

Figure S1. Estimated response surfaces for each response variable, and their corresponding Standardized Pareto charts: **A)** Extraction yield (%); **B)** TPC (mg GAE/mL); **C)** IC₅₀ ROS (µg/mL); **D)** IC₅₀ AChE (µg/mL).

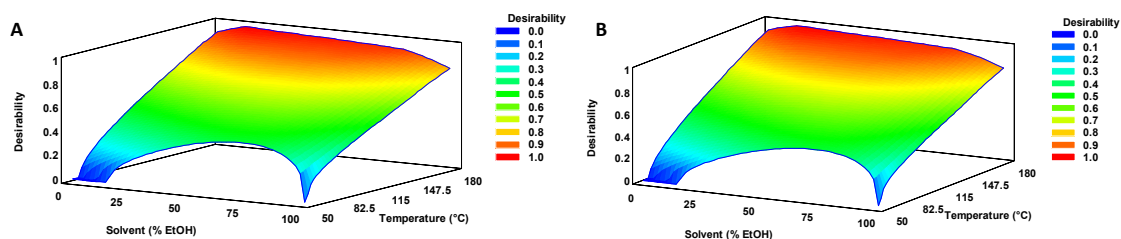


Figure S2. Desirability response surface to optimize response variables: **A)** including extraction yield as response variable; **B)** excluding extraction yield as response variable.

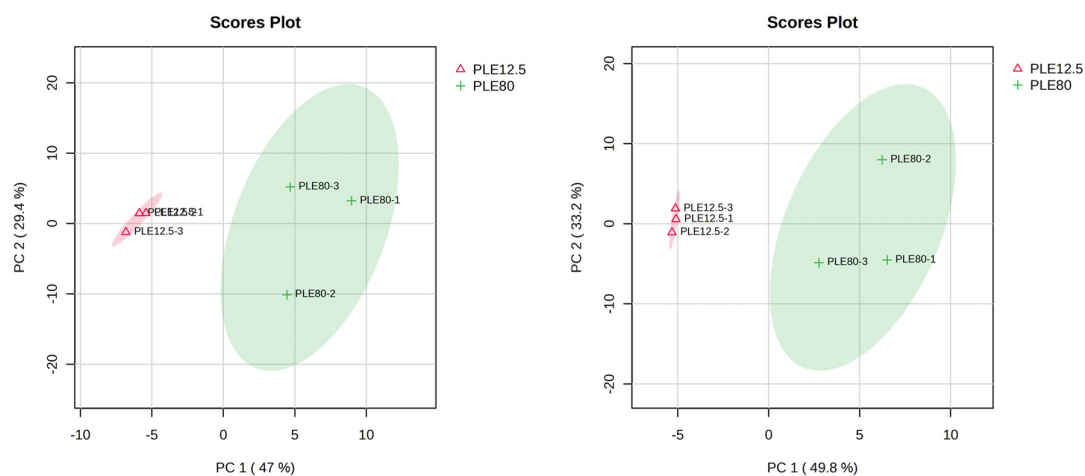


Figure S3. PCA score plots of pracaxi nuts PLE extracts data obtained by: **A)** HPLC-C18-Q-TOF MS/MS ESI (+); **B)** HPLC-C18-Q-TOF MS/MS ESI (-).

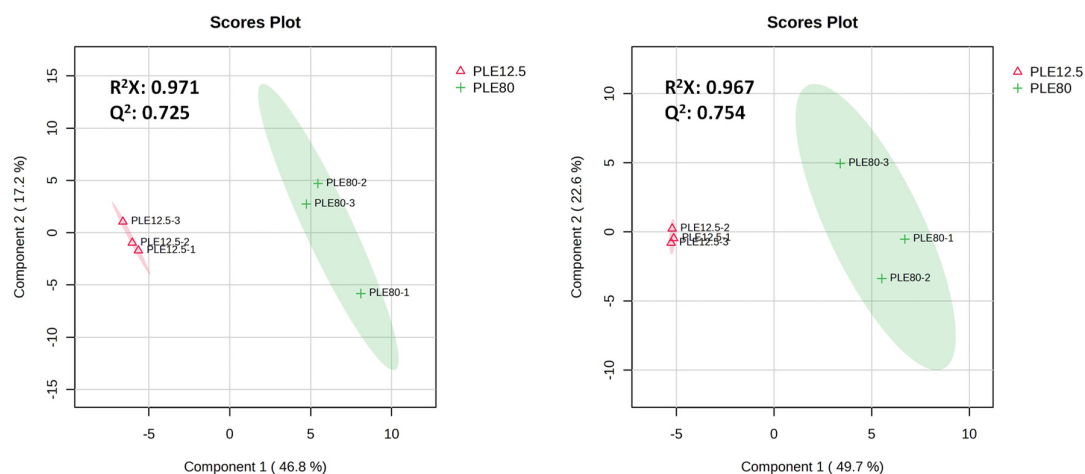


Figure S4. PLS-DA score plots of pracaxi nuts PLE extracts data obtained by: **A)** HPLC-C18-Q-TOF MS/MS ESI (+); **B)** HPLC-C18-Q-TOF MS/MS ESI (-).

Table S1. Analysis of Variance of extraction yield variable for response surface modeling showing linear, quadratic and interaction relations, and coefficient for model prediction.

Source	Sum of Squares	Df	CE	F-Ratio	P-Value
Model			β_0	-1.84655	
Solvent composition (% EtOH)	94.4067	1	β_1	0.0556026	90.56
Temperature (°C)	213.607	1	β_2	0.106144	204.9
Solvent composition ²	0.135	1	$\beta_{1,1}$	-9.00×10^{-5}	0.13
Solvent composition x Temperature	3.4225	1	$\beta_{1,2}$	2.85×10^{-4}	3.28
Temperature ²	0.735	1	$\beta_{2,2}$	-1.24×10^{-4}	0.71
Lack-of-fit	7.84833	3		2.51	0.2349
Pure error	3.1275	3			
Total (corr.)	323.627	11			

Df (degree of freedom)

CE (coefficients of regression equation)

* Denotes statistical differences ($p < 0.05$)

R-squared = 96.6085 percent

R-squared (adjusted for d.f.) = 93.7822 percent

Standard Error of Est. = 1.02103

Mean absolute error = 0.888889

Durbin-Watson statistic = 2.14667 ($P=0.5543$)

Lag 1 residual autocorrelation = -0.189627

Asterisk indicates statistical significance (p -value < 0.05).

Table S2. Analysis of Variance of TPC variable for response surface modeling showing linear, quadratic and interaction relations, and coefficient for model prediction.

Source	Sum of Squares	Df	CE	F-Ratio	P-Value
Model			β_0 58.4568		
Solvent composition (% EtOH)	299.627	1	β_1 0.992372	0.93	0.4068
Temperature (°C)	7661.23	1	β_2 0.206933	23.69	0.0166*
Solvent composition ²	207.682	1	$\beta_{1,1}$ -3.53×10^{-3}	0.64	0.4816
Solvent composition x Temperature	792.422	1	$\beta_{1,2}$ -4.33×10^{-3}	2.45	0.2155
Temperature ²	281.535	1	$\beta_{2,2}$ $-.43 \times 10^{-3}$	0.87	0.4197
Lack-of-fit	379.968	3		0.39	0.7692
Pure error	970.388	3			
Total (corr.)	10472.6	11			

Df (degree of freedom)

CE (coefficients of regression equation)

* Denotes statistical differences ($p < 0.05$)

R-squared = 87.1059 percent

R-squared (adjusted for d.f.) = 76.3608 percent

Standard Error of Est. = 17.9851

Mean absolute error = 8.39028

Durbin-Watson statistic = 1.96499 ($P=0.3927$)

Lag 1 residual autocorrelation = -0.0617368

Asterisk indicates statistical significance (p -value < 0.05)

Table S3. Analysis of Variance of ROS variable for response surface modeling showing linear, quadratic and interaction relations, and coefficient for model prediction.

Source	Sum of Squares	Df	CE	F-Ratio	P-Value
Model			β_0 20.5195		
Solvent composition (% EtOH)	16.9277	1	β_1 −0.0880672	28.37	0.0129*
Temperature (°C)	58.7251	1	β_2 −0.184977	98.43	0.0022*
Solvent composition ²	1.16998	1	$\beta_{1,1}$ -2.65×10^{-4}	1.96	0.2559
Solvent composition x Temperature	20.9444	1	$\beta_{1,2}$ 7.04×10^{-4}	35.1	0.0096*
Temperature ²	9.2964	1	$\beta_{2,2}$ 4.42×10^{-4}	15.58	0.029*
Lack-of-fit	11.3316	3		6.33	0.0819
Pure error	1.78989	3			
Total (corr.)	119.02	11			

Df (degree of freedom)

CE (coefficients of regression equation)

* Denotes statistical differences ($p < 0.05$)

R-squared = 88.9754 percent

R-squared (adjusted for d.f.) = 79.7882 percent

Standard Error of Est. = 0.772419

Mean absolute error = 0.876167

Durbin-Watson statistic = 2.3977 ($P=0.7609$)

Lag 1 residual autocorrelation = −0.234766

Asterisk indicates statistical significance (p -value < 0.05)

Table S4. Analysis of Variance of AChE variable for response surface modeling showing linear, quadratic and interaction relations, and coefficient for model prediction.

Source	Sum of Squares	Df	CE	F-Ratio	P-Value	
Model			β_0	366.498		
Solvent composition (% EtOH)	176474	1	β_1	-6.48654	641.92	0.0001*
Temperature (°C)	178193	1	β_2	3.48097	648.17	0.0001*
Solvent composition ²	333468	1	$\beta_{1,1}$	1.41×10^{-1}	1212.98	0.0001*
Solvent composition x Temperature	57121	1	$\beta_{1,2}$	-3.68×10^{-2}	207.78	0.0007*
Temperature ²	16590	1	$\beta_{2,2}$	-1.87×10^{-2}	60.35	0.0044*
Lack-of-fit	123530	3			149.78	0.0009*
Pure error	824.75	3				
Total (corr.)	874174	11				

Df (degree of freedom)

CE (coefficients of regression equation)

* Denotes statistical differences ($p < 0.05$)

R-squared = 85.7746 percent

R-squared (adjusted for d.f.) = 73.92 percent

Standard Error of Est. = 16.5806

Mean absolute error = 77.4722

Durbin-Watson statistic = 2.00322 (P=0.4261)

Lag 1 residual autocorrelation = -0.00284093

Asterisk indicates statistical significance (p -value < 0.05)

Table S5. Annotated compounds and their total compound contribution (%) in pracaxi SFE extract after HPLC-CSH-Q-TOF MS/MS ESI (-) analysis.

<i>Average Mz</i>	<i>Average RT (min)</i>	<i>Metabolite name</i>	<i>Adduct type</i>	<i>MSI Level</i>	<i>MSI Level</i>	<i>Molecular Formula</i>	<i>Compound subclass</i>	<i>Total compound contribution (%)</i>
281.24976	2.73	FA 18:1; (oleic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C18H34O2	Fatty acids and conjugates	37.81
339.32681	4.59	FA 22:0; (behenic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C22H44O2	Fatty acids and conjugates	14.28
279.23251	2.07	FA 18:2; (linoleic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C18H32O2	Linoleic acids and derivatives	11.61
367.35602	5.31	FA 24:0; (lignoceric acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C24H48O2	Fatty acids and conjugates	10.43
283.26358	3.34	FA 18:0; (stearic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C18H36O2	Fatty acids and conjugates	9.85
255.23288	2.51	FA 16:0; (palmitic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C16H32O2	Fatty acids and conjugates	8.92
309.27914	3.42	FA 20:1; (eicosenoic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C20H38O2	Fatty acids and conjugates	1.76
337.30914	3.98	FA 22:1; (erucic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C22H42O2	Fatty acids and conjugates	1.64
311.29413	3.94	FA 20:0; (arachidic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C20H40O2	Fatty acids and conjugates	1.02
395.39133	6.12	FA 26:0; (cerotic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C26H52O2	Fatty acids and conjugates	0.89
365.34146	4.61	FA 24:1; (nervonic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C24H46O2	Fatty acids and conjugates	0.35
253.21912	1.86	FA 16:1; (palmitoleic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C16H30O2	Fatty acids and conjugates	0.29
353.34186	4.96	FA 23:0	[M-H]-	2b	<i>m/z</i> , MS/MS	C23H46O2	Fatty acids and conjugates	0.18
277.21735	1.58	FA 18:3; (linolenic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C18H30O2	Linoleic acids and derivatives	0.16
227.20163	1.63	FA 14:0; (myristic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C14H28O2	Fatty acids and conjugates	0.15
269.24841	3.00	FA 17:0; (margaric acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C17H34O2	Fatty acids and conjugates	0.14
381.37344	5.72	FA 25:0	[M-H]-	2b	<i>m/z</i> , MS/MS	C25H50O2	Fatty acids and conjugates	0.09
295.22772	0.82	FA 18:2;O	[M-H]-	2b	<i>m/z</i> , MS/MS	C18H32O3	Linoleic acids and derivatives	0.06
241.21724	2.04	FA 15:0; (pentadecylic acid)	[M-H]-	2a	<i>m/z</i> , RT	C15H30O2	Fatty acids and conjugates	0.05
267.23019	2.25	FA 17:1	[M-H]-	2b	<i>m/z</i> , MS/MS	C17H32O2	Fatty acids and conjugates	0.04
325.31213	4.26	FA 21:0	[M-H]-	2b	<i>m/z</i> , MS/MS	C21H42O2	Fatty acids and conjugates	0.04
439.35886	4.17	FA 30:6	[M-H]-	2b	<i>m/z</i> , MS/MS	C30H48O2	Fatty acids and conjugates	0.04
225.18394	1.22	FA 14:1; (physeteric acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C14H26O2	Fatty acids and conjugates	0.04
199.16656	1.05	FA 12:0; (lauric acid)	[M-H]-	2a	<i>m/z</i> , RT	C12H24O2	Fatty acids and conjugates	0.04
574.49921	6.07	Ceramide d34:0	[M+Cl]-	2a	<i>m/z</i> , RT	C34H69NO3	Ceramides	0.03
307.2627	2.95	FA 20:2; (eicosadienoic acid)	[M-H]-	1	<i>m/z</i> , MS/MS, RT	C20H36O2	Fatty acids and conjugates	0.02
415.35745	5.07	FA 28:4	[M-H]-	2b	<i>m/z</i> , MS/MS	C28H48O2	Fatty acids and conjugates	0.02
251.19859	1.37	FA 16:2	[M-H]-	2b	<i>m/z</i> , MS/MS	C16H28O2	Fatty acids and conjugates	0.02
335.2966	3.54	FA 22:2; (docosadienoic acid)	[M-H]-	2a	<i>m/z</i> , RT	C22H40O2	Fatty acids and conjugates	0.01
143.10736	0.57	FA 8:0; (caprylic acid)	[M-H]-	2a	<i>m/z</i> , RT	C8H16O2	Fatty acids and conjugates	0.01

Table S6. Annotated compounds and their total compound contribution (%) in pracaxi SFE extract after HPLC-CSH-Q-TOF MS/MS ESI (+) analysis.

