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Data Article

Chemical characterizations dataset of flavonoid glycoside isomers and other constituents from *Ficus deltoidea* Jack

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ABSTRACT

Phytochemical data for *Ficus deltoidea* Jack, a plant widely studied for its anti-hyperglycemic effect, are scarce. In the pursuit of characterizing the chemical constituents of this species, extraction and purifications were conducted using multiple chromatographic procedures on selected varieties (var. *deltoidea*, var. *kunstleri* and var. *trengganuensis*). Twenty-two constituents were unambiguously identified through NMR, MS and UV data. These included gallocatechin (**S1**), afzelechin-4–8″-gallocatechin (**S2**), catechin (**S3**), afzelechin-4–8″-catechin (**S4**), afzelechin (**S5**), epicatechin (**S6**), hovetrichoside C (**S7**), 6,8-di-*C*-glucopyranosylapigenin (vicenin-2) (**S8**), afzelechin-4–8″-epiafzelechin (**S9**), epiafzelechin (**S10**), 6-*C*-xylopyranosyl-8-*C*-glucopyranosylapigenin (vicenin-1) (**S11**), orientin (**S13**), schaftoside (**S14**), 6-*C*-glucopyranosyl-8-*C*-xylopyranosylapigenin (vicenin-3) (**S16**), vitexin (**S17**), vitexin 2″-*O*-rhamnoside (**S19**), isovitexin 2″-*O*-rhamnoside (**S20**), 6,8-di-*C*-arabinopyranosylapigenin (**S21**),

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6,8-di-*C*-xylopyranosylapigenin (**S22**), 6-*C*-arabinopyranosyl-8-*C*-xylopyranosylapigenin (**S23**), rhoifolin (**S24**) and cerberic acid A (**S26**). The presented phytochemical data can assist ethnobotanists, chemists, and natural product researchers in investigating the medicinal properties of *F. deltoidea* by facilitating the dereplication of its constituents.

Specifications Table

Subject	Chemistry
Specific subject area	Natural products isolation and characterization of its chemical constituents
Type of data	Table, Figure Raw, Processed, Analysed
Data collection	NMR, MS, and UV data were acquired to unambiguously elucidate the chemical structures of 22 constituents purified from *F. deltoidea* Jack varieties. The NMR were recorded on a 500 MHz Varian Inova spectrometer or CryoProbe Bruker 600 MHz spectrometer. The MS and UV data were obtained from an Acquity UHPLC coupled to a Micromass LCT Premier Time-of-Flight Mass Spectrometer (TOF–MS) and photodiode array detector (Waters, Milford, USA).
Data source location	*F. deltoidea* leaves were sourced from Johor, Malaysia, at a Latitude of 1°55′25.8″ N and a Longitude of 102°48′09.7″E. All instrument data files are stored at the Phytochemistry and Bioactive Natural Products Laboratory, University of Geneva, Switzerland.
Data accessibility	Repository name: Mendeley Data Data identification number: doi: 10.17632/xgs4vs2b79.1 Direct URL to data: https://data.mendeley.com/datasets/xgs4vs2b79/1 Instructions for accessing these data: NMR, MS and UV spectra for each isolated compound can be accessed directly from the pdf files.
Related research article	Noraini Kasim, Adlin Afzan, Ahmed Mediani, Kah Hin Low, Abdul Manaf Ali, Nashriyah Mat, Jean-Luc Wolfender, Nor Hadiani Ismail, Correlation of chemical profiles obtained from ^{1}H–NMR and LC–MS metabolomics with α-glucosidase inhibition activity for varietal selections of *Ficus deltoidea*, Phytochemical Analysis. 2022; 33(8): 1235–1245. https://doi.org/10.1002/pca.3175 [1]

1. Value of the Data

- Currently, the phytochemical profile and chemical information of *F. deltoidea* Jack lacks comprehensive documentation.
- The NMR, MS and UV datasets address this knowledge gap by providing detailed characterizations of 22 chemical constituents from the leaves.
- By employing taxonomically informed scoring with the available phytochemical data, researchers can enhance their confidence in annotations when dereplicating *F. deltoidea* extracts.
- The NMR spectral data serves as a valuable and updated resource, especially for elucidating similar flavonoid glycoside isomers, a task that can be challenging with sole reliance on MS fragmentation data.
- The chromatographic protocols can assist researchers in extracting and purifying flavan-3-ols, proanthocyanidins, flavone glycosides, aurone glycoside and pulvinone.

2. Background

F. deltoidea Jack (Moraceae) has been widely studied for its glucose-lowering effects [2,3]. Nevertheless, phytochemical data of this species is not exhaustive, with only a few available

literatures. Most research predominantly focused on isovitexin and vitexin, the main flavone *C*-glycosides found in leaves. Another low-resolution MS profiling work annotated multiple isomers and proanthocyanidins without full structural assignments [4]. Furthermore, the occurrence of unambiguously identified compounds for this species is unavailable, even in common natural product resources, e.g., Dictionary of Natural Products [5] and LOTUS [6]. Given the reported chemotypes and differences in biological effects linked to different varieties, the reported phytochemical data of *F. deltoidea* becomes imperative for unambiguous metabolite identifications [1,7]. This data presents the purification methods for 22 chemical constituents and their characterizations through spectroscopic data.

3. Data Description

This article describes the spectroscopic data of chemical constituents purified from common *F. deltoidea* varieties (var. *kunstleri*, var. *deltoidea* and var. *trengganuensis*) using high-speed counter-current chromatography, vacuum liquid chromatography, medium-pressure liquid chromatography, preparative high-performance liquid chromatography, and preparative recycling high-performance liquid chromatography. The dataset consists of nuclear magnetic resonance (NMR), high-resolution mass spectrometry (HRMS) and ultraviolet (UV) spectra, fundamental for unequivocal structural elucidations of the purified flavan-3-ol monomers (**S1, S3, S5, S6, S10**), proanthocyanidin dimers (**S2, S4, S9**), flavone *C*-glycosides (**S8, S11, S13, S14, S16, S17, S19, S20, S21, S22, S23**), the flavone *O*-glycoside (**S24**) and aurone glycoside (**S7**) as well as pulvinone (**S26**) (Fig. 1).

Based on the spectroscopic data, the flavan-3-ols were identified as gallocatechin (**S1**), catechin (**S3**), afzelechin (**S5**), epicatechin (**S6**), and epiafzelechin (**S10**) (Table 1). The proanthocyani-

Table 1
NMR data for flavan-3-ol monomers.

