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Supplementary

LC-ESI-QTOF-MS/MS characterisation of phenolics in herbal tea infusion and their antioxidant potential

Osbert Chou[1], Akhtar Ali[1], Vigasini Subbiah[1], Colin J. Barrow[2], Frank R. Dunshea[1,3] and Hafiz A.R. Suleria[1,2,*]

[1] School of Agriculture and Food, Faculty of Veterinary and Agricultural Sciences, The University of Melbourne, Parkville, VIC 3010, Australia; ochou@student.unimelb.edu.au (O.C.); akali@student.unimelb.edu.au (A.A.); vsubbiah@student.unimelb.edu.au (V.S.); fdunshea@unimelb.edu.au (F.R.D.)

[2] Centre for Chemistry and Biotechnology, School of Life and Environmental Sciences, Deakin University, Waurn Ponds, VIC 3217, Australia; colin.barrow@deakin.edu.au

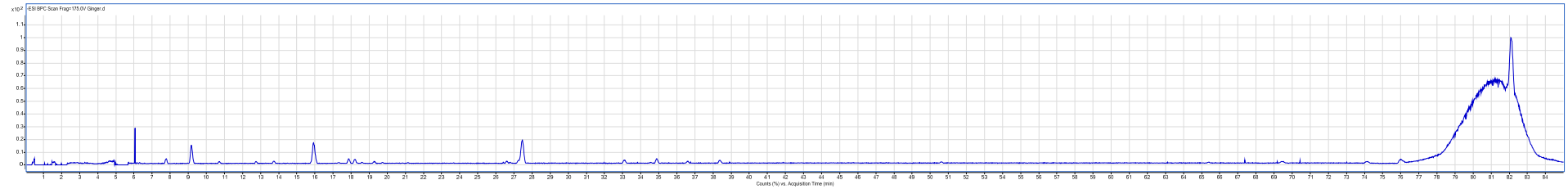
[3] Faculty of Biological Sciences, The University of Leeds, Leeds LS2 9JT, UK

* Correspondence: hafiz.suleria@unimelb.edu.au (H.A.R.S.); Tel.: +61-470-439-670

Abstract: Ginger (*Zingiber officinale* R.), lemon (*Citrus limon* L.) and mint (*Mentha sp.*) are commonly consumed medicinal plants that have been of interest due to their health benefits and purported antioxidant capacities. This study was conducted on the premise that no previous study has been performed to elucidate the antioxidant and phenolic profile of the ginger, lemon and mint herbal tea infusion (GLMT). The aim of the study was to investigate and characterise the phenolic contents of ginger, lemon, mint and GLMT, as well as determining their antioxidant potential. Mint recorded the highest total phenolic content, TPC (14.35 ± 0.19 mg gallic acid equivalent/g) and 2,2′-azino-bis(3-e-thylbenzothiazoline-6-sulfonic acid), ABTS (24.25 ± 2.18 mg ascorbic acid equivalent/g) antioxidant activity. GLMT recorded the highest antioxidant activity in the reducing power assay, RPA (1.01 ± 0.04 mg ascorbic acid equivalent/g) and hydroxyl radical scavenging assay, •OH-RSA (0.77 ± 0.08 mg ascorbic acid equivalent/g). Correlation analysis showed that phenolic content positively correlated with the antioxidant activity. Venn diagram analysis revealed that mint contained a high proportion of exclusive phenolic compounds. The liquid chromatography coupled to electrospray ionisation and quadrupole time of flight tandem mass spectrometry (LC-ESI-QTOF-MS/MS) characterised a total of 73 phenolic compounds, out of which 11, 31 and 49 were found in ginger, lemon and mint respectively. These characterised phenolic compounds include phenolic acids (24), flavonoids (35), other phenolic compounds (9), lignans (4) and stilbene (1). High-performance liquid chromatography photometric diode array (HPLC-PDA) quantification showed that GLMT does contain relatively high concentration of phenolic compounds. This study presented the phenolic profile and antioxidant potential of GLMT and its ingredients, which may increase the confidence in developing GLMT into functional food products or nutraceuticals.

