**ONLINE-ONLY SUPPLEMENTAL MATERIAL**

**SUPPLEMENTAL METHODS**

*Ambulatory BP*

Prior to the test-food intake, baseline Ambulatory blood pressure (ABP) was confirmed with 3 measures (each separated by 3 min) performed in a seated position; differences of ≥10% systolic or diastolic BP between the second and third measure, resulted in further assessments until BP stabilized. Participants recorded an ABP monitoring diary, which documented activities / interactions which may have affected BP, and the timing of sleep and waking; the latter was used to partition ABP data into *day* and *night* periods for analysis. The ABP was removed whilst other vascular measures (i.e. office BP, FMD, PWV, AIx) were performed. A quality assurance (QA) threshold of ≥ 10 day, and ≥ 5 night measures was implemented. *N* = 7 participants failed this QA step, with intolerance to overnight assessments the reported cause for non-compliance.

**Supplemental Table 1. Reference Standard list, identifiers and number of qualitative MS transitions utilized**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Full name1** | **CAS** | **Abbreviation** | **Reference Standard** | **Relative Quantifier** | **Transi-tions** | **Mode** | **InChI Key** | **Monoisotopic Mass (units)** |
| dihydroxyphenylacetic acid | x | diOH-PAA | x | 3-hydroxyphenylacetic acid | 1 | - | N/A | \*168.8 |
| 3-hydroxybenzyl alcohol | 620-24-6 | 3-OH-Balc |  | reference standard | 3 | - | OKVJCVWFVRATSG-UHFFFAOYSA-N | 124.0524 |
| 4-hydroxymandelic acid | 1198-84-1 | 4-OH-Man |  | reference standard | 3 | - | YHXHKYRQLYQUIH-UHFFFAOYSA-N | 168.0423 |
| 3,5 dihydroxybenzyl alcohol | 29654-55-5 | 35-diOH-Balc |  | reference standard | 4 | - | NGYYFWGABVVEPL-UHFFFAOYSA-N | 140.0473 |
| 3,4,5-trihydroxybenzoic acid | 149-91-7 | 345-triOCH-BA |  | reference standard | 3 | - | LNTHITQWFMADLM-UHFFFAOYSA-N | 170.0215 |
| 4-hydroxybenzyl alcohol | 623-05-2 | 4-OH-Balc |  | reference standard | 2 | - | BVJSUAQZOZWCKN-UHFFFAOYSA-N | 124.0524 |
| 3,4,5-trihydroxybenzaldehyde | 13677-79-7 | 345-triOH-Bald |  | reference standard | 3 | - | RGZHEOWNTDJLAQ-UHFFFAOYSA-N | 154.0266 |
| benzoic acid-diglucuronide | x | BA-diGlcA | x | 3-methoxybenzoic acid-4-O-glucuronide | 4 | - | N/A | \*505 |
| 1,2-dihydroxybenzene | 120-80-9 | 12-diOH-B |  | reference standard | 3 | - | YCIMNLLNPGFGHC-UHFFFAOYSA-N | 110.0368 |
| 3,4-dihydroxybenzoic acid | 99-50-3 | 34-diOH-BA |  | reference standard | 3 | - | YQUVCSBJEUQKSH-UHFFFAOYSA-N | 154.0266 |
| 4-hydroxyhippuric acid | 2482-25-9 | 4-OH-HA |  | reference standard | 3 | - | ZMHLUFWWWPBTIU-UHFFFAOYSA-N | 195.0532 |
| alpha-hydroxyhippuric acid | 16555-77-4 | alpha-OH-HA |  | reference standard | 4 | - | GCWCVCCEIQXUQU-UHFFFAOYSA-N | 195.0532 |
| 3-hydroxyhippuric acid | 1637-75-8 | 3-OH-HA |  | reference standard | 4 | - | XDOFWFNMYJRHEW-UHFFFAOYSA-N | 195.0532 |
| 3-methoxybenzoic acid-4-O-glucuronide | synthetic | 3-OCH-BA-4-OGlcA |  | reference standard | 3 | - | MBNPZIKKKDDLLL-QGZCQISNSA-N | 342.0951 |
| 4-methoxybenzoic acid-3-O-glucuronide | synthetic | 4-OCH-BA-3-OGlcA |  | reference standard | 3 | - | HATMKBLUSXVYDS-JLERCCTOSA-N | 344.0743 |
| trihydroxybenzaldehyde-sulfate | x | triOH-Bald-Sulf | x | benzoic acid-4-sulfate | 4 | - | N/A | \*232.95 |
| dihydroxybenzoic acid-sulfate | x | diOH-BA-Sulf | x | benzoic acid-4-sulfate | 4 | - | N/A | 233.9834 |
| 3,4-dihydroxybenzaldehyde | 139-85-5 | 34-diOH-Bald |  | reference standard | 3 | - | IBGBGRVKPALMCQ-UHFFFAOYSA-N | 138.0317 |
| 3,5-dihydroxybenzaldehyde | 26153-38-8 | 35-diOH-Bald |  | reference standard | 2 | - | HAQLHRYUDBKTJG-UHFFFAOYSA-N | 138.0317 |