Position	S1	S3	S5	S6	S10
H-2	4.53, d (7.3)	4.56, d (7.5)	4.59, d (7.8)	4.82, br s	4.87, br s
H-3	3.96, td, (7.3, 5.3)	3.97, td (7.9, 5.4)	3.98, td (8.2, 5.6)	4.18, ddd (4.6, 3.0, 1.5)	4.18, ddd (4.5, 2.6, 1.4)
H-4α	2.81, dd (16.2, 5.3)	2.85, dd (16.1, 5.4)	2.88, dd (16.1, 5.6)	2.86, dd (16.8, 4.6)	2.88, dd (16.8, 4.5)
H-4β	2.50, dd (16.2, 7.3)	2.50, dd (16.1, 7.9)	2.51, dd (16.1, 8.5)	2.74, dd (16.8, 3.0)	2.74, dd (16.8, 2.6)
H-6	5.92, d (2.3)	5.93, d (2.3)	5.93, d (2.2)	5.94, d (2.3)	5.95, d (2.3)
H-8	5.86, d (2.3)	5.85, d (2.3)	5.85, d (2.2)	5.92, d (2.3)	5.92, d (2.3)
H-2′	6.40, s	6.84, d (2.0)	7.22, d (8.6)	6.97, d (2.0)	7.32, d (8.5)
H-3′	–	–	6.79, d (8.6)	–	6.78, d (8.5)
H-5′	–	6.76, d (8.2)	6.79, d (8.6)	6.76, d (8.2)	6.78, d (8.5)
H-6′	6.40, s	6.72, dd (8.2, 2.0)	7.22, d (8.6)	6.80, dd (8.2, 2.0)	7.32, d (8.5)
C-2	82.6	83.0	82.9	79.7	79.9
C-3	68.5	69.0	68.8	67.3	67.5
C-4	27.8	28.7	28.9	29.1	29.4
C-5	157.6	157.7	157.6	157.7	157.7
C-6	95.9	96.4	96.3	96.2	96.4
C-7	157.4	158.0	157.6	158.1	157.8
C-8	95.2	95.7	95.5	95.7	95.9
C-9	156.5	157.1	157.0	157.5	157.4
C-10	100.4	101.0	100.9	100.1	100.0
C-1′	131.2	132.4	131.5	132.2	131.6
C-2′	106.9	115.4	129.6	115.1	129.1
C-3′	146.6	146.4	116.0	145.7	115.7
C-4′	133.6	146.4	158.4	146.0	157.9
C-5′	146.6	116.2	116.0	115.7	115.7
C-6′	106.9	120.2	129.6	119.2	129.1

Notes: All spectra were obtained at 500 MHz for protons and 125 MHz for carbon and were recorded in CD_3OD. Chemical shifts are in ppm. The coupling constant reported in brackets is in Hz.

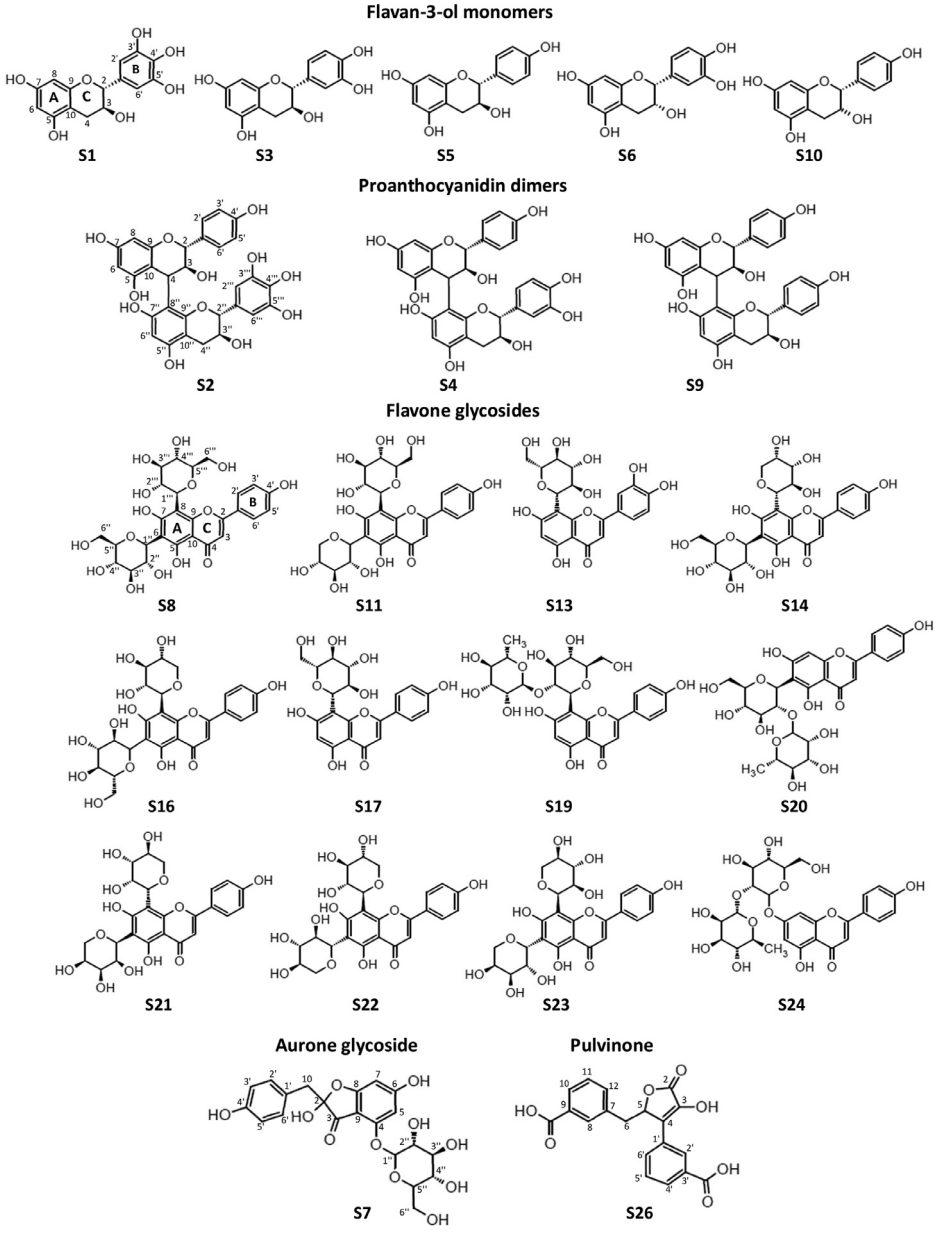

Fig. 1. Chemical structures of 22 compounds purified from *F. deltoidea* leaves.

dins were identified as afzelechin-4–8″-gallocatechin (**S2**), afzelechin-4–8″-catechin (**S4**) and afzelechin-4–8″-epiafzelechin (**S9**) (Table 2). Table 3 shows the NMR data for all the flavone glycosides purified from var. *deltoidea* and var. *kunstleri*. These flavone *C*-glycosides were assigned as orientin (**S13**), vitexin (**S17**), vitexin 2″-*O*-rhamnoside (**S19**), isovitexin 2″-*O*-rhamnoside (**S20**) and the flavone *O*-glycosides was identified as rhoifolin (**S24**). The flavone glycosides purified from var. *trengganuensis* were identified as 6,8-di-*C*-glucopyranosylapigenin (vicenin-

Table 2
NMR data for proanthocyanidins dimers.

