Supporting Informations

Optimization of Microwave-Assisted Extraction of Antioxidant Compounds from Spring Onion Leaves using Box-Behnken Design

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Table S1. Extraction Yield (%) and DPPH assay values.[80]

Run	Factors				Yield (%) *	DPPH*# (μM TE g^{-1} dw)
	A-Temp	B-Time	C-Extr. Vol.	D-EtOH		
1	-1	-1	0	0	26.97 ± 1.46	19.04 ± 0.90
2	0	-1	-1	0	22.93 ± 1.23	21.60 ± 0.54
3	0	-1	0	-1	22.10 ± 0.79	22.57 ± 0.88
4	0	-1	0	+1	23.30 ± 0.30	22.97 ± 0.38
5	0	-1	+1	0	14.83 ± 1.00	22.61 ± 0.26
6	+1	-1	0	0	19.17 ± 0.26	23.03 ± 0.46
7	-1	0	-1	0	19.37 ± 1.20	20.45 ± 0.65
8	-1	0	0	-1	28.63 ± 1.00	20.31 ± 0.49
9	-1	0	0	+1	25.10 ± 1.05	21.91 ± 0.37
10	-1	0	+1	0	20.93 ± 1.52	23.24 ± 0.44
11	0	0	-1	-1	26.60 ± 0.26	19.32 ± 0.08
12	0	0	-1	+1	21.57 ± 0.70	20.41 ± 0.37
13	0	0	0	0	23.87 ± 1.60	17.67 ± 0.03
14	0	0	0	0	20.57 ± 0.75	22.47 ± 3.34
15	0	0	0	0	29.20 ± 0.26	20.73 ± 0.97
16	0	0	0	0	22.80 ± 1.04	23.90 ± 0.34
17	0	0	0	0	22.63 ± 1.30	20.30 ± 0.30
18	0	0	+1	-1	16.63 ± 1.56	21.42 ± 1.88
19	0	0	+1	+1	27.50 ± 1.40	21.03 ± 0.20
20	+1	0	-1	0	20.47 ± 1.28	22.12 ± 0.27
21	+1	0	0	-1	25.20 ± 0.36	20.95 ± 0.11
22	+1	0	0	+1	22.67 ± 1.53	24.51 ± 1.82
23	+1	0	+1	0	20.73 ± 1.45	17.28 ± 1.42
24	-1	+1	0	0	24.77 ± 1.55	21.40 ± 0.23
25	0	+1	-1	0	24.40 ± 1.06	20.76 ± 0.23
26	0	+1	0	-1	22.67 ± 0.64	21.26 ± 0.29
27	0	+1	0	+1	20.20 ± 1.47	21.61 ± 0.13
28	0	+1	+1	0	21.40 ± 1.20	21.67 ± 0.14
29	+1	+1	0	0	23.30 ± 0.66	21.15 ± 0.24
Optimal extract	60°C	22 in	11 mL	51 v/v	22.90 ± 0.76	22.85 ± 0.15

** Mean ± SD (n=3)*

The results were expressed as μM Trolox equivalents/g dried extract.

Table S2. Analysis of variance (ANOVA) for DPPH radical scavenging activity of CN extracts.

Source	Sum of Squares	df	Mean Square	F-value	*p*-value
Model	69.58	14	4.97	11.97	< 0.0001*
A-Temp.	4.80	1	4.80	11.56	0.0043*
B-Time	35.19	1	35.19	84.77	< 0.0001*
C-Extr. Vol.	3.20	1	3.20	7.72	0.0148*
D-EtOH	24.31	1	24.31	58.56	< 0.0001*
AB	1.17	1	1.17	2.81	0.1159
AC	0.0002	1	0.0002	0.0005	0.9818
AD	0.0144	1	0.0144	0.0347	0.8549
BC	0.6642	1	0.6642	1.60	0.2266
BD	0.0784	1	0.0784	0.1888	0.6705
CD	0.0784	1	0.0784	0.1888	0.6705
A^2	0.0129	1	0.0129	0.0311	0.8626
B^2	0.0237	1	0.0237	0.0570	0.8147
C^2	0.0221	1	0.0221	0.0532	0.8210
D^2	0.0024	1	0.0024	0.0057	0.9407
Residual	5.81	14	0.4151		
Lack of Fit	5.26	10	0.5264	3.84	0.1033
Pure Error	0.5482	4	0.1371		
R^2	0.9229				
Adjusted R^2	0.8458				
Predicted R^2	0.5865				