| 4-hydroxybenzoic acid | 99-96-7 | 4-OH-BA |  | reference standard | 2 | - | FJKROLUGYXJWQN-UHFFFAOYSA-N | 138.0317 |
| benzoic acid-4-sulfate | synthetic | BA-4-Sulf |  | reference standard | 2 | - | N/A | 217.9885 |
| 3-methoxybenzoic acid-4-sulfate | synthetic | 3-OCH-BA-4-Sulf |  | reference standard | 3 | - | TXRKUXPAEPOCIX-UHFFFAOYSA-N | 247.9991 |
| 4-methoxybenzoic acid-3-sulfate | synthetic | 4-OCH-BA-3-Sulf |  | reference standard | 3 | - | N/A | 247.9991 |
| hippuric acid-sulfate | x | HA-Sulf | x | benzoic acid-4-sulfate | 4 | - | N/A | \*257.9 |
| hippuric acid | 495-69-2 | HA |  | reference standard | 3 | - | QIAFMBKCNZACKA-UHFFFAOYSA-N | 179.0582 |
| 3-(3,4-dihydroxyphenyl)propanoic acid | 1078-61-1 | 34-diOH-PPA |  | reference standard | 3 | - | DZAUWHJDUNRCTF-UHFFFAOYSA-N | 182.0579 |
| 3-hydroxyphenylacetic acid | 621-37-4 | 3-OH-PAA |  | reference standard | 3 | - | FVMDYYGIDFPZAX-UHFFFAOYSA-N | 152.0473 |
| dihydroxybenzenediol-sulfate | x | diOH-Bdiol-Sulf | x | benzoic acid-4-sulfate | 1 | - | N/A | \*205.1 |
| hydroxybenzenediol-sulfate | x | OH-Bdiol-Sulf | x | benzoic acid-4-sulfate | 1 | - | N/A | \*189.1 |
| 3-hydroxybenzoic acid | 99-06-9 | 3-OH-BA |  | reference standard | 3 | - | IJFXRHURBJZNAO-UHFFFAOYSA-N | 138.0317 |
| 2,5-dihydroxybenzoic acid | 490-79-9 | 25-diOH-BA |  | reference standard | 3 | - | WXTMDXOMEHJXQO-UHFFFAOYSA-N | 154.0266 |
| 4-hydroxybenzaldehyde | 123-08-0 | 4-OH-Bald |  | reference standard | 3 | - | RGHHSNMVTDWUBI-UHFFFAOYSA-N | 122.0368 |
| 3-hydroxybenzaldehyde | 100-83-4 | 3-OH-Bald |  | reference standard | 3 | - | IAVREABSGIHHMO-UHFFFAOYSA-N | 122.0368 |
| 3-(4-methoxyphenyl)propanoic acid-3-sulfate | 1258842-21-5 | 4-OCH-PPA-3-Sulf |  | reference standard | 3 | - | QZIYZVFIROFZCV-UHFFFAOYSA-N | 276.0303 |
| 5-O-caffeoylquinic acid | 906-33-2 | 5-CQA | x | 2-hydroxycinnamic acid | 4 | - | CWVRJTMFETXNAD-NXLLHMKUSA-N | 354.0951 |
| 2,4-dihydroxybenzoic acid | 89-86-1 | 24-diOH-BA |  | reference standard | 3 | - | UIAFKZKHHVMJGS-UHFFFAOYSA-N | 154.0266 |
| 4-hydroxy-3-methoxybenzoic acid | 121-34-6 | 4-OH-3-OCH-BA |  | reference standard | 5 | - | WKOLLVMJNQIZCI-UHFFFAOYSA-N | 168.0423 |
| 3-hydroxy-4-methoxyphenylacetic acid | 1131-94-8 | 3-OH-4-OCH-PAA |  | reference standard | 2 | - | BWXLCOBSWMQCGP-UHFFFAOYSA-N | 182.0579 |
| n-benzoylglutamic acid | 6094-36-6 | N-Benzyglut A |  | reference standard | 4 | - | LPJXPACOXRZCCP-VIFPVBQESA-N | 251.0794 |
| 3,4-dihydroxycinnamic acid | 331-39-5 | 34-diOH-CIA |  | reference standard | 3 | - | QAIPRVGONGVQAS-DUXPYHPUSA-N | 180.0423 |
| catechin-O-glucuronide | x | Cat-OGlcA | x | myricetin-3-O-galactoside | 5 | - | N/A | \*465.05 |
| hydroxy-methoxybenzenediol-sulfate | x | OH-OCH-Bdiol-Sulf | x | benzoic acid-4-sulfate | 1 | - | N/A | \*219.1 |
| 4-hydroxy-3-methoxyphenylacetic acid | 306-08-1 | 4-OH-3-OCH-PAA |  | reference standard | 1 | - | QRMZSPFSDQBLIX-UHFFFAOYSA-N | 182.0579 |
| 2,6-dimethoxybenzoic acid | 1466-76-8 | 26-diOCH-BA |  | reference standard | 3 | - | MBIZFBDREVRUHY-UHFFFAOYSA-N | 182.0579 |
| 2,4-dihydroxybenzaldehyde | 95-01-2 | 24-diOH-Bald |  | reference standard | 4 | - | IUNJCFABHJZSKB-UHFFFAOYSA-N | 138.0317 |
| 3-O-caffeoylquinic acid | 327-97-9 | 3-CQA | x | 2-hydroxycinnamic acid | 3 | - | CWVRJTMFETXNAD-JUHZACGLSA-N | 354.0951 |
| 3-hydroxy-4-methoxybenzoic acid | 645-08-9 | 3-OH-4-OCH-BA |  | reference standard | 3 | - | LBKFGYZQBSGRHY-UHFFFAOYSA-N | 168.0423 |
| benzoic acid | 65-85-0 | BA |  | reference standard | 1 | - | WPYMKLBDIGXBTP-UHFFFAOYSA-N | 122.0368 |
| 3-(3-hydroxyphenyl)propanoic acid | 621-54-5 | 3-OH-PPA |  | reference standard | 2 | - | QVWAEZJXDYOKEH-UHFFFAOYSA-N | 166.063 |