<i>Average Mz</i>	<i>Average RT (min)</i>	<i>Metabolite name</i>	<i>Adduct type</i>	<i>MSI Level</i>	<i>MSI Level</i>	<i>Molecular Formula</i>	<i>Compound subclass</i>	<i>Total compound contribution (%)</i>
923.7563_907.7833_902.8348	11.03	TG 54:3 TG 18:1_18:1_18:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C57H104O6	Triacylglycerol	10.73
979.8079_963.8411_958.8925	11.81	TG 58:3 TG 22:0_18:1_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C61H112O6	Triacylglycerol	10.50
977.7941_961.8201_956.8676	11.53	TG 58:4 TG 18:1_22:1_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C61H110O6	Triacylglycerol	8.60
930.8611	11.41	TG 56:3 TG 18:1_18:1_20:1	[M+NH4]+	2a	m/z, RT	C59H108O6	Triacylglycerol	7.05
898.7927_903.7485	10.31	TG 54:5 TG 18:1_18:2_18:2	[M+NH4]+_[M+Na]+	1	m/z, MS/MS, RT	C57H100O6	Triacylglycerol	6.90
960.9102_965.8542_981.8278	11.98	TG 58:2 TG 22:0_18:1_18:1	[M+NH4]+_[M+Na]+_[M+K]+	1	m/z, MS/MS, RT	C61H114O6	Triacylglycerol	6.43
921.7391_905.7672_900.8184	10.69	TG 54:4 TG 18:1_18:1_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C57H102O6	Triacylglycerol	6.00
986.917	12.03	TG 60:3 TG 24:0_18:1_18:2	[M+NH4]+	2b	m/z, MS/MS	C63H116O6	Triacylglycerol	5.33
993.8839_1009.8556_988.9398	12.13	TG 60:2 TG 24:0_18:1_18:1	[M+Na]+_[M+K]+_[M+NH4]+	1	m/z, MS/MS, RT	C63H118O6	Triacylglycerol	4.31
932.8668_953.7968	11.75	TG 56:2 TG 20:0_18:1_18:1	[M+NH4]+_[M+K]+	1	m/z, MS/MS, RT	C59H110O6	Triacylglycerol	4.24
933.7853_949.7598_928.8427	11.10	TG 56:4 TG 18:1_20:1_18:2	[M+Na]+_[M+K]+_[M+NH4]+	1	m/z, MS/MS, RT	C59H106O6	Triacylglycerol	3.55
881.7598_897.7347_876.8074	10.99	TG 52:2 TG 16:0_18:1_18:1	[M+Na]+_[M+K]+_[M+NH4]+	1	m/z, MS/MS, RT	C55H102O6	Triacylglycerol	3.37
984.8951_1005.8330	11.87	TG 60:4 TG 18:1_24:1_18:2	[M+NH4]+_[M+K]+	1	m/z, MS/MS, RT	C63H114O6	Triacylglycerol	2.68
909.8022_925.7759_904.8306	11.42	TG 54:2 TG 18:0_18:1_18:1	[M+Na]+_[M+K]+_[M+NH4]+	1	m/z, MS/MS, RT	C57H106O6	Triacylglycerol	1.93
1037.889_1021.9243_1016.9614	12.22	TG 62:2	[M+K]+_[M+Na]+_[M+NH4]+	2a	m/z, RT	C65H122O6	Triacylglycerol	1.65
659.5071_643.5297_638.5728	7.12	DG 36:2 DG 18:1_18:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C39H72O5	Diacylglycerols	1.53
872.7745	10.29	TG 52:4 TG 16:1_18:1_18:2	[M+NH4]+	1	m/z, MS/MS, RT	C55H98O6	Triacylglycerol	1.22

895.7213_879.7 471_874.7914	10.63	TG 52:3 TG 16:0_18:1_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C55H100O6	Triacylglycerol	1.20
917.7013_901.7 272_896.7706	9.93	TG 54:6 TG 18:2_18:2_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C57H98O6	Triacylglycerol	1.15
657.4871_641.5 132_636.5561	6.58	DG 36:3 DG 18:1_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C39H70O5	Diacylglycerols	0.87
959.8052_954.8 490_975.7749	11.16	TG 58:5 TG 22:1_18:2_18:2	[M+Na]+_[M+NH4]+_[M+K]+	1	m/z, MS/MS, RT	C61H108O6	Triacylglycerol	0.81
947.7493_931.7 764_926.8237	10.74	TG 56:5 TG 20:1_18:2_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C59H104O6	Triacylglycerol	0.76
974.9140_979.8 685	12.08	TG 59:2	[M+NH4]+_[M+Na]+	2a	m/z, RT	C62H116O6	Triacylglycerol	0.66
878.8253	11.40	TG 52:1 TG 16:0_18:0_18:1	[M+NH4]+	1	m/z, MS/MS, RT	C55H104O6	Triacylglycerol	0.65
993.8309_977.8 547_972.8976	11.93	TG 59:3 TG 23:0_18:1_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C62H114O6	Triacylglycerol	0.58
962.9131	12.14	TG 58:1	[M+NH4]+	2a	m/z, RT	C61H116O6	Triacylglycerol	0.47
906.8511_927.7 825	11.74	TG 54:1 TG 18:0_18:0_18:1	[M+NH4]+_[M+K]+	1	m/z, MS/MS, RT	C57H108O6	Triacylglycerol	0.44
911.7518_895.7 775_890.8185	11.23	TG 53:2 TG 17:0_18:1_18:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C56H104O6	Triacylglycerol	0.44
934.8787	12.01	TG 56:1 TG 16:0_22:0_18:1	[M+NH4]+	2b	m/z, MS/MS	C59H112O6	Triacylglycerol	0.42
967.8142_951.8 406_946.8867	11.92	TG 57:2 TG 21:0_18:1_18:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C60H112O6	Triacylglycerol	0.41
1014.9418_1035 8682	12.16	TG 62:3	[M+NH4]+_[M+K]+	2a	m/z, RT	C65H120O6	Triacylglycerol	0.39
696.6494_701.6 060	8.97	DG 40:1 DG 22:0_18:1	[M+NH4]+_[M+Na]+	2b	m/z, MS/MS	C43H82O5	Diacylglycerols	0.38
853.7298_869.7 048_848.7749	10.61	TG 50:2 TG 16:0_16:1_18:1	[M+Na]+_[M+K]+_[M+NH4]+	1	m/z, MS/MS, RT	C53H98O6	Triacylglycerol	0.34
851.7112_867.6 879_846.7594	10.25	TG 50:3 A	[M+Na]+_[M+K]+_[M+NH4]+	2a	m/z, RT	C53H96O6	Triacylglycerol	0.30
976.8957	11.12	TG 58:2;10 TG 22:0_18:1_18:1;10	[M+NH4]+	2b	m/z, MS/MS	C61H114O7	Oxidized triglyceride	0.25
855.7427_850.7 925	10.99	TG 50:1 TG 16:0_16:0_18:1	[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C53H100O6	Triacylglycerol	0.25
909.7307_893.7 579_888.8032	10.86	TG 53:3 TG 17:0_18:1_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C56H102O6	Triacylglycerol	0.23

724.6851_729.6406	9.53	DG 42:1 DG 24:0_18:1	[M+NH4]+_[M+Na]+	2b	m/z, MS/MS	C45H86O5	Diacylglycerols	0.18
937.764_921.7919_916.8352	11.23	TG 55:3 TG 18:1_18:1_19:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C58H106O6	Triacylglycerol	0.17
918.8124	9.87	TG 54:3;1O TG 18:1_18:1_18:1;1O	[M+NH4]+	2b	m/z, MS/MS	C57H104O7	Oxidized triglyceride	0.15
972.8616	10.38	TG 58:4;1O TG 18:1_18:2_22:1;1O	[M+NH4]+	2b	m/z, MS/MS	C61H110O7	Oxidized triglyceride	0.14
633.4877_617.5115_612.5547	7.06	DG 34:1 DG 16:0_18:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C37H70O5	Diacylglycerols	0.14
655.472_639.4988_634.5423	6.04	DG 36:4 DG 18:2_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C39H68O5	Diacylglycerols	0.14
944.867	11.63	TG 57:3 TG 21:0_18:1_18:2	[M+NH4]+	2b	m/z, MS/MS	C60H110O6	Triacylglycerol	0.13
891.6811_875.7121_870.7532	9.90	TG 52:5 TG 18:1_16:2_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C55H96O7	Triacylglycerol	0.12
661.5183_645.5452_640.5891	7.73	DG 36:1 DG 18:0_18:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C39H74O5	Diacylglycerols	0.11
974.8779	10.74	TG 58:3;1O TG 18:1_18:1_22:1;1O	[M+NH4]+	2b	m/z, MS/MS	C61H112O7	Oxidized triglyceride	0.10
844.7417	9.90	TG 50:4 TG 14:1_18:1_18:2	[M+NH4]+	2b	m/z, MS/MS	C53H94O6	Triacylglycerol	0.09
970.8812	11.69	TG 59:4 TG 23:0_18:2_18:2	[M+NH4]+	2b	m/z, MS/MS	C62H112O6	Triacylglycerol	0.09
923.8068_918.8463	11.60	TG 55:2 TG 18:0_17:1_20:1	[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C58H108O6	Triacylglycerol	0.08
1012.926	12.06	TG 62:4 TG 26:0_18:2_18:2	[M+NH4]+	1	m/z, MS/MS, RT	C65H118O6	Triacylglycerol	0.08
982.8835	11.49	TG 60:5	[M+NH4]+	2a	m/z, RT	C63H112O6	Triacylglycerol	0.07
886.7846_907.7150	10.49	TG 53:4 TG 17:1_18:1_18:2	[M+NH4]+_[M+K]+	1	m/z, MS/MS, RT	C56H100O6	Triacylglycerol	0.06
722.6694_743.6091	9.09	DG 42:2 DG 24:0_18:2	[M+NH4]+_[M+K]+	2b	m/z, MS/MS	C45H84O5	Diacylglycerols	0.06
915.684_899.7114_894.7565	9.54	TG 54:7 TG 18:2_18:2_18:3	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C57H96O6	Triacylglycerol	0.06
631.476_615.4995_610.5392	6.52	DG 34:2 DG 16:0_18:2	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C37H68O5	Diacylglycerols	0.06
843.6837_827.7095_822.7546	10.59	TG 48:1 TG 14:0_16:0_18:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C51H96O6	Triacylglycerol	0.06
916.7979	9.46	TG 54:4;1O TG 18:1_18:2_18:1;1O	[M+NH4]+	2b	m/z, MS/MS	C57H102O7	Oxidized triglyceride	0.05
666.6044_671.5598	7.74	DG 38:2 DG 18:1_20:1	[M+NH4]+_[M+Na]+	2b	m/z, MS/MS	C41H76O5	Diacylglycerols	0.05