Subunit	Position	S2	S4	S9
Upper unit	H-2	4.26, d (9.4)	4.29, d (9.7)	4.36, d (9.2)
	H-3	4.35, dd (9.4,7.4)	4.34, dd (9.7,7.5)	4.33, dd (9.2, 6.8)
	H-4	4.37, d (7.4)	4.40, d (7.5)	4.46, d (6.8)
	H-6	5.87, d (2.4)	5.88, d (2.4)	5.91, d (2.4)
	H-8	5.84, d (2.4)	5.82, d (2.4)	5.96, d (2.4)
	H-2′	6.92, d (8.6)	6.91, d (8.6)	7.05, d (8.5)
	H-3′	6.69, d (8.6)	6.66, d (8.6)	6.78, d (8.5)
	H-4′	–	–	–
	H-5′	6.69, d (8.6)	6.66, d(8.6)	6.78, d (8.5)
	H-6′	6.92, d (8.6)	6.91, d (8.6)	7.05, d (8.5)
	C-2	83.7	82.5	83.8
	C-3	74.1	72.7	74.0
	C-4	38.5	37.3	38.7
	C-5	156.8	155.9	157.3
	C-6	97.3	96.1	97.6
	C-7	156.9	155.9	157.4
	C-8	96.9	95.6	96.9
	C-9	158.9	157.5	158.5
	C-10	107.4	106.0	107.2
	C-1′	132.2	131.0	132.1
	C-2′	130.1	129.0	130.0
	C-3′	115.7	114.5	115.6
	C-4′	158.3	156.9	158.0
	C-5′	115.7	114.5	115.6
	C-6′	130.1	129.0	130.0
Terminal unit	H-2″	4.33, d (7.9)	4.44, d (8.0)	4.85 (overlapped)
	H-3″	3.77, m	3.76, td (8.4, 5.9)	4.07, dt (5.0, 1.7)
	H-4″α	2.86, dd (16.3, 5.9)	2.84, dd (16.3, 5.9)	2.91, dd (17.0, 5.0)
	H-4″β	2.46, dd (16.3, 8.6)	2.48, dd (16.3, 8.6)	2.73, dd (17.0, 1,7)
	H-6″	6.08, s	6.08, s	6.11, s
	H-2‴	6.22, s	6.65, d (2.0)	6.86, d (8.5)
	H-3‴	–	–	6.59, d (8.5)
	H-5‴	–	6.74, d (8.2)	6.59, d (8.5)
	H-6‴	6.22, s	6.38, dd (8.2, 2.0)	6.86, d (8.5)
	C-2″	83.4	81.7	80.1
	C-3″	69.1	68.0	67.8
	C-4″	29.7	28.4	29.7
	C-5″	155.8	155.1	156.3
	C-6″	96.1	94.9	96.4
	C-7″	155.4	154.0	156.3
	C-8″	108.8	107.3	108.5
	C-9″	155.2	153.9	155.5
	C-10″	103.0	101.6	101.6
	C-1‴	131.1	130.6	131.1
	C-2‴	108.0	114.6	129.3
	C-3‴	146.6	144.9	115.6
	C-4‴	134.0	144.8	157.6
	C-5‴	146.6	114.9	115.6
	C-6‴	108.0	119.0	129.3

Notes: All spectra were obtained at 500 MHz for protons and 125 MHz for carbon and were recorded in CD_3OD. Chemical shifts are in ppm. The coupling constant reported in brackets is in Hz.

2) (**S8**), 6-*C*-xylopyranosyl-8-*C*-glucopyranosylapigenin (vicenin-1) (**S11**), schaftoside (**S14**), 6-*C*-glucopyranosyl-8-*C*-xylopyranosylapigenin (vicenin-3) (**S16**), 6,8-di-*C*-arabinopyranosylapigenin (**S21**), 6,8-di-*C*-xylopyranosylapigenin (**S22**) and 6-*C*-arabinopyranosyl-8-*C*-xylopyranosylapigenin (**S23**) (Table 4).

Table 3
NMR data for flavones with glucopyranosyl and rhamnopyranosyl units.

Subunit	Position	S17	S13[i]	S19	S20		S24
					A-Rotamer	B-Rotamer	
Apigenin or luteolin[i]	H-3	6.77, s	6.64, s	6.62, s	6.76, s	6.76, s	6.67, s
	H-6	6.27, s	6.26, s	6.29, s	–	–	6.46, d (2.2)
	H-8	–	–	–	6.51, br s	6.50, br s	6.80, d (2.2)
	H-2′	8.02, d (8.3)	7.48, br s	8.01, d (8.8)	7.92, d (8.4)	7.92, d (8.4)	7.89, d (8.8)
	H-3′	6.89, d (8.3)	–	6.96, d (8.8)	6.93, d (8.4)	6.93, d (8.4)	6.94, d (8.8)
	H-4′	–	–	–	–	–	–
	H-5′	6.89, d (8.3)	6.86, d (8.2)	6.96, d (8.8)	6.93, d (8.4)	6.93, d (8.4)	6.94, d (8.8)
	H-6′	8.02, d (8.3)	7.53, br d (8.2)	8.01, d (8.8)	7.92, d (8.4)	7.92, d (8.4)	7.89, d (8.8)
	5–OH	13.16	13.17	–	13.55	13.55	–
	C-2	163.9	164.0	165.4	163.2	163.2	166.8
	C-3	102.5	102.3	101.5	102.5	102.5	104.1
	C-4	182.1	182.0	182.8	–	182.6	184.0
	C-5	162.5	160.5	162.8	161.2	162.7	162.9
	C-6	98.1	98.1	97.7	109.0	108.5	101.0
	C-7	160.4	162.6	161.4	163.1	163.6	164.4
	C-8	104.5	104.5	156.5	92.9	94.2	95.9
	C-9	158.9	155.9	161.4	–	161.7	159.0
	C-10	104.0	104.0	104.6	103.5	104.0	107.1
	C-1′	121.6	121.9	122.2	120.9	120.9	123.0
	C-2′	128.9	114.0	128.8	128.4	128.4	129.7
	C-3′	115.8	145.7	115.6	116.0	116.0	117.2
	C-4′	161.1	149.6	161.4	161.3	161.3	162.9
	C-5′	115.8	115.6	115.6	116.0	116.0	117.2
	C-6′	128.9	119.3	128.8	128.4	128.4	129.7

(*continued on next page*)

Table 3 (*continued*)

Subunit	Position	S17	S13[+]	S19	S20		S24
					A-Rotamer	B-Rotamer	
Glucopyranosyl unit	H-1″	4.96, d (9,3)	4.68, d (9.7)	5.03, d (9.9)	4.63, d (9.8)	4.66, d (9.7)	5.21, d (7.6)
	H-2″	3.84, t (9.32)	3.83, t (9,4)	4.26, dd (9.9, 7.7)	4.38, t (9.3)	4.20, t (9.0)	3.70, dd (8.9, 7.6)
	H-3″	3.26, m	3.25, m	3.63, m	3.33 (overlapped)	3.36 (overlapped)	3.64, t (8.9)
	H-4″	3.38, m	3.37, m	3.63, m	3.13, m	3.13, m	3.41, t (9.4)
	H-5″	3.24, m	3.25, m	3.44, m	3.17, m	3.12, m	3.55, ddd (9.7, 5.9, 2.3)
	H-6″α	3.77, m	3.79, d (11.9)	3.96, dd (12.0, 2.3)	3.70, d (11.7)	3.70, d (11.7)	3.93, m
	H-6″β	3.53, m	3.55, dd (11.9, 6.4)	3.79, dd (12.0, 5.7)	3.35 (overlapped)	3.41 (overlapped)	3.70, m
	C-1″	73.3	73.3	72.3	71.2	71.2	99.8
	C-2″	70.8	70.8	76.8	74.5	75.7	79.2
	C-3″	78.6	78.7	80.2	80.1	79.6	79.0
	C-4″	70.5	70.6	71.1	–	71.9	71.4
	C-5″	81.8	81.9	81.5	81.4	81.5	78.3
	C-6″	61.3	61.6	61.6	61.7	61.2	62.4
Rhamnopyranosyl unit	H-1‴	–	–	5.10, d (1.7)	5.09, s	5.01, s	5.28, d (1.8)
	H-2‴	–	–	3.84, dd (3.2, 1.7)	3.60, br s	3.62, br s	3.95, dd (3.0, 1.8)
	H-3‴	–	–	3.39, dd (9.5, 3.2)	3.13, m	3.08, m	3.61, dd (9.4, 3.0)
	H-4‴	–	–	3.12, t (9.5)	2.92, m	2.92, m	3.41, t (9.4)
	H-5‴	–	–	2.45, dq (9.4, 6.2)	2.34, m	2.34, m	3.93, m
	H-6‴	–	–	0.65, d (6.2)	0.52, d (6.0)	0.61, d (6.1)	1.33, d (6.2)
	C-1‴	–	–	101.1	100.3	100.7	102.5
	C-2‴	–	–	68.6	70.6	70.6	72.2
	C-3‴	–	–	70.6	70.8	70.3	72.3
	C-4‴	–	–	72.2	71.6	71.6	74.0
	C-5‴	–	–	70.8	68.2	68.2	70.1
	C-6‴	–	–	16.7	17.8	17.6	18.3

Notes: S13, S19, and S20 proton spectra were obtained at 600 MHz, while S17 and S24 were obtained at 500 MHz. S17, S13, and S20 spectra were recorded in DMSO–d_6, while S24 and S19 spectra were recorded in CD_3OD. Chemical shifts are in ppm. The coupling constant reported in brackets is in Hz.