| 3-(4-hydroxyphenyl)propanoic acid | 501-97-3 | 4-OH-PPA |  | reference standard | 3 | - | NMHMNPHRMNGLLB-UHFFFAOYSA-N | 166.063 |
| methoxycinnamic acid-sulfate-O-glucuronide | x | OCH-CIA-Sulf-OGlcA | x | 4-methoxybenzoic acid-3-O-glucuronide | 5 | - | N/A | \*449.05 |
| 3,4-dimethoxybenzyl alcohol | 93-03-8 | 34-diOCH-Balc |  | reference standard | 3 | - | OEGPRYNGFWGMMV-UHFFFAOYSA-N | 168.0786 |
| 3,5-dihydroxybenzoic acid methyl ester | 2150-44-9 | M-35-diOH-BA |  | reference standard | 4 | - | RNVFYQUEEMZKLR-UHFFFAOYSA-N | 168.0423 |
| 3-hydroxy-4-methoxybenzaldehyde | 621-59-0 | 3-OH-4-OCH-Bald |  | reference standard | 3 | - | JVTZFYYHCGSXJV-UHFFFAOYSA-N | 152.0473 |
| 3,4-dihydroxybenzoic acid methyl ester | 2150-43-8 | M-34-diOH-BA |  | reference standard | 4 | - | CUFLZUDASVUNOE-UHFFFAOYSA-N | 168.0423 |
| 3-methylhippuric acid | 27115-49-7 | 3-M-HA |  | reference standard | 3 | - | YKAKNMHEIJUKEX-UHFFFAOYSA-N | 193.0739 |
| phenylvalerolactone-sulfate-O-glucuronide | x | phenyl-Val-Sulf-OGlcA | x | 3-methoxybenzoic acid-4-O-glucuronide | 5 | - | N/A | \*463.01 |
| 4-methylhippuric acid | 27115-50-0 | 4-M-HA |  | reference standard | 5 | - | NRSCPTLHWVWLLH-UHFFFAOYSA-N | 193.0739 |
| hydroxyhippuric acid | x | OH-HA | x | 4-hydroxyhippuric acid | 3 | - | N/A | \*194.201 |
| 5-(3'-hydroxyphenyl)-gamma-valerolactone-4'-O-glucuronide | x | OH-phenyl-Val-OGlcA | x | 3-methoxybenzoic acid-4-O-glucuronide | 6 | - | OTBJYBQGMPICIK-GHPVWUPISA-N | 384.1056 |
| 4-hydroxycinnamic acid | 7400-08-0 | 4-OH-CIA |  | reference standard | 3 | - | NGSWKAQJJWESNS-ZZXKWVIFSA-N | 164.0473 |
| 3-(4-hydroxy-3-methoxyphenyl)propanoic acid | 1135-23-5 | 4-OH 3-OCH-PPA |  | reference standard | 5 | - | BOLQJTPHPSDZHR-UHFFFAOYSA-N | 196.0736 |
| hydroxybenzoic acid-sulfate | x | OH-BA-Sulf | x | benzoic acid-4-sulfate | 1 | - | N/A | \*233.1 |
| phenylacetic acid | 103-82-2 | PAA |  | reference standard | 1 | - | WLJVXDMOQOGPHL-UHFFFAOYSA-N | 136.0524 |
| 2,6-dihydroxybenzoic acid | 303-07-1 | 26-diOH-BA |  | reference standard | 4 | - | AKEUNCKRJATALU-UHFFFAOYSA-N | 154.0266 |
| methylcatechol-sulfate | x | M-OH-Bdiol-Sulf | x | benzoic acid-4-sulfate | 1 | - | N/A | \*203.1 |
| 1,3-benzenediol | 108-46-3 | 13-diOH-B |  | reference standard | 3 | - | GHMLBKRAJCXXBS-UHFFFAOYSA-N | 110.0368 |
| 3-(3-hydroxy-4-methoxyphenyl)propanoic acid | 1135-15-5 | 3-OH-4-OCH-PPA |  | reference standard | 3 | - | ZVIJTQFTLXXGJA-UHFFFAOYSA-N | 196.0736 |
| 3-hydroxycinnamic acid (trans) | 14755-02-3 | t-3-OH-CIA |  | reference standard | 3 | - | KKSDGJDHHZEWEP-SNAWJCMRSA-N | 164.0473 |
| hydroxyphenylvalerolactone-sulfate | x | 3-OH-phenyl-Val-4-Sulf | x | benzoic acid-4-sulfate | 4 | - | WAXYAOJFDCCESK-UHFFFAOYSA-N | 288.0304 |
| 3-caffeoylquinic acid-O-glucuronide | x | CLGA-OGlcA | x | 3-methoxybenzoic acid-4-O-glucuronide | 6 | - | N/A | \*529.31 |
| hydroxybenzyldehyde-O-glucuronide | x | OH-Bald-OGlcA | x | 3-methoxybenzoic acid-4-O-glucuronide | 5 | - | N/A | \*313.121 |
| 2-hydroxybenzoic acid | 69-72-7 | 2-OH-BA |  | reference standard | 3 | - | YGSDEFSMJLZEOE-UHFFFAOYSA-N | 138.0317 |
| epicatechin-O-glucuronide | x | Ecat-OGlcA | x | myricetin-3-O-galactoside | 6 | - | N/A | \*466.1111 |
| 3,4 dimethoxybenzoic acid | 93-07-2 | 34-diOCH-BA |  | reference standard | 1 | - | DAUAQNGYDSHRET-UHFFFAOYSA-N | 182.0579 |
| 2,6-dimethoxyphenol | 91-10-1 | 26-diOCH-Phen |  | reference standard | 2 | - | KLIDCXVFHGNTTM-UHFFFAOYSA-N | 154.063 |
| 3-hydroxybenzoic acid methyl ester | 19438-10-9 | M-3-OH-BA |  | reference standard | 3 | - | YKUCHDXIBAQWSF-UHFFFAOYSA-N | 152.0473 |
| 4-hydroxy-3-methylbenzoic acid | 99-76-3 | M-4-OH-BA |  | reference standard | 3 | - | LXCFILQKKLGQFO-UHFFFAOYSA-N | 152.0473 |
