	2.9	3.1%			
Flaxseed oil 2 A	683.5751 ^a	2.4	(86347) 100%	751.6374 ^d	2.6	(23336956) 100%	819.6998 ^h	2.6	(260652) 100%
	684.5795 ^b	0.8	36.1%	752.6406 ^e	2.8	56.7%	820.7031 ⁱ	2.7	60%
				753.6439 ^f	2.8	16.4%	821.7064 ^j	2.7	6.5%
				754.6472 ^g	2.9	3.0%			
Flaxseed oil 2 B	683.5741 ^a	3.8	(184815) 100%	751.6376 ^d	2.3	(20521380) 100%	819.7023 ^h	0.5	(184815) 100%
	684.5789 ^b	1.7	38.8%	752.6409 ^e	2.4	56.1%	820.7036 ⁱ	2.1	60.9%
				753.6444 ^f	2.2	16.5%			
				754.6478 ^g	2.1	3.1%			
<i>Cecropia</i> leaves A	683.5759 ^a	1.2	(343346) 100%	751.6384 ^d	1.2	(57484518) 100%	819.7022 ^h	0.5	(293171) 100%
	684.5779 ^b	3.2	45.6%	752.6418 ^e	1.2	57.2%	820.7034 ⁱ	2.2	39.3%
	685.5813 ^c	3.2	1.4%	753.6450 ^f	1.4	16.6%			
				754.6479 ^g	2.0	3.0%			

SI Table S1 Cont.

Sample	PC-7			PC-8			PC-9		
	Measured value [<i>m/z</i>]	Deviation [ppm]	(Area) Ratio	Measured value [<i>m/z</i>]	Deviation [ppm]	(Area) Ratio	Measured value [<i>m/z</i>]	Deviation [ppm]	(Area) Ratio
<i>Cecropia</i> leaves B	683.5745 ^{a)}	3.2	(297000) 100%	751.6382 ^{d)}	1.5	(58415607) 100%	819.7005 ^{h)}	1.6	(321286) 100%
	684.5787 ^{b)}	2.0	54.4%	752.6416 ^{e)}	1.4	56.8%	820.7031 ⁱ⁾	2.7	65.7%
	685.5812 ^{c)}	3.2	4.4%	753.6450 ^{f)}	1.4	16.6%	821.7075 ^{j)}	1.4	5.0%
				754.6479 ^{g)}	2.0	3.2%			
Rapeseed oil A	683.5761 ^{a)}	0.9	(5601) 100%	751.6376 ^{d)}	2.3	(1087720) 100%	819.6999 ^{h)}	2.5	(2776) 100%
				752.6412 ^{e)}	2.0	64.1%			
				753.6449 ^{f)}	1.5	15.7%			
Rapeseed oil B	683.5759 ^{a)}	1.2	(6976) 100%	751.6377 ^{d)}	2.2	(1161067) 100%	819.7007 ^{h)}	1.5	(2552) 100%
				752.6407 ^{e)}	2.6	56.4%			
				753.6433 ^{f)}	3.6	7.4%			
Mustard oil 1 A ^{k)}	683.5747 ^{a)}	2.8	(81820) 100%	751.6373 ^{d)}	2.6	(24073838) 100%	819.6993 ^{h)}	3.2	(87502) 100%
	684.5787 ^{b)}	2.0	48.1%	752.6405 ^{e)}	2.9	56.5%	820.7033 ⁱ⁾	2.4	51.6%
				753.6436 ^{f)}	3.3	13.7%			
				754.6473 ^{g)}	2.7	2.2%			
Mustard oil 1 B ^{k)}	683.5752 ^{a)}	2.2	(77348) 100%	751.6371 ^{d)}	2.9	(18563860) 100%	819.6995 ^{h)}	3.0	(70196) 100%
	684.5779 ^{b)}	3.2	46.4%	752.6403 ^{e)}	3.1	51.4%	820.7032 ⁱ⁾	2.5	35.9%
				753.6437 ^{f)}	3.1	16.4%			
				754.6470 ^{g)}	3.2	2.5%			
Mustard oil 2 A ^{k)}	683.5742 ^{a)}	3.7	(42910) 100%	751.6373 ^{d)}	3.0	(13909397) 100%	819.6987 ^{h)}	3.9	(47692) 100%
	684.5775 ^{b)}	3.8	19.9%	752.6406 ^{e)}	3.7	56.2%	820.7023 ⁱ⁾	3.6	35.0%
				753.6439 ^{f)}	3.4	15.8%			
				754.6469 ^{g)}	3.0	1.9%			

SI Table S1 Cont.

