We obtained data regarding the metabolites from flowers, the skin pulp, green beans, and peaberry green beans of the robusta coffee plant (*Coffea canephora*). The beans were processed using a wet-hulled method. The volatile compounds from the flowers were extracted using a solid-phase microextraction. Secondary metabolites from the skin pulp, green beans, and peaberry green beans were extracted by a maceration method using methanol as a solvent. The separation and identification of metabolites were conducted using gas chromatography-mass spectrometry. The flower's volatile compounds were identified by matching the generated spectra with the NIST14 library as a reference, whereas the metabolites in the skin pulp, green beans, and peaberry green beans were identified using the WILLEY09TH library as a reference. The identified volatile compounds in flowers have been listed in Table 1, and the identified skin pulp, green bean, and peaberry green bean metabolite compounds have been listed in Table 2.

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1. Data description

These raw data include information on the volatile compounds of the robusta coffee flowers and the profiles on the secondary metabolites of the skin pulp, green beans, and peaberry green beans of the robusta coffee. The raw data have been provided in a Microsoft Excel Worksheet (Tables 1 and 2) and have been presented with retention times, identified volatile compounds, and peak areas.

2. Experimental design, materials, and methods

a. Preparation and analysis of the flower samples

All samples were collected from a low land robusta coffee orchard (at 680 m above sea level). Only fresh anthesis flowers were picked for analysis. Three sets of samples (10 fresh anthesis of the robusta coffee flowers, approximately 1.5 g) were placed in 22-mL clear glass bottles for SPME with PTFE/Silicon septa (Supelco Co., Bellefonte, PA, USA). After 24 h, the flowers were extracted and identified by
Table 1
Retention times, identified compounds, and relative peak areas (%) from the GC chromatogram of Robusta coffee flower.