| 3-methoxyphenylacetic acid | 1798-09-0 | 3-OCH-PAA |  | reference standard | 2 | - | LEGPZHPSIPPYIO-UHFFFAOYSA-N | 166.063 |
| gallocatechin-O-glucuronide | x | Gcat-OGlcA | x | myricetin-3-O-galactoside | 6 | - | N/A | \*481.212 |
| 3,4-dimethoxyphenylacetic acid | 93-40-3 | 34-diOCH-PAA |  | reference standard | 4 | - | WUAXWQRULBZETB-UHFFFAOYSA-N | 196.0736 |
| 3-hydroxy-4-methoxycinnamic acid | 537-73-5 | 3-OH-4-OCH-CIA |  | reference standard | 3 | - | QURCVMIEKCOAJU-HWKANZROSA-N | 194.0579 |
| 4-hydroxy-3-methoxycinnamic acid | 537-98-4 | 4-OH-3-OCH-CIA |  | reference standard | 3 | - | KSEBMYQBYZTDHS-HWKANZROSA-N | 194.0579 |
| 2-hydroxycinnamic acid | 614-60-8 | 2-OH-CIA |  | reference standard | 3 | - | PMOWTIHVNWZYFI-AATRIKPKSA-N | 164.0473 |
| phenylvalerolactone-sulfate | x | phenyl-Val-Sulf | x | benzoic acid-4-sulfate | 3 | - | DPRDYFJWDRNYAZ-UHFFFAOYSA-N | 272.0355 |
| 3-phenylpropanoic acid | 501-52-0 | PPA |  | reference standard | 1 | - | XMIIGOLPHOKFCH-UHFFFAOYSA-N | 150.0681 |
| 2-hydroxy-6-methoxybenzoic acid | 3147-64-6 | 2-OH-6-OCH-BA |  | reference standard | 2 | - | AAUQLHHARJUJEH-UHFFFAOYSA-N | 168.0423 |
| 2,4-dimethoxybenzoic acid | 91-52-1 | 24-diOCH-BA |  | reference standard | 1 | - | GPVDHNVGGIAOQT-UHFFFAOYSA-N | 182.0579 |
| 2,3,4-trimethoxyphenylacetic acid | 22480-91-7 | 234-triOCH-PAA |  | reference standard | 4 | - | ZMWCKCLDAQWIDA-UHFFFAOYSA-N | 226.0841 |
| 4-hydroxy-3,5-dimethoxycinnamic acid | 530-59-6 | 4-OH-35-diOCH-CIA |  | reference standard | 2 | - | PCMORTLOPMLEFB-ONEGZZNKSA-N | 224.0685 |
| 4-hydroxy-3-methoxybenzoic acid methyl ester | 3943-74-6 | M-4-OH-3-OCH-BA |  | reference standard | 4 | - | BVWTXUYLKBHMOX-UHFFFAOYSA-N | 182.0579 |
| myricetin-3-O-galactoside | 15648-86-9 | Myr-OGal |  | reference standard | 1 | - | FOHXFLPXBUAOJM-OPAWWROQSA-N | 480.0904 |
| 2-hydroxy-4-methoxybenzaldehyde | 673-22-3 | 2-OH-4-OCH-Bald |  | reference standard | 3 | - | WZUODJNEIXSNEU-UHFFFAOYSA-N | 152.0473 |
| trans-cinnamic acid | 140-10-3 | t-CIA |  | reference standard | 1 | - | WBYWAXJHAXSJNI-VOTSOKGWSA-N | 148.0524 |
| 4-methoxycinnamic acid | 830-09-1 | 4-OCH-CIA |  | reference standard | 4 | - | AFDXODALSZRGIH-UHFFFAOYSA-N | 178.063 |
| dihydroxybenzoic acid | x | diOH-BA | x | 2,4-dihydroxybenzoic acid | 3 | - | N/A | \*154.1204 |
| 2-hydroxy-4-methoxybenzoic acid | 2237-36-7 | 2-OH-4-OCH-BA |  | reference standard | 3 | - | MRIXVKKOHPQOFK-UHFFFAOYSA-N | 168.0423 |
| 3-(3,4,5-trimethoxyphenyl)propanoic acid | 25173-72-2 | 345-triOCH-PPA |  | reference standard | 6 | - | ZCYXGVJUZBKJAI-UHFFFAOYSA-N | 240.0998 |
| 3-(3-methoxyphenyl)propanoic acid | 10516-71-9 | 3-OCH-PPA |  | reference standard | 4 | - | BJJQJLOZWBZEGA-UHFFFAOYSA-N | 180.0786 |
| 3,5-dimethoxybenzoic acid | 1132-21-4 | 35-diOCH-BA |  | reference standard | 3 | - | IWPZKOJSYQZABD-UHFFFAOYSA-N | 182.0579 |
| methoxycinnamic acid-sulfate | x | OCH-CIA-Sulf | x | benzoic acid-4-sulfate | 2 | - | N/A | \*273.122 |
| 3-methoxycinnamic acid | 6099-04-3 | 3-OCH-CIA |  | reference standard | 3 | - | LZPNXAULYJPXEH-AATRIKPKSA-N | 178.063 |
| rosmarinic acid | 20283-92-5 | Rosm A |  | reference standard | 3 | - | DOUMFZQKYFQNTF-WUTVXBCWSA-N | 360.0845 |
| resveratrol | 501-36-0 | Res |  | reference standard | 5 | - | LUKBXSAWLPMMSZ-OWOJBTEDSA-N | 228.0786 |
| myricetin | 529-44-2 | Myr |  | reference standard | 4 | - | IKMDFBPHZNJCSN-UHFFFAOYSA-N | 318.0376 |
| 3-O-feruloylquinic acid | 62929-69-5; 1899-29-2 | 3-FQA | x | 2-hydroxycinnamic acid | 3 | - | RAGZUCNPTLULOL-KJJWLSQTSA-N | 368.1107 |
| 4-O-feruloylquinic acid | 2613-86-7 | 4-FQA | x | 2-hydroxycinnamic acid | 3 | - | VTMFDSJJVNQXLT-XQCMRRNBSA-N | 368.1107 |
