Data Article

LC-MS Data set on the Malayan Deer (Cervus timorensis) Antler Velvet and its antibiofilm activity against Candida species

LC-MS Data set on the Malayan Deer (Cervus timorensis) Antler Velvet and its antibiofilm properties against Candida species.

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A B S T R A C T

Deer antler velvet (DAV) has been traditionally used in Chinese medicine, including treatment on toothache [1]. Due to its rapid and regenerative capacity, deer antlers were proposed to be the good model for bone remodelling in mammals [2]. The data presented in this work is on the liquid chromatography and mass spectrometry (LC-MS) profile and bioactive potential of Malayan deer antler velvet (DAV) on different Candida species that has clinical importance.

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Aqueous extraction of DAV samples was subjected to Liquid chromatography quadrupole time of flight mass spectrometry (LC-QTOF-MS) profiling. Reverse phase (RP) separation was used due to the process extraction using water as a solvent to separate polar compound. The data was interpreted using Profile Analysis 2.1V. The DAV samples were also tested for the effect on the biofilm formation of seven Candida species in a 96 well plate [3]. The biofilms were developed for 72 h in aerobic environment. Following that, the biofilms biomass was determined using crystal violet assay.

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Specifications Table

| Subject | Type of data | How data were acquired | Data format | Parameters for data collection | Description of data collection | Data source location | Data accessibility | Related research article |
|---------|--------------|-------------------------|-------------|-------------------------------|-------------------------------|---------------------|----------------------|--------------------------|
| Specific subject area | Biology | Dentistry, Oral Surgery and Medicine | Data on biofilm was acquired by incubation of Candida species with DAV extract to produce biofilm, stained with crystal violet and assessed using Microplate reader (Tecan NanoQuant Infinite M200, CA). Secondary metabolites dataset was acquired from the LC–MS-Quadrupled time of flight mass spectrometer online database (Vion Ion Mobility QTOF MS, Waters, USA) using both positive and negative ionization mode and were assessed using Profile Analysis Software 2.1 (Bruker, Germany). Analysed data for Candida species biofilm and analysed data for LCMS identified compounds of DAV are presented within this article. Summary reports for LC-MS are provided in .pdf and Raw data for LCMS identified compounds are provided in. clx. Both data can be accessible at Mendeley repository. | Water extract was used for LC-MS analysis and Reversed phase column was used to separate polar compound. Mass spectrometer conditions: desolvation temperature (550 °C); desolvation gas (600 L/h); Source type (ESI); source temperature (120 °C); cone gas (50 L/h); Capillary voltage (2.50 kV); MS mode (High definition); Collision energy interval (4.00–40.00 eV). The Auto MS/MS mode was used to confirm the fragment ions. The liquid chromatography mass spectrometry (LC-MS) acquisition data were processed using Profile Analysis software (2.1) to extract the mass spectral features from samples raw data. Mono-species Candida biofilm reduction test was conducted in 96-well plate with nine replicates for each species (with and without DAV) cultured in RPMI-1640 media at 37 °C for 72 h. The media was replenished aseptically every 24 h at the same incubation condition. | DAV materials were diluted with water. Sample was analyzed with LC-ESI-QTOF-MS system and processed using Profile Analysis software (version 2.1) Candida biofilms were grown in 96-well plate and was performed at nine replicates for each Candida species. The well with crystal violet-stained biofilms attached on the surface were read using an absorbance microplate reader at 620 nm (Tecan NanoQuant Infinite M200, CA) | International Islamic University Malaysia (IIUM), Kuantan Pahang Malaysia (Latitude: 3.8425; Longitude: 103.2999) | Complete dataset can be accessible at Mendeley Repository 10.17632/mc7z2j7g4r.2 | Arzmi, M. H., Cirillo, N., Lenzo, J. C., Catmull, D. V., O’Brien-Simpson, N., Reynolds, E. C., Dashper, S., & McCullough, M. (2019). Monospecies and polymicrobial biofilms differentially regulate the phenotype of genotype-specific oral cancer cells. Carcinogenesis, 40(1), 184–193. 10.1093/carcin/bgy137 |
1. Data Description

Acquisition of data is possible from Liquid chromatography–mass spectrometry (LC–MS) analysis on Malayan deer antler velvet (DAV) water extract. Both Positive and negative ionization mode was analyzed. Raw OD values represents microbial biofilm density of different Candida species with or without DAV is presented in Table 1. LC-MS raw data was further scrutinized to identify different chemical compounds in DAV and its MS peak intensities is presented in Table 2.