| Retention Time (min.) (n = 3) | Compounds | Relative Peak Area (%) (n = 3) |
|-------------------------------|-----------|-------------------------------|
| 1.794                         | Ethanol   | 3.62 n.d 3.3                 |
| 4.309                         | Cyclobutylcarboxylic acid | n.d 0.34 n.d                |
| 6.450                         | Butanoic acid, 3-methyl, ethyl ester | 0.17 n.d 0.27               |
| 6.515                         | 1H-Indole, 5-methyl-2-phenyl- | n.d 0.05 n.d                |
| 7.009                         | 1-Butanol | n.d 0.04 n.d                 |
| 7.693                         | Carboxylic acid, methyl-, ethyl ester | n.d n.d 0.02               |
| 8.073                         | 2-Heptanol | n.d n.d 0.16                 |
| 8.076                         | 2-Pentadecanol | 0.11 n.d n.d                |
| 8.079                         | 4-Methyl-2-hexanol | n.d 0.04 n.d                |
| 10.303                        | Benzaldehyde | 0.23 0.13 1.0               |
| 11.308                        | β-Myrcene | 0.67 0.73 0.54               |
| 12.574                        | α-Limonene | 0.15 0.18 0.12               |
| 16.754                        | Benzyl alcohol | 4.92 3.23 3.09            |
| 14.073                        | Ethyl 2-(5-methyl-5-vinyltetrahydrofur-2-yl)propan-2-yl carbonate | 0.69 0.53 n.d        |
| 14.810                        | trans-Linalool oxide (furanoid) | n.d 0.60 0.48            |
| 15.440                        | Linalool | 2.70 1.15 1.62               |
| 15.642                        | Phenylethyl Alcohol | 22.29 27.03 22.23           |
| 15.993                        | 2,4,6-Octatriene, 2,6-dimethyl-, (E)- | 0.13 0.13 0.10            |
| 16.754                        | Benzyl nitrile | 14.56 0.04 n.d       |
| 17.135                        | 3,6-Dimethyl-2,3,3a,4,5,7a-hexahydrobenezofuran | n.d n.d 0.05      |
| 17.343                        | Benzoic acid, methyl ester | 1.50 0.88 1.37        |
| 17.498                        | Deltacyclene | 2.03 n.d n.d              |
| 17.509                        | 5H-1-Pyrindine | n.d 1.74 1.54             |
| 17.670                        | Indole | 1.50 1.33 1.17               |
| 17.896                        | α-Terpineol | 0.02 0.02 0.01          |
| 18.009                        | Methyl salicylate | n.d 0.29 n.d          |
| 18.027                        | Dodecane | 0.19 n.d 0.18               |
| 18.687                        | 6-Octen-1-ol, 7-methyl-3-methylene | 0.03 0.03 0.02       |
| 19.020                        | 2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- | 1.96 2.62 1.84        |
| 19.127                        | 3,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- | 0.20 0.10 0.19       |
| 19.317                        | 2,6-Octadienal, 3,7-dimethyl-, (Z) Citral | 0.15 0.22 0.12 |
| 19.418                        | Benzenacetic acid, ethyl ester | 0.24 n.d 0.38        |
| 19.781                        | Geraniol | 1.76 2.07 1.59               |
| 20.155                        | 2,6-Octadienal, 3,7-dimethyl-, (E) | 0.29 n.d 0.31        |
| 20.173                        | 2,6-Octadienal, 3,7-dimethyl- | n.d 0.38 n.d       |
| 20.322                        | 2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)- | 0.02 n.d n.d        |
| 20.405                        | 2,6-Octadienoic acid, 3,7-dimethyl-, methyl ester | n.d n.d 0.01       |
| 20.548                        | 5-Tridecene, (E)- | 0.04 n.d n.d         |
| 20.554                        | 6-Tridecene, (E)- | n.d 0.04 0.03            |
| 21.018                        | Tridecane | 5.50 5.01 5.46               |
| 21.291                        | Indole | 0.02 0.01 0.02               |
| 21.582                        | trans-Geranic acid methyl ester | 0.10 n.d 0.11       |
| 22.153                        | Methyl anthranilate | 0.76 0.65 0.58       |
| 22.278                        | Benzenepropanoic acid, ethyl ester | 0.14 n.d 0.11       |
| 23.087                        | 5-Tridecane, (E)- | n.d 0.02 n.d         |
| 23.087                        | 3-Tridecane, (Z)- | n.d n.d 0.01          |
| 23.081                        | 7-Tridecane, (Z)- | 0.01 0.00 n.d        |
| 23.331                        | 3-Tridecane, (E)- | 0.03 0.03 0.03        |
| 23.551                        | Tetradecane | 0.41 0.38 0.43          |
| 23.872                        | Benzoic acid, 2-(methylamino)-, methyl ester | 0.01 0.01 0.01          |
| 24.175                        | Caryophyllene | n.d 0.00 n.d         |

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an SPME connected with a GC-MS (GC: 7890A, MS: 5975C, Agilent) following the procedure reported by Syamsudin et al. [1]. Coffee flowers in the SPME bottles were extracted at 40 °C for 45 min. The extract was injected into a gas chromatograph at 250 °C for 5 min using a splitless mode. The oven temperature was initially set to 50 °C and held for 5 min. Then, the temperature was increased to 150 °C (5 °C/min for 2 min) and then to 250 °C (5 °C/min for 5 min). An HP-5MS (30 m × 250 μm × 0.25 μm) column was used to separate the volatile compounds with helium as the carrier gas injected at 0.8 mL/min. The flower volatile compounds were identified by matching the generated spectra with the spectra in the NIST14 library as references.