841.6709_825.6 935_820.7418	10.18	TG 48:2	[M+K]+_[M+Na]+_[M+NH4]+	2a	m/z, RT	C51H94O6	Triacylglycerol	0.05
914.8154	10.89	TG 55:4 TG 18:1_19:1_18:2	[M+NH4]+	2b	m/z, MS/MS	C58H104O6	Triacylglycerol	0.05
818.7216	9.90	TG 48:3 TG 14:0_16:1_18:2	[M+NH4]+	2b	m/z, MS/MS	C51H92O6	Triacylglycerol	0.04
1002.9177	11.36	TG 60:3;1O TG 18:1_20:1_22:1;1O	[M+NH4]+	2b	m/z, MS/MS	C63H116O7	Oxidized triglyceride	0.04
948.8986	12.08	TG 57:1	[M+NH4]+	2a	m/z, RT	C60H114O6	Triacylglycerol	0.04
1042.9739	12.23	TG 64:3	[M+NH4]+	2a	m/z, RT	C67H124O6	Triacylglycerol	0.04
883.7145_867.7 424_862.7841	10.84	TG 51:2 TG 16:0_17:1_18:1	[M+K]+_[M+Na]+_[M+NH4]+	1	m/z, MS/MS, RT	C54H100O6	Triacylglycerol	0.04
860.7714	10.51	TG 51:3 TG 15:1_18:1_18:1	[M+NH4]+	2b	m/z, MS/MS	C54H98O6	Triacylglycerol	0.04
892.8317	11.58	TG 53:1 TG 17:0_18:0_18:1	[M+NH4]+	1	m/z, MS/MS, RT	C56H106O6	Triacylglycerol	0.04
864.8019	11.22	TG 51:1 TG 16:0_17:0_18:1	[M+NH4]+	1	m/z, MS/MS, RT	C54H102O6	Triacylglycerol	0.04
694.6366	8.35	DG 40:2 DG 18:1_22:1	[M+NH4]+	2b	m/z, MS/MS	C43H80O5	Diacylglycerols	0.02
668.6227_673.5 733	8.38	DG 38:1 DG 20:0_18:1	[M+NH4]+_[M+Na]+	2b	m/z, MS/MS	C41H78O5	Diacylglycerols	0.02
946.8414	9.54	TG 56:3;1O TG 20:1_18:2_18:0;1O	[M+NH4]+	2b	m/z, MS/MS	C59H108O7	Oxidized triglyceride	0.02
920.8729	11.91	TG 55:1	[M+NH4]+	2a	m/z, RT	C58H110O6	Triacylglycerol	0.02
970.8424	10.03	TG 58:5;1O TG 18:2_18:2_22:1;1O	[M+NH4]+	2b	m/z, MS/MS	C61H108O7	Oxidized triglyceride	0.02
842.7237	9.50	TG 50:5	[M+NH4]+	2a	m/z, RT	C53H92O6	Triacylglycerol	0.02
914.7808	9.15	TG 54:5;1O TG 18:1_18:2_18:2;1O	[M+NH4]+	2b	m/z, MS/MS	C57H100O7	Oxidized triglyceride	0.02
664.5866	7.22	DG 38:3 DG 20:1_18:2	[M+NH4]+	2b	m/z, MS/MS	C41H74O5	Diacylglycerols	0.02
1044.9919	12.30	TG 64:2	[M+NH4]+	2a	m/z, RT	C67H126O6	Triacylglycerol	0.02
964.9267	12.21	TG 58:0	[M+NH4]+	2a	m/z, RT	C61H118O6	Triacylglycerol	0.02
202.1894	0.45	NAE 9:0	[M+H]+	2b	m/z, MS/MS	C11H23NO2	Amines	0.02
818.7230_823.6 804	9.75	TG 48:3 TG 12:0_18:1_18:2	[M+NH4]+_[M+Na]+	1	m/z, MS/MS, RT	C51H92O6	Triacylglycerol	0.02
794.7263_799.6 751	10.16	TG 46:1	[M+NH4]+_[M+Na]+	2a	m/z, RT	C49H92O6	Triacylglycerol	0.02
952.8367	10.78	TG 58:6	[M+NH4]+	2a	m/z, RT	C61H106O6	Triacylglycerol	0.01
752.7138	10.04	DG 44:1 DG 26:0_18:1	[M+NH4]+	2b	m/z, MS/MS	C47H90O5	Diacylglycerols	0.01
836.7705	10.81	TG 49:1	[M+NH4]+	2a	m/z, RT	C52H98O6	Triacylglycerol	0.01
884.7700_889.7 270	10.09	TG 53:5	[M+NH4]+_[M+Na]+	2a	m/z, RT	C56H98O6	Triacylglycerol	0.01
991.8675_1007. 8397	11.95	TG 60:3	[M+Na]+_[M+K]+	2a	m/z, RT	C63H116O6	Triacylglycerol	0.01
692.6197	7.85	DG 40:3 DG 22:1_18:2	[M+NH4]+	2b	m/z, MS/MS	C43H78O5	Diacylglycerols	0.01

912.7636	8.73	TG 54:6;10 TG 18:2_18:2_18:2;10	[M+NH4] ⁺	2b	m/z, MS/MS	C57H98O7	Oxidized triglyceride	0.01
374.3294	2.87	MG 18:1	[M+NH4] ⁺	2b	m/z, MS/MS	C21H40O4	Monoacylglycerols	0.01
356.3564	4.13	NAE 20:0	[M+H] ⁺	2b	m/z, MS/MS	C22H45NO2	Amines	0.01
608.5269	5.96	DG 34:3	[M+NH4] ⁺	2a	m/z, RT	C37H66O5	Diacylglycerols	0.01
694.6561	10.94	CE 20:2	[M+NH4] ⁺	2a	m/z, RT	C47H80O2	Steroid esters	< 0.01
856.7423	9.69	TG 51:5	[M+NH4] ⁺	2a	m/z, RT	C54H94O6	Triacylglycerol	< 0.01
816.7056	9.34	TG 48:4	[M+NH4] ⁺	2a	m/z, RT	C51H90O6	Triacylglycerol	< 0.01
851.7086	10.40	TG 50:3 B	[M+Na] ⁺	2a	m/z, RT	C53H96O6	Triacylglycerol	< 0.01
632.5263	5.59	DG 36:5	[M+NH4] ⁺	2a	m/z, RT	C39H66O5	Diacylglycerols	< 0.01

Table S7. Annotated compounds and their total compound contribution (%) in pracaxi SFE extract after GC-Q-TOF MS analysis.

<i>Average RT (min)</i>	<i>Metabolite name</i>	<i>MSI Level</i>	<i>MSI Level</i>	<i>Molecular Formula</i>	<i>Compound subclass</i>	<i>Total compound contribution (%)</i>
19.829	Oleic acid	1	MS, RT	C18H34O2	Fatty acids and conjugates	11.87
18.247	Palmitic acid	1	MS, RT	C16H32O2	Fatty acids and conjugates	11.34
20.054	Stearic acid	1	MS, RT	C18H36O2	Fatty acids and conjugates	6.94
9.355/9.572	Glycerol	1	MS, RT	C3H8O3	Carbohydrates and carbohydrate conjugates	6.63
24.122	1-monooleoylglycerol	1	MS, RT	C21H40O4	Monoacylglycerols	6.61
24.721	Lignoceric acid	1	MS, RT	C24H48O2	Fatty acids and conjugates	6.27
7.675	Alanine, N-methyl-N-allyloxycarbonyl-, undecyl ester	2	MS	C19H35NO4	Amino acids, peptides, and analogues	5.94
7.664	2-Pyrrolidinone	1	MS, RT	C4H7NO	Pyrrolidones	5.89
19.77	Linoleic acid	1	MS, RT	C18H32O2	Linoleic acids and derivatives	3.66
7.441/9.106	Oxalic acid	1	MS, RT	C2H2O4	Dicarboxylic acids and derivatives	3.29
16.58	Tagatose	2	MS	C6H12O6	Carbohydrates and carbohydrate conjugates	2.60
25.822	gamma-tocopherol	1	MS, RT	C28H48O2	Quinone and hydroquinone lipids	2.54
16.484	Uridine	2	MS	C9H12N2O6	Pyrimidine nucleosides	1.98
7.219/7.241	Hydroxylamine	1	MS, RT	H3NO	Homogeneous other non-metal compounds	1.45
9.887	Methylmalonic acid	2	MS	C4H6O4	Dicarboxylic acids and derivatives	1.23
9.905	Succinic acid	1	MS, RT	C4H6O4	Dicarboxylic acids and derivatives	0.96
24.585	Squalene	1	MS, RT	C30H50	Triterpenoids	0.82
27.695/28.082	Stigmasterol	2	MS	C29H48O	Stigmastanes and derivatives	0.78
11.103	4-aminobutyric acid	2	MS	C4H9NO2	Amino acids, peptides, and analogues	0.76
7.085	2-methyl-5-aminobenzoxazole	2	MS	C8H8N2O	Benzoxazoles	0.74
15.627	D-(+)-Glucuronic acid .gamma.-lactone, tris(trimethylsilyl) ether, methyloxime (anti)	2	MS	C16H35NO6 Si3	Gamma butyrolactones	0.69
16.482	D-(-)-Fructose	1	MS, RT	C6H12O6	Carbohydrates and carbohydrate conjugates	0.65
22.951	Behenic acid	2	MS	C22H44O2	Fatty acids and conjugates	0.64
6.274	L-norvaline	2	MS	C5H11NO2	Amino acids, peptides, and analogues	0.55
16.614/16.742	Gluconolactone	1	MS, RT	C6H10O6	Carbohydrates and carbohydrate conjugates	0.53
7.833	3-hydroxybutyric acid	1	MS, RT	C4H8O3	Beta hydroxy acids and derivatives	0.52
6.535	Lactic acid	1	MS, RT	C3H6O3	Alpha hydroxy acids and derivatives	0.49
10.307	2-oxohexanoic acid	2	MS	C6H10O3	Medium-chain keto acids and derivatives	0.47

26.763	alpha-tocopherol	1	MS, RT	C29H50O2	Quinone and hydroquinone lipids	0.45
22.175	(Z)-Docos-9-enenitrile	2	MS	C22H41N	Organic cyanides	0.42
17.82	7-Tetradecenal, (Z)-	2	MS	C14H26O	Fatty aldehydes	0.41
16.28	Myristic acid	2	MS	C14H28O2	Fatty acids and conjugates	0.39
24.341	Undec-10-ynoic acid, undec-2-en-1-yl ester	2	MS	C22H38O2	Fatty alcohol esters	0.38
17.13	Sedoheptulose	1	MS, RT	C7H14O7	Carbohydrates and carbohydrate conjugates	0.37
24.439	Methyl 22-methyl-tetracosanoate	2	MS	C26H52O2	Fatty acid esters	0.37
7.569	p-dichlorobenzene	2	MS	C6H4Cl2	Halobenzenes	0.36
22.857	1-monopalmitin	1	MS, RT	C19H38O4	Monoacylglycerols	0.35
28.629	Cycloartenol	2	MS	C30H50	Cycloartanols and derivatives	0.34
18.783	trans-13-Octadecenoic acid	2	MS	C18H34O2	Fatty acids and conjugates	0.33
26.073	Cerotic acid	2	MS	C26H52O2	Fatty acids and conjugates	0.29
14.456	D-xylulose	2	MS	C5H10O5	Carbohydrates and carbohydrate conjugates	0.27
8.231	D-(-)-Pantolactone	2	MS	C6H10O3	Gamma butyrolactones	0.27
12.059	5-Hydroxymaltol	2	MS	C6H6O4	Pyranones and derivatives	0.27
26.91	Propyl docosanoate	2	MS	C25H50O2	Fatty acid esters	0.27
12.76	L-Iditol	2	MS	C6H14O6	Carbohydrates and carbohydrate conjugates	0.27
17.989	Palmitelaidic acid	1	MS, RT	C16H30O2	Fatty acids and conjugates	0.26
24.293	Glycerol monostearate	2	MS	C21H42O4	Monoacylglycerols	0.26
9.022	Eupatoriochromene	2	MS	C13H14O3	1-benzopyrans	0.26
16.665	Andrographolide	2	MS	C20H30O5	Gamma butyrolactones	0.24
10.444	3,4-Dihydroxy-5-methyl-dihydrofuran-2-one	2	MS	C5H8O4	Gamma butyrolactones	0.24
12.562	L-pyroglutamic acid	1	MS, RT	C5H7NO3	Amino acids, peptides, and analogues	0.24
27.297	Benzoic acid, 2-heptafluorobutyryloxy-, tert.-butyldimethylsilyl ester	2	MS	C17H19F7O4Si	Benzoic acids and derivatives	0.23
8.624	1-methoxy-2-propanol	2	MS	C4H10O2	Alcohols and polyols	0.23
11.105	Ethanolamine	2	MS	C2H7NO	Amines	0.23
15.223	3,6-anhydro-D-galactose	1	MS, RT	C6H10O5	Tetrahydrofurans	0.23
8.509	3-hydroxyisovaleric acid	1	MS, RT	C5H10O3	Fatty acids and conjugates	0.22
9.054	Benzoic acid	1	MS, RT	C7H6O2	Benzoic acids and derivatives	0.20
14.135	Lauric acid	1	MS, RT	C12H24O2	Fatty acids and conjugates	0.20
16.738	Dihydroconiferyllic acid	2	MS	C10H12O4	Phenylpropanoic acids	0.20
10.694	Erythronic acid lactone	1	MS, RT	C4H6O4	Gamma butyrolactones	0.19
22.444	Methyl behenate	1	MS, RT	C23H46O2	Fatty acid esters	0.19