Keywords: Polyphenol, LC-ESI-QTOF-MS/MS, HPLC, medicinal plants, ginger, lemon, mint, herbal tea infusion, antioxidants

(a)



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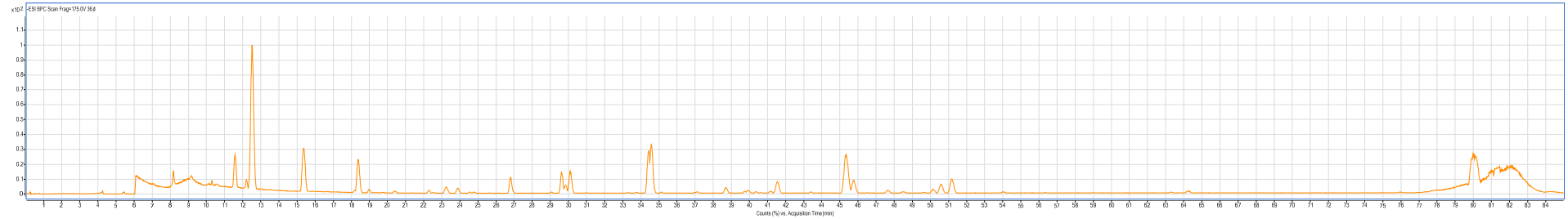

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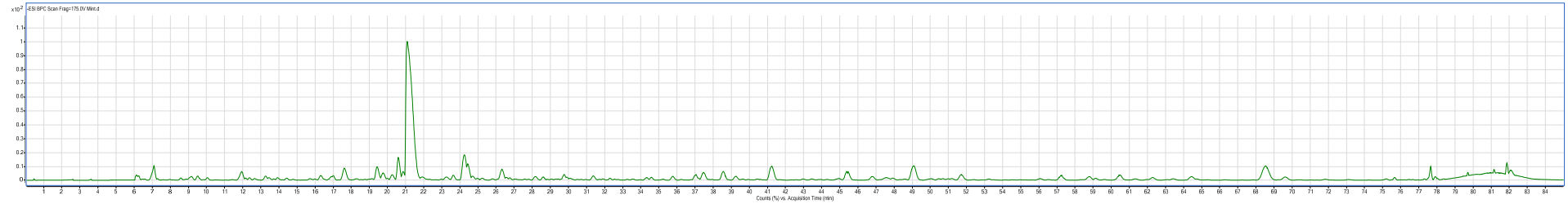
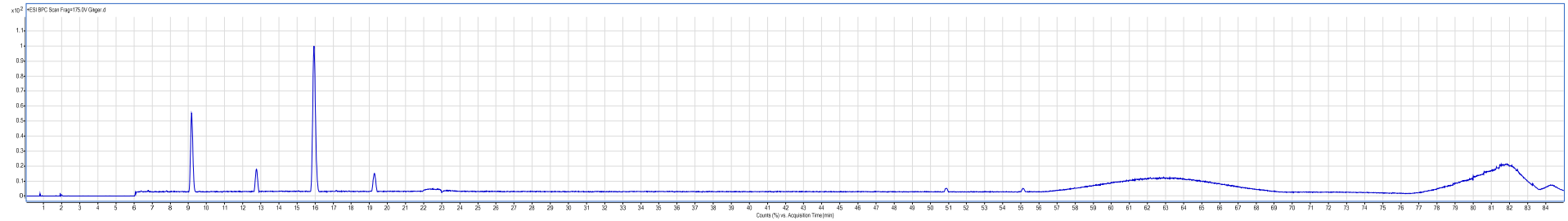


(d)



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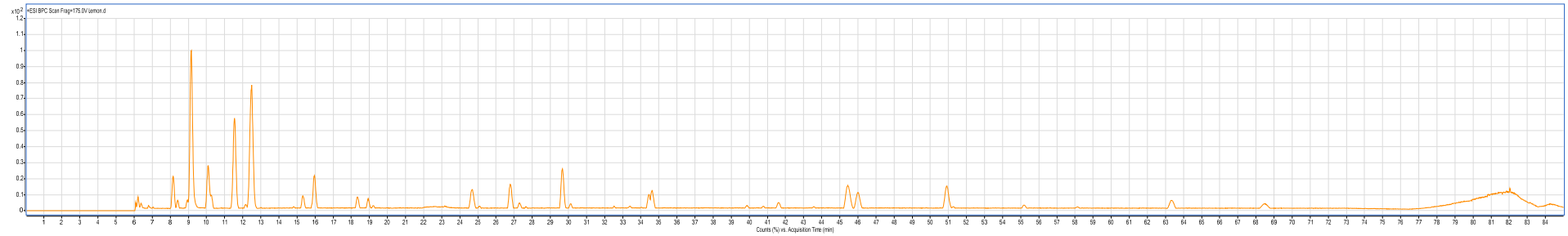