| Retention Time (min.) | Compounds | Relative Peak Area (%) |
|-----------------------|-----------|------------------------|
| (n = 3)               |           | (n = 3)                |
| 25.754 25.751 25.750 | 1-Tridecene | 4.56 4.36 4.60        |
| 25.858               | n-Tridecan-1-ol | 1.07 n.d n.d       |
| 25.858 25.857        | Cyclopentadecane | n.d 1.00 1.09      |
| 26.583 26.583 26.607 | Pentadecane  | 18.68 17.12 19.24    |
| 28.064               | Succinic acid, di(3-methylbut-3-enyl) ester | 0.00 n.d n.d |
| 28.069               | Succinic acid, hex-4-yn-3-yl 3-methylbut-3-en-1-yl ester | n.d n.d 0.00 |
| 28.064               | Supraene  | n.d 0.00 n.d          |
| 28.301               | Benzene, [2,2-dimethylcyclopropyl]methyl]- | 0.00 n.d n.d |
| 28.593 28.593 (3E,7E)-4,8,12-Trimethyltrideca-1,3,7,11-tetraene | 0.07 n.d 0.09 |
| 28.593               | Squalene | n.d 0.00 n.d          |
| 29.134 29.128 29.134 | Hexadecane | 0.07 0.05 0.06      |
| 29.532               | Pentadecanal | 0.03 n.d n.d         |
| 31.072 31.072 31.072 | 6,9-Heptadecadiene | 0.27 0.05 0.28 |
| 31.209               | 1,4-Cyclooctadiene, (Z,Z)- | 0.17 n.d 0.16 |
| 31.209               | Tricyclo[4.2.1.1(2,5)]decan-3-ol | n.d 0.18 n.d |
| 31.411 31.399 31.411 | 8-Heptadecane | 3.51 2.86 3.34 |
| 31.893 31.881 31.893 | Heptadecane | 1.21 0.95 1.22     |
| 32.089               | Pentadecfluorooctanoic acid, dodecyl ester | n.d 0.01 n.d |
| 32.095 32.243        | Cyclopentane, pentyl- | 0.01 n.d 0.00      |
| 32.244               | 3,6-Octadecen-3,7-dimethyl- | 0.01 n.d n.d |
| 32.244               | Cyclohexene, 4-methyl- | n.d 0.01 n.d |
| 32.434               | 3,4-Octadecen-7,7-methyl- | n.d 0.01 n.d |
| 32.440               | Cyclobaldecene, (E)- | 0.01 n.d n.d |
| 32.440               | E,E-10,12-Hexadecadien | n.d n.d 0.00 |
| 33.260 33.260 33.266 | ZZ-10,12-Hexadecadien | 0.00 0.00 0.00 |
| 34.241 34.247        | Octadecane | n.d 0.03 0.03 |
| 34.247               | Dodecane, 2,6,11-trimethyl- | 0.03 n.d n.d |
| 34.396 34.396        | cis-11-Hexadecenal | 0.00 0.01 n.d |
| 34.669 34.670        | Tetradecanol, (Z)- | 0.16 0.18 n.d |
| 34.669               | Hexadecanol | n.d n.d 0.17        |
| 34.872               | Isopropyl myristate | 0.00 n.d n.d |
| 35.692               | 9-Tetradecen-1-ol, acetate, (Z)- | n.d n.d 0.01 |
| 35.698               | 1,9-Tetradecadiene | 0.01 n.d n.d |
| 35.787               | Z-1,6-Tridecadiene | 0.01 n.d n.d |
| 35.787 35.787        | Cyclooctadecene | 0.01 n.d 0.01 |
| 35.924 35.924 35.924 | 9,12,15-Octadecatrien | 0.01 n.d n.d |
| 36.019 36.138        | 9-Nonadecene | 0.02 0.00 n.d |
| 36.019 36.019        | Z-5-Nonadecene | n.d 0.02 0.02 |
| 36.120               | Cyclotetradecane | n.d n.d 0.02 |
| 36.126               | 1-Nonadecene | 0.02 n.d n.d |
| 36.501 36.501 36.507 | Nonadecane | 0.47 0.46 0.55 |
| 38.546 38.540        | Eicosane | 0.01 0.01 0.01 |
| 40.479 40.479 40.479 | Heneicosane | 0.02 0.02 0.06 |
| 43.594 43.600 43.594 | 9-Tricosene, (Z)- | 0.00 0.00 0.00 |
Table 2
Retention times, identified compounds, and relative peak areas (%) in the GC chromatogram from skin-pulp, pea berry skin-pulp, green bean and pea berry green bean.