9.252	Octanoic acid	1	MS, RT	C8H16O2	Fatty acids and conjugates	0.19
8.894	Urea	1	MS, RT	CH4N2O	Ureas	0.18
24.958	Benzene, 1,2-bis(9-borabicyclo[3.3.1]non-9-yloxymethyl)-	2	MS	C24H36B2O2	Borinanes	0.16
18.972	1,4-Benzenediamine, N-(1-methylethyl)-N'-phenyl-	2	MS	C15H18N2	Amines	0.16
13.692	Glutaconic acid	2	MS	C5H6O4	Dicarboxylic acids and derivatives	0.16
23.862	2-monoolein	1	MS, RT	C21H40O4	Monoacylglycerols	0.16
28.103	beta-sitosterol	2	MS	C29H50O	Stigmastanes and derivatives	0.13
10.537	Pelargonic acid	1	MS, RT	C9H18O2	Fatty acids and conjugates	0.13
21.67	1-Pentadecyne	2	MS	C15H28	Acetylides	0.13
6.282	1,3-propanediol	1	MS, RT	C3H8O2	Alcohols and polyols	0.13
8.318	Malonic acid	1	MS, RT	C3H4O4	Dicarboxylic acids and derivatives	0.12
17.076	Methyl palmitate	1	MS, RT	C17H34O2	Fatty acid esters	0.12
18.675	Ferulic acid	1	MS, RT	C10H10O4	Hydroxycinnamic acids and derivatives	0.12
14.104	D-(+)-Ribono-1,4-lactone	2	MS	C5H8O5	Carbohydrates and carbohydrate conjugates	0.10
15.387	Arabinofuranose	2	MS	C5H10O5	Carbohydrates and carbohydrate conjugates	0.10
11.07	5-hydroxymethylfurfural	2	MS	C6H6O3	Carbonyl compounds	0.10
19.168	Margaric acid	1	MS, RT	C17H34O2	Fatty acids and conjugates	0.09
16.447	Senecioic acid	2	MS	C5H8O2	Fatty acids and conjugates	0.08
26.517	nonacosane	2	MS	C29H60	Alkanes	0.08
11.536	Reticuline, 6'-methyl	2	MS	C20H25NO4	Benzylisoquinolines	0.08
15.994	1-Tetradecyne	2	MS	C14H26	Acetylides	0.08
17.194/17.204	Coniferyl alcohol	2	MS	C10H12O3	Methoxyphenols	0.07
19.023	Methyl stearate	1	MS, RT	C19H38O2	Fatty acid esters	0.07
22.491	alpha-Lactose	1	MS, RT	C12H22O11	Carbohydrates and carbohydrate conjugates	0.07
23.221	Sucrose	1	MS, RT	C12H22O11	Carbohydrates and carbohydrate conjugates	0.07
15.547	D-(-)-Ribofuranose	2	MS	C5H10O5	Carbohydrates and carbohydrate conjugates	0.07
23.973	Methyl lignocerate	1	MS, RT	C25H50O2	Fatty acid esters	0.06
16.438	Methyl-beta-D-galactopyranoside	2	MS	C7H14O6	Carbohydrates and carbohydrate conjugates	0.06
8.86	2-butyne-1,4-diol	1	MS, RT	C4H6O2	Alcohols and polyols	0.06
13.314	3-phenyllactic acid	1	MS, RT	C9H10O3	Phenylpropanoic acids	0.05
25.154	delta-tocopherol	2	MS	C27H46O2	Quinone and hydroquinone lipids	0.04
18.719	Methyl linoleate	1	MS, RT	C19H34O2	Linoleic acids and derivatives	0.04
8.406	Aniline	1	MS, RT	C6H7N	Aniline and substituted anilines	0.04
17.209	4-hydroxycinnamic acid	1	MS, RT	C9H8O3	Hydroxycinnamic acids and derivatives	0.04

22.762	Brassicid acid	2	MS	C22H42O2	Fatty acids and conjugates	0.04
9.723	2-phenylacetic acid	2	MS	C8H8O2	Benzene and substituted derivatives	0.04
14.673	1,6-Anhydro-beta-D-glucose	1	MS, RT	C6H10O5	Oxepanes	0.03
15.934	Citric acid	1	MS, RT	C6H8O7	Tricarboxylic acids and derivatives	0.03
16.705	Glucopyranose	2	MS	C6H12O6	Carbohydrates and carbohydrate conjugates	0.03
17.282	Pentadecanoic acid	2	MS	C15H30O2	Fatty acids and conjugates	0.03
10.209	Uracil	1	MS, RT	C4H4N2O2	Pyrimidines and pyrimidine derivatives	0.03
17.555	D-lyxose	2	MS	C5H10O5	Carbohydrates and carbohydrate conjugates	0.03
9.298	1-(2-Ethyl-[1,3]dithian-2-yl)-3-methyl-butan-1-ol	2	MS	C11H22OS2	Dithioacetals	0.03
11.787	Capric acid	2	MS	C10H20O2	Fatty acids and conjugates	0.02
18.618	Oleonitrile	2	MS	C18H33N	Organic cyanides	0.02
15.478	D-(-)-Tagatofuranose	2	MS	C6H12O6	Carbohydrates and carbohydrate conjugates	0.02
22.308	L-(+)-Rhamnopyranose	2	MS	C6H12O5	Carbohydrates and carbohydrate conjugates	0.02
13.191	Tyrosol	1	MS, RT	C8H10O2	Tyrosols and derivatives	0.02
20.799	Methyl arachidate	1	MS, RT	C21H42O2	Fatty acid esters	0.01

Table S8. PLE conditions, desirability and predicted response values at the optimum conditions predicted by the model, and experimental response values for the selected optimum conditions.

	Including Extraction yield as response variable			Excluding Extraction yield as response variable	
	<i>Predicted</i>	<i>Experimental</i>	<i>Optimum</i>	<i>Predicted</i>	<i>Experimental</i>
	<i>Optimum</i>	<i>(80% EtOH at 180 °C)</i>		<i>Optimum</i>	<i>(12.5% ethanol at 180 °C)</i>
Temperature (°C)	180	180		180	180
Solvent composition (% EtOH)	80.2	80		12.6	12.5
Desirability	0.934953			1.0000	
Response variable					
Extraction yield	21.22	24.0 ± 3.0			
ROS	2.94	1.5 ± 1.0		1.98798	1.6 ± 1.0
TPC	168.86	91.9 ± 0.9		176.595	103.9 ± 0.5
AChE	247.00	276 ± 17		245.516	315 ± 29

Table S9. Tentative identified compounds in pracaxi nuts PLE extracts after HPLC-C18-Q-TOF MS/MS ESI (+/-) analyses.

			ESI (+)										ESI (-)									
			Peak area										Peak area									
Compound number	Tentative compound name	Molecular Formula	Retention time	m/z	Adduct type	MS/MS Spectra	PLE 12	PLE 12	PLE 12	PLE 80	PLE 80	PLE 80	Retention time	m/z	Adduct type	MS/MS Spectra	PLE 12	PLE 12	PLE 12	PLE 80	PLE 80	PLE 80
1	Agmatine	C5H14N4	0.497	131.12921	[M+H] ⁺	97.07, 72.08, 60.06, 55.05	202	173	186	115	275	201										
2	L-Arginine	C6H14N4O2	0.537	175.11766	[M+H] ⁺	70.07, 60.06	465	437	326	191	458	424										
3	Serine	C3H7NO3											0.545	104.02676	[M-H] ⁻	74.02	265	289	192	121	198	225
																	868	990	206	600	663	002
4	D-Asparagine	C4H8N2O3											0.552	131.04405	[M-H] ⁻	114.02, 113.03, 96.00, 72.01, 71.03,	113	114	327	351	629	118
																	270	454	167	796	49	587
																	1	3				1

5	Threonine	C4H9 NO3	0.5 54	120. 065 19	[M+H]+	74.06, 56.05	57.03,	163 989	167 612	142 685	108 232	234 263	142 659										
														70.03, 58.03									
6	D-Arabinonic acid	C5H1 OO6												0.5 71	165. 031 63	[M- H]-	87.01, 75.01, 72.99, 71.01, 59.01 195.05, 129.02, 99.01, 89.02, 87.01, 85.03, 75.01, 59.01	854 608	908 332	722 748	343 277	126 850 1	475 827
7	Galactonic acid	C6H1 2O7												0.5 72	195. 041 93	[M- H]-		609 254	683 445	607 868	209 021	106 441 7	429 571
8	Choline cation	C5H1 4NO	0.5 85	104. 099 43	[M]+	104.11, 60.08, 59.07, 58.06		181 161 85	107 880 31	186 397 26	146 694 55	175 193 03	153 260 08										
9	D-Lyxose	C5H1 OO5												0.6 11	149. 045 87	[M- H]-	71.01, 59.01	251 990	262 958	142 933	235 10	411 18	380 61
10	Glycerophosp hocholine	C8H2 ONOO P	0.6 16	258. 108 12	[M+H]+	258.11, 184.07, 125.00, 104.11		426 875	429 884	328 050	150 065	230 162	161 092										

11	L- Monomethyl arginine	C7H1 6N4O 2	0.6 18	116. 072 00	[M+H - C2H7 N3]+	116.07, 70.06	974 929 3	107 119 68	119 655 46	697 761 7	116 715 52	797 126 1																
											0.6 40	341. 110 05	[M- H]-	179.06 [M- H- C6H10O5]-, 119.04, 101.03, 89.03, 71.01, 59.01 377.08 [M+Cl]-, 341.11 [M- H]-, 179.06 [M-H- C6H10O5]-, 161.04, 143.03, 119.03, 101.02, 89.02, 71.01, 59.01	342 931 721 753 776 794 396	289 721 753 776 794 396	349 753 776 794 396	322 776 794 396	384 794 396	333 396								
											0.6 28	365. 107 76	[M+N a]+	365.10, 203.06, 185.04	127 340	101 456	159 954	104 812	946 75	116 973								
12	4-O-.beta.- Galactopyran osyl-D- mannopyrano se	C12H 22O1 1	0.6 40	360. 148 96	[M+N H4]+		123 010 1	145 824 5	166 522 0	125 802 8	139 293 9	135 687 5	0.6 34	377. 081 51	[M+ Cl]-	281 860 2	283 056 7	311 274 8	252 631 4	294 959 6	254 223 0							
											0.6 28	365. 107 76	[M+N a]+	365.10, 203.06, 185.04	127 340	101 456	159 954	104 812	946 75	116 973								
											0.6 40	360. 148 96	[M+N H4]+		123 010 1	145 824 5	166 522 0	125 802 8	139 293 9	135 687 5								

13	Trigonelline	C7H7NO2	0.652	138.055	[M+H] ⁺	138.06, 94.06	811	843	911	668	638	785	<div>341.11 [M-H]⁻, 179.06 [M-H-C6H10O5]⁻, 161.04, 592 494 609 538 580 581 119.03, 698 955 133 969 302 272 101.03, 89.02, 71.01, 59.01 683.23 [2M-H]⁻, 341.11 [M-H]⁻, 179.06 [M-H-C6H10O5]⁻</div>					
				56			3	4	4	3	9	0						
				275.101			334	374	412	301	260	448						
				93			839	713	408	762	385	491						
14	3-Hydroxypyridine	C5H5NO	0.656	96.0430	[M+H] ⁺	96.04, 78.03, 68.05	261	268	245	269	260	352						
				8			545	014	891	751	168	930						
							3	7	2	5	2	2						

15	5-Hydroxy-2-methylpyridine	C6H7NO	0.673	110.06235	[M+H] ⁺	110.06, 95.04, 94.03, 82.06, 81.06, 80.05, 67.04, 65.04	1834270	2084313	1773971	1477776	1304996	1977798											
16	Betaine	C5H11NO2	0.674	118.08470	[M+H] ⁺	118.09, 59.07, 58.06	1170165	1415371	1552937	1259719	2516723	1219785											
17	Malic acid	C4H6O5					0.677	133.01433	[M-H] ⁻	133.01, 115.01, 89.02, 72.99, 71.01, 59.02	7494537	7820892	6948604	8207084	10510066	7461399							
18	Cadaverine	C5H14N2	0.678	86.09517	[M+H] ⁺ [NH3] ⁺	86.10, 69.07	147777	145973	132977	438966	324936	386118											
19	His-Pro	C11H16N4O3	0.680	235.11913	[M+H] ⁺ [H2O] ⁺	235.12, 207.13, 166.06, 162.10, 110.07, 82.05, 70.07	860358	1048104	950386	877044	1061739	920442											
20	N-Methyl-L-leucine	C7H15NO2	0.681	100.11154	[M+H] ⁺ [CH2O2] ⁺	100.11, 58.07	45485	56696	30593	2218926	1025087	1120199											

[illegible]

[illegible]

37	L-Tryptophan	C11H12N2O2	2.846	205.09726	[M+H] ⁺	188.07 [M+H-NH3] ⁺ , 170.06, 159.09, 813 110 131 513 243 136 146.06, 164 297 036 464 467 033 144.08, 132.08, 131.07, 118.06
38	N-Acetyl-DL-valine	C7H13NO3	3.014	114.09003	[M+H] ⁺	188.11 [M+H-NH3] ⁺ , 170.06, 146.06, 219 327 102 325 720 136 144.08, 496 150 562 38 029 655 143.07, 118.06, 91.05
39	N-L-γ-Glutamyl-L-leucine	C11H20N2O5	3.061	261.14438	[M+H] ⁺	244.12, 198.11, 177 549 182 779 247 121 132.10, 190 550 891 884 387 949 130.05, 86.10, 2 7 1 3 84.04
40	3,4-Dihydroxybenzaldehyde	C7H6O3	3.033	137.02615	[M-H] ⁻	259.13132 [M-H] ⁻ , 241.12, 197.13, 490 477 461 268 581 378 130.08, 800 755 486 283 832 303 128.04