(f)

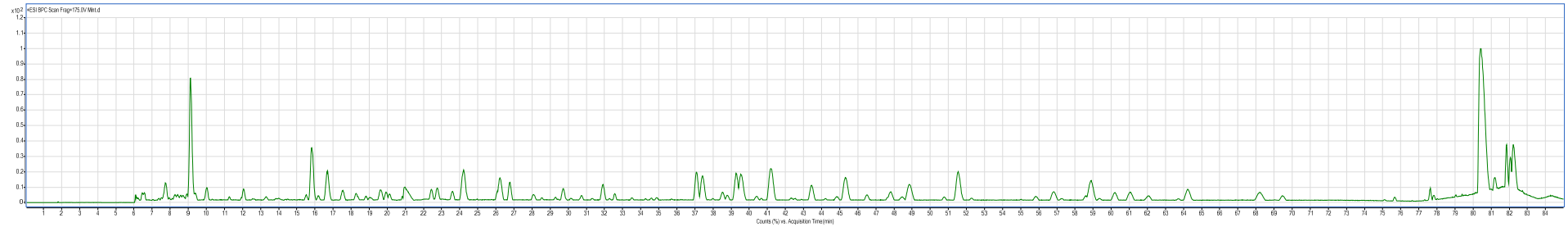
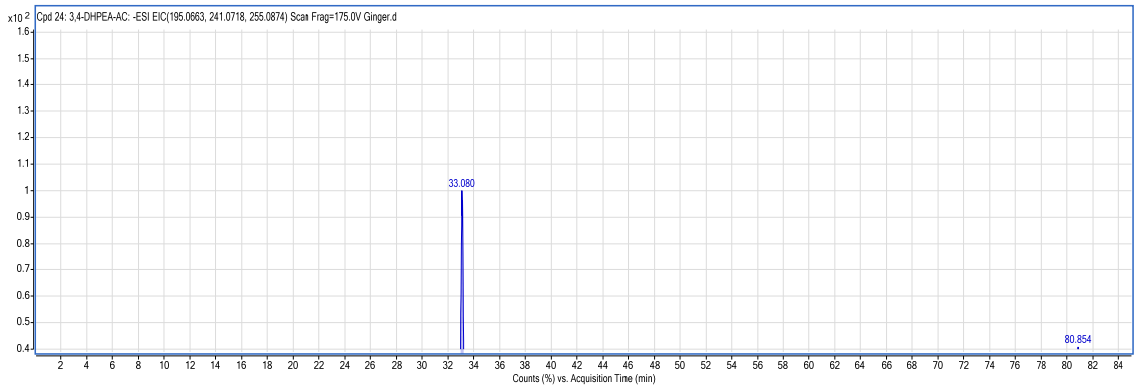
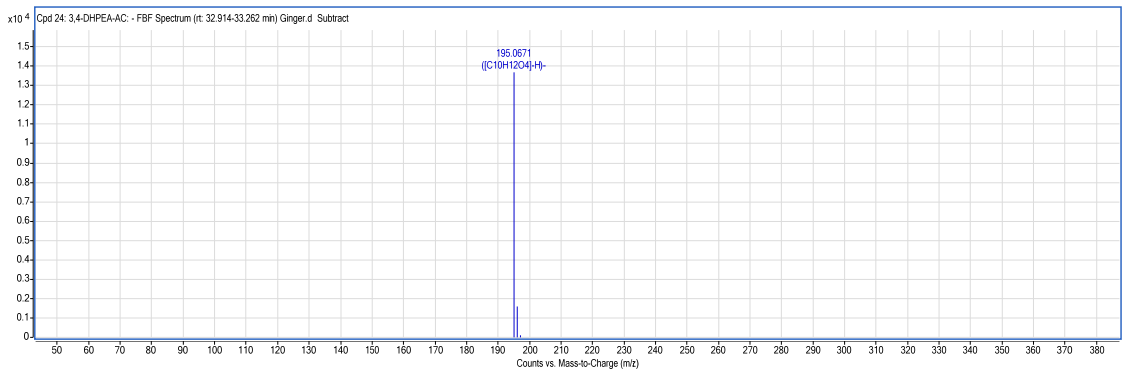


Figure (1S): LC-ESI-QTOF-MS/MS basic peak chromatograph (BPC) for characterization of phenolic compounds of herbal tea; **(a)** Ginger in negative ionization mode; **(b)** Lemon in negative ionization mode; **(c)** Mint in negative ionization mode; **(d)** Ginger in positive ionization mode; **(e)** Lemon in positive ionization mode; **(f)** Mint in positive ionization mode.