| 3-methoxyphenylacetic acid-4-sulfate | 38339-06-9 | 3-OCH-PAA-4-Sulf | x | benzoic acid-4-sulfate | 2 | - | IACOAKYXFIWAQN-UHFFFAOYSA-N | 262.0147 |
| kaempferol | 520-18-3 | Kae |  | reference standard | 5 | - | IYRMWMYZSQPJKC-UHFFFAOYSA-N | 286.0477 |
| myricetin-O-glucuronide | x | Myr-OGlcA | x | myricetin-3-O-galactoside | 6 | - | N/A | \*493.21 |
| hydroxy-methoxybenzoic acid-sulfate | x | OH-OCH-BA-Sulf | x | benzoic acid-4-sulfate | 1 | - | N/A | \*263.1 |
| methoxycinnamic acid-O-glucuronide | x | OCH-CIA-OGlcA | x | benzoic acid-4-sulfate | 1 | - | N/A | \*369.1 |
| 5-O-feruloylquinic acid | 40242-06-6 | 5-FQA | x | 2-hydroxycinnamic acid | 3 | - | RAGZUCNPTLULOL-KQJPBSFVSA-N | 368.1107 |
| epigallocatechingallate-O-glucuronide | x | EGCatG-OGlcA | x | myricetin-3-O-galactoside | 5 | - | N/A | \*633.31 |
| methylcatechol-O-glucuronide | x | diOH-Bdiol-OGlcA | x | 4-methoxybenzoic acid-3-O-glucuronide | 1 | - | N/A | \*301.1 |
| methoxyphenylacetic acid-O-glucuronide | x | OH-OCH-PAA-OGlcA | x | 3-methoxybenzoic acid-4-O-glucuronide | 5 | - | N/A | \*356.91 |
| phenylpropanoic acid-O-glucuronide | x | PPA-OGlcA | x | 4-methoxybenzoic acid-3-O-glucuronide | 5 | - | N/A | \*325.05 |
| malvidin acetyl glucoside | x | Mal-Acetyl-Gluc | x | myricetin-3-O-galactoside | 1 | + | N/A | \*535 |
| methoxybenzoic acid-sulfate | x | OCH-BA-Sulf | x | benzoic acid-4-sulfate | 5 | + | N/A | \*233.14 |
| petunidin-sulfate | x | Pet-Sulf | x | myricetin-3-O-galactoside | 1 | + | N/A | \*397 |
| methoxyphenylacetic acid-sulfate | x | OCH-PAA-Sulf | x | benzoic acid-4-sulfate | 4 | + | N/A | \*247.12 |
| dimethoxyphenylacetic acid-sulfate | x | diOCH-PAA-Sulf | x | benzoic acid-4-sulfate | 6 | + | N/A | \*293.1 |
| cyanidin-sulfate | x | Cya-Sulf | x | myricetin-3-O-galactoside | 1 | + | N/A | \*367 |
| ascorbic acid-sulfate | x | AA-Sulf | x | 3,4-dihydroxybenzoic acid | 6 | + | N/A | \*257.1 |
| methoxyphenylpropanoic acid-sulfate | x | OCH-PPA-Sulf | x | benzoic acid-4-sulfate | 4 | + | N/A | \*261 |
| malvidin-sulfate | x | Mal-Sulf | x | myricetin-3-O-galactoside | 2 | + | N/A | \*411 |
| methoxycinnamic acid-sulfate | x | OCH-CIA-Sulf | x | benzoic acid-4-sulfate | 4 | + | N/A | \*259 |
| methoxycinnamic acid-O-glucuronide | x | OCH-CIA-OGlcA | x | 4-methoxybenzoic acid-3-O-glucuronide | 6 | + | N/A | \*355.11 |
| phenylacetic-sulfate | x | PAA-Sulf | x | benzoic acid-4-sulfate | 4 | + | N/A | \*231.8 |
| delphinidin-sulfate | x | Del-Sulf | x | myricetin-3-O-galactoside | 1 | + | N/A | \*383 |
| 3,5-dihydroxybenzoic acid | 99-10-5 | 35-diOH-BA |  | reference standard | 3 | + | UYEMGAFJOZZIFP-UHFFFAOYSA-N | 154.0266 |
| methoxybenzaldehyde-sulfate | x | OCH-Bald-Sulf | x | benzoic acid-4-sulfate | 4 | + | N/A | \*233.2 |
| peonidin acetyl glucoside | x | Peo-Acetyl-Gluc | x | myricetin-3-O-galactoside | 1 | + | N/A | \*505 |
| 4-hydroxyphenylacetic acid | 156-38-7 | 4-OH-PAA |  | reference standard | 2 | + | XQXPVVBIMDBYFF-UHFFFAOYSA-N | 152.0473 |
| 4-methylcatechol | 452-86-8 | 4M-Cat |  | reference standard | 3 | + | ZBCATMYQYDCTIZ-UHFFFAOYSA-N | 124.0524 |
| hippuric acid methyl ester | 1205-08-9 | M-HA |  | reference standard | 5 | + | XTKVNQKOTKPCKM-UHFFFAOYSA-N | 193.0739 |
| 4-hydroxy-3,5-dimethoxybenzoic acid | 530-57-4 | 4-OH-35-diOCH-BA |  | reference standard | 3 | + | WBIZZNFQJPOKDK-UHFFFAOYSA-N | 198.0528 |
| 2-methoxybenzoic acid | 579-75-9 | 2-OCH-BA |  | reference standard | 4 | + | ILUJQPXNXACGAN-UHFFFAOYSA-N | 152.0473 |
| 4-hydroxy-3,5-dimethoxyphenylacetic acid | 4385-56-2 | 4-OH-35-diOCH-PAA |  | reference standard | 5 | + | BQBQKSSTFGCRQL-UHFFFAOYSA-N | 212.0685 |