41	N-(3-(Aminomethyl)benzyl)acetamidine	C10H15N3	3.125	178.13219	[M+H] ⁺	178.13, 161.11, 120.08	107	639	345	135	107	113										
						747	77	56	417	163	666											
42	Diethyl glutamate	L- C9H17NO4	3.164	158.08083	[M+H] ⁺	84.04, 56.05	506	101	768	965	798	128										
						282	0	009	048	311	022	4	3	8								
43	N-N'-bis-(dihydrocaffeoyl) spermidine-monoglucoside (+C6H10O5)	C31H45N3O11	3.766	636.31165	[M+H] ⁺	636.31 [M+H] ⁺ , 618.33 [M+H-H2O] ⁺ , 600.30 [M+H-H2O] ⁺ , 474.26 [M+H-C6H10O5] ⁺ , 457.23 [M+H-C6H10O5-NH3] ⁺ , 384.17, 293.19 [M+H-C6H10O5-NH3-dihydrocaffeo	224	270	557	306	102	527	3.6	634.29742	[M-H] ⁻	634.29 [M-H] ⁻ , 472.24 [M-H-C6H10O5] ⁻	490	368	352	175	138	942
						836	356	888	094	186	587	04	42	H] ⁻	00	43	07	967	176	56		

44	N-N'-bis-(dihydrocaffeoyl) spermidine isomer 1	C25H35N3O6	4.0 16	474.264 65	[M+H]]+	yl]+, 222.11, 112.11, 72.08 474.26 [M+H]+, 457.23 [M+H- NH3]+, 310.21 [M+H- dihydrocaffeoyl]+, 293.19 [M+H- dihydrocaffeoyl-NH3]+, 239.14, 222.11, 165.05, 123.04, 72.08	457	456	306	387	344	224	3.6 57	472.243 56	[M- H]-	472.24 [M- H]-, 350.21 [M-H-122]-, 308.20 [M- H- dihydrocaffeoyleyl]-, 186.16 [M- H-122- dihydrocaffeoyleyl]-, 121.03	138	155	167	204	377	195
							258	378	677	740	642	090					661	384	275	782	687	948
							87	99	25	55	16	77					80	75	29	62	59	69
4.0 16	496.241 15	[M+N a]+	496.24 [M+H+Na]+	104	108	101		428	896	561												
				221	807	813		472	164	891												
				3	0	1																
4.0 13	947.514 34	[2M+ H]+	474.25 [M+H]+, 457.23 [M+H- NH3]+	475	432	603	552	928	579													
				717	440	943	163	267	680													
4.0 07	969.491 70	[2M+ Na]+		191	193	484	387	366	433													
				214	510	195	584	225	901													

N-N'-bis-(dihydrocaffeoyl) spermidine-monoglucoside (+C ₅ H ₈ O ₄)	C ₃₀ H ₄₃ N ₃ O ₁₀	4.096	606.30280	[M+H] ⁺	606.30 [M+H] ⁺ , 588.29 [M+H-H ₂ O] ⁺ , 570.28 [M+H-H ₂ O-H ₂ O] ⁺ , 552.26 [M+H-H ₂ O-H ₂ O-H ₂ O] ⁺ , 474.25 [M+H-C ₅ H ₈ O ₄] ⁺ , 457.22 [M+H-C ₅ H ₈ O ₄ -NH ₃] ⁺ , 388.22 [M+H-H ₂ O-H ₂ O-dihydrocaffeoyl] ⁺ , 370.20 [M+H-H ₂ O-H ₂ O-dihydrocaffeoyl-H ₂ O] ⁺ , 293.18 [M+H-C ₅ H ₈ O ₄ -NH ₃ -dihydrocaffeoyl] ⁺ , 222.10, 204.11, 150.08	651 136 9	513 256 6	550 346 1	181 584 4	232 772 3	164 061 9	3.726	604.28595	[M-H] ⁻	604.29 [M-H] ⁻ , 586.28 [M-H-H ₂ O] ⁻ , 568.26 [M-H-H ₂ O-H ₂ O] ⁻ , 545.27, 514.25, 472.24 [M-H-C ₅ H ₈ O ₄] ⁻ , 350.21 [M-H-C ₅ H ₈ O ₄ -122] ⁻	542 631	768 687	541 977	329 814	190 147	248 694
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46	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+CH2)	C26H37N3O6	4.1	488.27515	[M+H] ⁺	488.27	770	682	612	280	140	276	3.7	486.63	[M-H] ⁻	486.26	281	853	243	325	412	460
						[M+H] ⁺ , 457.22 [M+H-CH5N] ⁺ , 324.23 [M+H-dihydrocaffeoyl] ⁺ , 293.18 [M+H-CH5N-dihydrocaffeoyl] ⁺ , 222.11, 165.05, 123.04, 86.10										[M-H] ⁻ , 364.22 [M-H-122] ⁻ , 322.21 [M-H-dihydrocaffeoyl] ⁻ , 200.18 [M-H-122-dihydrocaffeoyl] ⁻ , 121.03, 111.08						
47	N-N'-bis-(dihydrocaffeoyl) spermidine isomer 2	C25H35N3O6	4.2	474.25964	[M+H] ⁺	474.26	163	296	344	425	177	533	3.8	472.91	[M-H] ⁻	472.26	157	647	192	434	241	392
						[M+H] ⁺ , 457.23 [M+H-NH3] ⁺ , 310.21 [M+H-dihydrocaffeoyl] ⁺ , 293.19 [M+H-NH3-dihydrocaffeoyl] ⁺ , 222.11, 165.05, 123.04, 72.08										[M-H] ⁻ , 364.22 [M-H-122] ⁻ , 322.21 [M-H-dihydrocaffeoyl] ⁻ , 200.18 [M-H-122-dihydrocaffeoyl] ⁻ , 121.03, 111.08						

48	N-coumaroyl-N'-dihydrocaffeoyl spermidine	C25H33N3O5	4.231	456.24939	[M+H] ⁺	456.25	565690	980932	775209	305145	351	3.840	454.23425	[M-H] ⁻	454.23	4798	5257	2303	12960	4833	12107				
						[M+H-NH3] ⁺ , 293.19				5129	7841				3731							[M-H-122] ⁻ , 297.15,			
						[M+H-NH3-coumaroyl] ⁺ , 236.13, 221.13, 165.05, 123.04, 112.11, 84.08, 72.08				5129	7841				3731							249.20, 233.96, 192.02, 123.30, 95.06			
49	N-caffeoyl-N'-dihydrocaffeoyl spermidine-conjugate (+C5H2O)	C30H35N3O7	4.242	550.25385	[M+H] ⁺	550.25	641624	653916	257973	385389	108	3.886	548.24036	[M-H] ⁻	548.24	13543	17349	15386	1185	419	1071				
						[M+H-NH3] ⁺ , 455.22				342.13, 326.10, 285.08, 243.07, 222.11, 165.05, 112.11	6241				4							5	628	345	[M-H-NH3] ⁺ , 455.22
						[M+H-NH3-C5H5NO] ⁺ , 383.16, 342.13, 326.10, 285.08, 243.07, 222.11, 165.05, 112.11				6241	4				5							628	345	412.19, 326.09, 175.03, 135.04	
50	N-caffeoyl-N'-dihydrocaffeoyl spermidine isomer 1	C25H33N3O6	4.303	472.24429	[M+H] ⁺	472.24	147241	336653	364421	320904	681590	278	3.945	470.22711	[M-H] ⁻	470.23	345633	370403	195947	476301	827668	412308			
						[M+H] ⁺ , 457.23				282	1	350.20													
						[M+H-NH] ⁺ , 310.21				2	4	9				4							5	1	[M-H-120] ⁻ , 308.20

51	N-N'-bis-(dihydrocaffeoyl) spermidine-monoglucoside (+C6H10O4)	C31H45N3O10	4.327	620.31561	[M+H] ⁺	[M+H-caffeoyl] ⁺ , 293.19 [M+H-NH3-caffeoyl] ⁺ , 222.11, 165.05, 163.04, 123.04, 72.08 620.32 [M+H] ⁺ , 602.31 [M+H-H2O] ⁺ , 584.29 [M+H-H2O-H2O] ⁺ , 566.28 [M+H-H2O-H2O-H2O] ⁺ , 548.26 168 118 872 292 961 264								H-caffeoyl] ⁻ , 186.16 [M-H-caffeoyl-122] ⁻ , 161.02							
						474.26 [M+H-C6H10O4] ⁺ , 457.23 [M+H-C6H10O4-NH3] ⁺ , 293.18															
						[M+H-C6H10O4-NH3-dihydrocaffeoyl] ⁺ , 293.18															

52	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C2H4)	C27H39N3O6	4.334	502.28925	[M+H] ⁺	yl] ⁺ , 222.11, 164.11, 95.05	623	651	242	3520552	751	405	3.964	500.27341	[M-H] ⁻	500.27 [M-H] ⁻ , 455.22	781	216	139	378	465	524
						457.23 [M+H-C2H7N] ⁺ , 338.24 [M+H-dihydrocaffeoyl] ⁺ , 293.19 [M+H-C2H7N-dihydrocaffeoyl] ⁺ , 222.11, 165.05, 123.04, 100.11										214.20 [M-H-122-dihydrocaffeoyleoyl] ⁻ , 195.06, 135.04						
53	N-dihydrocoumaroyl-N'-dihydrocaffeoyl spermidine	C25H35N3O5	4.440	458.26361	[M+H] ⁺	458.26 [M+H] ⁺ , 441.24 [M+H-NH3] ⁺ , 310.21	160	171	203	129	261	140	4.061	456.24817	[M-H] ⁻	456.25 [M-H] ⁻ , 334.41 [M-H-122] ⁻ , 308.20 [M-H-dihydrocoumaroyl] ⁻ , 186.16 [M-H-122-dihydrocoumaroyl] ⁻ , 137.06,	898	101	101	110	322	995
						293.19 [M+H-NH3-dihydrocoumaroyl] ⁺ , 277.19 [M+H-NH3-										334.41 [M-H-122] ⁻ , 308.20 [M-H-dihydrocoumaroyl] ⁻ , 186.16 [M-H-122-dihydrocoumaroyl] ⁻ , 137.06,						

54	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C5H2)	C30H37N3O6	4.468	536.274	[M+H] ⁺	dihydrocaffeoyl] ⁺ , 236.13, 222.11, 206.12, 165.05, 123.04, 107.05, 100.07, 72.08 536.27 [M+H] ⁺ , 457.23 [M+H-C5H5N] ⁺ , 293.19 [M+H-C5H5N-dihydrocaffeoyl] ⁺ , 236.13, 222.11, 165,05, 72.08 472.25 [M+H] ⁺ , 455.22 [M+H-NH3] ⁺ , 310.21 [M+H-caffeoyl] ⁺ , 293.19 [M+H-NH3-caffeoyl] ⁺ ,												121.03, 58.03												
						246	215	221	452	470	401	293.19	781	276	292	287	501	129	2	1	0	8	3	4						
55	N-caffeoyl-N'-dihydrocaffeoyl spermidine isomer 2	C25H33N3O6	4.519	472.243	[M+H] ⁺	470.22 [M-H] ⁻ , 350.21 [M-H-120] ⁻ , 308.20 [M-H-caffeoyl] ⁻ , 186.16 [M-H-caffeoyl-122] ⁻ ,																								
						731	852	103	883	247	103	731	814	695	287	189	739	290	2	5	67	470.229	[M-H] ⁻	308.20	[M-H-caffeoyl] ⁻	323.08	604.39	180.04	848.04	356.884

56	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C4H6)	C29H41N3O6	4.538	528.30560	[M+H] ⁺	239.14, 222.11, 220.10, 163.04, 123.04, 72.08 528.31 [M+H] ⁺ , 457.23 [M+H-C4H9N] ⁺ , 293.19 [M+H-C4H9N-dihydrocaffeo yl] ⁺ , 222.11, 126.13										161.02, 58.03									
						21950	28759	10909	1502929	283047	515908														
57	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C5H2O) isomer 1	C30H37N3O7	4.634	552.27325	[M+H] ⁺	552.27 [M+H] ⁺ , 457.23 [M+H-C5H5NO] ⁺ , 293.18 [M+H-C5H5NO-dihydrocaffeo yl] ⁺ , 236.12, 222.11, 165.05, 123.04, 112.11										550.25 [M-H] ⁻ , 455.22 [M-H-C5H5NO] ⁻ , 333.18 [M-H-C5H5NO-122] ⁻ , 291.17 [M-H-C5H5NO-dihydrocaffeo yl] ⁻ , 279.14, 94.03									
						33058149	32452875	32943042	24444075	9156470	34298097	4.313	550.25287	[M-H] ⁻	550.25287	920226	1246058	818414	1368890	130470	1974136				

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60	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C4H3N)	C29H38N4O6	4.763	539.28522	[M+H] ⁺	C4H8N2-dihydrocaffeoyl] ⁺ , 236.13, 222.11, 165.05, 123.04, 112.11 539.28 [M+H] ⁺ , 457.23 [M+H-C4H6N2] ⁺ , 375.24 [M+H-dihydrocaffeoyl] ⁺ , 293.19 [M+H-C4H6N2-dihydrocaffeoyl] ⁺ , 236.13, 222.11, 165.05, 123.04, 112.11 560.29 [M+H] ⁺ , 457.23 [M+H-C4H9NO2] ⁺ , 396.25 [M+H-dihydrocaffeoyl] ⁺ , 378.24										537.27 [M-H] ⁻ , 373.22 [M-H-dihydrocaffeoyleyl] ⁻ 558.28 [M-H] ⁻ , 436.24 [M-H-122] ⁻ , 394.23 [M-H-dihydrocaffeoyleyl] ⁻ ,									
						1837799	1787123	1559406	1828513	8157001	1319551	4.374	537.27124	[M-H] ⁻	537.27	24938	26460	15184	17315	6234	20440				
61	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C4H6O2)	C29H41N3O8	4.834	560.29669	[M+H] ⁺	1666879										7558									
						1560483	1609421	3519999	5580890	2978043	4.425	558.28082	[M-H] ⁻	558.28	7558	14779	14826	185478	159345	129080					