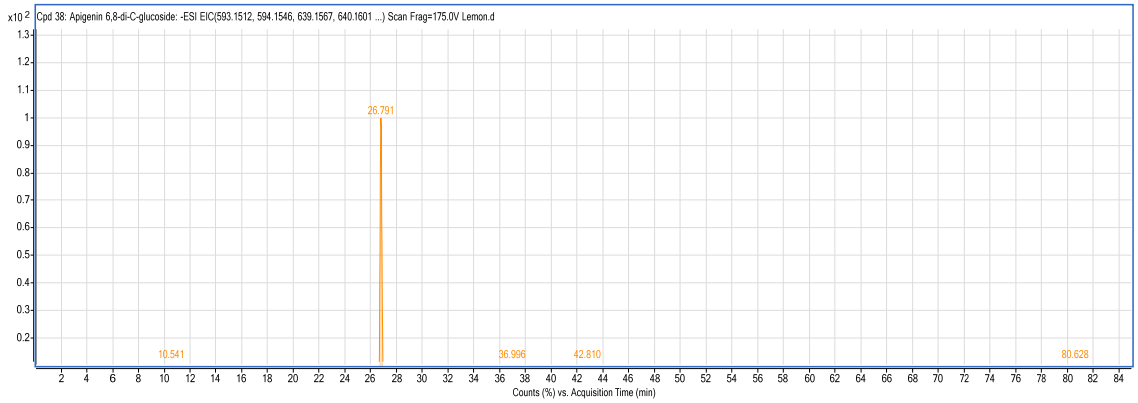
(a)


Cpd 24: 3,4-DHPEA-AC: -ESI EIC(195.0663, 241.0718, 255.0874) Scan Frag=175.0V Ginger.d
33.080
80.854
Counts (%) vs. Acquisition Time (min)

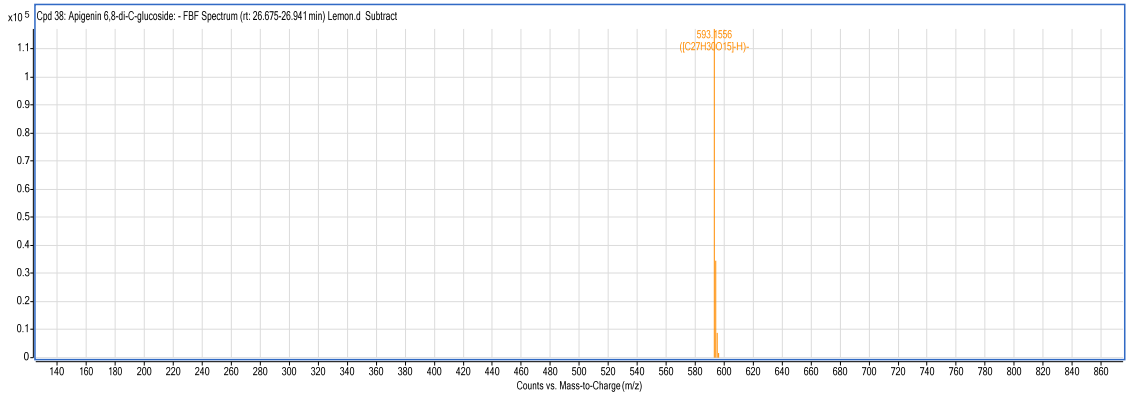
(b)


Cpd 24: 3,4-DHPEA-AC: - FBF Spectrum (rt: 32.914-33.262 min) Ginger.d Subtract
195.0671
([C10H12O4]-H)-
Counts vs. Mass-to-Charge (m/z)