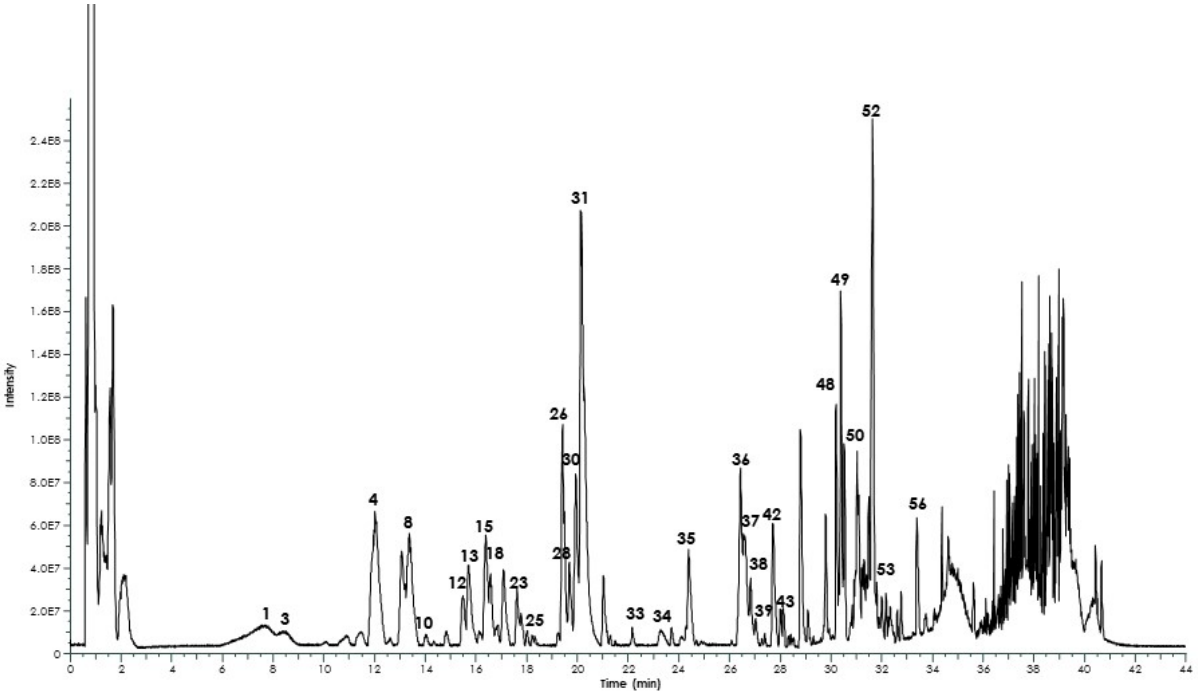
**Significant at $p < 0.05$.*

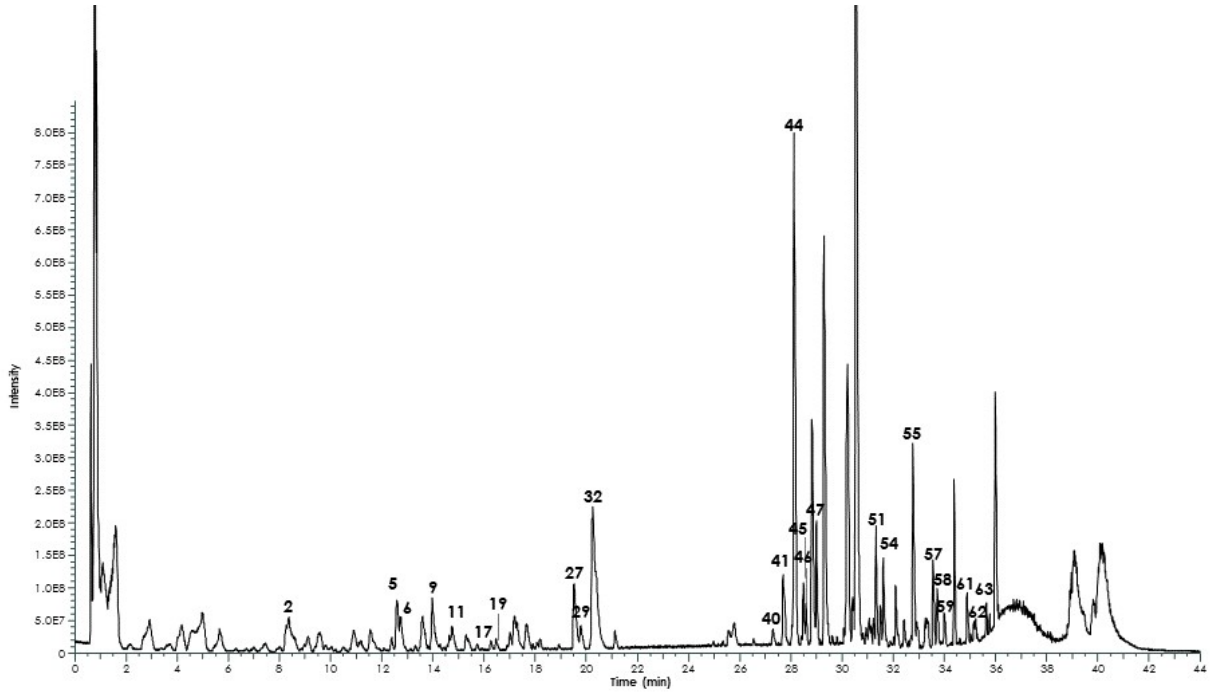
Table S3. Systematic classification of Allium sapogenins and substituents in related steroidal saponins.

Class	Subclass	Formula of $[M-H]^-$ ion	$[M-H]^-$ (Da)	Allium Sapogenins
III	III3	$C_{27}H_{41}O_4$	429	(25R/S)-furost-5(6),20(22)-diene-2α,3β,26-triols; 5β-furost-20(22),25(27)-diene-3β,12β,26-triol; furost-5(6),20(22)-diene-1β,3β,26-triol
				(25R)-5α-furost-20(22)-ene-6-one-3β,26-diol
				(22S,25S)-22,25-epoxy-furost-5(6)-ene-3β,22,26-triol
				(25R/S)-spirost-5(6)-ene-1β,3β-; 2α,3β-;3β,3β-diols; (25R)-spiros-25(27)-ene-2β,3β-;3β,12β-diols
				(25S)-spirostan-6-one-3-OH (laxogenin); (25R)-5α-spirostane-12-one-3β-ol (hecogenin)
	III4	$C_{27}H_{41}O_5$	445	(22S, 25R)-5α-furost-5(6),22(23)-dien1β,3β,20α,26-tetrol
				(25R)-furost-5(6)-ene-2-one-3β(α),22α(22),26-triol, (25R)-furost-25(27)-en-12-one3β,22,26-triol