2. Experimental Design, Materials and Methods

2.1. DAV collection and sample preparation

Male Malayan deer antler was collected from local company; D’Paradise Deer Valley and Exotic Farm Sdn. Bhd. Dried samples was powdered using variable speed laboratory blender (Waring®, USA). 10 g of powdered sample was soaked in 450 ml double distilled deionized water with periodic shaking for 30 min intervals for 8 h; then the mixture will be allowed to settle for 16 h. After filtration, the residue was washed with a small portion of water and followed by freeze-drying (Martin Christ, Germany).

2.2. Mono biofilm reduction test

A total of 7 Candida species (C. glabrata ATCC 90030, C. tropicalis ATCC 13803, C. krusei ATCC 14243, C. parapsilosis ATCC 22019, C. lusitaniae ATCC 64125, C. dubliniensis ATCC MYA-2975, C. albicans ATCC MYA-4901) were procured from American Type Culture Collection (ATCC). While ALC2 (isolate from HIV positive patient) and ALC3 (isolate from Oral cancer patient) representing Candida albicans isolates from Melbourne dental school, University of Melbourne, Australia were tested for biofilm formation with or without DAV extract of known concentration in RPMI-1640 media following the previously established procedure [3,4]. Nine replicates for each species were accessed in 96 well-plate. Samples were incubated at 37 °C for 72 h and the fungal density was determined using Microplate reader (Tecan NanoQuant Infinite M200, CA) at 620 nm wavelength (Table 1). All chemicals and reagents used were of analytical grade procured from Thermo Scientific.

2.3. LC-MS analysis

The DAV solution was prepared for LC–MS analysis by diluting the extract in aqueous solution. Samples were flow through on Column ACQUITY UPLC-BEH C18, 2.1 mm x 100 mm (Waters, USA) at the rate of 0.5 ml/min. The mobile phase was prepared using the binary solvent manager with solvent A and B. Briefly, the gradients elution were 99% A and 1% B (0.00 min) 99% A and 1% B (0.00–0.50 min), 65% A and 35% B (0.50–16.00 min), 0% A and 100% B (16.00–18.00 min), 99% A and 1% B (18.00–20.00 min), with the flow rate of 0.6 mL/min. The solvent A is made of 0.1% formic acid (Sigma Aldrich, Germany) plus water (Milli-Q grade, v/v). However, solvent B was acetonitrile at a seal wash time and highest-pressure limit of 5 min and 1800 psi, respectively. Positive and negative ionization mode was performed at the following setting: capillary voltage: 2.50 kV, nebulizer pressure: 1.2 bar, drying gas: 8 l/min at 200 °C, mass range: 50–1000 m/z [5]. The sample was analyzed using LC-ESI-QTOF-MS (Vion Ion Mobility QTOF MS, Waters, USA) and processed using Profile Analysis 2.1 (Bruker, Germany).
Table 1
Raw OD values of the different *Candida* species in RPMI 1640. OD represent *Candida* biofilm density and was recorded at 620 nm wavelength in Microplate reader.