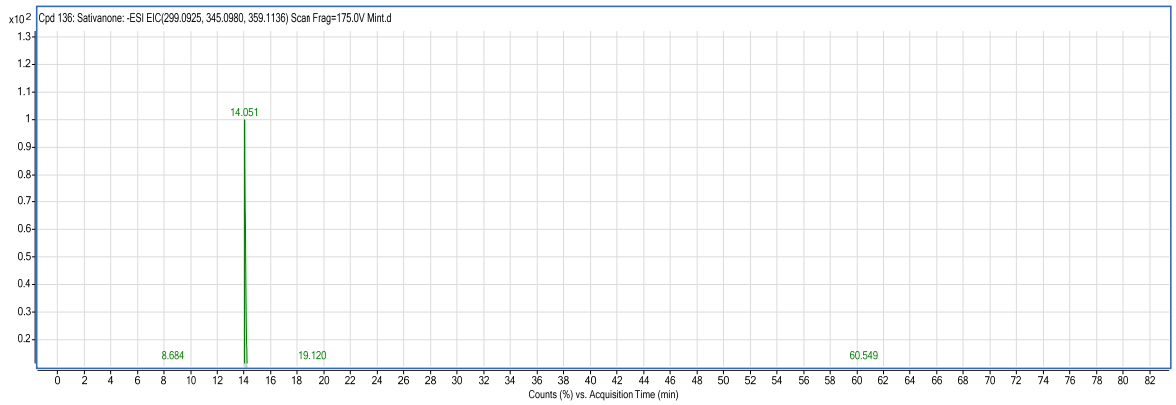
(c)


Cpd 38: Apigenin 6,8-di-C-glucoside: -ESI EIC(593.1512, 594.1546, 639.1567, 640.1601 ...) Scan Frag=175.0V Lemon.d
26.791
10.541
36.996
42.810
80.628
Counts (%) vs. Acquisition Time (min)

(d)


Cpd 38: Apigenin 6,8-di-C-glucoside: - FBF Spectrum (rt: 26.675-26.941 min) Lemon.d Subtract
593.1556
([C27H30O15]-H)-
Counts vs. Mass-to-Charge (m/z)

(e)



(f)

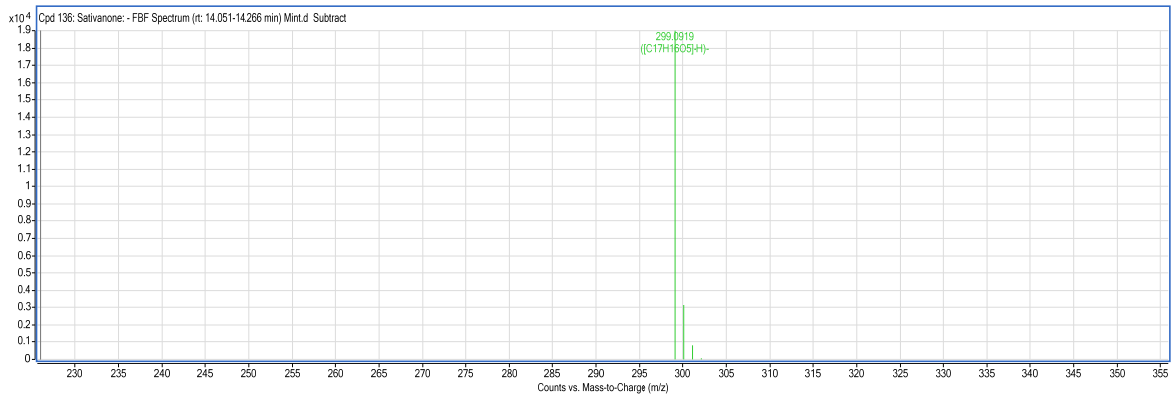


Figure (S2). Extracted ion chromatogram and their mass spectrum. (a) A chromatograph of 3,4-DHPEA-AC (Compound 66, Table 3), Retention time (RT = 33.080 min) in the negative mode of ionization ($ESI^-/[M-H]^-$) identified and characterized in ginger; **(b)** Mass spectra of 3,4-DHPEA-AC showing an observed *m*/*z* 195.0671 in ginger; **(c)** A chromatograph of Apigenin 6,8-di-C-glucoside (Compound 29, Table 3), Retention time (RT = 26.791 min) in the negative mode of ionization ($ESI^-/[M-H]^-$) identified and characterized in lemon sample; **(d)** Mass spectra of Apigenin 6,8-di-C-glucoside showing an observed *m*/*z* 593.1556 in lemon; **(e)** A chromatograph of Sativanone (Compound 52, Table 3), Retention time (RT = 14.051 min) in the negative mode of ionization ($ESI^-/[M-H]^-$) identified and characterized in mint sample; **(f)** Mass spectra of Sativanone showing an observed *m*/*z* 299.0919 in mint.