Table 4
NMR data for flavones with glucopyranosyl, xylopyranosyl and arabinopyranosyl units.

Subunit	Position	S8[ł,ł]	S11[ł,ł]	S14[ł,ŀ]	S16[ł,ł]	S21[ŀ,ŀ]	S22[ł,ł]	S23[ŀ,ł]
Apigenin	H-3	6.55, s	6.61, br s	6.75, s	6.64, s	6.64, s	6.47, s	6.72, s
	H-2′	7.93, d (8.5)	7.94, d (8.4)	8.08, d (8.1)	7.90, d (8,6)	8.10, d (8.8)	7.86, d (8.8)	7.92, d (8.8)
	H-3′	6.89, d (8.5)	6.90, d (8.4)	6.92, d (8.1)	6.95, d (8,6)	6.90, d (8.8)	6.90, d (8.8)	6.94, d (8.8)
	H-5′	6.89, d (8.5)	6.90, d (8.4)	6.92, d (8.1)	6.95, d (8,6)	6.90, d (8.8)	6.90, d (8.8)	6.94, d (8.8)
	H-6′	7.93, d (8.5)	7.94, d (8.4)	8.08, d (8.1)	7.90, d (8,6)	8.10, d (8.8)	7.86, d (8.8)	7.92, d (8.8)
	C-2	–	162.6	163.7	166.5	–	161.5	163.1
	C-3	102.1	102.0	101.9	104.0	101.7	101.7	102.1
	C-4	–	–	182.0	184.3	–	–	–
	C-5	–	159.5	159.3	161.0	–	159.6	158.0
	C-6	–	108.6	108.3	–	–	108.7	107.8
	C-7	–	–	161.5	163.2	–	–	–
	C-8	–	–	104.0	–	–	104.1	104.4
	C-9	–	–	154.1	157.1	–	155.1	154.6
	C-10	–	–	103.1	105.4	–	–	–
	C-1′	–	121.6	121.1	123.4	121.1	122.0	121.2
	C-2′	128.4	128.2	128.5	129.8	128.7	127.7	127.9
	C-3′	115.7	115.5	115.5	117.1	115.6	115.4	115.4
	C-4′	–	160.6	160.9	162.9	160.4	160.1	160.6
	C-5′	115.7	115.5	115.5	117.1	115.6	115.4	115.4
	C-6′	128.4	128.2	128.5	129.8	128.7	127.7	127.9
Sugar at C-6 (Glucopyranosyl unit[ł], xylopyranosyl unit[ŀ], arabinopyranosyl unit[ŀ])	H-1″	4.70, d (10.0)	4.60, d (9.8)	4.74, d (9.8)	5.00, d (9.9)	4.61, d (9.4)	4.55, d (9.8)	4.69, d (9.2)
	H-2″	3.83, m	3.97, br s	3.88, br s	–	4.12, br s	4.01, t (9.3)	3.92, m
	H-3″	3.27/ 3.32, m	3.20, m	3.28, m	3.52, m	3.42, d (8.7)	3.17 (overlapped)	3.46, dd (9.2, 2.3)
	H-4″	3.27/ 3.37, m	3.45, m	3.28, m	3.54, m	3.78, br s	3.41, m	3.82, t (2.3)
	H-5″α	3.24/ 3.30, m	3.80, dd (10.9, 5.3)	3.28, m	3.47, m	3.80, d (12.5)	3.76, dd (10.9, 5.5)	3.85, dd (11.9, 2.3)
	H-5″β	–	3.19, m	–	–	3.55, d (12.5)	3.08, t (10.7)	3.62, d (11.9)
	H-6″α	3.67, d (11.7)	–	3.69, m	3.87, dd (12.2, 2.3)	–	–	–
	H-6″β	3.55, m	–	3.53, m	3.81, dd (12.2, 4.8)	–	–	–
	C-1″	74.3	74.6	73.1	76.0	74.2	75.0	73.9
	C-2″	71.8	70.6	70.5	–	–	70.8	68.9
	C-3″	79.0/79.2	78.9	78.2	79.5	74.3	79.1	73.6
	C-4″	70.3/70.8	69.7	69.6	71.2	68.7	69.9	68.1
	C-5″	81.0/81.6	70.1	80.8	82.7	69.8	70.0	69.7
	C-6″	61.1	–	60.5	62.0	–	–	–

(*continued on next page*)

Table 4 (*continued*)

Subunit	Position	S8[i,l]	S11[i,l]	S14[i,1]	S16[l,i]	S21[1,1]	S22[i,i]	S23[1,i]
Sugar at C-8 (Glucopyranosyl unit[i], xylopyranosyl unit[i], arabinopyranosyl unit[1])	H-1‴	4.85, d (10.5)	4.89, brs	4.80, d (9.7)	4.96, d (9.9)	4.74, d (9.5)	4.73, d (9.9)	4.75, d (10.0)
	H-2‴	3.83, m	3.73, m	4.09, t (9.7)	4.05, t (9.9, 8.4)	4.22, t (9.5, 8.3)	3.81, dd (9.9, 8.7)	3.96, t (10.0, 8.7)
	H-3‴	3.27/ 3.32, m	3.35, m	3.53, m	3.40, t (8.9)	3.48, d (8.3)	3.25, t (8.7)	3.27, td (8.7, 3.2)
	H-4‴	3.27/ 3.37, m	3.40, m	3.87, br s	3.78, m	3.85, br s	3.53, m	3.58, m
	H-5‴α	3.24/ 3.30, m	3.35, m	3.92, dd (12.1, 2.2)	4.10, dd (11.1, 5.5)	3.89, dd (12.2, 2.0)	3.88, dd (10.9, 5.4)	3.91, dd (11.0, 5.4)
	H-5‴β	–	–	3.69, m	3.40, t (11.1)	3.61, d (12.2)	3.20 (overlapped)	3.21, t (11.0)
	H-6‴α	3.74, d (11.6)	3.73, d (11.6)	–	–	–	–	–
	H-6‴β	3.55, m	3.59, d (11.6)	–	–	–	–	–
	C-1‴	74.6	74.5	74.6	–	74.8	75.7	74.1
	C-2‴	71.8	71.6	68.6	73.1	68.7	71.9	70.6
	C-3‴	79.0/79.2	78.6	74.0	80.2	74.9	79.1	78.7
	C-4‴	70.3/70.8	69.7	68.3	71.7	68.8	70.1	69.7
	C-5‴	81.0/81.6	81.2	70.2	71.9	70.5	70.3	70.0
	C-6‴	61.4	60.7	–	–	–	–	–

Notes: All spectra were obtained at 600 MHz for protons and 150 MHz for carbon and were recorded in DMSO–d_6 at 60 °C, except for S16, which was recorded in CD_3OD at ambient temperature. Chemical shifts are in ppm. The coupling constant reported in brackets is in Hz.

Table 5
NMR data for an aurone glycoside (**S7**) and a pulvinone (**S26**).