| Retention Time (min.) (n = 2) | Compounds | Relative Peak Area (%) (n = 2) |
|-------------------------------|-----------|-------------------------------|
| Skin-Pulp                    | Pea berry skin-pulp | Green bean | Pea berry green bean |
| 1.919                        | 1.989     | 1.728 | 2.032 | 2.005 | 1.935 | 2.162 | 1.905 |
| 2.330                        | 2.345     | 2.379 | 2.387 | 2.531 | 2.787 | 2.842 | 2.917 |
| 3.119                        | 3.120     | 3.471 | 3.441 | 4.771 | 7.282 | 5.080 | 5.135 |
| 5.166                        | 5.080     | 5.135 | 5.123 | 5.098 | 5.098 | 5.071 | 5.414 |
| 6.215                        | 6.194     | 6.141 | 6.216 | 6.372 | 6.315 | 6.372 | 6.577 |
| 7.252                        | 7.247     | 8.019 | 5.098 | 5.071 | 5.135 | 5.123 | 5.098 |

(continued on next page)
| Retention Time (min.) | Compounds | Relative Peak Area (%) |
|----------------------|-----------|------------------------|
| Skin-Pulp skin-pulp | 1 2 1 2 1 2 1 2 | 1 2 1 2 1 2 1 2 |
| Pea berry skin-pulp  | 1 2 1 2 1 2 | 1 2 |
| Green bean | 1 2 1 2 1 2 | 1 2 |
| Pea berry green bean | 1 2 1 2 1 2 | 1 2 |
| 7.962 | 9.004 | 12.12 12.12 | 0.60 n.d n.d n.d n.d n.d n.d n.d |
| 8.378 | 9.411 | 8.244 8.336 8.340 8.440 | 8.604 8.449 8.453 | 9.18 7.71 5.36 6.62 1.07 0.6 2.59 1.23 |
| 8.587 | 9.611 | n.d n.d | 0.78 n.d n.d n.d n.d |
| 9.966 | 10.726 | 9.779 9.983 9.684 | 9.731 9.620 9.779 | 7.87 n.d n.d 6.93 n.d n.d n.d n.d |
| 10.510 | 10.810 | 4-Ethylcatechol | 0.43 n.d n.d n.d n.d n.d n.d n.d 0.14 |
| 11.578 | 11.613 | 1,2-Benzenediol, 4-methyl- | 7.87 n.d n.d 6.93 n.d n.d n.d n.d |
| 12.12 | 12.12 | 1,3-Dimethyl-5-(isopropyl)pyrazole | n.d n.d n.d n.d n.d n.d 0.24 n.d |
| 15.540 | 15.575 | 14.618 | n.d n.d n.d n.d n.d n.d n.d n.d 0.76 |
| 15.891 | 15.805 | 2,1,3-Benzothiadiazole | n.d n.d n.d n.d n.d n.d n.d n.d 0.14 |
| 16.715 | 16.664 | 2,1,4-Dimethyl-3,5,6-trimethylpyrazin-2-yl) ethanol | n.d n.d n.d n.d n.d n.d n.d n.d 0.32 |
| 17.730 | 17.676 | 12-Octadecadienoic acid, methyl ester | n.d n.d n.d n.d n.d n.d n.d |
| 18.263 | 18.468 | 18.285 | 15.14 5.12 5.12 5.12 5.12 5.12 5.12 5.12 | 1.64 5.12 5.12 5.12 5.12 5.12 5.12 5.12 | 6.04 1.43 1.43 1.43 1.43 1.43 1.43 1.43 | 3.41 1.43 1.43 1.43 1.43 1.43 1.43 1.43 | 8.05 1.43 1.43 1.43 1.43 1.43 1.43 1.43 | 5.4 1.43 1.43 1.43 1.43 1.43 1.43 1.43 | 2.20 1.43 1.43 1.43 1.43 1.43 1.43 1.43 | 2.63 1.43 1.43 1.43 1.43 1.43 1.43 1.43 |