62	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C6H5N) isomer 1	C31H40N4O6	4.831	565.30200	[M+H] ⁺	[M+H-dihydrocaffeoyl-H2O] ⁺ , 293.19 [M+H-C4H9NO2-dihydrocaffeoyl] ⁺ , 236.13, 222.11, 165.05, 158.12, 130.09, 84.08 565.30 [M+H] ⁺ , 457.23 [M+H-C6H8N2] ⁺ , 293.19 [M+H-C6H8N2-dihydrocaffeoyl] ⁺ , 236.13, 222.11, 165.05, 123.04, 112.11 585.33 [M+H] ⁺ , 105 541.30 [M+H-C2H4O] ⁺ , 457.24 [M+H-										362.20, 320.19, 121.02, 58.02					
						293.19	118	124	130	310	237	119									
						978	556	045	932	388	937										
						2	1	8	3	6	6										
63	N-N'-bis-(dihydrocaffeoyl) spermidine-	C31H44N4O7	4.888	585.32916	[M+H] ⁺	[M+H] ⁺ , 105 541.30 [M+H-C2H4O] ⁺ , 457.24 [M+H-															
						541.30	362	763	787	102	118	109									
								137	317	042	551	622									
							7			6	6	1									

[illegible]

66	N-dihydrocoumaroyl-N'-dihydrocaffeoyl spermidine conjugate (+C5H2O)	C30H37N3O6	5.065	536.275	[M+H] ⁺	177.06,	165.05,	145.03,	123.04,	117.03, 72.08	536.27	[M+H] ⁺ ,	441.24 [M+H-C5H5NO] ⁺ ,	293.18 [M+H-C5H5NO-dihydrocoumaroyl] ⁺ ,	608.876	623.342	578.968	205.867	513.238	499.545	4.719	534.259	[M-H] ⁻	534.26 [M-H] ⁻ ,	439.22 [M-H-C5H5NO] ⁻ ,	386.20 [M-H-dihydrocoumaroyl] ⁻ ,	665.10	923.62	499.89	500.44	458.2	470.30
						222.11,	220.13,	206.12,	165.05,	123.04,	112.11,	107.05, 100.07	551.29	[M+H] ⁺ ,	122.717	888.2	111.40	317.9	231.2	260.9	4.749	549.271	[M-H] ⁻	549.27 [M-H] ⁻ ,	427.23 [M-H-122] ⁻ ,	385.22 [M-	540	100.38	208.3	123.004	108.497	644.05
67	N-N'-bis-(dihydrocaffeoyl) spermidine-	C30H38N4O6	5.078	551.286	[M+H] ⁺	551.29	[M+H] ⁺ ,	122.717	888.2	111.40	317.9	231.2	260.9	4.749	549.271	[M-H] ⁻	549.27 [M-H] ⁻ ,	427.23 [M-H-122] ⁻ ,	385.22 [M-	540	100.38	208.3	123.004	108.497	644.05							
						551.29	[M+H] ⁺ ,	122.717	888.2	111.40	317.9	231.2	260.9	4.749	549.271	[M-H] ⁻	549.27 [M-H] ⁻ ,	427.23 [M-H-122] ⁻ ,	385.22 [M-	540	100.38	208.3	123.004	108.497	644.05							

[illegible]

70	spermidine-conjugate (+C5H8O2)												C3H6O2]+, 457.22 [M+H-C5H11NO2]+, 410.25 [M+H-dihydrocaffeoyl]+, 392.24 [M+H-dihydrocaffeoyl-H2O]+, 336.21 [M+H-C3H6O2-dihydrocaffeoyl]+, 293.17 [M+H-C5H11NO2-dihydrocaffeoyl]+, 222.11, 172.12, 98.08 567.32 [M+H]+, 457.23 [M+H-C6H10N2]+, 293.19 [M+H-C6H10N2-dihydrocaffeoyl]+, 236.13, 222.11,										C3H6O2]-, 450.26 [M-H-122]-, 408.25 [M-H-dihydrocaffeoyleoyl]-, 376.23 [M-H-C3H6O2-122]-, 334.22 [M-H-C3H6O2-dihydrocaffeoyleoyl]-, 135.05, 121.03 565.30 [M-H]-, 443.26 [M-H-122]-, 423.06, 401.25 [M-H-dihydrocaffeoyleoyl]-,									
	N-N'-bis-(dihydrocaffeoyleoyl) spermidine-conjugate (+C6H7N)	C31H42N4O6	5.344	567.31769	[M+H]+	762485	654957	820331	2194086	3881258	1282542	4.951	565.30200	[M-H]-	423.06, 401.25	3145	3478	3835	25994	38462	7839											

71	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C ₆ H ₅ N) isomer 2	C ₃₁ H ₄₀ N ₄ O ₆	5.351	565.30212	[M+H] ⁺	1650.5, 123.04, 112.11 565.30 [M+H] ⁺ , 457.23 [M+H-C ₆ H ₈ N ₂] ⁺ , 401.25 [M+H-dihydrocaffeoyl] ⁺ , 383.24 [M+H-dihydrocaffeoyl-H ₂ O] ⁺ , 293.19 [M+H-C ₆ H ₈ N ₂ -dihydrocaffeoyl] ⁺ , 236.13, 222.11, 123.04 502.25 [M+H] ⁺ , 474.26 [M+H-CO] ⁺ , 338.21 [M+H-dihydrocaffeoyl] ⁺ , 320.20 [M+H-dihydrocaffeoyl-H ₂ O] ⁺ ,	747 672 564 176 131 141 219 220 623 298 892 701 7 4 2	4.984	563.28424	[M-H] ⁻	121.03, 109.08	593 443 514 461 119 123 5 3 9 19 24 99
72	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+CO)	C ₂₆ H ₃₅ N ₃ O ₇	5.388	502.25519	[M+H] ⁺	500.24 [M-H] ⁻ , 378.20 [M-H-122] ⁻ , 336.19 [M-H-dihydrocaffeoyleoyl] ⁻ , 214.15 [M-H-122-dihydrocaff	157 162 151 134 215 258 521 756 267 332 680 333 7 4 8 6 5 7	5.339	500.23798	[M-H] ⁻	500.24 [M-H] ⁻ , 378.20 [M-H-122] ⁻ , 336.19 [M-H-dihydrocaffeoyleoyl] ⁻ , 214.15 [M-H-122-dihydrocaff	483 548 391 156 858 131 696 974 409 763 250 6 657 0

73	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C8H7N)	C33H42N4O6	5.395	591.31757	[M+H] ⁺	222.11, 165.05, 157.14, 123.04, 100.07, 72.08 591.32 [M+H] ⁺ , 457.23 [M+H-C8H10N2] ⁺ , 293.19 [M+H-C8H10N2-dihydrocaffeoyl] ⁺ , 236.13, 222.11, 165.05, 123.04 593.33 [M+H] ⁺ , 457.23 [M+H-C8H12N2] ⁺ , 293.19 [M+H-C8H12N2-dihydrocaffeoyl] ⁺ , 236.13, 222.11, 165.05, 123.04, 112.11	257 207 5	216 297 9	211 657 3	792 934	124 966 2	203 237 5
						eoyl]-, 186.16, 121.03, 115.09						
74	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C8H9N) isomer 1	C33H44N4O6	5.543	593.33429	[M+H] ⁺	274 576 2	242 342 3	235 302 4	748 643 9	584 246 8	468 578 4	

75	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C2H2O)	C27H37N3O7	5.563	516.26849	[M+H] ⁺	516.27								514.26	[M-H] ⁻							
						[M+H] ⁺ , 457.23 [M+H-C2H5NO] ⁺ , 352.22 [M+H-dihydrocaffeoyl] ⁺ , 334.21 [M+H-dihydrocaffeoyl-H2O] ⁺ , 293.19 [M+H-C2H5NO-dihydrocaffeoyl] ⁺ , 222.11, 171.15, 165.05, 123.04, 114.09, 100.07	6835322	6959581	6878591	3708138	4616669	4237937	514.25507	350.21		[M-H] ⁻	1815931	2023693	1460453	1552007	1225567	1487164
76	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C4H2O3)	C29H37N3O9	5.747	572.26086	[M+H] ⁺	572.26								570.24	[M-H] ⁻							
						[M+H] ⁺ , 408.21 [M+H-dihydrocaffeoyl] ⁺ , 390.20 [M+H-dihydrocaffeoyl-H2O] ⁺ , 227.14,	1271795	1197199	780446	4933818	1152121	4358162	570.24347	570.24		[M-H] ⁻	506724	566490	352522	3367120	519363	2349849

77	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C8H9N) isomer 2	C33H44N4O6	5.756	593.33380	[M+H] ⁺	222.11, 213.12, 165.06, 123.04							dihydrocaffeoyl]-, 279.13, 135.04, 121.03									
						593.33 [M+H] ⁺ , 457.23 [M+H-C8H12N2] ⁺ , 293.19 [M+H-C8H12N2-dihydrocaffeoyl] ⁺ , 236.13, 222.11, 165.06, 137.11, 123.04, 112.11 630.27 [M+H] ⁺ , 466.22 [M+H-dihydrocaffeoyl] ⁺ , 448.21 [M+H-dihydrocaffeoyl-H2O] ⁺ , 285.14 [M+H-dihydrocaffeoyl-H2O] ⁺ ,																
78	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C6H4O5)	C31H39N3O11	5.824	630.26556	[M+H] ⁺	816 672 255 230 527 128 861 083 571 663 038 252 9							628.25 [M-H] ⁻ , 610.24 [M-H-H2O] ⁻ , 566.25 [M-H-62] ⁻ , 472.25 [M-H-C6H4O5], 456.21,									
						747 613 467 382 192 281 402 016 903 8 5 7							5.7 628.24738 [M-H] ⁻ 580 774 396 458 188 317 698 116 297 6 4 7									

79	N-dihydrocoumaroyl-N'-dihydrocaffeoyl spermidine-conjugate (+C2H2O)	C27H37N3O6	yl-dihydrocaffeoyl-NH3]+, 271.13, 222.11, 165.05, 123.04										444.21[M-H-62-122]-, 402.20 [M-H-62-dihydrocaffeoyl]-, 322.18 [M-H-62-122-122]-, 280.17 [M-H-62-122-dihydrocaffeoyl], 163.04, 121.03										
			500.27 [M+H]+, 352.22 [M+H-dihydrocoumaroyl]+,										498.26 [M-H]-, 376.22 [M-H-122]-, 350.21 [M-H-										
			6.0	500.	[M+H	334.21	[M+H-	146	151	135	414	491	506	6.0	498.	[M-	H-	128	129	965	633	518	613
			58	275]+	334.21	[M+H-	257	646	155	085	667	333	10	260	H]-		340	794	81	28	07	43

80	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C8H6O3)	C33H41N3O9	6.160	624.29431	[M+H] ⁺	222.11,											157.10,										
						206.11,											121.03										
81	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C4H2O2)	C29H37N3O8	6.230	556.26532	[M+H] ⁺	165.05, 123.04, 112.11											554.25 [M-H] ⁻ , 536.24 [M-H-H2O] ⁻ ,										
						556.26 [M+H] ⁺ , 392.22 [M+H-dihydrocaffeoyl] ⁺ , 374.21 [M+H-dihydrocaffeoyl-H2O] ⁺ ,											432.21 [M-H-122] ⁻ , 390.20 [M-H-dihydrocaffeoyleoyl] ⁻ ,										
						222.11, 211.15, 206.12,	511.63	344.89	571.19	508.995	121.004	439.669					268.38 [M-	178.214	195.918	120.070	516.415	105.072	421.122				

82	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C3H2O2)	C28H37N3O8	6.233	544.26624	[M+H] ⁺	197.13, 165.05, 154.09, 123.04								6.188	542.24951	[M-H] ⁻	H-122-dihydrocaffeoyl]-, 163.04, 124.75, 98.05 542.25 [M-H]-, 420.21 [M+H-122] ⁺ , 378.20 [M+H-dihydrocaffeoyl] ⁺ , 279.14, 256.16 [M+H-122-dihydrocaffeoyl] ⁺ , 167.12, 129.10, 121.03 580.26 [M-H]-, 550.26 [M-H-30] ⁻ , 458.23 [M-H-122] ⁻ ,							
						544.26 [M+H] ⁺ , 380.22 [M+H-dihydrocaffeoyleyl] ⁺ , 362.21 [M+H-dihydrocaffeoylel-H2O] ⁺ , 222.11, 199.14, 185.13, 123.04											669164	576949	226231	420269	325429	799669	140758	226740
83	N-N'-bis-(dihydrocaffeoyl) spermidine-	C31H39N3O8	6.944	582.28229	[M+H] ⁺	582.29 [M+H] ⁺ , 564.27 [M+H-H2O] ⁺ , 536.28 [M+H-								6.896	580.26270	[M-H] ⁻								
						243 240 258 334 277 367 176 175 509 693 097 284 3 5 2 2 3 2											911159	1011736	881257	2446	1316	2158		

conjugate
(+C6H4O2)