Position	S7		Position	S26	
	^{1}H	DEPTQ		^{1}H	DEPTQ
2	–	107.7/107.7	2	–	170.8
3	–	196.8/196.8	3	–	140.8
4	–	158.5/158.3	4	–	129.1
5	6.02, d (1.7)/6.01, d (1.7)	97.9/97.6	5	5.81, dd (5.6, 3.7)	79.8
6	–	172.7/172.7	6α	3.43, dd (14.5, 3.7)	40.0
7	5.90, d (1.7)/5.90, d (1.7)	93.4/93.3	6β	3.06, dd (14.5, 5.6)	40.0
8	–	174.6/174.6	7	–	136.7
9	–	103.2/103.2	8	7.68, br s	132.2
10a, 10b	3.10, d (13.9)/3.10, d (13.9), 3.06, d (13.9)/3.06, d (13.9)	42.2/40.0	9	–	132.4
1′	–	125.6/125.6	10	7.85, d (7.7)	129.3
2′, 6′	6.98, d (8.5)/6.98, d (8.5)	132.5/132.5	11	7.31, t (7.7)	129.1
3′, 5′	6.57, d (8.5)/6.55, d (8.5)	115.8/115.7	12	7.23, d (7.7)	135.3
4′	–	157.3/157.3	13	–	170.2
1″	4.84 (overlapped)	101.7/101.7	1′	–	134.1
2″	3.53, dd (9.2, 7.8)/3.49, ddd (9.2, 7.6)	74.1/74.0	2′	8.35, br s	129.6
3″	3.45, t (8.8)/3.45, t (8.8)	77.4/77.3	3′	–	132.4
4″	3.40, m/3.40, m	71.2/71.2	4′	8.03, d (7.8)	130.6
5″	3.41, m/3.41, m	78.4/78.3	5′	7.58, t (7.8)	129.9
6″a	3.86, dd (12.2, 2.0)/3.86, dd (12.2, 2.0)	62.3/62.3	6″	7.94, d (7.8)	132.4
6″b	3.68, dd (12.2, 5.0)/3.67, dd (12.2, 5.4)		7′	–	170.5

Notes: All spectra were obtained at 600 MHz for protons and 150 MHz for carbon and DEPTQ. All spectra were recorded in CD_3OD. Chemical shifts are in ppm. The coupling constant reported in brackets is in Hz. S7 was isolated as a mixture of diastereoisomers.

In the case of 6,8-di-*C*-glycoside derivatives hydroxylated at C-5 and C-7, positioning the sugars at C-6 and C-8 is particularly difficult. Fortunately, after identification of each sugar using 2D NMR experiments (HSQC, COSY and TOCSY), the observation of a dipolar correlation (NOESY or ROESY) between the anomeric proton of the sugar at C-8 and the protons of the aromatic ring at C-2 provides an answer to this question (Fig. 2). It should also be noted that some compounds had to be recorded at 60 °C due to slow exchanges between rotamers leading to broad spectra at 25 °C. Apart from flavonoids, the aurone glycoside and pulvinone were identified as hovetrichoside C (**S7**) and cerberic acid A (**S26**), respectively (Table 5).

For comprehensive characterization, HRMS and UV data were obtained, as detailed in Table 6 and visualized in Fig. 3 and Fig. 4. Two methods were developed: a short 10-minute gradient (Method A) and a longer 55-minute gradient (Method B), each serving specific purposes. Method A was ideal for high-throughput metabolomics analysis, enabling the establishment of chemical and bioactive markers associated with *F. deltoidea* varieties [1,7]. Alternatively, peak resolutions are enhanced in Method B, making it more effective for dereplicating crude extracts with complex matrices. Altogether, the NMR, MS and UV spectra for all isolated compounds are supplemented in Mendeley Data [8].

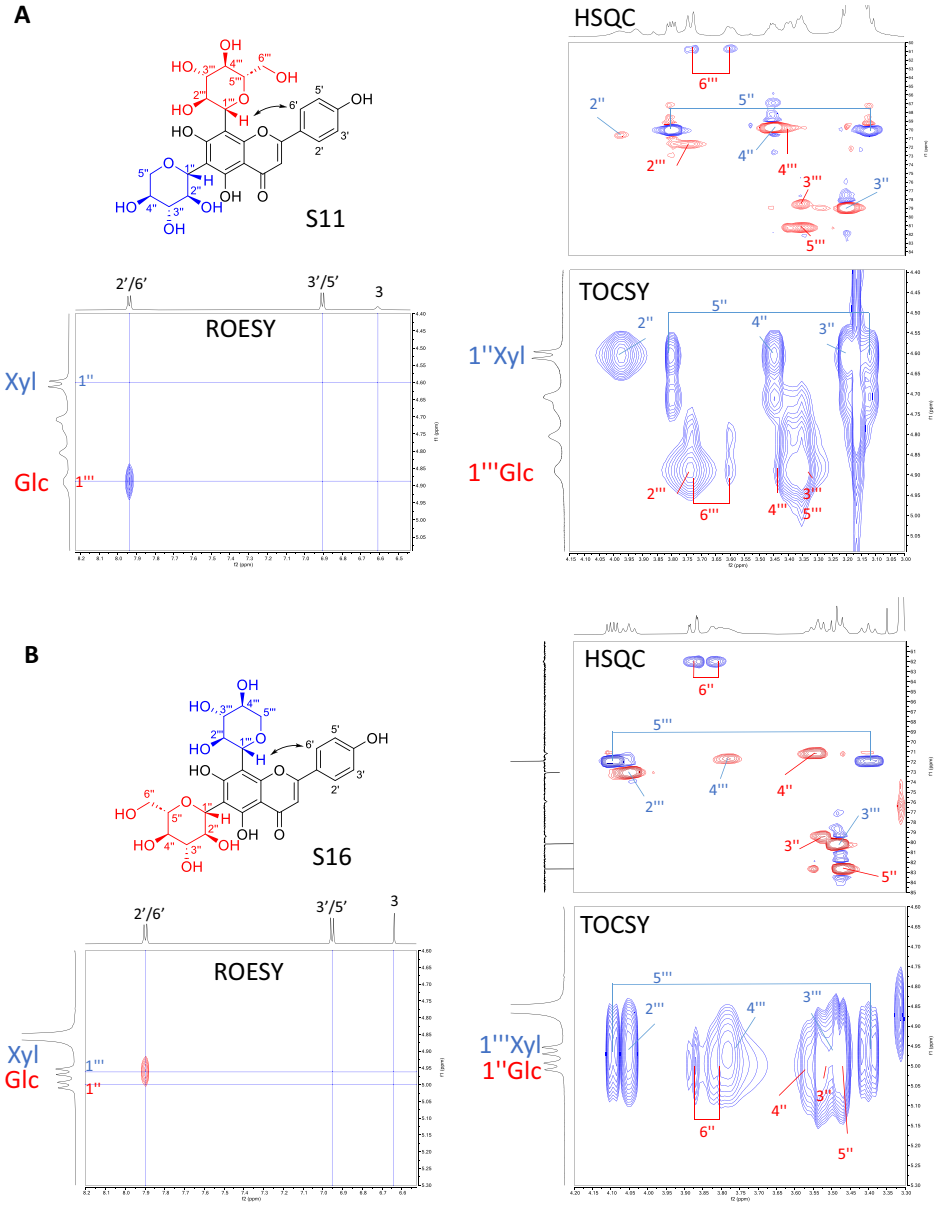

Fig. 2. HSQC and TOCSY spectra of S11 (vicenin-1) (**A**) and S16 (vicenin-3) (**B**) were used to assign the protons of the glucopyranosyl (red) and xylopyranosyl (blue) sugars. The ROESY correlation between H-2′/H-6′ and the anomeric proton of the C-8 sugar was used to position each sugar on the apigenin (the double-headed arrow indicates this ROESY correlation).

Table 6
LC–HRMS electrospray negative ionization mode and UV absorbance data.