				(25R)-spirost-5(6)-ene1β,3β,24-triol, (20S,25S)-spirost-5(6)-ene-3β,11α(12β),21-tiols, (24S,25R)-spirostS(6)-ene-β(2α),3β,24-triol
				(25R/S)-5α-spirostan-2-one-3β,6β-diol; (25S)-5α-spirostane-6-one2α,3α-diol; (25R)-5αspirostane-12-one3β,6β-diol
				(25R)-5α-spirostane2α,5α-epoxy-2α,3β,6βtriol
IV	IV4	$C_{27}H_{43}O_5$	447	(25R/S)-furost-5(6)-ene-1β(2α),3β,22α(β),26-tetraols; (25S,20R)-5α-furost-22(23)-ene-2α,3β,20,26-tetrol; 5α(β)-furost-25(27)-ene-3β,12β,22,26-tetraol
				(25R)-5α-furostane-6-one-3β,22,26-triol
				(25R/S)-spirostan-2α (β),3β,6β(α); 2,3,27-; 2,3,24-; 2,3,5-; 3,5,6-triol; (24S,25S)-5β-spirostan-2β,3β,24-triol

Neutral Loss	Abbreviations	Formula	Neutral Loss	Example Substituents
hexosyl	Hex	$C_6H_{10}O_5$	162.0528	glucosyl, galactosyl, mannosyl
deoxyhexosyl	dHex	$C_6H_{10}O_4$	146.0579	rhamnosyl, deoxymannosyl, quinovosyl
pentosyl	Pen	$C_5H_8O_4$	132.0422	arabinosyl, xylosyl
formic acid	FA	CH_2O_2	46.0055	