CH2O2]+, 400.22 [M+H-H2O-dihydrocaffeoyl]+, 382.21 [M+H-H2O-dihydrocaffeoyl-H2O]+, 222.11, 219.15, 162.09, 134.10, 123.04										428.22 [M-H-30-122]-, 416.22 [M-H-dihydrocaffeoyle]-, 386.21 [M-H-30-dihydrocaffeoyle]-, 124.03, 94.03 580.26 [M-H]-, 416.22 [M-H-dihydrocaffeoyle]-									
6.9 43	604.263 00	[M+N a]+	604.26 [M+Na]+	907 705	869 736	117 832 5	101 343 7	105 086 3	126 193 9	6.8 97	616.239 87	[M+ Cl]-		107 137	125 844	108 022	250 874	151 213	230 961
6.9 45	564.270 81	[M+H - H2O] +	564.27 [M+H-H2O]+, 546.26 [M+H-H2O-H2O]+, 536.28 [M+H-CH2O2]+, 400.22 [M+H-H2O-dihydrocaffeoyl]+, 382.22	588 594	590 243	635 962	956 986	659 198	943 461	6.8 98	643.262 21	[M- H+ HN O3] -	580.27 [M-H]-, 550.26 [M-H-30]-, 416.22 [M-H-dihydrocaffeoyle]-	351 773	389 616	349 118	732 630	448 512	647 050

84	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C ₈ H ₈ O ₅)	C ₃₃ H ₄₃ N ₃ O ₁₁	[M+H-H ₂ O-dihydrocaffeoyl-H ₂ O] ⁺ , 222.11, 162.09, 134.10																			
			6.9 43	620. 238 28	[M+K]] ⁺	620.24 [M+K] ⁺	186 727	178 355	204 348	216 042	225 335	268 871										
			7.2 17	658. 296 88	[M+H]] ⁺	658.30 [M+H] ⁺ , 494.25 [M+H-dihydrocaffeoyl] ⁺ , 476.24 [M+H-dihydrocaffeoyl-H ₂ O] ⁻ , 313.18, 299.16, 222.11, 165.05, 123.04	590 90	851 98	258 19	268 093 5	773 268	137 655 7	7.1 69	656. 279 97	[M-H] ⁻	656.28+ [M-H] ⁻ , 638.27 [M-H-H ₂ O] ⁻ , 592.23 [M-H-64] ⁻ , 568.23 [M-H-88] ⁻ , 470.19 [M-H-64-122] ⁻ , 428.17 [M-H-64-dihydrocaffeoyleoyl] ⁻ , 402.20 [M-H-656.28 [M-H-88] ⁻ , 638.27 [M-H-H ₂ O] ⁻ ,	261 34	792 3	470 5	134 912 2	265 693	526 236
			7.2 12	680. 279 24	[M+N a] ⁺	680.28 [M+Na] ⁺	416 5	167 08	473 4	978 626	372 088	570 602	7.1 69	692. 257 45	[M+Cl] ⁻	656.28 [M-H] ⁻ , 638.27 [M-H-H ₂ O] ⁻ ,	246 3	105 0	101 4	197 544	379 11	937 30

85	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C6H5N) isomer 3	C31H40N4O6	7.219	696.25415	[M+K] ⁺	696.25	[M+K] ⁺	694	1720	1329	192742	76191	116388	7.169	719.27820	H+ HN O3]	592.23 [M-H-64]-, 402.20 656.28 [M-H]-, 638.27 [M-H-H2O]-, 592.23 [M-H-64]-, 402.20	5521	4426	749	507438	130829	256045
			7.359	565.30371	[M+H] ⁺	565.30 [M+H] ⁺ , 548.28 [M+H-NH3] ⁺ , 401.25 [M+H-dihydrocaffeoyl] ⁺ , 383.24 [M+H-dihydrocaffeoyl-H2O] ⁺ , 222.11, 163.15, 134.09, 123.04	74645	81394	32070	314627	102601	221023	7.423	563.28552	[M-H]-	563.28 [M-H]-, 441.25 [M-H-122]-	4008	3813	3211	15112	6689	22681	
86	N-N'-bis-(dihydrocaffeoyl) spermidine-	C30H37N3O8	7.603	568.26349	[M+H] ⁺	568.27 [M+H] ⁺ , 404.22 [M+H-dihydrocaffeoyl-H2O] ⁺	419697	470919	319114	342688	119068	274259	7.563	566.24799	[M-H]-	566.25 [M-H]-, 444.21 [M-H-122]-, 402.21 [M-	133210	121418	78234	1515507	325068	906257	

conjugate
(+C5H2O2)

yl]+, 386.21
[M+H-
dihydrocaff
yl-H2O]+,
223,.14,
222.11,
209.13,
165.05, 123.04

7.6	590.	[M+N	590.25	165	184	129	905	450	770
11	244	a]+	[M+Na]+	243	563	420	692	065	007
	93								
7.6	606.	[M+K	606.22 [M+K]+	129	371	434	189	813	168
15	223]+		50	24	9	282	92	735
	45								

H-
dihydrocaff
eoyl]-,
322.18 [M-
H-122-
122]-,
280.16 [M-
H-122-
dihydrocaff
eoyl]-,
135.04,
121.03
566.25 [M-
H]-, 444.21
[M-H-122]-,
402.21 [M-
H-
dihydrocaff
eoyl]-,
322.18 [M-
H-122-
122]-,
121.03
566.25 [M-
H]-, 444.21
[M-H-122]-,
402.20 [M-

7.5	602.	[M+	H-	916	565	300	477	269	730
63	225	Cl]-	dihydrocaff	8	6	8	15	08	63
	10		eoyl]-,						
			322.18 [M-						
			H-122-						
			122]-,						
			121.03						
			566.25 [M-						
7.5	629.	[M-	H]-, 444.21	373	666	428	479	161	354
60	245	H+	[M-H-122]-,	72	04	83	591	001	644
	79	HN	402.20 [M-						

87	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C5H2O) isomer 2	C30H37N3O7																				
			7.929	552.27155	[M+H] ⁺	552.27 [M+H] ⁺ , 524.28 [M+H-CO] ⁺ , 388.22 [M+H-dihydrocaffeoyl] ⁺ , 370.21 [M+H-dihydrocaffeoyl-H ₂ O] ⁻ , 360.23 [M+H-CO-dihydrocaffeoyl] ⁺ , 342.22 [M+H-CO-dihydrocaffeoyl-H ₂ O] ⁺ , 222.11, 207.15, 165.05, 123.04	612 968 4	630 463 6	621 436 5	720 435 6	245 046 9	928 640 2	7.885	550.25378	[M-H] ⁻	550.25 [M-H] ⁻ , 428.22 [M-H-122] ⁻ , 386.21 [M-H-dihydrocaffeoyl] ⁻ , 333.18, 157.10, 121.03, 94.03	151 721 9	159 138 4	135 258 6	281 180 8	320 559 718	320 574 0
			7.930	574.25171	[M+Na] ⁺	574.25 [M+Na] ⁺	178 770 5	182 029 6	199 256 7	175 295 3	727 796	237 004 8	7.887	586.23016	[M+Cl] ⁻	550.25 [M-H] ⁻ , 428.22 [M-H-122] ⁻ , 386.21 [M-	870 73	472 10	746 91	157 080	365 65	185 074

88	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C4H2)	C29H37N3O6																				
			7.930	590.227	[M+K] ⁺	590.23	[M+K] ⁺	316862	334163	343111	330874	141230	455153	7.885	613.24902	H ⁺ HN O3]	H-dihydrocaffeoyl]-, 550.25 [M-H]-, 428.22 [M-H-122]-, 386.21 [M-H]-, 511851	508241	460759	859058	233582	1023360
			8.247	524.27649	[M+H] ⁺	524.28 [M+H] ⁺ , 360.23 [M+H-dihydrocaffeoyl] ⁺ , 342.22 [M+H-dihydrocaffeoyl-H2O] ⁺ , 222.11, 165.05, 123, 122.10	931261	924013	1110526	2118503	966497	2278672	8.224	522.25897	[M-H]-	H-dihydrocaffeoyl]-, 236.18 [M-H-122-dihydrocaffeoyl]-, 121.03, 66.03	437379	425774	456261	1951869	613278	1766210

89 N-N'-bis-
(dihydrocaffe
oyl)
spermidine-
conjugate
(+C₆H₄O)

C31H
39N3
O7

8.2 45	546. 260 13	[M+N a]+	546.26 [M+Na]+	172 468	170 417	226 919	252 968	170 548	292 422	8.2 23	558. 234 86	[M+ Cl]-	315 11	329 95	308 03	934 88	355 91	853 40	
8.2 46	562. 235 35	[M+K]+		403 68	344 58	547 36	733 55	437 53	817 58	8.2 24	585. 256 41	[M- H+ HN O3] -	522.26 [M- H]-, 400.22 [M-H-122]-, 358.21 [M- H- dihydrocaff eoyl]-, 236.18 [M- H-122- dihydrocaff eoyl]-, 163.04, 121.03 564.27 [M- H]-, 442.22 [M-H-122]-, 424.22 [M- H-122- H2O]-, 400.22 [M- H- dihydrocaff eoyl]-, 348.81,	176 578	181 274	199 754	489 940	196 914	465 218
8.2 57	566. 286 80	[M+H]+	566.28 [M+H]+, 538.29 [M+H- CO]+, 524.27 [M+H-42]+, 402.24 [M+H- dihydrocaffeo yl]+, 384.23 [M+H- dihydrocaffeo yl-H2O]+,	139 574 8	157 475 3	160 762 8	129 254 0	641 791	177 129 6	8.2 33	564. 270 63	[M- H]-	394 675	360 191	368 369	492 456	210 512	585 041	

90	N-dihydrocoumaroyl-N'-dihydrocaffeoyl spermidine-conjugate (+C5H2O)	C30H37N3O6	8.278	588.27073	[M+Na] ⁺	222.11, 165.05, 136.11, 123.04	294	314	371	210	147	294	8.236	600.24597	[M+Cl] ⁻	280.20, 157.10, 117.93	327	293	317	360	174	401			
						588.27	717	772	007	146	673	214													
			8.257	604.24597	[M+K] ⁺	604.04	663.49	788.87	454.25	285.93	605.05	8.235	627.26727	H ⁺ HN O3]	564.27 [M-H] ⁻ , 442.22 [M-H-122] ⁻	149.767	147.974	160.479	148.258	759.04	177.725				
			8.278	536.27673	[M+H] ⁺	536.28 [M+H] ⁺ , 388.22 [M+H-dihydrocoumaroyl] ⁺ , 370.21 [M+H-dihydrocoumaroyl-H2O] ⁺ , 354.22 [M+H-dihydrocoumaroyl-H2O2] ⁺ , 222.11, 206.12, 165.05, 107.05	568	617	679	347	125	602	8.254	534.26086	[M-H] ⁻	534.26 [M-H] ⁻ , 386.21 [M-H-dihydrocoumaroyl] ⁻ , 333.80, 264.14 [M-H-H-dihydrocoumaroyl-122] ⁻ , 121.03, 94.03	717.58	683.55	682.81	671.55	198.52	849.00			

91	N-N'-bis-(dihydrocaffeoyl) spermidine-conjugate (+C8H8O2)	C33H43N3O8	8.2	558.25879	[M+N a]+	558.26	136	148	175	733	383	116	8.2	570.23633	[M+ Cl]-	18405	8804	17932	10942	3524	13177	
			8.4	610.31274	[M+H]+	610.29 [M+H]+, 564.27 [M+H-46]+, 536.27 [M+H-74]+, 400.22 [M+H-46-dihydrocaffeoyl]+, 382.21 [M+H-46-dihydrocaffeoyl-H2O]+, 222.11, 162.09, 134.10	218021	287287	194199	581056	67628	599814	8.4	608.29578	[M-H]-	608.30 [M-H]-, 486.26 [M-H-122]-, 444.25 [M-H-dihydrocaffeoyl]-, 122.02	105831	94074	71122	271473	27886	242147
92	Hederagenin-tetraglucoside	C53H86O22	8.8	1075.56775	[M+H]+	1075.55 [M+H]+, 455.35 [M+H-C6H10O5-C6H10O5-C6H10O4-C5H8O4-H2O]+, 309.11, 279.11	113194	125668	143942	95924	112689	104260	8.8	1073.55347	[M-H]-	1073.55 [M-H]-, 911.50 [M-H-C6H10O5]-, 765.44 [M-H-C6H10O5-C6H10O4]-, 749.45 [M-	1884968	1759630	2083888	1612647	1740375	1604058

										H- C6H10O5- C6H10O5]-, 603.39 [M- H- C6H10O5- C6H10O5- C6H10O4]-, 585.37 [M- H- C6H10O5- C6H10O5- C6H10O4- H2O]-, 471.35 [M- H- C6H10O5- C6H10O5- C6H10O4- C5H8O4]- 1109.53									
8.8	109	[M+N a]+	1097.55	170	173	193	128	163	149	8.8	110	[M+ Cl]-	[M+Cl]-, 1073.55 [M-H]-	448	436	519	356	413	370
65	7.55 151		[M+Na]+	462	768	264	957	609	822	35	9.53 284			036	518	788	744	383	140
8.8	913.	[M+H - C6H1	913.50 [M+H- C6H10O5]+,	257	283	298	192	228	204	8.8	113	[M- H+ HN	1136.55 [M- H+HNO3]-,	546	526	727	357	477	377
53	516 72		751.47 [M+H-	862	121	902	389	184	402	34	6.54 944			390	631	042	434	111	209