Compound No.	Chemical name	t_R (min)		*m/z*	Molecular formula	Mass error (ppm)	UV (nm)
		Method A	Method B				
S1	Gallocatechin	0.69	2.03	305.0620	$C_{15}H_{13}O_7$	−13.4	270
S2	Afzelechin-4–8″-gallocatechin	1.13	4.49	577.1365	$C_{30}H_{25}O_{12}$	−1.0	273
S3	Catechin	1.20	4.79	289.0686	$C_{15}H_{13}O_6$	−9.0	278
S4	Afzelechin-4–8″-catechin	1.49	7.06	561.1385	$C_{30}H_{25}O_{11}$	−2.1	277
S5	Afzelechin	1.67	8.42	273.0727	$C_{15}H_{13}O_5$	−13.2	272
S6	Epicatechin	1.72	9.79	289.0686	$C_{15}H_{13}O_6$	−9.0	278
S7	Hovetrichoside C	1.77	10.14	449.1087	$C_{21}H_{21}O_{11}$	0.7	293
S8	Vicenin-2	2.07	ND	593.1547	$C_{27}H_{29}O_{15}$	6.9	215, 270, 334
S9	Afzelechin-4–8″-epiafzelechin	2.13	12.99	545.1459	$C_{30}H_{25}O_{10}$	2.0	272
S10	Epiafzelechin	2.24	14.00	273.0737	$C_{15}H_{13}O_5$	−9.5	272
S11	Vicenin-1	2.37	16.85	563.1412	$C_{26}H_{27}O_{14}$	−6.4	216, 270, 334
S13	Orientin	2.49	17.05	447.0923	$C_{21}H_{19}O_{11}$	−0.9	212, 254, 268, 348
S14	Schaftoside	2.51	17.72	563.1405	$C_{26}H_{27}O_{14}$	0.7	215, 270, 336
S16	Vicenin-3	2.76	19.42	563.1373	$C_{26}H_{27}O_{14}$	−5.0	216, 270, 335
S17	Vitexin	2.90	ND	431.0959	$C_{21}H_{19}O_{10}$	−4.4	214, 267, 337
S19	Vitexin 2″-*O*-rhamnoside	2.97	20.17	577.1570	$C_{27}H_{29}O_{14}$	2.3	214, 268, 339
S20	Isovitexin 2″-*O*-rhamnoside	3.02	20.61	577.1587	$C_{27}H_{29}O_{14}$	5.2	213, 269, 338
S21	6,8-di-*C*-arabinopyranosylapigenin	3.11	21.44	533.1268	$C_{25}H_{25}O_{13}$	−5.1	216, 270, 335
S22	6,8-di-*C*-xylopyranosylapigenin	3.17	21.96	533.1318	$C_{25}H_{25}O_{13}$	4.3	218, 270, 334
S23	6-*C*-arabinopyranosyl-8-*C*-xylopyranosylapigenin	3.45	23.81	533.1306	$C_{25}H_{25}O_{13}$	2.1	221, 270, 333
S24	Rhoifolin	3.93	26.99	577.1569	$C_{27}H_{29}O_{14}$	2.1	211, 266, 337
S26	Cerberic acid A	4.90	30.20	353.0641	$C_{19}H_{13}O_7$	−5.7	226, 283

Notes: ND: not determined. The *m/z*, molecular formula and mass error were determined from Method A. The acceptable mass error tolerance was <15 ppm, slightly higher for HRMS since older TOF–MS model was used for this analysis. All *m/z* were identified as $[M-H]^-$ ion. For retention time information, refer to UHPLC conditions detailed in Section 4.3.

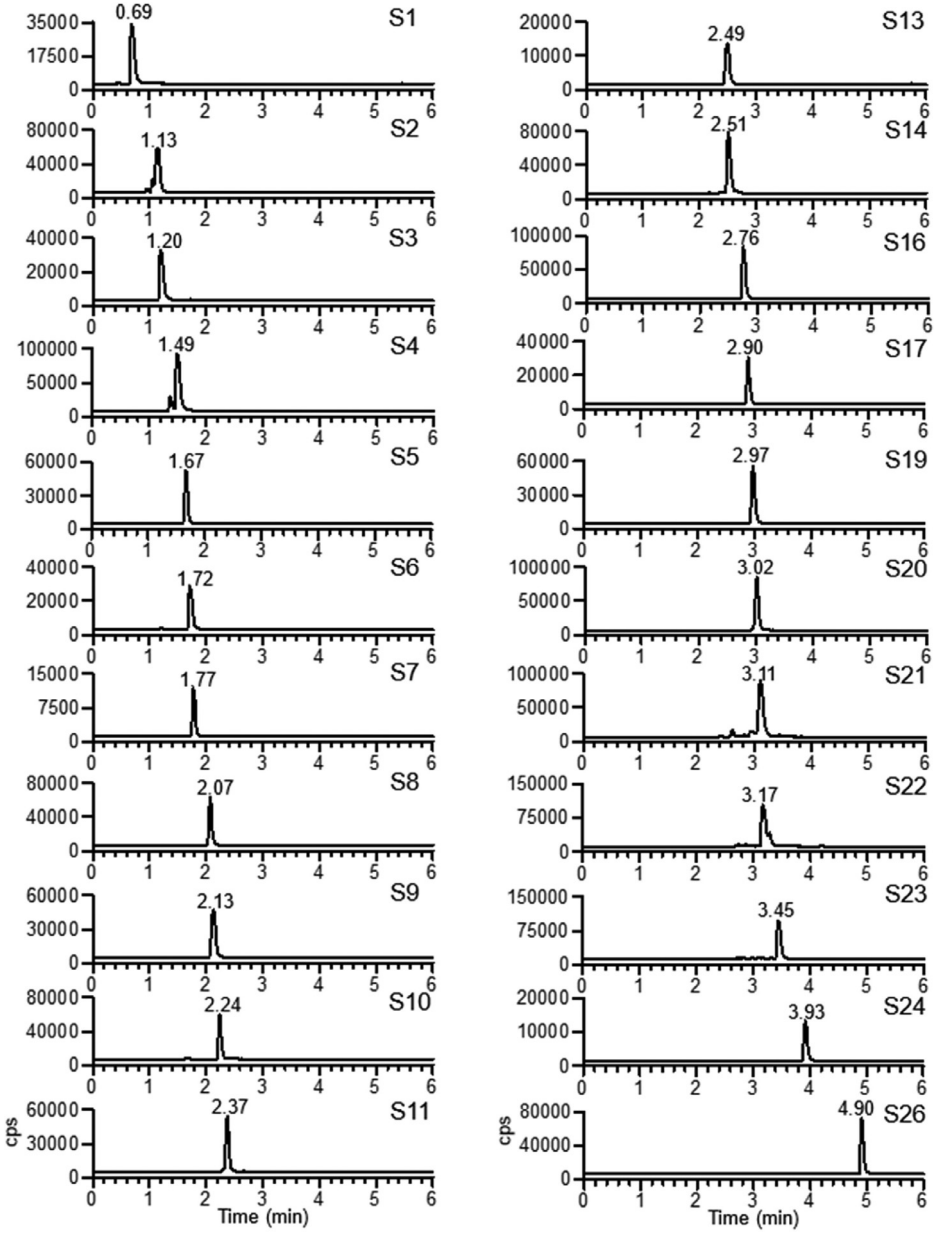

Fig. 3. Retention time comparisons of the isolated compounds (Method A).