| Species | Replicate 1 | Replicate 2 | Replicate 3 | Replicate 4 | Replicate 5 | Replicate 6 | Replicate 7 | Replicate 8 | Replicate 9 | Mean | SD |
|---------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|------|----|
| CG      | MONO        | 0.5872      | 0.4024      | 0.7382      | 0.5863      | 0.4023      | 0.7337      | 0.584       | 0.402       | 0.7308 | 0.574 | 0.144 |
|         | POLY DAV    | 0.3748      | 0.2548      | 0.2572      | 0.3723      | 0.2557      | 0.255       | 0.374       | 0.2549      | 0.2555 | 0.295 | 0.059 |
| CT      | MONO        | 0.4536      | 0.4284      | 0.4673      | 0.4546      | 0.4289      | 0.4689      | 0.4582      | 0.4328      | 0.4754 | 0.452 | 0.018 |
|         | POLY DAV    | 0.3047      | 0.1857      | 0.248       | 0.3033      | 0.1853      | 0.2475      | 0.3058      | 0.187       | 0.2495 | 0.246 | 0.051 |
| CK      | MONO        | 0.2597      | 0.459       | 0.639       | 0.2589      | 0.4571      | 0.634       | 0.2582      | 0.4541      | 0.6312 | 0.450 | 0.163 |
|         | POLY DAV    | 0.2725      | 0.2468      | 0.4187      | 0.2707      | 0.2374      | 0.4148      | 0.2721      | 0.2368      | 0.4169 | 0.310 | 0.082 |
| CP      | MONO        | 0.4112      | 0.3615      | 0.8658      | 0.413       | 0.3621      | 0.866       | 0.416       | 0.3645      | 0.8749 | 0.548 | 0.241 |
|         | POLY DAV    | 0.5348      | 0.5738      | 0.4972      | 0.5371      | 0.5764      | 0.4996      | 0.5404      | 0.5785      | 0.5002 | 0.538 | 0.034 |
| CL      | MONO        | 0.4756      | 0.5582      | 0.4184      | 0.472       | 0.5508      | 0.4126      | 0.4716      | 0.5499      | 0.4111 | 0.480 | 0.060 |
|         | POLY DAV    | 0.3807      | 0.3231      | 0.3052      | 0.3786      | 0.3214      | 0.3045      | 0.3801      | 0.3219      | 0.3056 | 0.336 | 0.034 |
| CD      | MONO        | 0.5983      | 0.4833      | 0.3347      | 0.6014      | 0.4845      | 0.3358      | 0.6109      | 0.4885      | 0.3393 | 0.475 | 0.116 |
|         | POLY DAV    | 0.4949      | 0.2333      | 0.3469      | 0.4926      | 0.2326      | 0.3453      | 0.4961      | 0.2343      | 0.3478 | 0.358 | 0.113 |
| ATCC    | MONO        | 0.1498      | 0.1121      | 0.1379      | 0.1489      | 0.1112      | 0.1373      | 0.1489      | 0.1112      | 0.1371 | 0.133 | 0.017 |
|         | POLY DAV    | 0.303       | 0.434       | 0.4623      | 0.301       | 0.4342      | 0.4595      | 0.302       | 0.4348      | 0.4615 | 0.399 | 0.074 |
| ALC2    | MONO        | 0.1064      | 0.2382      | 0.1975      | 0.1064      | 0.239       | 0.1974      | 0.1069      | 0.2429      | 0.199   | 0.182 | 0.059 |
|         | POLY DAV    | 0.2903      | 0.3473      | 0.2608      | 0.29        | 0.3472      | 0.2603      | 0.2925      | 0.35        | 0.2618 | 0.300 | 0.038 |
| ALC3    | MONO        | 0.4025      | 0.3486      | 0.6585      | 0.3935      | 0.3455      | 0.6491      | 0.3985      | 0.3461      | 0.6473 | 0.466 | 0.141 |
|         | POLY DAV    | 0.279       | 0.2667      | 0.2723      | 0.2771      | 0.2656      | 0.2706      | 0.2778      | 0.2673      | 0.2714 | 0.272 | 0.005 |

*Note*: Mono represents *Candida* monoculture while poly represents *Candida* cultured with DAV supplement. CG: *C. glabrata*, CT: *C. tropicalis*, CK: *C. krusei*, CP: *C. parasilopsis*, CL: *C. lusitaniae*, CD: *C. dubliniensis*, ATCC: *C. albicans* MYA-4901, ALC2: *C. albicans* HIV isolates, ALC3: *C. albicans* oral cancer isolates.
**Table 2**
Chemical compounds identified in DAV and its MS peak intensities of the LC-QTOF-MS.