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C6H10O5-C5H8O4]+, 455.35 [M+H-C6H10O5-C6H10O4-C5H8O4-H2O]+, 437.34 [M+H-C6H10O5-C6H10O4-C5H8O4-H2O-H2O]+, 309.12, 279.11										H-C6H10O5-C6H10O4]-, 471.35 [M-H-C6H10O5-C6H10O4-C5H8O4]-									
8.965	935.49963	[M+N a]+	935.50	359	383	451	243	358	303	8.936	947.47931	[M+ Cl]-	947.48						
			[M+Na]+	316	199	234	333	409	273				[M+Cl]-, 911.50 [M-H]-	410	395	471	356	396	361
8.950	751.46436	[M+H-C6H10O5-C6H10O4-C5H8O4-H2O]+, 437.34 [M+H-C6H10O5-C6H10O4-	751.46							8.937	957.50531	[M+ FA-H]-	957.49						
			455.35	671	743	884	538	675	590				[M+FA-H]-, 911.50 [M-H]-, 749.45 [M-H-C6H10O5]-	156	147	177	145	162	142
				696	290	280	614	127	384					169	603	535	788	273	580
														4	1	3	3	0	4

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[illegible]

[illegible]

[illegible]

96	alpha-hederin	C41H66O12	9.200	1076.59875	[M+N H4]+	1076.58 [M+NH4]+	126022	140139	149344	96845	120269	109310	9.178	1093.53284	[M+ Cl]-	1093.54 [M+Cl]-, 1057.56 [M-H]-, 895.51 [M- H- C6H10O5]-, 733.45 [M- H- C6H10O5- C6H10O5]-	459164	464705	456746	423076	449883	417159
			9.179	1120.56090	[M- H+ HN O3]	1120.56 [M- H+HNO3]-, 1057.56 [M-H]-	703335	688708	741978	585145	628334	604024										
			9.179	1175.49622	[M- H+1 18]-	1175.49622 [M- H+1 18]-	426819	379660	386386	455765	464107	417635										
			9.245	749.44702	[M- H]-	749.45 [M- H]-, 603.38 [M-H- C6H10O4]-, 585.38 [M- H- C6H10O4- H2O]-,	346400	338034	222958	229029	205696	333044										
			9.243	751.46484	[M+H]+	751.45 [M+H]+, 455.35 [M+H- C6H10O4- C5H8O4- H2O]+, 437.34 [M+H- C6H10O4-	1879338	2128350	2466941	1709793	2082227	1882934										

C5H8O4-H2O-H2O]+, 409.35, 279.11										471.35 [M-H-C6H10O4-C5H8O4]- 785.42 [M+Cl]-, 749.45 [M-H]-, 471.35 [M-H-C6H10O4-C5H8O4]- 795.45 [M+FA-H]-, 749.45 [M-H-C6H10O4]-, 585.38 [M-H-C6H10O4-H2O]-, 471.35 [M-H-C6H10O4-C5H8O4]-									
9.2	773.	[M+N	773.45	272	295	352	231	282	267	9.2	785.	[M+	749.45 [M-H]-, 471.35	305	407	433	297	326	310
50	448	a]+	[M+Na]+	777	699	754	083	464	967	51	424	Cl]-	[M-H-C6H10O4-C5H8O4]- 795.45 [M+FA-H]-, 749.45 [M-H-C6H10O4]-, 585.38 [M-H-C6H10O4-H2O]-, 471.35 [M-H-C6H10O4-C5H8O4]-	792	156	484	751	960	018
	18										56								
619.42 [M+H-C5H8O4]+, 455.35 [M+H-C6H10O4-C5H8O4-H2O]+, 437.34 [M+H-C6H10O4-C5H8O4-H2O-H2O]+																			
9.2	619.	[M+H	C6H10O4-C5H8O4-	224	239	289	195	234	218	9.2	795.	[M+	585.38 [M-H-C6H10O4-H2O]-, 471.35 [M-H-C6H10O4-C5H8O4]-	266	255	280	260	268	254
47	423	-	C5H8O4-H2O]+, 437.34	161	607	053	140	562	245	45	451	FA-	H-	832	029	192	924	818	011
	22	C5H8O4]+	[M+H-C6H10O4-C5H8O4-H2O-H2O]+								48	H]-	C6H10O4-H2O]-, 471.35 [M-H-C6H10O4-C5H8O4]-	0	6	5	0	3	1

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97	Oleanolic acid-triglucoside	C47H76O16																				
			9.351	897.51782	[M+H] ⁺		15075	44097	25101	20301	31588	24277	9.336	895.50769	[M-H] ⁻	895.51 [M-H] ⁻ , 749.45 [M-H-C ₆ H ₁₀ O ₄] ⁻ , 733.46 [M-H-C ₆ H ₁₀ O ₅] ⁻ , 587.39 [M-H-C ₆ H ₁₀ O ₅ -C ₆ H ₁₀ O ₄] ⁻ , 455.36 [M-H-C ₆ H ₁₀ O ₅ -C ₆ H ₁₀ O ₄ -C ₅ H ₈ O ₄] ⁻ , 931.48 [M+Cl] ⁻ , 895.51 [M-H] ⁻ , 733.45 [M-H-C ₆ H ₁₀ O ₅] ⁻ , 455.34 [M-H-C ₆ H ₁₀ O ₅ -C ₆ H ₁₀ O ₄ -C ₅ H ₈ O ₄] ⁻	205853	173985	268712	188947	185756	149469
			9.341	919.50067	[M+N a] ⁺	919.50 [M+Na] ⁺	231830	277325	272146	221850	296007	250369	9.389	931.48492	[M+Cl] ⁻	931.48 [M-H-C ₆ H ₁₀ O ₅] ⁻ , 455.34 [M-H-C ₆ H ₁₀ O ₅ -C ₆ H ₁₀ O ₄ -C ₅ H ₈ O ₄] ⁻	495612	445526	475282	674421	709021	658544

98	Hederagenin-monoglucoside	C35H56O8	9.359	914.54871	[M+N H4]+	914.55 [M+NH4]+, 439.36 [M+H-C6H10O5-C6H10O4-C5H8O4-H2O]+, 279.11	892122	2192853	1159181	2641671	2324891	2894213	9.353	941.51050	[M+FA-H]-	941.51 [M+FA-H]-, 895.51 [M-H]-, 733.45 [M-H-C6H10O5]-, 587.41 [M-H-C6H10O5-C6H10O4]-, 455.35 [M-H-C6H10O5-C6H10O4-C5H8O4]-	3104724	1586626	1861677	2543019	2937999	2426224
98	Hederagenin-monoglucoside	C35H56O8	9.360	439.35159	[M+H C17H30O14]+	439.35 [M+H-C6H10O5-C6H10O4-C5H8O4-H2O]+, 203.18, 191.18	1933752	2150995	2347072	1727169	2379941	1997828	9.384	958.50183	[M+HN O3]-	958.50 [M+HN O3]-, 1013.44 [M-H+118]-	158242	1499828	1745771	1867823	2291349	1807070
98	Hederagenin-monoglucoside	C35H56O8	9.393	605.40674	[M+H]+	25507	22809	29619	6903	440	15124	9.396	603.39038	[M-H]-	603.39 [M-H]-	308124	309225	289670	100702	1564	157633	

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99	Oleanolic acid-diglucoside	C41H66O12	9.563	773.44318	[M+N a] ⁺	773.44 [M+Na] ⁺	2229534	1141274	1055202	1377595	308757	1804257	9.544	749.44763	[M-H] ⁻	749.45 [M-H] ⁻ , 587.38 [M-H-C6H10O5] ⁻ 785.43 [M+Cl] ⁻ , 749.45 [M-H] ⁻ , 587.39	226468	255352	370782	348035	109064	425504
			9.565	768.49200	[M+N H4] ⁺	768.49 [M+NH4] ⁺ , 439.36 [M+H-C6H10O5-C5H8O4-H2O] ⁺	12232098	13406362	14540392	4947224	366553	7677270	9.543	785.42419	[M+Cl] ⁻	[M-H-C6H10O5] ⁻ , 455.35 [M-H-C6H10O5-C5H8O4] ⁻ 795.45 [M+FA-H] ⁻ , 749.45 [M-H] ⁻ , 587.39	344241	341507	377438	247076	50881	276535
			9.569	439.35754	[M+H C11H20O1] ⁺	439.36 [M+H-C6H10O5-C5H8O4-H2O] ⁺ , 203.18	2056654	2361282	2619927	726548	331800	1447377	9.544	795.45117	[M+FA-H] ⁻	[M-H-C6H10O5] ⁻ , 455.35 [M-H-C6H10O5-C5H8O4] ⁻	2720882	2553061	2791875	1584504	383074	1965191
			9.543	812.44202	[M-H+HN] ⁻	812.44 [M-H+HNO3] ⁻	1882175	1782059	2010240	768792	204173	1219075										

100	1,2-dioleoyl-sn-glycero-3-phosphatidylcholine	C44H84NO8P	9.665	786.60046	[M+H] ⁺	786.60											9.539	867.38489	[M-H+18] ⁻						
						[M+H] ⁺ , 184.07 [M-C39H70O4+H] ⁺ , 86.10 [M-C39H73O8P+H] ⁺	108657	134247	198916	170153	166469	135990	733617	614872	674423	469300				119943	555091				
101	Beta-hederin	C41H66O11	9.734	752.49518	[M+N H4] ⁺	752.50											9.762	733.45026	[M-H] ⁻						
						[M+NH4] ⁺ , 439.36 [M+H-C6H10O4-C5H8O4-H2O] ⁺ , 279.11	419886	106921	443420	288945	183271	440599	733.45 [M-H] ⁻ , 689.46, 587.39 [M-H-C6H10O4] ⁻ , 455.35 [M-H-C6H10O4-C5H8O4] ⁻	827032	811144	861977				937187	1519889	820387			
			9.731	457.37094	[M+H-C11H18O8] ⁺	457.35											9.798	769.43079	[M+Cl] ⁻						
						[M+H-C6H10O4-C5H8O4] ⁺ , 439.36 [M+H-C6H10O4-C5H8O4] ⁺	46981	131126	77405	39102	81312	122430	769.43 [M+Cl] ⁻ , 733.45 [M-H] ⁻ , 455.35 [M-H-]	342840	453944	472249				200670	391732	224230			

[illegible]

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104	1-Palmitoyl-sn-glycero-3-phosphocholine	C24H50NO7P	9.836	967.69879	[2M+Na]+	[M+H-H2O-H2O]+, 207.18																			
						967.70																			
						[2M+Na]+, 495.35																			
						[M+Na]+, 496.34																			
105	Oleanolic acid-monoglucoside	C35H56O7	10.002	606.44220	[M+NH4]+	[M+H-H2O]+, 184.07																			
						[C19H36O3+H]+, 104.11																			
						[C19H37O6P+H]+, 606.43																			
						[M+NH4]+, 439.36																			
105	Oleanolic acid-monoglucoside	C35H56O7	10.002	611.39447	[M+N a]+	[M+H-H2O]+, 393.36, 247.17																			
						[M+H-H2O]+, 393.36, 247.17																			
						[M+H-H2O]+, 393.36, 247.17																			
						[M+H-H2O]+, 393.36, 247.17																			

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107	1-Oleoyl-sn-glycero-3-phosphocholine	C26H52NO7P	10.689	522.35638	C14H29NO2+H]+ 522.35 [M+H]+, 504.34 [M+H-H2O]+, 184.07 [M-C21H38O3+H]+, 104.11 [M-C21H39O6P+H]+ 326.31 [M+H]+, 308.30 [M+H-H2O]+, 135.12 [M-C10H25NO2-H]+, 121.10 [M-C11H27NO2-H]+, 109.10 [M-C12H27NO2-H]+, 95.09 [M-C13H29NO2-H]+, 83.08 [M-C14H29NO2-H]+								121	864	273	109	210	673	970	9
108	N-Oleylethanolamine	C20H39NO2	10.700	326.30621	C14H29NO2+H]+ 522.35 [M+H]+, 504.34 [M+H-H2O]+, 184.07 [M-C21H38O3+H]+, 104.11 [M-C21H39O6P+H]+ 326.31 [M+H]+, 308.30 [M+H-H2O]+, 135.12 [M-C10H25NO2-H]+, 121.10 [M-C11H27NO2-H]+, 109.10 [M-C12H27NO2-H]+, 95.09 [M-C13H29NO2-H]+, 83.08 [M-C14H29NO2-H]+								489	533	607	249	492	526	165	4

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112	ethylhexanoate)			10.835	425.28665	[M+N a] ⁺	425.29 [M+Na] ⁺	2874561	3785995	4256551	5454772	6430159	5640178												
				10.833	420.33414	[M+N H4] ⁺	171.14 [M+H-C10H16O6] ⁺ , 57.07	19366511	23400948	25315765	26917560	31291395	29321350												
				10.833	171.13455	- C10H16O6] ⁺	171.14 [M+H-C10H16O6] ⁺ , 73.03, 57.07	2398409	3025630	3197590	4258554	4777309	4308624												
				12.202	433.33344	[M+H - CH2] ⁺	149.02, 85.10, 71.08, 57.07	84538	105520	231255	1156054	1125710	1073544												
														11.195	281.24533	[M-H] ⁻	281.25 [M-H] ⁻	304499	290691	347554	273556	245309	285611		
														11.708	605.40302	[M+FA-H] ⁻	605.41 [M+FA-H] ⁻ , 559.39 [M-H] ⁻	186555	182882	132048	12424	374	31104		