4. Experimental Design, Materials and Methods

4.1. Plant source and extraction

The fresh leaves of three varieties (var. *kunstleri*, var. *deltoidea*, var. *trengganuensis*) were purchased from a small orchard in Johor, Malaysia. Plant authentications have been described in

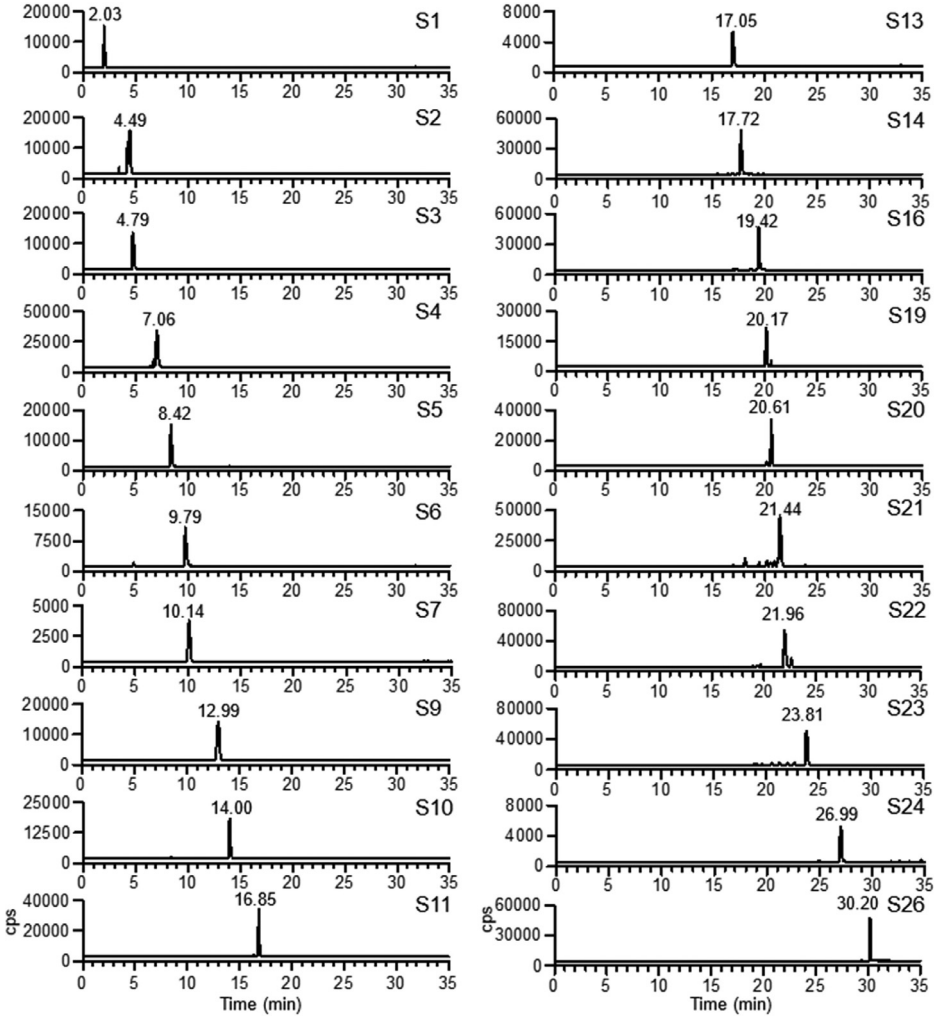

Fig. 4. Retention time comparisons of the isolated compounds (Method B).

previous work [7]. The leaves were washed, oven-dried at 40 °C, and pulverized into powder. The extraction method for var. *kunstleri* and var. *deltoidea* involved defatting with hexane (3 kg in 12 L, repeated thrice) for 24 h at room temperature with continuous stirring. The hexane extract was filtered and dried under reduced pressure using a rotary evaporator. Subsequently, the marc was macerated in methanol using a volume and extraction time similar to the first step. The methanol extract yields were 473.23 g for var. *kunstleri* (15 % recovery) and 251.06 g for var. *deltoidea* (8 % recovery). For var. *trengganuensis*, the dried powdered leaves (804.61 g) were soaked in methanol at room temperature for three days and concentrated using a rotary evaporator. This extraction yielded 90.42 g methanol extract (11.24 % recovery). Only a portion of methanol extract from each variety was used for purifications. The remaining was stored at 4 °C for other experiments outside the context of this article.

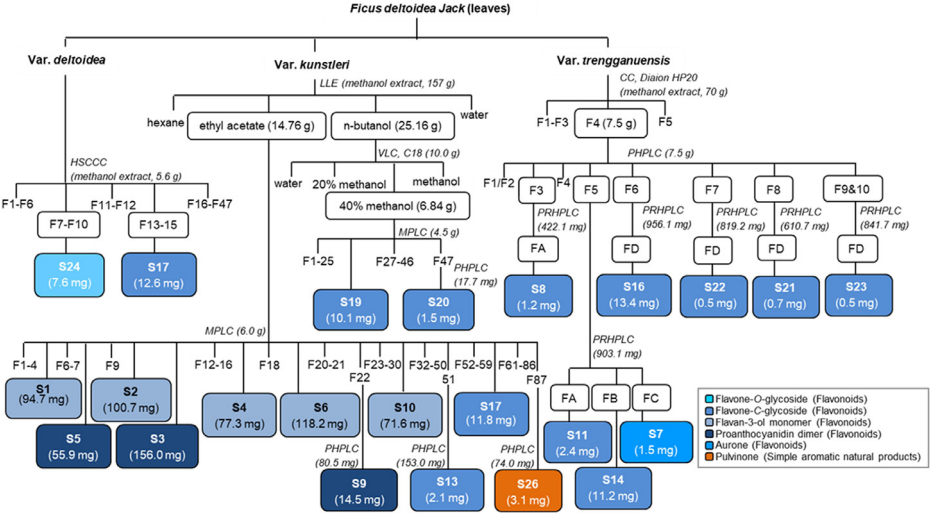

Fig. 5. Schematic diagram for the purification of 22 constituents from *F. deltoidea* varieties by multiple chromatographic techniques (HSCCC: High-speed counter-current chromatography, LLE: Liquid-liquid extraction, VLC: Vacuum liquid chromatography, MPLC: Medium pressure liquid chromatography, PHPLC: Preparative high-performance liquid chromatography, PRHPLC: Preparative recycling high-performance liquid chromatography.

4.2. Chromatographic procedures for compound purification

The purification workflow from var. *deltoidea*, var. *kunstleri* and var. *trengganuensis* extracts involved several separation techniques (Fig. 5). Compounds **S17** and **S24** were isolated from the methanol extract of var. *deltoidea* using TBE300B high-speed counter-current chromatography (HSCCC) (Shanghai Tauto Biotech, China) equipped with LC-10AD pump (Shimadzu, Kyoto, Japan), K-2001 UV–vis detector (Knauer, Berlin, Germany), Büchi C-660 fraction collector (Büchi, Flawil, Switzerland) and 260 mL coil column. The extract was separated using a biphasic system of ethyl acetate, n-butanol and water mixture (4:1:5; v/v). The column was loaded with the upper phase (UP) at 3 mL/min and 800 rpm speed, followed by equilibration with the lower phase (LP). About 277.5 mg/mL methanol extract was introduced into the 50 mL sample loop through sandwich injection with half the volume in UP and half in the LP. Elution was performed in descending mode for 7 h, and the effluent was monitored at 280 nm. The remaining content of the HSCCC column was extruded by pumping the organic mobile phase at 3 mL/min for 2 h.