| cyanidin-3-galactoside | 27661-36-5 | Cya-3-OGal |  | reference standard | 1 | + | YTMNONATNXDQJF-QSLGVYCOSA-N | 449.1084 |
| 4-hydroxy-2-methoxybenzaldehyde | 18278-34-7 | 4-OH-2-OCH-Bald |  | reference standard | 3 | + | WBIZZNFQJPOKDK-UHFFFAOYSA-N | 152.0473 |
| petunidin-3-O-glucoside | 6988-81-4 | Pet-3-OGluc |  | reference standard | 1 | + | HBKZHMZCXXQMOX-YATQZQGFSA-N | 479.119 |
| delphinidin-3-O-glucoside | 6906-38-3 | Del-3-OGluc |  | reference standard | 1 | + | ZJWIIMLSNZOCBP-BTTVDUMLSA-N | 465.1033 |
| peonidin-3-O-galactoside | 28148-89-2 | Peo-3-OGal |  | reference standard | 1 | + | VDTNZDSOEFSAIZ-HVOKISQTSA-N | 463.124 |
| 3,5-dimethoxybenzyl alcohol | 705-76-0 | 35-diOCH-Balc |  | reference standard | 4 | + | AUDBREYGQOXIFT-UHFFFAOYSA-N | 168.0786 |
| 4-methoxyphenylacetic acid | 104-01-8 | 4-OCH-PAA |  | reference standard | 3 | + | NRPFNQUDKRYCNX-UHFFFAOYSA-N | 166.063 |
| 3-methoxybenzoic acid | 586-38-9 | 3-OCH-BA |  | reference standard | 4 | + | XHQZJYCNDZAGLW-UHFFFAOYSA-N | 152.0473 |
| malvidin-3-galactoside | 30113-37-2 | Mal-3-OGal |  | reference standard | 1 | + | YDIKCZBMBPOGFT-IEQOHONMSA-N | 493.1346 |
| 3,4-dimethoxybenzaldehyde | 120-14-9 | 34-diOCH-Bald |  | reference standard | 5 | + | WJUFSDZVCOTFON-UHFFFAOYSA-N | 166.063 |
| peonidin-O-glucoside-O-glucuronide | x | Peo-OGluc-OGlcA | x | petunidin-3-O-glucoside | 6 | + | N/A | \*639.21 |
| 3,4,5-trimethoxybenzaldehyde | 86-81-7 | 345-triOCH-Bald |  | reference standard | 4 | + | OPHQOIGEOHXOGX-UHFFFAOYSA-N | 196.0736 |
| pyridoxic acid-sulfate | x | pyridoxic acid-Sulf | x | benzoic acid-4-sulfate | 5 | + | N/A | \*264 |
| 3,5-dimethoxybenzaldehyde | 7311-34-4 | 35-diOCH-Bald |  | reference standard | 3 | + | VFZRZRDOXPRTSC-UHFFFAOYSA-N | 166.063 |
| 3,4-dimethoxybenzoic acid methyl ester | 2150-38-1 | M-34-diOCH-BA |  | reference standard | 3 | + | BIGQPYZPEWAPBG-UHFFFAOYSA-N | 196.0736 |
| malvidin-O-glucoside | 7228-78-6 | Mal-OGluc | x | myricetin-3-O-galactoside | 1 | + | PXUQTDZNOHRWLI-OXUVVOBNSA-O | 493.1 |
| malvidin-O-galactoside-O-glucuronide | x | Mal-OGal-OGlcA | x | myricetin-3-O-galactoside | 1 | + | N/A | \*669 |
| methoxyphenylpropanoic acid-O-glucuronide | 1187945-72-7 | OCH-PPA-OGlcA | x | 4-methoxybenzoic acid-3-O-glucuronide | 4 | + | OSJGZCUHTGTJHT-JHZZJYKESA-N | 372.1056 |
| peonidin-O-glucuronide | x | Peo-OGlcA | x | myricetin-3-O-galactoside | 1 | + | N/A | \*477 |
| peonidin-O-glucoside | x | Peo-OGluc | x | myricetin-3-O-galactoside | 2 | + | N/A | \*463.124 |
| malvidin-O-glucuronide | x | Mal-OGlcA | x | myricetin-3-O-galactoside | 4 | + | N/A | \*507 |
| kaempferol-O-glucuronide | x | Kae-OGlcA | x | myricetin-3-O-galactoside | 1 | + | N/A | \*463.1 |
| cyanidin-O-glucuronide | 683208-13-1 | Cya-OGlcA | x | myricetin-3-O-galactoside | 1 | + | N/A | \*463.0871 |
| methoxybenzyldehyde-O-glucuronide | x | OCH-Bald-OGlcA | x | 4-methoxybenzoic acid-3-O-glucuronide | 4 | + | N/A | \*329.21 |
| petunidin acetyl glucoside | x | Pet-Acetyl-Gluc | x | myricetin-3-O-galactoside | 1 | + | N/A | \*521 |
| petunidin-disulfate | x | Pet-diSulf | x | myricetin-3-O-galactoside | 1 | + | N/A | \*477 |
| cyanidin-O-glucoside | 7084-24-4 | Cya-OGluc | x | myricetin-3-O-galactoside | 1 | + | RKWHWFONKJEUEF-UNJWAJPSSA-O | 449.1 |
| petunidin-O-glucoside-sulfate | x | Pet-Gluc-Sulf | x | myricetin-3-O-galactoside | 2 | + | N/A | \*558 |
| petunidin-O-galactoside | x | Pet-OGal | x | myricetin-3-O-galactoside | 1 | + | CCQDWIRWKWIUKK-UHFFFAOYSA-O | 479.1 |
| peonidin-O-galactoside-O-glucuronide | x | Peo-OGal-OGlcA | x | myricetin-3-O-galactoside | 2 | + | N/A | \*639.37 |
| hydroxy-methoxycinnamic acid-sulfate | x | diOH-OCH-CIA-Sulf | x | benzoic acid-4-sulfate | 6 | + | N/A | \*291 |