| No. | Component name                                      | Formula     | Identification status | Observed neutral mass (Da) | Observed m/z | Mass error (mDa) | Mass error (ppm) | Observed RT (min) | Response | Adducts | Observed CCS (Å²) | Total Fragments Found |
|-----|-----------------------------------------------------|-------------|-----------------------|----------------------------|--------------|------------------|------------------|-------------------|----------|---------|------------------|-----------------------|
| 1   | Benzopyran derivative                              | C32H30O7   | Identified            | 526.2009                   | 525.1936     | 1.7              | 3.3              | 1.11              | 2075     | -H      | 213.32           | 0                     |
| 2   | Meliadanoside A                                    | C16H24O10  | Identified            | 376.1359                   | 421.1341     | -1.0             | -2.4             | 1.22              | 2374     | +HCOO   | 195.83           | 0                     |
| 3   | Octahydrocurcumin                                  | C21H28O6   | Identified            | 376.1859                   | 421.1841     | -2.6             | -6.3             | 2.12              | 1304     | +HCOO   | 198.21           | 0                     |
| 4   | 3’,4’-Dimethoxy-isoflavan-7,2’-di-O-β-D-glucoside  | C29H38O15  | Identified            | 626.2216                   | 671.2198     | 0.5              | 0.8              | 2.38              | 1090     | +HCOO   | 254.40           | 0                     |
| 5   | 4’-Hydroxyacetophenone                             | C8H8O2     | Identified            | 136.0521                   | 181.0503     | -0.3             | -1.8             | 2.87              | 1848     | +HCOO_,-H_     | 144.29           | 1                     |
| 6   | Methyl-β-orsellinate                               | C9H10O4    | Identified            | 182.0576                   | 181.0503     | -0.3             | -1.8             | 2.87              | 1848     | -H      | 144.29           | 3                     |
| 7   | Didemethoxycurcumin                                | C19H16O4   | Identified            | 308.1024                   | 353.1006     | -2.5             | -7.0             | 5.08              | 1230     | +HCOO   | 171.99           | 0                     |
| 8   | Moracin E                                          | C19H16O4   | Identified            | 308.1024                   | 353.1006     | -2.5             | -7.0             | 5.08              | 1230     | +HCOO   | 171.99           | 0                     |
| 9   | Moracin E                                          | C19H16O4   | Identified            | 308.1024                   | 353.1006     | -2.5             | -6.9             | 5.51              | 4981     | +HCOO   | 239.37           | 1                     |
| 10  | Didemethoxycurcumin                                | C19H16O4   | Identified            | 308.1024                   | 353.1006     | -2.5             | -6.9             | 5.51              | 17118    | +HCOO   | 196.06           | 3                     |
| 11  | Apocynin                                           | C9H10O3    | Identified            | 166.0627                   | 165.0554     | -0.3             | -1.9             | 5.51              | 1099     | -H      | 201.32           | 2                     |
| 12  | 2’-Hydroxy-3’,4’-dimethoxy-isoflavan-7-O-β-D-glucoside | C23H28O10 | Identified            | 464.1635                   | 509.1617     | -4.7             | -9.3             | 16.49             | 1066     | +HCOO   | 224.36           | 0                     |
| 13  | Feralolide                                          | C18H16O7   | Identified            | 344.0886                   | 343.0813     | -1.0             | -2.9             | 16.69             | 2460     | -H      | 179.09           | 1                     |
| 14  | (3R,4R)-3,4-trans-7,2’-Dihydroxy-4’-methoxy-4’-[3R]-2’,7’-dihydroxy-4’-methoxy-isoflavan-5’-yl-isoflavan | C32H3O8 | Identified            | 542.1936                   | 587.1918     | -0.5             | -0.9             | 18.52             | 1177     | +HCOO_,-H_     | 242.15           | 1                     |