The methanol extract from var. *kunstleri* was further enriched using liquid-liquid extraction (LLE) and vacuum liquid chromatography (VLC) to remove free sugars and concentrate the targeted flavonoids (Fig. 5). The ethyl acetate fraction was then subjected to medium-pressure liquid chromatography (MPLC). The MPLC system consisted of a 681 pump, a C-640 UV detector and a C-684 fraction collector (Büchi, Flawil, Switzerland). The column's inner diameter (ID) was 49 mm with 460 mm length. The column was loaded with a ZEOprep® C18, 15–25 µm particle size (Zeochem, Rüti, Switzerland). A dry loading sample was prepared by packing 6 g of ethyl acetate fraction with 33 g of ZeoPrep C18, 40–63 µm particle size (ZeoCHEM, Rüti, Switzerland) and 6 g of 50–70 mesh sand (Sigma Aldrich, Germany). The mobile phase consisted of MiliQ water (A) and methanol (B), added with 0.1 % formic acid. The mobile phase gradient was 10 % B for 56 min, 10–30 % B from 56 to 1097 min, 30 % B isocratic from 1097 to 1192 min and 30–95 % B from 1192 to 1471 min. Throughout this gradient, the flow rate was 20 mL/min. The column temperature was 45 °C, and UV monitoring was 270 nm. Eight compounds (**S1, S2, S3, S4, S5, S6, S10** and **S17**) were obtained directly from MPLC fractions. Other fractions were purified using

preparative HPLC on a C18 X-bridge column with 19 mm ID, 150 mm length and 5 µm particle size (Waters®, Milford, MA, USA) at 10 mL/min flow rate. The separation using 12 % acetonitrile in isocratic conditions afforded **S9**, while 10 % acetonitrile in isocratic conditions afforded **S13** and **S26**. In addition, MPLC separation was performed for a fraction obtained from VLC named 40 % methanolic (see Fig. 5) to obtain **S19** and **S20**. The gradient for this separation consisted of 5 % B (methanol in 0.1 % formic acid) for 56 min, 5–30 % B from 56 to 103 min, 30–30.5 % B from 103 to 955 min, 30.5–40 % B from 955 to 1050 min and 40–100 % B from 1050 to 1097 min.

The enrichment of flavonoids from the methanol extract of var. *trengganuensis* was performed using column chromatography with Diaion HP20 resin (Mitsubishi Chemical, Tokyo, Japan) and water–methanol mixtures (100:0, 80:20, 60:40, 40:60, 20:80, v/v). Fraction 4, containing the targeted flavonoids, was further fractionated using the PLC 2020 preparative HPLC system (Gilson, Saint-Avé, France). The LC method consisted of an XBridge C18 column measuring 19 mm ID × 250 mm length, 5 µm particle size (Waters®, Milford, MA, USA), 18 mL/min flow rate and 1 mL injection volume. The mobile phase gradient was 5–30 % acetonitrile from 0 to 24 min, 30–95 % acetonitrile from 24 to 25 min and 95 % acetonitrile from 25 to 31 min. The sub-fractions were subjected to recycling HPLC on JAIGEL SP-120–15 ODS-AP column measuring 20 mm ID × 250 mm length (Japan Analytical Industry, Tokyo, Japan). Different percentages of acetonitrile (12 %, 16 % and 18 %) in isocratic conditions (4 mL/min) and multiple cycles were used to purify **S7, S8, S11, S14, S16, S23, S21** and **S22**.

4.3. Chemical characterization

NMR spectroscopic data were recorded on a Varian INOVA 500 MHz spectrometer (Palo Alto, CA, USA) or Bruker 600 MHz spectrometer equipped with a 5 mm CryoProbe™ (Mannheim, Germany). Chemical shifts (δ) are reported in parts per million (ppm) using the residual deuterated methanol (CD_3OD) signals (δ_H 3.31; δ_C 49.0) or dimethyl sulfoxide-d_6 (DMSO–d_6) signals (δ_H 2.50; δ_C 39.5) as internal standards. Coupling constants (J) are reported in Hertz (Hz) and the multiplicity are represented as singlet (s), broad singlet (br s), doublet (d), triplet (t), doublet of quartet (dq), doublet of doublets (dd), doublet of triplets (dt), doublet of doublet of doublets (ddd) and multiplet (m). All NMR spectra were processed using Mnova software *ver.* 14 (Mestrelab Research, SL, Spain). The complete spectral assignments were achieved using combinations of 1D (^{1}H, ^{13}C-APT or DEPTQ) and 2D (COSY, HSQC, HMBC, TOCSY, NOESY and ROESY) NMR. When available, the spectral assignments were validated with literature. These included a report by Gleńsk et al. for **S5** [9], Camargo et al. for **S20** [10], Zhang et al. for **S26** [11], Xie et al. for **S8, S14, S21** and **S23** [12], Thuy et al. for **S7** [13], Davis et al. for **S1, S3, S6** and **S10** [14], Ragab et al. for **S6, S9** and **S10** [15], Liu et al. for **S13** and **S17** [16] as well as Katagiri et al. for **S24** [17].

The MS and UV data for all isolated compounds was acquired on an Acquity UHPLC system coupled with a Micromass LCT Premier Time-of-Flight mass spectrometer coupled to a photodiode array detector (Waters, Milford, USA). The short gradient method (Method A) has been described in previous work [7]. In brief, the separation was performed on an Acquity C18 BEH column (WATERS, MA, USA) with 2.1 mm ID × 100 mm length and 1.7 µm particle size. The mobile phase comprised 0.1 % formic acid in water (A) and 0.1 % formic acid in acetonitrile (B) and this was delivered at 0.75 mL/min flowrate as follows: 5–20 % B from 0 to 4 min; 20–95 % B from 4 to 7 min; 95 % B isocratic from 7 to 8 min; 95–5 % B from 8 to 8.5 min and equilibrated at 5 % B from 8.5 to 10 min. Given that the flow rate exceeded the typical rate of 0.3 mL/min for 100 mm column, we opted for a column temperature of 60 °C to lower the column pressure. The long gradient (Method B) was optimized using the same mobile phase and column conditions as the short gradient, except the column length was 150 mm. The gradient was delivered at 0.46 mL/min and consisted of 4 % B isocratic for 2 min, 4–10 % B from 2 to 16 min (Curve 7-concave change), 10–15 % B from 16 to 27 min, 15–95 % B from 27 to 37 min, isocratic at 95 % B from 37 to 44 min, returned to 4 % B from 44 to 45 min and equilibration step for 5 min.

Limitations

Constraints on measurement time hindered the acquisition of carbon-13 NMR spectra for all compounds. In these instances, complete carbon assignments were unattainable, and the chemical shift values were determined using HSQC and HMBC experiments in place of the carbon-13 NMR data that was unavailable.

Ethics Statement

The authors have read and followed the ethical requirements for publication in Data in Brief. This research does not involve human subjects, animal experiments, or any data collected from social media platforms.

Declaration of Generative AI in Scientific Writing

During the preparation of this work, the authors used ChatGPT in order to improve readability and language. After using this tool/service, the authors reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

Data Availability

Supplementary files for "Chemical characterizations of isomeric flavonoid glycosides and other constituents from *Ficus deltoidea* Jack" (Original data) (Mendeley Data).

CRediT Author Statement

Adlin Afzan: Conceptualization, Methodology, Formal analysis, Investigation, Data curation, Writing – original draft, Visualization, Project administration; **Laurence Marcourt:** Formal analysis, Investigation, Supervision, Data curation, Writing – review & editing; **Hidayatul Atiqah Abd Karim:** Conceptualization, Methodology, Investigation, Project administration; **Noraini Kasim:** Methodology, Investigation, Project administration; **Emerson Ferreira Queiroz:** Conceptualization, Methodology; **Che Puteh Osman:** Formal analysis, Supervision; **Nor Hadiani Ismail:** Conceptualization, Resources, Supervision, Funding acquisition; **Jean-Luc Wolfender:** Conceptualization, Resources, Writing – review & editing, Supervision.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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