1Ordered by retention time within ionization mode (-or +)

N/A: InchiKey not available

\*m/z provided where monoisotopic mass are not available in online databases

**Supplemental Table 2. Ambulatory blood pressure in participants with validated monitoring periods (n = 21 blueberry group; n = 17 placebo group) 1, 2**.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Placebo**  **(n = 17)** | | **1 cup blueberries**  **(n = 21)** | |  |
|  | **n =** | **Mean (95% CI)** | **n =** | **Mean (95% CI)** | **p-value** |
| **Systolic BP (SBP), *mmHg*** |  |  |  |  |  |
| Mean 24 h SBP | 17 | 125 (114, 136) | 21 | 125 (114, 136) | 0.92 |
| 24h SBP variability | 17 | 14.5 (12.0, 16.9) | 21 | 14.8 (12.5, 17.2) | 0.51 |
| Mean SBP during waking hours | 17 | 130 (118, 141) | 21 | 130 (119, 141) | 0.78 |
| Mean SBP during sleeping hours | 17 | 110 (97.8, 122) | 21 | 111 (99.2, 123) | 0.83 |
|  |  |  |  |  |  |
| **Diastolic BP (DBP), *mmHg*** |  |  |  |  |  |
| Mean 24 h DBP | 17 | 74.4 (69.4, 79.5) | 21 | 75.5 (70.6, 80.4) | 0.97 |
| 24h DBP variability | 17 | 11.4 (9.6, 13.2) | 21 | 10.9 (9.1, 12.7) | 0.63 |
| Mean DBP during waking hours | 17 | 78.2 (73.1, 83.3) | 21 | 78.6 (73.7, 83.6) | 0.68 |
| Mean DBP during sleeping hours | 17 | 63.4 (57.1, 69.7) | 21 | 65.5 (59.4, 71.6) | 0.56 |
|  |  |  |  |  |  |
| **Mean Arterial Pressure (MAP), *mmHg*** |  |  |  |  |  |
| Mean 24 h MAP | 17 | 91.8 (85.9, 97.6) | 21 | 91.7 (86.0, 97.3) | 0.68 |
| 24h MAP variability | 17 | 12.1 (10.2, 14.0) | 21 | 11.3 (9.5, 13.2) | 0.51 |
| Mean MAP during waking hours | 17 | 95.6 (89.9, 101) | 21 | 94.9 (89.3, 101) | 0.42 |
| Mean MAP during sleeping hours | 17 | 80.5 (73.4, 87.6) | 21 | 81.7 (74.8, 88.6) | 0.74 |
|  |  |  |  |  |  |

BP, blood pressure.