Figure S1. Representative TIC of CN extract analyzed in negative (up) and positive (down) ionization mode. 1. Quercetin 7,4′- dihexoside; 2. Herniarin; 3. Kaempferol 3,7-O-dihexoside; 4. Kaempferol 3,7-O-dihexoside (isomer I); 5. Quercetin 3,4′- dihexoside; 6. Cyanidin 3-laminaribioside; 7. Quercetin 3,4′- dihexoside (isomer I); 8. Quercetin 3-O-hexoside; 9. Kaempferol; 10. Phenethyl rutinoside; 11. Quercetin; 12. Kaempferol 3,7-O-dihexoside (isomer II); 13. Kaempferol 3-O-hexoside; 14. Quercetin 3-O-hexoside (isomer I); 15. Kaempferol 3-O-hexoside (isomer I); 16. Isorhamnetin-O-hexoside; 17. Kaempferol (isomer I); 18. Quercetin-3-O-feruloyl-sophoroside-7-O-D-glucoside; 19. Petunidin 3-hexoside; 20. Quercetin-3-O-feruloyl-sophoroside-7-O-D-glucoside (isomer I); 21. Kaempferol-3-O-coumaroyldiglucoside-7-O-glucoside; 22. Isorhamnetin-O-hexoside (isomer I); 23. Kaempferol-3-O-feruloyldiglucoside-7-O-glucoside; 24. Kaempferol-3-O-coumaroyldiglucoside-7-O-glucoside (isomer I); 25. Kaempferol-3-O-feruloyldiglucoside-7-O-glucoside (isomer I); 26. Saponin 3-IV4-1 (447+dHex+2 Hex + FA); 27. Neohecogenin-3- Oβ-Dglucopyranosyl (1→2)-β-D-glucopyranosyl (1→4)-β-D-galactopy-ranoside; 28. Saponin 3-IV4-1 (isomer I) (447+ dHex+2 Hex + FA); 29. Neohecogenin-3- Oβ-Dglucopyranosyl (1→2)-β-D-glucopyranosyl (1→4)-β-D-galactopy-ranoside (isomer I); 30. 7-Hydroxy-2’,4’,5-trimethoxyflavanone; 31. Saponin 3-IV4-2 (447+Pen + dHex +Hex + FA); 32. Pennogenin-3-O-α-L-arabinofuranosyl(1→4)[α-L-rhamnopyranosyl(1→2)]-β-D-glucopyranoside; 33. Quercetin-3-O-feruloyl-sophoroside; 34. Kaempferol (isomer II); 35. Oxo-dihydroxy-octadecenoic acid (oxoDiHODE); 36. 9,12,13-trihydroxy octadeca-7-enoic acid (TriHODE); 37. 9,12,13-trihydroxy octadeca-7-enoic acid (TriHODE) (isomer II); 38. Saponin 2-III4 (445+dHex + Pen + FA); 39. 9,12,13-trihydroxy octadeca-7-enoic acid (TriHODE) (isomer III); 40. Palmitoylglycine; 41. Palmitoylglycine (isomer I); 42. 2'-Hydroxy-4,4',6'-trimethoxychalcone; 43. 5,6,7,4'-Tetramethoxyflavanone; 44. Dehydrophytosphingosine; 45. Palmitoylglycine (isomer II); 46. Dehydrophytosphingosine (isomer I); 47. Phytosphingosine; 48. Tigogenin; 49. Saponin 2-III3 (429+dHex + Pen + FA); 50. Hydroxyoctadecatrienoic acid (HOTrE); 51. LysoPC(16:0); 52. 13-hydroxyoctadecadienoic acid (13-HODE); 53. 13-hydroxyoctadecadienoic acid (isomer I); 54. α-Linolenoyl ethanolamide; 55. Linoleoyl ethanolamide; 56. Hydroxy-hexadecanoic acid; 57. 3-dehydrosphinganine (C20); 58. Hexadecanamide; 59. Sphingosine ; 60. Pheophorbide a; 61. Octadecanamide; 62. 1,3-dilinolenoylglycerol (DG(18:3n6/0:0/18:3n6)); 63. 1,3-dilinolenoylglycerol (DG(18:3n6/0:0/18:3n6)) (isomer I)




Intensity
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