|     |     |     | 1,2-Epoxy-1-vinylcyclododecene | 9,12,15-Octadecatrienoic acid, (Z,Z,Z)- | Octadecanoic acid | Eicosanoic acid | Palmitoyl chloride | Glycerol 1-palmitate | Nonadecanoic acid | 7,9-Dimethoxy-8-isopropyl-4-methyl-1H-phenalen-1-one | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | Benzene, (1-methyl-1-butanyl)- | (R)-(-)-14-Methyl-8-hexadecn-1-ol | 2-Methyl-ZZ-3,13-octadecadienol | 1,3,12-Nonadecatriene | 5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)- | 9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 6-methyl-2,3-dihydro-1H-imidazo[1,2-a]pyrimidin-7-one | 1H-Purin-2-amine, 6-methoxy-Vitamin E | Ergost-5-en-3-ol, (3,β,)-2-[(4-tert-butylphenyl)methyl]propane-1,3-diol |
|-----|-----|-----|-------------------------------|------------------------------------------|-------------------|-----------------|-------------------|---------------------|-----------------|-----------------------------------------------|-----------------------------------------------|---------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| 18.297 | 18.290 | n.d | n.d | n.d | n.d | n.d | n.d | n.d | n.d | n.d |
| 18.302 | 18.290 | n.d | n.d | 2.02 | n.d | 1.58 | n.d | n.d | n.d | n.d |
| 18.420 | 18.407 | 18.423 | n.d | 2.88 | n.d | 2.39 | n.d | 1.73 | n.d | 0.09 |
| 20.041 | 20.044 | 20.054 | n.d | 0.45 | n.d | n.d | n.d | 0.38 | n.d | 0.14 |
| 21.319 | 21.337 | 21.216 | 0.46 | n.d | 0.47 | 0.44 | n.d | n.d | n.d | n.d |
| 21.787 | 21.658 | 21.663 | n.d | n.d | 0.59 | n.d | n.d | n.d | n.d | n.d |
| 21.787 | 21.658 | 21.663 | 23.195 | 0.53 | 1.85 | n.d | 0.73 | n.d | n.d | 4.92 | n.d |
| 22.571 | 21.219 | 22.563 | 21.216 | n.d | n.d | n.d | 0.45 | 0.93 | 1.75 | 0.61 | 0.33 |
| 22.571 | 21.219 | 22.563 | 21.216 | n.d | n.d | n.d | n.d | n.d | n.d | 0.28 | n.d |
| 22.672 | 21.219 | 22.563 | 21.216 | n.d | n.d | n.d | n.d | n.d | n.d | n.d | n.d |
| 22.672 | 21.219 | 22.563 | 21.216 | n.d | 0.61 | n.d | n.d | n.d | n.d | n.d | n.d |
| 22.672 | 21.219 | 22.563 | 21.216 | n.d | n.d | 0.59 | n.d | n.d | n.d | n.d | n.d |
| 22.685 | 21.219 | 22.563 | 21.216 | n.d | n.d | 0.64 | n.d | n.d | n.d | n.d | n.d |
| 22.685 | 21.219 | 22.563 | 21.216 | n.d | n.d | n.d | n.d | n.d | n.d | n.d | n.d |
| 23.370 | 21.219 | 22.563 | 21.216 | n.d | n.d | n.d | 0.27 | n.d | n.d | n.d | n.d |
| 24.785 | 22.576 | 22.576 | n.d | n.d | n.d | n.d | 0.99 | 4.24 | n.d | n.d |
| 24.785 | 22.576 | 22.576 | n.d | n.d | n.d | n.d | 1.03 | n.d | n.d | n.d |
| 24.987 | 22.576 | 22.576 | n.d | n.d | n.d | n.d | n.d | n.d | 0.15 | n.d | n.d |
| 24.987 | 22.576 | 22.576 | n.d | n.d | n.d | n.d | n.d | n.d | n.d | n.d | n.d |
| 25.803 | 25.803 | n.d | n.d | n.d | n.d | 0.94 | n.d | n.d | n.d | n.d | n.d |
| 25.975 | 25.975 | n.d | n.d | n.d | n.d | n.d | 0.51 | n.d | n.d | n.d | n.d |
| 27.111 | 26.899 | 27.115 | 26.891 | 26.877 | 26.733 | 0.78 | n.d | n.d | n.d | 0.45 | 1.07 | 0.87 | 0.62 | n.d | 0.32 | n.d | n.d | n.d | n.d |