1 Values are mean (95% CI) adjusted for age, sex, BMI, and use of statins or blood pressure medication. Cup, relates to the equivalent number of US cups of fresh blueberries.

2*P =* linear regression analysis; *treatment* as predictor.

**Supplemental Table 3. Baseline adjusted postprandial serum levels (of total anthocyanin-related metabolites and phase II conjugates following the intake of an energy-dense test meal challenge, with / without 1 cup of blueberries1, 2**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Placebo: mean (95% CI)** | | | | | | **1 cup blueberries: mean (95% CI)** | | | | | | **P =** |
| **Pre-dose** | **Hours (h)** | | | | | **Pre-dose** | **Hours (h)** | | | | |
| **1 h** | **2 h** | **3 h** | **6 h** | **24 h** | **1 h** | **2 h** | **3 h** | **6 h** | **24 h** |
| Total serum  metabolites (*uM*) | 13.05  (11.9, 14.2) | 17.21  (15.7, 18.8) | 15.91  (14.3, 17.5) | 15.12  (13.5, 16.7) | 12.02  (10.5, 13.6) | 12.4  (10.9, 14.0) | 13.05  (11.9, 14.2) | 15.83  (14.3, 17.4) | 15.29  (13.7, 16.8) | 14.84  (13.3, 16.4) | 14.56  (13.0, 16.1)\* | 15.36  (13.8, 16.9)\* | 0.00 |

1 Values are means (95% CI) adjusted for age, sex, BMI, and plate number.

2 *P=* values for the time point x treatment interaction calculated using a constrained linear mixed-effect model (adjusting for baseline values).

3 total serum calculations excluded 4-Hydroxy-3-methoxybenzaldehyde (vanillin), as it was a component of the placebo beverage.

\* indicates a significant difference between groups, at a specific time point.

**Supplemental Table 4. Baseline adjusted postprandial urinary recovery levels (*mg*) of total anthocyanin-related metabolites and phase II conjugates following the intake of an energy-dense test meal challenge, with / without 1 cup of blueberries1,2**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Placebo: mean (95% CI)** | | | | **1 cup blueberries: mean (95% CI)** | | | | **P=** |
| **Pre-dose** | **Hours (h)** | | | **Pre-dose** | **Hours (h)** | | |
| **0-3 h** | **3-6 h** | **6-24 h** | **0-3 h** | **3-6 h** | **6-24 h** |
| Total urinary  metabolites (*mg*) | 10113  (4857, 15370) | 9731  (1883, 17580) | 22499  (13044, 31954) | 70938  (53154, 88723) | 10113  (4857, 15370) | 13698  (3578, 23817) | 35505  (25604, 45407) | 144057  (114625, 173489)\* | 0.00 |

1 Values are means (95% CI), of urinary recovery (in *mg*), adjusted for age, sex, BMI, and plate number.

2 *P=* values for the time point x treatment interaction calculated using a constrained linear mixed-effect model (adjusting for baseline values).

\* indicates a significant difference between groups, at a specific time point.

**Supplemental Table 5. Exploratory correlations (p < 0.10) in the 1 cup blueberry group, between postprandial (0 to 24 h) iAUCs of anthocyanin-related metabolites and phase II conjugates (urinary recoveries and serum levels) and iAUCs of cardiometabolic outcomes which significantly differed by treatment group1,2**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Outcome | Urinary metabolites | Metabolite assessment | r= | p= |
| Apo-A1 (g/L) | 3-Methoxyphenylacetic acid-4-sulfate | serum | 0.44 | 0.04 |
| 3,4-Dihydroxyphenylacetic acid (DOPAC) | urinary | 0.41 | 0.06 |
| Glucose (mmol/L) | 3-(3,4-Dihydroxyphenyl)propanoic acid | urinary | 0.47 | 0.05 |
| HDLC (mmol/L) | Benzoylglutamic acid | urinary | 0.50 | 0.02 |
| 3-Methoxyphenylacetic acid-4-sulfate | serum | 0.40 | 0.06 |
| Total cholesterol (mmol/L) | Benzoylglutamic acid | urinary | -0.48 | 0.03 |
| Benzoic acid-4-sulfate | urinary | -0.49 | 0.03 |
| 4-Methoxybenzoic acid-3-glucuronide (Isovanillic acid-glucuronide) | urinary | -0.42 | 0.07 |
| 4-Hydroxyhippuric acid | serum | -0.37 | 0.09 |
| XLHDLP (x10-6) | Hippuric acid-sulfate | serum | 0.45 | 0.03 |
| Hippuric acid | serum | 0.43 | 0.04 |
| 3-(3,4-Dihydroxyphenyl)propanoic acid | urinary | 0.45 | 0.05 |
| 3,4-Dihydroxyphenylacetic acid (DOPAC) | urinary | 0.40 | 0.06 |

1 R = correlation coefficient from Spearman's Rank Order Correlation (non-parametric correlation)

2 iAUC of biochemical measurements (30 60 90 120 180 360 1440 minutes) & iAUC of cumulative metabolite value (calculated from pre-dose to 1440 min)