*(continued on next page)*
| No. | Component name                                                                 | Formula         | Identification status | Observed neutral mass (Da) | Observed m/z | Mass error (mDa) | Mass error (ppm) | Observed RT (min) | Response | Adducts | Observed CCS (Å²) | Total Fragments Found |
|-----|--------------------------------------------------------------------------------|-----------------|-----------------------|---------------------------|--------------|-----------------|-----------------|-----------------|----------|---------|-------------------|-----------------------|
| 15  | Dichotomitin                                                                   | C18H14O8        | Identified            | 358.0708                  | 381.06      | 2               | 5.1             | 0.81            | 2004     | +Na, +K | 183.78           | 1                     |
| 16  | 6-Aldehydo-7-methoxy-isophiopogonone A                                         | C20H16O7        | Identified            | 368.0919                  | 391.0811    | 2.3             | 5.9             | 0.97            | 2090     | +Na     | 181.97           | 2                     |
| 17  | Dichotomitin                                                                   | C18H14O8        | Identified            | 358.071                   | 381.0603    | 2.2             | 5.7             | 0.98            | 1279     | +Na     | 184.29           | 0                     |
| 18  | Bavachinin                                                                      | C21H22O4        | Identified            | 338.1506                  | 361.1398    | -1.2            | -3.3            | 1.81            | 1161     | +Na     | 181.66           | 0                     |
| 19  | Mirificin                                                                       | C26H28O13       | Identified            | 548.1485                  | 549.1557    | -0.45           | -8.3            | 2.02            | 2036     | +H, +Na | 258.43           | 0                     |
| 20  | Naringenin-4’-glucoside-7-rutinoside                                           | C33H42O19       | Identified            | 742.1467                  | 765.1286    | -2.7            | -3.5            | 2.02            | 1049     | +Na     | 225.46           | 1                     |
| 21  | 5-Hydroxyauranetin                                                              | C20H20O8        | Identified            | 388.1159                  | 395.1313    | 0.1             | 0.2             | 2.54            | 1504     | +Li     | 194.15           | 0                     |
| 22  | (-)-Epiafzelechin-3-O-(6''-O-acetyl)-β-D-allosepyranoside                       | C23H20O10       | Identified            | 478.1467                  | 479.1539    | -0.9            | -1.8            | 5.07            | 3463     | +H      | 225.46           | 1                     |
| 23  | Silymonin                                                                       | C25H22O9        | Identified            | 466.122                    | 473.1375    | -4.3            | -9.2            | 5.07            | 2073     | +Li     | 224.21           | 0                     |
| 24  | Daidzin_1                                                                       | C21H20O9        | Identified            | 416.1114                  | 439.1006    | 0.7             | 1.6             | 5.33            | 1112     | +Na     | 196.33           | 0                     |
| 25  | 3,4,2’-Trihydroxychalcone-4’-O-beta-D-glucopyranoside                          | C21H22O10       | Identified            | 434.1225                  | 457.1118    | 1.2             | 2.7             | 5.33            | 1272     | +Na     | 199.28           | 0                     |
| 26  | Pinnatifinoside B                                                              | C23H20O10       | Identified            | 456.1045                  | 457.1118    | -1.2            | -2.5            | 5.33            | 1272     | +H      | 199.28           | 1                     |
| 27  | Bavachalcone                                                                   | C20H20O4        | Identified            | 324.1343                  | 347.1235    | -1.9             | -5.5            | 6.01            | 4354     | +Na     | 182.22           | 0                     |
| 28  | Corylifolinin                                                                  | C20H20O4        | Identified            | 324.1343                  | 347.1235    | -1.9             | -5.5            | 6.01            | 4354     | +Na     | 182.22           | 0                     |
| 29  | Hibiscetin-3-O-glucoside                                                        | C21H20O14       | Identified            | 496.0851                  | 497.0923    | -0.2            | -0.5            | 7.47            | 6132     | +H      | 217.13           | 0                     |
| 30  | Norcimifugin                                                                   | C15H16O6        | Identified            | 292.094                   | 299.1094    | -0.7            | -2.4            | 11.86           | 1429     | +Li     | 167.93           | 0                     |
| 31  | 5-Hydroxy-7,8-dimethoxy-6-methyl-3’-(3’,4’-dihydroxybenzyl) chroman-4-one       | C19H20O7        | Identified            | 360.1207                  | 367.1362    | -0.2            | -0.5            | 14.98           | 1037     | +Li     | 177.93           | 0                     |