(continued on next page)
### Table 2 (continued)

| Retention Time (min.) (n = 2) | Compounds | Relative Peak Area (%) (n = 2) |
|--------------------------------|-----------|--------------------------------|
| Skin-Pulp | Pea berry skin-pulp | Green bean | Pea berry green bean | Skin-Pulp | Pea berry skin-pulp | Green bean | Pea berry green bean |
| 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 | 1 | 2 |
| 27.242 | 27.242 | (24S)-ergosta-5,22(E)-dien-3β-ol | n.d | 0.58 | n.d | n.d | n.d | n.d | n.d | 0.23 |
| 27.780 | 4,7-Methano-1H-indene, octahydro- | n.d | n.d | n.d | n.d | n.d | n.d | n.d | 0.13 |
| 28.186 | 27.953 | 28.186 | 27.917 | 32.445 | β-Sitosterol | 1.61 | 2.82 | 2.50 | n.d | 2.02 | 0.52 | 0.73 | n.d |
| 29.025 | 29.000 | β-Tocopherol | n.d | n.d | n.d | n.d | 0.20 | n.d | 0.22 | n.d |
| 30.154 | 30.111 | dl-α-Tocopherol | n.d | n.d | n.d | n.d | 0.33 | n.d | 0.34 | n.d |
| 31.718 | 31.676 | Campesterol | n.d | n.d | n.d | n.d | n.d | n.d | 0.23 | n.d |
| 32.496 | 34.488 | Stigmasterol | n.d | n.d | n.d | n.d | 0.73 | n.d | 0.54 | n.d |
| 32.770 | 32.700 | γ-Sitosterol | n.d | n.d | n.d | n.d | 0.69 | n.d | n.d | n.d |
| 34.488 | 9,19-Cyclolanostan-3-ol, 24-methylene-, (3β)-Fucosterol | n.d | n.d | n.d | n.d | 0.33 | n.d | n.d | n.d |
Preparation and analysis of skin pulp and bean samples

Only red fruits of the coffee plants were included in this analysis. All fruits (‘normal’ beans and peaberries) were picked by hand from the orchard and processed using the wet-hulled method. Washed coffee fruits were then peeled to obtain the skin pulp. The seeds (beans) were fermented anaerobically for 12 h in a sealed plastic bag, and the mucilage was then washed away. The skin pulp and beans were dried in a screen house (temperature: 32.90 °C ± 5.87 °C; relative humidity: 46.14% ± 16.26%) for 3 weeks. According to standard agricultural practices, the skin pulp and beans were kept at room temperature (24–26 °C). Then, the skin pulp and beans were freeze dried for 24 h and crushed using a coffee grinder (Cyprus International 200W). Next, 100 mg powder of each sample (skin pulp beans, skin pulp peaberry beans, green beans, and peaberry green beans) was macerated for 4 × 24 h using methanol. All extracted samples were evaluated in duplicate. The extract was filtered (Whatman paper No. 91) then evaporated with a rotary evaporator. The macerated samples were redissolved in 1 mL methanol (chromatography-grade; Merck LiChrosolv Reag. Ph Eur). Before injecting into the GC-MS, the sample was filtered with a 0.22-μm/25 mm PTFE filter syringe (Axiva Sichem Biotech Pvt. Ltd. India).

Extraction of the skin pulp and beans was performed with the Sunarharum method [2] using GC-MS with some modifications. The extract was injected into the GC-MS (GC: 6890N, MS: 5973; Agilent Technologies Inc.) at 290 °C using a split mode. The initial oven temperature for green bean and peaberry green bean extracts was set to 50 °C. The temperature was increased to 220 °C (10 °C/min) and then to 290 °C (5 °C/min for 10 min). For ‘normal’ bean skin pulp and peaberry skin pulp extracts, the temperature was increased to 290 °C at 10 °C/min for 15 min. An HP-5MS (30 m × 250 μm × 0.25 μm) column was used to separate volatile compounds with helium as the carrier gas at 1.0 mL/min. The compounds were identified by matching the generated spectra with the spectra from the WILLEY09TH library database.

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Conflict of 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.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2020.105219.

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