Sample	PC-7			PC-8			PC-9		
	Measured value [<i>m/z</i>]	Deviation [ppm]	(Area) Ratio	Measured value [<i>m/z</i>]	Deviation [ppm]	(Area) Ratio	Measured value [<i>m/z</i>]	Deviation [ppm]	(Area) Ratio
Mustard oil 2 B ^{k)}	683.5749 ^{a)}	2.7	(51542) 100%	751.6371 ^{d)}	3.0	(13768958) 100%	819.6987 ^{h)}	3.3	(53030) 100%
	684.5790 ^{b)}	1.6	28.8%	752.6399 ^{e)}	3.7	48.9%	820.7023 ⁱ⁾	3.9	56.3%
				753.6435 ^{f)}	3.4	12.9%			
				754.6472 ^{g)}	3.0	2.2%			
Candle nut oil A ^{k)}	683.5752 ^{a)}	2.2	(110880) 100%	751.6370 ^{d)}	3.1	(21898468) 100%	819.7001 ^{h)}	2.2	(212190) 100%
	684.5792 ^{b)}	1.2	32.8%	752.6412 ^{e)}	2.0	50.3%	820.7032 ⁱ⁾	2.5	55.4%
				753.6445 ^{f)}	2.1	13.6%	821.7064 ^{j)}	2.7	22.9%
				754.6478 ^{g)}	2.1	2.6%			
Candle nut oil B ^{k)}	683.5753 ^{a)}	2.1	(157956) 100%	751.6385 ^{d)}	1.1	(1161067) 100%	819.7005 ^{h)}	1.7	(235370) 100%
	684.5782 ^{b)}	2.7	54.3%	752.6409 ^{e)}	2.3	59.4%	820.7031 ⁱ⁾	2.7	47.9%
				753.6442 ^{f)}	2.4	14.4%	821.7093 ^{j)}	0.8	6.2%
				754.6476 ^{g)}	2.3	2.9%			
Camelina oil A ^{k)}	683.5754 ^{a)}	1.9	(36165) 100%	751.6376 ^{d)}	2.3	(9731566) 100%	819.6995 ^{h)}	3.0	(12019) 100%
				752.6412 ^{e)}	2.0	69.1%			
				753.6449 ^{f)}	1.5	19.4%			
Camelina oil B ^{k)}	683.5755 ^{a)}	1.8	(66024) 100%	751.6377 ^{d)}	2.2	(13013310) 100%	819.6990 ^{h)}	3.6	(8339) 100%
				752.6407 ^{e)}	2.6	53.1%			
				753.6433 ^{f)}	3.6	14.7%			

a) [¹²C₄₈¹H₇₄¹⁶O₂+¹H]⁺, b) [¹²C₄₇¹³C₁¹H₇₄¹⁶O₂+¹H]⁺, c) [¹²C₄₆¹³C₂¹H₇₄¹⁶O₂+¹H]⁺

d) [¹²C₅₃¹H₈₂¹⁶O₂+¹H]⁺, e) [¹²C₅₂¹³C₁¹H₈₂¹⁶O₂+¹H]⁺, f) [¹²C₅₁¹³C₂¹H₈₂¹⁶O₂+¹H]⁺, g) [¹²C₅₀¹³C₃¹H₈₂¹⁶O₂+¹H]⁺

h) [¹²C₅₈¹H₉₀¹⁶O₂+¹H]⁺, i) [¹²C₅₇¹³C₁¹H₉₀¹⁶O₂+¹H]⁺, j) [¹²C₅₆¹³C₂¹H₉₀¹⁶O₂+¹H]⁺

k) measurements taken on another day as a second set of measurements