(continued on next page)
| No. | Component name                                         | Formula      | Identification status | Observed neutral mass (Da) | Observed m/z          | Mass error (mDa) | Mass error (ppm) | Observed RT (min) | Response | Adducts       | Observed CCS (Å²) | Total Fragments Found |
|-----|--------------------------------------------------------|--------------|-----------------------|-----------------------------|-----------------------|------------------|------------------|-------------------|----------|---------------|------------------|-----------------------|
| 32  | Sophoranodichromane D                                 | C25H28O5     | Identified            | 408.1961                    | 415.2115              | 2.4              | 5.7              | 16.67             | 12569    | +Li, +H       | 205.99           | 17                    |
| 33  | (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane        | C18H18O5     | Identified            | 314.1151                    | 337.1043              | -0.3             | -0.9             | 16.7              | 100608   | +Na, +Li     | 179.5            | 5                     |
| 34  | Ophiopogonanone B                                     | C18H18O5     | Identified            | 314.1151                    | 337.1043              | -0.3             | -0.9             | 16.7              | 100608   | +Na, +Li     | 179.5            | 6                     |
| 35  | Kuwanon S                                             | C25H26O5     | Identified            | 406.1777                    | 407.185               | -0.3             | -0.8             | 16.71             | 1296     | +H, +Li, +Na | 209.9            | 42                    |
| 36  | Neokurariminol                                         | C27H34O7     | Identified            | 470.2297                    | 471.237               | -0.1             | -0.2             | 16.72             | 1267     | +H           | 219.52           | 31                    |
| 37  | Glabrol                                               | C25H28O4     | Identified            | 392.1994                    | 393.2067              | 0.0              | 0.6              | 16.72             | 2413     | +H, +Li      | 195.67           | 34                    |
| 38  | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethylchroman-4-one | C18H18O5 | Identified            | 314.1147                    | 337.1039              | -0.8             | -2.3             | 16.95             | 10015    | +Na          | 178.84           | 0                     |
| 39  | (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane        | C18H18O5     | Identified            | 314.1151                    | 337.1043              | -0.4             | -1.2             | 17.28             | 15479    | +Na          | 179.31           | 0                     |
| 40  | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethylchroman-4-one | C18H18O5 | Identified            | 314.1151                    | 337.1043              | -0.4             | -1.2             | 17.28             | 15479    | +Na          | 179.31           | 0                     |
| 41  | (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane        | C18H18O5     | Identified            | 314.1153                    | 337.1045              | -0.1             | -0.3             | 18.03             | 12092    | +Na          | 179.64           | 0                     |
| 42  | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethylchroman-4-one | C18H18O5 | Identified            | 314.1153                    | 337.1045              | -0.1             | -0.3             | 18.03             | 12092    | +Na          | 179.64           | 0                     |
| 43  | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethylchroman-4-one | C18H18O5 | Identified            | 314.1173                    | 321.1327              | 1.8              | 5.7              | 18.46             | 1800     | +Li          | 181.35           | 1                     |
| 44  | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethylchroman-4-one | C18H18O5 | Identified            | 314.1154                    | 321.1309              | 0                 | 0                 | 18.6              | 1458     | +Li, +H      | 178.4            | 0                     |
Ethics Statement

This research work does not require ethical approval.

CRediT Author Statement

Arzmi M.H: Conceptualization, Methodology; John B.A.: Data interpretation, Writing - manuscript; Rismayuddin N.A.R, Kenali N.M: Laboratory analysis; Arzmi M.H: Supervision; Darnis D.S: Validation; Arzmi M.H, John B.A., Rismayuddin N.A.R: Writing - Reviewing and Editing. All authors equally contributed to this manuscript.

Declaration of Competing Interest

Authors have no competing interest.

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